Spectroscopic Properties of Inorganic and Organometallic Compounds

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Volume 38

A Specialist Periodical Report

Spectroscopic Properties of Inorganic and Organometallic Compounds

Volume 38

A Review of the Literature Published up to Late 2004

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ISBN-10: 0-85404-451-5
ISBN-13: 978-0-85404-451-1
ISSN 0584-8555

A catalogue record for this book is available from the British Library

Published by The Royal Society of Chemistry,
Thomas Graham House, Science Park, Milton Road,
Cambridge CB4 0WF, UK

Registered Charity Number 207890

For further information see our web site at www.rsc.org

Typeset by Macmillan India Ltd, Bangalore, India
Printed by Henry Lings Ltd, Dorchester, Dorset, UK

Preface

It gives me great pleasure to introduce the thirty-eighth volume in the series of Specialist Periodical reports on the ‘Spectroscopic Properties of Inorganic and Organometallic Compounds’. The NMR chapters have now returned, with a coverage now limited to those publications where the spectroscopic data have been significant in structural or mechanistic terms. I am most grateful to my fellow Reporters for their accuracy and promptness, and to the staff of the Royal Society of Chemistry for all their assistance.

George Davidson
November 2005

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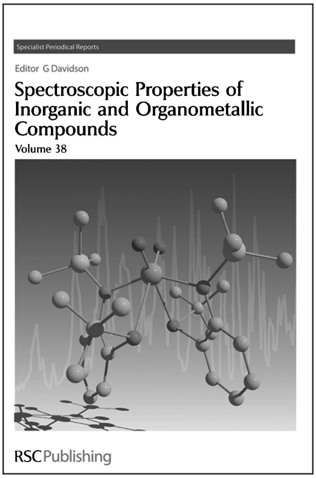

Cover
Cover shows molecular structure of molybdenum dioxocomplex with thioester functionalised amido ligands superimposed on a spectral background. Adapted from image reproduced by permission of Nadia C. Mösch-Zanetti.

NMR Spectroscopy in the Liquid and Gas Phases 1

G. Davidson

NMR Spectroscopy in the Liquid and Gas Phases

BY G. DAVIDSON
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1 Introduction

The format of this Chapter will be slightly different from that for earlier years. Papers dealing with essentially static situations will be dealt with first – with each Group of the Periodic Table discussed in turn. Results on dynamic systems will then follow – again on the basis of the Periodic Groups, with papers on paramagnetic compounds being dealt with last.

2 Stereochemistry

2.1 Compounds of Group 1. – (^{6}Li, ^{15}N) and (^{6}Li, ^{13}C) couplings were observed for mixed complexes formed between LiCH$_2$CN and chiral lithium amides (^{1}H, ^{6}Li, ^{13}C, ^{15}N data).[1] ^{7}Li and ^{31}P{^{1}H} HMQC experiments were used to assign the structures of benzyllithium complexes of *N*-methyl-*N*-benzylphosphinamide, *e.g.* (1).[2] ^{1}H and ^{13}C NMR and ^{13}C-^{1}H correlation spectra were used to confirm the presence of a C-Si-Ni-Li 4-membered heterocycle in [benzylbis(dimethylamino)-methylsilyl-κ^2-*C,N*](*N, N, N′,N′* -tetramethylenediamine-κ^2-*N,N*)lithium(I).[3]

The ^{7}Li NMR spectra of (CpAr$_5$)Li(thf)$_2$ and (CpAr$_5$)Li, where Ar = 3,5-^{t}Bu$_2$C$_6$H$_3$, suggest the presence of more than one species in solution, *e.g.* in thf/C$_6$D$_6$ the monomer and [(CpAr$_5$)$_2$Li][Li(thf)$_x$].[4] ^{2}H NMR spectroscopy was used to study cation π-interactions between LiCl, NaCl, KCl, RbCl, CsCl and AgNO$_3$ solutions with C$_6$D$_6$.[5] The complex (2) gives a ^{119}Sn resonance as a quartet at -819.8 ppm, due to ^{119}Sn^{-7}Li coupling, confirming the covalent Sn–Li bond in solution, even at room temperature.[6]

The ^{6}Li, ^{15}N and ^{13}C NMR spectra of the α-aminoalkoxide-LiHMDS mixed dimer, where LiHMDS = lithium hexamethyldisilazide, showed the presence of a pair of conformers.[7] ^{6}Li and ^{15}N couplings and ^{6}Li, ^{1}H HOESY data gave structural information for chiral lithium amides with chelating sulfide groups, *e.g.* (3).[8]

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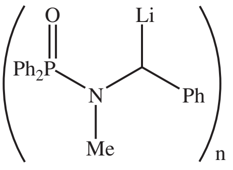

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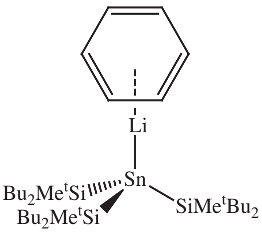

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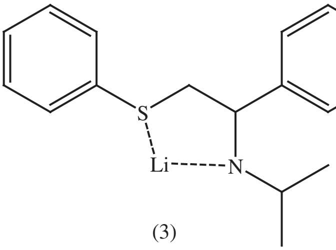


(3)

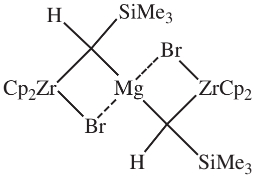
^{7}Li pulsed gradient spin-echo (PGSE) measurements on $LiPPh_2$ in thf or Et_2O solutions show that the compound is a monomer in the former, but a dimer in the latter solution.[9] Proton NMR chemical shifts have been used to examine perturbations in water structure in LiOH, KF or KCl solutions.[10]

Other lithium-containing systems studied by NMR included: alkyne lithium compounds with ligands tethered at C_2 (^{13}C);[11] *n*-[$CMe_2\{CHMeN(R)_2\}.Li$], where R = 2,6-$^iPr_2C_6H_3$ (^{1}H, ^{7}Li, ^{13}C);[12] $(Et_2O)LiSnPh_2Ar^*$, $(LiSnPh_2Ar^*)_2$, where Ar* = C_6H_3-2,6-$Trip_2$, Trip = C_6H_2-2,4,6-$^iPr_3$, (^{1}H, ^{7}Li, ^{13}C, ^{119}Sn);[13] $[Ph_2PTe][Li(TMEDA)_{1.33}(thf)_{1.33}]$, $[Ph_2PTe_2][Li(thf)_{3.5}(TMEDA)_{0.25}]$ and related (^{1}H, ^{13}C, ^{31}P);[14] $[1\text{-}LiNPhCHPh\text{-}2\text{-}NMe_2C_6H_4]_2$, $[1\text{-}LiNPhCHPhCH_2\text{-}2\text{-}NMe_2C_6H_4]_2$ (^{1}H, ^{7}Li, ^{13}C);[15] $[(R_fN)_2NLi(solv)_2$, where R_f = C_6F_5, solv = Et_2O, thf (^{1}H, ^{13}C, ^{19}F);[16] $(R\text{-}NP)Li(thf)_2$, where H(R-NP) = *N*-(2-diphenylphosphinophenyl)-2,6-di-R-aniline, R = Me, ^{i}Pr (^{7}Li{^{1}H}, ^{31}P{^{1}H});[17] $MeSi(2\text{-}C_5H_4N)_3Li(X)$, where X = 0.8Cl,0.2Br (^{1}H, ^{7}Li);[18] $Li[P(NH^tBu)_2(N^tBu)\text{-}(NSiMe_3)]$ and related (^{1}H, ^{7}Li, ^{13}C, ^{31}P);[19] $[\{Ph_2P(O)N(CH_2Ph)\text{-}CH_3\}.LiOC_6H_2\text{-}2.6\text{-}\{C(CH_3)_3\}_2\text{-}4\text{-}CH_3).C_7H_8]_2$ (^{1}H, ^{7}Li, ^{13}C, ^{31}P).[20]

Proton NMR data have established that Na^+ or K^+ can be encapsulated into a range of new calix[4]crowns-4 and calix[4]crowns-5.[21] Similar data show that Na^+ and K^+ can bind to a calix[4]semitube having urea functionality.[22] The solution ^{1}H NMR spectrum of $Na_{11}(O^tBu)_{10}(OH)$ includes a peak at 3.21 ppm due to the hydroxyl group.[23] Samples in the $NaF\text{-}AlF_3\text{-}Al$ system at 1030°C were characterised by ^{19}F, ^{23}Na and ^{27}Al NMR spectroscopy.[24] Proton and ^{133}Cs NMR spectroscopy gave evidence for complexation of Cs^+ by a *p-tert*-butylcalix[6]arene hexaacetamide derivative.[25]

2.2 Compounds of Group 2. – ^{9}Be chemical shift data were used to study hydrogen-bonding between $Be(H_2O)_4{}^{2+}$ and water in the second coordination sphere.[26]

Evidence was found (^{1}H and ^{31}P NMR) for the formation of (neopentyl)$Mg(HMPA)_2{}^{+}$ and (neopentyl)$_3Mg^{-}$ in solutions containing Mg(neopentyl)$_2$ and hexamethyphosphoramide (HMPA).[27] Proton NMR spectra of C_6D_6 solutions showed the presence of two isomers of (4).[28] The complex (5) was characterised by ^{1}H, ^{13}C and ^{31}P NMR.[29] Characteristic ^{1}H and $^{13}C\{^{1}H\}$ data were reported for Br(thf)Mg[oxam(R)$_2$]Mg(thf)Br, where oxam(R)$_2$ = (6), R = OMe or NMe_2.[30] ^{1}H and ^{13}C NMR, with (^{1}H, ^{1}H) COSY and (^{1}H,^{13}C) HETCOR data on $[Mg(L)]^{2+}$, where the ligands are bis(pendant arm) macrocyclic Schiff bases, suggest that there is approximately pentagonal bipyramidal coordination at the magnesium.[31]



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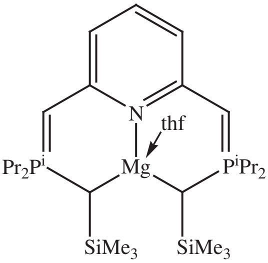
Calculated inter- and intramolecular indirect NMR spin-spin coupling constants and chemical shifts gave predicted values associated with inner- and outer-sphere binding of Mg^{2+} or Zn^{2+} to a guanine base.[32] NMR spectra (^{2}H, ^{23}Na and ^{31}P) were used to study the interaction of M^{2+} (=Mg, Cd or Ni) with liquid crystalline NaDNA solutions.[33] *Ab initio* and DFT methods were used to calculate ^{17}O NMR shieldings for $OM_6(OH)_{12}{}^{2-}$, where M = Mg, Ca or Sr.[34]



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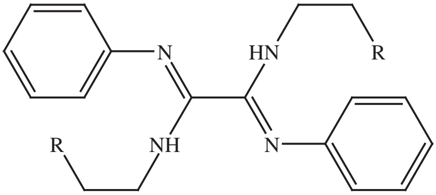

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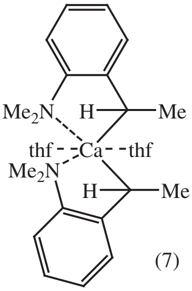

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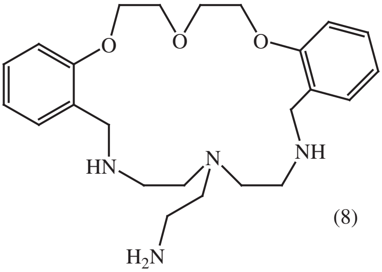


(8)

The ^1H NMR spectrum of (7) at low temperatures shows the presence of two diastereoisomers.[35] *Ab initio* calculations have been made of ^{15}N chemical shift differences induced by Ca^{2+} binding to EF-hand proteins.[36] ^1H and ^{13}C NMR spectra were used to characterise calcium pyrrolates, [Ca{(2-dimethylamino-methyl)pyrrolyl}$_2$(D)$_n$], where D = thf, py, n = 2, D = dmf, TMEDA, n = 1.[37] The ^1H NMR spectra of (η^5-Gaz)M(thf)$_2$, where M = Ca or Yb, and (η^5-Gaz)Yb(py)$_2$, where Gaz = 1,4-dimethyl-7-isopropylazulene, show exclusive formation of N_2-*ansa*-metallocenes.[38] ^1H-^{15}N heteronuclear single quantum coherence spectra were used to study and compare the binding of Ca^{2+} and La^{3+} to calmodulin and a calmodulin-binding peptide.[39]

^1H and ^{13}C NMR spectra of M^{2+} (M = Ca, Ba, Pb) complexes with the Schiff base formed from gossypol and 5-hydroxy-3-oxapentylamine show the formation of 1 : 1 complexes.[40] Complexes $[M(L)]^{2+}$, where M = Ca, Ba, Zn, Cd, Pb, L = (8) were characterised by ^1H NMR.[41] An NMR study has been made of the binding of Ca^{2+} to synthetic hexasaccharide models of modified heparin.[42]

^1H and ^{13}C NMR spectra were used to study $[M(thd)_2(L)_n]_m$, where M = Ba, L = Hpz, Hpz*, m = 2, n = 2; M = Sr, L = Hpz, Hpz*, m = 1, n = 3; Hthd = 2,2,6,6-tetramethylheptane-3,5-dione, Hpz = pyrazole, Hpz* = 3,5-dimethylpyrazole.[43]

2.3 Compounds of Group 3 (Yttrium, Lanthanides, Actinides).

– The ^{13}C NMR spectrum of $(Y_2C_2)@C_{82}$ in CS_2 solution is consistent with encapsulation of Y_2C_2 in a C_{82}–$C_{3v}(8)$ cage.[44] The complex $Y[CH(SiMe_3)(SiMe_2OMe)]_3$ gives ^1H, ^{13}C and ^{29}Si NMR spectra in solution consistent with the presence of two isomers.[45] ^1H, $^{13}C\{^1H\}$ and ^{89}Y spectra were reported and assigned for $[\{(\eta^5\text{-}C_5Me_4SiMe_2R)Y\}_4(\mu\text{-}H)_4(\mu_3\text{-}H)_4(thf)_2]$.[46]

^1H, ^{11}B and ^{13}C NMR data were used to characterise [1,1′-{5,6-(μ-H)$_2$-*nido*-2,4-(SiMe$_3$)$_2$-2,4-C$_2$B$_4$H$_4$}-2,2′,4,4′-(SiMe$_3$)$_4$-1-1′-*commo*-Ln(2,4-C$_2$B$_4$H$_4$)$_2$, where Ln = Dy, Er, and related species.[47] DFT calculations have been reported for ^{13}C chemical shifts for uranyl sulphene complexes and anions in the gas-phase.[48]

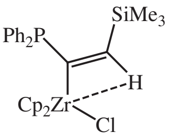
2.4 Compounds of Group 4.

– The ^1H NMR spectra of $(R_2NO)_2Ti(CH_2Ph)_3$, where R = CH_2Ph or Et, show that the hydroxylaminato ligands exhibit both η^1- and η^2- binding modes.[49] The ^1H and ^{13}C NMR spectra of (Me$_2$PMEN)-Ti(CH$_2$Ph)$_2$, where H$_2$(Me$_2$PMEN) = *N,N′*-dimethyl-*N,N′*-bis[(*S*)2-methyl-pyrrolidine]ethylene diamine, show that C_2 symmetry is retained on the NMR time-scale between −80 and +30°C.[50]

^1H and ^{13}C NMR data for $(L)Ti(NEt_2)_2$ and $(L)Zr(NEt_2)(thf)$, where H_2L = 2,2′-di(3-methylindolyl)methane, have been reported. The zirconium complex is 5-coordinate, with a coordinated thf molecule, as shown.[51] ^1H and $^{31}P\{^1H\}$ spectra forTiI$_4$[*o*-C$_6$H$_4$(EMe$_2$)], where E = P or As, are consistent with *cis*, 6-coordinate octahedral geometries.[52] The anion $Ti_2Cl_9^-$ in solution has $^{47,49}Ti$ NMR spectra showing that it comprises two face-sharing octahedra.[53]

^{1}H NOESY and ^{1}H,^{19}F NOESY spectra were used to determine the solution-phase structures of metallocenium homogeneous catalyst ion-pairs, *e.g.* $[Cp_2ZrMe]^+[MeB(C_6F_5)_3]^-$ and related systems.[54] Cation-like intermediates formed by activation of zirconocenes, L_2ZrCl_2 (L = Cp, indenyl, fluorenyl) with methylaluminoxane, have been characterised using ^{1}H NMR.[55]

Detailed ^{1}H and $^{13}C\{^1H\}$ assignments were used to deduce the geometry for the substituted salicylaldimine derivatives of zirconium alkyls, $Zr(L)R_2$, where R = CH_2Ph or $CH_2{}^tBu$, H_2L = derivatives of 2,2′-diamino-6,6′-dimethylbiphenyl.[56]



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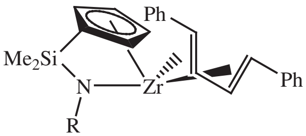
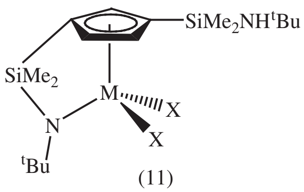


(10)

^{1}H, ^{13}C and ^{31}P NMR data for (9) and similar complexes gave evidence for the agostic interaction shown.[57] Solution ^{1}H NMR spectra of (10) show that for R = ^{i}Pr the supine isomer is formed exclusively, while for R = ^{t}Bu a 2 : 1 mixture of the supine and prone isomers is formed.[58] Mesoporous SiO_2-ZrO_2 aerogels were studied by ^{29}Si liquid-state NMR.[59] The ^{13}C and ^{31}P solution NMR spectra have been reported for $\{Zr[\mu,\mu'\text{-}O_2P(\mathit{cycl}\text{-}C_6H_{11})_2](O^tBu)_3\}_2$ and $Zr_3[\mu,\mu'\text{-}O_2P(O^tBu)_2]_5(O^tBu)_7$. The latter shows the presence of three phosphorus environments (ratio approximately 2 : 2 : 1).[60]

NMR data were also reported for: $CpTiX_3$, Cp^*TiX_3 (X = Cl, Br) and related (^{47,49}Ti);[61,62] $[Ti(\eta^5{:}\eta^1\text{-}C_5H_4SiMe_2N^tBu)Me(NC_5H_5)]^+$ (^{1}H);[63] (11), where M = Ti, Zr, X = NMe_2, CH_2Ph; (^{1}H, ^{13}C);[64] $Ti[\eta^5{:}\eta^1\text{-}(C_5H_4)B(NR_2)NPh](NMe_2)_2$ (^{1}H, ^{11}B, ^{13}C, ^{29}Si);[65] $Ti[\eta^5{:}\eta^1$-2-methylindenyl)-$SiMe_2NCMe_3]_2[CH_2]_n$ (n = 6, 9, 12) (^{1}H, ^{13}C);[66] $[Ti(N_3)_n]^{(n-4)-}$, n = 4, 5, 6 (^{14}N);[67] (12), R = Cl or Me (^{1}H, ^{13}C);[68] (13), E = C or Si, (^{1}H, $^{13}C\{^1H\}$);[69] $[(2,6\text{-}Ph_2\text{-}C_6H_3\text{-}\eta^5\text{-}C_5H_4)Zr(NEt_2)_3]$ (^{1}H, $^{13}C\{^1H\}$);[70] silsesquioxane-tethered fluorene ligand and their zirconium η^5-complexes, *e.g.* $Cp^*[(c\text{-}C_5H_9)_7Si_8O_{12}\text{-}X\text{-}Flu]ZrCl_2$, where Flu = fluorene, X = CH_2, $(CH_2)_3$ or $C_6H_4CH_2$ (^{13}C, ^{29}Si);[71] (14) and related complexes, (^{1}H, ^{13}C);[72] and $Cp^{\P}{}_2Zr(OOCCH_2S\text{-}\kappa^2\text{-}O,S)(\mu\text{-}O\text{-}OOCCH_2S\text{-}\kappa^1\text{-}O,\kappa^2\text{-}O,S)(MoCp'_2)$, where $Cp^{\P}$ = C_5EtMe_4, Cp′ = C_5Me_4H.[73]



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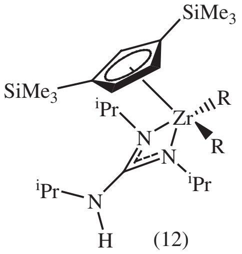

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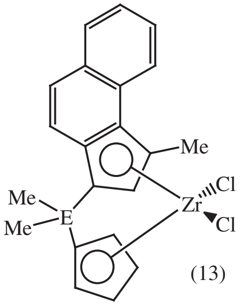

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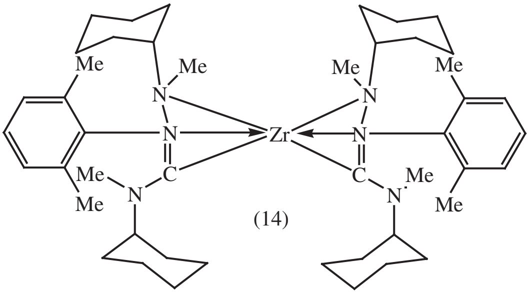

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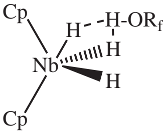
2.5 Compounds of Group 5. – NMR data (^{1}H, ^{13}C, ^{31}P, ^{51}V) were reported for ^{t}BuN=V^{III}Cp(PR$_3$)$_2$, where R = Me, Et, ^{n}Bu, OMe, OPh; R$_3$ = Me$_2$Ph, MePh$_2$ – characteristic ^{51}V chemical shifts, J(^{51}V^{31}P) and J(^{51}V^{14}N) coupling constants were determined.[74] The ^{51}V NMR data for VOL(hq), where Hhq = 8-hydroxyquinoline, H$_2$L = dibasic tridentate ONO Mannich bases, all show a single signal, *i.e.* only one isomer is present.[75] The ^{1}H, ^{13}C and ^{31}P NMR of VO(acac)L, VOCl$_2$L, and VOClL$_2$, where HL = HN(PPh$_2$NR)$_2$, R = Ph, SiMe$_3$, show that they are all monomers, with bidentate L$^-$.[76] Coordination interactions between K$_3$[VO(O$_2$)C$_2$O$_4$].H$_2$O and imidazole or substituted imidazoles were probed by ^{1}H, ^{13}C and ^{51}V NMR.[77]

The ^{51}V NMR spectra of aqueous solutions of [VO(O$_2$)*cmaa*(H$_2$O)]$^{2-}$ and [VO(O$_2$)(H*cmaa*)(H$_2$O)]$^-$, where H$_3$*cmaa* = (*R,S*)-*N*-(carboxymethyl)aspartic acid, gave evidence for the presence of both *exo*- and *endo*- forms.[78] DFT calculations gave a predicted ^{51}V chemical shift for [VO(O$_2$)$_2$(Im)]$^-$, where Im = imidazole.[79] ^{51}V NMR data for [VO(O$_2$)$_2$(phen)]$^-$ show that it is substantially more inert to ligand substitution than the bipy analogue.[80] ^{1}H, ^{13}C and ^{51}V NMR, with NOESY experiments, were used to determine the solution structures of VO(OR)(ONNO), where R = ^{i}Pr, ^{t}Bu or CH$_2$CF$_3$, H$_2$[ONNO} = bis(phenoxy)amine ligand.[81] The ^{51}V NMR spectra of aqueous solutions of [VO(O$_2$)(oxalate)(L)]$^-$, where L = bipy or phen, show that they are stereochemically rigid.[82]



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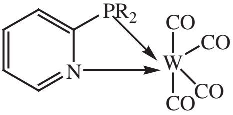
Proton NMR spectra of solutions of Cp_2NbH_3 and fluorinated alcohols gave evidence for hydrogen bond formation, *i.e.* (15).[83] The proton NMR spectrum of $[(L)Ta(\mu\text{-}H)_2(\mu\text{-}O)Ta(L)]^-$, where L = 2,6-bis(3-*tert*-butyl-5-methyl-2-hydroxybenzyl)-4-*tert*-butyl phenol, includes resonances at 10.3 and 12.1 ppm due to bridging hydrides.[84]

NMR data were also reported for: *cis*-VO_2L (L = salicylaldehyde semicarbazone and related) (^1H, ^{13}C);[85] $VO(O_2)(bpa)$, $[VO(O_2)(heida)]^-$ (Hbpa = bis(picolyl-β-alanine, H_2heida = *N*-(2-hydroxyethyl)iminodiacetic acid) (^{17}O, ^{51}V);[86] $[V_2O_2(O_2)_2(R,S\text{-mand})_2]^{2-}$ (mand = mandelato) (^{51}V);[87] $ClV[S_2P(OR)_2]_2$ (R = Pr, Ph), cyclic $ClV[S_2POGO]_2$ (G = $–CH_2CMe_2CH_2–$, $–CMe_2CMe_2–$, $–CH_2CEt_2CH_2–$);[88] $[MNb_{12}O_{40}]^{16-}$ (^{17}O);[89] $NbCl_5$-(LiCl/KCl), $NbCl_5$-NaCl and $NbCl_5$-CsCl melts;[90] and Ta(V)-1,2,3-triazolato complexes, *e.g.* $Cp^*TaPh_3[N_3C_2(COOMe)_2]$.[91]

2.6 Compounds of Group 6. – The ^1H, ^{13}C and ^{14}N NMR spectra of $M(N^tBu)_2(dpma)$, where M = Cr, Mo or W, dpma = *N,N*-di(pyrrolyl-α-methyl)-*N*-methylamine, show that the axial (bent) alkylimido appears to be more electron-rich than the equatorial (linear) ligand.[92]

The complex $CpMoMnPt(PPh_3)_2(CO)_5(\mu_3\text{-}Se)_2$ has a single resonance in the $^{31}P\{^1H\}$ spectrum , with J_{Pt-P} 2762 Hz.[93] NMR data (^1H, $^1H\{^{11}B\}$, ^{11}B, $^{11}B\{^1H\}$, ^{13}C) for $[CpMo(CO)_3I.Ag\text{-}(\textit{closo}\text{-}(CB_{11}H_{11}Br)]_2$ show that the Cp ligands are equivalent, with $CB_{11}H_{11}Br^-$ resonances very similar to those for the free ion.[94] The ^1H NMR spectra of $[CpMo(L)]Cl_2$, where L = 6-mercaptopurine, 6-mercaptopurine ribose, and related ligands, are consistent with coordination in solution *via* S(6) and N(7) or N(1).[95] ^{31}P NMR data were reported for the unstable complex $CpMo(PPh_2)_2$.[96] Similar data show that $Na_{24}[Na_4(H_2O)_6\{(Mo_2O_4)_{10}(O_3PCH_2PO_3)_{10}(CH_3COO)_8(H_2O)_4\}]$ and related species are stable in solution at room temperature.[97]

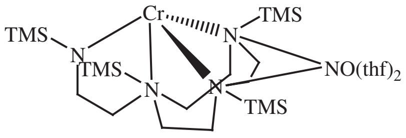


(16)

The complexes (16), where R = Ph or NMe_2, showed large values for J_{PC} for the CO ligand *trans* to P.[98] The first μ-silyleneditungsten complex, $(\mu\text{-}SiPh_2)W_2(CO)_{10}$ has been characterised by ^1H, $^{13}C\{^1H\}$ and $^{29}Si\{^1H\}$ NMR.[99] The ^{13}C NMR spectrum of $Cp(CO)(CN\text{-benzyl})FeNCW(CO)_5$ showed that it was possible to differentiate the isocyanide from the bridging cyanide (the latter gave characteristic coupling to ^{183}W).[100] The ^1H NMR spectrum of Tp*WOS(pyS), where Tp* = hydridotris(3,5-dimethylprazol-1-yl)borate, shows that the molecule has C_1 symmetry.[101] DFT calculations have been made of NMR parameters for the cluster WAu_{12}.[102] There have been a number of NMR studies of a wide range of polytungstate complexes in solution.[103–112]

NMR data were also reported for $[\{\eta^5\text{-}MeC_5H_4Cr(CO)_2\}_2Se]$, where R = Me, MeCH(OH) or PhCH=CMe (^1H, ^{77}Se);[113] $(OC)_5M{=}C$

$(NMeCH_2CH{=}CHCH_2OH)R$ (M = Cr, W; R = Me, Ph) (^1H, ^{13}C, ^{29}Si, $^1H/^1H$ COSY, $^1H/^1H$ NOESY, $^{13}C/^1H$ HETCOR);[114] $(OC)_4Cr{=}C(\eta^2\text{-}NMeCH_2\text{-}CH{=}CHCH_2OH)R$ (R = Me, Ph) (^1H, ^{13}C, ^{29}Si, ^{31}P, $^1H/^1H$ COSY, $^{13}C/^1H$ HETCOR, $^{31}P/^{31}P$ EXSY);[115] $\{\eta^5\text{-}RC_5H_4)_4Cr_4Se_4$ (R = MeCO, MeO_2C) (^{77}Se);[116] vinylferrocene (vfc) and $M(CO)_5(\eta^2\text{-vfc})$ (M = Cr, Mo or W) (^1H, ^{13}C);[117] (17) (^1H, ^{13}C);[118] (18) (^1H, ^2H);[119] (19) (M = Mo,



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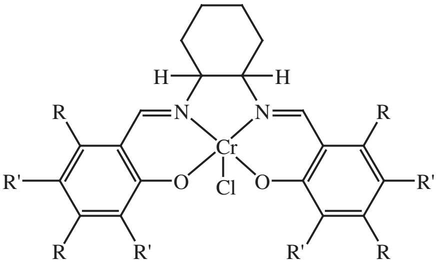

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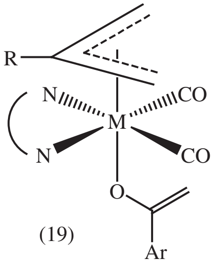

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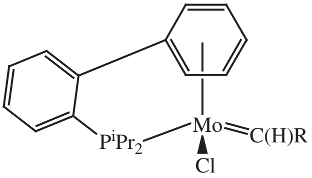
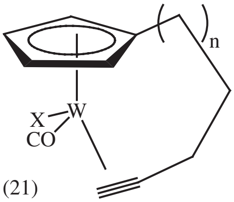


(20)

R = H, Me, Ar = Ph, naphthyl; M = W, R = H, Ar = phenyl) (^1H, ^{13}C);[120] (20) (R = Ph, $SiMe_3$) (^1H, ^{13}C, ^{31}P);[121] $Cp(OC)_3W(CH_2)_nMo(CO)_3Cp$ (n = 3–6) (^1H, ^{13}C, with COSY, HETCOR, HSQC);[122] 1,3-[*cis*-$Mo(CO)_4(PPh_2)_2N]_2C_6H_4$ (^1H, ^{13}C, ^{31}P);[123] $(\eta^5\text{-}C_5H_4R)_2Mo_2(CO)_6$ (R = MeCO, MeO_2C) (^1H, ^{13}C, ^{31}P);[124] $Cp_2Mo_2Fe_2(RNC)(CO)_6(\mu_3\text{-}E)(\mu_3\text{-}E')$, where R = ^{i}Pr, ^{t}Bu, E = E′ = Se, E = S, E′ = Te) (^1H, ^{13}C, ^{77}Se, ^{125}Te);[125] *mer*-$[(\eta^2\text{-}C_{60})M(CO)_3\{(+$ or $-)$DIOP}], where M = Mo or W, DIOP = 2,3-*O,O′*-isopropylidene-2,3-dihydroxy-1,4-bis(diphenylphosphanyl)butane (^1H, ^{13}C, ^{31}P);[126] *cis*-$Mo(CO)_4$ (L-L′), *cis*-$Mo(CO)_2(L\text{-}L')_4$ (L-L′ = *N*(1)-methyl-2-(*p*-X-phenylazo)imidazoles, X = MeO, Me, H, Br, CF_3, NO_2) (^1H, ^{13}C, ^{95}Mo);[127] $MoCl(NAr)_2R$ (Ar = 2,6-$^iPr_2C_6H_3$, R = CH_2CMe_2Ph, CH_2CMe_3);[128] $M(N^tBu)_2\{(3,5\text{-}^tBu_2)_2salen\}$ (M = Mo, W) and related (^1H, $^{13}C\{^1H\}$);[129] MoO_2L_2 (HL = β′-hydroxy-β-enaminones) (^1H, COSY, HMQC);[130] $[MoO(O_2)_2(H_xL)]^{2-}$, where H_xL = oxalic, tartaric, glycolic, malic acids, and $[MoO_2(O_2)(L)]^-$ (L = oxalate) (^{13}C);[131] $MoO_2Cl_2(L\text{-}L)$, where L-L = $(OPMe_3)_2$, $Ph_2P(O)CH_2P(O)Ph_2$, $Ph_2P(O)CH_2CH_2P(O)Ph_2$, *o*-$C_6H_4[P(O)Ph_2]_2$ (^1H, $^{31}P\{^1H\}$, ^{95}Mo);[132] $Mo_2O_2(\mu\text{-}S_2)[S_2P(OR)_2]_2.L$, where R = Me, Et, ^{i}Pr, L = dmso, dmf, py;[133] $[MS_4(CuBp)_4]^{2-}$, where M = Mo, W; Bp = anionic bis(pyrazolyl)borate, $BPz_2^{[2-]}$);[134] (21) (n = 1, X = Cl; n = 2, X = Cl, I) (^1H, ^{13}C);[135] $Tp^*W(S_2CNEt_2\text{-}\kappa\text{-}S)(\eta^2\text{-}PhC{\equiv}CH)(CO)$ and related (Tp* = hydridotris

(3,5-dimethyl-pyrazol-1-yl)borate) (^{1}H, ^{13}C);[136] $Ph_3E\text{-}CH{=}WCl_2(O^tBu)_2$ (E = Si, Ge, Sn) (^{1}H, ^{13}C, ^{29}Si);[137]



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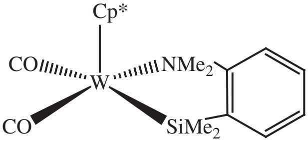

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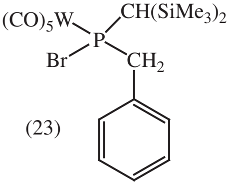

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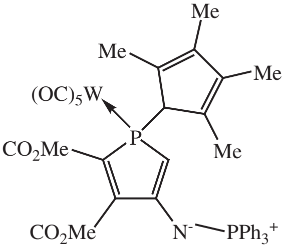

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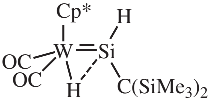


(25)

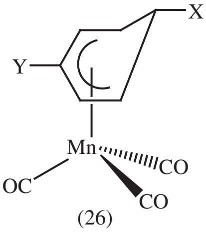
$W(NC_4Me_4)L_2$ (L = Cl, CH_3) (^{1}H, ^{13}C{^{1}H});[138] (22) (^{1}H, ^{29}Si{^{1}H});[139] $W(CO)_5(PCy_3)$, *trans*-$W(CO)_4(PCy_3)_2$ (^{1}H, ^{13}C, ^{31}P);[140] $(OC)_5W\text{-}P(R){=}C(H)NMe_2$ (R = *c*-C_3H_5, *c*-C_5H_9) (^{1}H, ^{13}C, ^{31}P);[141] (23) (^{1}H, ^{13}C{^{1}H});[142] (24) and related (^{1}H, ^{13}C, ^{31}P);[143] $W(\eta^2\text{-}PhC{\equiv}CPh)_3(\eta^1\text{-}Ph_2PC{\equiv}CPPh_2)$ (^{31}P{^{1}H});[144] (25) (^{1}H, ^{29}Si);[145] and $[(PO_4)\{WO(O_2)_2\}_4]^{3-}$ and related (^{31}P).[146]

2.7 Compounds of Group 7. – Trends in the quadrupole coupling constants of ^{55}Mn, ^{59}Co and ^{187}Re have been analysed for $(\eta^5\text{-}Me_nC_5H_{5-n})M(CO)_3$ (M = Mn, Re) and $(\eta^5\text{-}Me_nC_5H_{5-n})Co(CO)_2$ (n = 0–5).[147]

The proton NMR spectrum of *fac*-$Re(CO)_3(dpkbh)Cl$ in dmf is consistent with strong complex/solvent interactions (dpkbh = di-2-pyridylketonebenzoylhydrazone).[148] ^{31}P{^{1}H} NMR results reveal *cis*-chelate bidentate ligand coordination in *fac*-$Re(CO)_3Br[Ph_2P(CH_2)_nPPh_2]$ (n = 1, 2 or 3).[149] NMR data (^{1}H, ^{13}C) of $Re(CO)_3(L)$, where HL = *N*-(2′-hydroxybenzyl)-2-amino-2-deoxy*d*-glucose, show that L^- is coordinated *via* amino N, phenolate O and C-3 hydroxyl O.[150] Similar experiments on $(OC)_4Re\{\eta^2\text{-}C(Me)C(CO_2Me)C(NRR')\}$, where R = R′ = Et, R = H, R′ = Ph, $(CH_2)_2OH$, *p*-tol, show that these have less carbene-like character than do alkoxy analogues.[151] NMR data confirmed the stereochemistry of $[Re_2X_3(\mu\text{-dppm})_2(CO)(CN\text{–}Xyl)(L)]^+$, where X = Cl, Br, L = 3,4-Me_2py or PEt_3.[152] The ^{31}P NMR spectrum of $ReOCl(P\text{–}O)_2$, where P–OH = 2-[bis(ethoxyethyl)phosphino]phenol, is consistent with a *cis*-PP, twisted octahedral complex (^{1}H, ^{13}C{^{1}H} also reported).[153] ^{31}P{^{1}H} data for $ReOX_2(OR)(dppe)$, where X = Cl or Br, R = Me, Et, Pr, Ph, Cy, CH_2CH_2OH, show that the OR group is *trans* to the Re=O bond.[154]

The complex $[ReH_2(O)(Cyttp)]^+$, where Cyttp = $PhP(CH_2CH_2CH_2PCy_2)_2$, has proton resonances at δ −1.04 (hydride *trans* to O), −12.62 (hydride *cis* to O).[155] ^{1}H and ^{13}C NMR spectra show that $[ReO(cyclen\text{-}H)X]^+$, where X = Cl or I, cyclen = 1,4,7,10-tetraazacyclododecane, exist as single isomers in solution.[156] Three isomers of $Re_2(\mu\text{-}PP)_2(O\text{-}N\text{-}O)Cl_2$, where PP = dppm, O–N–O = pyridine-2,6-dicarboxylate, show distinct ^{31}P{^{1}H} NMR spectra – showing *cis,cis*-, *trans,trans*- and *trans,cis*-coordination of the μ-dppm ligands.[157] Such spectra for *fac*-$Re(CO)_3Br_2[R_2P(S)P(S)\text{-}PR_2]$, where R = Me, Et, ^{n}Pr, ^{n}Bu or Ph, are consistent with *cis*-chelated ligands.[158]

The ^{13}C NMR spectrum of ^{13}C-labelled $[Re_4Os_2Se_8(CN)_{16}]^{2-}$ is consistent with the presence of a mixture (1 : 2) of *cis*- and *trans*-isomers in dmso solution.[159] ^{1}H and ^{31}P NMR. spectra show retention of the solid state stereochemistry in solution for $[Re_6(\mu_3\text{-}Se)_8(PEt_3)_nL_{6-n}](SbF_6)_2$, where L = nicotinamide, n = 3, 4 or 5.[160]



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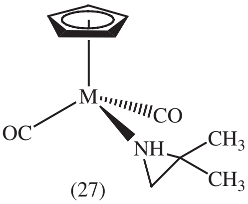
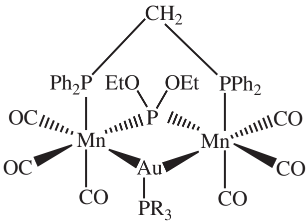


(27)

NMR data have also been reported for $Mn(CO)_3[CymB(pz)_3]$, $Mn(CO)_3[CymB(pz)_2(OH)]$ (Cym = cymantryl, $Mn(CO)_3$, pz = pyrazolyl) (^{1}H, ^{11}B, ^{13}C);[161]



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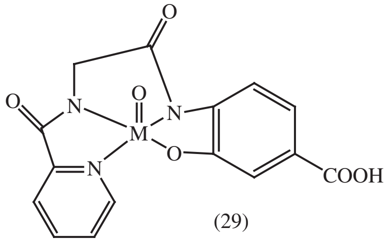

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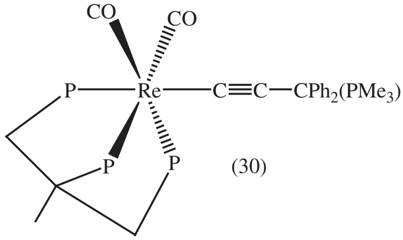

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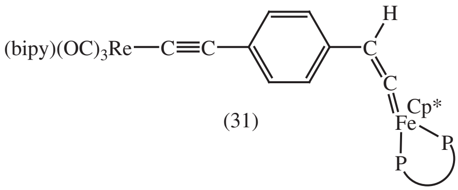

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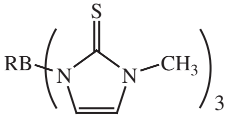
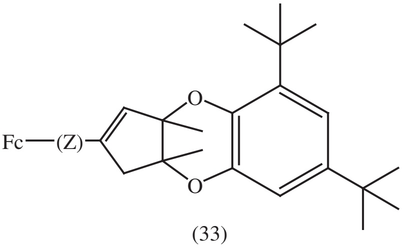


(32)

(26) (X = Cl, Y = Me; X = Me, Y = Cl) (^{1}H);[162] (27) (M = Mn, Re) (^{1}H, ^{13}C{^{1}H});[163] $[Mn(CO)_5(L)]^+$ (L = tris(1-cyclohepta-2,4,6-trienyl)phosphane) (^{1}H, ^{13}C, ^{31}P);[164] $[1\text{-}(\mu\text{-}B)\text{-}4\text{-}H\text{-}(NC_5H_5)\{(C_5H_4Me)Mn(CO)_2\}_2]$ (^{1}H, ^{11}B, ^{13}C);[165] (28) (R = Ph, *p*-tolyl) (^{31}P{^{1}H});[166] $Tc(CO)_3{}^+$ complexes of [(5-aminopentyl)-pyridi-2-yl-methylamino]acetic acid and related ligands;[167] (29) (M = ^{99g}Tc, Re) (^{1}H, ^{13}C);[168] $[Re(CN^tBu)_3(Cyttp)]^+$, where Cyttp = $PhP(CH_2CH_2CH_2PCy_2)_2$, (^{1}H, ^{13}C{^{1}H}, ^{31}P{^{1}H});[169] *fac*-$[Re(ClCH_2Cl)(CO)_3L]^+$ (L = 1,2-bis(diphenylphosphinite)ethane) and *fac*-$Re(OTf)(CO)_3L$ (^{1}H, ^{13}C{^{1}H}, ^{31}P{^{1}H}, ^{19}F{^{1}H});[170] (30) and related species (^{1}H, ^{13}C{^{1}H}, ^{31}P{^{1}H});[171] (31) (^{1}H, ^{13}C, ^{31}P{^{1}H});[172] $[(bipy)Re(CO)_3L]^+$ (L = aza-15-crown-5 linked to alkenyl or alkynyl spacer groups (1-D and 2-D ^{1}H);[173] chiral chelate complexes of Re(I), Pd(II) and Pt(II) with 1,5-(*R,R*)- and 1,5-(*S,S*)-bis(2-methylbenzyl)-3,7-diphenyl-1,5-diaza-3,7-diphosphacyclooctane (^{1}H, ^{13}C, ^{31}P);[174] $[Re(XQ^+)(CO)_3(NN)]^{2+}$ (NN = bipy, 4,4′-di-Me-bipy; XQ^+ = *N*-methyl-4,4′-bipyridinium) (^{1}H, including 2-D NOESY);[175] $Re[RB(tim^{Me})_3\text{-}\kappa^3\text{-}S,S,S](CO)_3$, where $RB(tim^{Me})$ = (32) (^{1}H, ^{11}B);[176] and $[Re(O)X_2(3,5\text{-}Me_2pzH)_2]_2(\mu\text{-}O)$ (X = Cl, Br) (^{1}H, ^{31}P).[177]

2.8 Compounds of Group 8. – ^{1}H and ^{13}C NMR experiments (1-D and 2-D – COSY, HSQC, HMBC) gave data on the stereochemistry of (33), where Z = no atom or –C≡C–, and related species.[178] ^{1}H and ^{13}C, with ^{1}H/^{1}H NOESY, data have been reported for enantiopure chiral bis-ferrocenes with S or N substituents.[179] The structure of (34), with only a single P-B bond, was confirmed by ^{11}B and ^{31}P measurements.[180] The complexes (35), with R = H, Me, R′ = H, Me or Cl, were characterised by ^{1}H and 2-D ^{13}C{^{1}H}-COSY-NMR – showing the presence of two 5-membered mercuriocycles fused with ferrocenyl fragments.[181] ^{1}H and ^{11}B spectra show that the adduct $FcP.BBr_3$ (where FcP = 3,4-dimethyl-1-phosphaferrocene), unlike $FcP.BBr_2Fc$, is stable in $CDCl_3$ solution.[182] Detailed 1- and 2-D NMR heteronuclear double resonance spectra were reported and assigned for (36), together with ^{13}C, ^{15}N, ^{29}Si and ^{119}Sn data.[183]



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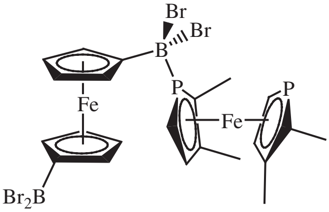

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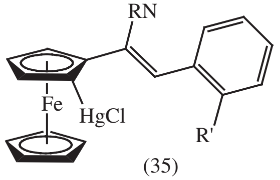

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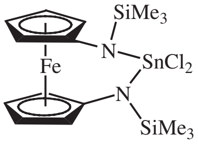

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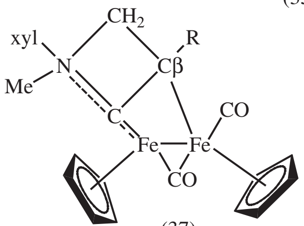

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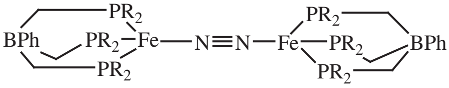


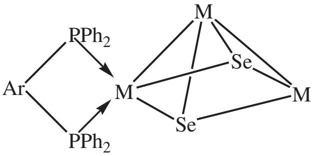
(38)

Low-temperature ^{1}H, ^{13}C and ^{29}Si NMR data for (37), where R = R′ = Et, R = Me, R′ = CH_2Ph, R = Et, R′ = Ph, show that B-N π-bonding depends upon the nature of R and R′.[184] Detailed ^{13}C NMR assignments, using an INEPT pulse sequence, have been made for a range of 1-sila-[1]ferrocenophanes.[185] ^{1}H and ^{13}C NMR data were given for a conformationally rigid 1 : 1 fullerene: ferrocene *ansa*-derivative of C_{60} and 1,1′-bis(diazoacetyl)ferrocene.[186] A correlation has been observed between Hammett σ-parameters and ^{13}C NMR chemical shifts for the metal-coordinated vinyl carbon atoms in $CpFe(CO)_2[\eta^2\text{-}CH_2C(H)NH(p\text{-}C_6H_4X)]^+PF_6^-$, where X = OMe, Me, H, Br, COMe, CN, NO_2.[187]

^{1}H and ^{11}B NMR data for 9-$[Fe(CO)_2(\eta^5\text{-}C_5H_5)]$-*nido*-7,8-$C_2B_9H_{12}$ and 7-$[Fe(CO)_2(\eta^5\text{-}C_5H_5)]$-*nido*-$As_2B_9H_{10}$ confirm the *nido* cage configurations in each case.[188] NMR spectra (^{1}H, $^{13}C\{^{1}H\}$, $^{29}Si\{^{1}H\}$) show that $[Cp(OC)_2Fe\text{-}Si(R)(R')OGaR''_2]_2$ remains as a dimer in C_6D_6 solution (R, R′, R″ = alkyl, aryl groups).[189] The complexes (38), where R = H, ^{n}Bu, COOMe, Ph, CH_2OH, Me, $SiMe_3$, tol, all show ^{1}H and ^{13}C NMR spectra corresponding to the presence of two isomers (due to orientations of the Me and Xyl groups with respect to the Ga–N vector).[190] The presence of a bridging Fe-N_2-Fe unit in (38, R = ^{i}Pr) is confirmed by ^{1}H, ^{15}N and ^{31}P NMR spectroscopy.[191]

The low-temperature ^{1}H NMR spectra of $L^{R}FeNHAr$, where L^{R} = methyl or *tert*-butyl –substituted diketiminate ligands; Ar = *p*-tolyl, 2,6-$C_6H_3Me_2$, 2,6-$C_6H_3{}^{i}Pr_2$, gave evidence for the presence of agostic interactions.[192] The proton NMR spectra of the complexes $[ML]^+$, where M = Fe or Ru, L = tris-chelating ligand (+)-(7*S*,10*R*)-X, where X comprises three 4,5-pinenopyridine subunits connected through a mesityl spacer, show that only one diastereoisomer is formed in each case.[193] $^{11}B\{^{1}H\}$ NMR data enabled a distinction to be made between $Fe\{(\mu\text{-}NC)B(C_6F_5)_3\}(\eta\text{-}C_5H_5)(CO)_2$ and $Fe\{(\mu\text{-}CN)B(C_6F_5)_3\}(\eta\text{-}C_5H_5)(CO)_2$.[194]

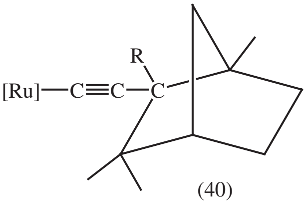
^{31}P NMR spectroscopy was used to differentiate *cis*- and *trans*-$[Fe(NCS)_2$(*rac*-$prP_4)]$ and *trans*-$[Fe(NCS)_2$(*meso*-$prP_4)]$, where prP_4 = 1,1,4,8,11,11-hexaphenyl-1,4,8,11-tetraphosphaundecane.[195] ^{1}H and $^{13}C\{^{1}H\}$ NMR data were given for *cis*-$Fe(NO)(E_2CNR_2)_2X$, where R = organic substituent, E = S, Se, X = Cl, Br, I, and ^{15}N data for E = S, R = Et, X = I. The data were consistent with structural rigidity.[196] ^{1}H and ^{31}P NMR data for $Fe[S_2C_2(CN)_2](^{t}BuNC)_4$ showed that there is strong Fe-C π-back-donation.[197] ^{1}H COSY and NOESY experiments gave detailed assignments for (39), where M = Fe, Ru, Ar = –$CH_2C_6H_4CH_2$–, and related species.[198]



(39)

NMR (^{1}H, ^{13}C, ^{15}N) data show that there is a haem-histidine cross-link in cyanobacterial haemoglobins from *Synechocyctis* sp. PCC 6803 and *Synechococcus* sp. PCC 7002.[199] Proton NMR spectroscopy was used to study the interaction of cytochrome *c* with micelles of sodium dodecyl sulfate.[200] The transient HNO (‘nitroxyl’) species can be trapped as an adduct with deoxymyoglobin, *i.e.* Mb-HNO, with a proton chemical shift of the iron-bound HNO at 14.8 ppm.[201] ^{1}H and ^{31}P NMR spectroscopy was used to probe the role of myoglobin as a scavenger of cellular NO in myocardium.[202]

^{13}C NMR data suggest significant carbene character for the acyl carbon in $[RhRu(OSO_2CF_3)(CO)_2\{\mu\text{-}C(CH_3)O\}(dppm)_2]^+$.[203] The complexes (40), where [Ru] = (η^5-C_9H_7)Ru-$(PPh_3)_2$, R = H, CN, Me or C≡CPh, have ^{1}H, ^{13}C{^{1}H} and ^{31}P{^{1}H} NMR spectra showing that each exists as only a single diastereoisomer.[204] (41), where R = Me or Ph, give ^{31}P NMR spectra showing that all of the phosphorus atoms are equivalent.[205] The single ^{31}P resonance for (42) shows that the structure is symmetrical.[206]



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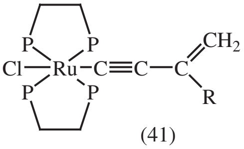

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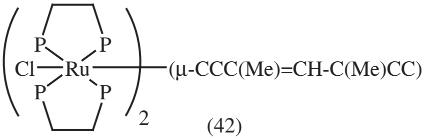

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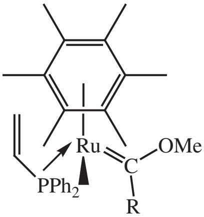

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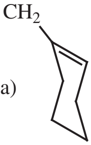

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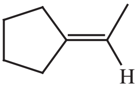

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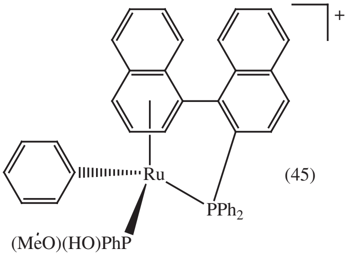

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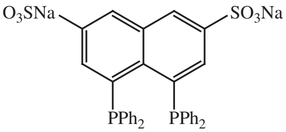

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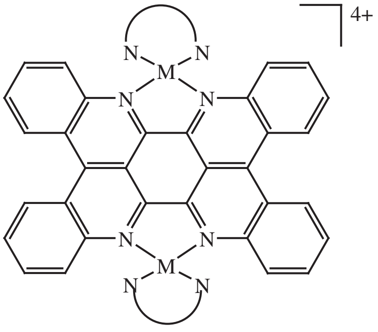
Encapsulation of the prochiral complex [CpRu(*p*-cymene)]$^+$ by a chiral host Ga_4L_6, where L = 1,5-bis(2′,3′-dihydroxybenzamido)naphthalene, gives ^{1}H NMR spectra showing that enantiotropic protons have become diastereotropic.[207] ^{1}H, ^{13}C{^{1}H} and ^{31}P{^{1}H} NMR spectra were used to characterise (43), where R = (44a or b). The Ru = C_α and C = CH carbons show ^{13}C peaks at 301.58, 137.90 and 133.62 ppm respectively.[208] The ^{1}H and ^{13}C{^{1}H} NMR spectra of the racemic mixture of $RuCl_2(1,2,4{-}C_6H_3Me_3)(PPh_3)$ only show an averaged signal for the enantiomers.[209] The solution ^{13}C NMR spectrum for Ru(II) complexes, *e.g.* (45), show that they have strongly distorted η^6-coordination.[210] The high-pressure ^{31}P NMR spectrum of the hydroformylation of 1-octene by $RuH(CO)_2$(sulfoxantphos), where sulfoxantphos = (46), gave evidence for *ee* and *ea* isomers of the catalyst.[211]

^{31}P{^{1}H} NMR data for $Ru(CO)_2$(P-S), where P-S = $Ph_2P(CH_2)_nP(S)Ph_2$, show that for n = 1, the ligand is *P,S*-chelating, while for n = 2–4, they are unidentate.[212] The ^{29}Si INEPT NMR spectrum of $Ru_2H_4(\mu\text{-}\eta^2{:}\eta^2{:}\eta^2{:}\eta^2\text{-}SiH_4)(PCy_3)_4$ shows the bridging coordination of SiH_4 *via* four σ-Si-H bonds to the Ru atoms.[213] The ^{1}H{^{11}B}, ^{11}B and ^{31}P{^{1}H} NMR spectra of RuX[7,8-$(PPh_2)_2$-7,8-$C_2B_9H_{10}](PPh_3)_2$, where X = H or Cl, reveal octahedral geometry with the carbaborane unit acting as a tridentate ligand.[214] ^{1}H, 2-D COSY, 1-D TOCSY and 1-D NOESY NMR spectra give detailed assignments for the ^{1}H resonances in bis(2,2′-bipyridyl)ruthenium complexes of di(2-pyridyl)methane and a number of multidentate derivatives.[215]

The ^{1}H NMR spectra of (47), where M, M′ = Ru or Os, N–N = bipy, show that for M = Ru, M′ = Os, the data are consistent with the presence of two diastereoisomers, ΔΔ/ΛΛ and ΔΛ/ΛΔ.[216] Proton NMR data produced evidence for positional isomerism of 9-EtGua (=9-ethylguanine) in α-[Ru(azpy)(bipy)(9-EtGua)$(H_2O)]^{2+}$, where azpy = 2-phenylazopyridine (*trans* to azo-N or to bipy respectively).[217] The ^{1}H NMR spectrum of Ru(ttp)(HNO)(1-MeIm), where ttp = tetratolyl-porphyrinato, shows a downfield resonance at 13.64 ppm from the HNO ligand.[218] A complete elucidation of the diastereoisomerism of (48) was obtained from 1-D and 2-D ^{1}H NMR spectra.[219] ^{1}H-^{1}H COSY data gave detailed assignments for Ru(dppt)(dien)$^{2+}$, where dppt = 3-(1,10-phenanthrolin-2-yl)-5,6-diphenyl-*as*-triazine.[220]



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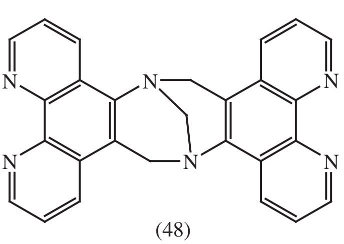

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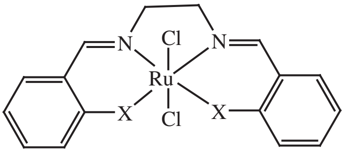

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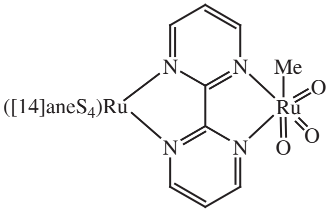

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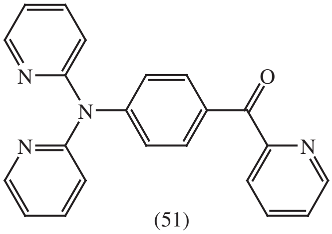


(51)

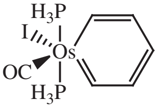
The ^{1}H NMR spectrum of δ-[Ru(azpy)$_2$Cl$_2$], where azpy = 2-phenylazopyridine, shows that only the all-*trans* isomer is present.[221] Similar data for [Ru(L)(4,7-dpphen)]$^{2+}$. where dpphen = diphenyl-1,10-phenanthroline, L = tetradentate bis-1,10-phenanthroline ligand, show C$_2$ symmetry for the complex in solution.[222] 1-D and 2-D ^{1}H NMR spectra were used to determine distinctive structural features for the (ΛΛ/ΔΔ)-*rac* and (ΛΔ/ΔΛ)-*meso* stereoisomers of [(bipy)$_2$M(pzdc)M(bipy)$_2$]$^{+}$, where M = Ru or Os, pzdc = pyrazole-3,5-dicarboxylate.[223] The *trans*-configuration of (49), where X = S(O)Me, was confirmed by ^{1}H NMR[224] ^{1}H NMR data confirm the bridging bidentate ligand in (50).[225]

^{1}H, ^{13}C and ^{31}P NMR spectra were able to differentiate *trans*- and *cis*-isomers of RuCl$_2$(L)(PPh$_3$), where L = 2,2′:6′,2″-terpyridine or 4,4′,4″-tri-*t*-butyl-2,2′:6′,2″-terpyridine.[226] The complex [Ru(bipy)$_2$(L)]$^{2+}$, where L = (51), gave very complex ^{1}H and ^{13}C NMR spectra which could only be assigned by using 2-D methods.[227] Detailed assignments were proposed for [Ru(tpy)(acac)(PPh$_4$-cyd)][PF$_6$], where tpy = 2,2′6′,2″-terpyridine, PPh$_4$cyd = 4-triphenylphosphoniophenyl cyanamide, from ^{1}H-^{1}H COSY and ^{1}H-^{13}C HMQC and HMBC experiments.[228] Proton NMR data were able to differentiate α- and β-isomers of [Ru(sazpy)$_2$Cl$_2$]$^{2-}$, where Hsazpy = 2-phenylazapyridine-5-sulfonic acid.[229]

^{1}H, ^{13}C and ^{31}P NMR spectra showed the coordination of P$_4$X$_3$ in [CpRu (L-L)(P$_4$X$_3$)]$^{+}$, where X = S or Se. For X = Se, coordination occurred *via* basal P, for X = S *via* basal or apical P.[230] The ^{31}P NMR spectrum of [Ru$_3$O(OAc)$_6$-(py)$_2$(L)]$^{+}$. where L = bis(diphenylphosphino)-acetylene, included signals from coordinated and non-coordinated P atoms of L.[231] ^{1}H, ^{13}C, ^{31}P, with ^{1}H DPFGSE TOCSY, 2-D ^{1}H-^{1}H{^{31}P} COSY DQF and ^{13}C-^{1}H correlated spectra gave very detailed assignments and structural information for RuH$_2${η^{2}-(*O,S*)-C$_6$H$_{10}$OS}(PCy$_3$)$_2$.[232] The ^{19}F and ^{31}P{^{1}H} NMR spectra of Ru(S$_2$CSR)$_2$ (PMe$_2$Ph)$_2$, where R = C$_6$H$_4$F-4, show that the solution-phase structure is the same as that in the solid.[233] ^{1}H, ^{19}F and ^{31}P{^{1}H} NMR spectra for [Ru$_2$

$(\mu\text{-F})_3(PR_3)_6][F(HF)_n]$ gave assignments to δ^1H (FHF) 11.5–11.7 ppm, δ^{19}F (FHF) −176.2 – −170.5 ppm and δ^{19}F (μ-F) −346.0 – −354.5 ppm.[234]

For the complex $(\mu\text{-H})Os_3(\mu\text{-OCNH-(}R\text{)-CHMePh})(CO)_{10}$, and related species, the relative positions of hydride resonances correlate with the cluster-fragment configuration.[235] NMR data for $[CpOs(PPh_3)L]^+$, where L = bipy, phen, show that the cyclopentadienyl protons are deshielded by comparison with the parent $[CpOs(PPh_3)_2(CH_3CN)]^+$.[236] NMR chemical shift data were calculated by *ab initio* methods for (52).[237] The silicon-bound proton in $[Cp^*(^iPr_3P)(H)_2Os{=}Si(H)(trip)]^+$, where trip = 2,4,6-$^iPr_3C_6H_2$, gives a resonance at very low field (+11.5 ppm). The ^{29}Si resonance is characteristically downfield (315 ppm).[238] Similar data were found for $[Cp^*(Me_3P)_2Os{=}SiR_2]^+$, where R = Me, ^{i}Pr.[239] ^{1}H, ^{13}C, ^{31}P and ^{119}Sn NMR data for $Os(SnMe_3)H(CO)_2(PPh_3)_2$ gave evidence for 4 geometrical isomers.[240]



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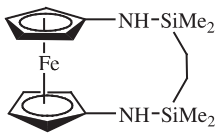
^{1}H and ^{31}P{^{1}H} NMR spectra were used to characterise three isomers of $Os_3(CO)_8(\mu\text{-SePh})_2(\mu\text{-dppm})$.[241] The pH-dependence of the ^{1}H NMR spectrum of $[Os_3(CO)_{10}(\mu\text{-}\eta^2\text{-Bz})(\mu\text{-H})L^+]$, where HBz = quinoxaline, $L^+ = P(OCH_2CH_2NMe_3)_3I_3$, shows that the extent of protonation affects the degree of aggregation in aqueous solution.[242] The ^{1}H, ^{15}N and ^{31}P NMR spectra of $\{OsH(ArN{=}NH)[PPh_2(OEt)]_4\}^+$, where Ar=Ph, 4-$MeC_6H_4$, suggest the presence of two isomers, with *N*-bonded or π-bonded ArN=NH.[243] Complete ^{1}H NMR chemical shift assignments were made for $[Os(bipy)_2(CO)(X)]^+$, where X = H or Cl, from 1-D and 2-D NMR experiments and DFT calculations.[244] The ^{13}C NMR spectrum of *cis*-$Os(CO)_4(FSbF_5)_2$ shows two resonances, as expected for *cis*-geometry.[245]

NMR data were also reported for: indenyl ferrocenes (^{1}H, ^{13}C, ^{31}P);[246] (53) (^{1}H, ^{13}C, ^{29}Si);[247] (ferrocenylmethyl)-imidazolium and –triazolium room-temperature ionic liquids (^{1}H, $^{!3}$C, ^{19}F);[248] *trans*-$[(dppe)_2Fe(\eta^2\text{-H}_2)(RCN)]^{2+}$, where R = Me, Et, ^{n}Pr, $CH_2{=}CH$, Ph, *p*-$MeC_6H_4CH_2$;[249] $\{\mu_3\text{-H(Ph)C=C}\}FeCo_2(CO)_8(EPh_3)$ (E = P or As), $\{\mu_3\text{-H(Ph)C=C}\}Fe(CO)_7(dppe)$ (^{1}H, ^{31}P);[250] $[Cp^*(\eta^2\text{-dppe})FeC{\equiv}C\text{-2,5-}C_4H_2S\text{-}C{\equiv}CFe(\eta^2\text{-dppe})Cp](PF_6)_2$ (^{1}H, ^{31}P);[251]



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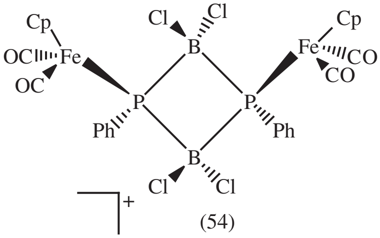

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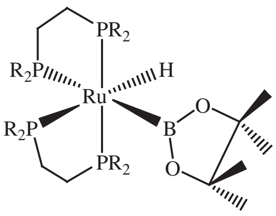
$Fe_2(L)_4(CO)_2(C_2S_4)$ (L = $P(OPh)_3$, $P(OEt_3)_3$, $P(O^iPr)_3$, $PPh(OEt)_2$, $PPh_2(OEt)$) (^{13}C, ^{31}P);[252] 1-Cp-*closo*-1,2,3,8- or −1,10,2,4-$FePC_2B_8H_{10}$ (^{1}H, ^{11}B, ^{13}C, ^{31}P);[253] sodium salt of azidotris(2*H*-tetrazolato)(5*H*-tetrazolato)iron(0) (^{13}C);[254]

$[M(trpn)(abpt)]^{2+}$ (M = Fe, Ni, trpn = tris(3-aminopropyl)amine, abpt = 4-amino-3,5-bis(pyridine-2-yl)-1,2,4-triazole) (^{1}H);[255] $(acac)_2Fe(\mu\text{-}ox)Fe(acac)_2$ (H_2ox = oxalic acid) (^{1}H);[256] $[Fe_4(TBA)(\mu\text{-}O)_2(\mu_4\text{-}suc)](ClO_4)_4(OH)_2$ (^{1}H, 2-D ^{1}H-^{13}C HMQC);[257] (54) (^{11}B, ^{31}P);[258] a novel 2×[4Fe-4S] ferredoxin from *Desulfovibrio desulfuricans ATCC27774* (1-D and 2-D ^{1}H);[259] $RuH(CO)(PPh_3)_2(L)$, where H_2L = *N,N′*-bis(salicylidine)hydrazine or *N,N′*-bis(salicylidine)-*p*-phenylenediamine (^{1}H, ^{13}C, ^{31}P);[260] *cis*- and *trans*-(55) (^{11}B, ^{31}P);[261] $RuH(CO)(PPh_3)[HB(mt)_3$ (mt = methimazolyl) (^{1}H, ^{13}C{^{1}H}, ^{31}P{^{1}H};[262] $Ru(H)_2(CO)(TPPMS)_3$, where TPPMS = $Ph_2P(m\text{-}C_6H_4SO_3Na)$ (^{1}H, ^{31}P{^{1}H});[263] $Ru_3(\mu\text{-}H)(\mu\text{-}N{=}CPh_2)(CO)_{10}$, $Ru_3(\mu\text{-}H)(\mu\text{-}N{=}CPh_2(CO)_8(L)$, where L = bis(dimethyphosphino)ethane, 4,5-bis(diphenylphosphino)-4-cyclopentene-1,3-dione (^{1}H, ^{31}P);[264] $H_4Ru_4(CO)_{10}[\mu\text{-}(S)\text{-}BINAP]$, $H_4Ru_4(CO)_9[\mu_3\text{-}(S)\text{-}BINAP]$, where BINAP = 2,2′-bis(diphenylphosphino)-1,1′-binaphthyl (^{1}H, ^{31}P, ^{1}H COSY, NOESY);[265] $Ru(OC_6F_5)_2(cdcypb)({=}C{=}CH^tBu)$, where dcypb = $Cy_2P(CH_2)_4PCy_2$ (^{1}H, ^{13}C, ^{31}P);[266] (56), where X = H, Cl, Me, OMe (^{1}H, ^{13}C{^{1}H});[267]



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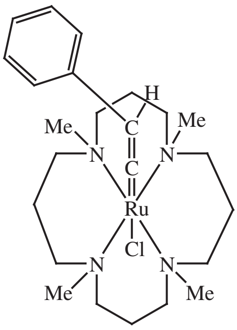

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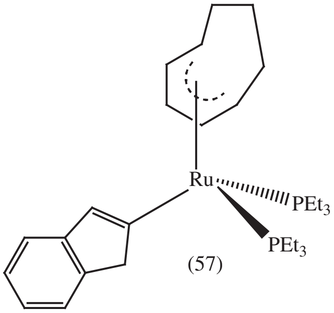

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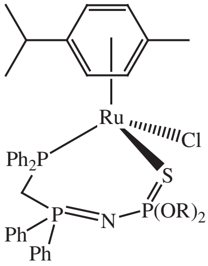
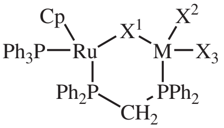


(58)

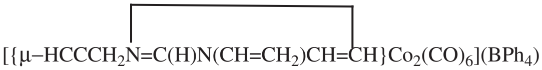
$Ru_3(\mu_3\text{-}\eta^2\text{-}R^1\text{-}4\text{-}C_6H_4CCR^2)(\mu\text{-}dppm)(\mu\text{-}CO)(CO)_7$ (R^1 = H, NO_2, CHO, CN, OMe, R^2 = Ph; R^1 = NO_2, R^2 = Fc) and related (^{31}P);[268] $Ru_2(CO)_6(\mu\text{-}bppm)$ (bppm = 2,3-bis(diphenylphosphino)-*N*-phenylmaleimide) and related (^{1}H, ^{31}P);[269] $(\mu\text{-}H)Ru_3(\mu_3\text{-}\eta^3\text{-}CHCHCMe)(CO)_7(bpcd)$ (bpcd = 4,5-bisdiphenylphosphino)-4-cyclopenten-1,3-dione) (^{1}H, ^{31}P);[270] $CpRu(P)_2SnX_2Cl$ (X = F, Br; P = PPh_3, 1/2dppe) (^{1}H, ^{13}C, ^{31}P, ^{119}Sn);[271] (57), where X = S or O, and related (^{1}H, ^{31}P{^{1}H}, ^{1}H-^{1}H COSY);[272] $(\eta^6\text{-}arene)Ru(PPh_3)(SiMeX_2)$ (X = Me, Cl, arene = benzene, toluene, xylenes) (^{29}Si{^{1}H}, ^{31}P{^{1}H});[273] (58) (R = Et, Ph) (^{1}H, ^{13}C{^{1}H}, ^{31}P{^{1}H});[274] $[(\eta^6\text{-}p\text{-}cymene)Ru(L)(3,5\text{-}Hdmpz)]^{2+}$ (L = 1-methylcarbaldimino-3, 5-dimethylpyrazole, 3,5-Hdmpz = 3,5-dimethylpyrazole) (^{1}H, 2-D COSY);[275] $[(\eta^6\text{-}C_6Me_6)Ru^{II}(bipy)H]^+$ (^{1}H, ^{2}H);[276] (η^6-arene)$RuCl_2(Cy_2PCH{=}CH_2)$, where arene = MeC_6H_5, *p*-$Me_2C_6H_4$, *p*-$MeC_6H_4CHMe_2$, 1,2,4,5-$Me_4C_6H_2$) (^{1}H, ^{31}P{^{1}H}, ^{13}C{^{1}H});[277] η^2-$C_{60}[Ru(NC)(PPh_3)]_n$ (^{13}C, ^{31}P);[278] linear multiporphyrin arrays with mono- and di-phosphine substituted porphyrins as ligand donors and Ru(II) or Rh(III) porphyrins as ligand acceptors (^{1}H, ^{31}P);[279] Ru(TTP)(NO)(L) (TTP = tetra-*p*-tolylporphyrin, L = ONO, ONO_2) (^{1}H);[280] $RuCl_3(NO)(P)$ (P = TPPMS, TPPTS) (^{1}H, ^{31}P);[281] $MH(NH_2OH)(P)_4$ (M = Ru, Os), $Ru(NH_2OH)(P)_4{}^{2+}$ (P = $P(OEt)_3$, $PPh(OEt)_2$) (^{1}H, ^{13}C, ^{31}P);[282] $[Ru(phen)_2(L)]^{2+}$ (L = 2-(4-methoxyphenyl)imidazo[4,5-*f*][1,10]phenanthroline and related) (^{1}H);[283] $Ru(terpy)(phen)L^{2+}$ (L = unidentate ligands, *e.g.* Cl^-, NC^- *etc.*) (^{1}H – COSY, ROESY);[284] $[Ru(phen)(H_2O)([9]aneS_3)]^{2+}$ (1-D, 2-D (COSY, NOESY) ^{1}H);[285] $[Ru(L\text{-}L)_2(actatp)]^{2+}$, where L–L = bipy, phen, actatp = acenaphthereno[1,2-*b*]-1,4,8,9-tetraazacriphenylene (^{1}H);[286] $[Ru(bipy)_3]_3\text{-}[P_2W_{18}O_{62}]$ (^{31}P);[287] $[Ru_2(terpy)_2(L)]^{4+}$, where L = bis-tridentate bis(benzimidazolyl)pyridine derivatives, (^{1}H);[288] *cis*-$RuX_2(L\text{-}L)_2$ (L–L = dppm, dppen, X = Br, I, and related) (^{1}H, ^{31}P{^{1}H});[289] (59)



(59)

(M = Pd, Pt; X^1, X^2, X^3 = Cl, I, Me) (^{1}H, ^{31}P{^{1}H});[290] $[CpRu(\eta^2\text{-}L\text{-}L)(CH_3CN)]^+$, $[\{CpRu(CH_3CN)_2\}_2(\mu\text{-}\eta^{1:1}\text{-}L\text{–}L)]^+$ (L–L = dppe and related diphosphines) (^{1}H, ^{31}P{^{1}H});[291] $CpRu(dppf)SnBr_3$ (dppf = 1,1′-bis(diphenylphosphino)ferrocene) (^{1}H, ^{13}C, ^{31}P, ^{119}Sn);[292] poly-nuclear ruthenium clusters derived from 1,2,3,4-tetraphenyl-1,2,3,4-tetraphospholane and $Ru_3(CO)_{12}$ (^{1}H, ^{31}P{^{1}H});[293] tris(pyrazolyl)borate/ruthenium complexes containing bidentate phosphine ligands (^{1}H, ^{13}C{^{1}H}, ^{31}P{^{1}H});[294] $[(BPPY)_2Ru(MeOH)_2(H_2O)_2]^{3+}$, $[Ru(BBuPY)\text{-}Cl_2(S)_2]^+$, where BPPY = $Ph_3PCHCOPh$; BBuPY = $^nBu_3PCHCOPh$ (^{1}H, ^{13}C, ^{31}P);[295] $(L)_2Ru(L')_2$, where L = 4,4′- or 5,5′-diethylester phosphonate-2,2′-bipyridine, L′ = CN, NCS (^{1}H, ^{13}C);[296] $Ru^{II}Cl_2(dmso)_2L$. where L = 5-nitro-2-furaldehyde semicarbazone or similar (^{1}H, ^{13}C);[297] $(\mu\text{-}H)Os_3(CO)_{10}(L)(SnR_3)$. where L = NMe_3, pyrrolidine, piperidine, morpholine; R = Me, Bu (^{1}H, ^{13}C, ^{119}Sn);[298] $(\eta^2\text{-}C_{60})Os(CO)(^tBuNC)(PPh_3)_2$ (^{1}H, ^{31}P);[299] 2,2,2-$(Ph_3P)_2(CO)$-*nido*-2-OsB_4H_7-3-(BH_2.dppe) and related (^{1}H, ^{11}B, ^{13}C);[300] $Os^{IV}(TPP)(NHNPh_2)_2$, $Os^{IV}(TPP)(NPh_2)(OH)$, $Os^{VI}(TPP)(NNPh_2)_2$, $Os^{VI}(TTP)(N)(OH)$ (^{1}H).[301]

2.9 Compounds of Group 9. – ^{31}P and ^{59}Co NMR spectra show that $HCo(CO)_3[P]$ and $HCo(CO)[P]_2$ are the only detectable hydrido cobalt complexes present in hydroformylations catalysed by $Co_2(CO)_6[P]_2$, where [P] = $P(p\text{-}CF_3C_6H_4)_3$.[302] The ^{1}H and ^{13}C NMR spectra of $(CpCo)_2[Fe(L)_2(\mu_3\text{-}S)(\mu_3\text{-}C_2S_3)]$, where L_2 = $(CO)(PPh_3)$, $CO[P(OPh)_3]$, $(CO)(P^nBu_3)$, $(CNMe)_2$, $(CNMes)_2$, show that all are chiral and do not racemise on the NMR timescale.[303] The ^{31}P NMR spectrum of the bppm + $PhCCo_3(CO)_9$ system show formation of the intermediate cluster $PhCCo_3(CO)_7(bppm)$, where bppm = 2, 3-bis(diphenylphosphino)-*N*-phenylmaleimide.[304] The ^{11}B NMR spectra of derivatives of Cs[3,3′-Co($C_2B_9H_{11}$)$_2$] containing alkyl substituents at B(8), B(8′) show that the spectra of the two halves are superimposed.[305]



$[\{\mu\text{–HCCCH}_2\text{N=C(H)N(CH=CH}_2\text{)CH=CH}\}\text{Co}_2\text{(CO)}_6](\text{BPh}_4)$

(60)

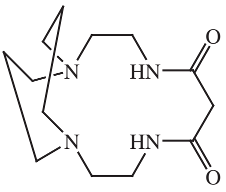
NMR data (^{1}H, ^{13}C{^{1}H}, ^{31}P{^{1}H}) for (60) show that cation-anion contacts (C–H . . . π) persist in solution.[306] The structure of [(methoxycarbonyl)methyl]cob(III)alamin was determined by ^{1}H,^{13}C and ^{1}H, ^{1}H ROESY experiments.[307] ^{59}Co chemical shifts were used to study hydrogen-bonding interactions in ([12]aneN$_4$)[Co(CN)$_6$] and related supramolecular complexes.[308] *Ab initio* calculations of the ^{59}Co chemical shift for $Co(NH_3)_6{}^{3+}$ have been reported.[309] NMR data (^{1}H, ^{31}P) have been used to follow the interaction of $Co(NH_3)_6{}^{3+}$ with the metal-ion-binding motif in hammerhead enzymes, showing outer-sphere complexation of the cation.[310] The *syn*- and *anti*-NH protons were assigned for *trans*-$[Co(en)_2(L)(N_3)]^{2+}$, where L = OSMe$_2$, NH$_3$, using 2-D NMR techniques.[311]

There have been several reports of 1-D and 2-D NMR experiments to probe intramolecular interaction in Co(III) complexes of *R,R*-picchxn (*N,N*′-di(2-picolyl)-1,2-diaminocyclohexane.[312–315] ^{1}H and ^{13}C NMR data for (py)-Co(dpgh)$_2$R, where R = Cl, CH$_3$, Et, ^{i}Pr, ^{t}Bu, CH$_2$SiMe$_3$, CH$_2$CMe$_3$, ^{n}Pr, ^{n}Bu, CH$_2$CH=CH$_2$, CH$_2$Ph, CF$_3$, dpgh = diphenylglyoximato, show that the dpgh is less electron-donating than dimethylglyoximato.[316] ^{1}H and ^{13}C spectra for $Co(MPz3Hex)_2{}^+$, where HMPz3Hex = 5-methyl-3-formyl-pyrazole 3-hexamethyleneiminyl thiosemicarbazone, are consistent with tridentate, *N,N,S*-coordination by the uninegative ligand.[317] 1-D and 2-D ^{1}H and ^{13}C NMR studies have been made of 4 (out of a possible 10) isomers for Co(pema)(ampy)Cl^{2+}, where pema = *N*-(2-anilinomethylpyridyl)ethylene diamine, ampy = 2-aminomethylpyridine.[318] Similar results were obtained for two isomers of Co(ptma)(ampy)Cl^{2+}, where ptma = *N*-(2-pyridylmethyl)-1,3-diaminopropane. In this case there was evidence for C–H . . . π interactions.[319]

The pH-dependent characteristics of the ^{1}H NMR spectra of Co^{III}(polyamine)aqua and Co^{III}(polyamine)(polyalcohol) complexes were due to cobalt-centred spin-orbit effects on the proton nuclear shielding.[320] The ^{1}H NMR spectrum of Co(L)(H$_2$O), where H$_2$L = (61), shows that this is a low-spin d^6 complex. ^{1}H and^{13}C resonances were assigned using COSY and HETCOR spectra.[321] The high-resolution ^{1}H and ^{13}C NMR spectra of the linkage isomers $[(H_3N)_5CoOC(S)NHMe]^{2+}$ and $[(H_3N)_5CoS(O)NHMe]^+$ show that both the *O*- and *S*-bonded forms exist as mixtures of *Z*- and *E*-isomers, due to restricted rotation about the C–N bond.[322]

A review has been published on the applications of ^{103}Rh NMR spectroscopy in structural chemistry.[323] The complex $[CpRh(dmpm)(HD)]^+$, where dmpm = bisdimethyldiphosphinomethane, gives a ^{1}H{^{31}P} spectrum showing that it is a dihydrogen complex.[324] High-pressure NMR spectroscopy was used to identify RhH(CO)(L)$_3$ and RhH(CO)$_2$(L)$_2$ under 40 bar of CO/H$_2$ (L = P

$(C_6H_4\text{-}4\text{-}OCH_2C_7F_{15})_3)$.[325] High-pressure $^{31}P\{^1H\}$ NMR spectra were also reported for $RhH(CO)(TPPTS)_3$ in the presence of methylated cyclodextrins (TPPTS = trisulfonated triphenyl-phosphine.[326]



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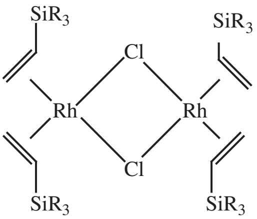

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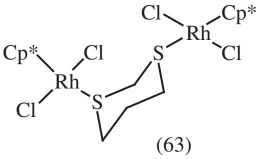

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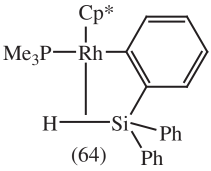

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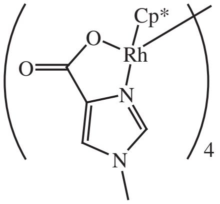


(65)

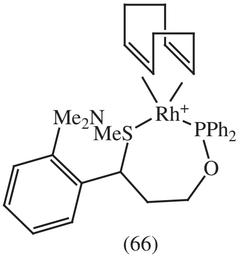
^1H and $^{31}P\{^1H\}$ NMR spectra were reported and assigned for $RhCl(CH_2{=}CH_2)_2(PMe_3)_2$ and $RhCl(CH_2{=}CH_2)(PMe_3)_2$.[327] ^1H, ^{13}C and ^{29}Si NMR spectra were reported for (62), where $R_3 = Me_3$, Me_2Ph, $MePh_2$, Ph_3, $Me_2(OSiMe_3)$. $J(^{13}C\text{-}^{103}Rh)$ coupling constants were assigned for the vinyl carbons.[328] The ^1H NMR spectrum of (63) showed that two isomers were present.[329] The complex Rh(PyP)(CO)Cl, where PyP = 1-(2-diphenylphosphino)ethylpyrazole, has a $^{13}C\{^1H\}$ spectrum with a CO resonance at 188.7 ppm, and $^1J(Rh\text{-}C)$ 71.2 Hz.[330] The low-temperature $^{31}P\{^1H\}$ NMR spectrum of $[Rh(CO)_2L_2]^+$, where $L = R\text{-}C_6H_4\text{-}(OCH_2CH_2)\text{-}PPh_2$ (R = *tert*-octyl), is consistent with very weak *P,O*-coordination.[331] Isomers of $Rh(\kappa^2\text{-}Tp^{PhCl})(CO)_2$, where Tp = hydridotris(pyrazolyl)-borate, were identified by ^1H NMR spectra.[332]

The non-classical silane complex (64) gave characteristic ^1H and ^{13}C NMR spectra.[333] The ^1H and ^{13}C NMR spectra of (65) show that it has a very symmetrical structure.[334] The ^1H NMR spectra of $[Rh(COD)(L)]^+$, where L = tris[2-(1-{pyrazolyl)methyl]amine or tris[(3,5-dimethyl-1-pyrazolyl)methyl]amine, show that each exists as two isomers in solution (involving κ^2- and κ^3-coordination).[335] The ^1H NOESY and $^{19}F\{^1H\}$ HOESY spectra for $[M(N\text{-}N)(CO)_2]^+X^-$, where M = Rh, Ir, N–N = bis(1-methylimidazol-2-yl)methane or bis(1-pyrazolyl)methane, gave evidence for strong interionic contacts.[336] ^1H, ^{13}C

and ^{31}P NMR spectra were used to identify possible diastereoisomers for Cp*M(Cl)(NHMeCHRCO$_2$), M = Rh, Ir, R = H, Me, and related systems.[337]

2-D (COSY, ROESY) NMR spectra gave assignments to all proton resonances for $[Rh_2(OAc)_2(bipy)(9\text{-}EtGH)(H_2O)_2(CH_3SO_4)]^+$, where 9-EtGH = 9-ethylguanine.[338] The structures of Et-[Rh]-ER$_n$-CH$_2$CH$_2$-ER$_n$-[Rh]-Et, where [Rh] = Rh(dmgH)$_2$, H$_2$dmg = dimethylglyoxime, ER$_n$ = NH$_2$, PPh$_2$, PMe$_2$, SMe, were assigned unambiguously using ^{1}H, ^{13}C and ^{31}P NMR spectra.[339] Experimental ^{103}Rh chemical shifts were reported for mono- and binuclear Rh(I) complexes containing *s*- or *as*-hydroindacenide and indacendiide bridging ligands, with a range of ancillary ligands.[340] A detailed ^{1}H NMR study has been made of the binding of 3 stereoisomers (ΔΔ, ΛΛ, ΔΛ) of $[\{Rh(Me_2bipy)_2\}_2(\mu\text{-}bpm)]^{2+}$, where bpm = bipyrimidine, to a tridecanucleotide.[341]

^{103}Rh chemical shifts were reported for 62 compounds: Rh(X)(PPh$_3$)$_2$, where X = Cl, N$_3$, NCO, NCS, N(CN)$_2$, NCBPh$_3$, CN, and related species.[342] ^{1}H, ^{13}C and ^{31}P NMR spectra, with several 2-D experiments gave a detailed assignment of the NMR parameters for $[(triphos)Rh(\eta^1{:}\eta^2\text{-}P_4RR')]^+$, where triphos = MeC(CH$_2PPh_2$)$_3$, R = H, alkyl, aryl, R′ = H, Me or lone pair of electrons.[343] The ^{31}P NMR spectrum of (66) confirms the *P,S*-bidentate bonding, with no *N*-interaction.[344] ^{1}H and ^{31}P{^{1}H} NMR spectra for (67), where M = Rh or Ir, were reported. For M = Rh, J_{Rh-P} at 162 HZ was diagnostic of a *cis*-phosphine-*cis*-thioether structure.[345]



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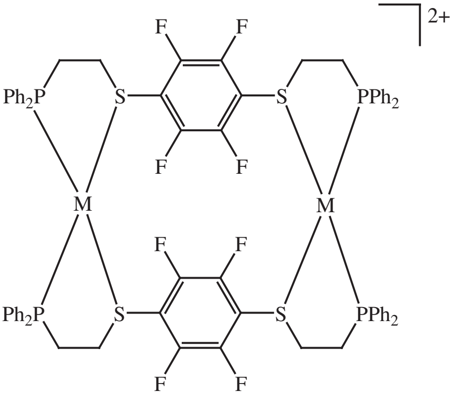

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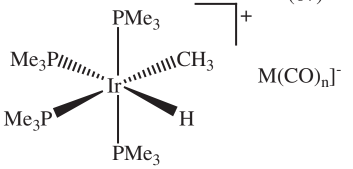


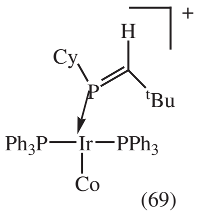
(68)

^{1}H and ^{13}C{^{1}H} NMR spectra for (*S*)-$[H_3Ru_3\{C_6H_5[CH(CH_3)CH_2)OH]\}(C_6Me_6)_2(O)]^+$ show a strong intramolecular hydrogen bond between the μ_3-oxo cap and the hydroxyl function in acetone solution.[346] ^{1}H, ^{13}C and ^{15}N chemical shifts were used to probe the coordination of substituted pyridines and aminides to Rh$_2$(O$_2$CCF$_3$)$_4$.[347] The ^{1}H, ^{13}C, ^{31}P and ^{103}Rh NMR spectra have been reported for phosphine-phosphonite ferrocenediyl dinuclear rhodium complexes.[348] ^{31}P NMR data were able to discriminate between enantiomers of $Rh_2[(R)\text{-}MTPA]_4$, where (*R*)-MTPA = *R*-$O_2CC(CF_3)Ph(OMe)$.[349] The ^1H COSY and ^1H-{^{13}C} HSQC spectra were used to characterise and differentiate isomers of $Rh_6(CO)_{14}[\mu\text{-}\kappa^2\text{-}PhP(2\text{-thienyl})_2]$.[350]

The ^{15}N NMR data for $Rh_2(OAc)_4(Tu)_2$, where Tu = thiourea, suggest some involvement by N as well as S in coordination.[351] The ^1H and $^{31}P\{^1H\}$ NMR spectra of (68), where M = Mn, n = 5; M = Co, n = 4, are all consistent with the *cis*-hydridomethyl cation structure.[352] The ^{31}P chemical shifts in $(Et_3P)_2Ir(H)(Cl)X$, where X = $Si(^tBu)_2(OH)$, $Si(^iPr_2)(OH)$, $Si(SEt)_3$, $Si(SEt)_2(OH)$, $Si(SEt)_2(OTf)$, follow the expected trends in silicon-group electronegativity.[353] 2-D NMR experiments enabled a full characterisation of 4 isomers of $[Ir(H)_2\{(S)\text{-}(R)L\}(L')]^+$, where L = *S*-1-[(*R*-2-diphenylphosphanyl)ferrocenyl] ethyldi(3,5-xylyl)phosphane; L′=2,6-dimethylphenyl-1′-methyl-2′-methoxy-ethylimine.[354] ^1H and ^{31}P NMR spectra show two isomeric forms for the cluster $Ir_4H_4(\mu\text{-}H)_4(CO)_4(PPh_3)_4$, with no interchange between them, in CD_2Cl_2 solution at room temperature.[355] ^1H, ^{13}C, ^{19}F and 2-D (COSY, ROESY, TOCSY) NMR data gave detailed assignments for several trinuclear iridium complexes containing C_2H_4, $C_2H_2F_2$, C_2HF_3 and C_2F_4 ligands (η^2- or bridging).[356]

The ^1H and $^{13}C\{^1H\}$ NMR spectra of $(COD)IrBr(\mu,\kappa^1{:}\eta^6\text{-}Ar)Ir(COD)$, where Ar = 2,4,6-$Me_3C_6H_2$, are consistent with an aromatic ring coordinated in π-fashion to an iridium atom.[357] The ^1H and ^{13}C NMR spectra of $\{[Bu_4N]\}\{[(1,5\text{-}COD)Ir.HPO_4]\}_n$ show that the symmetry is probably C_2 or C_s.[358] ^1H NMR evidence has been found for the agostic intermediate $[H_2Ir\{py\text{-}N(Me)CH_2\text{-}H\}L_2]^+$, where L = PPh_3, py-NMe_2=2-(dimethylamino)pyridine.[359] 1-D (^1H, ^{13}C) and 2-D (^1H-^1H, ^1H-^{13}C) NMR experiments were used to elucidate the solution-phase structure of *mer*-$Ir(ppy)_2(vppy)$, where ppy = 2-phenylpyridine, vppy = 2-(4-vinylphenyl)pyridine.[360] The complex (69) has an $^{31}P\{^1H\}$ spectrum showing chemically-equivalent PPh_3 groups, and a typical signal for η^1-phosphaalkenes.[361]

NMR data have also been reported for: $Co_3(CO)_6[\mu_2,\eta^2,\eta^1\text{-}C(Ph)C{=}C(PPh_2C(O)SC(O)](\mu_2\text{-}PPh_2)$ (^{31}P);[362] $Co_3(CO)_9[\mu_3\text{-}CCO_2CH_2CCH\{Co_4(CO)_{10}\}]$ (^1H);[363] substituted μ_3-carbido-capped tricobalt carbonyl clusters (^1H, ^{13}C);[364] Co(III) complexes of NH_3, en, 1,2-propylenediamine or 1,2-cyclohexanediamine (^1H, ^{13}C, ^{59}Co);[365] $[Co(CO)_3(L)]^-$ (L = *N,N*-diethyl-1,2-ethanediamine, *N,N*-bis(2-chloroethyl)-1,2-ethanediamine and related) (^1H, $^{13}C\{^1H\}$);[366] *cis*-$[Co(en)_2(N_3)_2]SCN$ (^1H, ^{13}C);[367] (70), where R = *n*-octyl, *n*-dodecyl, *n*-hexadecyl (^1H, ^{13}C);[368] $[CH_2ClCo(tmsalen)]_2$,



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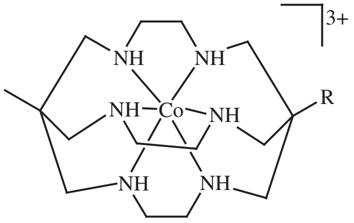

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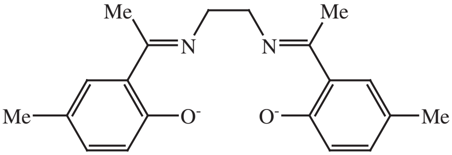

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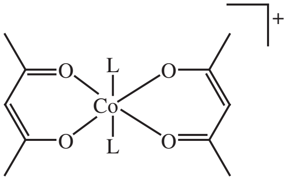

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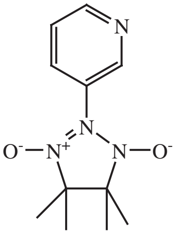
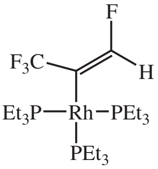


(73)

where tmsalen = (71) (^{1}H, ^{13}C);[369] ML_2 (M = Co(II), Ni(II), Cu(II), Zn(II); HL = bidentate Schiff bases;[370] $[Co(Rac)(cyclam)]^{2+}$ (cyclam = 1,4,8,11-tetrazacyclotetradecane; Rac = β-diketonates) (^{1}H, ^{13}C);[371] (72), where L = (73) and related (^{2}H);[372] $[Co(EtN_4S_2amp)]^{3+}$, where EtN_4S_2amp = 2,2,9,9-tetra(methylene-amine)-4,7-dithiadecane (^{1}H, ^{13}C);[373] $\{Rh(H)(PR_3)_2[o\text{-}C_6H_4(R')C{=}NN(H)\text{-}CONH_2]\}^+$, where R_3 = Ph_2(*p*-tolyl), Ph_2Me; R′ = Me, Et (^{1}H, ^{31}P{^{1}H});[374] $[(Bpm^*)Rh(CO)(L)]^+$ (Bpm = $H_2C(3,5\text{-}Me_2pz)_2$; L = CO, PPh_3, $PMePh_2$, $P(OMe)_3$) (^{1}H, ^{13}C, ^{31}P);[375] $Rh(CO)(PPh_3)(\eta^5\text{-}C_5H_4R)$, $RhMo(CO)_4(PPh_3)_2(\eta^5\text{–}C_5H_4R)$ (R = H, COMe) (^{1}H);[376] $[Rh(CO)L\{HC(pz')_3\}]^+$ (L = PPh_3, $AsPh_3$, P(*o*-tolyl)$_3$; $HC(pz')_3$ = tris(3,5-dimethylpyrazolyl)methane) (^{1}H, ^{13}C{^{1}H});[377] *trans*-$Rh(CO)LL'_2$ (L = κ^1*P*- or κ^2*P,O*- $PR_2\{NC_4H_3C(O)Me\text{-}2\}$, where R = Ph or NC_4H_4) (^{31}P{^{1}H});[378] (74) (^{1}H, ^{31}P, ^{1}H{^{13}C)-^{13}C HMQC, ^{19}F{^{1}H}-^{13}C HMQC/HMBC);[379] $Rh_6(CO)_{15}$(4-Vpy), $Rh_6(CO)_{14}(\mu,\eta^2\text{-}PPh_2CH_2CH{=}CH_2)$ (4-Vpy = 4-vinylpyridine) (^{1}H);[380] (P)RhIn(P′) (P, P′ = OEP, TPP, β-Cl_4TPP, β-Cl_8TPP, TPyP) (^{1}H, ^{13}C);[381] $[Rh(\mu\text{-}Pz)(CO)(T\text{-}PPMS)]_2$, where Pz =pyrazolate, T-PPMS = $Ph_2P(m\text{-}C_6H_4SO_3Na)$ (^{1}H, ^{1}H{^{31}P}, ^{31}P);[382] (75) and related (^{1}H, ^{13}C{^{1}H}, ^{31}P{^{1}H});[383]



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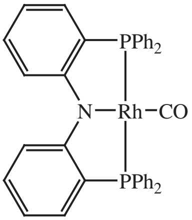

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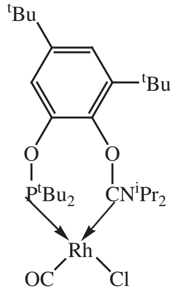

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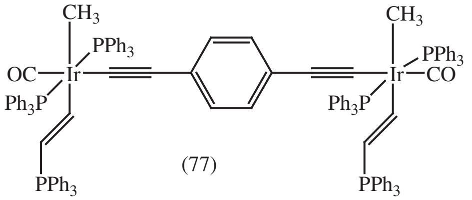

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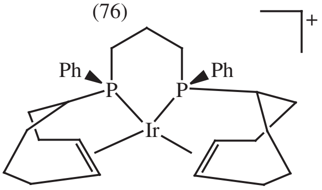

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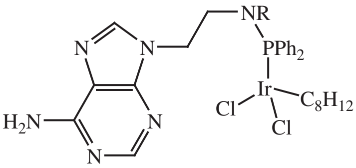
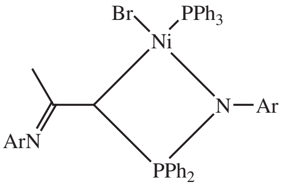


(79)

trans-RhCl[P(OH)Ph$_2$](PPh$_3$) and related (^{1}H, ^{31}P;[384] (76) (^{13}C, ^{31}P);[385] Cp*Ir(PMe$_3$)[C$_6$H$_3$(CO$_2$)(CO$_2$H)] (^{1}H, ^{13}C);[386] (77) (^{1}H, ^{13}C, ^{31}P, ^{1}H-^{13}C 2-D COSY);[387] IrCl$_2$(η^{1}-CH$_2$Ar)(CO)(PPh$_3$)$_2$ (Ar = Ph, *p*-tolyl), IrCl$_2$[C(O)CH$_2$CMe$_3$](PPh$_3$)$_2$ (^{1}H, ^{13}C, ^{31}P);[388] Ir$_4$(CO)$_3$(μ$_4$-CH)(PMe$_3$)$_2$(μ-PMe$_2$)(CNCH$_2$Ph)(μ-η^{2},η^{2}-C$_{60}$)(μ$_4$-η^{1},η^{1},η^{2},η^{2}-C$_{60}$) ^{1}H, ^{31}P{^{1}H});[389] *meso*- and *rac*-forms of (78) (^{1}H, ^{13}C);[390] (79) (R = H, ^{n}Pr) (^{31}P{^{1}H});[391] and [Ir(H){PhCH$_2$N=CH(*o*-C$_6$H$_4$)}(PPh$_3$)$_2$(L)]$^{+}$, where L = Me$_2$CO or PhCH$_2$NH$_2$ (^{1}H, ^{31}P{^{1}H}).[392]

2.10 Compounds of Group 10. – The complex (80), where Ar = C$_6$H$_3{}^{i}$Pr$_2$, gives ^{13}C{^{1}H} features showing metallation of the central ligand carbon atom.[393] ^{1}H NMR spectroscopy was used to differentiate (81) and (82) in solution.[394] The ^{1}H and ^{31}P NMR spectra of (83), η where dtppe = 1,2-bis(di-*tert*-butylphosphino)ethane, dmp = dimesitylphenyl, show characteristics of a 4-membered cyclo-species.[395] The ^{31}P NMR spectra of Ni(dnpdtc)(PPh$_3$)X, where X = NCS, CN, dnpdtc = di-*n*-propyldithiocarbamate, show more pronounced back bonding for X = CN than for NCS.[396] Low-temperature (−80°C) ^{1}H and ^{29}Si NMR spectra gave evidence for a tris(silyl)(hydrido)nickel(IV) complex, (84).[397]



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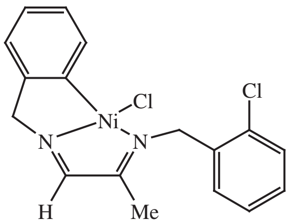

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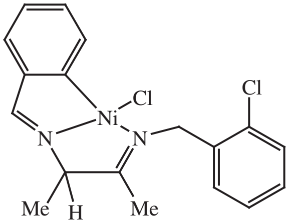

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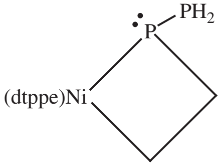

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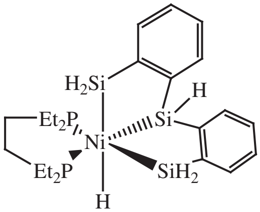


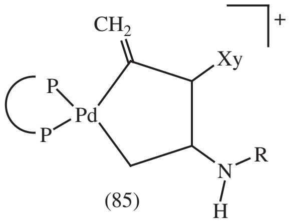
(84)

The ^{31}P NMR spectra of nickel and zinc complexes of tetrakis(ethylphenylphosphinate)-substituted phthalocyanines showed the presence of several constitutional isomers.[398] The formation of trimetallic (Ni_2Pt) complexes by the reaction of nickel *meso*-tetratolylporphyrin derivatives with $PtCl_2$-containing species has been shown by ^{1}H and ^{13}C NMR spectroscopy to be diastereoselective.[399] The ^{1}H NMR spectrum of nickel(II) umecyanin (a stellacyanin with an axial Glu ligand, demonstrates the unidentate coordination of Glu *via* the side-chain amode oxygen atom.[400]

The complexes $Ni^{II}(L)$, where L = 3,10-di(*p*-X-benzoyl)-2,4,9,11-tetramethyl-1,5,8,12-monobenzotetraazcyclo[14]annulene, X = Me, H, Cl, NO_2, OMe, show ^{1}H deshielding effects due to the benzoyl groups.[401] The ^{1}H and ^{13}C NMR spectra of Ni(II) and Zn(II) complexes with the Schiff base from 1,2-bis(*o*-aminophenoxy)ethane and salicylaldehyde are consistent with *O,N,N,O*-coordination of the ligand.[402] The ^{1}H NMR spectra of aqueous solutions of $[Ni(L\text{-}O)]^{+}$ and $[Ni(L\text{-}NH)(H_2O)_3]^{2+}$, where L = flexidentate 5-substituted salicylaldimino Schiff bases based on 1-(2-aminoethyl)piperazine, show that these exist as planar and octahedral forms in equilibrium.[403] ^{1}H NMR signals from the *ortho*-protons in bis[2-(2,4-dichlorophenylmethyleneamino)benzenethiolato]nickel(II) are consistent with Ni . . . H–C interactions in solution.[404]

^{31}P NMR data indicate the existence of a relatively unstable monomer $Pd(dpph)Me_2$.[405] Solution NMR (^{1}H, ^{13}C, ^{31}P) spectra were used to probe interactions between $[PdCl(\eta^3\text{-}C_3H_5)]_2$ and 1,1′,2,2′-tetrakis(diphenylphosphino)-4,4′-di-*tert*-butyl ferrocene.[406] ^{1}H, ^{13}C and ^{31}P NMR spectra for $[Pd(\eta^3\text{-}C_3H_4R)(\eta^2\text{-}Ph_2PCH_2CH(Ph)NHAr)]^{+}$, where R = H, Me, Ph, Ar = Ph, 2,6-$^{i}Pr_2C_6H_3$, show highly diastereoselective coordination at the N atom.[407] The ^{31}P NMR spectra of (85), where P–P = dppe, E = O, R = Et, Ph; E = S, R = Ph, show that the two phosphorus atoms in the coordinated dppe are non-equivalent.[408] The ^{1}H and ^{13}C{^{1}H} NMR spectra of (86), where R = ^{n}Pr, ^{i}Pr, CHPh$_2$, are all consistent with C$_1$ symmetry and bidentate ligands.[409]

The ^{31}P{^{1}H} NMR spectrum of [Pd(*N,C*-dmba)(dppf)]NO$_3$, where dmba = *N,N*-dimethylbenzylamine, dppf = 1,1′-bis(diphenylphosphino)ferrocene, in solution shows that 3 cyclopalladated species are present – with two having bridging and one chelating dppf.[410] ^{1}H and ^{31}P NMR data were used to characterise the first 16-electron, trigonal-planar Pd(0) carbonyl complex, (tbpx)Pd(CO), where tbpx = 1,2-(CH$_2$P^{t}Bu$_2$)$_2$C$_6$H$_4$.[411] ^{1}H NMR spectra, including DQF-COSY and NOESY 2-D experiments, were used to characterise Pd and Pt porphyrins with *cis*- configurations at the metal centre (forced by tmeda or bipy ligands).[412]



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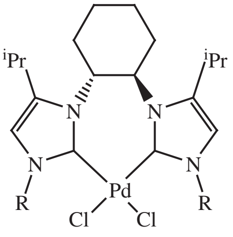

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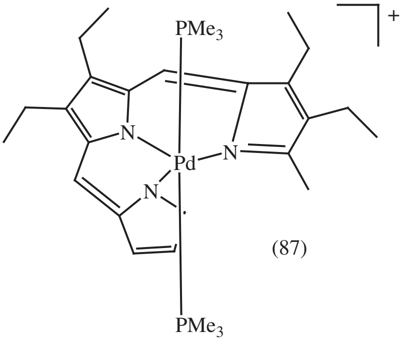

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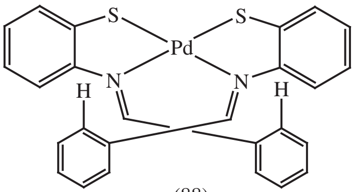
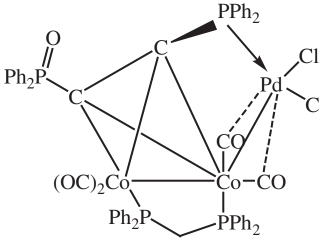


(88)

The ^{1}H, ^{13}C, ^{19}F and ^{31}P NMR spectra for (87) show that the 5-coordinate structure is stable in solution.[413] ^{1}H and ^{13}C{^{1}H} NMR spectra (including NOESY data) gave detailed assignments for PdCl$_2$(L)$_2$, where L = 1-hydroxymethyl-, 1-(2-hydroxymethyl) or 1-(3-hydroxymethyl)-pyrazole, which exist as *anti*- and *syn*-conformers in solution, because of restricted rotation about the Pd–L bond.[414] The ^{1}H NMR spectra of Pd(II) and Pt(II) dien complexes of isocytosine show a distinct preference of the metal for the N(3) site.[415] The ^{1}H NMR spectrum of (88) shows significant Pd . . . H–C interaction involving the CH bonds shown.[416] DFT calculations have been made of the ^{31}P chemical shifts for [Pd{Ph$_2$P(CH$_2$)$_n$PPh$_2$}X]$^-$, where n = 3–6, X = Cl, OAc.[417]

The ^{31}P NMR spectrum of (89) includes a resonance due to the Pd-coordinated phosphorus at high field (δ 33.92 ppm).[418] Detailed 1- and 2-D homo- and heteronuclear NMR spectra, including ^{1}H, ^{13}C, ^{1}H-^{1}H COSY, ^{1}H-^{13}C COSY, were reported for *trans*-PdL$_2$X$_2$, where X = Cl, Br; L = 2- or 8-diethylquinolyl methylphosphonates.[419] Similar experiments were reported to give full assignments of [Pd(μ-κ^2-OAc)(μ-κ^1-OAc)(κ*P*, κ*C*^{14}-phenop)]$_2$, where phenop = chiral pentacyclic phosphine, and related complexes.[420] For $[Pd(L)]^{2+}$, where L = (90), the $^3J_{H,H}$ coupling constants (derived from 2-D ^{1}H J-resolved NMR spectra, gave information on S-C-C-S torsional angles.[421]

A characteristic hydrido signal in the ^{1}H NMR spectrum of $Pt_3H(\mu\text{-}PPh_2)_3(PEt_3)_3$ at δ −7.98 ppm is split by both H-P and H-Pt coupling.[422] DFT calculations gave ^{205}Tl and ^{295}Pt chemical shifts and spin-spin coupling constants for $[(NC)_5Pt\text{-}Tl(CN)_n]^{n-}$ (n = 0–3) and $[(NC)_5Pt\text{-}Tl\text{-}Pt(CN)_5]^{3-}$.[423,424] ^{1}H chemical shifts were consistent with strong π-back donation to ethene in $[PtMe(\eta^2\text{-}C_2H_4)(DPCB\text{-}Y)]^+$, where DPCB-Y = 1,2,-diaryl-3,4-bis[(2,4,6-tri-*tert*-butylphenyl)-phosphinidene] cyclobutenes, aryl = 4-methoxyphenyl, 4-trifluoromethylphenyl *etc.*[425] 1- and 2-D ^{1}H NMR spectra for PtMe(olefin)(*N,N′*-imino-amide chelate), where olefin = ethane, propene, styrene, allyl alcohol, methyl vinyl ketone, methyl acrylate, show only one isomer in solution (square-planar Pt, *cis*-geometry).[426]



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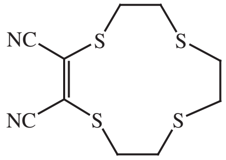

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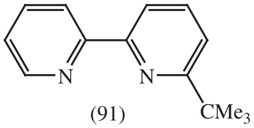

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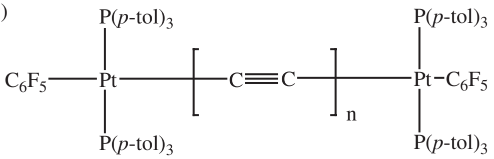
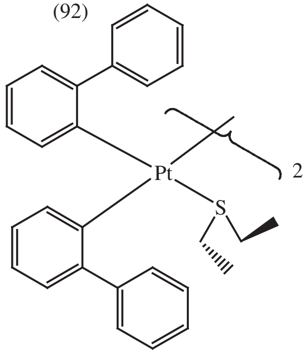


(92)

trans-[PtCl$_2${N=C(CH=CHPh)O-N(Me)-CHPh}$_2$]

(93)



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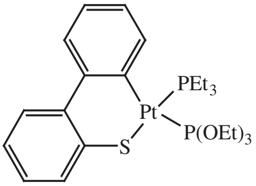

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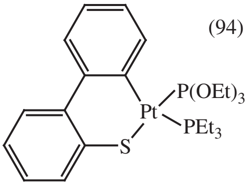


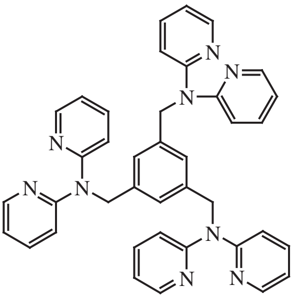
(96)

The complex PtMe(L)(dmso), where L = (91), had a $^{13}C\{^1H\}$ spectrum showing aromatic C bound to Pt ($^1J_{PtC}$ 1086 Hz).[427] Characteristic PtC≡,

PtC≡C and Pt–C≡C–C ^{13}C chemical shifts were reported for (92) and related complexes.[428] A typical ^{195}Pt resonance was observed (−2180 ppm) for (93).[429] A detailed analysis of ^{1}H and ^{13}C{^{1}H}resonances (from 2-D COSY and ^{13}C, ^{1}H HMQC experiments) has been made for (94) and related systems.[430] ^{1}H and ^{31}P{^{1}H} NMR spectra for *cis*-[PtCl{L-κ^{3}*C,P,P*}], where L = sterically constrained diphosphonite ligands, gave characteristic Pt–P coupling constants.[431] ^{31}P NMR spectroscopy was used to differentiate the isomers (95) and (96).[432]

^{31}P NMR spectroscopy revealed the formation in ionic liquid solution of complexes $PtCl(SnCl_3)(bdpp)$ and $Pt(SnCl_3)_2(bdpp)$, where bdpp = 2,4-bis(diphenylphosphino)pentane.[433] The ^{1}H NMR spectrum of *meso*-tetrakis(4-*t*-butylphenyl)porphyrinatoplatinum(II) gave no evidence for long-range ^{1}H-^{195}Pt coupling.[434] ^{15}N chemical shifts reveal *N*-coordination in $PtCl_2(L)_2$, $PtCl_2(NH_3)(L)$, where L = 5,7-disubstituted-1,2,4-triazolo[1,5-α]-pyrimidines.[435] A ^{195}Pt NMR study of *cis*- and *trans*-$Pt(amine)_2I_2$, where amine = RNH_2 (R = Me, Et, ^{n}Pr, ^{n}Bu, ^{i}Pr, ^{i}Bu, *sec*-Bu) or R_2NH (R = Me, Et) showed a lower field chemical shift for secondary amines.[436]

The ^{1}H NMR spectrum of Pt_3LCl_6, where L = (97), shows that the three dipyridylamine fragments are equivalent.[437] ^{1}H and ^{195}Pt NMR spectra show that *trans*-$[\{Pt(NH_3)_2Cl\}_2(\mu\text{-dpzm})]^{2+}$, where dpzm = 4,4′-dipyrazolylmethane, forms a 1,2-GG interstrand cross-link with the oligonucletide d(ATGCAT)$_2$.[438] ^{1}H, ^{13}C and ^{195}Pt NMR spectra were used to characterise $Pt(R_2SO)(pyrazine)Cl_2$, where R_2SO = dmso, tmso, dbzso, dphso. The values of $^{3}J(^{195}Pt–^{1}H)$ were consistent with *trans* geometry.[439]



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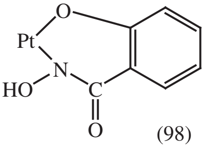

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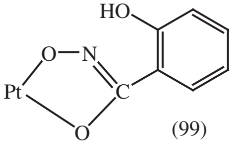
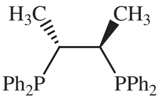


(99)

A ^{195}Pt NMR study was used to determine the influence of the *para*-substituent on the electronic properties of the metal centre in PtX(NCN-Z), where X = Cl, Br or I, NCN-Z = $2,6\text{-}(CH_2NMe_2)_2C_6H_4\text{-}4\text{-}Z$; Z = NO_2, COOH, SO_3H, $PO(OEt)_2$, PO(OH)(OEt), CH_2OH, SMe or NH_2.[440] ^{195}Pt NMR spectra were also used to characterise platinum(II) complexes with L-serine.[441] ^{13}C{^{1}H} and ^{31}P{^{1}H} spectra were reported for a range of platinum(II) salicylhydroxamate complexes, to distinguish between the binding modes (98) and (99).[442] ^{1}H, ^{13}C and ^{15}N NMR spectra all support square-planar coordination for the dimeric complexes $LPtCl_2PtL$, where L = (*E*)-Cl-*p*- or (*Z*)-CH_3O-*o*-$C_6H_4CH{=}NNHC(S)NH_2$, *i.e.* *N,S*-bidentate ligands.[443] ^{1}H, ^{13}C and ^{195}Pt{^{1}H} NMR spectra for $(H_2OOSPz)PtCl_2$, where H_2OOSPz = octakis(octylthio)porphyrazine, reveal *S,N*-coordination.[444] A ^{19}F-^{195}Pt HMQC experiment was used to differentiate conformers of $(C_6F_5)_3Pt(\mu\text{-}PPy_nPh_{3-n})RhL_2$, where n = 2, 3; L_2 = $(CO)_2$, diene *etc.*[445] The ^{31}P NMR spectra of $[PtCu_2(tdt)(\mu\text{-}SH)(dppm)_3]^+$, where tdt = 3,4-toluenedithiolate, and related, all show Pt satellite peaks.[446]

Chemical shifts and spin-spin coupling constants were obtained from the ^{31}P NMR spectra of $Pt_2(\mu\text{-}S)_2(P\text{-}P)$, $[Pt_2(\mu\text{-}S)(\mu\text{-}SH)(P\text{-}P)_2]^+$ *etc.*, where P–P = dppe, dppp.[447] The ^{13}C NMR spectrum of $[Pt([9]aneS_3(R,R\text{-chiraphos})]^+$, where *R,R*-chiraphos = (100), shows the effect of the chirality of the diphosphine chelate.[448] For PtX_2(eddp), where eddp = ethylenediamine-*N,N′*-di-3-propionate, X = Cl, Br, the ^{1}H NMR spectra show a very large diastereotropic splitting of the propionate protons.[449] ^{195}Pt chemical shifts for $[Pt(9S3)(NN)]^+$, where NN = bipy, phen or substituted analogues, 9S3 = thiacrown ligand, are consistent with a *cis*-PtS_2N_2 coordination sphere.[450] Similar data for $[Pt(12S3)_2]^{2+}$, where 12S3 = 1,5,9-trithiacyclododecane, are consistent with alternating positions for the 4 S lone pairs on the coordinated thioethers.[451]



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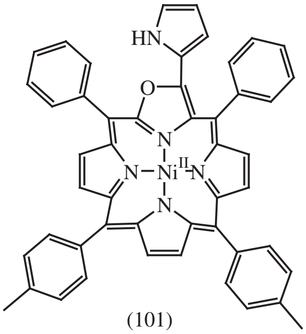

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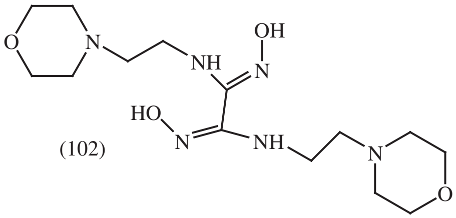

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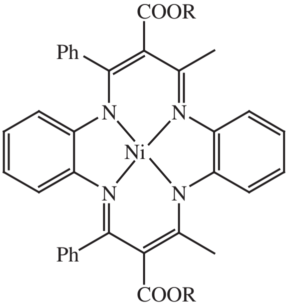
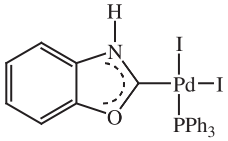


(103)

NMR data were also reported for: (101) (^{1}H).[452] [(6-Ph_2TPA)Ni(CH_3CN)(CH_3OH)]$^+$ (TPA = tris((2-pyridyl)methyl)amine and related) (^{1}H);[453] M(L)$^{2+}$ (M = Ni, Zn, Cd, Pb; L = Me_2[28]py_2N_6 macrocycle) (^{1}H);[454] (*E,E*)-Ni(HL)$_2$, (*E,E*)-$NiL_2(BPh_2)$ (H_2L = (102)) (^{1}H, ^{13}C);[455] (103) (R = Et, ^{i}Pr, ^{t}Bu, CH_2Ph) (^{1}H, ^{13}C);[456] [$NiBr_4${PhP(CH_2NHEt_2)$_2$}$_2$][$NiBr_4$] (^{1}H, ^{13}C, ^{31}P);[457] cationic Ni(II) complexes with dithiocarbamate and mixed-donor bidentate ligands, *o*-$Ph_2PC_6H_4$-CH=NR (R = Me, Et, ^{i}Pr, ^{t}Bu) (^{1}H, ^{31}P{^{1}H});[458] [MCl_2(med)]$_2$ (M = Ni, Pd, Pt; Hmed = *N*-(2-mercaptoethyl)-3,5-dimethylpyrazole) (^{1}H, ^{13}C, inc. HMQC, NOESY);[459] Ni(II) and Pd(II) salicyaldiminato complexes also containing the water-soluble phosphine 1,3,5-triaza-7-phosphaadamantane (^{1}H, ^{13}C, ^{31}P);[460] planar [Ni(dnpdtc)(P)$_2$]$^+$, where P = PPh_3, 1/2(dppe); dnpdtc = *N,N*-dipropyldithiocarbamate (^{13}C, ^{31}P);[461] a nickel complex of all-*trans* retinoic acid (^{1}H);[462] [(C_6F_5)$_2$Ni{S(S)P(OR)(ferrocenyl)]$^+$ (R = Et, ^{i}Pr) (^{1}H, ^{19}F, ^{31}P);[463] [(η^3-Me-allyl)Pd(η^2-*S,N*-$MeSC_6H_4N$=CHC_6H_4(X)Y)]$^+$, where X = H, F, Me; Y = H; X = H, Y = Cl, NMe_2NO_2 (^{1}H, ^{19}F{^{1}H}, ^{13}C{^{1}H}, ^{31}P{^{1}H}, including ^{1}H–^{1}H COSY, HSQC, HMBC);[464] [(COD)M$^+$(Cl)($PPh_2CH_2CH_2Sn^-Cl_4$)] (M = Pd, Pt) (^{31}P, ^{119}Sn);[465] (η-Ind)Pd(PR_3)Cl (Ind = indenyl, R = Ph, Cy, Me, OMe) (^{1}H, ^{13}C);[466] (η^2-$Ar_5C_{60}H$)M(PPh_3)$_2$ (M = Pd, Pt; Ar = Ph, substituted Ph) (^{1}H, ^{31}P);[467] $Au_2Pd_{21}(CO)_{20}(PEt_3)_{10}$ (^{31}P{^{1}H});[468] [Pd{$C_4(COOMe)_4$}(imidate)L]$^-$ (L = PPh_3, P(*p*-C_6H_4F)$_3$, PBu_3, py; imidate = succinimidate *etc.* (^{1}H, ^{13}C, ^{19}F, ^{31}P);[469] (104) (^{31}P);[470] (105) (R = CF_3, CF_2CF_3, $CF_2CF_2CF_3$) (^{1}H, ^{13}C, ^{19}F);[471] (106) (L^1=Cl, PEt_3. L^2 = Cl, z = 0; L^1 = L^2 = NCMe *etc.*, z = +1; R$^\alpha$, R$^\beta$ = CO_2Et, Ph) (^{19}F, ^{31}P);[472] *trans*-[Pd_2(μ-Cl)$_2${CH(CO_2Me)$CH_2C_6F_5$}$_2$(tht)$_2$] and related (tht = tetrahydrothiophene) (^{1}H, ^{19}F);[473] (107) and related (^{1}H, ^{13}C, ^{31}P);[474] (108) (^{1}H, ^{13}C, ^{31}P{^{1}H});[475]



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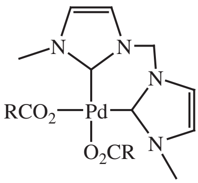

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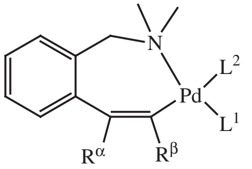

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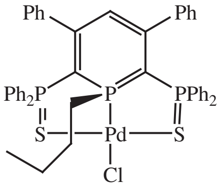

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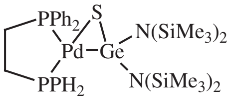

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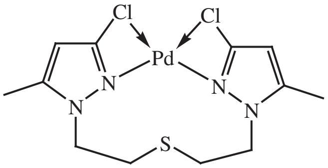

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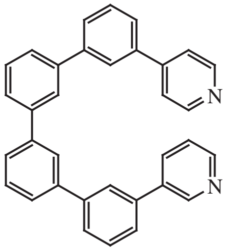

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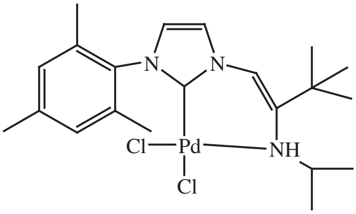

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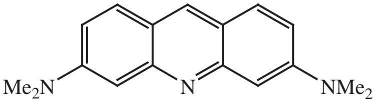
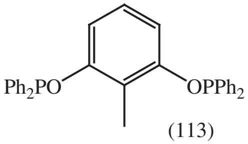


(112)

Pd(en)(3,4-NCNsq), where 3,4-NCNsq = 3,4-bis(cyanamide)squarate (^{13}C);[476] (109) and related (^{1}H, $^{13}C\{^{1}H\}$);[477] $[M]_2$(ttab) (ttab = tetrakis(7-azaindolyl)benzene; [M] = $PdCl_2$, $Ag(NO_3)$, $ZnCl_2$) (^{1}H, ^{13}C);[478] Pd_2L_2 (L = (110)) (^{1}H);[479] (111) and similar (^{1}H, $^{13}C\{^{1}H\}$);[480] *cis*-MCl_2(diamine) (M = Pd, Pt; diamine = 2,3- or 3,4-diaminotoluene, 4,5-diaminoxylene, 2,3-diaminophenyl) (^{1}H, $^{13}C\{^{1}H\}$, ^{195}Pt);[481] $MCl_2(L)$ (M = Pd, Pt; L = methyl-3,4-diamino-2,3,4,6-tetradeoxy-α-L-*lyxo*-hexapyranoside);[482] Pd(X)(py)(PPh_3)(L) (X = Cl, L = 8-methylthiotheophylline; X = Br, L = 8-benzylthiotheophylline) (^{1}H, $^{31}P\{^{1}H\}$);[483] *cis*-$[M(A)_n(Cl)(AO)]^+$ (M = Pd, Pt; A = en (n = 1), NH_3 (n = 2); AO = (112) (^{1}H);[484] $[Pd(\eta^1,\eta^5\text{-5-OMe-}C_8H_{12})(L)]^+$ (L = α-iminoketone *N,O*-ligands) (^{1}H, ^{13}C, ^{19}F, ^{19}F, ^{1}H NOESY);[485] $PdCl_2(L\text{-}\kappa^2\text{-}P,P)$ (L = $Ph_2PCH_2P\text{-}(NC_4H_8)_2$ and related) (^{1}H, $^{31}P\{^{1}H\}$);[486] $[Pd_2Cl_2(\mu\text{-}Cl)_2\{Ph_2P(CH_2CH_2O)_nCH_2CH_2PPh_2\text{-}P,P')$ (n = 3, 4) (^{1}H, $^{31}P\{^{1}H\}$);[487] *trans*-$PdCl(PPh_3)_2(HL)$ and *trans*-$[PdCl(PPh_3)_2]_2L$ (H_2L = bis(8-thiotheophylline)alkane derivatives) (^{1}H, $^{13}C\{^{1}H\}$, $^{31}P\{^{1}H\}$);[488] MX_2L_2 (M = Pd, Pt; X = Cl, Br, I; L = $As(CH_2\text{-}CH{=}CH_2)_3$ and similar) (^{1}H, ^{13}C, ^{195}Pt);[489] Pd(oxalate)(pyridoxine)$_2$ (^{13}C);[490] $Pd(OPh)(CO_2Ph)(PPh_3)_2$ (^{1}H, $^{13}C\{^{1}H\}$, $^{31}P\{\{^{1}H\}$);[491] M(ESDT)(Am)Cl (M = Pd, Pt; ESDT = $EtO_2CCH_2(CH_3NCS_2Me$; Am = chiral amino-alcohols) (1- and 2-D NMR);[492] $Pd_4(\mu\text{-}OOCCF_3)_4(\mu\text{-}L)_2$ (L = (113)) (^{1}H, $^{13}C\{^{1}H\}$, ^{31}P);[493] $Pd_2(\mu\text{-}SO_2)(\mu\text{-}PPh_2py)(PBz)_3$, $Pd_3(\mu\text{-}PPh_2py)_2(\mu\text{-}SO_2)\text{-}(PBz_3)_2$ ($^{31}P\{^{1}H\}$);[494] *cis*-M(L-*S,O*)$_2$, where M = Pd, Pt; HL = *N,N*-dialkyl-*N*′-(2,2′-dimethyl-propyl)thioureas (^{1}H, ^{13}C, ^{195}Pt);[495] *cis*-MX_2L (M = Pd, Pt; L = [18]aneO_4Te_2, X = Cl or Br) (^{1}H, ^{63}Cu, $^{125}Te\{^{1}H\}$, ^{195}Pt);[496] MCl_2([n]aneS_2Te), where M = Pd or Pt, n = 11, 12 (^{1}H, $^{13}C\{^{1}H\}$, $^{125}Te\{^{1}H\}$, ^{195}Pt);[497] $Pt(CF_3)_3(PPh_3)^-$, $Pt(CF_3)_4{}^{2-}$ (^{13}C, ^{19}F, ^{31}P, ^{195}Pt, $^{13}C(^{19}F$ DEPT));[498] $[PtX_n(CF_3)_{6-n}]^{2-}$ (X =F, OH, Cl, CN; n = 0–5) (^{19}F, ^{195}Pt);[499] *trans*-$[PtPh_{3-n}(C_6F_5)_n]_2PtCl_2$ (n = 1, 2) (^{1}H, ^{19}F, ^{31}P);[500] $[Pt(C_6Cl_5)(C_6F_5)_3]^{2-}$ and related (^{1}H, ^{19}F);[501] *trans*-$PtCl_2$(coe)(L) (coe = cyclo-octene, L = coe, MeOH, MeCN) (^{1}H, ^{195}Pt);[502] *trans*-$[PtCl_2(coe)]_2(L)$ (L = ArC(H) = NCH_2CH_2-N = C(H)Ar, Ar = 3- or 4-C_6H_4Bpin, pin = 1,2-$O_2C_2Me_4$) (^{1}H, ^{11}B, ^{13}C);[503] (114a and b) (L = PMe_2Ph) ($^{31}P\{^{1}H\}$);[504] (115) (X = range of linking groups) (^{1}H, ^{31}P);[505]

$PtCl_n(1\text{-}S\text{-}C_2B_{10}H_{11})_{2-n}(N\text{–}N)$, where N–N = bipy, phen, n = 1 or 0 (^{1}H, ^{11}B, ^{13}C, ^{195}Pt);[506]



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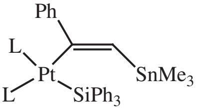
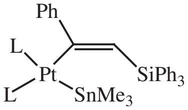


(114a)



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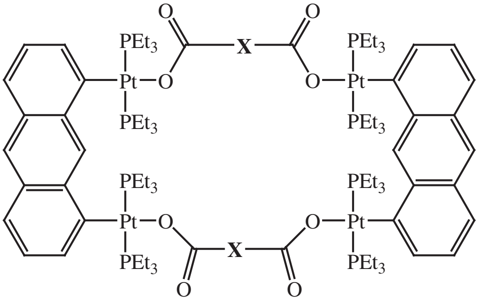

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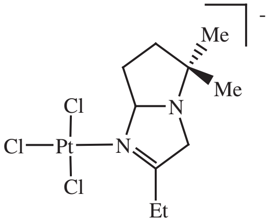
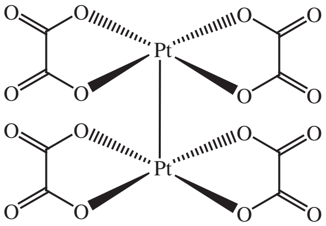


(116)

$[Pt(NH_2CH_2COO\text{-}N,O)\{cyclo\text{-}[NH_2CH(CH_2C_6H_4)]COO\text{-}N,C\}]^-$ and related (^{195}Pt);[507] $Pt(H)(PPh_3)_2\{Si(CH_2SPh)_2R\}$ (R = Me, CH_2SPh) (^{1}H, ^{13}C, ^{29}Si, ^{195}Pt);[508] $[Pt(SnB_{11}H_{11})_4]^{6-}$ (^{1}H, ^{11}B, ^{119}Sn);[509] $[Pt(\mu\text{-}Cl)(SnR_2Cl)(L)]_2$ (L = PEt_3, PBu_3, PMe_2Ph, PPh_3; R = $N(SiMe_3)_2$, $CH(SiMe_3)_2$) (^{31}P);[510] *cis*- and *trans*-$Pt(RNH_2)(NO_3)_2$ (R = Me, Et, ^{n}Pr, ^{n}Bu, ^{i}Pr, ^{i}Bu);[511] $[Pt\{2,6\text{-}(NMe_2CH_2)_2C_6H_2\text{-}4\text{-}COOH\}]$ (^{1}H, ^{13}C, ^{195}Pt);[512] $PtCl_2(NCNR_2)_2$ (R_2 = Me_2, Et_2, C_5H_{10}, C_4H_8O) (^{1}H, ^{13}C{^{1}H});[513] *trans*-$PtCl_2\{NH{=}C(OMe)NR_2\}_2$ (R = Me, Et) (^{1}H, ^{13}C{^{1}H});[514] *trans*-$[PtCl_2\{NH{=}C(Et)ON{=}C(Me)\text{–}C(Ph){=}NN{=}CH(C_6H_3\text{-}2\text{-}OH\text{-}5\text{-}NO_2)\}_2]$ and related (^{1}H, ^{13}C{^{1}H}, ^{195}Pt);[515] (116) and similar (^{1}H, ^{13}C, ^{195}Pt);[516] [{*cis*-$Pt(NH_3)_2Cl\}(\mu\text{-}pzn)]Cl_2$ (pzn = pyrazine) and other azine-bridged complexes (^{1}H, ^{195}Pt);[517] *trans*-$[Pt(\mu\text{-}NH_2)_2(ampy\text{-}N^1,N^2,N^2)_2\{(en)Pd\}_2Pd(H_2O)]^{4+}$ (^{1}H);[518] *cis*-$[Pt(NH_3)_2(9\text{-}made\text{-}N6)(9\text{-}made\text{-}N7)]^{2+}$ (made = methyladenine) (^{1}H, ^{195}Pt);[519] $PtCl_5$(9-MeAH) (9-MeAH = 9-methyladeninium cation) (^{1}H, ^{13}C, ^{195}Pt);[520] $Pt(L)I_2$ (L = *cis*-1,2-bis(methoxyamino)cyclohexane, and related) (^{1}H, ^{13}C, ^{195}Pt);[521] $Pt^{IV}(dach)L_3L'$, $Pt^{IV}(dach)L_2L''_2$ (dach = *trans*-(±)-1,2-diaminocyclohexane, L = acetate, propionate, L′ = acetate, propionate, valerato, pivalato, L″ = trifluoroacetato) (^{1}H);[522] $[Pt^{IV}$(*cis*-1,4-dach)(L)(*trans*-X)$_2$Cl]$^+$ (^{1}H, ^{195}Pt);[523] isomeric structures of Pt(dach) complexed to tamoxifen or hydroxyltamoxifen (2-D NMR study);[524] oestrogen-tethered , Pt(IV) complexes (^{1}H);[525] *trans*-$PtCl_2$(Ala-*N*)(Phe-*N*) and *ortho*-metalated [Pt(*S*)-Ala-*N*)][(*S*)-Phe-*N,Cl*] (Ala = alanine, Phe = phenylalanine) (^{1}H, ^{13}C, ^{195}Pt, ^{1}H-^{1}H COSY);[526] $(MCl_n)_m$(dippf) (M = Pt, Zn, Cd, Hg, n = 2, m = 1; M = Au, n = 1, m = 1) (^{1}H, ^{13}C, ^{31}P);[527] *trans*-$Pt(Cab^{P,Si})_2$, where $Cab^{P,Si}$ = $\eta^2\text{-}[(SiMe_2(PR_2)C_2B_{10}H_{10}\text{-}P,Si]$, R = Me, OEt (^{1}H, ^{31}P);[528] (117) (^{195}Pt);[529]

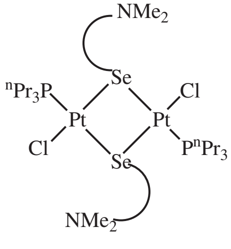


(117)

supramolecular assemblies derived from 1,4-bis(4-pyridyl)tetrafluoro-benzene and diphosphine Pt(II) and Pd(II) triflates (^{1}H, ^{31}P{^{1}H}, ^{19}F, ^{195}Pt{^{1}H}),[530] [(bis(phosphonomethyl)amino-κ*N*)acetate-κ*O*(2-)]-platinum(II) complexes attached to a range of 1,2-diamines (^{1}H, ^{13}C, ^{31}P);[531] Pt(II) and Au(III) complexes of bile acids (^{1}H, ^{13}C, ^{195}Pt);[532] *trans,trans*-$Pt(R_2SO)Cl_2$(μ-pyrazone)$Pt(R_2SO)Cl_2$ (R = Me, Pr, Bu, Bz; R_2=$(CH_2)_4$) (^{195}Pt);[533] [Pt(μ-*N,S*-8-TT)$(PPh_3)_2]_2$ (8-TTH$_2$ = 8-thiotheophylline) (^{1}H, ^{31}P{^{1}H}),[534] *cis*-$PtCl_2$(L) (L = 4,5-bis(diphenylphosphine)-9,9-dimethyl-xanthene) (^{31}P);[535] Pt(dppf)(2-Spy)$_2$, [Pt(dppf)(2-Spy)](BF$_4$) (dppf = 1,1′-bis(diphenylphosphino)ferrocene; 2-Spy = 2-mercaptopyridine) (^{1}H, ^{13}C{^{1}H^{31}},P{^{1}H},^{195}Pt{^{1}H}),[536] $[Pt_3(\mu\text{-SR})_4(dppm)_2]^{2+}$, $[Pt_2(\mu\text{-ER})_2(dppm)_2]^{2+}$ (E = S, Se; R = alkyl, aryl) (^{1}H, ^{13}C, ^{31}P, ^{195}Pt);[537] and (118) and its *cis*-isomer, where Me$_2$N-Se = [Me$_2$N(CH$_2$)$_3$Se]$_2$ (^{1}H, ^{13}C, ^{31}P, ^{77}Se, ^{195}Pt).[538]

2.11 Compounds of Group 11

2.11 Compounds of Group 11. – Detailed ^{1}H and ^{13}C NMR spectra were used to determine the structures of $[Cu(L)]^{+}$, where L = (119) (R = H, Me or Ph). All involve η^{2}-coordination between Cu^{I} and the phenyl ring of the ligand side-arm.[539] ^{1}H NMR data were used to structurally characterise new copper [3]rotaxanes. Rings contained either a single phen chelate or two different chelates (phen, terpy).[540] The complex $[Cu_3(\mu_3\text{-Br})_2(\mu\text{-pz*})_3Br_3]^{2-}$, where pz* = 4-O$_2$N-pz, pz = pyrazolato anion, shows magnetic equivalence of the 3 pyrazole rings, with an average D$_{3h}$ symmetry in solution.[541] ^{1}H NMR experiments for M$_2$(Indo)$_4$(dmf)$_2$, where M = Cu(II), Zn(II), Indo = (120), show greater lability (lower thermodynamic stability) for M = Zn compared to Cu.[542]



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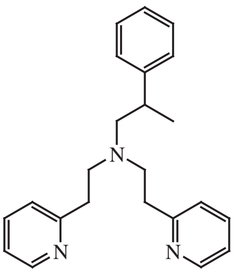

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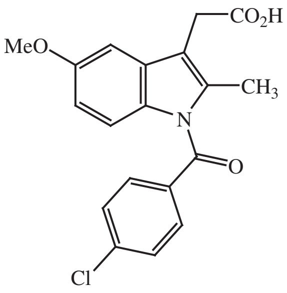
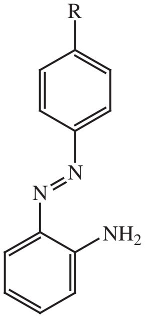


(120)

A review has appeared on NMR studies on copper proteins.[543] NMR studies (^{1}H,^{15}N) were used to probe the structure of the Cu-bound form of protein

Menkes ATPase.[544] The tight ion-pair $[Cu(PCy_3)_2][CuMe_2]$ gives a ^{13}C signal due to C_1 of PCy_3 which is a triplet, due to virtual coupling to two P atoms – confirming the formation of this species.[545] ^1H, ^{31}P and ^{77}Se NMR data were reported for $Cu_{11}(\mu_9\text{-}Se)(\mu_3\text{-}Br)_3\{Se_2P(OR)_2\}_6$, where R = Et, ^nPr, ^iPr. The two inequivalent Se nuclei of the diselenophosphate ligand show different scalar coupling patterns to adjacent phosphorus nuclei.[546] The ^1H NMR spectra of MX_nL, where M = Cu^I, Ag^I, Hg^{II}, L=*o*-tellurated *p*-bromoacetanilide derivatives, X = Cl, NO_3, n = 1 or 2, show that L is coordinated *via* the Te atom.[547]

^1H and ^{13}C NMR data allowed the determination of enantiomeric abundances of chiral olefinic compounds using the fragment (chiral diamine)Ag^+.[548]



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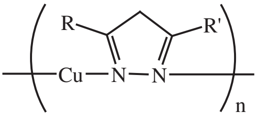
Proton NMR spectra were used to characterise a range of diazoketiminato complexes of gold(III), $(L)AuCl_2$, where L = (121), R = H, Me or Cl.[549] The $^{31}P\{^1H\}$ NMR spectra of $[Au_2(NP_3)_2]X_2$, where $NP_3 = N(CH_2CH_2PPh_2)_3$, X = Cl, Br, are consistent with the formation of mononuclear forms in solution.[550] ^{31}P NMR spectra show that $[Au(PR_2)]_n$, where $PR_2 = PMes_2$, PCy_2, PPhMes *etc*, exist in solution as mixtures of different oligomers.[551] ^{31}P NMR data were also reported for the 42-membered ring species $[Au_4(\mu\text{-}PP)(\mu\text{-}L)_2]^{4-}$, where PP = $Ph_2P(CH_2)_3PPh_2$, L = 1,2-$C_6H_4(NHCO\text{-}4\text{-}C_5H_4N)_2$.[552] The ^3C and ^{31}P NMR spectra for $[(R_3P)Au(Seu)]^+$, where Seu = selenourea, R = Cy, Et, Me, *p*-tol, *m*-tol, Ph, are consistent with Se-coordination to Au.[553]

NMR data have also been reported for: $[Cu\{1,2\text{-}C_6H_4(CH_2SbMe_2)\}_2]^+$ and similar (^1H, ^{63}Cu);[554] DmpCu ← L, where Dmp = 2,6-$Mes_2C_6H_3$, L = PPh_3, $C\{N(^iPr)CMe\}_2$ (^1H, ^{13}C, ^{31}P);[555] $M_2(bipy)_2(tsdb)$, where M = Cu, Zn, H_4tsdb = *N,N′,N″,N‴*-tetrasalicylidene-3,3′-diaminobenzidine (^1H, ^{13}C, ^1H-^1H COSY);[556] $[M(bipy)(LH_2)Cl_2]_n$, where M = Cu, Zn, LH_2 = 5-cyano-6-(4-pyridyl)-2-thiouracil;[557] (122) (n = 3, R = R′ =^iPr; n = 4, R = R′ = ^tBu, R = ^tBu, R′ = ^iPr (^1H, ^{13}C);[558] polymeric (123) (^1H, ^{13}C);[559] $[Cu^I(L)_2]^+$, where L = (124), n = 2, 3 or 4 (^1H);[560] $[Cu(dppz)_2]BF_4$, where dppz = dipyrido[3,2-a:2′,3′-c]phenazine (^1H);[561] coordination complexes formed by Cu^I with phosphines, phosphates in liquid NH_3 solutions($^{63,65}Cu$);[562] $[Cu(diphosphine)_2](RCOO)$, where R = C_2F_5, C_4F_9, C_6F_{13}, C_8F_{17}, C_9F_{19}, diphosphine = 1,3-bis(diphenylphosphino)propane, 1,2-bis(diphenylphosphino)benzene (^1H, ^{13}C, ^{19}F, ^{31}P, ^{63}Cu);[563] $[Cu(dppe)(NO_3(MeCN)]_n$, $[Cu(dppe)(NO_3)]_n$ (dppe = 1,2-bis(diphenylphosphino)ethane);[564]



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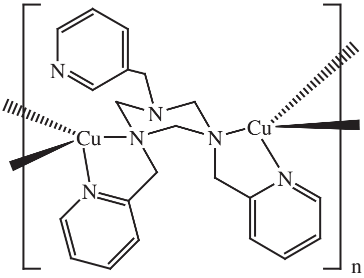

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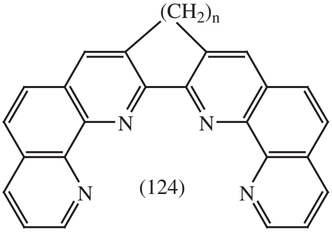

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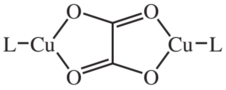

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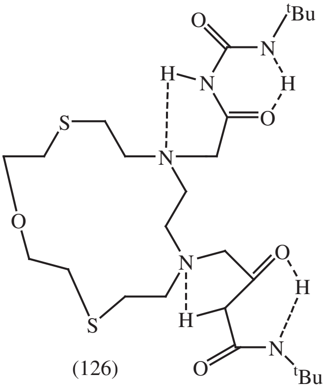

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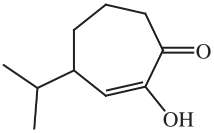
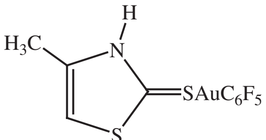


(127)

(125), where L = $H_2C{=}C(H)\text{-}SiMe_2tBu$, $H_2C{=}C(H)SiEt_2Me$, norbornene (^{13}C);[565] $[Ag_4(L)_n(dppm)_4]^{2+}$ (L = *N,N,S*-mercapto-benzimidazolate, n = 1), or $[Ag_2(L)(dppm)_2]_2$ (L = *O,S*-mercaptonicotinate);[566] Ag(L), where L = (126) and related (^1H);[567] diphosphine adducts with $Ag^I(NO_2)$ (^1H, ^{31}P);[568] $[Ag(L)]_2$, $Al(L)_3$, where HL = (127);[569] $\{Ag_8(\mu_8\text{-}X)[Se_2P(OR)_2]_6\}PF_6$, where R = Et, ^{n}Pr, ^{i}Pr, X = Cl or Br (^{31}P);[570] [Au(Hdamp-C^1)Cl(FcTSC)]Cl, where Hdamp = 2-(dimethylaminomethyl)phenyl, FcTSC = formylferrocene thiosemicarbazones {^1H, ^{13}C);[571] $[Au(\mu\text{-}3,5\text{-}{}^tBu_2\text{-}pz)]_4$ (^1H, ^{13}C);[572] Au(ppy)X (ppy = 2-phenylpyridine, X = (SCN)(NCS), thiolactate, thiosalicylate, 2,3-dimercapto-1-propanol, 2,3-dimercaptosuccinic acid (^1H, ^{13}C);[573] $(Ph_3P)AuPh$, $C_6H_5[Au(PPh_3)]_2BF_4$ (^1H);[574] $Au(PPh_3)(Hxspa)$, $Au(PPh_3(xspa)^-$ (H_2xspa = 3-(2-aryl)-2-sulfanyl-propenoic acids, aryl = phenyl, furyl, thienyl) (^1H, ^{13}C, ^{31}P);[575] $Au(Tp^x)(PR_3)$, where Tp^x = Tp, Tp*, *i.e.* hydrotris(pyrazol-1-yl)borate and 3,5-dimethylpyrazol-1-yl analogue, R = Ph, ^{t}Bu (^1H, $^{31}P\{^1H\}$);[576] Au(ppy)X, where ppy = 2-phenylpyridine, X = $OOCCH_3^-$, $OOCPh^-$, $(^-OOC)_2CH_2$, $(^-OOC)_2C_6H_4$ (^1H, ^{13}C, ^1H-^1H COSY);[577] $Au(L)(PPh_3$. where HL = mercaptonicotinic or mercaptopropionic acid (^1H, ^{13}C, ^{31}P);[578] (128) and related (^1H,^{13}C, ^{19}F);[579] and $Au_{38}(PhCH_2SCH_2S)_{24}$ (^1H, $^{13}C\{^1H\}$).[580]

2.12 Compounds of Group 12. – A $^{31}P\{^1H\}$ NMR study of the interaction of DBP^- (=dibenzyl phosphate) with $\{(bpapa)Zn\}^{2+}$ and $\{(tpa)Zn\}^{2+}$ (where bpapa = *N,N*-bis(2-pyridylmethyl)-*N*-(6-amino-2-pyridylmethyl)amine; tpa = tris(2-pyridylmethyl)amine) shows that bridging, η^2-coordination by phosphate occurs.[581] There is ^1H NMR evidence for complexation between Zn^{2+} and a terpyridyl ligand linked to a pyrene fragment.[582] Similar data for $[Zn(L)(d_6\text{-}dmso)]^{2+}$, where L = (2*R*,3*R*)-bis(2,2′-dipyridyl-5-methoxy)butane, show C_1 symmetry, *i.e.* distorted trigonal bipyramidal coordination at the Zn.[583] Proton NMR spectroscopy was used to probe the strength of N–H . . . Cl–N hydrogen bonding in $(L)ZnCl^+$ and $(L)ZnCl_2$, where L = range of polydentate ligands, *e.g.* 6-NHCO^{t}Bu-2-pyridylmethyl-bis(2-pyridylmethyl)amine.[584]



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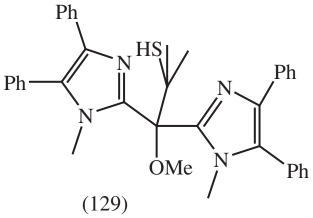


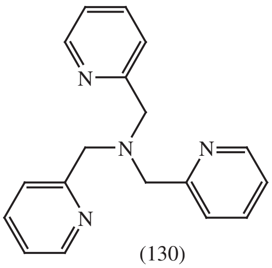
(129)

Mono- and di-zinc complexes of diporphyrins (two halves linked by $-(CH_2)_n$ spacers, n = 2–4) were characterised by 1-D and 2-D COSY and NOESY ^1H NMR studies.[585] ^1H and ^{31}P NMR specta were used to study interaction of tris-3-pyridylphosphine and mesophenyl zinc(II) porphyrin in $CDCl_3$ solution. The results were consistent with complete encapsulation of the former by 3 molecules of the latter.[586] Interaction of Zn^{2+} with *N′,N″,N‴*-tris(3-aminopropyl)amine or *N′,N″,N‴*-tris(3-dimethylaminopropyl)amine.[587] The proton NMR spectrum of $L_2Zn_2Br_2$, where HL = (129), shows coordination of L^- in bidentate *N,S*-fashion.[588] Similar data for M(SNNS), where M = Zn, Cd, H_2SNNS = 2,6-diacetylpyridinebis(*S*-benzyldithiocarbazate), show coordination *via* py N, azomethine N and mercaptide S atoms.[589] The ^1H and ^{31}P NMR spectra of Zn^{2+} complexes with phen-bridging polyaza ligands and ATP reveal multiple interactions (coordination, π-stacking *etc.*) in the Zn(II)-L-ATP system.[590]

There is ^1H and ^{13}C NMR evidence for agostic interactions in Cd(II) and Hg(II) complexes of *m*-benziporphyrin.[591] ^{113}Cd NMR spectroscopy was used to probe complexation of Cd^{2+} by 15-crown-5 and dibenzo-15-crown-5.[592] The binding of Cd(II) to 4-thiouridine or 4-thio-2′-deoxythymidine was follwed by ^1H and ^{113}Cd NMR spectroscopy.[593]

Proton NMR spectroscopy was used to characterise isotopically-enriched (^{199}Hg, ^{13}C) MeHgCl.[594] The ^{199}Hg NMR spectrum of $[Hg(TMIMA)_2]^{2+}$, where TMIMA = tris[(1-methylimidazol-2-yl]methylamine, shows a chemical shift of −1496 ppm, *i.e.* upfield from *N*-coordinated complexes of lower coordination number.[595] $^1J_{HgP}$ coupling constants were reported for $[(L)(O_2CR)_4(OPPh_2HgX_2)_4]$, where L = $(PhCH_2CH_2CHC_6H_2)_4$, R = OCH_2Ph, Cy, 4-C_6H_4Me, OCH_2CCH, X = Cl, Br or I.[596] The $P^{31}\{^1H\}$ NMR spectra of Pt(C-P)(μ-$O_2CR)_2HgX$, where C–P = $-CH_2C_6H_4P(o\text{-tolyl})_2$-κ*C,P*, R = CH_3, CF_3, X = Cl, Br, I, all show ^{199}Hg-P coupling consistent with a strong Pt–Hg bond in solution.[597] ^{1}H, ^{31}P{^{1}H} and ^{199}Hg{^{1}H} data have been reported for RHg[E-$P^iPr_2)_2N$], where R = Me, Et or thienyl, *e.g.* for R = thienyl, J(Se-Hg) 737 Hz, J(P-Hg) 179 Hz.[598]

NMR data have also been reported for: $Zn(L)Cl_2$ (L = *p*-R-C_6H_4-N=N-C_3H_2NNR', R = H, Me, Cl; R′ = Me, Et, CH_2Ph (^{1}H);[599] $[Zn(RSO_2N{=}CS_2)2]^{2-}$ (R = Ph, 4-MeC_6H_4) (^{1}H, ^{13}C);[600] $[(bppapa)Zn]^{2+}$ and $[(bppapa)ZnCl]^+$, where bppapa = (130) (^{1}H, ^{13}C);[601] 12 zinc(II) complexes containing semicarbazone and thiosemicarbazone ligands(^{1}H, ^{13}C);[602] $[\{N(PPh_2NR)_2\}M(OAc)$ and $\{N(PPh_2NR)_2M$ (M = Zn, Cd, Hg, R = Ph, $SiMe_3$) (^{1}H, ^{13}C, ^{31}P);[603] $[M\{Et_2NP(O)F_2\}_4]^{2+}$ (M = Zn, Cd) (^{19}F, ^{31}P, ^{113}Cd);[604]



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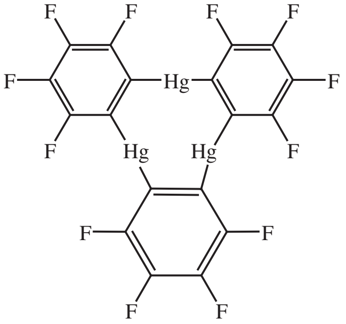


(131)

trimeric (131) (^{199}Hg);[605] $HgLCl_2$ (L = 1,2-bis-[(5-H/Me/Cl/NO_2)-1*H*-benzimidazol-2-yl)]-1,2-ethanediols) (^{1}H, ^{13}C);[606] $PhHg[(XPR_2)(YPR'_2)N]$, where X = O, Y = S, R = Me, Ph, OEt, R′ = Ph; X = Y = O, R = OEt, R′ = Ph (^{1}H, ^{13}C, ^{31}P);[607] and $[2\text{-}(Me_2NCH_2)C_6H_4]Hg[S(S)PR_2]$ (R = Me, Et or Ph) and related (^{1}H, ^{13}C, ^{31}P).[608]

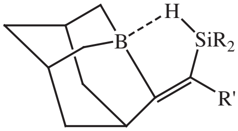
2.13 Compounds of Group 13.

– A review has appeared of NMR studies on Group 13 elements in systems of biological importance.[609]

2.13.1 Boranes and Heteroboranes. DFT calculations have been made for ^{1}H, ^{11}B, ^{13}C and ^{14}N NMR parameters for $(HCNBH)_n$, $(BH_2CN)_n$, where n = 1–6.[610] ^{1}H and ^{11}B chemical shifts have been reported and assigned (using DFT calculations) for $(CpRe)_2B_nH_n$ (n= 7–10).[611] An NMR study (^{1}H, ^{11}B, ^{13}C, ^{31}P) of 6-R-*arachno*-6,8,9- or -6,5,7-$PC_2B_7H_{11}$ confirm the *arachno* structures.[612] The ^{1}H and ^{13}C NMR spectra of $[(py\text{-}py)B_8H_{11}NH^iPr]$, where py-py = *trans*-1,2-di-(4-pyridyl)ethane, revealed the existence of *cis* and *trans* isomeric forms.[613] For 8-R-*nido*-7,8,9-$C_3B_8H_{11}$, where R = NH_2, NH^tBu, NMe_2, all of the cluster ^{1}H and ^{11}B resonances were identified by ^{11}B-^{11}B COSY and/or ^{1}H{^{11}B(selective)} experiments.[614] The ^{11}B and ^{13}C NMR data for the new 11-vertex species $[1,6,7\text{-}C_2SB_8H_{11}]^-$ were assigned with the aid of *ab initio* calculations.[615] ^{1}H, ^{11}B and ^{13}C NMR data were used to characterise 1,12-$[(CH_2)_3NH_2BH_2X]_2$-1,12-$C_2B_{10}H_{10}$ (X = CN, COOMe, CONHEt *etc.*);[616] and a novel low-melting ionic species [*N*-pentylpyridinium]$^+$[*closo*-$CB_{11}H_{12}]^-$.[617]

2.13.2 Other Boron Compounds. ^{1}H, ^{11}B and ^{13}C NMR data were also used to characterise $[(RC{\equiv}C)BNH]_3$ (R = H, $SiMe_3$).[618] ^{11}B and ^{19}F NMR data for $Cl_2BCF = CF_2$ show that there is significant π-character in the C–F bonds.[619] The ^{11}B NMR spectrum of $[B(CF{=}CF_2)_4]^-$ shows a quintet of quintets of quintets ($^{2}J_{BF}$ 21.5 Hz, $^{3}J_{BF}$ 3.2 and 2.2 Hz).[620] ^{1}H, ^{11}B, ^{13}C and ^{29}Si NMR data for (132) (R = Me, R′ = $SiMe_3$, Ph, Bu; R = ^{i}Pr, R′ = $SiMe_3$, $SiHPh_2$, Fc, are consistent with the presence of an Si–H . . . B bridge.[621] Assignments of ^{13}C and ^{29}Si NMR parameters for (133) were supported by DFT calculations.[622]

Other NMR data were reported for: (134) and related species (^{1}H, ^{11}B, ^{13}C, ^{29}Si, ^{119}Sn);[623] (135) (^{1}H, ^{11}B, ^{13}C, ^{15}N, ^{119}Sn);[624] (136) (R = H, Me, Ph, (H,Me); R′=$SiMe_3$, all = allyl) (^{11}B, ^{13}C, ^{29}Si);[625]



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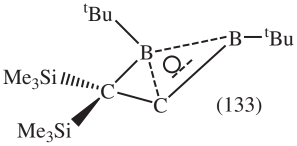

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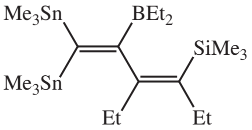

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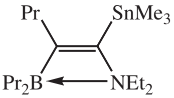

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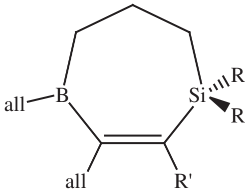

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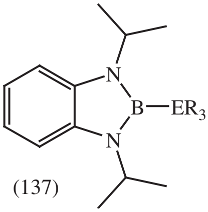


(137)

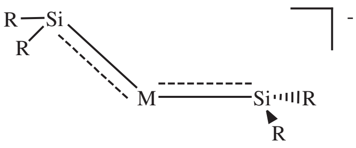
$X^+[R_fBF_3]^-$ (X = Li, NEt_4, 1-ethyl-3-methylimidazolium; R_f = C_2F_5, *n*-C_3F_7, *n*-C_4F_9) (^{1}H, ^{7}Li, ^{11}B, ^{19}F);[626,627] Ar_2BF, Ar_3B, $Ar_2B(OH)$ *etc*., where Ar = 2,4,6-$(CF_3)_3C_6H_2$, 2,4- and 2,6-$(CF_3)_2C_6H_3$;[628] (137), where ER_3 = CMe_3, $SiPh_3$, $GePh_3$, $SnMe_3$, $SnPh_3$, $PbPh_3$ (^{11}B);[629] CpB(N^{i}Pr$_2$)N(H)Cy and related (^{1}H, ^{11}B, ^{13}C);[630] four-membered BNCN ring compound {^{t}BuN(H)(Ph)B (μ-N^{t}Bu)$_2$C^{n}Bu} (^{1}H, ^{11}B, ^{13}C);[631] borosilicate glasses melted at 5 GPa (^{11}B, ^{17}O);[632] heterobimetallic complexes containing $[M(O^{i}Pr)_n]^-$ (M = B, Al, n = 4; M = Ti, n = 5, M = Nb, n = 6) and In(L)Cl (H_2L = $HOC_6H_4CH{=}NCH_2CH$-MeOH) (^{1}H, ^{11}B, ^{13}C, ^{27}Al);[633] and *cyclo*-borotetrasiloxanes $(RBO)(Me_2SiO)_3$ (R = ^{n}Bu or substituted phenyl groups).[634]

2.13.3 Compounds of Other Group 13 Elements. A review of ^{19}F and ^{27}Al NMR studies of organoaluminium fluorides has appeared.[635]

Proton NMR spectroscopy shows the presence of two isomers: {$C_4H_3N(CH_2NMe_2)$-2-[C(=O)NPh]-1}$AlMe_2$(*O*-bonded)and {$C_4H_3N(CH_2NMe_2)$-2-[CO(=NPh)]-1}$AlMe_2$ (*N*-bonded) in solution.[636] The proton NMR spectrum of Me_2Al[2,5-bis(*N*-aryliminomethyl)pyrrolyl] shows C_s symmetry in solution.[637] NMR studies (^1H, ^{13}C, ^{27}Al, ^{31}P) were used to study interactions of dihydronicotinamide adenine dinucletide (NADH) and Al(III), and their effects on conformation of the coenzyme.[638] ^{27}Al NMR spectroscopy was used to characterise aqueous aluminate-borate complexes, including $Al(OH)_4{}^-$, $Al(OH)_3OB(OH)_2{}^-$, $Al(OH)_2O_2[B(OH)_2]_2{}^-$ *etc.*[639] Similar data suggest five-coordination around Al(III) for $Et_2Al(O\text{-}R\text{-}NR^1NR^2)$ and $EtAl(OR\text{-}NR^1R^2)_2$, where R = $(CH_2)_2$, R^1=R^2=H; R = $(CH_2)_3$, R^1=R^2=H, Me, R^1=H, R^2=Me; R = CH_2CHEt, R^1=R^2 =H.[640]

The ^{29}Si NMR spectra of (138), where M = Ga, In, R = $SiMe^tBu_2$, are consistent with preferential localisation of negative charge on the terminal silicon atom.[641] The 1-D and 2-D ^1H NMR studies on the indium(III)-bleomycin A_2 (InBLM) show that the BLM is coordinated to In(III) through five N atoms, to give a distorted tetragonal pyramidal structure.[642]

NMR studies have also been reported for the following: *O*-(AlMeY)-2-(1,3,5-dithiazinan-5-yl)ethanolates (Y = Me or Cl) (^1H, ^{13}C, ^{27}Al);[643] $(R_2MONMe_2)_2$ (R = Me, ^tBu; M = Al, Ga) (^1H, ^{13}C, ^{15}N, ^{17}O, ^{27}Al);[644] 3,3,6,6-tetra-*tert*-butyl-1,4-dimethyl-3,6-dialumina-1,4-diazanorbornane (^1H, ^{13}C, ^{27}Al);[645] $Et_3Bi\text{-}M(^tBu)_3$ (M = Al, Ga), $[Me_2MSbR_2]_3$ (R = Me, M = Ga or In; R = ^iPr, M = Ga) (^1H, ^{13}C);[646] (Me-NP)AlR_2 (Me-NP^- = *N*-(2-diphenylphosphinophenyl)-2,6-dimethylanilide; R = Me, Et) (^1H, ^{13}C, ^{27}Al, ^{31}P);[647] (139) (R = Me, Ph, octyl, ^iPr, Cy, H) (^{13}C);[648]



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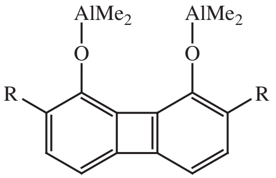

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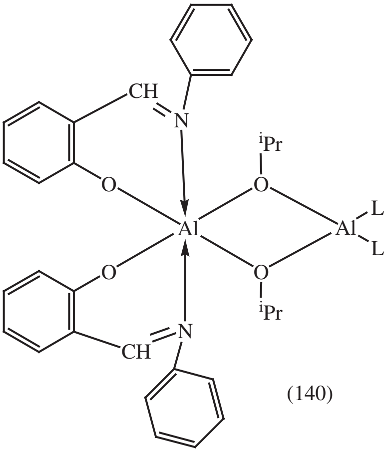

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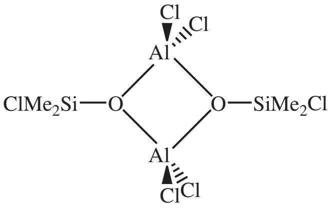

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$[(^{i}Pr_2Si)\{P(H)\text{-}MEt_2\}_2]_2$ (M = Al, Ga, In) (^{1}H, ^{13}C{^{1}H}, ^{31}P);[649] $[^{t}Bu_2MON = CMe_2]_2$ (M = Al, Ga) (^{1}H, ^{13}C, ^{27}Al);[650] (dmap)MR_3 (MR_3 = $AlMe_3$, $GaMe_3$, $InMe_3$, $TlMe_3$, $AlCl_3$, $Al^{t}Bu_3$) (^{1}H, ^{13}C{^{1}H});[651] $(AlMe_3)\{Ph_2P(8\text{-}CH_2C_9H_6N) = N^{t}Bu\}$, $(AlMe_2)\{CH(8\text{-}C_9H_6N)(Ph_2P{=}N^{t}Bu)\}$ (^{27}Al);[652] $[ArN(CH_2)_3NAr]\text{-}AlX(NMe_3)$ (Ar = 2,6-$^{i}Pr_2C_6H_3$, X = H, F) (^{1}H, ^{19}F);[653] X–H_2O-$NaAlO_2$ systems (X = triethanolamine, diethanolamine, di-isopropanolamine) (^{1}H, ^{13}C, ^{27}Al);[654] (140) (L = RR′C=NOH, R = R′ = Me, R = Me, R′ = C_4H_3S-2, C_4H_3O-2, C_5H_4N-2) (^{1}H, ^{13}C, ^{27}Al);[655] $[(acac)_2Al(\mu\text{-}O^{i}Pr)_2Al(\mu\text{-}O^{i}Pr_2Al\text{-}O\text{-}R\text{-}NR^1R^2)(O^{i}Pr)$ (R = $(CH_2)_3$, CH_2CMe_2, $(CH_2)_2$, R^1, R^2 = H, Me) (^{27}Al);[656] $BuMeSnO_2Al_2(O^{i}Pr)_{4-n}L_n$ (n = 1,2, L = heterocyclic acids based on indole) (^{1}H, ^{13}C, ^{27}Al, ^{119}Sn);[657] $Ga(L)_2B(O^{i}Pr)_2$, $Ga(L)_2Al(O^{i}Pr)_2$ (LH_2 = $HOC_6H_4CMe = NCH_2CHMeOH$) (^{1}H, ^{11}B, ^{13}C, ^{27}Al);[658] (141) (^{1}H, ^{13}C{^{1}H});[659] $(2,6\text{-}Mes_2C_6H_3)_2GaMe$ and related species (^{1}H, ^{13}C{^{1}H});[660] organometallic In-As cage compounds (^{1}H, ^{13}C);[661] $Me_2Tl(4\text{-}CF_3pymS)$ (4-CF_3pymSH = 4-trifluoromethylpyrimidine-2-thione) (^{1}H, ^{13}C, ^{205}Tl);[662] thallium tris(pyrazol-1-yl)borates (^{1}H, ^{13}C, ^{15}N);[663] $TlCl_2(L)(HL))$ (HL = picolinic or nicotinic acids) (^{1}H, ^{13}C, ^{205}Tl);[664] and $Tl(\mu\text{-}F)_3Ru(PPh_3)_3$ (^{19}F, ^{31}P).[665]

2.14 Compounds of Group 14. – *2.14.1 Carbon Compounds*. The proton and ^{13}C NMR spectra of the $C_5SiMe_7^{+}$ cation were consistent with rapid equilibration of $SiMe_2$ groups among different positions.[666] A review has been published on the use of ^{13}C NMR spectroscopy to study a wide range of [60]fullerene derivatives.[667] The ^{13}C and ^{19}F NMR spectra of the new fluorofullerene, $C_{60}F_{24}$ show that only one isomer is present, with T_h symmetry.[668] Mild hydrogenation of C_{60} produced $C_{60}H_n$ (n = 38, 40, 42, 44) – which were characterised by ^{1}H and ^{13}C NMR spectra.[669] ^{13}C NMR spectra, and *ab initio* calculations, gave evidence for the dimerisation of [5,6]-$C_{60}O$ to form $C_{120}O_2$ (C_2 symmetry).[670] ^{1}H and ^{13}C NMR data show C_s symmetry for a new fullerene-substituted phenanthroline ligand.[671] Proton NMR spectra were reported for hydrogenated and/or methylated fullerenes formed by CVD methods.[672] DFT calculations have been made of indirect NMR spin-spin coupling constants in C_{70}.[673] The ^{1}H NMR spectrum of the bis-oxide $C_{76}Me_4O_2$ shows that it has C_2 symmetry.[674]

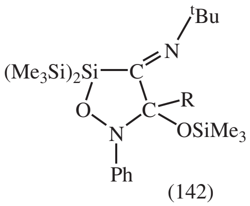
NMR data were also reported for: FC(O)OOOC(O)F (^{13}C, ^{19}F);[675] $CS_2N_3^{-}$, $CH_3CS_2N_3$ (^{1}H, ^{13}C, ^{14}N);[676] CCl_3^{+}, CBr_3^{+}, $C(OTeF_5)_3^{+}$ (^{13}C, ^{19}F);[677] a soluble C_{60}-TPP complex (^{13}C);[678] $C_{60}F_{17}OF$, $C_{60}F_{17}O(OH)$ (^{19}F);[679] $C_{60}(CF_3)_n$ (n = 2, 4, 6) (^{19}F);[680] C_{60} derivatives bearing one or more diphosphonate and hydroxyl substituents (^{31}P{^{1}H});[681] *e, trans*-1, *trans*-2, *trans*-3, *trans*-4 regioisomers of phosphorylated bismethanofullerenes (^{1}H, ^{13}C, ^{31}P);[682] C_{60}-containing polyphosphazenes (^{1}H, ^{13}C);[683] mono- and bis-adducts of C_{70} with 1,1,2,2-tetraphenyl-1,2-di-*tert*-butyl-1,2-disilane (^{1}H, ^{13}C, ^{29}Si);[684] and C_{70}NH isomers.[685]

2.14.2 Silicon Compounds. ^{29}Si NMR chemical shift tensors were calculated by *ab initio* methods for 21 simple silylenes, R_2Si:.[686] The proton NMR spectra of (Trip)SiH_3 and (Trip)AsH_2 (Trip = triptycene) included a characteristic signal of the single bridge proton of triptycene at 5.4 ppm.[687] ^{1}H, ^{13}C and ^{29}Si NMR spectra were used to characterise the relatively unstable 5-membered heterocyclic ring systems (142) (R = adamantyl, ^{t}Bu).[688] The ^{29}Si NMR data for the adduct $F_3Si(C{\equiv}CPh).py_2$ show that the only isomer present in solution is (143).[689] ^{29}Si spin-lattice relaxation times have been measured (32–100°C) for $MeSi(OMe)_3$.[690]

NMR spectra (^{1}H, $^{29}Si\{^{1}H\}$) were used to identify oligomeric primary alkyl silanes with up to 5–6 silicon atom chains.[691] The ^{29}Si NMR spectra for $^{t}Bu_2PhSiM$, where M = Li, Na or K, benzene and thf adducts are consistent with monomeric adducts, and increased negative charge on the silicon centre.[692] ^{1}H, ^{11}B, ^{13}C and ^{29}Si NMR data were obtained for a range of sila-2,4-cyclopentadienes (siloles).[693] NMR (^{1}H, ^{13}C and ^{29}Si) spectra were reported for $Si(SiMe_3)_3^{-}$ ions in solution.[694] The ^{1}H and ^{29}Si NMR spectra of complexes of tri- and diorganosilicon(IV) with sulfonamide imine are consistent with bidentate ligand coordination and 5- (tri-) and 6 (diorgano) coordination numbers.[695]

Analysis of ^{1}H 2-D COSY, ^{29}Si 2-D DOSY and $^{1}H\{^{29}Si\}$ 3-D DOSY-HMQC spectra was carried out for mixtures of cyclic dimethylsiloxanes.[696] ^{29}Si NMR spectra were analysed for octa-hydrosilsesquioxane cages containing a range of pendant groups.[697] *Ab initio* calculations of ^{29}Si NMR chemical shifts were carried out for complexes of silicates with carbohydrates, amino acids and polycarboxylic acids.[698] Low-temperature ^{1}H NMR data for $(thd)_2SiX_2$ (thd = 2,2,6,6-tetramethyl-3,5-heptanedionato, X = Me, ^{t}BuO, ^{t}AmO) show that *cis* six coordination is maintained in solution.[699]

NMR data were also reported for: silylarenes, $Ar(SiH_3)_n$, where Ar = phenyl, tolyl, xylyl, n = 1, 2 (^{1}H, ^{29}Si);[700]



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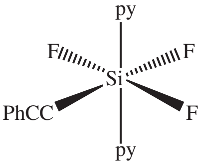

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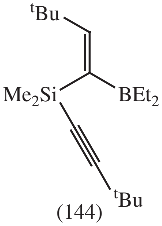

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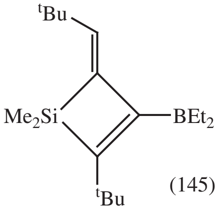

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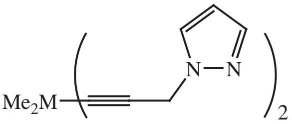

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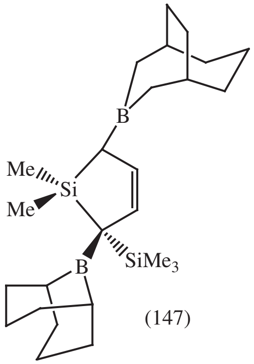

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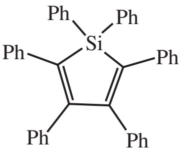

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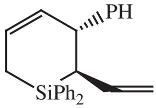

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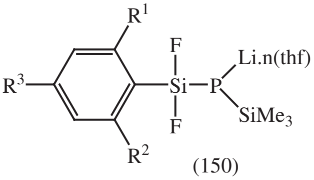
(144), (145) and related species (^{1}H, ^{11}B, ^{13}C, ^{29}Si);[701] (146) (M = Si, Sn) (^{1}H, ^{13}C, ^{29}Si, ^{119}Sn);[702] (147) and related species (^{1}H, ^{11}B, ^{13}C, ^{29}Si);[703] $R_nM(L)_{4-n}$ (M = Si, Sn; R = Me, Ph; HL = 2-acetylfuransulfaguanidine; n = 2, 3) (^{1}H, ^{13}C, ^{29}Si, ^{119}Sn);[704] (148) (^{29}Si);[705] new silacyclic compounds, *e.g.* (149) (2-D ^{1}H,^{13}C);[706] $(Me_5Si_3)_2Se_3$ (^{1}H, ^{13}C, ^{29}Si, ^{77}Se);[707] $(R^1R^2{}_2SiCH_2CH_2Si\text{-}MeH)_2.H_4bigR$ (H_6bigR = 1-propyl- or 1-phenylbiguanide; R^1, R^2 = Me, Et, Ph) (^{1}H, ^{13}C, ^{29}Si);[708] (aryl)ECl_3, (aryl)$_2ECl_2$ (aryl = 2,4,6-$(CF_3)_3C_6H_2$, 2,6- or 2,4-$(CF_3)_2C_6H_3$, E = Si, Ge, Sn) (^{19}F, ^{119}Sn);[709] (6-Me-Apy)$_2$(μ-SiMe)$_2$ (6-Me-Apy = 6-methyl-2-aminopyridine) (^{1}H, ^{13}C, ^{29}Si);[710] PhRSiCl(L), PhRSi(L)$_2$ (R = range of alkyl, aryl groups, HL = cyclic alcohols) (^{1}H, ^{13}C, ^{29}Si);[711] $(Me_3Si)_2HCP(=X)Cl_2$, where X = O, S, Se (^{1}H, ^{13}C, ^{31}P{^{1}H}, ^{77}Se);[712] (150) ($R^1 = R^2$ = 2,4,6-$^{i}Pr_3C_6H_2$ or 2,4,6-$Me_3C_6H_2$, R^3 = H, n = 2; $R^1 = R^2 = R^3 = {}^{t}Bu$, n = 3) (^{7}Li, ^{19}F, ^{29}Si, ^{31}P);[713] (151) (^{1}H, ^{13}C, ^{29}Si);[714] $F_3SiN(R)NMe_2$ (R = Me, $SiMe_3$, $SnMe_3$) (^{1}H, ^{13}C, $^{14/15}$N, ^{19}F, ^{29}Si, ^{119}Sn);[715] $R_3SiN[(CH_2)_nX]_2$ (R_3 = Me_2H, Me_2Cl, MeCl(H), n = 3, X = NMe_2, n = 2, X = OMe) (^{1}H, ^{13}C, ^{29}Si);[716]



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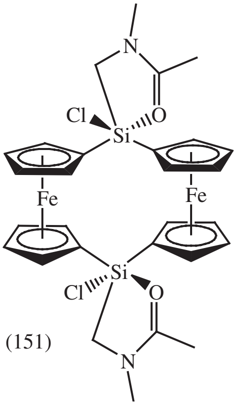

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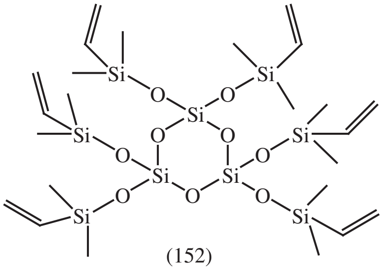

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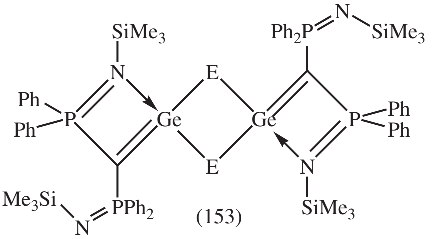
tert-butyldimethylsilyl derivatives of *N*,*O*-diacylhydroxylamines (^{1}H, ^{13}C, ^{15}N, ^{29}Si);[717] $R_2SiCl(L)$, $R_2Si(L)_2$, $R_3Si(L)$ (R = Me, Ph, L = sulfonamide-imine ligand) (^{1}H, ^{29}Si);[718] $R_2SiCl(SB)$, $R_2Si(SB)_2$ (R = CH_3, Ph), $Ph_3Si(SB)$ (SB = anion of Schiff base of sulfonamide) (^{1}H, ^{13}C, ^{29}Si);[719] $FSi(PH_2)_3$ (^{19}F, ^{19}F{^{1}H}, ^{29}Si, ^{29}Si{^{1}H});[720] polysiloxanes containing sulfonyl side-chains (^{1}H);[721] (152) and related species (^{1}H, ^{13}C{^{1}H},^{29}Si);[722] soluble tetra-branched polydimethylsiloxanes with terminal 2′-ethyl-4-cyclohexanyl-1,2-epoxide groups (^{1}H, ^{13}C, ^{29}Si);[723] cage-like silsesquioxanes (^{1}H, ^{13}C, ^{29}Si);[724] $[(O_2N)_2PhSiO_{1.5}]_8$ (^{1}H, ^{13}C);[725] and $MeRSi(OSnBu_3)_2$ (R = Me, CH_2CH_2CN) (^{29}Si).[726]

2.14.3 Germanium Compounds. NMR data (^{1}H, ^{13}C, and, where applicable, ^{77}Se and ^{125}Te) were all consistent with solid state structures of (153) (E = S, Se, Te) persisting in solution.[727] ^{31}P NMR data show that among the products of reaction of $GeCl_4$ with $CyPH_2$ is $CyP(H)GeCl_3$.[728] Proton and ^{13}C NMR spectra are consistent with tetrahedral geometry around the germanium atom in $(^iPrO)_{4-n}Ge(OCH_2CH_2OR)_n$, where R = Me, Et or Bu, n = 1–4.[729] NMR data were also reported for (154) (^{1}H, ^{13}C, ^{73}Ge);[730] $MeN(CH_2CH_2O)_2GeX_2$ (X = Cl, Br Me) (^{1}H, ^{13}C).[731]



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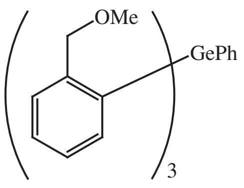

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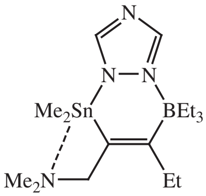

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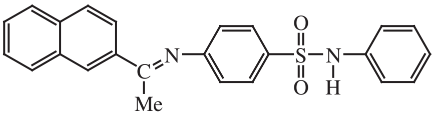
2.14.4 Tin Compounds. The ^{1}H, ^{13}C and ^{119}Sn NMR spectra of $Ph(Et)SnCl_2$ (phen) in dmso-d_6 suggest that the complex is at least partially undissociated in this solvent.[732] The ^{119}Sn NMR spectra of $[Bu_2Sn(L)_2]_n$, where L = pyridine mono- and dicarboxylates, show that the polymeric structures are not retained in solution.[733] ^{1}H, ^{11}B, ^{13}C, $^{14/15}$N and ^{119}Sn NMR results for (155) and related species gave evidence for strong N-Sn interaction.[734] The solution NMR spectra (^{1}H, ^{13}C, ^{119}Sn) of $[SnR_2(MePN\text{-}H]I$, where R = Me, Et, Bu, Ph; MePN = *N*-methylpyridoxine, show the presence of dimeric cationic units.[735] ^{1}H and ^{119}Sn NMR spectra of $[H_2B(im)_2]R_nSnCl_{4-n-1}$, where$[H_2B(im)_2]^-$ =

dihydrobis(1-imidazolyl)borate, n = 1–3, are all consistent with five-coordination at tin.[736]

The ^{1}H NMR spectrum of $[Ph_2SnCl(\mu\text{-}OH)]_2(quin)$, where quin = quinoline, is consistent with distorted trigonal-bipyramidal, five-coordination at Sn.[737] The ^{1}H, ^{13}C and ^{119}Sn NMR spectra of $R_2Sn(L)$, where R = ^{n}Bu, L = dianions of glycyl-tyrosine, leucine-tryptophan *etc*, show that all L^{2-} ligands are tridentate (*via* COO^-, NH_2, $N_{peptide}$).[738] The ^{119}Sn NMR spectra of $Bu_2Sn(L)A$, where HL = $RCOC{=}C(OH)N(Ph)N{=}CCH_3$ (R = Ph, Et, Me); AH = $C(O)C_6H_4C(O)NCHR'COOH$ (R′ = H, Me, ^{i}Pr, CH_2Ph), suggest that there are 6-coordinate tin centres in some cases.[739]

NMR data (^{1}H, ^{13}C, ^{15}N, ^{119}Sn) for $R_2Sn(L)$, where R = Me, Ph, L = 2-$OC_6H_4CH{=}N{-}N = C(O)Ph$, suggest five-coordination at Sn.[740] The ^{1}H, ^{13}C and ^{119}Sn NMR data for organotin(IV) complexes of (156) show that the ligand is bidentate, *via* nitrogen atoms.[741] The ^{1}H NMR spectra of $SnX_4(DMPP)$ and $R_2SnX_2(DMPP)$, where DMPP = (157), X = Cl, Br or I, R = Me, Et, Bu, Ph, indicate that there is significant dissociation in solution.[742] The ^{1}H and ^{119}Sn NMR spectra of $Me_2Sn(aptsc)$, where X = Cl, Br, Haptsc = acetone *N*(4)-phenylthiosemicarbazone, show that the ligand is *N,S*-bidentate, and the tin 5-coordinated.[743]



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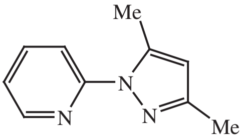

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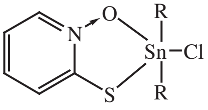

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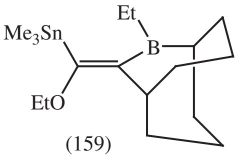
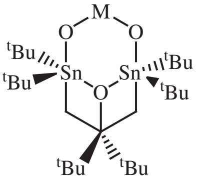


(159)

^{119}Sn NMR data were used to characterise a very complex (48-membered) tin macrocycle derived from di-*n*-butyltin chloride and the sodium salt of 2-mercaptonicotinic acid.[744] ^{1}H, ^{13}C and ^{119}Sn NMR results for $^nBu_3Sn(OOCAr)$, where Ar = $C_6H_3(NH_2)_2$-3,4 or −3,5, $C_6H_4N{=}NC_6H_4NMe_2$-4, reveal distorted tetrahedral coordination at the tin atom in CH_2Cl_2 solution, but trigonal bipyramidal geometry in strongly coordinating solvents.[745] ^{119}Sn data show 5-coordinate tin in solution for (158), where R = Me, Et, Bu, Ph, Bz.[746]

NMR data were also reported for: Me_3SnX, where X = $OTeF_5$, $N(SO_2F)_2$, $N(SO_2CF_3)_2$ (^{1}H, ^{13}C, ^{19}F, ^{119}Sn, ^{125}Te);[747] $R_3Sn(ceph)$, $R_2Sn(OH)(ceph)$ (R = Me, ^{n}Bu; Hceph = deacetoxy-cephalosporin antiobiotic) (^{1}H, ^{13}C, ^{119}Sn);[748] $R_nSn(OSO_2C_6H_4CH_3\text{-}4)_{4-n}$ (n = 2, 3; R = Et, ^{n}Pr, ^{n}Bu);[749] $(Ph_3Sn)_2(\mu\text{-oxalato})$ (^{119}Sn);[750] (159) and related Si and Ge species (^{1}H, ^{13}C, ^{11}B, ^{29}Si, ^{119}Sn);[751] R_3SnL, R_2SnL_2 (R = Bu, Ph, $PhCH_2$, $n\text{-}C_8H_{17}$; HL = 2-[(2,3-dimethylphenyl)-amino]benzoic acid) (^{1}H, ^{13}C, ^{119}Sn);[752] $^nBu_3Sn(L)$ (L = C_6H_4SEt-2, CHMe(SPh)) (^{1}H, ^{13}C, ^{119}Sn);[753] *n*-butyltin monomers containing 1, 2 or 3 chloride ligands;[754] $R_{4-n}SnL_n$ (n = 1, 2; L = 2-(2-fluoro-4-biphenyl)-propanoate (^{1}H, ^{13}C, ^{119}Sn);[755] di- and triorganotin(IV) complexes of 2′-hydroxy-acetophenone semicarbazone and thiosemicarbazone (^{1}H, ^{13}C, ^{119}Sn);[756] $R_{4-n}SnL_n$ (n = 1, 2; L = 2-[*N*-(2,6-dichloro-3-methylphenyl)amino]benzoate) (^{1}H, ^{13}C, ^{119}Sn);[757] $Ph_2SnCl(L)$, $Ph_3Sn(L)$, $Bu_2Sn(L)_2$ (HL = 2-*N*-ethyl- or 2-*N*-butyl-amino-1-cyclopentene-1-carbodithioic acid) (^{1}H, ^{119}Sn);[758] $[Me_2Sn(HTDP)(H_2O)]Cl$ (H_3TDPCl = thiamine diphosphate hydrochloride) (^{1}H, ^{13}C, ^{31}P, ^{119}Sn);[759] $[^nBu_2Sn(L)]_2O$, $^nBu_2Sn(L)_2$ (HL = 4′/2′-nitrobiphenyl-2-carboxylic acids) (^{1}H, ^{13}C, ^{119}Sn);[760] $Ph_2SnCl(MNBT)$, $Bz_2Sn(MNBT)_2$, $^nBu_2Sn(MNBT)_2$ (HMNBT = 2-mercapto-6-nitrobenzothiazole) (^{1}H, ^{13}C, ^{119}Sn);[761] $SnMeX_2(PMP)$ (X = Cl, Br; PMP = 2-(pyrazol-1-ylmethyl)pyridine) (^{1}H, ^{13}C);[762] (160) (M = Me_2Si, Ph_2Si, MesB, Ph_2P^+, X = OH; M = Ph_2Si, X = F) (^{1}H, ^{13}C, ^{31}P, ^{119}Sn);[763] $[R_2Sn(O_2CR')OSO_2Me]_2$ (R = ^{n}Pr, ^{n}Bu; R′ = C_9H_6N-2 or −1, 4-$MeOC_9H_5N$-2) (^{1}H, ^{13}C, ^{119}Sn);[764] R_2SnL_2, $R_2Sn(L)(L')$ (L, L′ = 4-X-benzohydroxamic acids, X = Cl, OMe) (^{1}H, ^{13}C, ^{119}Sn);[765] $R_2SnR'_2$, R_3SnR' (R = Me, Bu, Ph, Bz; R′ = n-C_7H_{15} (^{1}H, ^{13}C, ^{119}Sn);[766] $^nBu_2Sn(FcCOS)_2$ (Fc = ferrocenyl) (^{1}H, ^{13}C, ^{119}Sn);[767] $\{[^nBu_2Sn(O_2CCH_2CS_2NR_2)]_2O\}_2$ (R = Me, Et) (^{1}H, ^{119}Sn);[768] $R_2Sn(PN\text{-}2H)$ (PN = pyridoxine; R = Me, Et, Bu) (^{1}H, ^{13}C, ^{119}Sn).[769]



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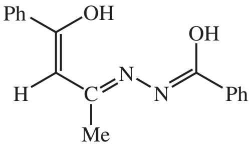

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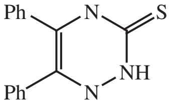

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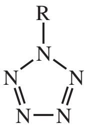
$R_2Sn(L)$ (R = Me, Ph; H_2L = (161)) (^{1}H, ^{13}C, ^{15}N, ^{119}Sn – inc. 2-D COSY, HMQC, HMBC for ^{1}H, ^{13}C);[770] R_2SnX_2 (R = ^{n}Bu, Ph, Bz; HL = 2-pyridinethiol-*N*-oxide) (^{1}H, ^{13}C, ^{119}Sn);[771] *trans*-$Me_2Sn(L)_2$ (L = MeO-*p*-$C_6H_4C(O)NHOH$) (^{1}H, ^{13}C, ^{119}Sn);[772] $Me_2Sn(aptsc)X$ (X = Cl, Br; Haptsc = acetone N(4)-phenylthiosemicarbazone) (^{1}H, ^{119}Sn);[773] $R_2Sn(L)$ (R = Me, Bu; H_2L = 2,2′-dihydroxyazobenzene) (^{1}H, ^{13}C{^{1}H}, ^{119}Sn{^{1}H});[774] $Me_2Sn(OAr)_2$, $BuSn(OAr)_3$ (Ar = range of aryl groups) (^{1}H, ^{13}C, ^{119}Sn);[775] $[R_2Sn(H_2O)_2(OPPh_3)_2](O_3SCF_3)_2$ (R = Me, Bu) (^{1}H, ^{13}C, ^{31}P, ^{119}Sn);[776] $SnPh_2(L)Cl$, $SnMe_2(L)_2$ (HL = (162)) (^{1}H, ^{13}C, ^{119}Sn);[777] homo- and heterobimetallic tri- and di-ethanolaminate derivatives cotaining Bu_2Sn^{IV} (^{1}H, ^{27}Al, ^{119}Sn);[778] 4-, 5- and 6-coordinate unsymmetrical diorganotin hydrides (^{1}H, ^{13}C, ^{119}Sn);[779] diorganotin(IV) derivatives of L-cysteine (^{1}H, ^{13}C, ^{119}Sn);[780] $[(MeCN)_4(RSn(CH_2)_nSn(R)(MeCN)_4]^{2+}$ (R = CH_2SiMe_3, n = 3, 4, 8, 10) (^{119}Sn);[781] organo-tin(IV) complexes of 2-maleimidoacetic acid (^{1}H, ^{13}C, ^{119}Sn);[782] $(BrMe_2SnCH_2CH_2)_2P(O)Ph$ (^{1}H, ^{13}C, ^{31}P, ^{119}Sn);[783] $[(SnNBu^t)_4(\mu\text{-}OSO_2)]_2$.thf (^{1}H, ^{119}Sn);[784] tetrakistin(IV) alkoxides (^{1}H, ^{13}C, ^{119}Sn);[785] and $ROP(S)[SSnR'_3]_2$ (R = Me, ^{i}Pr, Ph; R′ = ^{n}Pr, ^{n}Bu, Ph), $RSP(O)S_2SnR'_2$ (R = Me, ^{i}Pr; R′ = Me, Et, Ph) (^{1}H, ^{31}P, ^{119}Sn).[786]

2.14.5 Lead Compounds. NMR data (^{1}H, ^{13}C, ^{31}P, ^{207}Pb) were used to characterise $PbPh_2Cl_4^{2-}$ and $PbPh_3Cl_2^-$. For the latter, the phenyl groups are all equatorial in a trigonal bipyramidal configuration.[787] Other NMR data were reported for $[Pb(4,4'\text{-bipy})(NO_3)(SCN)]_m$ (^{1}H, ^{13}C, ^{207}Pb);[788] and $Pb^{II}(dmphen)X_2$ ($X = NO_3^-$, ClO_4^-, OAc^-; dmphen = 2,9-dimethyl-1,10-phenanthroline) (^{1}H, ^{13}C, ^{207}Pb).[789]

2.15 Compounds of Group 15. – Proton NMR spectra were used to characterise NO^+ trapped in solutions of a 1,3-alternate bis-calix[4]arene tube.[790] *Ab initio* calculations have been made of NMR parameters for pentazoles RN_5 ($R = H$, F, CH_3, CN).[791] ^{15}N data were reported for these systems, (163).[792]

The ^{31}P{^{1}H} NMR spectrum of $[HP(\mu\text{-N}^t\text{Bu})_2PN^t\text{Bu}]^-$ confirms the formation of a P–H bond.[793] *Ab initio* and DFT calculations have been reported for λ^3-phospha-alkynes, $RC{\equiv}P$ (R = H, Me, ^{t}Bu, Ph, $SiMe_3$ *etc*.).[794,795] New cage isomers of $P_6C_4{}^t\text{Bu}_4$ have been fully characterised by ^{1}H and ^{31}P{^{1}H} NMR spectra.[796] The ^{1}H, ^{13}C and ^{31}P NMR spectra of (164) and related P^{III},P^V and P^V,P^V related species, show that there is strongly hindered rotation about P–C bonds.[797] The ^{1}H, ^{13}C{^{1}H} and ^{31}P{^{1}H} NMR spectra of $Ph_2PC(NR)(NHR)$ (R = Cy, ^{i}Pr) show that the E_{syn} isomer is present in solution.[798]

The ^{31}P NMR spectrum of $[(^t\text{BuN})_2PK]_\infty$ is consistent with the presence of the monoanion $[(^t\text{BuN})_2P]^-$.[799] NMR chemical shifts were calculated by DFT methods for the phosphatranes (165), where E = NH, NMe or O, X = lone pair, O or S.[800] NMR data (^{1}H, ^{13}C, ^{31}P) were used to characterise the cone, partial cone, 1,2-alternate and 1,3-alternate isomers for the cyclophosphazene $[Ph(Me)PN]_4$.[801] ^{1}H, ^{13}C and ^{31}P NMR spectra show only the chair conformation for (166).[802]



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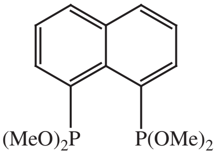

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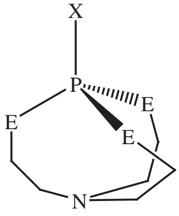

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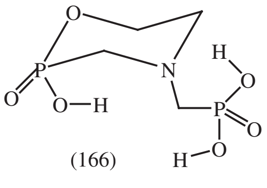

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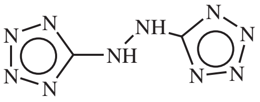

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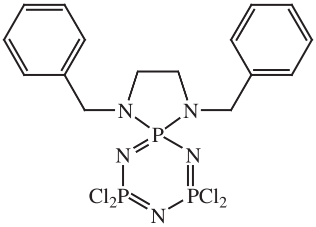

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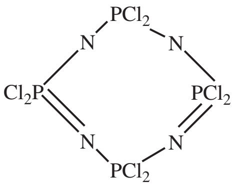
Calculated values have been reported for ^{1}H, ^{13}C, ^{17}O and ^{31}P NMR parameters for $PhP(O)(OH)_2$.[803] *Ab initio* calculations gave ^{17}O NMR electric field gradient parameters for the bridging oxygen in the model system $H_4P_2O_7$.[804] Similar calculations gave NMR shielding constants for PF_3, PF_5 and ClF_3.[805] ^{14}N NMR data have been reported for $E(N_3)_3$, where E = As or Sb, including chemical shifts for the N_α, N_β and N_γ atoms.[806]

NMR data were also reported for: hydrazinium nitroformate (^{1}H, ^{13}C);[807] (167) (^{1}H, ^{13}C, ^{14}N);[808] $Ph(C_{12}H_8)P(C_4H_3O\text{-}2)_2$ (^{31}P);[809] new *spiro*-phosphazenes, *e.g.* (168) (^{1}H, ^{13}C, ^{31}P);[810] N_3P_3(2-thienyl)$_6$ and related species (^{1}H, ^{13}C, ^{31}P);[811] octa-alkoxy-substituted phosphorus(V) triazabenzcorroles (^{1}H, ^{31}P);[812] $(R_2PN)_3$ (R = 2- or 3-thienyl, 3,3′-bithienyl-2,2′-ylene) (^{1}H, ^{13}C, ^{31}P);[813] $\{NP(NHCH_2CO_2Et)_{0.6}[N(CH_2CH_2Cl)]\}_n$ (^{13}C, ^{31}P);[814] (169), (170) and related species ($L = NC_5H_{10}$) (^{1}H, ^{13}C, ^{31}P);[815] (indenyl)$_x$Ph$_{3-x}$PE (E = O, x = 1 – 3; E = S, x = 3; E = Se, x = 1,2) (^{1}H, ^{13}C);[816] $(Me_3SiO)_2P_2)_3F_2$ (^{19}F, ^{31}P);[817] $(RC_6H_4\text{-}NH_3^+)(O^-)P(=O)_2H$ (R = H, *o*-, *m*- or *p*-Me) (^{1}H, ^{31}P);[818]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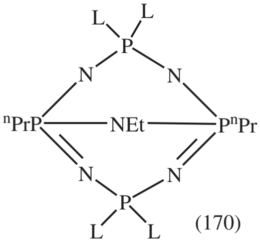
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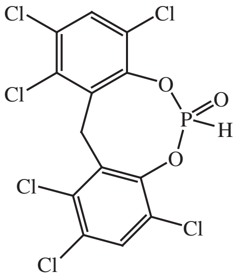
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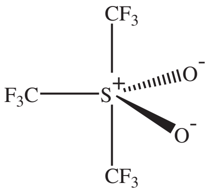
(171) (^{1}H, ^{13}C, ^{31}P);[819] a chain octaphosphate prepared by hydrolysis of cyclo-octa-phosphate (^{31}P);[820] $(C_6F_5)_3As^VXY$ (X = I, Y = Cl; X = Y = NCS), $(C_6F_5)_3M(N_3)(NCS)$ (M = As, Sb) (^{19}F);[821] poly(vinylenearsenic) polymers (^{1}H, ^{13}C);[822] 1,2-, 1,3- and 1,4-$C_6H_4(CH_2SbMe_3)_2$ (^{1}H, ^{13}C{^{1}H});[823] $[(C_6F_5)_2SbL_3]^{2+}$ (L = dmso, Ph_3AsO, pyO, dmf, α-, β- or γ-picoline) (^{1}H, ^{19}F);[824] $[N(PPh_2NR)_2SbOGO]$ (R = Ph, $SiMe_3$; G = $–CHMeCH_2–$, $–CHMeCH_2CMe_2–$ *etc.*) (^{1}H, ^{13}C, ^{31}P);[825] $PhBi[RC(NC_6H_4S)CH_2(NC_6H_4S)C\text{-}COOCH_3]$ (R = Ph, 4-Cl-, 4-Br-, 4-CH_3-C_6H_4) (^{1}H, ^{13}C);[826] $PhBi[RC(NC_6H_4S)CH_2(NC_6H_4S)CR']$ (R = Me, R′ = Me, Ph, 4-MeC_6H_4; R = CF_3, R′=CF_3, 2-C_4H_3S) (^{1}H, ^{13}C, ^{19}F);[827] $[Bi(dmtsc)(NO_3)]_2$ (H_2dmtsc = 2,3-diacetylpyridinebis(^{4}N-morpholinyl thiosemicarbazone) (^{1}H, ^{13}C);[828] and $Bi(Se_2CNRR')_3$ (R = R′ = Et, Bu; R = Me, R′ = Bu, Cy) (^{1}H, ^{13}C).[829]

2.16 Compounds of Group 16. – DFT calculations gave ^{17}O chemical shifts for gaseous and liquid H_2O.[830] ^{17}O and ^{33}S chemical shifts were reported for gaseous SO_2 – showing increased ^{17}O and decreased ^{33}S shielding due to intermolecular interactions (*i.e.* increased pressure).[831] NMR parameters were calculated by *ab initio* methods for dimethyl sulfur di-imide.[832] ^{13}C NMR spectroscopy was used to characterise the structure of (172). No axial/equatorial CF_3 exchange was detected.[833]

There has been an *ab initio* calculation of ^{77}Se chemical shifts for $S_xSe_{4-x}{}^{2+}$ (where x = 0–3).[834] The ^{77}Se NMR spectra of PhSeCH = C(SePh)R (R =

CO_2Me, CH_2NMe_2,CH_2OH, Ph) were assigned using results of *ab initio* calculations.[835] ^{77}Se NMR data were assigned for $X_3C_6H_2SeY$, where X = Me, CF_3, ^tBu; Y = Cl, Br, CN. Distinct $^{77}Se–^{35}Cl$ and $^{77}Se–^{37}Cl$ resonances were seen.[836] Theoretical ^{77}Se chemical shifts may be useful in assigning experimental spectra for selenoenzymes and selenoamino acids.[837]



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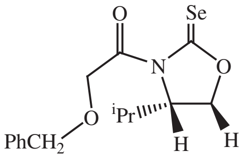

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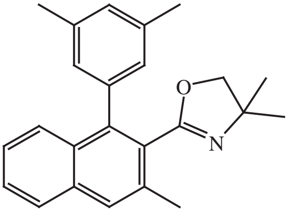

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^{77}Se NMR spectra were used to identify the two regioisomers ArC(Cl)=C (SePh)Fc and ArC(SePh)=C(Cl)Fc, where Ar = Ph, substituted phenyl.[838] (173) and its ^{13}C and ^{77}Se enriched analogues were characterised by ^1H, ^{13}C and ^{77}Se NMR. ^1H-^1H NOESY experiments in the titanium complex of the enolate were used to establish the solution-state orientation.[839] ^1H, ^{13}C and ^{77}Se NMR data were also reported for RSeX, where X = Cl, Br or I; R = (174),[840] while ^{77}Se data were used to characterise $Cs_4Mo_6Br_{12}Se_2$ and some cyano-seleno halide derivatives.[841]

The $^{31}\{^1H\}$ spectrum of $Te[N(SP^iPr_2)(SePPh_2)]_2$ contained two sets of doublets indicative of the presence of two isomers (*cis, trans*)[842] ^{125}Te and ^1H chemical shifts were reported for $(p\text{-}RC_6H_4COCH_2)_2TeBr_2$ (R = H, Me, OMe).[843] ^1H, $^{13}C\{^1H\}$ and $^{125}Te\{^1H\}$ NMR spectra were reported and assigned for *m*- and *p*-$C_6H_4(CH_2TeMe)_2$.[844] ^1H and ^{125}Te NMR data were given for organotellurium compounds derived from 4,5-diphenylimidazole.[845] Characteristic ^{125}Te chemical shifts were reported for $Te[S(CH_2)_nC(O)OCH_3]_2$, where n = 2, 3 or 4.[846]

2.17 Compounds of Group 17. – *Ab initio* calculations gave values for $^{19}F–^{19}F$ spin-spin coupling constants for a pair of HF molecules.[847] Similar calculations were reported for ^1H and ^{19}F magnetic shielding tensors for $[FHF]^-$.[848] The ^1H NMR spectra of Me_4NF-mHF melts (m = 3.0–5.0) gave evidence for the formation of anionic complexes $(FH)_xF^-$ (x = 1–3).[849] Solvent-induced temperature dependence was reported for ^1H and ^{19}F chemical shifts and $^2J_{FF}$ (across the hydrogen bridge) for $(FH)_2F^-$ in CDF_3/CDF_2Cl solution.[850]

Ab initio calculations gave values for ^{17}O and ^{19}F chemical shifts for $FOH_3{}^{2+}$ and $F_2OH_2{}^{2+}$.[851] ^{13}C and ^{19}F NMR parameters were assigned for FC(O)I.[852] The ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of the liquid formed from 1-methylimidazole (mim) and anhydrous HBr show the formation of $Hmim^+$, together with Br^-, $HBr_2{}^-$ and $H_2Br_3{}^-$.[853]

2.18 Compounds of Group 18. – β-NMR measurements gave a value for the magnetic moment of ^{17}Ne.[854] Theoretical calculations have been made of ^{129}Xe NMR shielding parameters for Xe–CO_2, Xe–N_2, Xe–CO, Xe–CH_4 and Xe–CF_4 gas mixtures.[855] The linearity of the C≡C–Xe–F unit was established by ^{19}F–^{13}C correlation spectra for RC≡CXeF (R = Me, ^{n}Bu, Ph).[856] The ^{13}C, ^{19}F and ^{129}Xe data obtained for $[CF_3C{\equiv}CXe][BF_4]$ included $^{1}J(^{3}C–^{129}Xe)$ of 343 Hz.[857] Other NMR data were reported for $[CF_2{=}C(CF_3)Xe][BF_4$ (^{19}F, ^{129}Xe), $[CF_2{=}CHXe][BF_4]$ (^{1}H, ^{19}F, ^{129}Xe);[858] $[CF_2{=}CFXe]^+$, *cis*- and *trans*-$[ClCF{=}CFXe]^+$ (^{19}F, ^{129}Xe).[859]

3 Dynamic Systems

3.1 Fluxional Molecules. – *3.1.1 Compounds of Group 2.* Variable-temperature ^{1}H NMR spectra of $Mg(L)(ClO_4)$, where L = tripodal di-imine ligand, reveal that Δ and Λ isomers interconvert in the intermediate to slow time scale.[860] Proton NMR data for D_2O solutions of Ca(II) and La(III) 1 : 1 complexes of *p*-sulfonatocalix[4]arene gave data on kinetics of ring inversion for the ligand.[861] ^{1}H and ^{13}C NMR spectra gave evidence for room-temperature fluxionality in solution for $[M(thd)_2(L)_n]_m$, where M = Sr, Ba, L = Hpz, Hpz*, n, m = 1, 2 or 3 (Hthd = 2,2,6,6-tetramethyl-heptane-3,5-dione, Hpz = pyrazole, Hpz* = 3,5-dimethylpyrazole).[862]

3.1.2 Compounds of Group 3. Relatively fast dissociation of thf for $(L)M[N(SiHMe_2)_2](thf)$ (M = Sc, Y, L = tetradentate 1,ω-dithiaalkanediyl-bridged bis(phenol)) is shown by ^{1}H and ^{13}C NMR data.[863] Variable-temperature ^{1}H NMR spectra of (*R,S*)-[Ln(biphen){$N(SiHMe_2)$}(thf)]$_2$ (H_2biphen = 3,3′-di-*tert*-butyl-5,5′,6,6′-tetramethyl-1,1′-biphenyl-2,2′-diol) show intramolecular exchange of the 2 different phenolate groups, leading to their equivalence on the NMR timescale.[864]

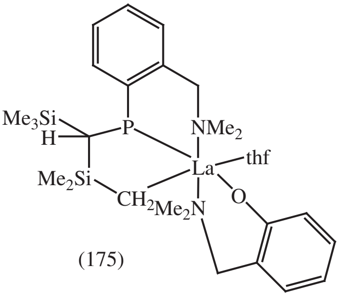
Variable-temperature ^{11}B NMR spectra for $(Nacac)ScCl(NHAr)(HBEt_3)$ (where $Nacac^-$ = $ArNC(CH_3)CHC(CH_3)NAr$; Ar = 2,6-$^{i}Pr_2C_6H_3$, showed a doublet, with J(BH) = 53 Hz (70°C).[865] Variable-temperature NMR data show that (175) (R = CH_2Ph, CH_2SiMe_3, $CH(SiMe_3)_2$) are subject to dynamic processes, due to rapid, reversible inversion at P. La–C cleavage is slow on the NMR timescale.[866] A temperature-dependent ^{13}C study has been made of tumbling motions of Ce atoms inside the C_{80} cage in *i*-Ce_2C_{80}.[867]

3.1.3 Compounds of Group 4. Variable-temperature ^{1}H, ^{13}C and ^{31}P NMR spectra probed the dynamic behaviour of $[\eta^5,\eta^1\text{-}O\text{-}C_5Me_4CH_2CH_2OMe]TiCl_3$

and $[\eta^5,\eta^1\text{-}P\text{-}C_5H_4CH_2CH_2PPh_2]TiCl_3$.[868] Proton NMR studies show the fluxional behaviour of the η^2-coordinated benzyl ligand in $[Ti(\eta^5{:}\eta^1\text{-}C_5Me_4SiMe_2NR)(CH_2Ph)]^+$ (R = Me, ^{i}Pr, ^{t}Bu).[869] Fluxionality in $CpTiCl_2(L)$, where HL = (176)[870] and in (177) (R = ^{i}Pr)[871] was studied by variable-temperature ^{1}H NMR.

The ^{1}H and ^{13}C NMR spectra for $[Ti(mdea)(O\text{–}O)]_2$, where mdea = tridentate *N*-methyl-diethoxoamine ligand, O–O = $OC(CH_3)_2CH_2CH(CH_3)O$ or $OC(CH_3)_2C(CH_3)_2O$, gave evidence for bridging bond scission and reformation, leading to an apparent increase in symmetry.[872] The NMR data (^{1}H, $^{13}C\{^1H\}$ and ^{77}Se) for $TiX_4(L)$, where X = Cl, Br, L = $MeC(CH_2EMe)_3$ (E = S,Se) show bidentate L, with rapid pyramidal inversion and exchange between free and coordinated chalcogen donors at room temperature.[873]

The 500 MHz ^{1}H NMR spectrum of $(L)Zr_2Cp_2H_4$, where L = (178), shows equivalence of all 4 protons, giving effective C_{2v} symmetry for the complex on the NMR timescale.[874] Dynamic solution-phase behaviour of a triple hydrogen-bridged dizirconium complex containing aromatic ligands and a bridging lithium-containing species was probed by ^{1}H and ^{7}Li NMR spectroscopy.[875]



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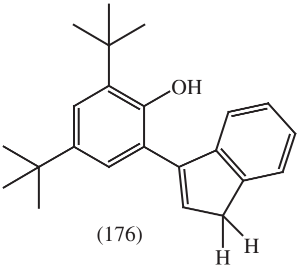

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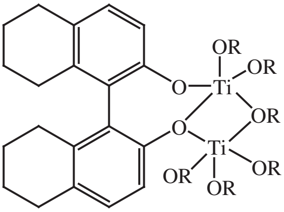

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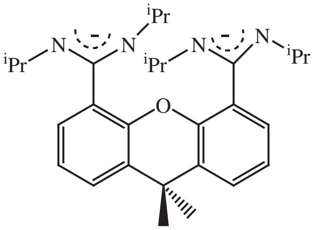

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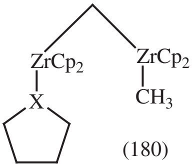
$[Cp_2Zr^-{}_2S^+CH(Ph)CH{=}CPPh_2]_2$

(179)



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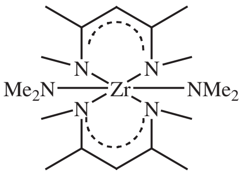

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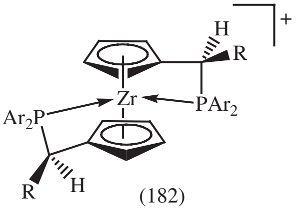

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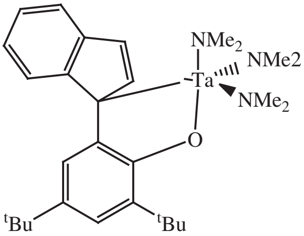

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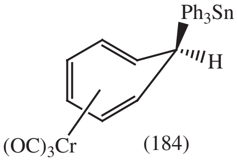

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Variable-temperature ^{1}H NMR spectra of $(C_5R_5)ZrCl_3$ (R = *m*-tolyl) show rapid rotation of the phenyl rings.[876] The molecular dynamics of (179) were followed in solution by variable-temperature ^{1}H NMR spectra.[877] Similar studies were reported for $[\eta^5:\eta^1$-*N*-$C_5Me_4CH_2CH_2N$-$Me_2]ZrCl_3$.[878] ^{1}H NMR line-shape analysis for bis(2-arylindenyl)zirconocenes was used to determine rotation rates for the indenyl ligand.[879] (180), where X = O or S, both gave ^{1}H NMR evidence for symmetrisation *via* methyl exchange.[880] Variable-temperature ^{1}H NMR data were used to probe the molecular dynamics of (181).[881]

The NMR study of molecular dynamics of (182), where R = Me, Ph; Ar = Ph, *p*-tolyl, stabilised by pendant (diarylphosphanyl)alkyl groups on the cyclopentadienyl rings, gave values for free energies for a number of intramolecular equilibration processes.[882] 2-D EXSY studies of solutions containing $[Zr_2(dhpta)_2]^{2-}$, where H$_5$dhpta = 1,3-diamino-2-propanol-*N,N,N′,N′*-tetraacetic acid, gave evidence for exchange of lgands at 298 K.[883] NMR studies on $Hf_4O_2(OMe)_{12}$ show that the ligands are highly dynamic even at −80°C.[884]

3.1.4 Compounds of Group 5. Variable-temperature ^{1}H NMR spectra were used to follow the dynamic behaviour of NbCl$_2$(dpmpza)(RC≡CR′), where R = R′ = Me, SiMe$_3$, R = Ph, R′ = Me, Et; dpmpza = (3,5-diphenylpyrazol-1-yl-3′,5′-dimethylptrazol-1-yl)acetate, and to determine barriers to alkyne rotation.[885] There is ^{1}H NMR evidence for fluxionality in (183), involving NMe$_2$ groups.[886]

3.1.5 Compounds of Group 6. The proton NMR spectrum of (184) shows that the Cr(CO)$_3$ group acts as an 'electronic lock', blocking [1,5]Sn migrations of cycloheptatrienyl tin – but allowing a slower [1,3]Sn/[1,2]Cr rearrangement.[887] Variable-temperature ^{1}H NMR data for [(9-indenyl)triptycene]Cr(CO)$_3$ show that the barrier to rotation of the ligand is 13 kcal mol^{-1}.[888] Variable-temperature ^{1}H NMR spectra gave evidence for a series of interconverting isomers for Cr$_2$(DpyF)$_4$ in solution (DpyF = *N,N′*-di(2-pyridyl)formamidinate).[889]

The low-temperature ^{1}H NMR spectrum of $[(\eta\text{-}C_5H_4)_2CMe_2Mo(H)(H_2)]^+$ shows that the bound dihydrogen ligand has hindered rotation ($\Delta^{\ddagger}{}_{150} = 7.4$ kcal mol^{-1}) but rapid H atom exchange down to at least 130 K.[890] The 2-D ^{1}H and ^{13}C NMR spectra of $[\{Mo(\eta^3\text{-}C_3H_5)(CO)_2(2,2'\text{-bipy})\}_2(\mu\text{-}4,4'\text{-bipy}))]$ and related species show fluxional behaviour in solution with interconverting *endo* and *exo* forms of the equatorial isomers.[891]

Variable-temperature ^{1}H NMR spectra were used to probe the fluxional behaviour of $Mo(\eta^3\text{-}C_3H_4Me)(\eta^2\text{-}S_2CNC_4H_8)(CO)(\eta^2\text{-diphos})$, where diphos = dppm, dppe. Detailed assignments to *endo*- and *exo*-isomers were made from ^{1}H–^{1}H and ^{1}H–^{13}C COSY experiments.[892] Dynamic ^{1}H, ^{13}C{^{1}H} NMR spectra identified conformers (*endo*-, *exo*-allyl ligand) for $[\eta^5\text{-}C_9H_6(CH_2)_3N(SiMe_3)_2]Mo(CO)_2(C_3H_5)$.[893]

Variable-temperature ^{1}H NMR spectra showed that MoO(mnt)(Bu$_2$bipy) had a rigid structure, but that MoO(mnt)(Me$_4$en) showed dynamic conformational inversion involving the en unit (mnt = *cis*-1,2-dicyano-1,2-ethylenedithiolate; Bu$_2$bipy = 4,4′-di-*tert*-butyl-2,2′-bipyridine; Me$_4$en = *N,N*′-tetramethylethylenediamine).[894] The ^{1}H NMR spectra of $CoMoO_2(NCS)(L)_3(H_2O)$, where L = diethyldithiocarbamate, 4-morpholinocarbodithoate, reveal restricted rotation of the alkyl side chain of the bidentate dithiocarbamate.[895] ^{17}O and ^{95}Mo NMR data for $[Mo_6O_{18}(N_2Ar)]^{3-}$ were consistent with stereochemical non-rigidity in solution (Ar = range of aryl groups).[896]

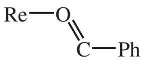
For $W(D_2)(CO)_3(PCy_3)_2$ and related species, ^{2}H T$_1$ relaxation data in solution were used to identify fast-spinning dihydrogen ligands.[897] Variable-temperature ^{1}H and ^{31}P NMR for (L)W(CO)$_4$ (L = [μ-*P,P*-Ph$_2$PCH$_2$PPh$_2$] Co$_2$(CO)$_4$[μ-Ph$_2$PC≡CPPh$_2$]) and related species showed that fluxional behaviour of each dppm unit depended on the bite angle of L in each complex.[898] ^{13}C NMR fluxionality studies were used to probe CO exchange mechanisms for $WIr_3(CO)_{11}Cp$ and $W_2Ir_2(CO)_{10}Cp_2$.[899] The solution-phase ^{1}H NMR spectrum of $W(OC_6H_4Me_2Ph\text{-}\eta^6\text{-}C_6H_4)(OC_6HPh_2\text{-}2,6\text{-}Me_2\text{-}3,5)(PMe_3)$ shows exchange of *ortho* and *meta* protons at higher temperatures *via* phosphine rather than π-arene dissociation.[900] The ^{1}H and ^{13}C NMR specta of $[W_2(COT)(OR)_4]_2$, where COT = cyclooctatetraenyl, R = Me, Et, Pr, show no evidence of fluxionality in the temperature range −60 to +65°C.[901]

3.1.6 Compounds of Group 7. Water exchange in $[(OC)_3Mn(H_2O)_3]^+$ is shown by ^{17}O NMR to be 4 orders of magnitude faster than for the rhenium analogue.[902] Variable-temperature ^{1}H NMR gave evidence for fluxional behaviour for $Cp_3Fe_3Mn_3(CO)_5(\mu_3\text{-}S_2)(\mu_4\text{-}S_2)_2$ above about 40°C.[903]

Proton exchange processes in $Cp'Ru(\mu\text{-}H)_3ReH_2Cp'$, $Cp'Ru(\mu\text{-}H)_3ReH$(triphos) (Cp′ = C$_5$EtMe$_4$, triphos = MeC(CH$_2$CH$_2$PPh$_2$)$_3$) were followed by variable-temperature ^{1}H NMR.[904] Variable-temperature ^{1}H and ^{13}C NMR followed fluxional behaviour in Cp(OC)$_2$Re{OC(Me)Ph} in solution, showing that acetophenone is coordinated in both σ (η^1) and π (η^2) fashions, (185a and b).[905] 2-D, difference NOE and variable-temperature NMR experiments (^{1}H, ^{13}C) show that for Re(CO)$_3$Br[(L)$_2$CH$_2$], where L = 3(5)-(1-pyrenyl)pyrazole and related species, isomers exist in solution due to restricted rotation about the pyrazolyl-pyrenyl bond.[906]

3.1.7 Compounds of Group 8. ^1H and ^{31}P NMR spectra of $FeH(H_2)(PP_3)^+$, where $PP_3 = P(CH_2CH_2PMe_2)_3$, show dynamic behaviour, with rapid exchange between η^2-H_2 and η^1-H protons.[907] Dynamic processes were also studied (^{15}N NMR) for ^{15}N-labelled $[Fe(H)(N_2)(PP)_2]^+$ (PP = dppe, depe, dmpe).[908]

Variable-temperature ^{31}P NMR spectra for Cp*(dppe)Fe-$(C{\equiv}C)_2$-Fe(dppe)Cp* gave a value for the barrier to rotation of the two organometallic fragments about the Fe . . . Fe axis.[909] Variable-temperature ^1H NMR data gave values for the kinetic and thermodynamic parameters for regioisomerisation of 2-methyl- and 2,6-dimethyl-derivatives of tricarbonyl(η^4-tropone)iron.[910]



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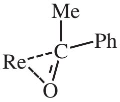

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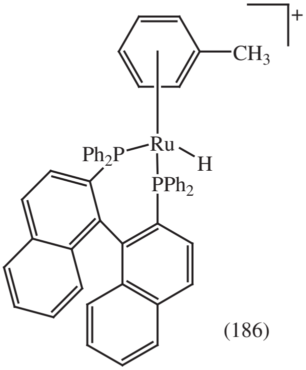

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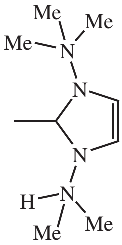


(187)

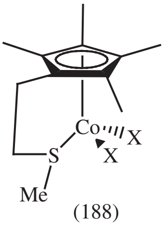
Detailed ^1H and ^{31}P, with NOESY NMR experiments for (186) show restricted rotation about the P–C bond.[911] Variable-temperature ^1H NMR spectra gave evidence for fluxional exchange of coordinated *tert*-butyl groups in $H_2Ru(PPh_3)_2L$, where L = (187).[912] Proton NMR spectroscopy was used to probe exchange couplings between hydrido and dihydrogen protons in $RuH(H_2)(X)(P^iPr_3)_2$, where X = 2-phenylpyridine, benzoquinoline, phenylpyrazole.[913] Variable-temperature ^1H NMR was used to follow the dynamical behaviour of $H_4Ru_4(CO)_{11}L$, where L = $P(C_6F_5)_3$, PMe_2Ph, $P(OMe)_3$, $P(OEt)_3$, involving transformations between a number of possible isomers.[914] Molecular exchange processes in $\{CpRu[(R)\text{-BINOP-F}]\}^+$, where (*R*)-BINOP-F = product of reacting (*R*)-BINOL with $(C_6F_5)_2PBr$, were followed by variable-temperature ^1H, ^{17}O and ^{31}P NMR, and by variable-pressure ^{17}O, ^{31}P NMR.[915]

A number of variable-temperature NMR studies were reported for $[Cp^*(DPVP)_2Ru{=}C{=}CH_2]^+$ (DPVP = $Ph_2PCH{=}CH_2$), showing that the barrier to vinylidene rotation was very low ($\leq$6.7 kcal mol^{-1}).[916] The barrier to rotation about the P–C(aryl) bond in *nido*-$Ru_3(CO)_9[\mu\text{-P-}C_6H_2\text{-2,4,6-}(CF_3)_3]_2$ ($\Delta G^{\ddagger}$) was shown by variable-temperature ^{19}F NMR to be 82.3 kJ mol^{-1} at 141°C.[917] Variable-temperature ^{13}C NMR examined the fluxional characteristics of $(\eta^1,\eta^5\text{-}CH_2C_5Me_4)Ru_2(CO)_6$. Five carbonyl ligands interchange in a rapid process, with the sixth only participating at a slower rate.[918] $[Ru(tpap)]^{2+}$ gave a ^{1}H NMR spectrum in solution showing exchange between non-coordinated and equatorially coordinated pyridines (tpap = *N,N,N′,N′*-tetrakis(2-pyridylmethyl)-2,6-bis(aminomethyl)pyridine).[919]

The variable-temperature ^{1}H NMR spectrum for RuL(napy-κ^{2}*N,N*)$(dmso)]^{n+}$, where L = *N*-methyl-3,5-di(2-pyridyl)-4-(pyridyl); n = 2; L = 2,6-di(2-pyridyl)phenyl, n = 1, napy = 1,8-naphthyridine, show fluxionality of the chelated napy in solution.[920] Proton NMR data gave information about intramolecular rearrangements in $RuCl_2[PPh_2(2,6\text{-}Me_2C_6H_3]_2$.[921] Variable-temperature ^{1}H NMR data for $[Ru(OAc)(CO)_2(dpa)]_2$, where dpa = di(2-pyridyl)amine, show fluxionality at room temperature.[922] Similar data (plus $^{31}P\{^{1}H\}$ spectra) for $Ru(RCOO)_2(dppf)$ (R = Me, Et, Ph; dppf = 1,1′-bis(diphenylphosphino)ferrocene) show uni- and bidentate exchange behaviour of the carboxylate ligands.[923]

Variable-temperature ^{1}H and ^{31}P NMR spectra for $\{Os(\eta^{2}\text{-}H_2)(bipy)[P]_3\}^{+}$, where [P] = $P(OEt)_3$, $PPh(OEt)_2$, confirmed the presence of the dihydrogen ligand.[924] Variable-temperature ^{1}H NMR spectroscopy was used to study the hydride dynamics in $[H_5Os_{10}(CO)_{24}]^{-}$, showing that μ_2-hydrides are much more mobile than μ_3-.[925]

3.1.8 Compounds of Group 9. Variable-temperature ^{1}H NMR spectra of $(py)(L)_2CoCH_2\text{-}R\text{-}CH_2Co(L)_2(py)$, where L = dmgh or other dioximes, R = $-C_6H_4-$, $-C_6H_4-C_6H_4-$ *etc*, show restricted rotation about the Co–C bond.[926] The proton NMR spectra of (188), where X = I, Me, gave signals due to the diastereotropic methyl groups below room temperature.[927] The ^{13}C NMR spectra of (189), where R = Ph, ^{t}Bu, are consistent with restricted rotation about the $C_5H_4\text{–}CHR^{+}$ bond.[928] Variable-temperature ^{1}H and ^{13}C NMR spectra showed racemisation of (190) and related complexes.[929]



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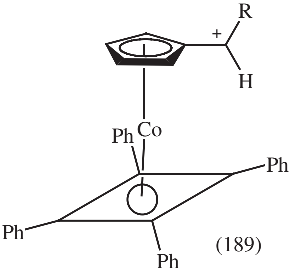

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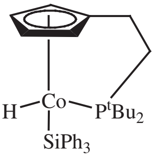

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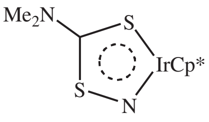
Variable-temperature ^{31}P (with high-pressure data) NMR spectra for Co $[C(O)C_5H_9]\text{-}(CO)_3(LIM\text{-}18)$, where LIM-18 = (4*R,S*-4,8-dimethyl-2-octadecyl-2-phosphabicyclo[3.3.1]nonane, suggest that racemisation can occur.[930] Solution structure and dynamic behaviour of the cluster $[Co_4(CO)_{11}]^{2-}$ in $\{(Et_2O)_3Ln[Co_4(CO)_{11}]\}_{\infty}$ (Ln = Yb, Eu) were followed by variable-temperature ^{13}C and ^{59}Co NMR.[931] ^{1}H and ^{13}C NMR spectra of (py)-[Co]-$C_6H_{10}F$, where py = py itself or substituted derivatives, [Co] = $Co(dmgh)_2$, $C_6H_{10}F$ = 2-fluorocyclohexyl, show hindered rotation of the 2-fluorocyclohexyl ligands.[932]

$^{1}H\text{-}^{19}F$ NOESY and inverse ^{103}Rh NMR were used to probe positional anion effects for [Rh(1,5-COD)(Biphemp)]X, where Biphemp = [(6,6′-dimethylbiphenyl)-2, 2′-diyl]bis(diphenyl-phosphine; X = BF_4^-, PF_6^-, $CF_3SO_3^-$.[933] Variable-temperature 1-D and 2-D ^1H NMR spectra for Tp″Rh(COD), where Tp″ = hydrobis(3-phenyl-5-isopropyl-pyrazolyl)(3,5-dimethylpyrazolyl)-borate, show that the Tp″ ligand is coordinated in κ^2 fashion.[934] Broad peaks in the $^{31}P\{^1H\}$ NMR spectrum of Rh(COD)Cl(Ph_2PNHNH-py-*P*) suggest the possibility of fluxional chelation.[935]

The proton NMR spectrum of CpRh(pesa)Cl, where pesa = (+)-*N*-[(*S*)-1-phenylethyl]salicylaldimine, gave data on the rate of epimerisation of this complex.[936] Variable-temperature $^{31}P\{^1H\}$ NMR spectra of [3,3-$(PPh_3)_2$-8-L-*closo*-3,1,2-$RhC_2B_9H_{10}$], where L = SEtPh, were used to follow fluxional behaviour.[937] Variable-temperature ^1H NMR spectra of [Rh(L)(CO)]PF_6 (where L = 2,6-bis(benzylthiomethyl)pyridine) showed fluxional behaviour typical of *S,N,S*-donor ligands, due to pyramidal inversion at S centres.[938] The fluxional behaviour of [Rh(CO)L$(PPh_3)_2$]ClO_4, where L = bis(benzimidazol-2-ylmethyl)methylamine, was studied similarly.[939]

Variable-temperature ^1H NMR, together with ^1H–^1H EXSY, were used to probe the dynamic properties of $Rh_6(CO)_{14}\{\mu,\ \kappa^3$-PV), where PV = $Ph_2P(CH{=}CH_2)$.[940] Solution structure and dynamic behaviour of $Rh_6(CO)_{14}(\mu,\eta^2$-P-P), where P-P = dppm, dppe, perfluoro-dppe, were examined using 1-D ^{13}C and ^{31}P NMR, 2-D $^{13}C\{^{103}Rh\}$-$^{31}P\{^{103}Rh\}$ HMQC and ^{13}C EXSY experiments.[941] The ^1H and ^{31}P NMR spectra of [Rh(dippe)(μ-SR)$]_2$, where R = H, Me, Cy, biphenyl, phenyl, or $(SR)_2$ = $S(CH_2)_3S$, dippe = $^iPr_2PCH_2CH_2P^iPr_2$, show that both ring inversion and S inversion can occur.[942] ^{17}O NMR studies were used to probe water exchange mechanisms in the binuclear aqua-ion $[Rh_2(\mu\text{-}OH)_2(OH_2)P_8]^{4+}$.[943]

The ^1H NMR spectrum of (191) shows that rotation about the C–N bond is fast on the NMR timescale even at −40°C.[944] Variable-temperature ^1H and ^{13}C NMR spectra of cationic Ir(I) cyclo-octadiene complexes containing binaphthalene templated sulfide ligands show that in all cases the ligand chelation is stereoselective, and only one stereoisomer is produced.[945]



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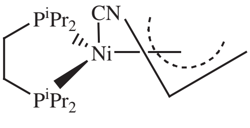

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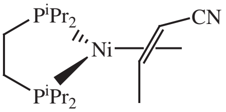

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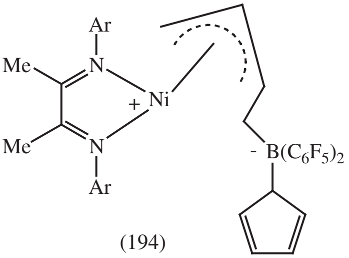
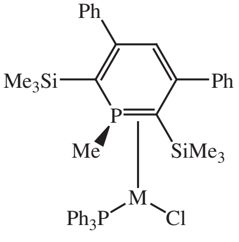


(194)

3.1.9 Compounds of Group 10. Dynamic ^{1}H NMR spectra for (192) and (193) gave measurements of barriers to π–σ allyl conversion.[946] Similar studies were made on (dippe)Ni(η^3-allyl)(CN), where dippe = bis(di-isopropylphosphino) ethane.[947] All 4 diastereotropic isopropyl groups in the *Z*-conformer of (194) (Ar = 2,6-^{i}Pr$_2$C$_6$H$_3$) give separate resonances. TOCSY experiments gave evidence on *Z*/*E* isomerisation.[948] Variable-temperature ^{1}H NMR spectra for [2-(η^2:η^2-diene)-*closo*-2,1,7-NiC$_2$B$_9$H$_{11}$], where diene = COD, norbornadiene, C$_5$H$_5$Me, COT *etc*., show that the {Ni(diene)} fragments are freely rotating even at 193 K.[949]

Variable-temperature ^{1}H NMR data were used to follow dynamic processes for isomers of M(L)$_2$, where M = Ni, Pd, L = η^3-N(SiMe$_3$)C(Ph)CH(SiMe$_3$). The isomers were characterised by a range of NOE, 2-D and saturation transfer NMR experiments.[950] Proton NMR studies on 14-, 15- and 16-membered nickel(II) cyclidene macrocycles appended with 2-aminoethyl(2-pyridine) receptors were used to determine the coordination stoichiometry and elucidate molecular inetrconversions.[951] The variable-temperature ^{31}P NMR spectrum of Ni(PPP)(HTMT), where PPP = PhP(CH$_2$CH$_2$PPh$_2$)$_2$; HTMT = 2,4,6-trimercaptotriazine, showed 2 conformers in solution at low temperature, although exchange is fast at room temperature.[952]

Variable-temperature ^{1}H and ^{31}P NMR spectra were used to follow ^{31}P environment exchange processes for Pd$_2$(H)X$_3$(dppm)$_2$, where X = Br or I.[953] Similar data for the η^2-complexes (195) (M = Pd, Pt) show that the MCl(PPh$_3$) fragment exchanges rapidly between two P–C bonds in solution ($\Delta G^\ddagger$ 43.7 (Pd), 55.5 (Pt) kJ mol^{-1}).[954] Proton NMR data show fluxional behaviour for (196), with exchange of coordinated *cis* nitriles.[955] For (197) (X = Cl, Br), fluxional behaviour was studied by ^{1}H NMR – giving parameters for 2-site exchange.[956] Variable-temperature ^{1}H NMR for (198) (M = Pd, Pt; R = CH$_2$CH$_2$OH, CH$_2$CH$_2$CH$_2$OH) revealed fluxionality.[957] Similar experiments for [Pd(OAc)$_2$]$_3$ (tdat), where tdat = 2,4,6-tris(di-2-pyridylamino)-1,3,5-triazine, show that at low temperature the solid structure is maintained in solution. At ambient temperature, however, flipping of the orientation of the Pd(OAc)$_2$(py)$_2$ units occurs.[958]



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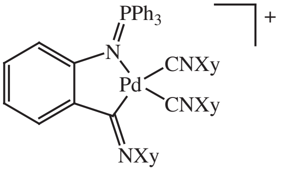

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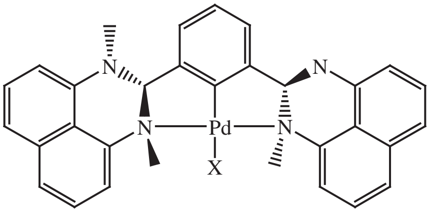

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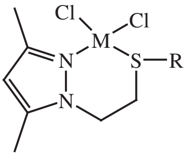

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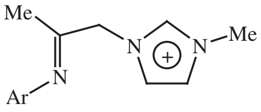

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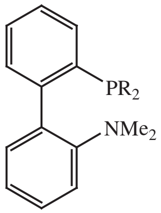

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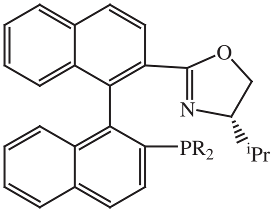

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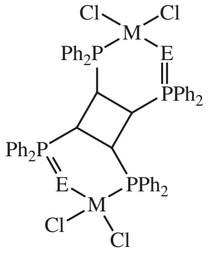

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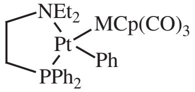

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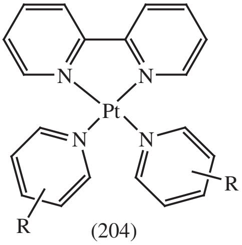

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Variable-temperature, EXSY and NOESY ^{1}H NMR spectra of (C–N)PdCl(X), where H(C–N)$^+$ = (199) (Ar = 2,6-^{i}Pr$_2$C$_6$H$_3$) provided a detailed analysis of the molecular dynamics, *e.g*. for X = Cl, there was evidence for a 'flip' of the boat conformation.[959] The dynamic behaviour of [(η^3-allyl)Pd(L)]$^+$, where L = (200) (R = Ph, Cy) was followed by variable-temperature ^{1}H experiments.[960] Variable-temperature and 2-D ^{1}H and ^{31}P NMR spectra for PdC$_2$(L), where L = (201), reveal restricted rotation about a number of P–C$_{ipso}$ aryl bonds.[961]

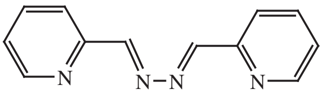
^{31}P{^{1}H} NMR spectra show that [M(P$_2$O$_9$)(PR$_3$)$_2$]$^-$, where M = Pd, Pt; PR$_3$ = PPh$_3$, PMePh$_2$, are fluxional in solution.[962] Proton and ^{31}P NMR spectra were used to probe the dynamics of [Pd{PPh$_2$(C$_{10}$H$_{15}$)}Cl$_2$]$_2$ in solution. The fluxional process involves isomerisation between *pseudo*-*trans* and *cis* conformations.[963] All of the complexes [P]MR$_2$ (M = Pd, R = C$_6$F$_5$; M = Pt, R = Me, Et, Pr, Bu, CH$_2$Ph, Ph, F-C$_6$H$_4$, C$_6$F$_5$; [P] = tris(1-cyclohepta-2,4,6-trienyl)phosphane, P(C$_7$H$_7$)$_3$) were shown to be fluxional in solution at room temperature on the NMR timescale.[964] Variable-temperature ^{31}P NMR spectra were reported for (202) (M = Pd, E = Se; M = Pt, E = S).[965]

^{1}H EXSY NMR experiments on *cis*-(Cy$_3$P)$_2$Pt(H)SiHMes$_2$ show that exchange of silicon and platinum hydrides occurs *via* reductive elimination-oxidative addition, and not *via* a silylene intermediate.[966] Proton and ^{31}P{^{1}H} NMR spectra for (Me$_3$P)(Ar$_2$ClSi)Pt(μ-H)(μ-η^2-HSiAr$_2$)-Rh(PMe$_3$)$_3$ show exchange between hydrido and Si-H hydrogen.[967] The dynamic behaviour of $[Pt_2(P\text{-}P)_2(\mu\text{-}H)(\mu\text{-}CO)]^+$, where P–P = dppe, dppb, dppp, was followed by ^1H and ^{195}Pt NMR spectroscopy. There was evidence for mutual exchange of P atoms with respect to bridging ligands.[968] The ^1H, ^{31}P and ^{195}Pt NMR spectra of $[Pt_2(dcype)(\mu\text{-}CO)(\mu\text{-}H)]^+$ show fluxional behaviour on the NMR timescale (dcype = 1,2-bis(dicyclohexylphosphanyl)ethane).[969] The variable-temperature ^1H NMR spectra of (203) (M = Mo, W) reveal reversible partial dissociation of the Pt–N bond.[970]

Analysis of the ^1H and $^{13}C\{^1H\}$ NMR spectra of (204) gave values for the activation energies for anisotropic rotational motion of *n*-Rpy (n = 3, 4; R = alkyl).[971] The temperature-dependent proton NMR spectrum of [Pt$_2$(*N,N,N′,N′*-tetrakis(2-pyridylmethyl)-1,3-propane-diamine)Cl$_2$]$^{2+}$ was used to probe conformational equilibria.[972] For *trans*-$[Pt\{SiNN(Cl)\}_2(SiNN)_2]$, where SiNN = $Si[(NCH_2{}^tBu)_2C_6H_4\text{-}1,2]$, variable-temperature ^1H and $^{29}Si\{^1H\}$ NMR spectra show the occurrence of three separate fluxional processes in solution.[973] The rates of dmso exchange for *cis*-$[Pt(Me)_2(dmso)(PR_3)]$, where R = 4-MeO-, 4-Me, 4-F-, 4-Cl-, 4-CF_3-C_6H_4, C_6H_5, were determined by ^1H isotopic labelling experiments.[974] The variable-temperature ^{19}F NMR spectra of *cis*-$[Pt(SC_6F_5)_2(R_fSCH_2CH_2R_f)]$, where R_f = *o*-, *m*- or *p*-SC_6H_4F, and related species, show the presence and interconversion of *syn* and *anti* isomers, consistent with fast flipping of the metallocycle ring, and slow inversion of conformation at the S atoms of the dithioether.[975]

3.1.10 Compounds of Group 11. The ^1H and ^{31}P NMR spectra of $[Cu_4(\mu\text{-}dppm)_4(\mu_4\text{:}\eta^1,\eta^2\text{-}C{\equiv}C\text{–})]^{2+}$ show 2 fluxional processes in solution, *i.e.* oscillation of the $C{\equiv}C^{2-}$ unit inside the Cu_4 rectangle, and flipping of the diphosphines.[976] Dynamic solution behaviour has been found using variable-temperature ^{31}P NMR spectra for a number of crown clusters of copper and silver, based on resorcinarene, $(PhCH_2CH_2CHC_6H_2)_4$.[977] The proton NMR spectrum of $[\{Cu(L)\}\{PF_6\}]_n$, where L = (205), is consistent with fluxional processes involving the pyridine-H_3 proton at room temperature.[978]

Rates for intramolecular Λ/Δ isomerisations have been reported for $Cu(L)_2{}^+$, where L = atropoisomer of di-imine benzimidazole-pyridine ligands.[979] ^1H, ^{13}C and ^{31}P NMR spectra suggest that $MX[P(C_7H_7)_3]$, where M = Cu or Ag, X = Cl, Br, are non-rigid in solution at room temperature.[980] Dynamic ^{31}P NMR spectroscopy was used to follow fluxional processes in [(3,5-di-*tert*-butyl-1,2,4-triphospholyl)Cu(PPh$_3$)]. The preferred coordination mode at room temperature is η^5-π coordination of copper. At low temperatures, two σ-isomers are seen.[981]



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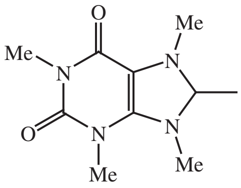

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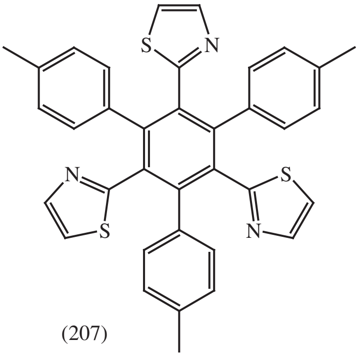

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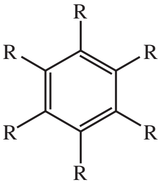

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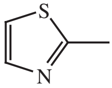

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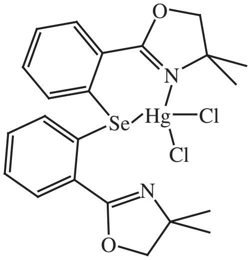
Ag(L)$_2$, where L = (206), has a ^{13}C NMR spectrum consistent with fluxional behaviour.[982] Variable-temperature ^{1}H NMR spectra of the trinuclear sandwich complex (L$_1$)Ag$_3$(L$_2$), where L$_1$ = (207), L$_2$ = (208), R = (209), show that metal-ligand exchanges take place at the three silver centres in concert.[983] Variable-temperature ^{31}P NMR spectra were reported, to study molecular dynamics for $Ag_2(R_fCOO)_2(dppm)$ ($R_f = CF_3$, C_2F_5 *etc.*);[984] ('P$_4$')$Ag_4I_5(HgI)$ ('P$_4$' = $(PhCH_2CH_2CHC_6H_2)_4(O_2CR)_4(OPPh_2)_4$, R = Cy, 4-$C_6H_4Me$ *etc*);[985] $[AgL]_2^{2+}$ (L = $(CH_2NHCOC_2H_4PPh_2)_2$).[986]

Variable-temperature ^{1}H NMR spectra for dinuclear Au^I complexes of bridging bidentate carbene ligands show that cyclophane-based ligands give rigid complexes, but otherwise they are fluxional.[987] ^{1}H and ^{13}C{^{1}H} NMR spectra of $[(Ph_3P)Au(Me_2NCH_2CH_2NMe_2)]^+$ show fluxionality, which is rapid on the NMR timescale.[988] Variable-temperature ^{1}H NMR spectra of gold(I) halide (= Cl, Br and I) derivatives of tetrakis(diphenylphosphinite)tetraester resorcinarene compounds show the existence of 2 different boat conformers, and followed the equilibrium between them.[989]

3.1.11 Compounds of Group 12. The proton and ^{13}C NMR spectra of $[Zn_2(X)_{4-n}(L)]^{n+}$, where X = Cl, n = 0, X = NO_3, n = 2; L = hexaazamacrocyclic ligands, show fluxional behaviour in solution, and structures different from those in the solid state.[990] Similar data were reported for [ML].3H_2O, where M = Cd(II), Hg(II), Pb(II), H_2L = 1,7-bis(carboxymethyl)-4,10-bis (1-methylimidazol-2-ylmethyl)-1,4,7,10-tetrazacyclododecane, showing that at 273 K, both of the dangling groups and the ethylenic fragments of the macrocycle ring are in fixed conformations. At higher temperatures, however, the ^{13}C data show ring inversion processes, and rate data were reported.[991]

^{13}C, ^{15}N and ^{199}Hg NMR data were reported for (3,5-$Cl_2C_6H_3$)HgCN and PhC≡CHg(CN) in dmso-d_6 solution. Evidence was found for re-orientation rates of these complexes in solution.[992] Variable-temperature ^{1}H NMR spectra of (210) gave evidence for fast exchange between Hg and two N atoms, resulting in higher apparent symmetry.[993]



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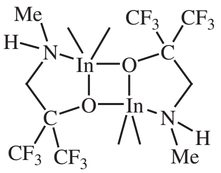
3.1.12 Compounds of Group 13. Proton NMR spectra and *ab initio* calculations were used to probe conformational equilibria of 2,5-substituted 1,3,2-dioxaborinane molecules.[994] A dynamic NMR study of [2,6-bis(ethylthiomethyl)phenyl]diethylborane shows rapid dissociation of the intramolecular B–S bond.[995]

The ^{31}P NMR spectrum of $\{(thf)_2Li\}_3Me_2Al\{(PhNH)_2(PhN)_4P_3N_3\}$ gave evidence for fluxional behaviour of the Li^+ ions – which oscillate between mono- and bidentate coordination sites.[996] 1-D and 2-D ^{1}H and ^{13}C NMR spectra of $AlMe_3[SiMe_2(NR_2)(NR'_2)]$ and related species, where NR_2, $NR'_2 =$ NH^iPr, NH^tBu, NC_4H_8, $NHCH_2CH_2NMe_2$, gave details on molecular structure and dynamics.[997] The variable-temperature ^{1}H NMR spectrum of $Al(Et)(Q)_2$, where Q = 2-methyl-8-quinolinato, shows 2 α-CH_2 peaks of Al-Et at low temperatures, collapsing due to fluxionality (simultaneous rotation of two Q ligands) at higher temperature.[998]

The variable-temperature ^{1}H NMR spectrum of $[GaSBr(3,5\text{-}Me_2C_5H_3N)]_3$ showed signals for all-*cis* and *cis*, *cis*, *trans*-isomers, with a coalescence temperature of -5°C for the signals of the two.[999]

Variable-temperature ^{1}H NMR data for (211) gave evidence for *cis*/*trans* isomerisation, involving N–Me groups.[1000] Similar data for $In_2Cl_6(L)_6$, where H_2L = *N*-substituted diethanolamines, gave evidence for non-dissociative topomerisation processes.[1001] Proton NMR data show that In(DOTA-AA), where DOTA-AA = 1,4,7,10-tetraazcyclododecane-1,4,7,10-tetraacetic acid mono(*p*-aminoanilide), is fluxional at room temperature.[1002]

3.1.13 Compounds of Group 14. Dynamic NMR (^{1}H, ^{13}C, ^{119}Sn) spectroscopy was used to follow the enantiomerisation of (212) and related compounds.[1003] A variable-temperature ^{1}H NMR study of the dynamics of Berry pseudorotation for the 5-coordinate complex (213) showed that the activation barrier between pseudo-rotamers was $\Delta^{\ddagger}_{298} = 15.5$ kcal mol^{-1}.[1004] A proton NMR study has been made of the diaxial-diequatorial equilibrium for silylated derivatives of *trans*-1,4- and *trans*-1,2-dihydroxycyclohexane.[1005] NMR data for (214), where R = Me, $SiMe_3$, showed coalescence of the signals from the two C-bound $SiMe_3$ groups.[1006]



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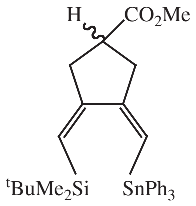

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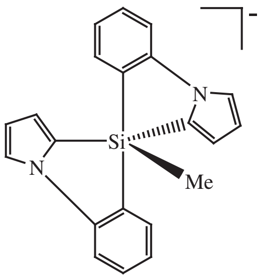

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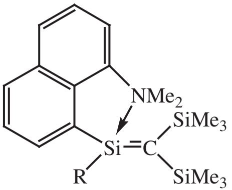

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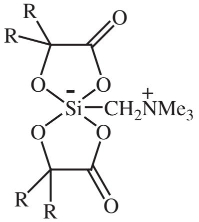

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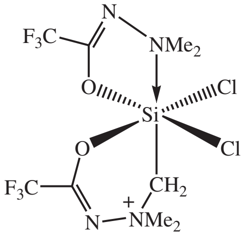

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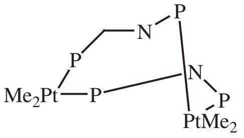

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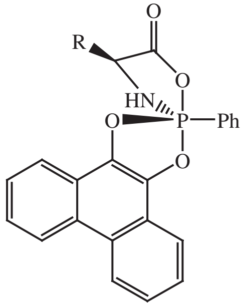

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Variable-temperature ^{1}H NMR data for bis[*cis*-1,2-piphenylethene-1,2-diolato(2-)][2,2,6,6-tetramethylpiperidino)methyl]silicate gave information on its dynamic behaviour.[1007] Variable-temperature ^{1}H solution NMR spectroscopy was used to probe the dynamic behaviour of (215), where R = H, Me, (Λ/Δ enantiomerisation).[1008] NMR evidence was found for two intramolecular ligand-site exchange processes for (216), leading to interchange of *N*-methyl groups.[1009]

3.1.14 Compounds of Groups 15 and 16. Variable-temperature ^{31}P NMR spectrum of (217) (where P-N-P = $Ph_2PNHPPh_2$) shows that at low temperatures, all phosphorus atoms are non-equivalent.[1010] ^{31}P NMR spectra were used to follow diastereoisomeric transformations in (218), where R = $CHMe_2$, CHMeEt.[1011]

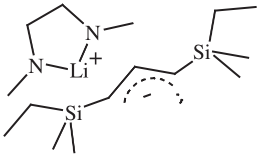
Variable-temperature ^{1}H and ^{13}C NMR spectra were obtained – to follow solution dynamic processes for R_2SbX (X = Cl or Br), $RSbX_2$ (X = Cl, Br, I), where R = 2-(Me_2NCH_2)C_6H_4 – involving interactions between Sb and N atoms on the pendant arm.[1012] Similar data (for ^{1}H and ^{31}P) gave evidence for fluxional behaviour in solution for (R)BiCl[[(XPR$'_2$)(YPR$''_2$)N], where R$'$ = Me, R = Ph, X = O, Y = S; R$'$ = R$''$ = Ph, X = Y = S, Se.[1013]

DFT calculations of the Berry pseudorotation mechanism in SF_4 was used to give ^{19}F chemical shifts for various points along the pseudorotation trajectory.[1014]

3.2 Equilibrium Processes. – A review has been published on studies of interionic and intermolecular solutions structures of transition metal complexes by NMR spectroscopy.[1015]

3.2.1 Group 1 Systems. ^{1}H NMR spectroscopy was used to follow the binding of alkali metal ions to the Ga(III) complex of the hexadentate ligand formed by linking 3 sets of 3-hydroxy-4(1*H*)-pyridinone and ethylenoxy chains to tris(carboxyethoxymethyl)ethane.[1016] ^{31}P NMR data revealed that alkali metal ions (Li – Cs) coordinate with nitrilotris(methylenephosphonic acid) (H_6L), to form MHL^{4-} and ML^{5-} in solution.[1017]

^{1}H, ^{6}Li, 2-D ^{1}H,^{6}Li HOESY and ^{6}Li,^{6}Li COSY spectra were used to study the formation of aggregates between MeLi and LiBr in toluene. All signals of $(MeLi)_n(LiBr)_{4-n}$ were assigned unambiguously.[1018] ^{1}H, ^{7}Li and ^{13}C NMR spectra showed the formation in solution of an unsolvated 1 : 2 heterocubane complex of *u*-[(Me_2{CHMeN(R$'$)$_2$}$_2$.Li_2] and *n*-BuLi (R$'$ = 2,6-$^{i}Pr_2C_6H_3$).[1019] Ion- and solvent-diffusion and ion conduction of $LiN(SO_2CF_3)_2$ in propylene carbonate and diethyl carbonate solutions were studied by ^{1}H, ^{7}Li, ^{19}F multinuclear pulsed field gradient spin-echo experiments.[1020] ^{1}H and ^{13}C NMR spectra showed the formation of 1 : 1 complexes of Li^+, Ca^{2+} or Ba^{2+} with the Schiff base of gossypol and *n*-butylamine.[1021] ^{1}H, ^{6}Li, ^{13}C and ^{15}N NMR line-shape studies on (219) gave evidence for the dynamics of three fast equilibrium reorganisation processes.[1022]



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^{13}C NMR relaxation time measurements were used to obtain association constants between Na^+ (from $NaClO_4$) and benzo[15]crown-5 and benzo[12]crown-4.[1023]

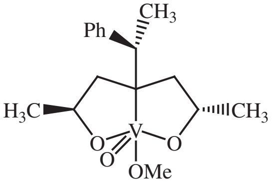
3.2.2 Group 2 Systems. ^{1}H, ^{13}C, ^{25}Mg and ^{27}Al NMR spectra were able to identify components in thf solutions containing Bu_2Mg and $EtAlCl_2$. Species included $MgCl^+$, $MgCl_2$, Et_4Al^-, Et_2Cl-Al-Cl-$AlCl_2Et_2^-$ *etc.*[1024] Interactions between Ca^{2+} and Fc-C(O)CH=CHC_6H_4-NEt-*p* were followed by ^{1}H and ^{13}C NMR.[1025] Variable temperature ^{19}F NMR spectra gave information on the complexation equilibrium of Ba^{2+} in [Ba{(Cp^*)$_2Ti_2F_7$}$_2$(hmpa)](thf) with hmpa, as well as Ba^{2+} dynamics with respect to the Ti core.[1026]

3.2.3 Group 3 Systems. Variable temperature ^{1}H NMR spectra of $\mathrm{Ln(CH_2SiMe_3)_3}$(12-crown-4), where Ln = Sc, Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, reveal labile coordination of the crown ether in thf solution.[1027] Similar data showed the existence of an equilibrium between $[\mathrm{Y(tmhd)_3}]_2$-(tmeda) and $\mathrm{Y(tmhd)_3}$(tmeda), where tmeda = *N,N,N′N′*-tetramethylethylene diamine, tmhd = 2,2,6,6-tetramethyl-3,5-heptanedionate;[1028] and for thf dissociation in solution for $[\eta^3:\eta^1\text{-}((3,6\text{-}^t\mathrm{Bu_2C_{13}H_6})\mathrm{SiMe_2N}^t\mathrm{Bu})\mathrm{Y(CH_2SiMe_3)(thf)_2}]$.[1029]

The proton NMR spectrum of $[(\eta_5\text{-}\mathrm{C_5H_2(SiMe_3)_3}\text{-}1,2,4]\mathrm{LaI_2(thf)_2}$ shows that the thf molecules are very labile, and easily removed under vacuum.[1030] The variable temperature ^{1}H NMR spectrum of $\mathrm{La_2(OAr)_6}$, where Ar = $2,6\text{-}^i\mathrm{Pr_2C_6H_3}$, shows that the bridging and terminal OAr groups can interchange while maintaining the dimeric structure. For $\mathrm{La_2(NHAr)_6}$, however, there was evidence for monomer/dimer equilibrium.[1031] The variable temperature ^{1}H NMR spectra of $[\{\mathrm{YbCp_2}(\mu\text{-}\mathrm{OCH_2CH_2NR_2})\}_2]$, where R = Me or Et, show a solution-state equilibrium between dimers and complexes where N is not bound to Yb.[1032] Proton NMR spectroscopy was used to study the equilibria between $\mathrm{M(C_5H_4R)_3}$, L and $\mathrm{M(C_5H_4R)_3L}$, where R = ^{t}Bu, $\mathrm{SiMe_2}$; L = py, pic; M = Ce, U.[1033]

3.2.4 Group 4 Systems. Proton and ^{13}C NMR spectra of the catalytic system $\mathrm{Cp^*TiMe_3}$/MAO, where MAO = methylaluminoxane, show the formation of a 'cation-like' intermediate $\mathrm{Cp^*Me_2Ti^+ \leftarrow Me^-Al{\equiv}(MAO)}$.[1034] ^{13}C data are consistent with an equilibrium between $[\mathrm{Ti(H_2cit)_3}]^{2-}$ and free citrate ions ($\mathrm{H_2cit}$ = citrato) in solution.[1035]

3.2.5 Group 5 Systems. ^{51}V NMR spectroscopy was used to follow the α-*cis* to β-*cis* isomerisation of the $\mathrm{V^V}$- propylenediaminetetraacetate complex.[1036] The presence of isomerisation equilibria for (220) was studied by ^{1}H, ^{13}C and ^{51}V NMR spectroscopy in solution,[1037] ^{51}V solution NMR spectra were used to determine the species present in the systems $\mathrm{H^+/H_2VO_4^-/H_2O_2}$/L-(+)-lactate or picolinate.[1038,1039]



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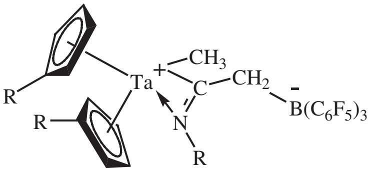
Proton and ^{51}V NMR spectra were used to speciate the vanadate/Hdmpp (= bis (3-hydroxy-1,2-dimethyl-4-pyridinonic acid) system as a function of metal/ligand ratio and pH.[1040] Multinuclear 1-D and 2-D NMR spectra probed interactions between $\mathrm{K_3[OV(O_2)_2(C_2O_4)].H_2O}$ and pyridine in solution. There was evidence for the new species $[\mathrm{OV(O_2)_2py}]^-$.[1041] Binding of $\mathrm{VO_2}^+$ and $\mathrm{VO(O_2)}^+$ to proteins, such as bovine apo-transferrin, was studied using ^{51}V NMR.[1042] The stabilities in solution of $\mathrm{V_2O_2(O_2)_3L_3}$ and $[\mathrm{VO(O_2)_2L}]^-$, where L = amino-acid ligands, were followed by ^{51}V NMR.[1043] The pH-dependence of the ^{51}V NMR spectrum of the 1 : 1.2 $\mathrm{VO_2}^+$-*D*-saccharic acid system determined the complex species formed.[1044]

The proton NMR spectra of $Tp^{Me2}Nb(X)(R)(MeC{\equiv}CMe)$, where Tp^{Me2} = hydrotris(3,5-dimethylpyrazolyl)borate; X = Cl; R = c-C_5H_9 or c-C_6H_{11}, show a temperature dependence due to an equilibrium between the major α-agostic species and a minor, non-agostic one.[1045] ^{1}H NMR spectroscopy was used to follow reactions between complexes such as $M(Q)CpX_2$, where M = Nb, Ta; Q, X = di- and monoanionic ligands respectively – involving ligand exchange processes.[1046] ^{1}H NMR data were used to follow isomerisation of (221), R = H, Me; R = ^{t}Bu, Cy, from *N-out* to *N-in* isomers.[1047]

3.2.6 Group 6 Systems. Kinetic and structural studies were reported using ^{1}H and ^{13}C NMR, including 2-D NOESY, TOCSY, COSY and EXSY experiments to monitor the equilibria (222), where M, M′ = $Cr(CO)_3$, $Mo(CO)_3$, $W(CO)_3$, $Ru(CO)_2$.[1048] Variable temperature ^{1}H NMR spectra gave a value for the equilibrium constant for the reaction of *trans*-$Mo(dmpe)_2(H)(NO)$ (dmpe = bis(dimethylphosphino)ethane) with PhCH=N(1-naphthyl).[1049] An NMR study has been reported of hydrogen-bonding and proton transfer involving $Cp^*M(dppe)H_3$ (M = Mo, W) and fluorinated alcohols.[1050]



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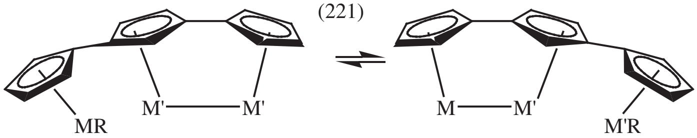

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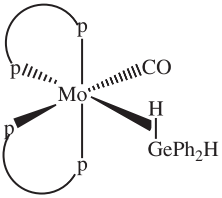

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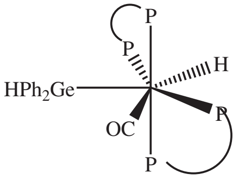

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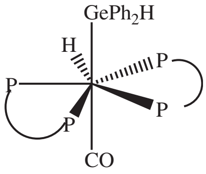

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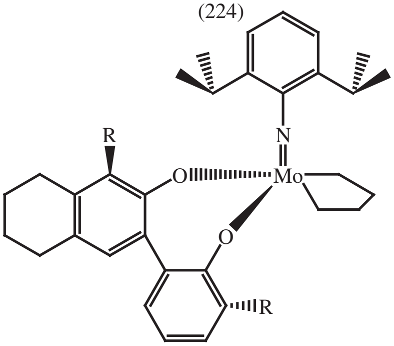

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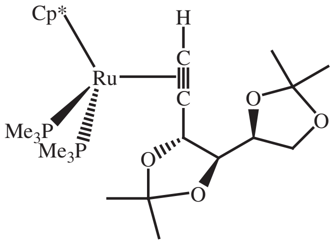
There is ^1H and ^{31}P NMR evidence for the formation in solution of a tautomeric equilibrium involving (223), (224) and (225) (P–P = $Et_2PCH_2CH_2PEt_2$).[1051] Variable temperature ^{13}C NMR spectra were used to follow interconversions between square pyramidal and trigonal bipyramidal forms of (226).[1052] ^{95}Mo NMR spectroscopy was used to speciate molybdates in solutions which are precursors in the formation of $(MoVW)_5O_{14}$, *e.g.* $Mo_7O_{24}{}^{6-}$, $Mo_8O_{26}{}^{4-}$.[1053] ^{31}P NMR spectroscopy was used to determine equilibria and dynamics for some aqueous peroxomolybdophosphate catalysts. Chemical exchange processes were detected by ^{31}P 2-D EXSY experiments.[1054] Redistribution and fluxional processes involving $[PM_4]^{3-}$ systems, where $PM_4 = [PO_4\{M_2O_2(\mu\text{-}O_2)_2(O_2)_2\}_2]$, M = Mo or W.[1055] Variable temperature ^{31}P NMR solution data for $K_5[Cl(P_2O_7Mo_{12}S_{12}O_{12}(OH)_{12}(H_2O)_4].22H_2O$ show that a supramolecular interaction between Cl^- and the dodecanuclear ring persists in solution.[1056]

The variable temperature ^1H NMR spectra for $W_2(\mu\text{-}RCCR')(OCH_2{}^tBu)_8$, where R = H, R′ = Ph, Me, Me_3Si; R = Me, R′=Me, Ph, show that several of these complexes exist as a mixture of alkyne-bridged and η^2-alkyne bonded isomers. There was evidence for rapid exchange of alkoxy groups, but slow $\mu\text{-}\eta^2$ alkyne exchange.[1057] A review has appeared on the use of ^{183}W NMR in studies of polyoxotungstates in solution.[1058] A ^{17}O NMR study of aqueous peroxotungstates (pH range 0.5–9.0) shows the presence of many different species.[1059]

3.2.7 Group 7 Systems. ^{99}Tc NMR data allowed the calculation of formation constants of complexes formed by $[Tc(CO)_3(H_2O)_3]^+$ with X^- (X = F, Cl, Br, I).[1060] Variable temperature ^1H and ^{13}C NMR spectra showed that η^1- and η^2-forms of $Cp(OC)_2Re\{OC(Me)Ph\}$ were in equilibrium in solution.[1061] The ^1H NMR spectrum of $[Re(9\text{-}MeG)_2(H_2O)(CO)_3]^+$, where 9-MeG = 9-methylguanine, is consistent with rapid equilibrium between HH and HT conformations of the bases in solution (H = head, T = tail).[1062]

3.2.8 Group 8 Systems. Multinuclear (^1H, ^{11}B, ^{13}C, ^{31}P) NMR soectra gave evidence for rapid equilibrium between $Ru(\eta^2\text{-}BH_4)(CO)H(PMe_2Ph)_2$, C_2H_4 and $Ru(\eta^1\text{-}BH_4)(CO)(\eta^2\text{-}C_2H_4)H(PMe_2Ph)_2$, with slower conversion to $Ru(\eta^2\text{-}BH_4)(CO)Et(PMe_2Ph)_2$.[1063] The kinetics of isomerisation of (227) and the corresponding vinylidene species was followed by variable temperature ^{31}P NMR.[1064] $[Ru(CO)_2(L)](BF_4)$, where L = bis[2-(3,5-dimethyl-1-pyrazolyl)-ethyl]ether, has variable temperature ^1H NMR spectra showing 2 isomers in rapid equilibrium on the NMR timescale.[1065]



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^{1}H, ^{13}C{^{1}H} and ^{31}P{^{1}H} NMR spectra were used to probe the binding modes of 2-aminopyridine to Ru(II) fragments.[1066] The variable temperature ^{1}H NMR spectrum of $[Ru(bipy)_2(L)]^+$ in solution (L = 4,4′-biquinazoline) gave evidence for the presence of enantiomeric pairs ($\Delta\delta,\Lambda\lambda$) and ($\Delta\lambda,\Lambda\delta$).[1067]

The variable temperature ^{1}H and ^{13}C NMR spectra for the stable radical anions $[Os_3(CO)_9(\mu_3\text{-}\eta^2\text{-}L)(\mu\text{-}H)]$, where HL = phenanthridine, 5,6-benzoquinoline, quinoxaline and their one-electron reduction products, showed that electron transfer between neutral and uninegative species occurs on the NMR timescale.[1068] Proton NMR studies have been reported for isomerisation between the three known isomers of $OsCl_2(dmso)_4$.[1069]

3.2.9 Group 9 Systems. The NMR spectra of $Co(DH)_2(SCN)L$, where DH_2 = dimethylglyoxime, L = py or substituted derivative, show that they exist in solution as mixtures of neutral species, $[Co(DH)_2(L)_2]^+$ and $[CO(DH)_2(SCN)_2]^-$.[1070] Proton NMR spectra were used to follow *trans* to *cis* isomerisation reactions for $[Co(dtc)_2\{P(OMe)_{3-n}Ph_n\}_2]^+$, where dtc^- = *N,N*-dimethyldithio-carbamate.[1071]

There is ^{1}H NMR evidence for two isomers of $[Rh(CO)_2(bdtp)]^+$, where bdtp = 1,5-bis(3,5-dimethyl-1-pyrazolyl)-3-thiapentane, *i.e.* κ^2-*N,N*- and κ^3-*N,N,S*-forms.[1072] Variable temperature ^{1}H NMR spectra for $[\kappa^2\text{-}PhBP'_3]Rh(PMe_3)_3$, where $PhBP'_3 = [PhB(CH_2P^iPr_2)_3]^-$, show a dynamic equilibrium involving dissociation of PMe_3 ligands and reversible migration of a CH_2 group in the ligand backbone, from B to Rh.[1073]

3.2.10 Group 10 Systems. Proton NMR spectra gave values for association constants for the formation of inclusion complexes of mononucleotides and the metallacalix[3]arene species, $[(R,R\text{-}1,2\text{-diaminocyclohexane})Pd(phen)]_3^{6+}$.[1074] Similar experiments were used to probe the binding of palladium(II) complexes, *e.g.* $[Pd(en)(H_2O)_2](NO_3)_2$, to guanine, guanosine and guanosine-5′-monophosphate in aqueous solution.[1075]

Variable temperature ^{1}H NMR data have been reported, and dmso exchange kinetics quantified, for $[(R\text{-}iso\text{-}BIPY)Pt(CH_3)L]^+X^-$, where R-*isi*-BIPY = *N*-(2-pyridyl)-R-pyridine-2-ylidene (R = 4-H, 4-^{t}Bu, 4-NMe_3, 5-NMe_2), L = dmso, X = OTf and/or BPh_4^-.[1076] [^{1}H, ^{15}N] HSQC 2-D NMR was used to follow the kinetics of formation of cross-links between $^{15}N\text{-}[\{trans\text{-}PtCl(NH_3)_2\}_2\{\mu\text{-}trans\text{-}Pt(NH_3)_2(H_2N(CH_2)_6NH_2)_2\}]^{4+}$ and oligonucleotides.[1077] The binding of Pt(II) complexes, including square planar complexes with methylated derivatives of phen, to the oligonucleotide $d(GTCGAC)_2$ was studied by 2-D ^{1}H NMR.[1078]

^{195}Pt NMR spectra were employed to study the nature of $Pt(bipy)_2^{2+}$ in aqueous alkaline solutions. The data were consistent with formation of a conformationally mobile pseudo-five-coordinate complex involving OH^- co-ordination.[1079] The time dependence of Pt(II) complexation with poly(amidoamine)dendrimers was established by ^{195}Pt NMR spectroscopy.[1080] The ^{1}H and ^{13}C NMR spectra for solutions of *cis*-$[L_2Pt\{9\text{-}MeAd(\text{-}H)\}]_3(NO_3)_3$ show dissociation to a mononuclear species, *e.g.* *cis*-$[L_2Pt\{9\text{-}MeAd(\text{-}H)\}]^+$, where L

= $PMePh_2$, 9-MeAd = 9-methyladenine.[1081] There is ^1H NMR evidence for stepwise isomerisation of $Pt(SCN)_2$(bipy) to $Pt(NCS)_2$(bipy).[1082]

3.2.11 Group 11 Systems. ^{63}Cu and ^{65}Cu NMR spectra were used to identify interactions of 0.064M $CuClO_4$ with a number of organic nitriles.[1083] Variable temperature ^1H NMR studies of a trimeric thiacalix[4]crown-6 encapsulating Ag^+ show that the silver ion oscillates through the central thiocalix spacer *via* Ag^+-π inetractions.[1084]

3.2.12 Group 12 Systems. ^1H NMR solution spectra of heterodinuclear complexes $MM'(NCDPP)_2$, where M,M′ = Zn, Cd, Hg; NCDPP = *N*-confused 5,20-diphenylporphyrin, gave values for equilibrium constants for monomer exchange reactions.[1085] Variable temperature ^1H NMR spectra for (L)ZnCl in solution (where L = tris(3-*tert*-butylpyrazolyl)methanesulfonate) show two sets of resonances, consistent with two isomers, one having *N,N,O*- and the other *N,N,S*-coordination (C_{3v}, C_s symmetry respectively).[1086] Coordination of 3-Ac-AMP (3-acetamido-5-methylpyrazole) to Zn^{2+} and Cd^{2+} was followed by ^1H NMR spectroscopy.[1087] Proton NMR spectroscopy was also used to follow complexation of Zn^{2+} by quercitin, (+)-catechin and related derivatives.[1088] The variable temperature ^{31}P NMR spectra of $Zn[Se_2P(OR)_2]_2$, R = Me, ^iPr, show that monomer and dimer are in equilibrium in solution.[1089]

^1H NMR spectroscopy was used to follow the complexation of Cd^{2+} to the phytochelatin (γ-GlU-Cys)$_2$-Gly.[1090] ^{113}Cd NMR spectra were used to examine bonding between Cd^{2+} and protein residues modelling calmodulin-dependent protein kinase I.[1091] Solution ^{113}Cd NMR data for $Cd(S_2CNHR)_2$, where R = *n*-C_5H_{11}, are temperature- and concentration dependent – consistent with dimer formation *via* Cd . . . S intermolecular bridges (as found in the solid state).[1092]

3.2.13 Group 13 Systems. There is ^{11}B NMR evidence for the formation of a diphenylboron cation by Cl^--abstraction from Ph_2BCl by $SbCl_5$ in CD_3NO_2 solution.[1093] The ^{13}C NMR spectra of BF_2L, where HL = $R^1COCH_2C(R^2)$=NMe, R^1 = R^2=Me; R^1 = Ph, R^2 = Me, Ph, show that ketoamine and enolimine tautomeric forms are present in approximately equal amounts.[1094]

^1H and ^{13}C NMR spectra were used in a quantitative study of Al(II)-glutamate complex equilibria in solution.[1095] ^{27}Al NMR spectroscopy was able to identify species present in an equimolar Al(III)-citrate solution.[1096] Complex formation equilibria were examined by ^1H, ^{13}C and ^{27}Al NMR spectra for the Al(III)-l-(+)-ascorbic acid system.[1097] An NMR (^1H, ^{13}C) study has been nade of the Al(III) binding abilities of D-saccharinic and mucic acids.[1098] ^{27}Al NMR data were used to characterise fulvic acid-Al^{3+} complexes under acidic aqueous solutions.[1099]

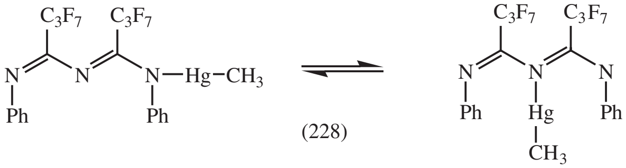
Multinuclear NMR (^1H, ^{13}C, ^{31}P, ^{27}Al), together with 2-D ^1H-^1H NOESY data, were used to study the complexation of coenzyme NAD^+ by Al^{3+}-evidence was found for $Al(LH_2)^{3+}$, $Al(LH)^{2+}$ and AlL_2^-.[1100] The liquid-state ^{27}Al NMR spectra were used to identify aluminium species formed by the interaction of $AlO_4Al_{12}(OH)_{24}(H_2O)_{12}$ with low molecular weight organic ligands.[1101]

The variable temperature ^1H NMR spectra of $GaMe_2L$, where L = $OC(CF_3)_2CH_2NHMe$, $OC(CF_3)_2CH_2NH^tBu$, indicated occurrence of rapid N → Ga bond breaking, followed by recombination with change of absolute configuration.[1102]

3.2.14 Group 14 Systems. The variable temperature ^1H, ^7Li and ^{13}C NMR spectra for the *N*-lithiated $Me_3SiCNNLi.TMEDA$ shows rearrangement at high temperature to the thermodynamically favoured *C*-lithiated isomer.[1103] The ^1H and ^{29}Si NMR spectra gave evidence for *trans* to *cis* isomerisation in solution for $[Si(CN)(Me)CH_2]_2$.[1104] The ^{13}C and ^{29}Si NMR spectra of aqueous solutions of alkaline silicates in the presence of furanoidic sugars show 5-coordinate silicon species, together with 2 containing 6-coordinate silicon.[1105]

^1H and ^{19}Sn NMR spectra for $[Et(Ph)Sn(H_2DAPTSC)]Cl_2$, where $H_2DAPTSC$ = 2,6-diacetylpyridinebis(thiosemicarbazone) show complete dissociation in dmso solution (to free $H_2DAPTSC$ and $Et(Ph)SnCl_2$).[1106] NMR data (^1H, ^{13}C) were used to determine the coordination properties of a dieptide (Ala-Gly) towards Me_2Sn^{2+}. Replacement of the terminal amino group of Ala by thiol leads to the formation of much more stable complexes.[1107]

3.2.15 Group 15 and 16 Systems. The equilibrium (228) was followed by ^{19}F NMR spectroscopy.[1108] Multinuclear (^1H, ^{13}C, ^{14}N, ^{19}F, ^{31}P) NMR spectra demonstrated the isomeric transformation of 2-(dimethylamino)ethyl dimethylphosphoramidofluoridate into (229).[1109]



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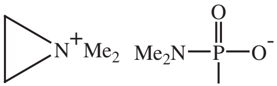

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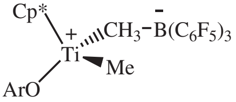
Successive deprotonation of $[P\{NH(Ph)\}]^+$ was followed by ^{31}P NMR spectroscopy.[1110] Formation constants for adducts of C_{60} and C_{70} with a number of phosphine oxides were calculated from ^1H chemical shift changes in the systems.[1111] Variable temperature ^1H NMR spectra of $[L]BiNO_3$, where L = porphyrin bearing ester pendant arms, suggest that the solution contains only monomer.[1112]

^{17}O and ^{133}Cs NMR spectra for the liquid $Cs_2S_2O_7$-$CsHSO_4$ are consistent with a temperature dependent equilibrium between HSO_4^- and $S_2O_7^{2-}$ anions.[1113]

3.3 Course of Reactions. – *3.3.1 Groups 1 and 2.* ^{6}Li, ^{13}C and ^{19}F NMR spectra were used to follow reactions of lithium phenylacetylide, PhC≡CLi, with quinazolines.[1114] ^{1}H NMR monitoring of reactions of R_2Mg with KOR′ shows the formation of the species $[R_2Mg(\mu\text{-}OR')_2MgR_2]^{2-}$, where R = hexyl, neopentyl, *sec*-butyl *etc.*, R′ = Me, Et, ^{t}Bu, Ph *etc.*.[1115]

3.3.2 Groups 3 and 4. ^{45}Sc NMR spectroscopy was used to follow the formation of complexes between $ScCl_3$ and podand ligands (inorganic esters of polyoxyethylene glycols).[1116]

^{1}H NMR spectra tracked the conversion of (230) to (231), where Ar = (232).[1117] ^{1}H and ^{13}C NMR spectra were able to identify the reaction products of Cp_2TiCl_2 and methylaluminoxane (MAO).[1118] ^{1}H NMR spectroscopy was used to follow the reactions of (233) with $M(NR_2)_4$, where M = Ti, R = Me; M = Zr, R = Me, Et; M = Hf, R = Et.[1119] ^{19}F and ^{31}P NMR spectra were used to study the solution phases in the formation of nanoporous titanium phosphate materials.[1120]



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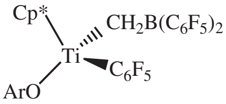

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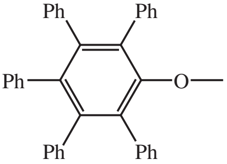

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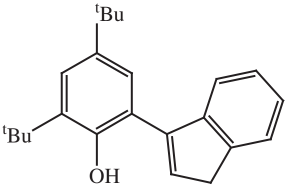

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3.3.3 Groups 5 and 6. The complexation of $V^VO_2^+$ by the Schiff base *N,N′*-ethylenebis(pyridoxyl-aminato) was followed by ^{1}H and ^{51}V NMR spectroscopy.[1121] ^{13}C, ^{14}N and ^{51}V NMR spectra were used to follow reactions of vanadate(V) with dipeptides (Val-Glu, Ala-Gly *etc.*).[1122] The reaction of TaF_5 with imidotetraphenyldiphosphinic acid was monitored by ^{19}F and ^{31}P NMR spectroscopy.[1123]

The reaction of *cis*-$Mo(CO)_4(2,2'\text{-}C_{12}H_8O_2PCl)_2$ and propylamine was followed by ^{31}P NMR spectra.[1124] ^{1}H, ^{13}C and ^{31}P NMR spectra were used to determine the relative affinity of Cp_2MoCl_2 for thiol, amino, carboxylate, phosphate and heterocyclic (N) donors in amino-acids and nucleotides.[1125] 1-D

(^{1}H, ^{13}C) and 2-D (COSY, HSQC, HMBC) NMR data gave detailed structural analysis of the reaction products of $Mo_2O_3(acac)_4$ and β′-hydroxy-β-enamines.[1126] ^{31}P NMR spectroscopy was used to study ligand (L) dissociation from $Mo_3S_4(DTP)_3(RCO_2)(L)$, where HDTP = *O,O*-diethyldithiophosphate, R = Me, CH_2Cl, CCl_3, L = py.[1127] The formation of $PW_xMo_{12-x}O_{40}{}^{3-}$ (x = 0–12) in acetonitrile solution was followed by ^{31}P NMR spectroscopy.[1128]

3.3.4 Groups 7 and 8. Complex formation in water between *fac*-$[(OC)_3Re(H_2O)_3]^+$ and *N*- or *S*-donor ligands has been studied by high-pressure ^{31}P NMR spectroscopy.[1129]

Degradation of pyClFe^{III}(*meso*-NH$_2$-OEP) and $[(py)_2Fe^{III}$(*meso*-NH$_2$OEP)$]^+$ in pyridine solutions was followed by ^{1}H NMR spectra.[1130] Dynamic ^{31}P NMR spectroscopy was used to determine the kinetics of $PO_4{}^{3-}$ exchange in Fe^{3+}.nFbp(PO$_4$, where nFbp = recombinant ferric binding protein from *Neuseria meningitides*.[1131] ^{1}H NMR spectroscopy shows that decomposition of $[Fe^{IV}(PaPy_3)OOH]ClO_4$, where HPaPy$_3$ = *N*-[bis(2-pyridylmethyl)aminoethyl]pyridine-2-carboxamide, leads to the substitution of a hydrogen atom by a solvent-derived OMe group.[1132] 2-D NOESY experiments were able to probe the behaviour of haem groups on oxidation of flavicytochrome c_3.[1133]

^{1}H{^{11}B}, ^{11}B and ^{13}C NMR spectra were used to study the structures of products and possible intermediates in the reaction of *nido*-1,2-$(Cp^*RuH)_2B_3H_7$ with methyl acetylene monocarboxylate.[1134] The formation of κ*O*-coordinated chelates was observed by ^{1}H NMR for $[\{\eta^6\text{-}C_6H_5(CH_2)_3COOH\}Ru(aq)]^{2+}$ and related complexes.[1135] ^{1}H and EXSY NMR experiments were used to follow the reversible olefin-hydride insertion reactions for $[(\eta^6\text{-}C_6H_5CH_2CH_2PR_2)RuH(CH{=}CH_2)]^+$ (R = Cy, Ph).[1136] Variable temperature ^{31}P spectra show that cyclopropanation reactions in the presence of CpRu[PPh$_2$N(R)PPh$_2$-κ*P*,κ*P*](PPh$_3$)Cl, proceed *via* CpRu(=CPh$_2$)[PPh$_2$N(R)PPh$_2$-κ*P*](PPh$_3$)Cl (R = Et, ^{n}Pr, ^{i}Pr, ^{n}Bu).[1137] Proton NMR spectroscopy was used to follow the reactions of $[(cymene)_2Ru_3S_2(MeCN)_3]^{2+}$ and [CpCo(CN)$_3$]-, showing the formation of several Co_4Ru_6 clusters.[1138]

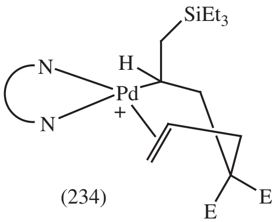
Variable temperature ^{1}H and ^{31}P NMR spectra have been reported for isomerisation reactions of Os(N)Ph(R)Cl(*S,S*-chiraphos), where R = CH$_2$SiMe$_3$, *S,S*-chiraphos = Me(PPh$_2$)HC-CH(PPh$_2$)Me.[1139]

3.3.5 Group 9. High-pressure *in situ* NMR experiments were used to follow the reaction of CO with $[Co(CO)_3L]_2$, where L = tertiary phosphine.[1140] Similar experiments (^{31}P) were used to monitor reactions of phosphine ligands derived from (*R*)-(+)-limonene with cobalt catalyst systems ($Co_2(CO)_8$, $HCo(CO)_4$.[1141]

Intermediates in the cobalt carbonyl-catalysed carbonylation of *o*-substituted benzyl halides have been identified by ^{1}H and ^{13}C NMR.[1142] High-pressure ^{1}H, ^{13}C and ^{31}P NMR spectra were used to detect intermediates during hydroformylation of 1-pentene in the presence of $Co_2(CO)_6[P(OPh)_3]_2$.[1143] Time-dependent ^{1}H NMR spectra followed the reactions of benzyl-, heteroaromatic-, methyl- and allyl-cobaloximes with aryldisulfonyl chlorides.[1144] ^{1}H NMR spectra to follow the reaction between methylcobalamin (MeCbl) and CN^- show the rapid formation of $(\beta\text{-}CH_3)(\alpha\text{-}CN)Cbl^-$ rather than, as previously suggested, $MeCBl.CN^-$.[1145] Solvolysis (including solvent exchange rates) was followed by ^{1}H NMR for *cis*- and *trans*-$[Co(tmen)_2(NCMe)_2](ClO_4)_2$ (tmen = tetramethylethylenediamine).[1146] ^{13}C NMR was used to study the hydration of $Co^{III}(1,10\text{-phenanthroline-5,6-dione})_3{}^{3+}$ in aqueous solution.[1147]

A ^{31}P NMR study of rhodium-catalysed asymmetric 1,4-addition of aryltitanate reagents to α,β-unsaturated ketones gave evidence on the stages of the process, and suggested intermediates.[1148] Detailed ^{1}H and $^{13}C\{^1H\}$ NMR studies revealed pathways by which $[Cp^*M(\eta^5\text{-}2,5\text{-}Me_2T)]^{2+}$ (M = Rh, Ir) react with H_2O/OH^- or $MeOH/MeO^-$ (T = thiophene).[1149] ^{1}H and ^{31}P NMR spectra were used to follow transformations of Rh(I) complexes of (1*S*,2*S*,5*R*-(+)-neomenthyldiphenylphosphine and (4*S*,5*S*)-(+)-2,2-dimethyl-4,5-bis(dimethylaminomethyl)-1,3-doxolane.[1150] ^{1}H, ^{13}C, ^{15}N and ^{103}Rh NMR spectra (including 2-D experiments) were used to study the (oxidative addition) reaction products of $Rh^I(Br)(Tpy^*)$ (Tpy* = 4′-(4-*tert*-butylphenyl)-2,2′:6′,2″-terpyridine) and alkyl bromides.[1151] Variable temperature ^{1}H and ^{31}P NMR spectra were able to characterise the adducts of four phosphorus chalcogenides with the chiral dirhodium complex. $Rh_2(O_2CR)_6$, R = $C(OMe)PhCF_3$.[1152] Proton and ^{13}C NMR spectra were used to monitor the diastereoselective formation of chiral tris-cyclometallated Ir(III) complexes, *e.g.* $Ir(pppy)_3$, where pppy = (8*R*,10*R*)-2-(2′-phenyl)-4,5-pinenepyridine.[1153] A time-dependent ^{1}H NMR study of the reaction between $[(\eta^5\text{-}Cp^*)Ir(acetone)_3](CF_3SO_2)_2$ and H-Tyr-Phe-OH reveals an initial kinetic preference for η^6-coordination of the *C*-terminal arene.[1154]

3.3.6 Groups 10–12. Proton NMR was used to characterise an intermediate η^1-allyl coordinated pincer complex in the palladium-catalysed allylation of aldehydes and imines.[1155] Low-temperature ^{1}H and ^{13}C NMR spectra, and ^{1}H NOESY data established the mechanism for palladium-catalysed cyclisation/hydrosilylation of dimethyl diallyl malonate, *via* (234, E = CO_2Me).[1156] High-pressure $^{31}P\{^1H\}$ NMR studies on coploymerisation of styrene with CO, catalysed by a Pd(II)-(*R*,*S*-BINAPHOS) complex, gave evidence for a number of active complex intermediates.[1157]



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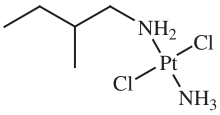

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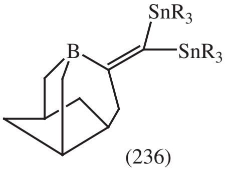
^{31}P and ^{119}Sn NMR spectra were used to follow reaction processes involving the formation of $Pt(R)(SnR_2Cl)$ complexes (R = alkyl).[1158] ^{31}P NMR monitoring of the thermolysis of *trans*-(dfmp)$_2$Pt(Me(X), where dfmp = (C$_2$F$_5$)$_2$MeP, X = O$_2$CCF$_3$, OTf, OSO$_2$F, shows that stability depends on the nature of X.[1159] Low-temperature ^{1}H NMR spectra identified hydride intermediates in reactions of Pt$_2$Me$_4$(L) and HCl, where L = 1,3- or 1,4-C$_6$H$_4$(CH=NCH$_2$CH$_2$CH$_2$NMe$_2$)$_2$.[1160] 2-D (^{1}H, ^{15}N) and 1-D (^{195}Pt) NMR spectra were used to follow the hydrolysis of, and to study the structures of products from, (235).[1161] ^{1}H NOESY techniques were used to monitor the formation of PtCl(PHCy$_2$){(PCy$_2$O)$_2$H}.[1162]

Proton NMR spectroscopy was employed to follow complex formation on titration of *N,N*-bis[{6-(hydroxymethyl)-pyridine-2-yl}methyl]-*p*-tosylamide (= L) with Cu(I) and Zn(II) salts (giving (L)Cu^I, (L)Zn^{II}).[1163] ^{31}P NMR spectra were used to follow oxidative-addition reactions of (L)AuX + X$_2$ (X = Cl, Br; L = phosphines, phosphates), showing a reluctance by very bulky L ligands to undergo such reactions.[1164] Similar data were obtained for redox reactions of (R$_3$P)$_2$AuBr with diselenides (R = Me, Et).[1165]

3.3.7 Groups 13–16. 1-D and 2-D NMR experiments were used to follow reactions of MeB=CR$_2$, where R = SiMe$_3$, SiMe$_2$Cl, with a range of reagents.[1166] The formation of boraadamantanes (236), where R = Me, Et, was monitored by ^{1}H, ^{11}B, ^{13}C and ^{119}Sn{^{1}H} NMR spectra.[1167] The reaction between Cs$_2$B$_{12}$H$_{12}$ and 30% H$_2$O$_2$ to form *closo*-Cs$_2$B$_{12}$(OH)$_{12}$ was followed by ^{11}B{^{1}H} NMR.[1168]



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Variable temperature ^{1}H, ^{13}C and ^{31}P NMR spectra gave information on the reactions of ^{t}BuP(NH$_2$)$_2$ with MR$_3$, where M = Al, Ga, In; R = Me, ^{t}Bu.[1169] A variable temperature ^{1}H NMR kinetic study has been made of the reaction of a β-diketiminate Al(III) complex with N$_3$Ar (Ar = 2,6-Ar$'_2$C$_6$H$_3$, Ar$'$ =2,6-^{i}Pr$_2$C$_6$H$_3$.[1170] ^{27}Al NMR spectra were used to follow the conversion of Al$_{13}$O$_4$(OH)$_{24}$(H$_2$O)$_{12}$$^{7+}$ to Al$_{30}$O$_8$(OH)$_{56}$(H$_2$O)$_{24}$$^{8+}$ in solution.[1171]

The dehydration of hydrolysates of PhSiCl$_3$, leading to the formation of poly(phenylsil-sesquioxane) was followed by ^{29}Si NMR spectroscopy.[1172] ^{29}Si DEPT NMR experiments were able to identify low molecular weight molecules during synthesis of poly(methylphenylsilane).[1173] The reactions of lithium hexamethyldisilazide with ketones was followed by ^{6}Li NMR, and complexes identified.[1174] ^{1}H and ^{29}Si NMR spectra were used to follow polycondensation of octyltriethoxysilane.[1175] ^{29}Si NMR data were used to elucidate the structures of the reaction products of octahydrosilsesquioxane with phenol and undec-1-ene or methyl 3,3-dimethylpent-4-enoate.[1176]

There was ^{29}Si and ^{119}Sn NMR evidence for the formation of the intermediate ClSiMe$_2$-^{t}Bu$_2$Sn-^{t}Bu$_2$Sn-SiMe$_2$Cl during the synthesis of [^{t}Bu$_2$Sn-SiMe$_2$]$_2$.[1177] ^{13}C NMR spectra were used to study the rate of disproportionation of MeSnCl$_3$

in different solvents. The data were consistent with a nucleophile-assisted electrophilic reaction.[1178] ^{31}P NMR spectra revealed the existence of intermediates in the formation of $[(^{n}BuSn)_2O\{O_2P(OH)^{t}Bu\}_4]_2$ from $^{n}BuSn(OH)_2Cl$ and ^{t}Bu-$P(O)(OH)_2$.[1179]

A ^{31}P NMR study of the reactions of phosphoryl halides and 4-(dimethylamino)phosphine (DMAP) shows the formation of $(DMAP)POX_2^{+}$, (DMAP)-PO_2X (X = Cl, Br), to give $(DMAP)_2PO_2^{+}$ and PX_5 as final products.[1180]

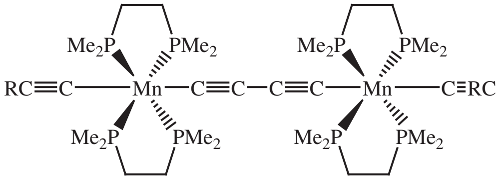
^{77}Se NMR spectra were used to monitor the thermal decomposition of $Se(NAd)_2$ (Ad = 1-adamantyl) to form, for example, the novel cyclic imide $Se_3(NAd)_2$.[1181]

4 Paramagnetic Complexes

4.1 The Transition Metals. – *4.1.1 Groups 4–6*. For the first time, individual (^{1}H, ^{13}C) NMR signals have been resolved for $[Ti(bipy)_m(solv)]^{3+}$, where m = 1–3.[1182] ^{19}F and ^{31}P NMR spectra were used to characterise $LV(OSO_2CF_3)_2$ and $LV(PPh_2)$, where L = *N,N′*-bis(2-diethylaminoethyl)-2,4-pentanedi-imineate(-1).[1183]

Paramagnetic NMR data were used to elucidate the solution structures and speciation for metal complexes containing 2,6-pyridinecarboxylic acid as ligand, with Cr^{3+} (d^3), Fe^{3+} (d^5), Fe^{2+} (d^6), Co^{2+} (d^7) and Ni^{2+} (d^8).[1184] Unpaired spin delocalisation within the odd-atom, non-benzenoid aromatic π-systems of $Cr(CNR)_6^{n+}$, where R = ferrocenyl, n = 1; L = cymantrenyl, n = 2, was studied by multinuclear, paramagnetic NMR (^{1}H, ^{13}C{^{1}H}, ^{14}N).[1185]

4.1.2 Group 7. The complexes $[RC{\equiv}C(dmpe)_2Mn(C{\equiv}CH)]^{+}$, where R = H, $SiMe_3$, were characterised by ^{1}H and ^{31}P NMR.[1186] Similar data were used to study a range of dinuclear manganese complexes containing a linear, bridging Mn-C≡C–C≡C–Mn unit, *e.g.* (237).[1187] The proton NMR spectrum of $[(6\text{-}Ph_2TPA)Mn(CH_3OH)_3]^{2+}$, where 6-$Ph_2$TPA = *N,N*-bis[(6-phenyl-2-pyridyl)methyl]-*N*-[(2-pyridyl)methyl]amine, is consistent with CH/π interactions.[1188] ^{1}H and COSY NMR experiments characterised $M(DAPATs)(H_2O)_n$, where H_2DAPATs = 2,6-bis[1-{2-(tosylamino)phenylimino}ethyl]pyridine; M = Mn, Fe, Cu, n = 3; M = Ni, Zn, n = 2; M = Co, Cd, n = 1.[1189] A proton magnetic relaxation study has been reported (−150 to +100°C) for aqueous solutions of $MnCl_2$ and $Cu(NO_3)_2$.[1190] The paramagnetic ^{1}H NMR spectra were fully assigned for the Re(III) complexes $[ReX_2(PPh_3)_2(bibzmH_2)]^{+}$, where $bibzmH_2$ = 2,2′-bibenzimidazole.[1191]



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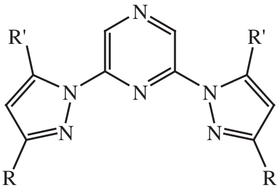

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4.1.3 Group 8. Proton NMR spectra gave evidence for the formation of a highly oxidised (Fe^{III}/Fe^{IV}) iron biliverdin complex.[1192] Solution ^{1}H NMR spectra of $[Fe(L)_2]^{2+}$, where L = (238), show that for R = H, Me, Mes, R′ = H, the complexes are completely low-spin (diamagnetic) at room temperature. For R = R′ =Me, however, there was evidence for a proportion of the high-spin (paramagnetic) form.[1193]

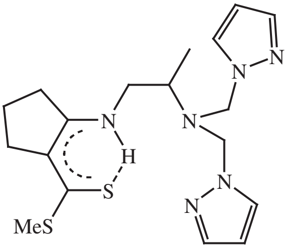
Proton NMR spectra characterised Fe^{III} complexes of heteropodand ligands with 8-hydroxyquinoline and catechol binding groups.[1194] NMR studies on $Fe^{II}(P)$, where P = 5,10,15,20-tetrakis(pentafluorophenyl)porphyrinate, show that the iron(II) is in an intermediate spin ($S = 1$) state.[1195] The proton NMR spectra of paramagnetic $(TPBPO)Fe^{III}X$ and $(TPBOH)Ni^{II}Cl$, where X = Cl, Br, I; $TPBPOH_2{}^{2+}$ = dication of hydroxybenziporphyrin, have been assigned.[1196] There have been several studies of ^{1}H (and in some cases ^{2}H and ^{13}C) NMR spectra of paramagnetic iron porphyrin complexes.[1197–1203] The first NMR evidence has been reported for a hydride-bonded porphyrin complex of $BH_4{}^{-}$, *i.e.* $(TPP)Fe^{III}(BH_4)$.[1204]

Proton NMR relaxation measurements have been made on ferric haem-human serum albumin (haem-HAS) – based on paramagnetic enhancement due to the paramagnetic Fe^{III}-haem.[1205] ^{1}H NMR spectra were used to characterise the paramagnetic oxidised (Fe^{III}) forms of recombinant FixL haem domains.[1206] A paramagnetic ^{1}H NMR study has been carried out on the thermodynamics of Cl^{-} binding to ferric haemoglobin of *Tokunagayusurika akamasi.*[1207] ^{1}H and ^{19}F NMR spectra were used to probe electron distributions in deoxymyoglobins containing fluorinated haem units.[1208] ^{1}H NMR spectra (1- and 2-D) gave details of the effects of mutation at Valine45 on the haem microenvironment of cytochrome b_5.[1209] High-field proton NMR data were used to probe the haem environment and ligand binding properties of paramagnetic cytochrome bo_3 and *bd* quinol oxidase.[1210] ^{1}H-^{15}N NOESY data were able to probe the stability of the cytochrome *c* scaffold in the presence of guanidine-HCl.[1211] Line-shape analysis of the NMR spectrum of *H. thermophilus* ferricytochrome c_{552} reveals fluxional behaviour of the haem axial methionine ligand.[1212] A detailed study has appeared of the NMR parameters for paramagnetic oxidised *Rhodapsendomonas palustris* cytochrome c_{556}.[1213] A strategy for the study of ^{1}H, ^{13}C and ^{15}N nuclei in paramagnetic proteins has been illustrated by reference to oxidised human [2Fe-2S] ferredoxin.[1214]

4.1.4 Groups 9 and 10. Paramagnetic NMR for cobalt-substituted amicyanin shows that the methionine side-chain residue interacts less strongly with the metal in *Paracoccus denitrificans* amicyanin than in the *P. versutus* variant.[1215] The ^{1}H NMR spectra of Co(P), where P = dodeca-substituted porphyrins, show $(d_{xz},d_{yz})^4(d_{xy})^1$ electron configurations.[1216] The paramagnetic ^{1}H NMR spectrum of the cobalt(II) derivative of spinach plastocyanin has been completely assigned.[1217]

Proton paramagnetic shifts have been measured for $[Cp_3Co_3(\mu_3\text{-}CPh)_2]^{+}$, and used to estimate the π-spin density on the sp^2 carbons.[1218] Paramagnetic ^{1}H

NMR spectra have been reported for $M_4(Piv)_4(Mq)_4$ (M = Co, Ni; HPiv = pivalic acid; Mq = 8-hydroxyquinoline).[1219]



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The complex [Ni(L)]ClO_4, where HL = (239), displays paramagnetic line broadening in the ^1H NMR spectrum, due to oligomerisation in solution.[1220] Proton NMR studies of oligonucleotides bound to $Ni(phen)_2(L)^{2+}$, where L = dipyridophenazine and related ligands, showed that it was possible to observe selective paramagnetic relaxation of the oligonucleotide proton resonances.[1221] ^1H and ^{15}N NMR studies have been made on electron relaxation rates in a paramagnetic Ni^{2+} metallo-protein.[1222] Paramagnetic NMR relaxation measurements were used to study the binding ability of a protein (*E. coli* thioredoxin) with a Ni^{2+} binding tag.[1223]

4.1.5 Group 11. Paramagnetic (^1H, ^{15}N) NMR spectra were used to study a Cu^{2+}-IDA (=iminodiacetic acid) complex localised on a protein surface.[1224] ^1H and ^{13}C NMR spectra were reported for copper(II) bis-benzimidazole complexes.[1225] Variable temperature ^1H NMR spectra of copper complexes of β-octafluorinated triarylcorroles reveal a thermally-accessible paramagnetic excited state, *i.e.* a Cu^{II} corrole π-cation radical.[1226] Copper(II) forms of stellacyanin from *Rhus vernicifera* were characterised by ^1H NMR.[1227]

A review has appeared of paramagnetic ^1H NMR studies of electron transfer copper sites in proteins.[1228] ^{13}C NMR (2-D experiments – ^{13}C-^{13}C COSY, COCAMQ and NOESY) were used to detect broad lines in paramagnetic oxidised copper zinc superoxide dismutase.[1229] The ^1H NMR spectrum of copper(II)-halocyanin from *Natronobacterium pharaonis* has been analysed and compared to copper(II) plastocyanins.[1230] A ^1H NMR study of copper(II) binding in the amyloid-β (Aβ) peptide shows that the Cu^{2+} binds to histidine residues, but not to Tyr^{10}.[1231] ^1H NMR spectra were used to characterise paramagnetic complexes formed by copper(II) and the amino-glycoside antibiotic, Kanamycin A.[1232] Detailed ^1H NMR studies (COSY, TOCSY, NOESY, ROESY) probed Cu(II) binding features of the APP(145-155) fragment of an amyloid precursor protein. Data were reported on paramagnetic relaxation enhancements.[1233]

4.2 Lanthanides and Actinides. – Paramagnetic shifts were reported in the NMR spectra of trivalent lanthanide chloride complexes with bipy.[1234]

Solutions of La@C_{82} in HMPA gave ^{31}P NMR spectra which reveal partial localisation of unpaired electron density outside the fullerene cage.[1235] ^1H, ^1H

NOESY NMR spectra were used to characterise the lanthanide complexes $Ln(L)^{3+}$, where L = tris[(2-pyridyl)methyl]amine or tris[6-{(2-*N,N*-diethylcarbamoyl)pyridyl}methyl]ketone, Ln = La – Lu except Pm.[1236] The ^{1}H NMR spectra of $Ln(L)Cl_3$, where L = N4O3 tripodal ligands, Ln = La – Lu, except Pm, show effective C_{3v} symmetry in solution.[1237] ^{1}H and ^{13}C NMR assignments, based on COSY, NOESY and HMQC data, have beeen made for $[LnL]Cl_3.nH_2O$, where Ln = La, Ce, Eu; L = chiral macrocycle derived from (1*R*,2*R*)-1,2-diphenylethylenediamine and 2,6-diformylpyridine.[1238]

The ^{1}H and ^{13}C NMR spectra were assigned, using COSY, HMQC and HMBC data, for $[M(L)]^{+}ClO_4^{-}$, where M = La, Sm; H_2L = lariat ether *N,N′*-bis(2-salicylaldiminobenzyl)-1,10-diaza-15-crown-5.[1239] The ^{1}H and ^{13}C NMR spectra of $[Ln(L)]^{3+}$, where Ln = La, Nd, Eu, Lu, Y, L = semi-rigid extended tripod podand, are consistent with the ligand wrapping around the metal ion to give a system with effective C_3 symmetry.[1240] Solution-phase NMR data enabled identification of LaEu, LaTb, PrEr and PrLu helicates containing unsymmetrical ditopic hexadentate ligands.[1241]

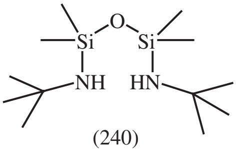
$^{31}P\{^{1}H\}$ NMR data were used to characterise $[LnCl_2(OPPh_3)_4]^{+}$, where Ln = La – Lu, except Pm).[1242] ^{13}C NMR spectra showed C_{2v} symmetry for $[M@C_{82}]^{-}$, where M = Pr, Ce.[1243] The ^{13}C NMR spectrum of $Ce@C_{82}$ shows temperature dependent shifts ascribed to f-electron density remaining on the Ce atom.[1244] ^{31}P NMR spectra were used to identify *syn*- and *anti*- forms and their interconversions for $[M^{n+}(\alpha_m\text{-}P_2W_{12}O_{61}]^{(20-n)-}$, where M = Ce(III), U(IV), Th(IV), m = 1.2.[1245]

^{1}H and ^{13}C NMR spectra gave structural characterisation of $[Ln(2,6\text{-}dhb)_5(H_2O)_2]^{2-}$, where Ln = Sm, Tb; Hdhb = 2,6-dihydroxybenzoic acid.[1246] ^{1}H NMR data have been reported and assigned for the paramagnetic complex $(C_5Me_4{}^{n}Pr)Sm(thf)$.[1247] ^{31}P NMR data show the formation of ternary complexes $[Ln(L)(ATP)]^{3-}$, where H_2L contains two bipyridyl carboxylate fragments linked to an aminobutyl chain; Ln = Eu, Tb.[1248] The ^{1}H NMR spectra of Eu and Er complexes of a dipartite ligand, including a 1,4,7,10-tetraazacyclododecane-1,4,7-triacetic acid and a phenanthroline unit, show nine-coordination of the metal in each case.[1249] A detailed analysis of the ^{1}H and ^{13}C NMR spectra has been carried out for M_2L_3 complexes, where H_2L = 1,3-bis(3-phenyl-3-oxopropanoyl)-benzene, M = Eu, Nd, Sm, Y, Gd.[1250]

Variable temperature ^{17}O NMR experiments on dmso solutions of $[Gd(dmso)_8]^{3+}$ show that dmso exchange is two orders of magnitude slower than the H_2O exchange in $[Gd(H_2O)_8]^{3+}$.[1251] Similar data for $[Gd_2(ohec)(H_2O)_2]^{2-}$, where ohec = octaazacyclohexacosane-1,4,7,10,14,17,20,23-octaacetate, show that water exchange is slow, and proceeds *via* an I_d mechanism.[1252] ^{17}O NMR chemical shifts in Ln(III) complexes of $en(DO3A)_2$ (*i.e.* *N,N*-bis(1,4,7-tris(carboxymethyl)-1,4,7,10-tetraazacyclododecan-10-yl)-methylcarbonyl)-*N,N′*-ethylenediamine) showed that they could be formulated as $[en\{Ln(DO3A)(H_2O)\}]$.[1253]

It was possible to assign the ^{13}C resonances for the strongly paramagnetic trimetallic sandwich complexes $[Ln_3(TACI\text{-}3H)_2(H_2O)_6]^{3+}$, where Ln = Tb – Yb.[1254] ^{171}Yb–^{19}F coupling was observed in the low-temperature ^{171}Yb NMR spectra of $[Yb(C_6F_5)(thf)_5]^+$ and $Yb(C_6F_5)_2(thf)_4$.[1255] The paramagnetic ^1H NMR spectrum of YbL^{3+}, where L is an enantiopure chiral macrocycle, hexaazapentacyclo $[25.3.1.1^{12,24}.0^{4,9}.O^{19,24}]$ ditriconta-1 (31),2,16,12,14,16 (32), 17,25,27,29-decaene, has been analysed in detail.[1256] Analysis of dipolar ^1H paramagnetic shifts was used to characterise complexes formed by common α-amino-acids with a chiral complex $(L)Yb(H_2O)_2$.[1257]

Paramagnetic ^1H NMR spectra were used to characterise the complexes $[(^{Ad}ArO)_3tacn]U^{III}$, $[(^{Ad}ArO)_3tacn]U^{III}(Me_4IMC)$ and $[\{Me_3Si)_2N]_3U^{III}(Me_4IMC)$, where $(^{Ad}ArO)_3tacn$ = adamantyl-derivatised tris-aryloxide tacn; Me_4IMC = tetramethylimidazol-2-ylidene.[1258] Paramagnetically shifted ^1H NMR spectra for the U(IV) complexes $[^{tBu}NON]UR_2$, where R = CH_2SiMe_3, $H_2{}^{tBu}NON$ = (240), and $[^{tBu}NON]U(Cp^*)(CH_3)$ showed U-CH_2 and U-CH_3 resonances at −148.9, −146.3 ppm respectively.[1259]



(240)

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Solid State NMR Spectroscopy

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1 Structure of Solids

1.1 Group 1. – ^{7}Li NMR spectroscopy was used to characterise a lithium/graphite intercalation compound with a formula close to LiC_3.[1] *In situ* solid-state ^{7}Li NMR data were reported for lithium inserted into disordered carbon. There was evidence for both $Li^{\delta+}$ and metallic lithium species.[2] ^{7}Li and ^{13}C solid-state NMR spectra were used to characterise a mesoporous tantalum oxide lithium fulleride (C_{60}) composite material.[3]

^{1}H and ^{7}Li variable-temperature NMR spectra were discussed for a microporous lithiosilicate [Li–Si–O]-MFI and its calcination products.[4] ^{1}H and ^{7}Li MAS-NMR spectra were obtained for $Li(Ni,Co,Al)O_2$ samples. On hydration, some Li^+ sites are replaced by H^+.[5]

The ^{13}C CP/MAS-NMR spectrum of *rac*-$[Li_4\{C_6H_4[CH(Me)NMe_2]\text{-}2\}_4]$ shows that it is a self-assembled tetranuclear aggregate comprising 2 dimeric units, derived from (*R*)- and (*S*)-enantiomers respectively.[6]

^{7}Li MAS-NMR spectra were used to study interactions between Li^+ and a styrene-maleic anhydride copolymer based on PEO-400.[7] Similar data could characterise an epoxide-crosslinked polysiloxane/polyether hybrid (SE55). They showed the formation of transient cross-links between Li^+ and the ether oxygen atoms of the polyether fragment.[8]

^{6}Li MAS-NMR for $xLi_2MO_3.(1-x)LiMn_{0.5}Nb_{0.5}O_2$, where M = Ti, Zr or Mn, revealed a 'composite' structure with short-range order.[9] Lithium coordination in partially reduced $Li_{1.1}Ti_{1.9}O_{4+\delta}$ spinels was probed using ^{6}Li MAS-NMR.[10] ^{7}Li NMR data were used to determine the lithium environments in solid electrolytes $Li_{3.75}Ge_{0.75}V_{0.35}O_4$ and $Li_{3.70}Ge_{0.85}W_{0.15}O_4$.[11] ^{7}LiMAS-NMR spectra for Li^+-ion conducting glasses $(LiCl)_x(LiPO_3)_{1-x}$, where $x \leq 0.45$, show a linear dependence of chemical shift on x.[12]

The chemical shifts in the ^{6,7}Li MAS-NMR of $Li_{2.5}V_2(PO_4)_3$ are consistent with short-range V^{3+}/V^{4+} order.[13] The ^{7}Li solid-state NMR spectrum of $Li_{1.2}Ti_{1.8}Al_{0.2}(PO_4)_3$ gave values for the quadrupole constant and the spin-spin relaxation rate. The data were used to probe the local and long-range motions of the Li^+ ions.[14]

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The ^{7}Li MAS-NMR spectrum of a mesoporous silica (BBA-15) composite with $LiClO_4$/poly(ethylene oxide) showed the existence of three types of Li^+ coordination.[15] ^{1}H and ^{7}Li NMR spectra were used to characterise the new solid polymer $(PEG)_xLiClO_4$, where PEG = polyethylene glycol.[16]

Ab initio calculations have been made of ^{23}Na NMR parameters for sodium-centred clusters, modelling crystalline and glassy sodium oxide systems.[17] ^{13}C and ^{23}Na solid-state NMR spectra were used to characterise Na_3C_{60}.[18] Anomalous superconducting properties of $(NH_3)_xNaK_2C_{60}$ fullerides, where $0<x<1$, have been probed by ^{2}H and ^{23}Na NMR spectroscopy.[19] ^{13}C and ^{23}Na solid-state NMR spectra were reported for $CPh_3^-Na(tmeda)^+$ and fluorenyl-$Na(L)^+$, where L = pmdta (pentamethyldiethylenetriamine) or tmeda (tetramethylethylenediamine). Chemical shifts and ^{23}Na quadrupole coupling constants were in agreement with the formation of contact ion-pairs.[20] A new homonuclear correlation NMR experiment has been used to determine distances between quadrupolar nuclei. It was tested on Na_2HPO_4 (^{23}Na, $S = 3/2$) and the molecular sieve $AlPO_4$-14 (^{27}Al, $S = 5/2$).[21]

A high-resolution ^{13}C and ^{39}K NMR study has been carried out on the non-ferroic phase transition of $KHCO_3$.[22] Proton NMR gave evidence on the nature of the hydride ions in KH–$KHCO_3$ and KH samples.[23] ^{1}H NMR spectra gave evidence for superprotonic and ferroelastic phase transitions in $K_3H(SO_4)_2$.[24] ^{27}Al and ^{39}K spin-lattice relaxation processes were studied for $KAl(SO_4)_2.12H_2O$ crystals, showing that there is a phase transition at 360 K.[25]

^{19}F, ^{87}Rb and ^{119}Sn NMR spectra were used to characterise the two-dimensional fluoride-ion conductor $RbSn_2F_5$.[26] Proton NMR studies helped to construct the P-T phase diagram (95–300 K, 0–800, MPa) for $Rb_{1-x}(NH_4)_xI$, where $x = 0.29$ or 0.77.[27]

A single-crystal ^{133}Cs NMR study of $Cs^+(15\text{-crown-}5)_2I^-$ yielded chemical shift tensor components and parameters for the quadrupolar interactions.[28] A ^{133}Cs NMR study has been carried out on the $S = 1/2$, quasi-two-dimensional ferromagnet Cs_2CuBr_4.[29]

1.2 Group 2. – Application of the quadrupolar Carr-Purcell-Meiboom-Gill (QCPMG) sequence gave the first natural abundance solid state ^{25}Mg NMR data for $(C_5H_5)_2Mg$. The experimental data were in good agreement with DFT calculations.[30] ^{1}H, ^{13}C and ^{15}N NMR spectra were used to study the effects of axial coordination of imidazole (Im) or 1-MeIm to the Mg(II) ion in Mg^{II}(OEP) and (bacterio)chlorophyll.[31]

DFT and *ab initio* calculations have been made of ^{17}O NMR shielding for the oxides MO (M = Mg, Ca or Sr) and the model species $OM_6(OH)_{12}^{2-}$ (central O).[32] Similar calculations were reported for magnesium and calcium oxides and aluminosilicates.[33] ^{17}O 3QMAS-NMR spectra were used to characterise a series of Ca–Mg and K–Mg silicate glasses.[34] Solid adducts of $MgCl_2$ with ethanol were studied by ^{13}CP/MAS-NMR and ^{1}H–^{13}C HETCOR experiments.[35]

^{43}Ca NMR data were reported for calcium peroxides formed in the disproportionation of H_2O_2 catalysed by $Ca(OH)_2$.[36] ^{19}F, ^{27}Al, ^{29}Si and ^{31}P MAS-NMR spectra were used to study the structures of samples in the

SiO_2–Al_2O_3–P_2O_5–CaO–CaF_2 system.[37,38] A method has been developed for probing the local structural environment of calcium by natural abundance ^{43}Ca NMR spectroscopy. The method was applied to, for example, sol-gel-prepared calcium silicate materials.[39]

^{31}P NMR spectra detected a hydrogen-bonded phosphate polymer in calcium phosphate composites.[40] ^{19}F MAS-NMR spectra were used to determine isotropic ^{19}F chemical shifts in various environments in CaF_2–AlF_3 and BaF_2–AlF_3 systems.[41] ^{137}Ba NMR data were used to probe the structure of a new clathrate, Ba_6Ge_{25}.[42]

1.3 Group 3. – ^{45}Sc NMR data were reported for solid solutions $ScBRh_3$–$ScRh_3$. The Knight shift decreased with increasing boron concentration.[43] ^{45}Sc and ^{207}Pb NMR studies of ferroelectric $Pb(Sc_{1/2}Nb_{1/2})O_3$ show that a phase transition occurs at about 360 K.[44]

An *ab initio* calculation has been made of spin-lattice relaxation rates for YH_2.[45] NMR evidence suggests that there is very little magnetic alignment in YD_3, whereas such alignment does occur in LnD_3 and $ZrBr_2(H,D)_x$.[46] The electronic properties of YB_6 were characterised using ^{11}B NMR.[47] ^{11}B NMR data were used to determine the local field distribution in a single crystal of YNi_2B_2C.[48] The ^{13}C NMR spectra of yttrium carbide (Y_2C_2) endohedral fullerenes show that there are three isomers of $(Y_2C_2)@C_{82}$, with symmetries of C_s, C_{2v} and C_{3v}.[49]

The ^{13}C, ^{15}N and ^{89}Y CP/MAS-NMR spectra of $[Y(Cp)_2\text{-}\mu\text{-}(R)\text{-}(-)\text{-}OCH_2CH(Et)NMe_2]_2$ showed the presence of two non-equivalent $\{Cp_2Y(OR)\}$ fragments, compared to solution phase data, which were consistent with at least C_2 symmetry.[50] ^{47,49}Ti NMR spectra were used to study orbital ordering in ferromagnetic $YTiO_3$.[51] ^{17}O MAS-NMR provided data on oxygen local environments in the anionic conductors $Y_2(M_{1-x}M'_x)_2O_7$, where M, M′ = Ti, Zr, Sn.[52] ^{13}C and ^{31}P solid-state NMR spectra were used to characterise the complex $\{[Y(OH_2)]_3(CO_3)(A\text{-}\alpha\text{-}PW_9O_{34})_2\}^{11-}$.[53]

^{89}Y NMR data were able to determine the local magnetic susceptibilities relating to defects in the chain complexes Y_2BaNiO_5[54] and $Y_2Ba(Ni,Zn)O_5$.[55] ^{89}Y NMR data were also reported for $Y_{1-x}Ca_xBa_2Cu_3O_y$[56] and (to study exchange coupling) $Ca_{2+x}Y_{2-x}Cu_5O_{10}$.[57] Phase changes on LnYSiAlO glasses (Ln = La, Ce) were probed using ^{27}Al MAS-NMR.[58] Substitutional order in the mixed garnets $Y_{3-x}Lu_xAl_5O_{12}$ was studied by ^{27}Al NMR, *via* spin-lattice relaxation imes.[59] The y-phase of $Y_2Si_2O_7$ was characterised by ^{29}Si NMR spectroscopy.[60] ^{29}Si MAS-NMR data for the Eu^{3+}-doped yttria-silica composite shows that yttria nanocrystals are coated by amorphous silica, with the formation of Y–O–Si bonds.[61]

^{11}B NMR spectroscopy was used to study the magnetic properties of MRh_3B_2, where M = La, Ce, Nd, Sm, Eu or Gd.[62] The solid complexes $Ln(pic)_3L$, where Ln = La, Nd, Eu, Gd, Er, Y, and L = 1,1′-(3,6,9-trioxaundecanedionyl)diphenothiazine, were studied by ^{1}H NMR.[63]

^{55}Mn and ^{139}La NMR studies have been reported on inhomogeneity of the ferromagnetic state of $(La_{1-x}Sr_x)_{1-\delta}MnO_3$ perovskites.[64] A ^{69,71}Ga NMR study of $LaGa_{1-x}Mn_xO_3$ (where $0 > x > 0.2$) gave data on spin/spin and spin/lattice relaxation.[65] Structural and magnetic inhomogeneities of $La_{0.7}Ba_{0.3-x}Sn_xMnO_3$ and related systems were studied by ^{55}Mn and ^{139}La NMR.[66] NMR studies on $LaCo_9Si_4$ gave evidence for an itinerant metamagnetic phase transition.[67] ^{17}O NMR spectroscopy was used to determine O/N ordering in the $La_3Si_8N_{11}O_{14}$ phase.[68] The temperature-dependent polymorphism of $LaPO_4$ was followed by ^{31}P solid-state NMR spectroscopy.[69]

Proton and ^{13}C NMR data were obtained, to analyse the polymeric forms of trihalophenolate cerium(IV) complexes.[70] The ^{13}C CP/MAS-NMR spectrum of $Eu(HnicO)_2(\mu\text{-}HnicO)(H_2O)$, where H_2nicO = 2-hydroxynicotinic acid, shows effects due to the interaction of the ^{13}C nuclei with paramagnetic Eu^{3+}.[71] Microporous lanthanide silicates, $Na_{1.08}K_{0.5}Ln_{1.14}Si_3O_8.1{,}78H_2O$, where Ln = Eu, Tb, Sm or Ce, were studied by ^{23}Na and ^{29}Si MAS-NMR.[72] $^{155,157}Gd$ NMR measurements showed hyperfine magnetic interactions in gadolinium iron garnet.[73] ^{11}B NMR spectra were used to study 4f-electron spin-dynamics in $HoNi_2B_2C$.[74] The magnetic properties of $YbInNi_4$ were studied by ^{115}In NMR spectroscopy.[75]

^{235}U NMR spectra were used to characterise uranium intermetallic compounds such as URh_3.[76] ^{73}Ge NMR studies have been carried out on the ferromagnetic superconductor UGe_2 at pressures of 1.2 GPa.[77] NMR data (Ga, Pt) were used to obtain evidence on the magnetic structures of $UPtGa_5$ and $UNiGa_5$.[78]

1.4 Group 4. – ^{13}C MAS-NMR spectroscopy was used to investigate the nature of the active species Cp^*TiCl_3/P, where P = functionalised 20% cross-linked chloromethylated polystyrene.[79] ^{27}Al NMR spectra were used to probe amorphisation processes in Al–Ti–Si composites, *e.g.* $Al_{30}Ti_{70-x}Si_x$, where x = 10, 20 or 30.[80]

^{13}C MAS-NMR data for solid $[(py)(RO)_3M]_2(\mu_4\text{-}DHP)$, where M = Ti, R = CH_2CMe_3, ^iPr; M = Ti or Zr, R = CMe_3, are consistent with octahedral geometry at M.[81] The structure and electronic environment of $KTiOPO_4$ were studied using ^{17}O, ^{39}K and $^{47,49}Ti$ solid-state NMR spectra.[82] ^1H MAS-NMR spectra were used to characterise monodisperse colloidal TiO_2 prepared by sol-gel synthesis from $Ti(OEt)_4$ in ethanol.[83] Interactions between TiO_2 nanoparticles and a silica sol-gel matrix were investigated by ^{29}Si NMR spectroscopy.[84] Titania-silica mixed oxides prepared from $Si(OEt)_4 + Ti(O^iPr)_4$ were studied similarly.[85] ^{17}O and ^{49}Ti MAS-NMR data were used to study the structure of $(TiO_2)_x(SiO_2)_{1-x}$ sol-gel glasses, where x = 0.08, 0.18, 0.41.[86]

The structural effects of TiO_2 substitution for Bi_2O_3 in $xNa_2O\text{–}xP_2O_5\text{–}yBi_2O_3\text{–}zTiO_2$ glasses were followed by ^{23}Na MAS-NMR and ^{27}Al double-quantum filtered MAS-NMR spectra.[87] Solid-state ^{17}O NMR data were reported for the nanocomposites PDMS–M_xO_y, where M = Ti(IV), Zr(IV), Ge(IV), Nb(V), Ta(V), PDMS = poly(dimethylsiloxane). There was evidence for the formation of M–O–M, M–O–Si and Si–O–Si bridges.[88] $^{47,49}Ti$ NMR data were obtained for cubic phases of $MTiO_3$, where M = Sr or Ba.[89] Similar results for $LaTiO_3$ indicate a large quadrupole splitting due to 3d electrons at titanium sites.[90]

^{1}H MAS-NMR spectra suggest that on $HTiNbO_5$, HTi_2NbO_7 and $HTiTaO_5$ nanosheets Ti(OH)M (M = Nb, Ta) units function as strong Brønsted acid sites.[91] ^{23}Na and ^{29}Si MAS-NMR spectra were used to probe cation environments and framework changes in silicotitanate materials $HNa_3Ti_4Si_2O_{14}.4H_2O$ and $HNa_3Ti_3NbSi_2O_{14}.4H_2O$.[92] ^{13}C solid-state NMR spectra show the presence of non-equivalent carboxylate groups in $Ti_6O_6(O^iPr)_6(OOC^tBu)_6$.[93]

^{91}Zr MAS-NMR spectra for Cp_2ZrCl_2 gave the first solid-state ^{91}Zr NMR data for an organometallic complex.[94] ^{13}C MAS-NMR spectra were used to characterise the silica-bound species $\equiv$Si–O–Zr$(CH_2CMe_3)_3$.[95,96] ^{13}C CP- and PD-MAS-NMR spectra were used to study triflic acid-functionalised mesoporous zirconium-containing molecular sieves.[97]

Ab initio calculations gave ^{29}Si NMR parameters for zircon, $ZrSiO_4$.[98] Natural-abundance ^{17}O solid-state NMR spectra showed the presence of bridging oxygen atoms in radiation-damaged zircon.[99] ^{29}Si and ^{31}P MAS-NMR spectra were used to characterise $SiO_2.xZr(HPO_4).yH_3PO_4$ composites.[100] Structures of novel small-pore metal silicates, $Na_{2.26}MSi_3O_9Cl_{0.26}.xH_2O$, where M = Zr, Hf or Sn, were determined using ^{23}Na, ^{29}Si and ^{119}Sn solid-state NMR spectra.[101] The structure of a highly-ordered, thermally stable meso-structured zirconium oxophosphate templated by tri-headgroup quaternary ammonium surfactants was probed by ^{31}P MAS-NMR.[102] ^{1}H, ^{27}Al and 2-D NMR were used to study the coordinative interactions between organoaluminium species (*e.g.* triethyl- and ethyl-aluminium sesquichlorides) and $ZrCl_4$.[103]

1.5 Group 5. – Solid-state ^{51}V NMR spectra were used to characterise the vanadium sites in $LiCo_xNi_{1-x}VO_4$.[104] The local structure of the vanadate material $LiMoVO_6$ was studied by ^{7}Li MAS-NMR spectroscopy.[105] A low-temperature phase transition (near 18 K) was detected by ^{23}Na NMR for $NaVGe_2O_6$.[106] ^{31}P and ^{51}V NMR spectra gave evidence for strong coupling between vanadium nuclei in $Sr_2VP_2O_9$ and $Sr_2V_3O_9$.[107]

^{51}V NMR data were used to characterise $[Ph_4P][\{(C_6H_5)_3SiO\}_2VO_2]_x[\{(C_6H_5)_3\text{-}SiO\}_2V\text{-}O(O_2)]_{1-x}$.[108] ^{31}P and ^{51}V NMR spectra of the high-pressure phase of $(VO)_2P_2O_7$ confirmed the presence of an alternating antiferromagnetic chain.[109] High-pressure and low-temperature ^{7}Li NMR measurements were used to study the spin dynamics of LiV_2O_4.[110,111] ^{7}Li static and MAS-NMR spectra were used to study the lithium environment in V_2O_5 xerogels with inserted Li^+.[112,113] A detailed study has been made of the ^{51}V MAS-NMR spectra of surface vanadia nanoparticles on titania. The data were consistent with vanadium in a distorted octahedral coordination environment.[114]

^{51}V NMR spectroscopy was used to characterise V_2O_5 supported on mesoporous SBA-15 catalysts.[115] ^{7}Li MAS-NMR spectra detected δ- and γ-LiV_2O_5 phase formation in the lithium vanadates $Li_xV_2O_5$, where x = 1.0, 1.2 or 1.4.[116] ^{51}V NMR spectra were used to follow the redox behaviour of vanadium in Ca^{2+}-doped magnesium vanadates (MgV_2O_6, $Mg_2V_2O_7$, $Mg_3V_2O_8$).[117] ^{51}V NMR spectra of $PbNi_{2-x}Mg_xV_2O_8$, where x = 0, 0.12, 0.24, show that VO_4 tetrahedra serve as superexchange bridges between Ni^{2+} chains.[118]

^{7}Li and ^{51}V MAS-NMR studies of electrochemical cycling of the layered battery material $Li_{1+x}V_3O_8$ were used to follow local structural and electronic changes.[119] ^{1}H NMR spectra were used to determine the spin dynamics of $(NHEt_3)_4[V^{IV}{}_8V^{V}{}_4As_8O_{40}(H_2O)].H_2O$.[120] EHMO calculations have been reported of ^{51}V, ^{95}Mo and ^{183}W chemical shifts for a large number of polyoxometalates.[121] ^{1}H nuclear spin-lattice relaxation rates were measured for a dodecanuclear polyoxovanadate cluster.[122] ^{51}V MAS-NMR data gave information on the redox behaviour of magnesium vanadate catalysts during oxidative dehydrogenation of propane.[123] ^{51}V NMR spectra of mesoporous vanadium-containing MCM-41 molecular sieves showed that calcinations followed by dehydration in air leads to transformation of T_d to O_h V^{5+} ions (due to coordination by water molecules).[124]

Mixed (Ru/V) sulfides were studied by ^{51}V NMR spectroscopy.[125] Variable-temperature ^{51}V NMR studies of spin relaxation rates show that the vanadium lattice in CuV_2S_4 behaves as a nearly antiferromagnetic metal.[126]

^{93}Nb 3QMAS-NMR was used to investigate the solid solutions $(1-x)Pb(Mg_{1/3}Nb_{2/3})O_3.xPb(Sc_{1/2}Nb_{1/2})O_3$, where x = 0, 0.1, 0.2, 0.6, 0.72, 0.9.[127] ^{93}Nb, ^{119}Sn and ^{207}Pb (single- and triple-quantum) solid-state NMR spectra were used to analyse non-stoichiometric mixed lead and tin niobates.[128] ^{31}P NMR spectra enabled the structures of Li_2O–Nb_2O_5–CaO–P_2O_5 glasses to be determined – showing the formation of Nb–O–P bonds.[129] Framework changes in Nb-exchanged $HNa_3Ti_4Si_{12}O_{14}.4H_2O$ with Cs^+ loading were followed by ^{93}Nb MAS-NMR.[130]

Wide-line ^{1}H NMR spectra of hydrated $Sr_6M_2O_{11}$ (M = Nb, Ta) and $Ba_4Ca_2Nb_2O_{11}$ show that there are three types of proton present: (i) relatively isolated OH groups; (ii) paired OH groups bound to the same M atom, and (iii) closely-spaced OH groups belonging to different octahedra and localised within a defect cluster.[131] Solid-state ^{1}H, ^{17}O MAS-NMR, ^{1}H-^{93}Nb TRAPDOR and ^{1}H 2-D MAS experiments were able to characterise O, OH and H_2O environments in $Na_7[HNb_6O_{19}].15H_2O$.[132] ^{29}Si MAS-NMR spectra were used to quantify the proportions of Keggin -1 and -2 structures in $Na_{16}[SiNb_{12}O_{40}].4H_2O$.[133]

Variable-temperature ^{31}P MAS-NMR spectra of $ANb_2P_2S_{12}$, where A = K, Rb, or Cs, suggest an increase in delocalised s-electron spin density with increasing temperature.[134]

Mesoporous tantalum oxide-sodium fulleride composites were characterised by the use of solid-state ^{13}C and ^{23}Na NMR spectra.[135]

1.6 Group 6. – The ^{29}Si MAS-NMR spectra of chromium catalysts on SiO_2, zeolite NaY and charcoal show chromium present in a range of oxidation states.[136] ^{95}Mo NMR spectra were used to characterise $Ln[CrMo_6O_{24}H_6]$, where Ln = La, Ce, Pr, Nd, Sm, Gd, Dy or Yb.[137]

^{13}C and ^{15}N CP/MAS-NMR spectra of $MoO_2{}^{2+}$ complexes of *trans-N,N′*-bis(R-salicylidene)-1,2-cyclohexanediamine (R = H, 3,5-Cl_2, 3,5-Br_2, 4,6-$(OMe)_2$) and related species gave evidence for coordination-induced changes in ligand conformation.[138] ^{95,97}Mo NMR data were used to probe the defect structures of Sr_2FeMoO_6, $Sr_{2-x}La_xFeMoO_6$ and $Sr_{1-3x}Ba_{1+x}La_{2x}FeMoO_6$.[139–141] ^{13}C and

^{29}Si MAS-NMR and CP/MAS-NMR spectra have been reported for mesoporous silica catalysts derivatised with bis(halogeno)dioxomolybdenum(VI) species.[142]

MAS-NMR spectra were employed to characterise a series of Ni–Mo–P/Al_2O_3 catalysts.[143] Solid-state ^{31}P MAS-NMR spectra of xerogels "$2MoO_{1.5}.2P_2O_5$" and "$2MoO_{1.5}.2P_2O_5.2SiO_2$" show that they retain structural features of the precursor molecules.[144] Solid-state NMR studies have been reported for a range of polyoxomolybdates[145–149] and polyoxotungstates.[150–156]

1.7 Group 7. – ^{55}Mn NMR data were reported for β-$Mn_{1-x}Os_x$ alloys.[157] ^{27}Al and ^{55}Mn NMR spectra were used to probe the magnetic behaviour of a decagonal pseudo-crystal, $Al_{69.8}Pd_{12.1}Mn_{18.1}$.[158] High-pressure ^{55}Mn NMR spectra were used to follow magnetic phase transitions in Mn_3GaC and MnAs to 19 kbar.[159] Evidence was found, from ^{55}Mn NMR data, for phase transitions for $Mn_3Ga_{0.98}Al_{0.02}C$.[160] ^{55}Mn NMR data were also reported for MnAs[161] and $Mn_{1-x}Ti_xAs$.[162]

Proton NMR spectra were used to study the effects of the antiferromagnetic phase transition (< 130 K) of α-$MnH_{0.06}$.[163] ^{13}C and ^{15}N MAS-NMR spectra were used to determine the spin density distribution in $Cs_2K[M(CN)_6]$, where M = Mn or Fe.[164]

^{2}H NMR studies on samples of γ-MnO_2 were able to investigate reduction and hydrogen insertion mechanisms in primary zinc batteries.[165] Conversion of layered $LiMnO_2$ to a spinel form on electrochemical cycling was followed by ^{6,7}Li NMR spectroscopy.[166] ^{6}Li MAS-NMR data were reported for the layered $Li_{1-x}Co_{1/3}Ni_{1/3}Mn_{1/3}O_2$ cathode material.[167] A single crystal of $LaMnO_3$ was characterised by ^{55}Mn NMR spectroscopy.[168] ^{55}Mn NMR spectra of ^{16}O- and ^{18}O-containing $La_{0.33}Nd_{0.33}Ca_{0.34}MnO_3$ gave information on the size of the ferromagnetic metallic regions.[169]

There have been several reports on ^{55}Mn NMR studies on $Pr_{1-x}Sr_xMnO_3$ samples.[170–172] ^{55}Mn NMR spectra were used to characterise single crystals of $La_{1-x}Sr_{1+x}MnO_4$.[173] ^{6}Li MAS-NMR shows 1:1 local ordering of Li and Mn atoms in the n = 2 Ruddlesden-Popper phase La_3LiMnO_7.[174] ^{55}Mn spin-echo NMR spectra (at 4.2 K) have been reported for single crystals of $La_{1.2}Sr_{1.8-x}Ca_xMn_2O_7$,where x = 0, 0.1 or 0.2.[175] ^{55}Mn NMR spectra for $La_{1.4}Sr_{1.6}Mn_2O_7$ (layered perovskite) gave evidence for localised Mn^{3+} and Mn^{4+} states.[176] A low-temperature ^{55}Mn NMR study of Mn_{12}-acetate molecular magnet has been carried out, at temperatures down to 20 mK.[177] ^{55}Mn NMR spectra were used to differentiate between relaxation processes in Mn_{12}-acetate and -benzoate.[178]

Static and MAS-NMR spectra (^{125}Te) for Re_6Te_{15} and related Re_6-Te clusters showed evidence of distortion of the magnetic field at Te sites by the Re_6 cluster unit.[179]

1.8 Group 8. – ^{29}Si NMR spectroscopy on FeSi at 900 K gave information on spin dynamic properties.[180] Temperature-induced phase changes were probed by ^{23}Na NMR spectroscopy for $NaFe_4Sb_{12}$, in the temperature range 4.2–290 K.[181] ^{1}H and ^{13}C MAS-NMR spectra were used to characterise Cp_2M, where M

= Fe or Ru, substituted in the 1- and 1′-positions by 2 nitronyl nitroxide radicals.[182] Similar data were also used to study cationic organometallic polymers, such as cyclopentadienyl-iron polyether-imines.[183] ^{13}C and ^{29}Si MAS-NMR spectra were reported for 1,5,3,2,4-diazooxadisila[5]ferrocenophane.[184]

^{2}H MAS-NMR spectra were used to study deuteriated goethite, α-FeOOD, both internal and surface structures.[185] ^{57}Fe NMR was used to study photomagnetic behaviour of $FeBO_3$.[186] Addition of ferromagnetic γ-Fe_2O_3 particles to liver tissue was used to obtain proton transverse relaxation rate images.[187]

^{29}Si CP/MAS-NMR spectra were used to characterise $(Ni_{0.5}Zn_{0.5}$-$Fe_2O_4)_{100-x}(SiO_2)_x$, where x = 5, 10 or 20.[188] Temperature dependence of ^{57}Fe NMR spectra was reported for $Fe_{3-x}Al_xO_4$, where x = 0, 0.005, 0.01, 0.02 or 0.03.[189] ^{57}Fe NMR spectroscopy was used to follow the effects of calcium-doping yttrium iron garnet films;[190] and to characterise yttrium iron garnet ($Y_3Fe_5O_{12}$) epitaxial films grown from BaO–B_2O_3–BaF_2 films.[191]

^{7}Li NMR nuclear spin relaxation rates (1.5–50 K) were measured for the molecular nanomagnet $[LiFe_6(OMe)_{12}(dbm)_6]BPh_4.5CH_2Cl_2$, where dbm = dibenzoylmethane.[192] Variable-temperature ^{57}Fe NMR spectra (4.2–295 K) for $BaFe_{12}O_{19}$ hexaferrite was used to probe the thermal behaviour of local magnetic fields.[193]

^{2}H MAS-NMR spectra of $[RuD(\eta^6$-toluene)(Binap)$]^+$ show that the structure is the same as in solution.[194] Solid-state ^{1}H NMR spectra were used to follow proton dynamics in solid $RuO_2.xH_2O$.[195] ^{99,101}Ru and ^{63,65}Cu NMR spectra were able to characterise superconducting and non-superconducting samples of $RuSr_2EuCu_2O_8$ and $RuSr_2GdCu_2O_8$.[196] The ^{6}Li NMR spectrum of Li_3RuO_4 suggests that about 10% of Li sites are occupied by Ru.[197] Ruthenium NMR studies on $Bi_3Ru_3O_{11}$ and $La_4Ru_6O_{19}$ show that there are three-dimensional linkages of edge-sharing pairs of RuO_6 octahedra.[198]

1.9 Group 9. – The ^{59}Co NMR spectrum of $ErCo_3$ gave evidence for a metamagnetic transition near 100 K.[199] ^{29}Si{^{1}H} CP/MAS-NMR and ^{59}Co NMR spectra were used to characterise mesoporous MCM-41 containing supported $Co(CO)_4^-$ units (which retained their geometry on deposition).[200] ^{59}Co NMR data were reported for (±)-$[Coen_3]Cl_3.3H_2O$ and its dehydrated analogues.[201]

There was NMR evidence for microscopic phase separation in Na_xCoO_2, where $0.65 \leq x \leq 0.75$).[202] There is ^{23}Na NMR evidence for charge order and magnetic susceptibility of oriented powder samples of Na_xCoO_2, where $0.50 \leq x \leq 0.70$.[203] ^{23}Na NMR spectroscopy was also used to follow magnetic fluctuations in the metallic state of $Na_{0.7}CoO_2$.[204] ^{1}H and ^{7}Li MAS-NMR spectra showed the existence of interphase layers in Li(Ni, Co, Al)O_2 samples.[205]

^{59}Co NMR spectra of $La_{1-x}Sr_xCoO_3$ are consistent with the presence of ferromagnetic regions, spin-glass regions and hole-poor low-spin regions at all x values from 0.1 to 0.5.[206] Similar data for $Nd_{1-x}Sr_xCoO_3$ ($0 \leq x \leq 0.5$) were used to study phase separation;[207] and for $Pr_{1-x}Ca_xCoO_3$ to construct a T–x phase diagram.[208] The spin state of Co ions was determined by ^{59}Co NMR spectroscopy for $EuBaCo_2O_{5-x}$, where x = 0.02 or 0.52.[209]

^{31}P solid-state NMR spectra were used to characterise SiO_2-tethered rhodium complexes derived from $RhCl(PPh_3)_3$ or $RhH(CO)(PPh_3)_3$.[210]

1.10 Group 10. – Defect structures were studied for binary intermetallic compounds Ni–M, where M = Al, Ga, In, Ti, using ^{27}Al, $^{47,49}Ti$, ^{61}Ni, ^{71}Ga and ^{115}In NMR spectroscopy, as appropriate.[211] ^{7}Li NMR spectra were used to determine the local distribution of transition metal ions in Fe- and Co-substituted $LiNiO_2$.[212] Similar experiments were used to characterise the cathode material $LiNi_{0.8}Co_{0.15}Al_{0.15}O_2$ in lithium-ion batteries.[213]

^{13}C MAS-NMR spectra characterised the octahedral coordination cage system $Na_4(Et_3NH)_{12}[(Pd_3L)_{18}(\mu\text{-bar})_{12}].xH_2O$, where H_5L = tris(2-hydroxybenzylidene)triaminoguanidine, bar^{2-} = 5,5-diethylbarbiturate.[214] Solid state ^{13}C NMR data were used to characterise $[PdCl_2L]_2$, $PdCl_2L_2$ and $[Pd(\mu\text{-}Cl)(L\text{-}H)]_2$, where L = diethyl-[α-(4-benzeneazoanilino)-2-hydroxybenzyl)-phosphonate.[215] One- and two-dimensional solid-state ^{31}P NMR characterised triphenylphosphine-phosphonic acid complexed to $PdCl_2$ on a zirconium phosphite network.[216]

Solid-state ^{31}P NMR spectra were used to determine the structures of $MPdPS_4$, where M = Na, Rb.[217] The structure of $Rb_2[Pd(Se_4)_2].Se_8$ was probed by ^{87}Rb MAS-NMR, ^{77}Se static and MAS-NMR. The results were consistent with the structural units $[Rb(Se_8)]_x^{x+}$ (columns) and $[Pd(Se_4)_2]_x^{2x-}$ (sheets).[218]

A ^{195}Pt NMR study has been made of the superconducting state of $CePt_3Si$.[219] Techniques for obtaining NMR spectra for heavy metal S = 1/2 nuclei in polycrystalline samples were tested on, for example, $(Ph_3P)_2Pt(C_2H_4)$, together with $PbCl_2$, $PbTiO_3$ and $Hg(OAc)_2$.[220] Assignments were proposed from ^{13}C NMR spectra for $Pt(PBu_3)_2L_2$, where L = an *o*-sydnone - C_6H_4–$C{\equiv}C$–$(C_6H_4$–$C{\equiv}C)_n$–H (n = 0, 1 or 2), especially for the alkyne carbons.[221]

1.11 Group 11. – ^{63}Cu NMR data were reported for $CeCu_{5.9}Au_{0.1}$.[222] Medium-range order and crystallisation were studied using ^{27}Al and ^{63}Cu NMR spectroscopy for $Cu_{20}Al_{10}Ni_8Ti_3$ and $Zr_{57}Cu_{20}Al_{10}Ni_8Ti_5$ metallic glasses.[223]

^{31}P MAS-NMR spectra were used to characterise a range of copper, silver and gold complexes containing scorpionate ligands (*i.e.* poly(pyrazolyl)borates).[224] The $^{31}P\{^1H\}$ CP/MAS-NMR spectra of Cu(dmppn)X, where X = Cl, Br or I, dmppn = 4,5-dimethyl-2-phenylphosphorin, show that there is strong back π-donation from Cu(I) to phosphorin.[225]

Temperature dependence has been observed for $^{63,65}Cu$ NMR spectra of the infinite-layer antiferromagnet $SrCuO_2$.[226] ^{63}Cu NMR spectroscopy was used to probe magnetic behaviour of $BaCuO_{2+x}$, where x = 0 or 0.14, containing $Cu_{18}O_{24}$ spherical clusters, Cu_6O_{12} ring clusters and CuO_4 isolated units.[227]

^{11}B NMR spectra were reported for the soliton lattice system CuB_2O_4 – including evidence for phase transitions.[228] ^{11}B NMR data for $SrCu_2(BO_3)_3$ showed that buckling of $CuBO_3$ layers had occurred.[229] Planar Cu and O hole densities in high-T_c cuprates, *e.g.* $La_{2-x}Sr_xCuO_4$, were probed by ^{17}O and ^{63}Cu solid-state NMR spectroscopy.[230,231]

Copper NMR spectra gave evidence on spin and charge structures of $Nd_{2-x}Ce_xCuP_{4-\delta}$.[232] ^{13}C NMR spectra were measured at high pressures to study the S = 12 antiferromagnetically coupled spin chain $[PM.Cu(NO_3)_2.(H_2O)_2]_n$, where PM = pyrimidine.[233] $^{63,65}Cu$ NMR spectra were measured in the temperature range 5–300 K for $RuSr_2GdCu_2O_8$.[234] There have been two reports of ^{65}Cu NMR spectra of $YBa_2Cu_3O_{6.5}$.[235,236] Several studies have been made of Cu NMR properties of long-range order and superconductivity in cuprates such as $Sr_{14}Cu_{24}O_{41}$,[237] $Sr_{13}LaCu_{24}O_{41}$,[238] $Sr_2Ca_{12}Cu_{24}O_{41}$[239] and $Sr_{14-x}Co_x$-$Cu_{24}O_{41+\delta}$.[240]

The electronic properties of the magnetic superconductor $CuFeS_2$ were studied using $^{63,65}Cu$ NMR spectroscopy.[241] ^{13}C CP/MAS-NMR data were used to characterise the alkylanthate complexes $[M\{S(S)COR\}_2]$, where M = ^{63}Cu, ^{65}Cu or Ni; R = Et, ^iPr, ^iBu, ^sBu or C_5H_{11}.[242] The ^{31}P MAS-NMR spectrum of $\{Cu_8(\mu_8\text{-}Se)[S_2P(OEt)_2]_6\}_{0.54}\{Cu_6[S_2P(OEt)_2]_6\}_{0.46}$ showed two closely spaced peaks – one from Cu_6 (100.7 ppm), and one from Cu_8 (101.1 ppm) clusters.[243] ^{63}Cu and ^{115}In NMR data were reported for $CuInSe_2$ crystals.[244]

The ^1H nuclear spin-lattice relaxation mechanism has been studied for the dense paramagnet $CuF_2.2H_2O$.[245] Copper NMR spectroscopy was used to study low-temperature phase transitions in the two-legged spin ladder NH_4CuCl_3.[246] Field-induced magnetic order and simultaneous lattice deformation were followed in $TlCuCl_3$ by Cu and Cl NMR spectroscopy.[247] Local structure of the fast solid-ion conductor $(CuI)_8P_{12}$, as well as those in related systems (*e.g.* $(CuI)P_4Se_4$), were all studied in detail by using $^{63,65}Cu$ and ^{31}P MAS-NMR spectra.[248,249]

The ^{119}Sn solid-state NMR spectrum of $LiAg_2Sn$ shows a narrow band, indicative of high local symmetry at the tin site.[250] Relaxation properties of silver in the crystalline ion conductor $Ag_7P_3S_{11}$ was probed in a multi-dimensional ^{109}Ag NMR study.[251] ^{109}Ag MAS-NMR spectra, with ^{109}Ag-^1H CP/MAS-NMR data where possible, have been reported for a range of solid inorganic silver-containing species: $AgNO_3$, $AgNO_2$, Ag_2SO_4, Ag_2SO_3, $AgCO_3$, AgCl, AgI *etc.*[252] ^{31}P CP/MAS-NMR data for $Ag_2(R_fCOO)_2(dppm)$, where $R_f = C_nF_{2n+1}$, n = 1, 2, 3, 4, 6, 9, demonstrated coupling between crystallographically inequivalent phosphorus atoms.[253]

Principal components of the ^{13}C, ^{31}P and ^{77}Se shielding tensors were determined from solid-state NMR data for the complex $[\{(Me_3P)Au(selenourea)\}_2{}^{2+}.2Cl^-]$.[254]

1.12 Group 12. – ^{15}N CP/MAS-NMR data were used in the structural characterisation of $[M(pyridazine)Cl_2]_n$, where M = Zn, Cd or Hg. Increased N shielding was observed on coordination, although this trend weakened with increasing atomic weight of M.[255] The ^{67}Zn solid-state NMR spectrum of human carbonic anhydrase suggests that the fourth ligand is OH^-.[256] ^{31}P MAS-NMR spectroscopy was used to study the solid polymer $(Zn[CH_2\{P(Ph)O_2\}_2])_n$.[257] ^1H MAS-NMR spectra led to the identification of different types of proton in $Zn(HINT)(HPO_4)$, where HINT = isonicotinate.[258]

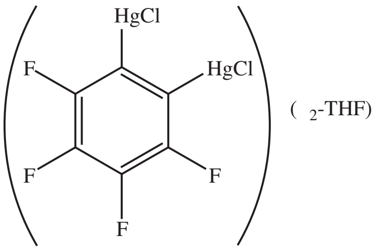
Characterisation of $ZnAl_2O_4$ powders was accomplished using ^{27}Al MAS-NMR spectroscopy.[259] ^{13}C and ^{31}P MAS-NMR spectra were used to study $Zn(O_3PPh)(phen)$, $Zn(O_3PR)_2(phen)$ (R = Me, Et, Bz) and

$Zn_2(O_3PR)_2(phen)(H_2O)$ (R = Ph, Bz).[260] The ^{31}P MAS-NMR spectra of several salts of $[Zn_3(HPO_3)_4]^{2-}$ were consistent with frameworks built up from strictly alternating ZnO_4 tetrahedra and HPO_3 pseudo-pyramids, sharing vertices.[261,262] ^{31}P MAS-NMR spectra yielded structural information for a range of zinc pyrophosphate glasses.[263]

^{67}Zn NMR spectra were used to measure electric field gradients at the metal site in ZnF_2, γ-$ZnCl_2$, $ZnBr_2$, ZnI_2 and Rb_2ZnCl_4.[264] DFT calculations have been made of ^{19}F magnetic shielding constants of MF_2 (M = Zn, Cd), β-PbF_2. MF_3 (M = Al, Ga or In), AMF_3 (A = K, Rb, Cs; M = Mg, Ca, Zn, Cd). $BaMgF_4$, $BaZnF_4$and Ba_2ZnF_6.[265]

MAS-NMR spectra have been reported and discussed for a microcrystalline cadmium-bacteriochlorophyll *d* analogue. The ^{113}Cd data suggested strong interaction with the fifth ligand.[266] ^{113}Cd MAS-NMR spectra were used to characterise $[Cd(O_2CMe)(O_2CPh)(H_2O)_2]_n$.[267] ^{113}Cd CP/MAS-NMR data for $CdX_2(C_5H_4NCOOR)$, where X = Cl, Br; R = Me, Et, ^nPr or ^iPr, gave values for chemical shift anisotropies due to distortions in the cadmium octahedra.[268]

The ^1H, ^{31}P CP/MAS-NMR spectra show that the cadmium phosphonate $Cd_2Cl_2(H_2O)_4(H_2L)$, where H_4L = ethylenediamine-*N,N′*-bis(methylenephosphonic acid contains the zwitterionic unit $NH_2^+CH_2P(O_2Cd)_2O^-$.[269] Two-dimensional ^{31}P 2Q and spin-echo NMR spectra were used to determine connectivity patterns of phosphorus atoms in $CdPS_3$ intercalated with K^+ and *N,N′*-dimethylviologen cations. ^{113}Cd data were also reported.[270] ^1H-^{113}Cd and ^1H-^{77}Se CP/MAS-NMR spectra were used to characterise Cd and Se sites in 2 nm.-hexadecylamine-capped CdSe nanocrystals.[271]



(1)

^{13}C CP/MAS-NMR spectra were reported for crystals of the complex (1).[272]

1.13 Group 13. – *1.13.1 Boron.*

^{11}B and ^{39}K MAS-, and ^{11}B 3Q MAS-NMR spectra for $K_{0.97}B_6$ were related to the structure of this species.[273] ^{11}B solid-state NMR spectra were reported for polycrystalline MgB_2;[274] ferromagnetic CaB_6 single crystals;[275] and $Al_{0.9}B_2$.[276] ^{11}B and ^{29}Si MAS-NMR spectra were used to study silicon boron oxycarbide (SiBOC) glasses based on SiO_xC_{4-x} and BO_yC_{3-y} mixed environments. There was evidence for some formation of a β-SiC phase.[277] Multinuclear MAS-NMR spectra were reported for SiBCN ceramics prepared by a number of routes.[278–280]

^{11}B NMR data were able to identify components due to hexagonal and rhombohedral phases in BN nanotubes.[281] ^{15}N CP/MAS-NMR spectra were reported for polymeric borazine derivatives.[282]

NMR data have been obtained giving information on B sites in $SrCu(BO_3)_2$.[283] ^{27}Al MAS-NMR spectra show the incorporation of boron as BO_4 units in $SrAl_{2-x}B_xO_4$ ($0<x<0.2$) and $Sr_4Al_{14-x}B_xO_{25}$ ($0<x<0.4$) in the presence of Eu^{II}/Dy^{III}.[284] ^{11}B MAS-NMR spectra were used to determine the structure of B_2O_3 in a B_2O_3/ZrO_2 catalyst.[285] Similar data were used to study the structure of the borate network in Na_2O–ZnO–B_2O_3 glasses.[286] ^{11}B, ^{27}Al and ^{29}Si MAS-NMR spectra were reported for $0.139MO(\text{or } M'_2O)-0.673SiO_2$-$(0.188-x)Al_2O_3.xB_2O_3$, where M = Mg, Ca, Sr, Ba; M′ = Na, K.[287] ^{7}Li, ^{11}B and ^{31}O high-resolution MAS-NMR spectra were used to gain structural information on glasses in the systems $xM_2O.(1-x)[0.5B_2O_3.0.5P_2O_5]$, where M = Li or Ag.[288]

^{11}B chemical shift anisotropies were determined for tetrahedral and trigonal boron sites in a range of borate systems, *e.g.* $CaB_2Si_2O_8$, $CaB_3O_4(OH)_3.H_2O$ *etc*. Tetrahedrally coordinated boron in borates shows anisotropies of less than 10 ppm.[289] ^{11}B NMR data for a single LiB_3O_5 crystal were analysed to give evidence on nuclear quadrupole interactions.[290] ^{11}B and ^{29}Si NMR spectra were used to determine alkali distribution in borosilicate glasses.[291] Boron-substituted molecular sieves, B-MCM-41, were characterised by ^{11}B MAS-NMR spectra.[292] A review has appeared on the use of multiple quantum (MQ) MAS-NMR spectra of quadrupolar nuclei (^{11}B, ^{17}O, ^{23}Na, ^{27}Al, $^{69,71}Ga$) in natural and synthetic clays.[293]

The ^{11}B NMR spectrum of $xLi_2S.(1-x)[0.5B_2S_3 + 0.5GeS_2]$ shows that approximately 80% of the boron is tetrahedrally coordinated.[294]

1.13.2 Aluminium. ^{27}Al NMR data have been reported for grain-aligned $CeNiAl_4$[295] and $PrNiAl_4$[296] samples. ^{27}Al NMR data gave evidence for differences between Mn-based magnetic features of icosahedral and decagonal forms of $Al_{69.8}Pd_{12.1}Mn_{18.2}$ quasi-crystals.[297]

^{1}H, ^{13}C, ^{27}Al and ^{29}Si solid-state NMR data were used to characterise Si–Al–C–N ceramics produced by thermolysis of $[Al(C_2H_4\text{-}SiHNH)_3]_n$.[298] A review has appeared on the use of CP/MAS-NMR (^{13}C, ^{27}Al, ^{29}Si) spectra to determine chemical order in Si–C–N–Al–Y nanopowders.[299] Si–C–Al–N–O ceramics containing a small amount of Al show a characteristic ^{27}Al MAS-NMR peak at 134.3 ppm.[300] Solid-state ^{27}Al and ^{29}Si NMR spectra were used to follow the degradation of an Si–Al–C–O ceramic under nitrogen at temperatures of up to 1700°C.[301]

^{27}Al MAS and 3Q MAS-NMR were used to monitor the decomposition path of solid $LiAlH_4$.[302] ^{27}Al and ^{133}Cs solid-state NMR data showed different orientation states of AlH_4^- in $CsAlH_4$ (120–360 K).[303] ^{1}H, ^{23}Na and ^{27}Al MAS-NMR spectra were used to obtain Ti-speciation in Ti-doped $NiAlH_4$.[304] ^{27}Al MAS-NMR data on alkyl-Al co-catalysts on a novel SiO_2-supported Ziegler-Natta catalyst were used to identify the nature of the Al^{3+} coordination sites.[305]

^{27}Al MAS-NMR spectroscopy was used to follow the formation of AlN by the thermal decomposition of $Al(NO_3)_3$ or $Al_2(SO_4)_3$ under nitrogen.[306] Solid-state ^{2}H NMR data gave information on the reorientation of the ND_3 group about the Al–N axis in $Me_3Al–ND_3$.[307] ^{27}Al MAS-NMR spectra can differentiate between solid polymorphs and between *fac*- and *mer*- isomers of AlQ_3, where Q = quinolin-8-olate.[308,309]

^{13}C and ^{27}Al MAS-NMR spectra were reported for $Mg_{0.86}Al_{0.3}(OH)_2(OAc)_{0.33}$.[310] ^{1}H, ^{7}Li and ^{27}Al NMR spectra were used to determine the structures of $[LiAl_2(OH)_6]_nX$, where X = Cl^-, Br^-, I^-, $1/2SO_4^{2-}$, $1/2C_6H_8O_4^{2-}$.[311] Solid-state ^{13}C, ^{27}Al and ^{31}P NMR spectra have been obtained for a new Al-O-P (aluminophosphonate) cluster $[Al_5(\mu_2\text{-}OH)_2(\mu_3\text{-}PhPO_3)_4(C_4H_9OH)_{12}]^{5+}$.[312] A Zn, Al layered double hydroxide (Zn/Al = 1.45) was characterised by ^{27}Al MAS-NMR.[313]

The structure of $CaTaOAlO_4$ was probed by ^{27}Al MAS-NMR spectroscopy.[314] The effects of adding B_2O_3 to albite ($NaAlSi_3O_8$) glass were investigated by using ^{17}O, ^{27}Al and ^{29}Si NMR spectra.[315] The transformation of a glass-like HAlO layer to Al/Al_2O_3 at 450°C was monitored using ^{27}Al MAS-NMR spectroscopy.[316] Boehmite-derived $\gamma\text{-}Al_2O_3$ was characterised structurally by ^{27}Al MAS-NMR.[317] NMR data were able to characterise a series of mesoporous Al_2O_3 and Cu/Al_2O_3 catalyst samples.[318] Multinuclear MAS-NMR spectra were used to characterise alumina and silica nanoparticles modified by methacryloxypropyl trimethylsilane and related species.[319]

^{27}Al MAS-NMR spectra were used to follow the conversion of 6- to 5-coordinate aluminium on dehydration of $Al_2(OH)_2(H_2O)_2(O_3PCH_2CH_2PO_3)$.[320] ^{27}Al dipolar solid-state NMR spectra were used to establish the nature of the aluminium atom ordering in $CsAl(SiO_3)_2$ and $3Al_2O_3.2SiO_2$. ^{27}Al homonuclear dipolar second moments were in good agreement with experiment.[321]

High-resolution ^{27}Al solid-state NMR data for $MAl_{12}O_{19}$ (M = Ca or Sr) show that the Al(2) sites are not 5-coordinate as previously thought, but distorted tetrahedrally 4-coordinate.[322] ^{27}Al MAS-NMR spectra gave structures of single- and two-phase yttria-alumina glasses (59.8–75.6% Al_2O_3).[323] The spatial ordering of Al atoms in $CsAl(SiO_3)_2$ and $3Al_2O_3.2SiO_2$ was probed by ^{27}Al dipolar solid-state NMR spectroscopy.[324] Site populations and short-range order in $Al_2Si_2O_5$ and $CaAl_2Si_2O_8$ were determined by ^{27}Al MQ-MAS-NMR.[325]

^{1}H, ^{27}Al and ^{29}Si MAS-NMR studies have been made of the structure of homogeneous binary $SiO_2–Al_2O_3$ glasses (0.4–12.0 wt% Al_2O_3).[326] ^{19}F and ^{29}Si MAS-NMR spectra were used to study the interaction between dissolved F^- and silicate glass in the $Na_2O–Al_2O_3–SiO_2$ system.[327] Structural units in glasses of the $Na_2Si_3O_7–Ma_2(NaAl)_3O_7$ system were investigated using ^{29}Si MAS-NMR spectra.[328] ^{27}Al, ^{29}Si and ^{31}P NMR studied were reported for Sr^{2+}-substituted glasses based on $4.5SiO_2–3Al_2O_3–1.5P_2O_5–3CaO–2CaF_2$.[329] ^{19}F, ^{27}Al and ^{29}Si MAS-NMR, with ^{27}Al MQ MAS-NMR experiments were used to determine Al/Si and F/OH ordering in the mineral zunyite, $Al_{13}Si_5O_{20}(OH,F)_{18}Cl$.[330]

Ab initio calculations have been made of ^{1}H, ^{17}O, ^{27}Al and ^{29}Si NMR parameters for sodium aluminosilicate glasses and hydrous silica.[331] Two-dimensional ^{17}O 3Q MAS-NMR experiments on sodium aluminosilicate glass gave evidence for Al–O–Al links.[332] ^{27}Al NMR spectra were used to study structural localisation of Al^{3+} in aluminosilicate clays.[333] ^{17}O MAS-NMR and MQ MAS-NMR experiments have been carried out on hybrid aluminosilicate xerogels, providing evidence for Si–O–Al and Si–O–Si sites.[334] Several other NMR studies have been made on aluminosilicate glasses and related systems.[335–338]

^{29}Si{^{1}H} CP/MAS-NMR, ^{27}Al and ^{23}Na MQ/MAS-NMR studies have been made of amorphous aluminium silicates, to determine local atomic structures.[339] ^{27}Al MAS-NMR (together with some other nuclei) studies have been carried out on novel porous sodium aluminophosphate-silicate and sodium ammonium fluorophosphates silicate;[340] an ordered hexagonal mesoporous silica material (JLU-30);[341] mesoporous Al-MSU-X aluminosilicate;[342] cubic mesoporous aluminosilicate AlMB48;[343] and mesoporous Al-SBA-15.[344]

^{27}Al NMR spectra of aluminium-rich microporous micelle-templated silicates show the absence of octahedral aluminium sites.[345] ^{19}F NMR spectra were used to determine the ordering of high-field strength cations at fluoride sites in aluminosilicate and silicate glasses.[346] ^{27}Al, ^{29}Si and ^{31}P MAS-NMR spectra were used to characterise PO_4-modified aluminosilicates.[347] Composite polymer-ceramic hybrids from poly(ethylene oxide)-block-poly(hexylmethacrylate) and aluminosilicates were studied using ^{13}C, ^{27}Al and ^{29}Si solid-state NMR spectroscopy.[348] ^{27}Al and ^{29}Si MAS-NMR spectra were used to study aluminosilica domains in organic/inorganic solid polymer electrolytes.[349]

It proved to be possible to identify ordered Si–O–Al environments in molecular sieves by {^{27}Al}-^{29}Si REAPDOR (*i.e.* rotational echo adiabatic passage double resonance) NMR techniques.[350] NMR studies have been reported for the following silicoaluminophosphate molecular sieves: SAPO-5;[351] SAPO-11 and -31;[352,353] H-SAPO-34 and -37;[354] and SAPO-44.[355]

Proton MAS-NMR spectra gave quantitative determination of hydrogen types in solid catalysts and supports, *e.g.* zeolites, silicoaluminophosphates *etc*.[356] ^{27}Al and ^{29}Si MAS-NMR data for zeolite catalysts used for the oxidative methylation of benzene with methane show the presence of extra-framework AlO_6 units, as well as the normal AlO_4 framework material.[357] ^{1}H MAS-NMR and ^{27}Al MQ- MAS-NMR spectra have been reported for zeolite-β. The ^{27}Al data were used to identify the distribution of aluminium in the original zeolite, its dealuminated and relauminated forms.[358,359] ^{27}Al MAS-NMR and two-dimensional 3Q MAS-NMR data were used to follow dealumination processes for zeolite-ω.[360]

There have been a number of NMR studies of zeolite-Y systems.[361–363] Other zeolites studied similarly include zeolite-HL;[364] zeolite-BEA;[365] zeolite-TNU-10;[366] and zeolite-USY.[367] ^{27}Al MAS-NMR spectra were used to probe the effects of simultaneous incorporation of Al and Ge into zeolite ZSM-5.[368] Related systems for which NMR structural studies have been made include Mo-ZSM-5;[369,370] and Cu-ZSM-5.[371] ^{13}C CP/MAS-NMR data were used to characterise MCM-41 with covalently grafted proline or benzylpenicillin.[372] Other studies of MCM-41-based mesoporous materials have been made.[373–378] ^{27}Al MAS-NMR spectra of mesoporous, cubic Na-Al-MCM-48 molecular sieve catalyst showed tetrahedrally-coordinated aluminium in both as-prepared and calcined samples.[379]

^{27}Al and ^{31}P MAS-NMR studies were used to probe the mechanism of formation of Al_2O_3–P_2O_5 glasses by sol-gel methods.[380] The novel microporous aluminophosphate $\{(CH_3NH_2)_4(CH_3NH_3{}^+)_4(OH^-)_4\}[Al_{12}P_{12}O_{48}]$ was characterised by ^{13}C, ^{27}Al and ^{31}P MAS-NMR spectroscopy.[381] Solid-state ^{27}Al and ^{31}P NMR experiments have been reported for aluminium polyphosphate gels.[382] Other aluminophosphate molecular sieves have been studied similarly: $AlPO_4$-5;[383] $AlPO_4$-31.[384] ^{27}Al MAS-NMR spectroscopy was used to follow the thermal decomposition of $AlPO_4$-HAD (where HAD = hexamethylenediammonium).[385] MAS-NMR spectroscopy (^{27}Al, ^{31}P) was able to characterise V- and/or Co-containing aluminophosphates: CoAPO-18, VAPO-18, VCoAPO-18.[386]

Characteristic ^{27}Al and ^{31}P NMR results for solid $Al_{1-x}Ga_xPO_4$ confirm that there are several phosphorus structural configurations throughout the range of $0<x<1$.[387] ^{29}Si 1-D MAS-NMR and 2-D ^{27}Al-^{29}Si HETCOR spectra were reported for the new sialon phase $Ba_2Al_3Si_9N_{13}O_5$.[388] ^{27}Al and ^{29}Si MAS-NMR spectra for the sialon S-phases $Ba_2Al_xSi_{12-x}N_{16-x}O_5$ gave evidence for Si/Al and O/N distributions.[389]

^{1}H and ^{31}P MAS-NMR and 2-D ^{31}P/^{1}H HETCOR-CP/MAS-NMR data were used to characterise plasma-sprayed hydroxyapatite coatings.[390] Solid-state NMR spectroscopy was used to follow the formation of a boehmite sol by hydrolysis of aluminium isopropoxide.[391] Mullite samples derived from different kaolinites were differentiated by ^{27}Al and ^{29}Si NMR data.[392] Ultra-high speed MAS-NMR, with ^{1}H-^{31}P cross-polarisation, was used to compare the chemical structure of human bone with hydroxyapatite, brushite and related mineral samples.[393] ^{27}Al MAS-NMR spectra have been obtained for mesoporous AlMSU-X, with a 'wormhole-like' framework.[394] ^{27}Al and ^{29}Si MAS-NMR spectra were able to follow the incorporation of aluminium into the framework of mesoporous silicas.[395]

^{13}C, ^{27}Al and ^{29}Si NMR spectra were used to characterise Al–Mg hybrids with phyllosilicate-like structures, especially the structural effects of replacing Mg + Si by 2Al.[396] The ^{27}Al and ^{29}Si MAS-NMR spectra of new inorganic polymeric composites based on kaolin or white clay showed a network of AlO_4 and SiO_4 tetrahedra.[397] Similar data were used to follow structural changes in a natural illite sample during acid-base titrations.[398] ^{27}Al NMR spectra of amorphous and paracrystalline Australian opals shows that all have 4-coordinate, T_d aluminium sites. The ^{29}Si NMR data are consistent with tetrahedral silicon, with 0, 1 or 2 Si–OH groups.[399]

Ground, granulated blast furnace slag was characterised using ^{27}Al and ^{29}Si solid-state NMR spectra.[400] The chemical structures of minerals in coal were investigated by ^{27}Al MQ/MAS-NMR.[401] ^{27}Al MAS-NMR spectra were obtained for aluminium-containing volcanic glasses.[402] ^{27}Al MAS-NMR spectroscopy confirms the incorporation of aluminium into the mesoporous framework of ethane-silica using Al(O^{i}Pr)$_3$.[403] ^{27}Al MAS-NMR and 2-D 3Q/MAS-NMR were used to determine the nature of aluminium coordination in fly-ash before and after grinding.[404]

Tetrahedral and octahedral aluminium sheets in montmorillonite were studied by ^{27}Al MQ/MAS-NMR spectroscopy.[405] ^{19}F, ^{27}Al and ^{29}Si MAS-NMR spectra were used to characterise montmorillonite with various contents of Mg(II) or Zn(II) substituted for aluminium in octahedral sheets.[406] Solid-state NMR spectra can be used to characterise and quantify the nanodispersion of variously modified montmorillonite clays in polystyrene matrices.[407] ^{27}Al and ^{29}Si MAS-NMR spectra were used to follow hydration processes for Portland cement.[408,409]

NMR chemical shifts (^{19}F, ^{27}Al) were calculated for the F and Al atoms of the mineral rosenbergite, $AlF[F_{0.5}(H_2O)_{0.5}]_4.H_2O$.[410] NMR measurements (^{23}Na, ^{27}Al) gave quadrupolar parameters in AlF_3, Na_3AlF_6 and $Na_5Al_3F_{14}$.[411] ^{19}F and ^{27}Al SATRAS (satellite transition spectroscopy) of solid aluminium chlorofluorides $AlCl_xF_{1-x}$ ($x = 0.05$–0.3) show a higher degree of disorder than in amorphous AlF_3, but no separate crystalline $AlCl_3$ phase.[412] ^{27}Al NMR spectra were used to determine the Al_{13}-content of nanosized poly-aluminium chloride samples.[413]

1.13.3 Gallium. ^{71}Ga MAS-NMR spectroscopy was used to probe nitrogen-deficiency in GaN powders.[414] Similar experiments were used to follow the formation of GaN by calcination of $Ga(NO_3)_3$ in flowing NH_3.[415] Laser-enhanced NMR spectra enabled the optical polarisation of nuclear spins in semi-insulating GaAs to be studied.[416] ^{69,71}Ga and ^{205}Tl NMR spectra were used to study thermal phase transitions in the layered semi-conductor $TlGaSe_2$.[417]

^{71}Ga MAS-NMR spectra for γ-Ga_2O_3 showed the presence of both 4- and 6-coordinate gallium. For α-Ga_2O_3, nearly all of the gallium was 6-coordinate.[418] A ^{71}Ga NMR study of the pyrochlore slab antiferromagnets $Ba_2Sn_2Ga_{10-7p}ZnCr_{7p}O_{22}$, where $p = 1, 0.93$, has been reported.[419] ^{1}H, ^{29}Si and ^{71}Ga MAS-NMR spectra were used to characterise the gallium-rich zeolite [Ga]beta, with a framework ratio $n_{Si}/n_{Ga} \approx 11.6$.[420] ^{71}Ga MAS-NMR shows isomorphous substitution of Ga for Si in the mesoporous gallosilicate Ga-MCM-48 (Si: Ga = 60).[421] The zeolites Ga-HZSM-5 and Ga-mordenite were characterised by ^{13}C CP/MAS-NMR, ^{1}H-^{13}C 2-D correlation spectra, and ^{71}Ga MAS-NMR.[422]

1.13.4 Indium. Homo- and heteronuclear indirect spin-spin interactions in InP semiconductors were studied by ^{31}P CP/MAS-NMR.[423] ^{31}P CP/MAS-NMR spectra were obtained for undoped and Fe-doped InP semiconductors.[424]

1.13.5 Thallium. ^{1}H NMR spectra of laser-irradiated TlH_3PO_4 gave values for NMR rotating frame spin-lattice relaxation times as a function of temperature.[425] ^{203,205}Tl NMR data for the ternary semiconductor $TlTaS_3$ were consistent with a chain structure.[426]

1.14 Group 14. – *1.14.1 Carbon.* There is ^{2}H and ^{13}C NMR evidence for a rigid skeletal structure in the fullerites $C_{60}D_x$.[427] Detailed structural information was obtained from the ^{13}C NMR spectrum of Li_4C_{60}.[428] ^{13}C MAS-NMR spectra of Ba_3C_{60} and Ba_6C_{60} showed one signal for the former, 3 for the latter, indicating the presence of three non-equivalent carbon sites.[429]

^{13}C MAS-NMR spectroscopy was used to quantify the different carbon species in synthetically produced nanodiamonds.[430] A ^{13}C study has been reported to study the modification of the electronic properties of SWCNT by alkali intercalation.[431,432] ^{13}C MAS-NMR data were used to study the structure of ^{13}C-enriched SWCNT, prepared by catalytic decomposition of CH_4.[433] ^{1}H, ^{13}C and ^{15}N MAS-NMR spectra of amorphous carbon nitride (a-CN_x) films were consistent with sp^2 hybridised nitrogen atoms in an aromatic carbon environment.[434]

1.14.2 Silicon. ^{2}H solid-state NMR spectra were used to determine the structural characteristics of macroporous silicon samples.[435] ^{29}Si chemical shift data gave structural information on solid solutions $Mg_2Si_xGe_{1-x}$, where $x = 0.1, 0.3, 0.4, 0.7, 0.8$ or 1.0.[436]

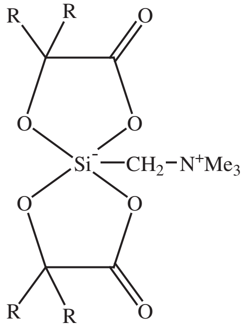
^{13}C and ^{29}Si MAS-NMR spectra of solid $Si(C{\equiv}CMe)_4$ showed the non-equivalence of the four propynyl groups.[437] Polycarbosilane-derived SiC fibres were characterised by ^{29}Si solid-state NMR.[438] Composition and short-range order were studied using ^{1}H and ^{29}Si MAS-NMR spectra for silicon oxycarbide, SiCO, glasses.[439] The ^{1}H, ^{13}C and ^{29}Si MAS-NMR spectra of self-assembled monolayers formed by reaction of $C_{18}H_{37}SiH_3$ and metal oxides show the formation of Si–O–Si and Si–OH . . . HO–Si units, but no bonds to metal oxide.[440]

Multinuclear NMR studies were used to characterise the structures of carbosilane polymers containing disilacyclobutane rings, $\text{-SiR(CH}_2)_2\text{SiR-}$ (R = Me or Ph), linked by $[\text{-(CH}_2)_2\text{CH=CH(CH}_2)_2\text{-}]$ or $[\text{-(CH}_2)_6\text{-}]$ units.[441] ^{1}H, ^{29}Si and $\{^{1}H\text{-}^{29}Si\}$ HETCOR NMR spectra were used to study σ-conjugated polysilanes with alkyl groups as side-chains.[442] ^{29}Si MAS-NMR spectra were able to follow the phase behaviour of a polymer containing SiC_4 sites, free C and traces of SiCO, prepared by pyrolysis of a polysilane (C:Si ratio 6.0).[443]

The ^{2}H NMR spectra of deuteriated guest chains of polydiethylsiloxane (PDES) in end-linked PDES networks gave data on their structure.[444] The ^{1}H, ^{13}C and ^{29}Si NMR spectra of poly(phenylsiloxane)s containing functional side groups show the presence of exactly alternating starting component units.[445] ^{29}Si NMR spectra were used to characterise copoly(dimethylsiloxane)(X-siloxane), where X = phenyl[446] or divinyl.[447] ^{13}C and ^{29}Si NMR spectra were reported for membranes comprising siloxane-methane polymers.[448] ^{13}C CP/MAS-NMR data were used to characterise $[S]\text{-(CH}_2)_3\text{-N(CH}_2\text{COOH)}_2$, where [S] = siloxane network.[449] ^{29}Si CP/MAS-NMR data for PEG-siloxane fibres showed that PEG is covalently bonded to the siloxane network.[450]

^{29}Si MAS-NMR data were used to characterise Si_2N_2NH crystals.[451] ^{13}C and ^{29}Si MAS-NMR spectra were able to determine the structures of

$(Et_4N)_2[Si(NCS)_6]$ and *cis*-$(acac)_2Si(NCS)_2$.[452] The solid-state structure of *cis*-$(acac)_2Si(NCO)_2$ was determined similarly.[453]



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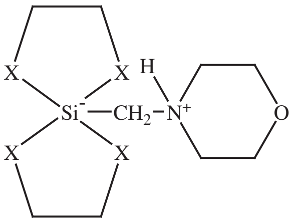

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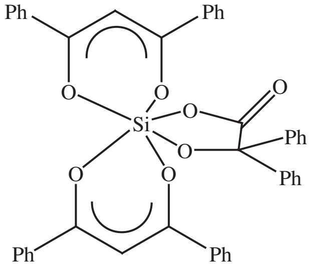

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^{29}Si CP/MAS-NMR spectra were used to characterise complexes of $[Si(catecholato)_3]^{2-}$ with Cr(III), Mn(II), Co(III), Ni(II) and Cu(II).[454] Solid-state ^{13}C, ^{15}N and ^{29}Si VACP/MAS-NMR spectra were used to determine the structures of (2), where $R = H$ or Me;[455] (3), where $X = O$ or S;[456] and (4).[457]

^{1}H and ^{29}Si MAS-NMR were used to determine the structure of the solid acid H_2SO_4–SiO_2.[458] Mesoporous silica-based spheres were studied by ^{1}H MAS-NMR spectroscopy.[459] Variable-temperature ^{29}Si MAS-NMR spectra were used to study the phase transition between low- and high-temperature forms of pure silica ferrierite.[460] High-resolution solid state NMR experiments were used to characterise SiO_2 aerogels.[461] Copper-containing hexagonal mesoporous silica gave characteristic ^{29}Si MAS-NMR spectra.[462]

The composites SiO_2.x(zirconium phosphate).y(H_3PO_4) were characterised by ^{29}Si and ^{31}P MAS-NMR spectroscopy.[463] ^{13}C MAS-NMR and ^{29}Si CP/MAS-NMR data were reported for a hydrothermally stable mesoporous ethane silica with long-rage hexagonal order (*p*6*mmm*).[464] ^{29}Si solid-state NMR spectra were used to characterise a molecularly-ordered mesoporous SiO_2 formed *via* phase transformation of silicate/surfactant composites.[465] Silyl-functionalised mesoporous silicas were studied by ^{13}C and ^{29}Si MAS-NMR spectra.[466] ^{29}Si CP/MAS-NMR data were used to characterise a novel anionic hydride derived from monomeric silsesquioxanes (‘silica hydride’).[467]

The conversion of native silica to a *p*-chlorobenzamide-bonded silica material was monitored by ^{13}C and ^{29}Si MAS-NMR spectroscopy.[468] Similar experiments were used to characterise a new mesoporous silica material (β-CD-silica 4%, where CD = cyclodextrin).[469] ^{29}Si MAS-NMR spectra showed the existence of Me_3Si- groups on the surface of a modified PTFE/SiO_2 hybrid.[470]The microstructure of SiO_2-PEG-vased proton-conducting membranes was investigated by ^{29}Si CP/MAS-NMR spectroscopy.[471] ^1H spin-spin relaxation times were measured for PEO/nano-SiO_2 composites.[472]

^{29}Si MAS-NMR spectra were used to determine the effects of attaching organometal carbonyl fragments covalently to SiO_2 nanoparticles.[473] SiO_2 modified by substituted propyltrimethoxysilane, and reacted with organic amines was characterised by VACP/MAS-NMR spectroscopy.[474] ^{13}C CP/MAS-NMR and ^{29}Si MAS-NMR spectra were employed to characterise silica-organic nanostructured materials from the hydrolysis and condensation of n-$C_nH_{2n+1}OSiCl_3$, where n = 12, 14, 16, 18 or 20. There was evidence for bimolecular layers of long-chain alcohols and thin silica layers.[475] Solid-state ^{13}C and ^{29}Si NMR spectra were used to characterise poly(vinylimidazole-co-methyl methacrylate)-silica hybrids.[476] ^{29}Si NMR data were able to characterise the reaction products of 3-methacryl-oxypropyltrimethoxysilane with tin oxide, antimony-doped tin oxide and silica nanoparticles.[477] Organic/inorganic hybrid materials based on 3-glycidoxypropyltrimethoxylsilane were studied by ^{13}C and ^{29}Si MAS-NMR spectroscopy.[478]

^{29}Si MAS-NMR and ^1H-^{29}Si CP/MAS-NMR studies were reported for layered sodium disilicate.[479] First principles calculations have been made of NMR parameters for crystalline and amorphous sodium silicate materials, including N_2SiO_3, α- and β-$Na_2Si_2O_5$. Good agreement was found with experimental data.[480] ^1H and ^{23}Na NMR data were reported for H_2O/H_2-bearing sodium silicate glasses.[481] ^1H, ^{23}Na and ^{29}Si solid-state NMR data were obtained for the one-dimensional sodium silicate phase Mu-29.[482] ^{17}O 3QMAS-NMR spectra of sodium silicate glasses quenched from 10GPa melts gave evidence for the units $^{(5,6)}Si$-O-$^{(4)}Si$ and Na-O-$^{(5,6)}Si$ sites.[483]

^{17}O and ^{29}Si MAS-NMR spectra were used to determine the structures of binary potassium silicate glasses containing 76.0–97.6 mol% SiO_2.[484]

^{29}Si MAS-NMR spectroscopy was used to probe the structure of calcium silicate hydrate (the main product of cement hydration).[485] ^{29}Si MAS-NMR spectra were used to follow the effects of incorporating a range of ions (*e.g.* K^+, Al^{3+}, Fe^{3+} *etc.*) on the stability and hydration of β-Ca_2SiO_4.[486] ^{29}Si MAS-NMR spectra were able to characterise the structures of NaF–CaO–SiO_2 glasses.[487] ^{19}F MAS-NMR spectra determined the coordination environment of F^- in CaO–SiO_2–CaF_2–Na_2O glasses.[488]

^{29}Si MAS-NMR spectra enabled a structural assignment to be given for $Na_5In_5Si_4O_{12}$.[489] ^{17}O MAS-NMR spectra gave evidence on the ordering of cation distributions in mixed-cation silicate glasses.[490] A ^{29}Si MAS-NMR study has been made of the structure of nanocrystalline α-Zn_2SiO_4.[491]

Xerogel polymers from the reaction of $(MeO)_3Si(CH_2)_3P{=}O(OEt)_2$ with $MeSi(OMe)_3$ were characterised using ^1H, ^{13}C, ^{31}P and ^{29}Si NMR spectra.[492]

^{29}Si CP/MAS-NMR was used to characterise mesoporous materials derived from sodium silicate and organotrialkoxysilanes.[493] Multinuclear NMR studies have been reported on periodic mesoporous organosilicas.[494,495] ^{13}C and ^{29}Si MAS-NMR spectra were used to characterise ordered macroporous organosilica materials.[496] A similar study has been made of mesoporous organosilica/clay heterostructures.[497]

Two-dimensional DQ ^{1}H MAS-NMR spectra were used to investigate the local structure of a surfactant-templated silicate thin film.[498] Silicalite-1 powders (20–1000 nm. crystals) were characterised by ^{29}Si MAS-NMR spectroscopy.[499] ^{13}C and ^{29}Si solid-state NMR data were used to characterise organic-inorganic mesoporous silica-based materials.[500]

^{19}F NMR spectroscopy was used to study the substitution of Ge for Si in fluoride-containing AST-type zeolites.[501] ^{29}Si and ^{31}P MAS-NMR spectra were used to characterise functionalised zeolite nanoparticles containing surface organic groups.[502] Several low-silica zeolites were studied by ^{29}Si MAS-NMR.[503] *Ab initio* calculations were reported for ^{1}H, ^{13}C and ^{15}N NMR chemical shift parameters to characterise Brønsted-acid sites in high-silica zeolites.[504] Algorithms have been derived for the assignment of peaks in high-resolution ^{29}Si MAS-NMR spectra of highly siliceous zeolites (*e.g.* ZSM-12, ZSM-5), based on 2-D ^{29}Si INADEQUATE spectra.[505]

^{1}H and ^{29}Si MAS-NMR spectra confirmed the covalent bonding of organics to the silicate framework for mesoporous silicas of the MCM-41 type, containing chiral binaphthyl, cyclohexadiyl moieties.[506] Quantitative studies on amino-functionalised mesoporous MCM-41 materials using ^{29}Si MAS-NMR spectroscopy provided an estimate of the proportion of Si atoms forming Si–C bonds.[507] ^{13}C, ^{29}Si and ^{31}P solid-state NMR spectra were used to follow the promoter (phosphate) enhanced crystallisation of siliceous MCM-41.[508] ^{15}N CP/MAS-NMR spectroscopy, can be used to study the interactions of pyridine-^{15}N with silanol groups of the inner surfaces of MCM-41 and SBA-15 ordered mesoporous silica.[509] Nanosized, luminescent Tb-MCM-41 was characterised by ^{29}Si MAS-NMR spectroscopy.[510] The solid-state NMR spectrum of MCM-48 coated by reaction with hexamethyldisilazane showed that the coating is chemically attached to the surface.[511] MoO_2^{2+}-modified mesoporous MCM-41 and MCM-48 silicas were studied by ^{13}C and ^{29}Si MAS-NMR spectroscopy.[512]

^{29}Si MAS-NMR spectra were reported for a new zeolite, ITQ-13. ^{19}F NMR data enabled the distribution of F and Ge atoms in the structure to be understood.[513] ^{13}C CP/MAS-NMR and ^{29}Si MAS-NMR spectra were used to characterise titanium-containing mesoporous silica SBA-15, formed in the presence of *n*-(trimethoxysilylpropyl)ethylenediamine triacetic acid.[514] ^{1}H, ^{19}F and ^{29}Si MAS-NMR spectra were reported for the fluoride-containing zeolite SSZ-44.[515]

^{29}Si CP/MAS-NMR data were reported for an 8-component system (CaO, SiO_2, Al_2O_3, Fe_2O_3, MgO, $CaSO_4$, $CaCO_3$, H_2O) – a model for Portland cement.[516] Ordered mesoporous titanosilicates were studied by ^{29}Si MAS-NMR spectroscopy,[517] as was mesoporous zirconium silicate.[518] ^{29}Si solid-state

NMR spectroscopy was used to follow structural changes on pyrolysis of organic/inorganic hybrids containing Si–O–Nb and Si–O–Ta units.[519]

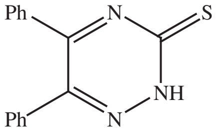
A phyllosilicate-rich clay was studied by ^{29}Si MAS-NMR spectroscopy.[520] ^{13}C CP/MAS-NMR and ^{29}Si MAS-NMR spectra were used to characterise silylated montmorillonites, and to estimate the extent of the silylation reaction.[521] *Ab initio* calculations have been made of ^{29}Si NMR chemical shifts for silicate complexes with carboxylates, amino acids and multicarboxylic acids.[522] Structural changes on thermal treatment of kaolinite were followed using ^{29}Si MAS-NMR spectra.[523]

Molecular orbital calculations of ^{29}Si shielding constants in the Li_2S–SiS_2 glass system were in good agreement with experimental data.[524] ^{29}Si and ^{19}F MAS-NMR data have been obtained for isolated $^{29}Si(^{19}F)_2$ and $^{29}Si(^{19}F)_3$ spin systems in $RR'SiF_2$ and $RSiF_3$ compounds, where R, R′ = organic ligands.[525] ^{29}Si MAS-NMR spectroscopy was used to characterise a NH_4Na-Y zeolite subjected to substitution of framework Al by Si, using crystalline $(NH_4)_2[SiF_6]$.[526] ^{19}F NMR data gave evidence for phase transitions in $[(CH_2OH)_3CNH_3]_2(SiF_6)$ in the temperature range 100–178 K.[527]

1.14.3 Germanium. ^{73}Ge (I = 9/2) NMR spectra of single germanium crystals were used to probe the electric-field gradient.[528] A new germanate zeolite framework, synthesised from isolated double-4-ring units, was characterised by ^{19}F MAS-NMR spectroscopy.[529] ^{31}P MAS-NMR spectra were obtained for $Ge_{2.5}PS_x$ glasses.[530]

1.14.4 Tin. Antiferromagnetic spin fluctuations in CeRhSn were studied using ^{119}Sn NMR.[531] ^{207}Pb chemical shifts were used to investigate powders of doped and undoped IV-VI semi-conductor crystals $Pb_{1-x}Sn_xTe$.[532]

Solid-state NMR data corroborate X-ray structural information for $[(Cp^*Sn)(Cp^*Sn)(O_3SCF_3)_2]$.[533] ^{119}Sn CP/MAS-NMR spectra for Ar_3SnCl, where Ar = phenyl, *o*-, *m*-, *p*-tolyl, 3,5-xylyl or mesityl, yielded values for indirect spin-spin coupling constants ($J(^{119}Sn-^{35}Cl)$), quadrupolar-dipolar shifts, and ^{119}Sn chemical shift tensors.[534] ^{31}P and ^{119}Sn MAS-NMR spectra were used to characterise $[Me_2Sn(OPPh_2)_2(O_3SCF_3)](O_3SCF_3)$.[535] The ^{119}Sn CP/MAS-NMR spectra for $SnPh_2(L)Cl$ and $SnMe_2(L)_2$, where HL = (5), confirm that tin is 5-coordinate in the phenyl derivative, and 6-coordinate for the methyl compound, with *S,N*-bidentate coordination by L^-.[536]



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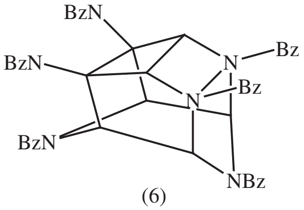
^{119}Sn solid-state NMR spectroscopy shows that the skew-trapezoidal bipyramidal organotin compounds of 2-quinaldate are always monomeric, because of the steric bulk of the carboxylate ligand.[537]

The structures of $xSnO.(100-x)P_2O_5$ glasses were investigated using ^{31}P and ^{119}Sn NMR spectra.[538] Aluminium-doped SnO_2 nanocrystals were characterised using ^{27}Al solid-state NMR.[539] The tin species formed by EtOH interaction with SnO_2 on a porous Vycor glass support was studied by ^{119}Sn NMR spectroscopy.[540] ^{29}Si and ^{119}Sn MAS-NMR spectra were obtained and analysed for $K_4M_2Si_6O_{18}$, where M = Sn or Ti.[541] ^{119}Sn CP/MAS-NMR data for tris(*N,N′*-diethyldithiocarbamato-*S,S′*)-3-methoxypropyltin(IV) show that the tin is seven-coordinate.[542]

1.14.5 Lead. ^{207}Pb NMR data were used to study the local structure of $PbMg_{1/3}Nb_{2/3}O_3$.[543] The local structure in the relaxor ferroelectrics $(1-x)[Pd(Mg_{1/3}Nb_{2/3})O_3].x[Pb(Sc_{1/2}Nb_{1/2})O_3]$ was investigated by ^{207}Pb MAS-NMR spectra and 2-D phase-adjusted spinning sidebands (PASS).[544] ^{17}O and ^{207}Pb NMR spectra were used to probe electron-density distribution in $BaPb_{1-x}Bi_xO_3$, where $0 \leq x \leq 0.33$.[545] Polycrystalline $[Pb\{S_2P(OR)_2\}_2]_n$, where R = ^{i}Pr, Cy, were characterised using ^{13}C and ^{31}P CP/MAS-NMR spectroscopy.[546]

Nanostructured PbF_2 samples were studied by ^{207}Pb MAS-NMR spectroscopy-to follow thermally-induced phase transformations.[547] ^{19}F solid-state NMR spectra were reported for glasses $60PbGeO_3.xPbF_2.yPbF_2$, where $x + y = 40$, $x = 10, 20, 30, 40$, in order to determine F . . . F distances.[548]

1.15 Group 15. – ^{15}N and ^{13}C MAS-NMR spectra gave structural information on ammonium dicyanamide, $NH_4[N(CN)_2]$.[549] Several cage-substituted hexaazawurtzitanes, *e.g.* (6) were studied by ^{15}N CP/MAS-NMR.[550]



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The local structure of the fast solid ion-conductor $Cu_2P_3I_2$, *i.e.* $(CuI)_8P_{12}$, was investigated by 1-D and 2-D ^{31}P and ^{65}Cu MAS-NMR spectroscopy.[551] ^{31}P NMR studies on $SmFe_4P_{12}$ show that the system remains in a paramagnetic state above the Curie temperature.[552] The silica-supported complex $\equiv Si\text{-}ORh(P^iPr_3)_2(H)_2$ was characterised by ^{31}P MAS-NMR.[553]

^{31}P CP/MAS-NMR data were used to characterise $UO_2(ReO_4)_2(TPPO)_3$, where TPPO = triphenylphosphine oxide.[554] The ^{31}P MAS-NMR spectra of $SbPO_4$ and $SbOPO_4$ gave evidence on the electron distributions.[555] The ^{31}P solid-state NMR spectrum of Na_3PO_3S shows a non-axially symmetric environment for the phosphorus atom at 20°C.[556] ^{31}P MAS-NMR spectroscopy was used to study the surface-anchored phosphates $[M\text{–}O]_x\text{-}PO(OH)_{3-x}$, where M = Si, Ti, x = 1 or 2, formed from Si- and TiMCM-41 mesoporous molecular sieves and $POCl_3$.[557]

^1H, ^{27}Al and ^{31}P MAS-NMR spectra have been reported for the iron aluminium phosphate $Fe_3Al_6(PO_4)_{12}.4tren.17H_2O$, where tren = tris(2-aminoethyl)amine. The ^{31}P spectrum could be interpreted in terms of three different phosphate environments.[558] ^{31}P MAS-NMR spectroscopy was able to detect a hydrogen-bonded phosphate polymer in calcium phosphate composites.[559] ^{31}P solid-state NMR spectra were used to study vitreous compositions in the system $(0.55-x)Na_2O.xSrO.0.45P_2O_5$, where $0 \leq x \leq 0.55$. A non-random distribution of cations was found, with Sr^{2+} preferentially near the chain ends.[560]

The structures of Na-Sr-phosphate glass and glass-ceramic samples were determined from ^{31}P NMR spectra.[561] NMR data have been reported for phosphate-based glasses in the system P_2O_5–CaO–Na_2O.[562] ^{31}P MAS-NMR spectra have been used to probe the structure of the phosphate network in $(40\text{-}y)Na_2O\text{-}yCdO\text{-}10PbO\text{-}50P_2O_5$, where $0 \leq y \leq 40$.[563] The new adduct $P_8O_{12}.2BH_3$ was characterised by ^{31}P MAS-NMR spectroscopy.[564]

^{31}P MAS-NMR spectra for $KPSe_6$ and $RbPSe_6$ crystals were consistent with the formation of infinite PSe_6^- chains.[565] A report has been made of measurements of longitudinal ^{31}P relaxation times for the selenophosphate compounds $M_2CdP_2Se_6$ (M = K, Rb) and $Ag_4P_2Se_6$.[566]

$^{13}C\{^1H\}$ CP/MAS-NMR spectroscopy was used to characterise the compounds $MeBi(S_2CNR_2)_2$, where R = Me, Et, $1/2C_4H_8N$.[567]

1.16 Group 16.

– MQ/MAS NMR measurements for ^{17}O of H_2O in Li_2SO_4–$H_2{}^{17}O$ were reported, using non-linear sampling techniques.[568]

Solid-state ^{31}P NMR spectra for $Rb_{0.33}P_{0.4}S_{2.23}O_x$ suggest the presence of $S_n{}^{2-}$ anions (n = 3, 4), and, possibly, $[P_4S_6O]^{6+}$ cation fragments.[569]

^{125}Te chemical shifts were reported from MAS-NMR data for Re_6Te_{15} and other Re_6-Te cluster species.[570]

1.17 Group 18.

– A ^3He NMR study has been made of line-broadening in solid ^3He-^4He mixtures below 50 mK.[571] ^2H NMR spectroscopy was used to study impurity-helium solids prepared by injecting deuterium atoms and molecules into superfluid ^4He.[572] Pulsed ^3He NMR data were reported for solid ^3He in a silver sinter down to temperatures of 400 pK.[573] He NMR was used to characterise ^3He nanoclusters embedded in h.c.p. ^4He.[574] Ferromagnetism of two-dimensional solid ^3He has been investigated by SQUID NMR.[575]

Solid-state ^{19}F and ^{129}Xe MAS-NMR data were reported for XeF_2, showing axially symmetric magnetic shielding tensors.[576]

2 Motion in Solids

A review has appeared on the use of MAS-NMR spectroscopy to study dynamic, electronic and magnetic properties of metal-ligand and metal-metal interacting systems.[577]

Cation dynamics in $Li_{1-x}Rb_xSO_3CF_3$, where x = 0.3, 0.45 or 0.8, were probed by ^7Li line-shape analysis, and ^7Li spin-lattice relaxation (T_1) measurements.[578] A ^7Li study has been made of lithium dynamics in the fast ion conductor $Li_{0.18}La_{0.61}TiO_3$.[579] $^{6,7}Li$ MAS-NMR spectra of Li_7TaO_5 yielded evidence for lithium exchange between tetrahedral and octahedral cavities even at ambient temperatures.[580] ^7Li NMR spectroscopy was used to investigate long- and short-range motions of lithium charge carriers in Li_6MoN_4–Li_7NbN_4 and Li_6WN_4–Li_7TaN_4.[581]

The ^7Li NMR spectrum of $Li_2(Mo_8ox)$. where Mo_8ox^{2-} = $Mo_8S_8O_8(OH)_8(C_2O_4)^{2-}$, confirms the mobility of Li^+ ions along the one-dimensional channels of this material.[582] The ^6Li NMR spectra of highly nuclear spin-polarised Li atoms on a Ru(001) surface gave details for the diffusion processes for these atoms.[583] Variable-temperature ^7Li NMR data on LiNiN were used to investigate Li^+ diffusion dynamics.[584] $^{6,7}Li$ NMR spectra gave evidence on dynamic behaviour in the spin-chain compound $LiCu_2O_2$.[585] Evidence for Li^+ mobility on the kHz timescale for the stannide Li_2AuSn_2 was obtained from ^7Li and ^{119}Sn NMR studies.[586] Variable-temperature solid state ^7Li NMR spectra were used to determine Li^+ mobility in polymer electrolytes based on P(VdF-HFP)/P(EO–EO) blends.[587]

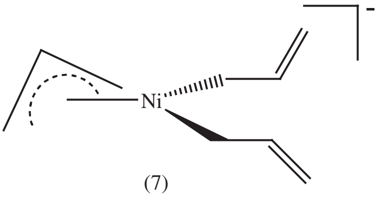
Molecular motion in $K_3H(SO_4)_2$ and $KHSO_4$ single crystals was followed by spin-lattice relaxation rates for ^1H and ^{39}K.[588] ^1H and ^{133}Cs solid state NMR spectra gave evidence for dynamic disorder in crystals of $GdZrCs_{1.5}(H_3O)_{0.5}(C_2O_4)_4.xH_2O$.[589] The ^2H NMR spectrum of $[Mg(H_2O)_6]$-$[SiF_6]$ was used to investigate the molecular dynamics and modulated structure.[590]

Spin-lattice relaxation times measured using ^1H NMR for $BaCe_{1-x}Y_xO_{3-\delta}$, where x = 0.01–0.10, were used to determine proton mobility in this system.[591] ^{139}La NMR data (T_1, linewidth) were reported for LaH_x ($2.0 \leq x\ 3.0$) in the temperature range 4 – 300 K could be related to the proton-hopping mechanism in the solid.[592] ^{11}B and ^{13}C pulsed NMR measurements on single crystals of $LuNi_2B_2C$ and $LuNi_2B_2{}^{13}C$ superconductors were used to analyse vortex dynamics.[593]

^2H NMR studies have been made of nuclear relaxation in TiD_x ($x = 1.91$) and HfD_x ($1.68 \leq x \leq 1.90$).[594] The diffusion of hydrogen isotopes in the monohydride phase of $Ti_{1-x}V_xH_xD_y$ was studied by ^1H and ^2H spin-lattice relaxation times.[595] There is NMR evidence for two frequency scales for the hydrogen-jump mechanism in Ti_2CoH_x, where x = 0.56, 0.77 or 1.34.[596] ^{17}O MAS-NMR (1-D and 2-D exchange spectroscopy, EXSY) data were used to study oxygen exchange in ZrW_2O_8.[597] Ion mobility was examined in tin fluorozirconate glasses in the SnF_2–ZrF_4–LiF and SnF_2–ZrF_4–HfF_4–SbF_3 systems by ^{19}F NMR measurements.[598]

Deuterium diffusion was studied in VD_x, where $0.4 \leq x \leq 0.6$, by means of ^2H NMR measurements.[599] ^1H and ^{51}V spin-lattice relaxation times for TaV_2H_x, where $x \leq 0.18$, were consistent with two co-existing proton-jump processes.[600] ^1H, ^2H and ^{51}V spin-lattice relaxation times were also determined for $NbVCrH_{0.3}$, $NbVCrD_{0.38}$ and $NbV_{1.4}Cr_{0.6}H_{0.6}$ in the temperature range 11–424 K.[601] A DFT/broken symmetry approach has been used to study exchange interactions in $VO(HPO_4).0.5H_2O$, and therefore to assign temperature-dependent ^{31}P chemical shift data.[602]

^1H MAS-NMR spectra were used to study the dynamics and local structure of water molecules in (±)-$[Co(en)_3]Cl_3.nD_2O$, where $0 \leq n \leq 4$.[603] ^1H spin-lattice relaxation times for Rh_2L_4, where HL = acetamide, were studied in the temperature range 4–300 K.[604] Variable-temperature ^{13}C CP/MAS-NMR spectra for (7) shows fluxionality in the solid state above −93°C.[605]



(7)

^{109}Ag solid-state NMR data were used to probe dynamics and local environment of silver cations in a series of silver-exchanged zeolites.[606] Solid-state ^2H NMR spectra gave evidence on the structure and dynamics in the clathrates $Gd(L)_2Ni(CN)_4.2C_4H_4NH$, where L = NH_3, 1/2en; C_4H_4NH = pyrrole.[607]

$^{23}Na\{^{11}B\}$ rotational echo double resonance data were used to analyse ionic motion in tetrahydroxoborate sodalite.[608] The effects of cation exchange on NaA zeolites were followed by ^{27}Al MAS and MQMAS NMR.[609] ^{71}Ga MAS-NMR data were used to investigate defect dynamics in GaN samples.[610] ^1H and ^{205}Tl relaxation times were reported for $Tl_3H(SO_4)_2$ at temperatures below 50 K, to give evidence for change in the mechanism of proton motion near 7 K.[611]

^{13}C NMR linewidths showed evidence for phase behaviour of the organic ferromagnet TDATE-C_{60} (4–290 K) in terms of motions of the C_{60}^- ions.[612] Solid-state ^{13}C and ^{23}Na NMR spectra were used to characterise Na_3C_{60} prepared by the direct reaction of Na with C_{60}. Variable-temperature ^{13}C MAS-NMR spectra revealed temperature-dependent motion of the C_{60}^{3-} anions.[613] C_{60}.2(ferrocene) gives CP/MAS-NMR spectra which show that both C_{60} and ferrocene are rotating at room temperature.[614] ^{13}C solid-state NMR spectra were used to follow the molecular dynamics in C_{60} doped with 0–10% C_{70}.[615] Variable-temperature ^{13}C NMR spectra of supramolecular complexes of C_{70} with a Rh(III) porphyrin cyclic dimer gave evidence of temperature-dependent C_{70} orientation change.[616]

^{13}C, ^{15}N and ^{29}Si solid-state NMR spectra were used to follow the dynamics of reaction of polychloromethylsilanes with NH_3 at various temperatures and pressures.[617] ^1H-^{29}Si CP experiments were used to study the dynamics of hydroxyl groups lying on the surface of nano-SiO_2 particles.[618] Variable-temperature ^2H NMR spectra gave information on conformational disorder and chain dynamics of *n*-alkyl chains attached to silica gels.[619]

^{13}C and ^{15}N CP/MAS-NMR spectra were used to follow the solid-state transformation of $NH_4[N(CN)_2]$ to $NCN{=}C(NH_2)_2$.[620] Polymeric $Pb[B(Im)_4]$ $(NO_3.xH_2O$, where Im = imidazole, was studied by ^{15}N and ^{207}Pb solid-state

NMR to monitor the stoichiometric exchange of $^{15}NO_3^-$ for NO_3^-, and of I^- for NO_3^-.[621]

^{19}F NMR has been used to study the internal mobility in $TlSb_4F_{13}$ and $TlSb_3F_{10}$ in the temperature range 210–450 K. There was evidence for phase transformations ($>$420 K, 385–425 K) in both cases.[622]

3 Atoms and Molecules Sorbed on to Solids

3.1 Water Sorbed on to Solids. – Solid-state ^1H NMR spectroscopy was used to determine the characteristics of H_2O adsorbed on TiO_2 photocatalytic systems.[623,624] The dynamics of water molecules in the deuteriated analogue of $H_3PW_{12}O_{40}.nH_2O$, where n = 5.5 or 0.1, were followed by solid-state ^2H NMR spectra.[625]

^1H, ^{13}C and ^{27}Al solid-state NMR spectra show that trapped water molecules in porous aluminium terephthalate interact with carboxylate groups *via* hydrogen-bonds.[626] Proton NMR studies have been reported for H_2O molecules confined within SWCNT (210–300 K).[627]

Pulsed-field gradient NMR spectra were used to measure restricted diffusion coefficients of water through porous silica.[628] Pulsed-field gradient-echo and nuclear Overhauser NMR spectra were used to study the interaction of water with soft segments in hard-soft segment block copolymers (polyethers).[629] Spin-lattice relaxation time measurements (^{19}F NMR) have been reported for $SF_6.17D_2O$ and $SeF_6.17D_2O$ clathrates, giving information on the dynamics of the guest molecules.[630]

3.2 Other Sorbed Atoms and Molecules. – ^2H NMR data were used to study the molecular dynamics of D_2 in SWCNT.[631] $^{1,2}H$ NMR spectra were used to follow H_2 adsorption on carbon nanotubes.[632] ^1H MAS spectroscopy was able to characterise molecular H_2 trapped inside an open-cage aza-thiafullerene, H_2@ATOCF.[633]

A lithium NMR study has been made of lithium atoms adsorbed on a Si(111)-(3 × 1)-Li surface.[634] ^{23}Na and ^{35}Cl NMR spectra were used to probe the distribution and state of Na^+ and Cl^- ions in tissues.[635]

^{13}C and ^{29}Si MAS-NMR spectra of MoO_2Cl_2(L-L), where L-L = $(MeO)_3Si(CH_2)_3N{=}C(Ph){-}C(Ph){=}N(CH_2)_3Si(OMe)_3$, adsorbed on mesoporous silica MCM-48 show that the complex remains intact on immobilisation.[636]

$^{29}Si\{^1H\}$ CP/MAS-NMR was used to probe interactions of transition metal carbonyl clusters ($Ru_3H(CO)_{11}^-$, $Os_2H(CO)_{11}^-$, $Co(CO)_4^-$) deposited in the mesoporous aluminosilicate material MCM-41.[637] A ^{29}Si MAS-NMR study has been made of rhodium-amine complexes on SiO_2 surfaces.[638] ^{31}P CP/MAS-NMR spectroscopy was able to characterise $Cu_6(TePh)_6(PPh_2Et)_5$ clusters in the pores of MCM-41.[639]

^1H PFG (pulsed field gradient) NMR data determined the diffusion coefficients of methane in 3 MFI-type siliceous zeolite silicalite samples.[640] The rotational motion of butane and pentane molecules adsorbed on zeolite ZK-5 was followed (130–320 K) by ^{13}C MAS-NMR.[641] *Ab initio* calculations have been made of NMR parameters for *n*-pentane trapped in zeolite silicalite-1.[642] ^{27}Al NMR spectroscopy was used to follow the fluorination reaction of $CHClF_2$ on alumina.[643] ^{2}H NMR data were used to determine pore-size distribution in mesoporous materials using confined C_6D_6 and C_6D_{12}.[644] ^{13}C and ^{27}Al MAS-NMR spectra characterised the interlayer alizarin S (ARS) and framework structure of Zn/Al and Mg/Al layered double hydroxides with interlayer ARS.[645]

^{1}H and ^{29}Si NMR spectra gave information on the interaction of adsorbed CO and pyridine on gallia-silica.[646] A detailed ^{13}C NMR study at low-temperature has been made of CO in a C_{60} matrix. There was evidence for both quantum and classical behaviour on the NMR timescale.[647] A ^{1}H and ^{2}H NMR study has been carried out on acetone molecules trapped in calix[4]hydroquinone supramolecular nanotubes.[648] A ^{13}C MAS-NMR study has been carried out to investigate the conformation of surfactant molecules in the interlayer of montmorillonite.[649]

^{13}C and ^{29}Si CP/MAS-NMR data were used to characterise the nature of gas-phase deposited γ-aminopropylalkoxysilanes on heat-treated SiO_2.[650] ^{29}Si solid-state NMR was used to characterise poly(methyloctylsiloxane) (PMOS) deposited on HPLC silica.[651,652]

^{15}N MAS-NMR spectra, with ^{23}Na-^{15}N and ^{27}Al-^{15}N TRAPDOR and ^{1}H-^{15}N CP/MAS-NMR experiments, gave details on NH_3 binding sites on 3A zeolite molecular sieves, and dynamics between two primary adsorbed NH_3 environments.[653] ^{2}H and ^{13}C solid-state MAS-NMR data were used to follow the dynamics of deuteriated *p*-nitroaniline molecules in zeolite ZSM-5 pores.[654,655] ^{1}H and ^{13}C CP/MAS-NMR spectra were able to probe host-guest interactions between $Me_3N^+(CH_2)_nN^+Me_3$ (where $n = 3 = 10$) and zeolites.[656]

The acidity of the internal surface of the zeolite MCM-22 was investigated by using ^{31}P MAS-NMR data for PPh_3 molecules adsorbed at the surface.[657] The ^{31}P NMR spectrum of PPh_3-capped gold nanoparticles, '$Au_{101}(PPh_3)_{21}Cl_5$', show rapid phosphine exchange.[658] ^{31}P high-power decoupled (HPDEC) MAS-NMR spectra showed the presence of $HPO_4{}^{2-}$ in highly-dispersed zirconium phosphate on cellulose acetate fibres.[659] Solid-state ^{31}P MR data for phosphonic acids intercalated in $[LiAl_2(OH)_6]Cl.H_2O$ show chemical shifts intermediate between those for mono- and di-anionic forms of the acids. There is therefore rapid proton exchange between intercalated anions.[660] ^{31}P NMR spectra showed that bulky triorganophosphines showed weaker coordination ability to palladium nanoparticles compared to that for PPh_3.[661]

Variable-temperature $^{29}Si\{^{1}H\}$ CP/MAS-NMR spectroscopy was used to study the effect of molecular oxygen on the location of sorbate molecules in highly-siliceous zeolite framework, *e.g.* ZSM-5 with adsorbed *p*-dibromobenzene.[662] ^{13}C MAS-NMR spectra were used to follow the conversion of methanol on weakly-dealuminated zeolite H-ZSM-5 – showing the formation of cyclic compounds and carbonium ions.[663] There is ^{13}C CP/MAS-NMR evidence for surface *n*-alkoxyl groups formed by the modification of the protonated perovskite $HCa_2Nb_3O_{10}$ by *n*-alcohols.[664] ^{13}C CP/MAS-NMR spectra were used to characterise 2-thiophenecarboxylate anions intercalated in layered double hydroxides.[665]

There has been a ^{3}He NMR study of liquid ^{3}He encapsulated in Grafoil.[666] Similar data were reported for superfluid phases of ^{3}He confined in 97.5% porous aerogel (at temperatures down to 0.3 mK);[667] and helium adsorbed in the pores of MCM-41 zeolite.[668]

The nature of xenon adsorbed on a metal single crystal surface (Ir(111)) was studied by ^{129}Xe NMR spectroscopy.[669] ^{2}H and ^{129}Xe NMR spectra were used to follow the sorption of CD_4 or Xe by a flexible microporous polymer, *catena*-bis(dibenzoylmethanato)(4,4′-bipy)nickel(II).[670]

Highly-polarised ^{129}Xe MAS-NMR spectra (including 2-D exchange experiments) were used to study surface interactions in AlPO-41 and ITQ-6 zeolites.[671] The pore structures of a range of microporous aluminophosphate (AlPO-5, -11, -31, -41) and silicoaluminophosphate (SAPO-5, -11, -31, -41) molecular sieves were investigated by ^{129}Xe NMR spectroscopy.[672] Similar experiments were also reported for xenon adsorbed on the ordered mesoporous aluminosilicate MAS-7;[673] on reduced platinum particles in mordenite channels;[674] on coke deposits on catalysts;[675] in a single crystal of silicalite;[676] on microporous materials such as HPLC column materials including XDB-C18;[677] on calcium montmorillonite and quartz sand;[678] confined on FSM-16 (pore diameters 1.9, 2.7 or 4.1 nm.);[679] and in cages of clathrate hydrates.[680,681]

^{129}Xe NMR spectra for a xenon layer frozen on EtOH or H_2O/EtOH were used to obtain time-resolve imaging of melting and dissociation processes.[682] ^{129}Xe NMR spectra gave information on the interaction of xenon with a dissymmetrical cryptophane ($(Xe)_2$@bis-cryptophane) complex.[683]

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Nuclear Quadrupole Resonance Spectroscopy

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1 Introduction

This chapter reports on pure nuclear quadrupole resonance (NQR) studies of quadrupolar ($I > 1/2$) nuclei in inorganic or organometallic solids. The number of references cited this year is very similar to the total last year, with no major conference specifically in this field having taken place; one change has been an increase in patent applications, particularly for NQR systems capable of detecting ^{14}N signals from explosives and/or drugs. While these applications are generally to organic systems, they have been listed because they are in principle applicable to inorganic nitrogen-containing systems as well. The theory and practice of modern 1D and 2D NQR and NQR imaging have been surveyed, including advantages of and problems with the method.[1] Hydrogen bonds in inorganic solids have been reviewed, including experimental techniques such as NQR used to study H-bonding.[2] A major review of magnetic ordering phenomena and dynamic fluctuations in cuprate superconductors and insulating nickelates, including NQR studies thereof, has appeared.[3] Similarities and differences between static and dynamic spin and charge properties of electron-doped and hole-doped high temperature (T) superconducting cuprates, including results from NQR data, have been surveyed.[4] Recent studies by means of NQR (^{63}Cu or ^{115}In) under pressure (P) on the heavy-fermion compounds $CeCu_2Si_2$, $CeRhIn_5$ and $CeIn_3$, including the effects of substitution of Ge for Si in the first compound, have been reviewed.[5] A similar review of NQR studies on unconventional superconductivity in these f-electron derived heavy-fermion systems has also been published.[6] A theoretical treatment of the complete range of quadrupole interactions, from NQR to NMR, for a spin 3/2 nucleus, as illustrated by ^{35}Cl NQR from $KClO_3$ in a weak magnetic field, has been presented.[7]

There have been patent applications for a wideband NQR system using multiple de-coupled radiofrequency (RF) coils,[8] for an apparatus and method of detecting NQR signals in the presence of incoherent noise,[9] and for a method and apparatus for improving the detection of NQR signals in coherent noise.[10]

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Patent applications have also been filed for an NQR apparatus and method,[11] for a method and apparatus for the detection and/or analysis of compounds simultaneously exhibiting NQR and NMR,[12] and for improvements in signal processing for the detection of NQR signals.[13] More specific applications have been for a SQUID NQR chemical sensor for noncontact cargo surveillance systems,[14] for land mine detectors with NQR-SQUID,[15] for a detector for the detection of explosives and drugs (which includes an NQR sensor),[16] for an NQR inspection system (used for explosives),[17] and for a method of substance identification performed in the RF range, using NMR, NQR, ESR or a combination of these methods.[18]

The usual format is followed in the more detailed sections, with results for main group elements preceding those for transition metals and lanthanides.

2 Main Group Elements

2.1. Group 1 (Lithium-8). – β-detected NQR has been observed for ^{8}Li implanted into a single crystal of $SrTiO_3$, using a beam of low-energy highly polarised radioactive $^{8}Li^{+}$ ions.[19] The resonances were detected by monitoring the β-decay anisotropy as a function of a small audio frequency magnetic field. A sharp resonance was observed, indicating that the implanted Li adopts well-defined crystal lattice sites. Results were also obtained for ^{8}Li implanted in α-Al_2O_3 and metallic Sr_2RuO_4. ^{8}Li was suggested as a sensitive probe of local magnetic and electronic environments in nanostructures and ultra-thin films, or in studying the diffusive motion of isolated Li in ionic conductors.

2.2. Group 13 (Boron-11 and -12, Gallium-69 and -71, and Indium-115). – A modification of a field-cycling method has been described which uses the ^{1}H NMR signal of a central transition at high field to detect zero-field quadrupole transitions indirectly.[20] The technique was used to obtain ^{11}B NQR signals of tetrahedral and trigonal planar boron species from a frozen solution of phenylboronic acid, and was sensitive enough to study boronic acid – protease inhibitors bound to proteins. A β-NMR and β-NQR spectrometer has been established in China, and used to measure the lifetime, magnetic moment and polarisation of ^{12}B nuclei.[21] The experimental results demonstrated the reliability of the system.

The microscopic magnetic properties of the itinerant 5f-electron antiferromagnet UGa_3 ($T_N = 67$ K) have been investigated in the paramagnetic state by means of the temperature (T)-dependence of its ^{69}Ga and ^{71}Ga NQR parameters, including the spin-lattice relaxation rate (SLR).[22] The SLR showed a striking increase above 230 K, including a strong component of nuclear quadrupole relaxation. Both the magnetic and quadrupolar relaxation rates were found to increase above 230 K. The NQR frequencies above this T also showed a clear deviation from the $T^{3/2}$-dependence found at lower T. The results were discussed in terms of a crossover from itinerant (lower T) to more localised spin fluctuations, and associated orbital fluctuations of the U

5f-electrons. A mechanism of transferred quadrupole interactions was proposed, through which fluctuations in the U 5f orbitals generate fluctuations among the Ga 4p orbitals, thereby causing quadrupolar relaxation of the Ga nuclear spins. The NQR signals were lost at *ca*. 300 K, because of a short T_1.

The *T*-dependence of the SLR for ^{115}In nuclei in $CeCoIn_5$ has been monitored at pressures up to 14 kbar.[23] In the normal state, the results indicated that $CeCoIn_5$ is located just at an antiferromagnetic (AF) instability at ambient pressure (*P*). The SLR decreased rapidly with increasing *P*, indicating that *P* moves the material away from the AF instability. In the superconducting state, the data demonstrated the appearance of an anisotropic superconductor with line nodes. Similar *T*-dependence studies of ^{115}In NQR, including the SLR, for $Ce_{1-x}Y_xRhIn_5$ and $Ce_{1-x}La_xRhIn_5$ have shown that the NQR frequency at the In(1) site varies linearly with the lattice parameter and dopant concentration for the Y- and La-substituted systems.[24] For $LaMIn_5$ (M = Co, Rh, or Ir) and $YRhIn_5$ the SLR was proportional to *T*, indicating that the system was in a Fermi liquid state over a wide *T*-range. In contrast, the SLR in $Ce_{0.1}La_{0.9}RhIn_5$ and $Ce_{0.5}Y_{0.5}RhIn_5$ had a power-law *T*-dependence, attributed to non-Fermi liquid behaviour near a quantum critical point, and expected from theory. For $Ce_{0.5}La_{0.5}RhIn_5$ and $Ce_{0.25}La_{0.75}RhIn_5$, the SLR was *T*-independent below 4.2 K and the signals broadened with decreasing *T*. This behaviour was associated with short-range magnetic order of Ce, expected from macroscopic measurements.

The *T*-dependence of ^{115}In NQR from $CeRhIn_5$ has been followed under an applied *P* of 1.75 GPa.[25] The onset of magnetic order was shown by a clear split in the spectrum due to a spontaneous internal field below $T_N = 2.5$ K. These and other results indicated that antiferromagnetism coexists homogeneously with superconductivity at a microscopic level. ^{115}In NQR SLR measurements under *P* up to 1.63 GPa have been carried out as a function of *T* for the heavy-fermion superconductor $CeCoIn_5$.[26] The value of the superconducting energy gap was found to increase slightly for $P < 0.45$ GPa, but it decreased significantly with further increase in *P*. In contrast, T_c increased monotonously up to 2.6 K as *P* increased up to 1 GPa, exhibiting saturation for *P* 1.0–1.5 GPa. No coherence peak was observed just below T_c, the results being consistent with the existence of line-nodes in the gap function. These measurements were subsequently extended up to 1.84 GPa.[27] The SLR was significantly suppressed by application of *P*, and was dominated by AF spin fluctuations specific to a quantum critical point. The suppression of spin fluctuations led to a reduction in the superconducting energy gap or in the coupling strength of the Cooper pair. T_c nevertheless increased with increasing *P*, due to an increase in the HF bandwidth.

New superconducting and magnetic phases on the verge of antiferromagnetism (AFM) have been discovered in $CeIn_3$ from ^{115}In NQR data under *P* up to 2.5 GPa.[28] A *P*-induced phase separation of AFM and paramagnetism (PM) was found, with no trace of a quantum phase transition. A new type of superconductivity (SC) under $P = 2.28$–2.5 GPa coexisted with AFM, mediated by a novel pairing interaction associated with the magnetic phase separation. This was magnetically separated from PM, where heavy fermion SC takes place. The highest value of T_c was observed for PM at $P = 2.43$ GPa, where the volume fractions of AFM and PM became almost identical. It was proposed that magnetic excitations, such as spin-density fluctuations, induced by first-order magnetic phase transitions, might mediate attractive interactions to form Cooper pairs in $CeIn_3$, which would be a new type of pairing mechanism. The T-dependence of the SLR for ^{115}In nuclei in $CeIrIn_5$ has been followed for various P up to 2.1 GPa.[29] Application of P suppressed dramatically the AF fluctuations that are strong at ambient P. T_c was increased by P (up to 0.8 K at $P = 2.1$ GPa). At this P the $T_1T =$ constant law was valid from 1–100 K. The results indicated that another superconducting phase existed in the absence of AF spin fluctuations, in addition to the superconducting phase that coexists below T_c with AFM. This behaviour was in sharp contrast with that in its Rh analogue. A systematic ^{115}In NQR investigation, including the T-dependence of the SLR, has been carried out for the heavy-fermion compounds $CeRh_{1-x}Ir_xIn_5$ (x = 0.25, 0.35, 0.45, 0.5, 0.55 or 0.75).[30] Substitution of Ir for Rh in the antiferromagnet $CeRhIn_5$ was found to act in the same way as applied P. The results provided strong evidence for the microscopic coexistence of AF order and SC in the range $0.35 \leq x \leq 0.55$. Detailed spectral analysis indicated that the same electrons participate in SC and AF order. The SLR showed a broad peak at T_N and followed a T^3 variation below T_c, indicating unconventional SC as in $CeIrIn_5$. T_c increased as the system penetrated deeper inside the AF ordered state. In the coexistence region the SLR showed a T-linear dependence below ~0.4 K. This could arise from magnetic excitations associated with the coexisting magnetism, in addition to the presence of crystal disorder that produces a residual density of states at the Fermi level.

2.3 Group 14 (Germanium-73). – ^{73}Ge NQR (and NMR) results as a function of T (0.01–100 K) and P up to 1.2 GPa have been described for UGe_2.[31] The T-dependence of the SLR demonstrated the onset of a SC transition at $T_c = 0.7$ K. The lack of a coherence peak just below T_c, followed by T^3-like behaviour, provided compelling evidence for the unconventional nature of the SC state that coexists with the ferromagnetic state on a microscopic scale. Further P-dependence studies on this compound revealed a first-order transition from a low-T and low-P ferromagnetic phase (FM2) to a high-T and high-P one (FM1), around a critical P_x of *ca.* 1.2 GPa.[32] The SLR exhibited a peak at the Curie T, as well as no coherence peak below T_c. The P-induced magnetic transition was first order around P_x, showing that there was no quantum critical point in this region.

2.4 Group 15 (Nitrogen-14, Arsenic-75, Antimony-121 and -123, and Bismuth-209). – The effects of "magic echo" multi-pulse sequences (MEMP) on ^{14}N NQR from polycrystalline $NaNO_2$ at 297 K have been investigated.[33] The time reversal effect was not observed, but the results added to the understanding of the dynamic properties of the quadrupolar spin system. Experimental data from applying MEMP and spin-locking sequences to the compound were presented. The behaviour of the ^{14}N NQR signal from $NaNO_2$ at 297 K has been studied in the ‘observation windows’ between RF pulses, after applying a multi-pulse sequence using a phase-cycling technique.[34] This system has a non-symmetric electric field gradient (efg) tensor. The experiments revealed some peculiarities in signal behaviour, which were important for understanding the dynamic properties of the spin system. Multi-pulse sequences consisting of one or more blocks of short-repetition phase alternated pulses have been applied to the ^{14}N spin system of polycrystalline $NaNO_2$ at room temperature (R*T*), permitting the detection of rotary echo signals in the effective field.[35] These echoes were then analysed.

A modification of the steady-state free precession (SSFP) multipulse technique, based on the use of the preparatory pulse in this sequence, has been devised.[36] It was applied to the detection of ^{14}N NQR signals from $NaNO_2$ at R*T*. Under certain conditions, the total intensity of the accumulated NQR signal could be increased, thus demonstrating its effectiveness. Various methods have been presented for cancelling magnetoacoustic and piezoelectric ringing signals in ^{14}N NQR, and have been applied to the ^{14}N resonance from a powdered $NaNO_2$ sample at R*T*.[37] These methods could be of practical value in detecting explosives or narcotics *via* ^{14}N NQR. The theoretical and practical aspects of using multi-pulse spin-locking and “strong off-resonant comb” (SORC) pulse sequences for detecting ^{14}N resonances have been examined.[38] Various optimum correlations between the parameters of the multi-pulse sequences and the relaxation characteristics of the substances under investigation were ascertained. The method was applied to the detection of ^{14}N signals from $NaNO_2$ and α-trinitrotoluene (TNT) at R*T*.

Quaternion algebra has been used to design composite pulses for spin-1 NQR nuclei, and applied to the ^{14}N resonance from powder samples of $NaNO_2$ at R*T*.[39] It was demonstrated theoretically and experimentally that consecutive noncommuting rotations applied at the same transition frequency are well described by a single rotation, given by quaternion parameterisation of the rotations in a fictitious spin-1/2 operator space. This new route was considered to have considerable advantages in computing time and effort. The approach was extended to design composite pulses that compensate for the effects of RF field inhomogeneity. The advantages of adiabatic half passage (AHP) for NQR detection of spin-1 nuclei in powder samples have been demonstrated theoretically and in practice for ^{14}N NQR signals from $NaNO_2$ and glycine at R*T*.[40] Under optimal conditions, AHP excitation provided 15% more signal than pulsed excitation. The results suggested that other excitation schemes based on adiabatic passage might be advantageous in NQR signal detection.

A correlation-based method for improvement of NQR signals utilising signal shape information has been developed, for the detection of weak signals hidden in noise.[41] It was applied to optimisation of the template for improved localisation of a noisy ^{14}N NQR line in $NaNO_2$ during repetitive scans by a superregenerative spectrometer at R*T*, and to ^{14}N signals from a mixture of hexamethylene tetramine with beet sugar. An NQR system has been developed for the detection of ammonium nitrate inside vehicles.[42] A novel high-Q resonant probe was designed, following studies of the penetration of RF fields inside metal enclosures, including vehicles. The probe was shaped not only for optimal penetration by RF fields, but also for optimal rejection of RF interferences and ease of shielding. It was demonstrated successfully using a full-scale model, and novel pulse sequences to generate and detect ^{14}N NQR signals from ammonium nitrate concealed in a car boot, or in the loading bay of a metal-sided van.

Tight binding calculations of the efg values at As sites in crystalline As and As chalcogenides have proved to be in good agreement with experimental results from ^{75}As NQR and high field broad-line NMR measurements.[43] Hence this approach could be used in future to quantify the local structural order in amorphous As and As chalcogenide glasses from NQR and NMR data. The *T*-dependence of ^{75}As NQR from CeRhAs has been monitored, including successive transitions occurring below T_K ($\sim$1500 K).[44] Some NMR results were also obtained. The efg tensor as well as the Knight shift at the As site was deduced in the respective phases. Three phase transitions were observed. A gap over the Fermi surface appeared in the ground phase, differing from the V-shaped one in isostructural CeRhSb and CeNiSn.

The *T*-dependence of the SLR for ^{123}Sb NQR from the filled-skutterudite compound $CeOs_4Sb_{12}$ showed a novel phase transition at $\sim$0.9 K.[45] In the range $1.3\ K < T < 25\ K$, the results suggested that the system was close to an AF critical point. Onset of spin-density-wave (SDW) order at $\sim$0.9 K was evidenced by broadening of the NQR spectrum, and a marked reduction in the SLR just below this *T*. The phase transition was deduced to be of the SDW type. The *T*-dependence of ^{121}Sb and ^{123}Sb NQR from the alkali metal-filled skutterudite $NaFe_4Sb_{12}$ has been monitored from 4.2–300 K.[46] Some ^{23}Na NMR data were also obtained. Two signals (two transitions) for ^{121}Sb and three (three transitions) for ^{123}Sb were observed at 300 K, enabling the asymmetry parameter η to be evaluated as 0.45. The results showed one Sb site in the compound. The NQR intensities decreased sharply below 90 K, attributed to the onset of a magnetic transition.

T-dependence studies of the ^{209}Bi NQR frequencies and SLR between 0.15 and 40 K for the heavy-fermion compound CeRhBi have shown no magnetic ordering.[47] The *T*-dependence plot of the SLR demonstrated a crossover from a localised regime at higher *T* to an itinerant ground state, with the Kondo temperature T_K of *ca.* 8 K. There was no trace of gap formation down to 0.2 K. The results revealed that the compound has a non-magnetic ground state, located close to a quantum critical point. Its behaviour differed from that of the Kondo semiconductors CeRhSb and CeRhAs. Previous work on detecting local magnetic fields in some bismuth compounds by means of ^{209}Bi NQR has been extended to $Bi_3B_5O_{12}$ and $Bi_2Ge_3O_9$.[48] The Zeeman–perturbed spectrum of an oriented single crystal of $Bi_3B_5O_{12}$ was examined, as well as the spin-echo envelopes for powdered samples of both compounds. Modelling of the spin-echo envelopes within the density matrix formalism supported the presence of a local ordered magnetic field of $\sim$65 G at the Bi atoms in $Bi_2Ge_3O_9$. Zero-field modulation of the ^{209}Bi spin-echo envelopes was also found in powdered $Bi_3B_5O_{12}$, indicating the presence of an internal source of line splitting. Considerable deviation in the resonance intensity ratios was found between the powder and single crystal samples, providing indirect evidence of a local ordered field in this compound also. The results were compared with earlier work on other Bi compounds.

2.5 Group 17 (Chlorine-35 and -37, Bromine-79 and -81, and Iodine-127). – Intramolecular barriers to CCl_3 group reorientation have been calculated for CCl_3PCl_4 (105.9 kJ mol^{-1}) and $(CCl_3)_2PCl_3$ (106.6 kJ mol^{-1}), by the Hartree–Fock method using the 6-31G(d) basis set.[49] The internal barriers were high enough to block reorientational motion of the CCl_3 groups, in agreement with ^{35}Cl NQR results for these compounds. Structural features in $RPCl_2$ (R = Me, CF_3, CCl_3, CH_2Cl, Et or Me_2CH) have been considered from ^{35}Cl NQR data at 77 K, and *ab initio* quantum-chemical calculations using RHF/6-31G* and MP2/6-31G* methods.[50] The degree of equivalence of the Cl atoms in the PCl_2 group was determined in each case. A correlation was found between the ^{35}Cl NQR frequencies for the PCl_2 group and the charges on the corresponding Cl atoms obtained by calculation. ^{35}Cl NQR frequencies at 77 K have been used to compare the coordinating abilities of the $Cl_3CSO_3^-$ (triclate) ion with those of chloroacetates $Cl_xCH_{3-x}CO_2^-$ (x = 1–3).[51] All frequencies were sensitive to the nature of the acceptor M ion or Lewis acid, particularly for monochloroacetates. In covalent derivatives, the average frequencies fell with the Pauling electronegativity of M. This trend was duplicated in *ab initio* Gaussian 98 computations at the B3LYP/6–311 ++ G (3df, 3pd) level for isolated XCH_2CO_2M (M = Li, Na or K; X = F or Cl), showing increased polarisation of the C–Cl bond and smaller electric field gradients for larger Group 1 ions. The dihydrate and monohydrate of Cl_3CSO_3H were also prepared. Although triclates normally have the highest ^{35}Cl frequencies in these salts, the NQR frequency for the acid dihydrate was lower than those of CCl_3COOH, suggesting that it is a strong acid, ionising in the solid to $H_5O_2^+$ and $Cl_3CSO_3^-$.

Various physical methods, including the *T*-dependence of the ^{35}Cl NQR frequencies, and the crystal structures at R*T*, have been used to investigate $[(PyO)D][AuCl_4]$ (1/1), $[(PyO)_4D_3][AuCl_4]_3$ (4/3) and $[(PyO)_3D_2][AuCl_4]_2$ (3/2), where PyO = pyridine-N-oxide.[52] The 4/3 salt gave five ^{35}Cl signals at 77 K, with one missing line since the crystal structure showed six non-equivalent chlorines. No phase transition was detected in the range studied (77–230 K). Four very broad ^{35}Cl resonances at 77 K were found for the 3/2 salt. Two ^{35}Cl lines, 1 at high and 1 at low frequency, were seen for the 1 : 1 salt at R*T*. The high frequency line split dramatically into 4 lines below 70 K, showing a phase transition (T_{c2}). A small thermal anomaly from DTA and DSC plots at 273 K was attributed to another phase transition (T_{c1}), but no anomaly was observed in the plot of ^{35}Cl frequency against *T* at this point. The *T*-dependence of the SLR showed an anomalous decrease with decreasing *T* for $T > T_{c2}$, suggesting dynamic disorder of the cations. These results were supported by ^1H NMR relaxation measurements. From the results, it was suggested that the cations may order below T_{c2}. Multi-photon resonances have been observed from ^{35}Cl nuclei in $KClO_3$ at 77 K, irradiated simultaneously by a multiple pulse RF sequence and a low frequency field swept in the range 0–80 kHz.[53] A theoretical description of the effect was presented, using both the rotating frame approximation and Floquet theory. The calculated magnetisation versus frequency of the low-frequency field agreed well with the experimental data. Multi-frequency spectra were considered to provide a means for studying slow atomic motion in solids.

Nuclear quadrupole moments for ^{35}Cl, ^{37}Cl, ^{79}Br, ^{81}Br and ^{127}I nuclei have been determined by comparison of experimental values for NQR frequencies in a range of inorganic halogeno-species with *ab initio* calculations of the electric field gradient at the halide site.[54] The values compared favourably with those recently obtained by independent quantum-chemical methods applied to atoms and small molecules. It was suggested that the generally accepted value for ^{127}I should be slightly corrected from the present results. The *T*-dependence of the signals from the bridging Br atoms in $[NiBr(chxn)_2]Br_2$ (chxn = 1R, 2R-diaminocyclohexane) has been monitored for a single crystal sample between 3.8 and 300 K.[55] A single ^{81}Br line was seen at 300 K and a pair of lines at 3.8 K (assigned from observation of the corresponding ^{79}Br signals), attributed to bridging Br atoms by comparison with the literature. The R*T* results were consistent with X-ray diffraction data. The signals disappeared on cooling around 130 K, and two resonances, separated by ~17 MHz, appeared below 40 K, the low *T* form having two non-equivalent bridging Br sites, thus suggesting a phase transition between 130 and 40 K. The results indicated that this was a spin-Peirls transition. The *T*-dependence of T_1 for ^{79}Br nuclei in Me_4NCdBr_3 has been monitored from 77–310 K, including the phase transition at 163 K.[56] In the paraelectric phase near the phase transition *T* relaxation was determined by critical fluctuations of the efg. In the ferroelectric phase, three different relaxation mechanisms were suggested, namely lattice vibrations, Me group reorientations and cation motions. From data analysis, the phase transition was concluded to be connected with the ordering of the cations, and the bromines were not directly involved.

^{127}I NQR frequencies at 77 K have been recorded for $Li_{1-x}H_xIO_3$ mixed crystals; some IR and Raman data were also reported.[57] For small HIO_3 concentration ($x < 0.06$), only one line was seen, invariant with x, and assigned to pure α-$LiIO_3$. Five lines were seen at higher x, one from pure α-$LiIO_3$ which decreased in intensity with increasing x, and four new lines which showed a corresponding increase in intensity. These resonances were observed up to $x = 0.22$, but no signals were detected for $0.22 \leq x \leq 0.35$. For $x > 0.35$, a single line was again apparent, attributed to pure α-HIO_3. From the results, it was suggested that the crystal retained hexagonal symmetry up to $x = 0.22$, but formed disordered solid solution crystals $Li_{1-x}H_xIO_3$ between $x = 0.22$ and 0.35. The incorporation of protons into the α-$LiIO_3$ lattice led to distortion of the IO_3^- pyramidal ions, due to H–bonding between different iodate anions.

3 Transition Metal and Lanthanides

3.1 Manganese-55. – The *T*-dependence of ^{55}Mn NQR from the Mn-II site in polycrystalline β-Mn, including the SLR and spin-spin relaxation rate, has been monitored up to 300 K.[58] Fine structure was newly observed below 100 K, indicating that a sufficiently large region of the sample had an AF moment with a small magnitude of $\sim 10^{-4}$ μ_B. Since the spectral shape depended on sample particle size, it was suggested that the surfaces of sample particles affected the electronic ground state, and that the staggered moment extended to within 3 μm depth from the surface. This staggered moment was proposed to be induced by release of the geometrical frustration of the Mn-II sites. The spin-lattice and spin-spin relaxation rates increased divergently above 200 K, implying quadrupolar relaxation arising from lattice vibrations becoming dominant at high *T*. In β-Mn metal, there are two crystallographically inequivalent sites in an 8:12 ratio, with 20 atoms per unit cell.[59] Preferential substitution of Os in β-$Mn_{1-x}Os_x$ alloys at site I has been confirmed by X-ray powder diffraction and other methods. NQR (and zero-field NMR) experiments have been performed on the alloys, to study the effects of substitution. The efg at site II was much larger than at site I. The intensity of the ^{55}Mn NQR signal for site II decreased with increasing x, without broadening of the signal. New signals were seen with increasing x, and these were the only ones observed for $x \geq 0.06$. The results suggested a local lattice expansion around the Os atom, and were consistent with the picture of an itinerant antiferromagnet.

Opposite trends in quadrupole coupling constants from the NQR of $[(\eta^5\text{-}Me_nC_5H_{5-n})M(CO)_3]$ (M = Mn or Re) and $[(\eta^5\text{-}Me_nC_5H_{5-n})Co(CO)_2]$ (n = 0–5) have been rationalised on the basis of a change of direction of the main efg axis.[60] In the Mn and Re compounds, the main axis was directed to the Cp ligand, thus showing an increase of π-back donation and electron population of the d_{xz} and d_{yz} metal orbitals with increase in Me substitution on the ring. In the Co complexes, with a planar $Co(CO)_2$ fragment, the main axis was orthogonal to this plane, featuring π electron transfer into the d_{xy} orbital. The result was an increase in e^2Qq for ^{55}Mn and ^{187}Re, and a decrease for ^{59}Co, with increase of Me substitution.

3.2 Cobalt-59.

– The SLR for ^{59}Co nuclei as a function of *T* has been followed for samples of $Na_xCoO_2.yH_2O$ with different x and y.[61] Two samples with different Na content (x = 0.348, $T_c = 4.7$ K and x = 0.339, $T_c = 4.6$ K) showed similar SLR values, except just above T_c. NQR spectra were also recorded for samples with different y, prepared from the x = 0.348 sample. A low-T_c sample with T_c 3.9 K had a larger residual density of states (DOS) in the SC state and a smaller increase of $1/T_1T$ just above T_c than a high-T_c sample with T_c 4.7 K. This behaviour was consistent with that observed in unconventional superconductors, and the results suggested a relationship between T_c and an increase in DOS just above T_c. This increase appeared to be associated with the two-dimensionality of the CoO_2 plane, and was considered to be one of the most important factors for the occurrence of superconductivity, *i.e.* the distance between the CoO_2 layers. Weak magnetic order has been found in a non-superconducting $Na_xCoO_2.yH_2O$ sample from the *T*-dependence of the SLR.[62] The SLR divided by *T* showed a prominent peak at 5.5 K, below which a ^{59}Co

NQR signal split, due to an internal field at the Co site. From spectral analysis at 1.5 K, this was evaluated as ~300 Oe, and in the *ab* plane. The ordered moment was deduced to be *ca.* 0.015 μ_B, From NQR measurements on various samples with different T_c, it was suggested that ν_Q could be a tuning parameter of the ground state in this system, and that the occurrence of superconductivity might be related to *c*-axis distortion of the tilted CoO_6 octahedron. Other results for ^{59}Co nuclei have been described in the sub-section on manganese-55.[60]

3.3 Copper-63 and -65. – The effect of *P* up to 1.68 GPa on ^{63}Cu NQR from $YbInCu_4$ has been studied.[63] The NQR frequency increased with *P*, caused mainly by shrinking of the cell volume. T_1 showed *T*-independent behaviour in the H*T* phase, and T_1T = constant behaviour in the L*T* phase, hardly affected by *P*, thus showing that the electronic states were little affected in either phase. The valence transition *T* was suppressed by *P*, and the high-*T* magnetic phase was stabilised. Various physical measurements, including the *T*-dependence of ^{63}Cu NQR, have been described for $BaCuO_{2.00}$ and $BaCuO_{2.14}$ samples.[64] For the latter, the intensity of the signal decreased with decreasing *T* and disappeared below 2.4 K. Anomalies observed in NMR and NQR data were concluded to be closely related to short-range ordering of the paramagnetic Cu_{18} cluster spins. ^{63}Cu relaxation as a function of *T*, together with NMR at various fields, has been monitored for $CeCu_{5.9}Au_{0.1}$, including the region around the quantum critical point.[65] The data in general confirmed previous neutron scattering results, but new aspects involving the effect of an external magnetic field were indicated. A ^{63}Cu NQR and Zeeman-perturbed NQR investigation, including *T*-dependence studies, of a $KCuF_3$ single crystal across T_N, has looked for evidence of a local rearrangement of the Cu unoccupied orbitals.[66] No change in NQR coupling was detected, but a gradual growth of the magnetic volume fraction for $T/T_N \geq 0.87$, previously detected by μSR, was confirmed.

A pulsed NQR technique involving the monitoring of ^{63}Cu signals from added Cu_2O powder (up to 20%) to polymers and composites for measuring internal stresses has been described.[67] It was applied to conventional (type A) and specially prepared (type B) fibreglass plastics. Internal stresses in type B composites were found to be lower, because of a lower glass transition *T*. The distribution of internal stresses in a sample was determined experimentally. The thermoelastic properties and spatial distribution of internal stresses were found to depend on the curing temperature. $^{63,65}Cu$ NQR methods have been used to investigate isomorphous CuS and CuSe.[68] An angle dependent NQR (AD-NQR) method has been devised to determine η in systems where the resonance line is so broad that the RF field can excite only a portion of the nuclear spins.[69] The method could be useful for single crystals and oriented powders. Its application was demonstrated experimentally for oriented $YBa_2Cu_3O_7$ powder, *via* ^{63}Cu NQR at R*T*. Calculations were not in exact agreement with the results, and possible causes for this were discussed.

^{63,65}Cu NQR (and ^{99,101}Ru NMR) investigations on the coexistence of magnetism and superconductivity on a microscopic scale for both superconducting and non-superconducting samples of magnetically-ordered $RuSr_2EuCu_2O_8$ and $RuSr_2GdCu_2O_8$ at 1.3 K have been described.[70] Cu NQR features were observed between 26 and 34 MHz, although with considerable line broadening. Two distinct peaks were resolved only for superconducting $RuSr_2GdCu_2O_8$, corresponding to ^{63}Cu and ^{65}Cu signals. The results were discussed in terms of the microscopic magnetic structure, mixed valence states for Ru, the occupancy of Ru sites, and the existence and role of impurity phases. The ^{63}Cu NQR frequency in $Pr_{2-x}Ce_xCuO_4$ ($x = 0.10$, 0.15 or 0.20) was found to be significantly lower than that observed in hole-doped high T superconducting cuprates.[71] This implied nearly complete cancellation of the Cu 3d, O 2p and nuclei contributions to the efg at the Cu nucleus. Some ^{63}Cu NMR data were also obtained. The SLR for Cu nuclei has been measured from 200–450 K in $CuYO_2$ and $CuYO_2$:Ca.[72] $CuYO_2$:Ca is a prototype transparent oxide exhibiting *p*-type semiconductivity. The relaxation rates in the Ca-doped material were enhanced by 1 or 2 orders of magnitude relative to those for the undoped compound, and exhibited a much stronger *T*-dependence. The relaxation contained approximately equal contributions from magnetic and quadrupolar mechanisms. In undoped $CuYO_2$, relaxation was purely quadrupolar, ascribed to interaction with lattice phonons. The magnetic contribution in the doped material was attributed to the hyperfine field of carriers. The dynamics of the hyperfine field were thought to be dominated by the hopping rate for carrier transfers between neighbouring atoms in the Cu planes. Comparison of the magnetic relaxation rates with DC conductivity enabled the carrier concentration and mobility to be estimated; the mobility was essentially independent of *T* above 200 K.

Cu NQR measurements, including the *T*-dependence of the frequencies and SLR, have been reported for optimally doped three layer high-T_c compounds $Hg_{0.8}Cu_{0.2}Ba_2Ca_2Cu_3O_{8+\delta}$ (Hg-1223) and $Hg_{0.8}Cu_{0.2}Ba_2Ca_2Cu_3O_{8+\delta}F$.[73] Above T_c, two Cu NQR line pairs were observed, corresponding to two inequivalent Cu sites. Below T_c, additional lines were found, leading to the well-known very broad spectrum at 4.2 K. From the SLR, complete removal of the Kramers degeneracy of the Cu quadrupole levels was deduced, indicating that the additional lines arise from Zeeman splitting of the Cu signals, due to the spontaneous formation of magnetic moments within the CuO layers. The spectra below T_c could be well fitted by six $^{63/65}$Cu line pairs. The magnetic moments were deduced to be parallel to the *c*-axis, with magnitude of the order of 1000 G (greater for the outer CuO layers, 400–1400 G, and approximately 200 G for the inner CuO_2 layer). The possible microscopic origin of the internal magnetic fields was discussed. Detailed ^{63}Cu NQR (and ^{17}O NMR) investigations have been reported for ^{63}Cu-enriched polycrystalline samples of $La_{2-x}Sr_xCuO_4$ ($0.04 \leq x \leq 0.16$), and high-quality single crystal samples for $x = 0.035$ and 0.15.[74] A patch-by-patch distribution of spatial variation with the patch radius as the only free parameter was used to fit the entire ^{63}Cu NQR spectrum. The implications of inhomogeneous electronic states to ^{63}Cu wipeout and stripe phenomena at lower *T* were discussed, and the generally believed view that hole doping is homogeneous across the CuO_2 plane was put into serious question.

The *T*-dependence of the SLR and NQR frequencies from 0–450 K has been monitored for $Y_{1-x}Ca_xBa_2Cu_4O_8$ (x = 0, 0.05 or 0.075) and $YBa_{2-y}La_yCu_4O_8$ (y = 0.05).[75] The carrier doping dependence of the pseudo-spin-gap was observed at the planar Cu(2) site but not at the chain Cu(1) site, showing that the hole carrier was exclusively doped into the CuO_2 planes. The magnetic phase diagram was drawn from the results. ^{63}Cu nuclear spin relation has been re-examined for $La_{2-x}Sr_xCuO_4$ with x = 0.13 (underdoped sample) and 0.18 (overdoped sample), using both NQR and NMR methods.[76,77] A remnant of the pseudo-spin-gap effect on the host Cu nuclear SLR was observed, and a finite contribution from inhomogeneous slow fluctuations around the optimally doped region, from analysis of the nonexponential curves. The magnetic phase diagram was constructed. These studies were subsequently extended to ^{139}La relaxation.[77] The slow spin fluctuations originated from a remnant of the spin freezing effect or the wipeout effect, more remarkable in less doped samples. The lower optimal T_c for this compound than for $HgBa_2CuO_4$ could possibly be attributed to the depairing effect caused by slow spin fluctuations. (A typographical error in the online version of this paper was later reported, but the printed version was correct.[78])

3.4 Lanthanum-139. – The SLR as a function of *T* has been recorded for ^{139}La nuclei up to 100 K for $LaRu_3Si_2$.[79,80] This compound shows superconductivity below $T_c \sim 6.5$ K. In the normal state, the SLR was proportional to *T*. The superconductivity was of the conventional BCS type, because the SLR showed a coherence peak just below T_c and an Arrhenius-type *T* dependence well below T_c. The relatively high T_c was attributed to a high density of states of conduction electrons at the Fermi surface, and strong electron-phonon interactions.[80] The *T*-dependence of ^{139}La NQR parameters including the SLR in the range 0–300 K has been monitored for $La_{2-x}Sr_xCuO_4$ (x = 0.01, 0.018 or 0.024).[81] At x = 0.018, the AF La NQR spectrum affected by internal fields emerged as *T* decreased below $T_N \sim 150$ K, whereas the nonmagnetic spectrum persisted down to $T_f \sim 20$ K, where the SLR had a pronounced peak. The results demonstrated that the phase separation of the nonmagnetic and AF phases occurred between T_N and T_f. This novel phase separation was suggested to arise from partial destruction of the AF phase caused by mobile holes, *via* formation of an extended spin-singlet state between Cu-derived spins and hole spins. Well below T_N, the characteristic energy scale for spin excitation was comparable with the gap of charge transport of mobile holes. Below T_f, localisation of holes made the spins freeze. Other results for ^{139}La nuclei have been described in the sub-section on Copper-63 and -65.[77,78]

3.5 Rhenium-187. – Results for this nucleus have been presented in the sub-section on Manganese-55.[60]

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Characteristic Vibrations of Compounds of Main Group Elements

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1 Group 1

A theoretical calculation has been made for the vibrational wavenumbers of H_2 trapped in 4H–SiC and 2H–GaN.[1] There is IR evidence for the formation of perturbed p-H_2 and o-H_2 molecules by laser ablation of normal H_2 during condensation at 3.8 K.[2] Raman data have been reported for small *para*-H_2 clusters formed in cryogenic free jets, $(p\text{-}H_2)_n$, where $n = 2$–8.[3] IR spectroscopic evidence has been obtained for the formation of $(H^-)(H_2)_{12}$ clusters in solid hydrogen – with a characteristic band at 3972 cm^{-1} (2869.8 cm^{-1} for the deuterio-analogue).[4]

Ab initio calculations gave values for the vibrational wavenumbers for Li_n clusters, where $n = 2$–10.[5] The IR spectrum of molten LiCl–KCl–LiH at 673 K showed a band in the range 1300–1600 cm^{-1} due to νLi^+-H^-.[6,7] The IR and Raman spectra of $LiMoVO_6$ gave bands at 263 (Raman)/252 (IR) cm^{-1}, and 290 cm^{-1} (IR), assigned to motions of the LiO_6 octahedron.[8]

Molecular dynamics calculations have been made on the motions of the Na^+ ion in mordenite zeolites.[9] Selenium clusters doped with Na (*i.e.* Na_2Se_n) show a Raman band in the range 165–225 cm^{-1} due to Na-Se motions.[10] Raman microspectra have been reported for caesium oxides, *e.g.* an a_{1g} mode of Cs_2O was seen at 103 cm^{-1}.[11]

2 Group 2

High-resolution IR emission spectra have been obtained for BeH/BeD and BeH_2/BeD_2, giving rotational analyses for several bands.[12] Laser-ablated Be atoms and MeOH react to give several matrix-trapped products, Table 1 summarises some vibrational assignments for MeOBeH, MeBeOH and MeBeOBeH.[13]

Raman bands at 215 and 535 cm^{-1} can be used to differentiate between Be-doped and pristine cubic BN.[14] The Raman spectra of Be-implanted GaN samples include bands at 168, 199, 320 and 346 cm^{-1} due to Be-related local symmetry modes.[15]

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Table 1 *Vibrational assignments for Be + MeOH reaction products (/cm^{-1})*

CH_3OBeH	νBe–H	2108.5
	δCH_3	1485.6
	νBe–O	1399.8
	δBe–H	542.5
CH_3BeOH	νO–H	3832.0
	νBe–O	1376.1
	δCH_3	685.4/683.4
$CH_3BeOBeH$	νBe–H	2089.0
	νBe–O–Be	1444.8
	δBe–H	558.5
(all data from ^{16}O form)		

The IR spectrum of $[BeCl(\mu_3\text{-}NPEt_3)]_4$ shows νBe_4N_4 at 677 cm^{-1}, and νBeCl at 598 cm^{-1}.[16] For $Be_3Cl_2(NPPh_3)_4$, νBeN_4 is at 888 cm^{-1}, and $\nu BeCl_2$ at 489 cm^{-1}.[17] IR spectra for $[Be_4X_4(\mu\text{-}N_3)_6]^{2-}$, where X = Cl or Br, have νBeN at 800 cm^{-1} (X = Cl), 790 cm^{-1} (Br), νBeX at 594, 579 cm^{-1} (Cl), 560 cm^{-1} (Br).[18] Raman spectra of BeTe thin films show features at 165 cm^{-1} for Te-rich, and 157 and 188 cm^{-1} for Be-rich samples.[19] The IR and Raman spectra of $BeCl_4{}^{2-}$ gave the following assignments: ν_1 (a_1) 293 cm^{-1} (Raman); ν_2 (e) 146 cm^{-1} (Raman); $\nu_3(t_2)$ 500 cm^{-1} (IR); ν_4 (t_2) 251 cm^{-1} (IR), 250 cm^{-1} (Raman). For $Be_2Cl_6{}^{2-}$, $\nu BeCl_2$ (terminal) modes were seen at 640 cm^{-1} (b_{3u}), 495 cm^{-1} (b_{1u}), with Be_2Cl_2 (bridging) modes at 336 and 286 cm^{-1}.[20]

FTIR emission spectra of MgH and MgD gave ω_e for ^{24}MgH, ^{24}MgD at 1492.776(7) cm^{-1}, 1077.298(5) cm^{-1} respectively.[21] A high-resolution IR study of gaseous $^{24}MgH_2$ showed that the band centre of ν_3 (σ_u, ν_{as}) was at 1588.67157(24) cm^{-1}, with an estimated value of 437 cm^{-1} for ν_2 (π_u).[22] Laser-ablated Mg atoms reacted with MeOH to give a range of matrix-trapped products, *e.g.* CH_3MgOH (νMg-OH 784.4 cm^{-1} (^{24}Mg), 777.2 cm^{-1} (^{25}Mg), 770.1 cm^{-1} (^{26}Mg)) and $CH_3MgOMgH$ (νMg–H 1541.4 cm^{-1}, ν_{as}Mg–O–Mg 940.4 cm^{-1} – both for the all-^{24}Mg form).[23]

Ab initio calculations gave values for vibrational wavenumbers for MgNC and MgCN.[24] IR bands with contributions from νMgN were seen at 440, 389 and 369 cm^{-1} for chlorophyll *d* from *Acerychlorus marina*.[25] DFT calculations of the vibrational wavenumbers for Mg(Pc) gave assignments to experimental νMgN bands.[26]

The IR spectrum of aqueous $MgSO_4$ showed $\nu Mg\text{–}OSO_3$ of ligated sulfate at 245 cm^{-1}, and of the $(H_2O)_5Mg(OSO_3)$ unit at 328 cm^{-1}.[27] Far-IR data for $Mg(H_2O)_6{}^{2+}$ and $M(H_2O)_6{}^{3+}$ (M = Al, Ga, In, Tl), together with earlier Raman values, gave full assignments to MO_6 fundamentals for the first time.[28] The far-IR spectra of $BaMg_{1/3}Nb_{2/3}O_3$ ceramics included characteristic O–Mg–O bending modes, and stretching modes of MgO_6 octahedra.[29]

IR emission spectra for CaH and SrH gave the following ω_e values: 1298.400(1) cm^{-1} (Ca) and 1207.035(1) cm^{-1} (Sr).[30] The Raman spectrum of $Er{:}Yb{:}YCa_4O(BO_3)_3$ showed bands due to CaO_6 octahedra and BO_3

triangles.[31] The Raman spectra of $xSrO.yAl_2O_3.(100–x–y)SiO_2$, where $33 \le x \le 40$; $0 \le y \le 2$, included a band at 330 cm^{-1} due to νSr–O.[32]

Variable-temperature Raman spectra of $[Me_4N][BaCl_4]$ gave evidence for two phase transitions, at 369.7 K and 411.3 K.[33] Similar experiments on copper-doped $[EtNH_3]_2[BaCl_4]$ showed that first-order phase transitions occurred at 362.7, 395.9 and 406.1 K.[34] The IR spectrum of $BaCl_5{}^{3-}$, as the $MeNH_3{}^+$ salt, has been reported and assigned.[35]

3 Group 13

3.1 Boron. – Raman spectroscopy was used to characterise ultrafine CaB_6 powder, prepared from $CaCl_2$ and $NaBH_4$ at 500°C.[36] *Ab initio* and DFT calculations of vibrational wavenumbers were reported for $M^+B_7{}^-$, where M = Li, Na, K, Rb, Cs.[37]

DFT calculations gave vibrational wavenumbers for $(HCNBH)_n$ and $(BH_2CN)_n$, where $n = 1 – 6$.[38] The high-pressure Raman spectrum of $BH_3.NH_3$ showed a phase transition near 8 kbar.[39] *Ab initio* calculations gave vibrational wavenumbers to assign experimental data for $BH_3.PF_3$.[40] The IR spectrum of $Me_2NH–PH_2–PPh_2–BH_3$ showed νNH at 3178 cm^{-1}, ν_{as}BH at 2337 cm^{-1} and ν_sBH at 2260 cm^{-1} – consistent with intermolecular H . . . H interactions.[41] Variable temperature (300–540 K) Raman spectra for MBH_4 (M = Li, Na, K, Rb, Cs) gave data on barriers to internal rotation of $BH_4{}^-$ ions.[42] The Raman spectra for MBH_4 (M = Li, Na, K) showed the general wavenumber order Li > Na > K for ν_1 (B–H stretch) and for the bending mode, except for ν_1 of $LiBH_4$.[43] The IR spectrum of the low-melting ionic species [*N*–pentylpyridinium]$^+[CB_{11}H_1]^-$ has νBH at 2571 cm^{-1}.[44]

Raman spectroscopy was used to characterise BCN nanotubes.[45] IR and Raman spectra of LiBC powder pellets gave the following assignments: (e_{1u}) 1252, 381 cm^{-1}; (e_{2g}) 1172, 174 cm^{-1}; (a_{2u}) 825, 545 cm^{-1}.[46] DFT calculations gave vibrational wavenumbers for LiBC, which were used to assign Raman spectra.[47,48]

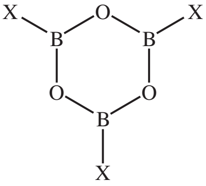
Boron atoms react with CO/N_2 mixtures to give a matrix-trapped product with IR bands at 1892.2 and 1884.7 cm^{-1}. Isotopic substitution suggests that these arise from a linear species, NNBCO.[49] *Ab initio* calculations gave vibrational wavenumbers for a hetero-diamond species, B_2CN,[50] Matrix-IR spectra of BBCO, together with DFT calculations, are consistent with a linear triplet ground state.[51] *Ab initio* calculations on BC_2P isomers gave values for vibrational wavenumbers, and indicated linear PBCC as the global minimum.[52] The FT Raman spectra of ^{10}B, ^{11}B and ^{13}C isotope-enriched samples of $B_{4.3}C$, $B_{6.5}C$ and $B_{10}C$ were assigned in terms of B_{12}, B_{11}, CBC, CBB and CCC units.[53] The IR and Raman spectra of sputtered boron carbide films gave evidence for the formation of intericosahedral chains at higher annealing temperatures.[54] The IR and Raman spectra of $[2\text{-}CB_{10}H_{11}]^-$ include low-wavenumber features due to deformations of the boron atom skeleton, *e.g.* a band at 227 cm^{-1} due to displacement of B(4,5,6,7) atoms.[55]

Raman spectra of cubic BN to 21 GPa, in the temperature range 300–723 K, were used to derive values for the isothermal bulk modulus at ambient and high temperature.[56] IR data (*v*BN of *c*–BN) were used to follow the formation of BN films by mass-selected B and N ion deposition.[57] Raman data were used to characterise BN single-walled nanotubes (SWNT), formed by substitution from SWCNT by B_2O_3/N_2 treatment.[58] Assignments for such species were made using the results of DFT and *ab initio* calculations.[59–61]

The IR spectra of BN MWNT included bands characteristic of *h*–BN, *i.e.* tangential (near 800 cm^{-1}) and longitudinal (near 1400 cm^{-1}) modes.[62] Raman spectra for BN and $B_xC_yN_z$ MWNT show that the latter are radially phase-separated into BN and C shells.[63] FTIR and Raman spectra of BN nanolayers coated on Fe (formed by heating Fe_2O_3/B under N_2) are predominantly of hexagonal structure.[64] The IR spectra of BN whiskers showed the presence of both σ-sp^2 and σ-sp^3 units.[65] Raman microspectroscopy was used to study BN and BN/C coatings on SiC.[66] High-pressure Raman spectra were obtained for *c*-BN up to 200°C and 32 GPa.[67]

The IR spectrum of $Ba_3[BN_2]_2$ shows low site symmetry for the BN_2^{3-} groups.[68] Vibrational data for $Eu_3[BN_2]_2$, however, were interpreted in terms of discrete BN_2^{3-} units of $D_{\infty h}$ symmetry.[69] IR data were reported for a 1,3,2-oxazaborolidine dimer derived from (*S*)-α,α-diphenylprolinol.[70] The IR and Raman spectra of the new adduct $P_8O_{12}.2BH_3$ included νPB at 565 cm^{-1} (IR), 574 cm^{-1} (Raman), as well as characteristic *v*BH bands.[71] High-pressure Raman spectroscopy was used to follow pressure-induced phase transitions for $B_{12}As_2$.[72]

Diode-laser spectroscopy of the radical BO ($X^2\Sigma^+$ state) gave vibrational band origins at 1915.30674(14) cm^{-1} (^{10}B), 1861.92409(13) cm^{-1} (^{11}B).[73] IR spectra were reported and assigned for $BF_3.EMe_2$ (E = O, S) in N_2 and Ar matrices at 17 K.[74] DFT calculations gave vibrational wavenumbers for (1), where X = F [75] or Cl.[76]

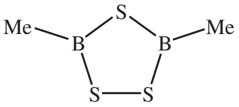


(1)

High-pressure Raman spectroscopy on B_2O_3 glass (to 57 GPa) gave evidence for phase transitions near 3 and 11 GPa.[77] Raman spectra were used to characterise β–B_2O_4, obtained by a polymeric precursor method.[78] IR data were reported and assigned for $Li_4CaB_2O_6$ – consistent with crystallographic data.[79] IR and Raman spectra of aqueous Cs_2CO_3/H_3BO_3 solutions revealed the presence of H_3BO_3, $B(OH)_4^-$, and a range of oligomeric species, such as $B_4O_5(OH)_4^{2-}$.[80,81] Modes of this anion were also assigned from IR and Raman spectra of $M_2Ca[B_4O_5(OH)_4]_2$, where M = Rb, Cs.[82,83] IR and Raman spectra of glasses in the system $SrSO_4$–KPO_3–$Na_2B_4O_7$ gave evidence for the structures of the borate and sulfate/phosphate lattices.[84] Vibrational spectra were calculated for the $Li_{10}B_8O_{17}H_6$ cluster, to help analyse the spectrum of crystalline $Li_2B_4O_7$.[85] There have been a number of other IR and Raman spectroscopic studies of the structures of borate glass systems.[86–93]

IR and Raman spectra gave assignments to modes of isolated BS_3^{3-} units in $Ba_7(BS_3)_4S$.[94] *Ab initio* calculations were reported for the vibrational modes of (2).[95] The IR and Raman spectra of ternary $xLi_2S + (1 - x)[0.5B_2S_3 + 0.5GeS_2]$ glasses showed characteristic structural features.[96]

Ab initio calculations have been made of vibrational wavenumbers for BF_3OH^- which were used to assign the IR and Raman spectra of $K[BF_3OH]$.[97] The IR spectra of matrix-isolated $BF_3.SO_2$ were compared to the results of *ab initio* calculations to differentiate between *trans*-*cis* and *cis*-*trans* forms.[98] Mode assignments, including νBCl near 500 cm^{-1}, were made from FTIR, RAIRS and SERS data for 2,3-borophthalocyanine chloride.[99] The phase behaviour of BBr_3 was followed (to 10 GPa) by Raman spectroscopy – no evidence was found of discontinuities.[100]



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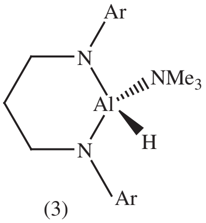


(3)

3.2 Aluminium. – Table 2 summarises vibrational assignments for $HAl(Cl)CH_3$, all of which were confirmed by D and ^{13}C substitution.[101] (3), where Ar = 2,6-$^iPr_2C_6H_3$, has νAlH at 1799 cm^{-1} in the IR spectrum.[102] Matrix-IR spectra were reported and assigned for $ClAlH_2$ – Table 3 (data refer to $^{35}ClAlH_2$).[103] DFT calculations have been reported for the vibrational wavenumbers of $(H_2AlN_3)_n$, where n = 1–4.[104,105] The species $(L)AlH_2$, where HL = 1-(NHAr)-2-(PPh_2=NAr′)C_6H_4 (Ar = 2,6-$^iPr_2C_6H_3$, Ar′ = 2,4,5-$Me_3C_6H_2$), has $\nu_{as}AlH_2$ at 1828 cm^{-1}, ν_sAlH_2 at 1780 cm^{-1}.[106]

Detailed Raman spectroscopic data were assigned for $NaAlH_4$ using *ab initio* calculations. The bands at 847, 812 and 765 cm^{-1} all involve Al-H motions.[107] A characteristic νAlH IR band was seen for solvent-free $Mg(AlH_4)_2$ (1835 cm^{-1}) – this was at higher wavenumber than for thf or Et_2O solvates.[108] Characteristic IR bands for matrix-trapped di-, tri- and tetra-alanes, $(AlH_3)_n$, n = 2, 3 or 4, produced by the reaction of laser-ablated Al atoms with H_2, have

Table 2 *Selected vibrational assignments for $HAl(Cl)CH_3$ (/cm^{-1})*

1905.2	νAl–H
604.4	νAlC
488.1/482.8	νAl–Cl
672.8	γ
421.4	ρAl–H
657.7	δCl–Al–H

Table 3 *Vibrational assignments for monomeric* $^{35}ClAlH_2$ *(/cm^{-1})*

$\nu_1(a_1)$	1915.9	ν_sAl–H
$\nu_2(a_1)$	769.9	δAlH_2
$\nu_3(a_1)$	549.9	νAlCl
$\nu_4(b_1)$	1928.1	ν_{as}Al–H
$\nu_5(b_1)$	518.6	ρCl
$\nu_6(b_2)$	604.9	γ

Table 4 *Vibrational assignments for the dibridged radical* Al_2H_5 *(/cm^{-1})*

Terminal AlH_2	1918
Terminal AlH	1845
Al–H–Al bridge	1363
Al–H–Al bridge (a″)	1307
Al–H–Al bridge (a′)	1228
AlH_2 bending	753

been reported, and assigned with the help of *ab initio* calculations. It was also possible to detect the Al_2H_5 radical – whose vibrational assignments are summarised in Table 4.[109] Vibrational wavenumbers for the cage compounds $H_6M_4(N_2H_2)_3$, where M = Al or Ga, were calculated by *ab initio* methods.[110]

IR spectroscopy shows significant differences between α- and δ-crystalline phases of $Al(Q)_3$, where Q = quinolin-8-olate, *e.g.* νAlN bands are at 423 and 397 cm^{-1} for the δ-form, 433, 415, 396 cm^{-1} for the α-form.[111] FTIR and Raman spectra (with DFT calculations) gave skeletal mode assignments for $[Al(Ser)(H_2O)_4]^{2+}$, where Ser = serine.[112] Raman spectroscopy was used to obtain a quantitative assessment of Al–N bonding in $Al_{0.33}Ga_{0.67}As_{1-y}N_y$ species.[113] DFT calculations gave vibrational wavenumbers for the clusters $Al_2As_2^n$, where n = −1, 0 or +1.[114]

Hartree–Fock–level calculations were made of the vibrational wavenumbers of $Al(H_2O)_6^{3+}$.[115] High-pressure Raman spectroscopy was used to follow the course of the C2/c to P2$_1$/c phase transition at 3.2 GPa for $LiAlSi_2O_6$ (spodumene).[116] IR and Raman spectra were used to follow the effects of water dissociation on the structure of boron-bearing aluminosilicate glasses based on albite, $NaAlSi_3O_8$.[117]

The νAl–O–Al IR band was used to study the effects of the caustic ratio on the structure of sodium aluminate solutions.[118] Variable-temperature Raman spectra of the spinel $MgAl_2O_4$ showed a band at 727 cm^{-1} for samples annealed above 800°C. This was ascribed to cation disorder in these samples.[119] The angular force constant method was used to analyse vibrational modes for MAl_2O_4, where M = Mg or Zn.[120] *Ab initio* calculations have been made of vibrational wavenumbers involving the OH group in topaz, $Al_2SiO_4(OH)_2$.[121]

Raman spectroscopy was used to investigate molten ceramic oxide materials formed in the CaO–Al_2O_3 system.[122] Raman spectroscopy showed characteristic AlO_4 and SiO_4 unit modes for $[Ca_{12}Al_{14}O_{32}][O_{1.5}]$ and related systems.[123] Information about the structural characteristics of molten Al_2O_3–Na_2O–SiO_2 samples was obtained by Raman spectroscopy.[124,125] An FTIR study (using ν_{as}T–O–Si, T = Al, Si) has been made of aluminosilicate particles produced by alkaline leaching processes.[126] The IR spectra of Mg^{2+}- or Ca^{2+}-doped $Y_3Al_5O_{12}$ showed features due to an O–ion vacancy-divalent ion complex.[127] FT Raman spectroscopy was used to study the porosity of the framework in the silicoalumino–phosphate-based molecular sieve SAPO-44 (using δT–O–T, where T = Al or Si).[128]

The Raman spectra of M_3AlF_6, where M = Na, K or Cs, and mixtures of AlF_3 in FLiNaK (46.5 mol% LiF, 11.5 mol% NaF, 42 mol% KF) and in CsF–KF eutectic confirmed the dissociation of AlF_6^{3-} to AlF_5^{2-} and AlF_4^{-}.[129] The IR spectra of crystalline and glassy specimens from the system AlF_3–BaF_2–MgF_2 all showed bands due to both AlF_4^- and AlF_6^{3-}.[130]

3.3 Gallium. – A theoretical treatment has been reported for a number of diatomic species, including GaH.[131] There is evidence for the presence of H in Mg–doped GaN, *i.e.* a Raman band at about 2200 cm^{-1}.[132] A band due to νGaH (1873 cm^{-1}) was seen in the IR spectrum of $HGaCl_2(3,5\text{-}Me_2py)_2$. Such a feature was at 1822 cm^{-1} for $H_3Ga(3,5\text{-}Me_2py)$.[133] Laser-ablated Ga atoms reacted with H_2 to give a range of matrix-trapped products. IR data showed that GaH was the main product, together with GaH_2, GaH_3, Ga_2H_2, GaH_2^- and GaH_4^-. Photolysis produced Ga_2H_n, where n = 4, 5 and 6. Assignments for Ga_2H_6 are given in Table 5.[134] Matrix-IR data were used to identify thermal fragmentation products of $[Me_2N(CH_2)_3]_2GaX$, where X = Cl or Br. These included GaH_3, $XGaH_2$, X_2GaH, GaH, GaX *etc.*[135]

Ab initio and DFT calculations have been reported for the vibrational wavenumbers of $GaMe_3$.[136] The Raman spectrum of $^tBu_2Ga(N_3)$ included νGaC at 386 cm^{-1}.[137]

IR and Raman spectra were used to characterise GaN nanocrystals grown by chloride–hydride vapour-phase epitaxy on oxidised silicon.[138] High-pressure Raman spectroscopy was used to follow the wurtzite to rock salt phase transition for epitaxial GaN.[139] The Raman spectrum of prism-shaped GaN nanorods included characteristic bands at 255 and 419 cm^{-1}.[140] Raman spectroscopy was used to characterise $GaN_{1-x}P_x$ alloys.[141–143]

The Raman spectra of GaN_xO_y films grown by nitridation of GaAs(100) substrates show expected GaN bands, together with features below 450 cm^{-1} which are related to the oxygen content of the films.[144] The IR spectrum of nitrogen-implanted GaAs shows a feature at 638 cm^{-1} due to Ga–N motion.[145]

Table 5 *Vibrational assignments for Ga_2H_6 (/cm^{-1})*

$\nu_8(b_{1u})$	1995
$\nu_{13}(b_{2u})$	1202
$\nu_{16}(b_{3u})$	1976
$\nu_{17}(b_{3u})$	1232

The IR spectra of hydrogenated $GaAs_{1-y}N_y$ show two weakly-coupled *v*NH modes.[146]

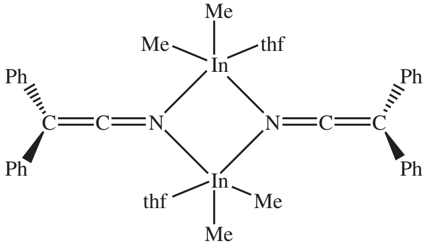
The micro-Raman spectra of GaAs nanoparticles include a characteristic feature at about 250 cm^{-1}.[147] The hydrogen-plasma treatment of GaAs has been probed by Raman spectroscopy. Characteristic bands were seen due to H_2 trapped at different types of site.[148] DFT calculations gave vibrational wavenumbers for the cluster Ga_8As_8.[149]

IR and Raman spectra gave assignments to *v*GaO, *v*TeO, *v*Ga–O–Te and *v*Te–O–Te modes for $KGaTeO_5$ and $K_3GaTe_2O_8(OH)_2$.[150] The IR spectrum of a PbO–Bi_2O_3–Ga_2O_3–GeO_2 glass doped with Tm^{3+} included a characteristic Ga–O–Ga band from linked GaO_4 tetrahedra.[151] Variable-temperature Raman spectra of a $La_{0.88}Sr_{0.12}Ga_{0.82}Mg_{0.18}O_{2.85}$ solid solution provided confirmation of a phase transition near 880 K.[152]

Force constant model calculations gave vibrational assignments for AGa_2X_4, where A = Zn, Cd, X = S, Se.[153] The Raman spectra of GeS_2–Ga_2S_3–CdS glasses were analysed in terms of $GaS_{4/2}$ modes.[154] The Raman spectra of GeS_2–Ga_2S_3–KCl glasses at room temperature gave evidence for structural changes induced by increasing concentration of K^+.[155] Addition of neodymium to MS–Ga_2S_3 glasses (M = Sr, Ba) leads to modifications of the networks of GaS_4 tetrahedra – these were followed by Raman spectroscopy.[156] The Raman spectra of glasses (1–x)[$CsGaS_{1.5}Cl$].x[$0.15Ga_2S_3.0.85GeS_2$] are consistent with tetrahedral Ga units with either corner- or edge-sharing.[157] Raman spectra gave evidence on the compositional dependence of the spectra for $Cu_yGa_ySe_z$ thin films.[158]

3.4 Indium. – Matrix-IR spectra have been reported and assigned for the reaction products of laser-ablated M (=In, Tl) atoms with H_2. Assignments to bands of MH_n species, where n = 1–3, are summarised in Table 6.[159,160]

IR and Raman spectra for (4) gave the following assignments: $v_{as}InC_2$ 536 cm^{-1}, v_sInC_2 493 cm^{-1}, vIn_2N_2 454, 298 cm^{-1}.[161] The Raman spectra of InGaAsN layers gave evidence for formation of isolated In–N bonds.[162]



(4)

Skeletal mode assignments were proposed from the IR spectra of [(MesInCl)$_4$(InCl)$_2$–(As^{t}Bu)$_4$], where Mes = mesityl, and related species, include *v*InAs 310 cm^{-1}, *v*InCl(br) + *v*InAs 210 cm^{-1}, *v*InCl(t) 536 cm^{-1} and *v*AsC 608

Table 6 *Vibrational assignments for indium and thallium hydrides (/cm^{-1})*

In, H_2	*In, D_2*	*Tl, H_2*	*Tl, D_2*	*Hydride*
1760.9	1266.2	1748.4	1254.6	MH_3
1628.9	1175.4	1520.0	1098.8	MH_2
1563.3	1126.3	1390.2	1007.5	MH_2
1393.4	997.7	1311	940	MH
979.6	709.9	909.7	652.9	M_2H_2

cm^{-1}.[163] High-pressure Raman spectroscopy (to 20 GPa) has been used to probe the phase behaviour of $M^{II}In^{III}{}_2S^{VI}{}_4$, where M = Mg, Mn, Cd.[164]

3.5 Thallium. – Laser-ablated Tl atoms and H_2 react to form a number of species, identified by matrix-IR – see Table 6.[165] The complex $[Tl(bipy)_3(dmso)]^{3+}$ has a Raman band at 456 cm^{-1} due to νTlN/νTlC.[166]

4 Group 14

4.1 Carbon. – *4.1.1 Small Carbon Clusters.* IR data have been reported for a C_3 molecule in a *para*-H_2 matrix, with a value of 2035 cm^{-1} for ν_3 ($^{12}C_3$).[167] *Ab initio* and DFT calculations have been made of vibrational wavenumbers for di-dodecahedral C_5N_{30}.[168]

The matrix-IR spectrum of $C_6{}^+$ includes a band at 2092 cm^{-1} from the linear, and at 1972 cm^{-1} from the cyclic, isomer.[169] The IR spectrum of C_7S in an argon matrix at 12 K includes bands at 2088.1 cm^{-1} (ν_2, σ), 1913.6 cm^{-1} (ν_3, σ), 1256.1 cm^{-1}(ν_5, σ). All are consistent with a linear structure, confirmed by ^{13}C substitution.[170] The argon matrix IR spectrum of linear GeC_7 shows ν_1 (σ) at 2063.6 cm^{-1}. For GeC_9, ν_4 (σ) is at 1928.3 cm^{-1}.[171]

DFT calculations have been made of vibrational wavenumbers for C_{20}-based clusters,[172] for a D_{2d}-symmetry dimer of C_{36},[173] and for the double-cage dodecahedrane $C_{35}H_{30}$.[174]

4.1.2 Fullerenes. A resonance Raman study of C_{60} in its first allowed electronic excited state shows that the ground state $h_g(1)$ mode splits into two components, 265, 281 cm^{-1}. The data are consistent with D_{5d} symmetry for the excited state.[175] Raman spectroscopy was used to characterise C_{60} units in a tantalum oxide lithium fulleride composite.[176] A group theoretical analysis has been made of the vibrational normal modes for the azafullerene $C_{48}N_{12}$.[177]

IR and Raman spectra were used to characterise $C_{50}Cl_{10}$.[178] IR spectra gave assignments for $C_{60}(CF_3)_n$, where n = 2, 4, 6, 8 or 10.[179] Raman data were reported for $C_{60}F_n$, with n = 18, 36 or 48.[180] For n = 24, the IR spectrum is consistent with the presence of a single isomer, of T_h symmetry.[181] There have been experimental and theoretical studies of the vibrations of $C_{60}X_n$, where X = Cl, Br, n = 6, 10; X = Br, n = 8, 24.[182–184] The IR spectra of

C_{60}-heterocyclic derivatives, *e.g.* C_{60}-pyrroline, -pyrazoline, gave assignments based on DFT calculations.[185]

IR were reported for the endohedral species $H_2@C_{60}$.[186] IR data for $Li@C_{60}$ gave evidence for two different species – one with much lower symmetry than the other. For $Li@C_{70}$, bands very similar to those of C_{140} were seen.[187,188]

The Raman spectrum of Na_3C_{60} included a band at 1447 cm^{-1}, from $C_{60}{}^{3-}$.[189] The Raman spectrum of Li_4C_{60} shows that this has a tetragonal structure, with intermolecular bonds formed by [2 + 2]–cycloaddition. Na_4C_{60}, however, has a monoclinic structure, with single C–C bonds between molecules.[190] The IR spectra of M_4C_{60}, where M = K. Rb or Cs, gave evidence for Jahn-Teller distortion of the C_{60} unit.[191] The Raman spectrum of Mg_4C_{60} was used to estimate the amount of Mg to C_{60} charge transfer.[192]

There have been numerous papers in which IR and Raman spectroscopies were used to follow thermally- and pressure-induced phase transitions, as well as irradiation effects, on C_{60} and C_{70}.[193–203]

The Raman spectra of C_{60}@SWCNT peapods included features due to coupling of C_{60} totally symmetric modes with fullerene translational mobility within the tube.[204] Raman data were reported for fullerene peapod species $C_{60}.C_{70}$@SWCNT.[205] Raman spectra were also reported for the charge-transfer species C_{60}@SWCNT and C_{70}@SWCNT.[206,207] High pressure resonance Raman spectra were reported for C_{60} and C_{70} peapods in SWCNT, at pressures of up to 9 GPa.[208] Raman spectroscopy was used to follow the transformation of C_{60} peapods into SWCNT,[209] and of C_{60}-SWCNT peapods into DWCNT.[210]

Raman spectroscopy showed characteristic wavenumber shifts in component bands on the formation of C_{60}-intercalated graphite.[211]

Structural changes in C_{70} caused by He^+ bombardment were monitored by FTIR and Raman spectra. There was no evidence for oligomer formation – simply direct degradation to amorphous carbon.[212] *Ab initio* calculations have been made of the vibrational wavenumbers for C_{115}, a coplanar double-C_{60} cage.[213] Semi-empirical AM1 calculations have been reported for the vibrational wavenumbers of the 'peanut-shaped' fullerenes C_{120}.[214]

4.1.3 Carbon Nanotubes. An FT Raman band at 146 cm^{-1} was assigned as a radial breathing mode for bundles of SWCNT with a tube diameter of 1.53 nm.[215] Oxidation of HipCO SWCNT (diameter 8–10 Å) leads to irreversible disappearance of Raman breathing modes below 220 cm^{-1}, in the temperature range 150–400°C.[216] The Raman spectra of SWCNT produced by plasma-enhanced CVD gave evidence for the formation of single tubes at quite low temperatures (*ca.* 550°C).[217]

Resonance Raman excitation profiles were measured for individually dispersed SWCNT in aqueous solution (excitation 695–985 nm.).[218] The IR and Raman spectra of SWCNT functionalised by long-chain hydrophobic groups show that the fundamental structure is unchanged on modification.[219] A review has appeared of Raman data for SWCNT and DWCNT, especially the conversion of C_{60}/SWCNT peapods into DWCNT at high temperatures.[220]

The Raman spectra of SWCNT (diameter 0.4 nm.) in a matrix of $AlPO_4$-5 zeolite single crystals gave dominant peaks due to (5,0), (4,2) and (3,3) structures.[221,222] SWCNT have been grown in MCM-41 molecular sieve templated with C_{12} or C_{16} alkyl chains. Their Raman spectra show that they are of uniform diameter (2.6 nm. for C_{12}, 3.3 nm. for C_{16} systems).[223] Raman spectra have been reported for superhard phases of SWCNT and C_{60}.[224]

Raman and/or IR spectra have been used extensively in the characterisation of other SWCNT systems.[225–253]Vibrational spectra were also used to follow the effects of chemical reactions and physical processing on SWCNT's.[254–265]

The Raman spectra of DWCNT's were analysed in terms of chiral, (*n,m*) assignments for these tubes.[266] The Raman spectrum of I_2-doped DWCNT gave assignments to radial breathing and tangential modes.[267] Resonance Raman spectra of DWCNT were analysed to probe diameters and chiralities.[268] The Raman spectra of DWCNT (from fullerene peapods annealed at high temperatures) show that the inner tubes are remarkably defect-free.[269] Very low levels of defects were also observed from the Raman spectra of DWCNT produced by the catalytic decomposition of benzene over Fe–Mo/Al_2O_3 catalysts at 900°C (*i.e.* very weak D-band at 1265.5 cm^{-1}).[270]

The Raman spectra of DWCNT produced by catalytic CVD show that the outer tube diameter is in the range 3–6 nm., with the inner tube about 0.36 nm.[271] Similar data for DWCNT formed by catalytic decomposition of *n*-hexane over Fe–Mo/MgO show that the outer/inner tube diameters are in the ranges 1.44–2.53 nm., 0.70–1.82 nm. respectively.[272] Other Raman studies of DWCNT were also reported.[273,274]

Raman data for MWCNT grown by hot-filament plasma-enhanced CVD include D– and G–band peaks at about 1370 cm^{-1} and 1590 cm^{-1} respectively.[275] The Raman spectra of MWCNT grown on Ni/Cr-deposited glass substrates below 580°C reveal a graphitic structure, and suggest that they are highly pure.[276] Raman data for MWCNT included a new feature at about 843 cm^{-1}.[277] The Raman spectra of MWCNT prepared in the presence of N_2 showed increased length and improved morphology compared to those prepared in the absence of N_2.[278]

Low-wavenumber Raman bands of MWCNT were assigned in terms of modes from coupling of radial breathing modes of individual tubes *via* van der Waals interactions.[279] The Raman spectra of MWCNT prepared at 470°C showed the coexistence of graphite and amorphous carbon units.[280] Micro-Raman spectra were used to characterise ^{13}C-labelled MWCNT.[281] The Raman spectra of MWCNT's subjected to plasma-etching were used to identify structural defects introduced thereby.[282] Raman spectroscopy was used to compare the structures of MWCNT's prepared by high-temperature arc and low-temperature CVD methods. The former had a more graphite-like structure.[283] Micro-Raman spectroscopy was used to characterise MWCNT obtained by electrophoretic deposition.[284]

4.1.4 Other Carbon Nanostructures. Raman spectroscopy was used to characterise single-walled carbon nanohorns (SWCNH).[285] Similar methods were used to characterise microporous carbon derived from boron carbide,[286] and polymer 'brushes' with SWCNT backbones, synthesised by atom transfer radical polymerisation.[287]

The Raman spectrum of the product of plasma spraying of nanodiamonds shows the formation of well-defined carbon onions (band at 1571 cm^{-1}) and defective carbon onions (1592 cm^{-1}).[288] Raman spectroscopy was used to follow the effects of heavy-ion irradiation on nanocomposite carbon films.[289] Laser-grown carbon microfibres were characterised by Raman microfibres,[290] as were giant fullerene-like hollow spheres generated from C_{60} by compression at 57 GPa.[291]

IR and Raman data were reported for carbon atom 'wires', $(=C=C=)_n$.[292] A polarised Raman study of nanographite ribbons gave evidence for anisotropic scattering.[293]

The Raman spectra of carbon nitride nanotubes show evidence for a high degree of graphitisation.[294] Raman spectroscopy was used to characterise CN_x nanotubes formed by the thermal decomposition of ferrocene/ethylenediamine mixtures.[295]

4.1.5 Diamond-like Phases and Carbon-based Films. Raman spectra were used to characterise ion-irradiated diamond samples.[296] Raman data could be used to identify features related to point defects in diamond.[297] There is Raman evidence for the formation of polycrystalline diamond from graphite at high pressures and temperatures.[298] Surface C–H groups on diamond nanocrystals were characterised by IR (νC–H) and *ab initio* calculations, *e.g.* the νC–H band on a C(111)–1 × 1 site is at 2834 cm^{-1}.[299]

Raman spectroscopy gave structural characterisation of nanocrystalline diamond films formed by pulsed laser deposition in an oxygen atmosphere.[300] Raman and IR spectra were used to follow diamond deposition on mirror-polished Si single crystal substrates.[301] Nanocrystalline diamond spheres were also characterised by Raman spectroscopy.[302]

The Raman spectra of DLC films were used to study the effects of the C_{60}-Ar ratio in their preparation.[303] Raman spectroscopy was used to characterise a-C:H amorphous hydrogenated carbon (DLC) films formed by vacuum arc deposition,[304] and DLC films prepared using a high power, high-frequency excimer laser.[305] Several other Raman and IR studies for the characterisation of DLC films have appeared.[306–309]

Raman spectroscopy was used to characterise the microstructure of ta:C films deposited by filtered arc, accelerated at different energies.[310] Similar data were used to examine a:C films incorporating Si, Ge and N;[311] and ta:C films (showing an amorphous sp^3 skeleton containing sp^2 clusters (sizes <1 nm.).[312] Raman spectra were used to follow the nanostructuring of ta:C films induced by ion-beam C implantation.[313]

A Raman spectroscopic study has been made of carbon films prepared on Al or Si substrates.[314] Raman spectra were used to characterise fluorinated amorphous carbon nanoparticle films (a-C:F NPs).[315] UV Raman spectra of templated carbon anodes showed a band at 1575 cm^{-1} (G band) and a broad, unsymmetrical feature at about 1600 cm^{-1}.[316] Raman spectra of 2-dimensionally-ordered linear chain carbon films included characteristic bands at about 1540 cm^{-1} and in the range 2000–2500 cm^{-1}.[317] The Raman spectrum of an MPCVD carbon film gave no evidence for the presence of nanocrystalline diamond.[318] The Raman spectra of nanostructured carbon films showed bands indicative of a high fraction of sp linear carbon chains.[319]

IR and Raman spectra were used to characterise ta-C : N : H films, as a function of the experimental formation conditions.[320] The FTIR spectra of a–CN_x:H films deposited in a CH_4/N_2 r.f. plasma showed νCH bands in the range 2800 – 3000 cm^{-1}, and *ν*CN at 2246 cm^{-1}.[321] IR spectroscopy was used to characterise a–C:H:N films deposited by r.f. magnetron sputtering of a graphite target in an $Ar/CH_4/N_2$ plasma. At high nitrogen concentrations, a *ν*C≡N band was observed at 2150 cm^{-1}.[322] The IR spectra of a-$C_{1-x}N_x$:H films show mainly C=N bands, but increasing C≡N with increasing x.[323]

The Raman spectra of CN_x films (with x values up to 1.22) show bands at 1098 cm^{-1}, 1950 cm^{-1}, due to *ν*C–N, *ν*C=N respectively.[324] CN_x films grown by a vacuum cathodic arc method (160–500°C) were characterised by IR and Raman spectra, in terms of sp^3, aromatic and non-aromatic sp^2 units.[325] The Raman spectra of CN_x films on a Co/Ni-covered substrate showed that they were mainly CN_x crystallites, diameter 20–30 nm.[326] Other reports have been made of characterisation of CN_x films by IR and Raman spectroscopy.[327,328]

The IR spectra of amorphous, graphite-like CO_x films included characteristic bands near 1700 cm^{-1} and 1605 cm^{-1}, with a Raman feature (G band) near 1605 cm^{-1}.[329]

4.1.6 Other Carbon Compounds. A high-resolution IR study (1800–2200 cm^{-1}) has been made of the radical $^{12}C^{14}N$.[330] *Ab initio* and DFT calculations have been reported for the vibrational wavenumbers of CH_2N_2, $CHDN_2$, CD_2N_2 and $CH_2N^{15}N$.[331] A high-resolution IR study of the $\nu_2 + \nu_9{}^1 – \nu_9{}^1$ hot band for $(HCN)_2$ showed that the band origin was at 3241.8210(11) cm^{-1}.[332]

The high-resolution FTIR spectra of $^{15}N^{12}C^{12}C^{15}N$ and $^{14}N^{13}C^{13}C^{14}N$ gave precise values for several fundamental, overtone and combination energy levels.[333] *Ab initio* calculations have given vibrational wavenumbers for N≡C–C≡C–C≡N ($D_{\infty h}$),[334] and for O=C=CH–N=C=O.[335] IR and Raman spectra were assigned for $(HOH_2C)_3C–NH_3{}^+X^-$, where X = F, Cl, Br or I.[336] *Ab initio* and DFT calculations gave vibrational wavenumbers for adamantane.[337]

The FTIR spectra of CO–CH_4 mixed thin solid films, below 50 K, gave evidence for the formation of a CO.CH_4 complex (*ν*CO 2136 cm^{-1}).[338] An *ab initio* calculation has been made of the vibrational wavenumbers for the formyl (HCO) radical.[339] A high-resolution IR study of ν_3 (*ν*CC) of the $\tilde{a}^1\Delta$ electronic state of the CCO radical showed that the band origin was at 1082.97894(94) cm^{-1}.[340] For the ground state the corresponding value was 1066.62407(54) cm^{-1}.[341]

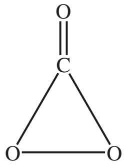
A detailed IR and Raman spectroscopic study of FC(O)I gave the assignments shown in Table 7 (confirmed by DFT calculations).[342] *Ab initio* calculations gave vibrational wavenumbers for the $Cl_2CO.H_2O$ complex.[343]

Table 7 *Vibrational assignments for FC(O)I (/cm^{-1})*

	IR (Ar matrix)	*Raman (solid)*
νC=O	1836.6	1778
νCF	1020.6	1008
δFCO	704.6	711
δ_{oop}	566.2	567
νCI		346
δFCO		294

A high-resolution matrix-isolation IR study of $^{13}CO_2$ in the ν_2 and ν_3 regions shows that (in a neon matrix) ν_2 is split (649.37, 648.73 cm^{-1}), while ν_3 shows as a singlet at 2282.15 cm^{-1}.[344] The phase behaviour of CO_2 was followed by *in situ* Raman spectroscopy up to 67 GPa and 1660 K.[345] A high-resolution IR study has been made of the (30^{0}1) band of CO_2 (6230–6250 cm^{-1}).[346] IR spectra and DFT calculations were used to probe the effects on CO_2 vibrations of adsorption on SWCNT.[347] IR spectra were also used to study CO_2 trapped in SWCNT bundles, *via* behaviour of the ν_{as} mode near 2330 cm^{-1}.[348]

High-resolution IR spectra were reported for the clusters $He_n.CO_2$[349] and $He_n.OCS$[350] (both with n up to about 20). Values of $\nu_{as}CO_2$ in the FTIR spectra of gaseous $X^-.CO_2$ (X = Cl, Br, I) were all at lower wavenumbers than for free CO_2.[351] There is matrix-IR evidence for the formation of a cyclic carbon trioxide isomer, (5) (X^1A_1) by addition of O atoms to CO_2.[352]



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High-pressure and −temperature Raman spectroscopy was used to study carbonate ions in aqueous solution in the ranges 1–30 GPa and 25–400°C.[353] IR and Raman spectra were used to study the pressure-induced phase transition (2.8 GPa) for $KHCO_3$.[354]

A detailed vibrational assignment was proposed for $ClC(O)OCF_3$, based on IR and Raman data. Only one conformer was found, of C_s symmetry, with a synperiplanar orientation of the O–C single bond with respect to the O=C double bond.[355] For $FC(O)OSO_2CF_3$, the IR and Raman spectra (together with *ab initio* calculations) suggest the presence of *trans*- and *gauche*-conformers in the gas phase.[356] The same type of data was consistent with two planar conformers for $CF_3OC(O)$-$C(O)OCF_3$, of C_{2v} and C_{2h} symmetry. Assignments were again supported by *ab initio* calculations.[357]

The assignments proposed from IR and Raman spectra for the C_2 rotamer of FC(O)OOOC(O)F are summarised in Table 8.[358] IR and Raman spectra, with DFT calculations, are consistent with the presence of several rotamers for the open-chain trioxide $CF_3OC(O)OOOC(O)OCF_3$.[359,360]

Table 8 *Some vibrational assignments for FC(O)OOOC(O)F (/cm^{-1})*

	IR (gas)	*Raman (solid)*
ν_{as}C=O	1921.7	1915
ν_{s}C=O		1890
ν_{s}CF	1207.1	1243
ν_{as}CF	1167.1	1166
ν_{as}CO	944.9	926
ν_{s}OOO	918.5	909
ν_{as}OOO	797.2	798

Table 9 *Vibrational assignments for CX_3^+ (/cm^{-1})*

Assignment	*X=*	*F*	*Cl*	*Br*	*I*
ν_1 (a$_1'$)	ν_sCX$_3$		554	321	
ν_2 (a$_2''$)	πCX$_3$	798.1			339
ν_3 (e$'$)	ν_sCX$_3$	1662.4	1036		739
ν_4 (e$'$)	δX–C–X		326.9	185	

The high-resolution IR spectrum of $CH^{35}Cl_2F$, in the region of ν_4 shows that the band origin is at 744.474290 cm^{-1}.[361] DFT calculations have given values for the vibrational wavenumbers of CX_2=CH–NNN, where X = F or Cl, for both *cis* and *trans* isomers.[362] A high-resolution IR study of CF_3CH_2F in a supersonic planar jet shows that ν_{14} is centred at 1203.60837(4).[363] Similar data for $CH_2{}^{79}BrCl$ gave ν_4 746.8809(1) cm^{-1}, ν_5 615.2271(1) cm^{-1}.[364] Raman bands have been obtained for the cations CX_3^+ where X = Cl or Br, and assignments given, Table 9.[365]

Raman spectroscopy was used to probe high-pressure phase transitions for CF_4 hydrate systems.[366] High-resolution tunable diode laser spectroscopy for CF_3Cl showed that the band origin for ν_1 was at 1108.35587(6) cm^{-1} (^{35}Cl) or 1108.0253(1) (^{37}Cl).[367] The following band origins were found, using high-resolution FTIR , for 2ν_3 for ICN: I^{12}C^{14}N 4332.83676(23) cm^{-1}; I^{13}C^{14}N 4235.73550(16) cm^{-1}; I^{12}C^{15}N 4274.28513(21) cm^{-1}.[368]

4.2 Silicon. – *Ab initio* calculations gave vibrational wavenumbers for the silicon clusters Si$_n$, where n = 12–20.[369] Micro-Raman spectroscopy was used to characterise polycrystalline silicon thin films.[370] A theoretical analysis has been carried out on the low-wavenumber Raman bands in nanosolid silicon samples.[371] Raman spectroscopy was used to analyse defects in polycrystalline silicon films, *e.g*. a band at 2000 cm^{-1} due to νSiH of dangling bonds at grain boundaries.[372]

Raman spectroscopy was used to monitor the effects of electron irradiation on the crystallisation of growing silicon film on a glass substrate.[373] Laser-crystallised amorphous silicon films were characterised by Raman spectra.[374] Localised vibrational modes of oxygen in ^{28}Si-, ^{29}Si- and ^{30}Si-enriched single crystals of silicon were studied by high-resolution IR absorption.[375] IR and Raman spectra were used to observe the effects of exposure of porous silicon to thermoelectrons, followed by H atoms, H_2O or O_3. The last two gave evidence for Si–O bond formation.[376]

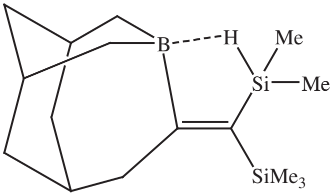
IR and Raman spectroscopy were used to characterise hydrogenated silicon thin films formed by magnetron r.f. sputtering,[377] or by hot-wire CVD.[378] An IR study (νSiH) has been made of the photoinduced changes in the structure of undoped hydrogenated amorphous silicon, a-Si:H.[379] IR bands due to Si–H–Si units were reported for silicon-isotopically enriched silicon crystals.[380]

Micro-Raman spectroscopy was used to characterise 4H–SiC layers grown from a variety of precursor systems.[381] FTIR data were able to characterise hydrogenated amorphous silicon nitride films with embedded nanoparticles. Oxidation leads to the appearance of an Si–O feature at 1070 cm^{-1}.[382] Raman spectra were used to determine the degree of micro-crystallinity of μc–Si:H layers, using the intensity ratio of bands at 520 cm^{-1} and 480 cm^{-1}.[383] IR and Raman spectra were used to determine the effects of neutron irradiation on a-SiC:H films.[384] A range of a-SiC_x:H and a-SiC_xN_y:H films were studied using IR spectroscopy;[385] similar experiments were carried out on a-$Si_{1-x}Ge_x$:H,F films.[386]

The nature of Si/H units in hydrogenated amorphous silicon prepared from H_2/SiH_4 was determined using IR spectra. Raman data gave evidence on the nature of the silicon network.[387] FTIR spectra were used to characterise SiCOH films (evidence for Si–Si, Si–CH_2–Si, Si–O–Si and Si–CH_2O–Si units).[388] DFT calculations gave vibrational wavenumbers for Si_3C_4, Si_4C_3 and Si_4C_4 clusters.[389] FTIR spectra were used to follow the formation of Si–O, Si–N and N–O bonds by treatment of Si(111) or Si(110) surfaces by O_2 and N_2O.[390]

The IR spectrum of the disilenyl radical, H_2SiSiH (X^2A) in an SiH_4 matrix showed ν_5 at 651 cm^{-1} (493 cm^{-1} in the d_3-analogue). In an SiD_4 matrix, ν_4 was seen at 683 cm^{-1}.[391] The Raman spectrum of $Mes_2Si{=}SiMes_2$ shows changes on forming solvates with toluene or thf.[392] The IR and Raman spectra of 1,1,2,2-$^tBu_4Si_2H_2$ were assigned with the help of *ab initio* calculations (νSiSi 484 cm^{-1}, νSiH 2080 cm^{-1} (IR), 2084 cm^{-1} (Raman)).[393] An *ab initio* calculation has been made of vibrational modes for $H_3SiSiMe_3$.[394]

The FTIR of an Si–D bending mode at the SiO_2/Si interface gave a value of 490 cm^{-1}.[395] ATR IR data were used to characterise a-Si : H surfaces subjected to interaction with SiH_3 radicals.[396] An *ab initio* calculation has been reported for the anharmonic force field of $SiHCl_3$.[397] The species (6) gave an IR band at 1849.0 cm^{-1} due to νSi–H . . . B, compared to νSiH of 2139.7 cm^{-1} for the parent silane.[398]



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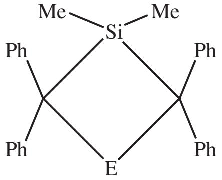
IR data (νSiH, δSiH, νSi–OH *etc.*) were used to follow the reactions of $(EtO)_3SiH$ with bis[3-triethoxysilylpropyl]tetrasulfane.[399] *Ab initio* calculations have been made of vibrational wavenumbers for SiH–B units as a model for p^+-type porous silicon.[400] High-resolution FTIR data have been reported for ν_6, ν_8 and ν_9 of Si_2H_6.[401,402] DFT calculations gave vibrational wavenumbers for $(SiH_3)_3CH$ and $(SiH_3)_4C$.[403] *Ab initio* and DFT calculations have been made for species involved in the reactions $AH_4 \rightarrow AH_2 + H_2$, where A = Si, Ge, Sn or Pb.[404] *Ab initio* calculations gave vibrational wavenumbers for the clusters Si_5H_3, Si_5H_6, Si_5Li_3 and Si_5Na_3.[405]

Raman and IR spectra were used to characterise spark-processed SiC.[406] Near-IR diode laser spectra of the radical HCSi showed that ω_2 (bending mode) was at 495.00698(30) cm^{-1}.[407] IR spectroscopy was used to characterise SiCN films. For films deposited at room temperature there was evidence for Si–C, Si–N and C≡N bonds.[408] DFT calculations gave vibrational wavenumbers for SiCS (linear triplet isomer).[409] Matrix-IR data have been obtained for the triplet carbene $HC–SiHCl_2$ (with assignments from *ab initio* calculations).[410]

IR and Raman data gave detailed assignments for $EtSiF_2(CH_3)$. *Trans*- and *gauche*-conformers were seen in fluid phases, but only *trans* in the solid.[411] New IR data have been reported for $(SiX_3)_2CH_2$, where X=H, D. They were assigned in detail with the help of *ab initio* calculations, including a_2 and b_2 torsional modes at 78.5, 133 cm^{-1} respectively.[412] Matrix-IR data were reported and assigned for $(MeO)_2SiMe_2$.[413]

The IR and Raman spectra of $CH_2{=}CHSiH(CH_3)Cl$ were assigned using *ab initio* calculations.[414] Similar results for $(CH_2{=}CH)(CH_3)_2SiH(D)$ suggested the presence of *syn*- and *gauche*-conformers.[415] There is matrix-IR evidence for the formation of $H_2C{=}Si(F)H$ and $MeF \rightarrow Si$ from the reaction of CH_3F with Si atoms.[416] A detailed IR and Raman study of $CH_2{=}CHSiF_2H$ showed that both *cis* and *gauche* conformers exist in fluid phases.[417] *Ab initio* and DFT calculations gave vibrational wavenumbers for $CH_3Si(C{\equiv}CH)_3$.[418]



(7)

The Raman spectra of (7), where E = O or S, have been reported and assigned with the aid of DFT and *ab initio* calculations.[419] IR and Raman spectra, with *ab initio* calculations, gave detailed vibrational assignments for cyclopropylbromosilane, $c\text{–}C_3H_5SiH_2Br$.[420] Time-resolved IR spectroscopy was used to monitor the formation of $(c\text{–}C_5H_9)Si(OH)_3$ by hydrolysis of $(c\text{–}C_5H_9)SiCl_3$.[421] Variable-temperature Raman spectroscopy gave evidence for complicated thermochromic phase transitions in the region 5–60° for $[(n\text{–}C_{10}H_{21})_2Si]_n$.[422]

Ab initio calculations gave vibrational wavenumbers for $CH_3C(O)OCH_2SiF_3$.[423] Detailed IR and Raman spectral studies, backed up by a range of calculations, have been reported for $CH_3CH_2SiH_2CH_3$;[424] $CH_3CH_2CH_2SiF_3$;[425] and $CF_3CH_2CH_2SiF_3$.[426] IR spectra gave some assignments for the new borazine derivatives, $[B(R)NH]_3$, where $R = CH_2(SiCl_3)$ or $CH_2(SiCl_2CH_3)$.[427] IR spectroscopy was used to characterise organo–silicon polymeric thin films derived from Me_3SiCl and an oxygen plasma.[428]

Vibrational wavenumbers were calculated for SiH_3GeH_3 by *ab initio* methods.[429] Raman data were used for the characterisation of strain and composition for as-grown and annealed self-assembled Si/Ge dot multilayers.[430] Characteristic low-wavenumber Raman bands were reported for a three-dimensional array of Ge_xSi_{1-x} quantum dots on a silicon substrate.[431]

DRIFT data for Si_3N_4 powders always included bands due to νSiH.[432] High-pressure Raman spectroscopy was used to follow phase transitions in ceramic silicon nitride.[433] IR spectra of nitrogen-rich silicon nitride films show that νSiN shifts to higher wavenumber with increased N–H concentration.[434] FTIR spectroscopy was used to characterise $Si_xO_yN_z$ layers formed by sequential implantation of O_2^+ and N_2^+ into crystalline n–type silicon.[435,436]

The IR spectrum of $FSi(PH_2)_3$ in an argon matrix included the following: νSiP 493.2, 488.8 cm^{-1}, νSiF 855.5 cm^{-1}, and νPH as 6 bands in the range 2307.1–2326.1 cm^{-1}.[437]

FTIR was used in the quantitative analysis of gas-phase SiO, including ^{28}Si, ^{29}Si and ^{30}Si isotopomers.[438] IR spectroscopy was used to characterise silicon suboxides at the SiO_2/Si(100) interface.[439] IR data were reported for thin SiO layers in amorphous SiO/SiO_2 superlattices. On annealing, νSi–O–Si shifts to higher wavenumbers on increasing the annealing temperature.[440]

DFT calculations of vibrational wavenumbers of the SiOH unit of trimethylsilanol were used to propose an assignment of experimental values.[441] The IR spectrum of argon-matrix isolated $Cl_3Si(OEt)$ includes $\nu_{as}SiCl_3$ at 600 cm^{-1} and νSiO at 1085 cm^{-1}.[442] IR spectra of SiO_2/Si nanowires show enhanced absorption near 1130 cm^{-1} compared to SiO_2 nanoparticles.[443]

Ab initio calculations of vibrational wavenumbers have been reported for small clusters with short range order, including SiO_2, GeO_2, As_2S_3 and GeS_2.[444] *Ab initio* calculations of Raman spectra for normal and compressed amorphous silica gave good agreement with experiment.[445] Raman data were used to follow the structural effects of ablation and compaction of amorphous SiO_2 irradiated by an ArF excimer laser.[446] The value of ν_{as}SiOSi of SiO_2 gave information on interfacial strain and the formation of substoichiometric silicon oxides at the SiO_2/Si interface.[447]

Raman spectroscopy was used to characterise quartzite samples shocked at pressures up to 28 GPa. Samples subjected to the highest pressures gave evidence for glassy SiO_2.[448] Raman spectroscopy was used to analyse structural changes in SiO_2 glass caused by β-irradiation.[449] IR data were reported for SiO_2 films grown under negative corona stress (characteristic bands at 935, 1074, 800 and 456 cm^{-1}).[450] IR data were used to study SiO_2 films formed by sol-gel processes.[451] The Raman spectrum of physisorbed H_2O in porous SiO_2 gave evidence for Si–OH species.[452] IR bands (ν_{as}SiOSi) were used to determine the local structure of porous silica xerogels.[453]

IR bands (ν_{as}SiOSi) were used to follow changes in nanosized TiO_2/SiO_2 particles with SiO_2 content.[454] Raman spectroscopy was used to probe the microstructure of SiO_2–GeO_2 sol-gel glass coatings.[455] The IR spectra of SiO_2/SnO_2 mixed oxides gave evidence for the formation of Si–O–Sn bonds.[456] The FTIR spectrum of ZSM – 5 zeolite with incorporated Ge gave assignments to features from ν_{as}Si–O–Ge near 950 cm^{-1}.[457] IR and Raman spectroscopy were used to follow the hydrolysis and condensation of Me_3SiCl in aqueous organic solvents. $Me_3Si(OH)$ was identified as an intermediate and $(Me_3Si)_2O$ as the final product.[458] IR analysis of plasma-deposited siloxane films showed the presence of 4 types of distorted tetrahedra: $Me_3SiO_{0.5}$, Me_2SiO, $MeSiO_{1.5}$ and SiO_2.[459]

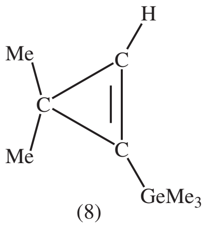
High-pressure Raman studies have been made to follow phase transitions of $MgSiO_3$.[460–462] Molecular dynamics calculations have been performed on the vibrational spectrum of $CaSiO_3$ over the melt to glass transition.[463]

Variable-temperature Raman data for $[C_3H_7NH_3]_2SiF_6$ were used to probe the phase transition at 223K.[464] The IR spectrum of the $SiCl_2.N_2$ adduct in Ar/N_2 matrices included ν_sSiCl (511.2, 508.9. 506.5 cm^{-1}) and ν_{as}SiCl (500.1, 496.9, 495.1 cm^{-1}). $Cl_2Si(N_2)_2$ shows features at 498.7 and 493.5 cm^{-1}. All data refer to the major isotopomers.[465]

4.3 Germanium. – Raman spectroscopy was used to characterise nanoparticles of Ge in mesoporous SiO_2 (especially a band near 300 cm^{-1}).[466] IR bands were reported for oxygen in vacancies in Ge. A band at 669 cm^{-1} was ascribed to a non-linear, symmetric Ge–O–Ge unit.[467]

Ab initio calculations have been made of vibrational wavenumbers for $Me_{3-n}H_nM(NXY)$, where M = Ge, Sn, Pb; XY = N=N, C=O, C=S; n = 0–3.[468] The Raman spectra of dilute GeC alloys (*i.e.* Ge–rich) contained a band at 530 cm^{-1} due to substitutional carbon.[469] *Ab initio* and DFT calculations have been reported for the vibrational wavenumbers of $Ge(C\equiv CH)_4$.[470]

IR and Raman spectra have been reported and assigned (using DFT calculations) for $^nPrMCl_3$, where M = Ge or Sn. There was evidence for both *trans* and *gauche* forms in the liquid. Variable-temperature Raman data suggest that the *trans* forms is more stable for M = Ge, the *gauche* for M = Sn.[471] The Raman spectra of $^nBuGeX_3$, where X = H or Cl, and $^nBu_2GeCl_2$ show significant differences between νGeC for *trans* and *gauche* conformations (ca. 65 cm^{-1}).[472] IR and Raman spectra were reported and assigned for (8).[473] Raman data were also reported and assigned for the cyclic germylene, (9), with νGeN at 574 cm^{-1}.[474]



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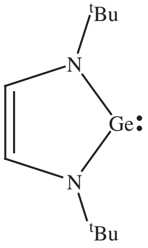

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High-pressure (to 40 GPa) Raman spectra were used to probe pressure-induced phase transitions for β-Ge_3N_4.[475]

The Raman spectra of $xEr_2O_3.(100–x)GeO_2$, where x = 1–10, show change on the Ge–O–Ge angle with increasing x.[476] The Raman spectra of lanthanum borogermanate glasses show differences between hot-extruded and non-extruded samples.[477]

The vibrational spectra of ordered and disordered phases of $MGeS_3$, where M = Sn, Pb, showed characteristic GeS_4 modes. The similarity of vibrational spectra for glasses in the Ge_2S_3–$SnGeS_3$–PbS_3 series suggests that they are isostructural.[478] Polarised Raman data for Pb_2GeS_4 single crystals were analysed in terms of intramolecular vibrations of GeS_4 tetrahedra.[479] The Raman spectra of Ge–Sb–S glasses showed the presence of GeS_4 tetrahedra and SbS_3 pyramids.[480] The Raman spectra of $Ge_{2.5}PS_x$ glasses were dominated by ν_s of $GeS_{4/2}$ tetrahedra, νP=S (near 700 cm^{-1}) was seen for ≥ 63.2 %S, together with some evidence for S–S bonding.[481] The Raman spectrum of thiogermanic acid, $H_4Ge_4S_{10}$ included $\nu_s GeS^-$ 405 cm^{-1}, ν_sGe–S–Ge 354 cm^{-1}, and an a_1 deformation mode at 186 cm^{-1}. IR and Raman bands were also seen for GeS_4 unit modes.[482] The IR and Raman spectra of adamantane-like $M_4Ge_4S_{10}$ crystals, where M = K, Rb or Cs, included νGe–S(terminal) at 473, 479 cm^{-1}.[483]

Variable-temperature Raman spectra gave evidence for temperature-induced phase transitions for $GeSe_2$.[484] A Raman study has been carried out on the structural effects of annealing amorphous Ge_xSe_{1-x}, where x = 0.22–0.28, thin films.[485] The Raman spectra of Ge_xSe_{1-x} glasses show characteristic shifts in the $GeSe_{4/2}$ breathing mode and in νSeSe with changes in germanium concentration.[486] The Raman spectra of melt-quenched $As_xGe_xSe_{1-2x}$ glasses ($0 < x < 0.26$) gave wavenumbers for $Ge(Se_{1/2})_4$ tetrahedral modes for a range of phase types.[487] A Raman spectroscopic study has been made of Ge–Se modes for $MSmGeSe_4$, where M = K. Rb or Cs.[488]

4.4. Tin. – Characteristic Raman bands for $Sn_4{}^{4-}$ units were seen for $A_{23.6}[Sn_4][SnO_3]_{3.4}[O]_3$, where A = Rb, Cs; a_1 modes were in the range 182–197 cm^{-1}, e modes 133–157 cm^{-1}, t_2 modes 92–112 cm^{-1}.[489]

A high-resolution IR study has been made of the ν_2/ν_4 region of $^{116}SnH_4$ (600–850 cm^{-1}).[490] *Ab initio* calculations have been reported for $Sn(C{\equiv}CH)_4$.[491] νSn–C modes were assigned from the IR spectra of $(Me_3Si)_3CSnR_2X$, where R = Me, Ph; X = F, Br, I, NO_3.[492]

IR and Raman spectra of SnX_4(DMPP), R_2SnX_2(DMPP), where X = Cl, Br, I; R = Me, Et, Bu, Ph; DMPP = 3,5-dimethyl-1-(2′-pyridyl)pyrazole, gave skeletal mode assignments. These were consistent with *cis* geometry for the SnX_4 compounds.[493] IR spectra gave assignments to νSnC (424–562 cm^{-1}) and νSnN (453–480 cm^{-1}) for $R_nSn(MNBT)_{4-n}$, where R = Me, n = 2; R=Me, ^{n}Bu, Ph, $PhCH_2$, n = 3; HMNBT = 2-mercapto-6-nitrobenzothiazole.[494]

$\nu SnC_2/\nu SnC_3$ and νSnS (near 310 cm^{-1}) were assigned for the non-linear, non-planar (respectively) units for R_nSnL_{4-n}, where HL = 1-(4-hydroxyphenyl)-1*H*-tetrazole-5-thiol, n = 2, 3; R = Me, Bu, Ph CH_2Ph.[495] Similar assignments were also reported for R_2SnX_2, where HL = 2-pyridinethiol-*N*-oxide, R = ^{n}Bu, Ph, Bz.[496] The IR and Raman spectra of $SnMe_2X_2$(PMP), where X = Cl, Br; PMP = 2-(pyrazol-1-ylmethyl)pyridine, are consistent with approximately linear SnC_2 units, with *ν*SnX modes in the expected ranges.[497] The IR spectra of $[^nBu_2Sn(L)]_2O$, $^nBu_2Sn(L)_2$, where HL = 4′/2′-nitrobiphenyl-2-carboxylic acids, however, show non-linear SnC_2 fragments.[498] Skeletal mode assignments have been proposed from IR and Raman spectra of $R_2(L)SnOSn(L)R_2$, where R = Me, Bu, Ph, and $Bu_2Sn(L)_2$ where HL = anti-inflammatory drug diclofenac.[499]

The Raman spectra of SnO_2 nanotubes include bands at 356 and 576 cm^{-1} not seen for bulk samples.[500] Skeletal (*ν*SnO, *ν*SnN) modes were assigned from IR spectra for $Ph_3SnOOCR$, where R = 2-furanyl, 2-pyridinyl, 3-indolyl, and related.[501] Raman spectra gave skeletal mode assignments (*ν*SnO, *ν*SnCl) for *cis*-$SnCl_4(H_2O)_2$ and $Sn_2Cl_6(OH)_2(H_2O)_2$. The latter has *ν*SnOSn at 482 cm^{-1}.[502] The complex $[Bu_2(DMPA)SnOSn(DMPA)Bu_2]_2$, where HDMPA = 2-[bis(2,6-dimethylphenyl)amino]benzoic acid, has two IR bands (470–490 cm^{-1}) for *ν*SnO – showing non-linear Sn–O–Sn, with *ν*SnO(carboxylate) 200–250 cm^{-1}.[503] The Raman spectra of Li_8MO_6 (M = Sn, Pb) and Li_7MO_6 (M = Sb, Bi), included ν_sMO_6 at 636 cm^{-1} (Sn), 603 cm^{-1} (Pb), 684 cm^{-1} (Sb), 618 cm^{-1} (Bi).[504]

The IR spectra of $SnBr_2[S_2CN(CH_2CH_2)_2O]_2$ and related complexes all show *ν*Sn–S bands in the range 455–462 cm^{-1}.[505]

Ab initio calculations of vibrational wavenumbers for $(SnCl_2)_n$, where n = 1, 2 or 3, are inconsistent with structures suggested earlier.[506]

4.5 Lead. – The Raman spectrum of the mineral laurionite, Pb(OH)Cl, includes *ν*PbO at 328 cm^{-1} and *ν*PbCl at 272 cm^{-1}.[507] IR and Raman spectra of $Pb_4Te_6M_{10}O_{41}$, where M = Nb, Ta, contain *ν*PbO/*ν*TeO modes in the range 670–770 cm^{-1}, and *ν*Pb–O–Tl 416–444 cm^{-1}.[508] Raman spectroscopy was used to characterise a large number of lead-containing minerals. Thus, perite, $PbBiO_2Cl$ has *ν*PbCl/*ν*BiCl 506 cm^{-1}, δClPb(Bi)Cl 157 cm^{-1}.[509]

5 Group 15

5.1. Nitrogen. – Raman spectroscopy was used to follow N_2 incorporation into hard fluorinated carbon films.[510] DFT calculations gave vibrational wavenumbers for the clusters $(HN_3)_n$, where n = 1 – 4.[511] *Ab initio* calculations gave vibrational wavenumbers for XN_3, where X = H, F, Cl or Br, which were used to assign earlier experimental data.[512]

High-resolution FTIR spectra for NH_2Br, in the region of ν_3 (amino wagging band) gave the band origins shown in Table 10.[513] *Ab initio* calculations were reported for the vibrational wavenumbers of $PhEH_2$, where E = N, P or As.[514] A DRIFT study has been made of the effect of the NH_3 environment on chlorinated diamond. There was evidence for δNH_2 and *ν*C=N modes.[515]

Table 10 *High-resolution vibrational assignments for ν_3 of NH_2Br (/cm^{-1})*

	$1^- \leftarrow 0$	$1^+ \leftarrow 0$
^{79}Br	993.4611(6)	993.3899(6)
^{81}Br	993.3200(47)	993.2499(8)

Table 11 *Vibrational assignments for $^{14}ND_2H$ (/cm^{-1})*

ν_{3a}	2430.7990(7)	(s)
	2434.6222(8)	(a)
ν_{3b}	2559.8069(8)	(s)
	2434.6222(8)	(a)
ν_1	3404.238(5)	(s)
	3404.316(5)	(a)

Low-temperature (25–110 K) FTIR spectra of NH_3 gave evidence for 3 solid phases (amorphous, metastable and crystalline).[516] A high-resolution IR study of $^{14}ND_2H$ gave the assignments to symmetric (s) and antisymmetric (as) sublevels shown in Table 11.[517] IR data show that HNCO and NH_3 form a 1:1 adduct in an argon matrix at 10 K. There was also evidence for the formation of $NH_4{}^+OCN^-$ in solid NH_3.[518] The IR spectra of the matrix-isolated photolysis products of formohydroxamic acid (HCONHOH) gave evidence for the formation of HNCO–H_2O and NH_2OH–H_2O complexes.[519] Matrix-IR evidence was also found for the formation of 3 isomeric complexes between HCONHOH and CO.[520]

Matrix-IR spectra of CO/N_2H_4 mixtures show the formation of 3 weak complexes, identified by comparison with *ab initio* and DFT calculations.[521] The variable-temperature IR spectra (-105 – 150°C) of Me_2NNH_2 in liquid krypton show that only the *gauche* conformer is present.[522] DFT calculations gave vibrational wavenumbers for $(XMYH)_n$ rings and clusters, where M = Al, Ga or In; Y = N, P or As; n = 1–6.[523]

Ab initio calculations gave vibrational wavenumbers for 9 isomers of CNNS.[524] A CARS study of the effects of 266 nm. pulsed laser photodissociation of NCNCS showed that the vapour contained both NCNCS and CNCN.[525] IR and Raman spectra, with factor group analysis, gave vibrational assignments for crystalline ammonium dicyanamide, $NH_4[N(CN)_2]$.[526] Variable-temperature Raman spectroscopy was used to follow the solid state transformation of $NH_4[N(CN)_2]$ into $NCN{=}C(NH_2)_2$.[527] *Ab initio* and/or DFT calculations gave vibrational wavenumbers for $CH_2{=}CH{-}N{=}C{=}X$ (X = O, Se);[528] NN–$C(CN)_2$;[529] nitroso-azide, NNN–N=O, and nitro-azide, NNN–NO_2.[530]

High-pressure and –temperature Raman data were used to construct a phase diagram for N_2O.[531] IR spectra have been reported for small N_2O clusters, as particles formed by collisional cooling.[532]

The FTIR spectrum of NO + O_2 co-adsorbed on H–ZSM-5 gave evidence for the formation of the novel species $[ONNO]^+$, with characteristic bands at 2000 and 1687 cm^{-1}.[533,534] IR and Raman spectra (gas, liquid, argon-matrix) of

CF_3ONF_2 were assigned, using *ab initio* calculations, to a single conformer (*syn*, nitrogen lone pair with respect to C–O bond).[535]

There is IR and Raman evidence for a phase transition for nitric acid hydrate, near 200 K.[536] RAIR and *ab initio* calculations gave information on the structure and vibrational wavenumbers for crystalline nitric acid.[537] A DRIFTS study has been performed on the interaction of gas-phase HNO_3 with ice and acid (HCl, HNO_3) hydrate surfaces.[538] An *ab initio* calculation of the vibrational wavenumbers of nitric acid hydrates, $HNO_3.(H_2O)_n$, where n = 1, 2 or 3, has been reported.[539]

The Raman spectrum of an aqueous $NaNO_3$ solution subjected to high-voltage pulsed electric discharge shows characteristic changes to the band position and width of ν_1 (a_1).[540] The IR spectra of magnesium nitrate thin films shows the formation of different hydrates, $Mg(NO_3)_2.nH_2O$, depending on the relative humidity.[541] High-pressure Raman spectroscopy of Na_3ONO_2 showed a cubic to rhombohedral phase transition at 0.79 GPa. Above 14 GPa, the material becomes amorphous.[542] *Ab initio* and DFT calculations of vibrational wavenumbers have been reported for isomers of $ClNO_3$ (showing $ClONO_2$ to be the most stable).[543] High-pressure and −temperature Raman spectroscopy of N_2O_4 showed the formation of the isomer $NO^+NO_3^-$ (above 15.3 GPa).[544]

Detailed IR (gas) and Raman (liquid) spectra gave assignments for $CF_3C(O)N{=}S(F)CF_3$ (supported by *ab initio* calculations), showing that the *anti-syn* conformer is dominant.[545] DFT calculations have been made for vibrational wavenumbers for $XN{=}CF_2$, where X = Cl[546] or Br.[547] The cation $[(Et_3PNI)_2I]^+$ has νN–I at 552 cm^{-1}, ν_{as}N–I–N 293 cm^{-1}.[548]

5.2 Phosphorus. – Resonance Raman spectroscopy gave the excitation profile for νP=P (622 cm^{-1}) for ArP=PAr, where Ar = bis[2,6-(m-xylyl)]phenyl.[549] The low-temperature Raman spectroscopy of P_4 gave the following assignments, corresponding to T_d symmetry: γ-phase – ν_1 599.8 cm^{-1}, ν_2 361.6 cm^{-1}, ν_3 459.0 cm^{-1}; α-phase – ν_1 598.8 cm^{-1}, ν_2 360.6 cm^{-1}, ν_3 458.0 cm^{-1}.[550]

The IR observation of a νP–H band at 2308 cm^{-1} for InP(001) – (2 × 1) shows that a single hydrogen atom is bonded to one end of a buckled phosphorus dimer.[551] IR data have been reported for $[^iPr_2Si\{P(H)Met_2\}_2]_2$, where M = Al, Ga or In, showing νP–H near 2305 cm^{-1} in all cases.[552] High-resolution IR data have been reported for PH_3 and PD_3, in the regions of a number of overtone and combination bands.[553,554]

Ab initio calculations of vibrational wavenumbers for compounds containing C≡P (*e.g.* HC≡P, FC≡P, ClC≡P), C=P (*e.g.* $H_2C{=}PCl$) or C–P (*e.g.* $MePCl_2$) bonds suggest the following 'intrinsic' wavenumbers: C≡P 1250 cm^{-1}, C=P 980 cm^{-1} and C–P 700 cm^{-1}.[555] IR data were reported and assigned for $R_2R'ML_2$, where M = P, As or Sb; R = C_6F_5, Ph; R′ = C_6F_5, $C_6H_5CH_3$-*p*; L = imidazole, indazole or related ligands.[556]

νP=N wavenumbers were assigned from IR spectra for $N_4P_4(NH^nPr)_2Cl_6$, $N_4P_4(NC_4H_8)_6(NH^nPr)_2$ and related systems.[557]

Ab initio calculations gave vibrational wavenumbers for $O{=}PX_iY_jZ_k$, where X, Y, Z = F, Cl, Br; i + j + k = 3,[558] while DFT calculations gave similar data for

O=P(SCN).[559] IR spectra gave the following assignments to νP=X modes for $(Me_3Si)_2HCP(=X)Cl$, where X = O (1252 cm^{-1}), S (673 cm^{-1}), Se (574 cm^{-1}).[560]

The Raman spectrum of $P(OPh)_3$ shows no hydrogen bonding in the liquid or glassy states.[561] *Ab initio* calculations gave vibrational wavenumbers for HPO_3 isomers.[562] IR and Raman spectra showed characteristic phosphite bands for $[Ga_{0.98}Cr_{0.02}(HPO_3)F_3]^{2-}$.[563] *Ab initio* calculations gave a set of predicted vibrational wavenumbers for $O_3PSO_3{}^{3-}$ and related species.[564]

IR and Raman spectra gave assignments to phosphate modes in Li_xFePO_4, where $0 \leq x \leq 1$.[565] DFT and molecular modelling calculations gave vibrational wavenumbers for $PO_4{}^{3-}$ in an aqueous environment.[566] *Ab initio* calculations enabled assignments to be proposed from IR and Raman spectra of various isomers of $PO_4{}^{3-}(H_2O)_n$, where n = 0 – 6, Na^+ or K^+ salts.[567] High-temperature Raman spectra of Na_3PO_4 crystals showed phase transitions, at 600 and 1773 K.[568] IR and Raman spectra were used to characterise a number of phosphate-containing minerals.[569,570] IR and Raman spectra were able to determine the structural behaviour within the system B_2O_3–Li_2O–$Zn_3(PO_4)_2$.[571]

Raman spectroscopy was used to identify several crystalline polymorphs of P_2O_5.[572] An *ab initio* calculation of vibrational wavenumbers for a lithium metaphosphate glass, Li_2O–P_2O_5, gave good agreement with experiment.[573] The IR spectra of xFeO.(1–x)P_2O_5 glasses show that the three-dimensional P_2O_5 network is replaced by a two-dimensional network on increasing the concentration of FeO.[574] Several studies have been made of IR and/or Raman spectra for systems containing $P_2O_7{}^{4-}$ anions.[575–578]

Ab initio and DFT calculations of vibrational wavenumbers for P_4O_{10} gave good agreement with experiment.[579] The IR and Raman spectra of $Li_6P_6O_{18}$ were assigned with the help of *ab initio* calculations for the P_6O_{18} ring unit.[580]

DFT calculations of vibrational wavenumbers have been carried out for *O*,*O′*-diethyl-*N*-(α-aryloxyacetyl)thiophosphoryl hydrazine molecules.[581] νPS and νSS features were assigned from the Raman spectrum of $Rb_4Ta_4P_4S_{24}$.[582]

Assignments to anion modes were proposed from the IR and Raman spectra of $[X][MF_6]$, where M = P, As or Sb, X = [poly(ethylene oxide)]$_6Li^+$ or related.[583] DFT calculations have been carried out on P_2Cl_4 (C_{2h} symmetry) to obtain values of vibrational wavenumbers.[584]

A high-resolution study of the $b^1\Sigma^+(b0^+) \rightarrow X^3\Sigma^-(X0^+)$ transition of PI gave the following values: $(X0^+)$ ω_e 371.296(4) cm^{-1}, $\omega_e x_e$ 1.3302(9) cm^{-1} and $(b0^+)$ ω_e 400.165(6) cm^{-1}, $\omega_e x_e$ 1.345(2) cm^{-1}.[585] *Ab initio* and DFT calculations of vibrational wavenumbers were reported for P_2I_4 (C_{2h} symmetry).[586]

5.3 Arsenic. – DFT calculations have been reported for the vibrational wavenumbers for the cage units As_n, where n = 4, 8, 20, 28, 32, 36 or 60.[587] The first report has been made of vibrational data for pure, solid $E(N_3)_3$, where E = As or Sb; some assignments are given in Table 12.[588]

Raman spectroscopy was used to characterise a range of arsenate minerals of the vivianite type.[589] IR and Raman spectra were assigned on the basis of factor group analysis for $Cd_2As_2O_7$, Table 13.[590] *Ab initio* calculations have given values for the vibrational wavenumbers for As_4O_6.[591]

Table 12 *Vibrational assignments for $E(N_3)_3$ (/cm^{-1})*

	$E =$	*As*	*Sb*
a	$\nu_s EN_3$	465	386
	$\delta_s EN_3$ in-phase	307	289
	δE–N–N in-phase	102	115
e	$\nu_{as} EN_3$	420	370
	δEN_3 out-of-phase	257	264/247
	δE–N–N out-of-phase	135	153/141

Table 13 *Vibrational assignments for $Cd_2As_2O_7$ (/cm^{-1})*

ν_{as}AsOAs	953 (IR)
$\nu_s AsO_3$	880 (Raman)
$\nu_{as} AsO_3$	854, 812 (IR), 810 (Raman)
$\delta_{as} AsO_3$	472, 393 (IR), 489, 358 (Raman)
ν_sAsOAs	423 (Raman)

Table 14 *Vibrational assignments for Sb_4O_6 (/cm^{-1})*

ν_1	ν_sSbOSb	451	(a_1)
ν_s	δ_sSbOSb	253	(a_1)
ν_7	νSbOSb	709	(t_2)
ν_8	νSbOSb	373	(t_2)

Structural units in glasses $(As_2S_3)_{100-x}(AsSe_{0.5}Te_{0.5}I)_x$ were characterised using IR and Raman spectroscopy.[592] Raman data have been reported for vacuum-evaporated layers of $As_{40}S_{60-x}Se_x$.[593]

IR and Raman spectra were reported and assigned for AsF_4^- as Na^+, Rb^+, Cs^+ and NMe_4^+ salts.[594] IR and Raman data for $M_2Cl_9^{3-}$, where M = As, Bi, included νAsCl 366, 325, 313 cm^{-1}; νBiCl 288, 238 cm^{-1}.[595] Lattice dynamics calculations gave vibrational wavenumbers for solid AsI_3.[596]

5.4 Antimony. – The complex (Fc)C(Me)=CH$(COO)_2SbPh_3$, where Fc = ferrocenyl, has νSbC at 461 cm^{-1}.[597]

νSbO bands were seen in the range 405 – 420 cm^{-1} in the IR spectrum of $[(C_6F_5)_2SbL_3]^{2+}$, where L = dmso, Ph_3AsO, pyO, dmf.[598] IR bands for $LaSb_3O_9$ include: νSbO 860, 804, 736 cm^{-1}; νSb–O–Sb 690, 653, 553, 526, 507 cm^{-1}, δO–Sb–O 484, 402 cm^{-1}.[599] Table 14 summarises some assignments made from the IR and Raman spectra of Sb_4O_6 (assisted by *ab initio* calculations).[600]

The IR and Raman spectra of $Ag^+(Sb_2F_{11})^-$ gave detailed anion mode assignments, including νSb–F–Sb 490, 475 cm^{-1}, νSb–F(eq) 585 – 692 cm^{-1}, νSb–F(ax) 697– 722 cm^{-1}.[601]

5.5 Bismuth. – FTIR data revealed first overtone bands from the very short-lived species BiH_3, near 3405 cm^{-1}.[602] νBiC modes were seen in the range

458 – 480 cm^{-1} for $Ar_3Bi(O_2CCHR^1CHR^2GePh_3)_2$, where Ar = Ph, 4-Me-, 4-F-, 4-Cl-, 4-Br–C_6H_4; R^1 = H,Me; R^2 = H, Ph.[603]

The Raman spectra of glasses from the systems xMnO.(100 − x)Bi_2O_3 and xMnO.(100 − x)[Bi_2O_3.MO] (MO = GeO_2, As_2O_3) contained features due to BiO_6 octahedra.[604] IR and Raman spectra of homogeneous glasses in the system MnO–Bi_2O_3–CdO gave evidence for BiO_3 and (predominantly) BiO_6 units.[605]

S–Bi–S modes were seen in the range 220–351 cm^{-1} in the IR spectra of $[Bi(dmit)_2]^-$, where H_2dmit = 4,5-dimercapto-1,3-dithiol-2-thione.[606]

6 Group 16

6.1 Oxygen. – IR spectroscopy was used to characterise O_2 molecules trapped in vacancies in silicon crystals.[607] The high-pressure Raman spectrum of O_2 (to 134 GPa) shows significant Raman intensity in the metallic phase, showing that this still retains molecular character.[608] High-resolution IR spectra were reported for a number of isotopomers of O_3 for a variety of fundamental and overtone/combination bands.[609–611]

Ab initio calculations of vibrational wavenumbers for D_2O gave detailed results on IR and Raman intensities.[612] High-resolution Raman spectra of vapour-phase H_2O, HOD and D_2O gave a very detailed interpretation of line intensities for ν_2 bands.[613]

High-pressure and −temperature Raman spectra of liquid H_2O gave evidence for hydrogen-bonding discontinuities.[614] Hydrogen-bond energy dispersion for dilute HDO in H_2O was determined from Raman intensities. Strong hydrogen-bonds give a feature near 2440 cm^{-1}, weak or broken hydrogen-bonds in the range 2650–2675 cm^{-1}.[615] Combined *ab initio* and molecular dynamics calculations have been reported for IR bands of dilute HOD in liquid H_2O or D_2O.[616] High-pressure Raman studies of the stretching band of liquid H_2O at 290 K were carried out to 6 kbar. The results were consistent with the known behaviour of the O . . . .O distance at increasing pressure.[617] Raman spectroscopy was used to probe the nature of water in aqueous solutions of zwitterionic surfactants.[618]

IR data were reported for size-selected $H^+(H_2O)_n$ clusters, where n = 6 – 27.[619] Argon photodissociation spectra gave νOH values for $Cl_2^-.nH_2O$. For n = 1 or 2, the presence of a single band suggests that the H_2O molecules bond symmetrically to the ion.[620] The IR spectra of argon-solvated X^-.HDO species, where X = F or I, show that they are preferentially F^-.HOD, I^-.DOH respectively.[621] DFT and *ab initio* calculations gave vibrational wavenumbers for $CsOH(H_2O)_n$, where n = 0 – 4.[622]

The IR spectrum of H_2O in solid neon gave assignments to $(H_2O)_2$ modes.[623] Matrix isolation studies of H_2O, D_2O and HOD in solid parahydrogen gave evidence for the formation of a range of cluster species.[624] Raman spectroscopy was used to study changes in low-density amorphous ice and hyperquenched glassy water, on annealing at 1 bar.[625] Variable-temperature and −pressure IR spectra of ice-VII, -VIII, -X in the ranges 12–298 K, 2–100 GPa, gave data in agreement with previous Raman data. A triple point was found at 100 K/62

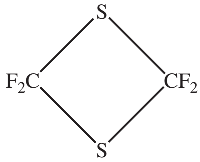
GPa.[626] Phase transitions of H_2O ice were investigated by IR spectroscopy (0.2–50 GPa, 20–298 K).[627]

A high-resolution FTIR study of ν_3 for HOBr gave band origins 620.22855(25) cm^{-1} (^{79}Br), 618.90606(25) cm^{-1} (^{81}Br).[628] IR data have been reported and assigned for the argon-matrix isolated complex $HOOH.O_3$.[629] Matrix-isolation IR data for the complex HOOH–HOO gave the following assignments: ν_1 3433 cm^{-1}, ν_2 1429 cm^{-1}, ν_3 868 cm^{-1}, ν_5 3574/3579 cm^{-1}, ν_6 1285 cm^{-1}.[630]

Oxygen-matrix IR data were reported and assigned (using *ab initio* calculations) for the radical CF_3OOO, for all-^{16}O and $^{16}O^{18}O^{18}O$ forms.[631] Assignments for H_2OOO^+ isolated in solid argon included $\nu_{as}OH$ 3430.7 cm^{-1}, ν_sOH 3341.7 cm^{-1} cm^{-1}, $\nu H_2O–O_2$ 731.0 cm^{-1}. For D_2OOO^+, νO–O was seen at 1601.1 cm^{-1}.[632]

Microwave discharge on HCOOH in a neon matrix gave IR bands assignable to *trans*-HOCO, *trans*-HCOOH and HCO_2^-.[633] Among products identified by IR spectroscopy from the effects of microwave discharge on an H_2/CO_2 mixture in a neon matrix are $HOCO^+/DOCO^+$.[634]

6.2 Sulfur. – *Ab initio* calculations gave vibrational wavenumbers for 8 isomers of S_4.[635] The irradiation of H_2S + CO in an argon matrix formed *trans*-HSCO, with νC=O 1823.3 cm^{-1}, δH–S–C 931.6 cm^{-1}, νC–S 553.3 cm^{-1} (confirmed by DFT calculations).[636] DFT calculations gave vibrational wavenumbers for (10).[637]



(10)

Experimental IR and Raman spectra and *ab initio* calculations gave vibrational wavenumbers for $CS_2N_3^-$ ions, and derivatives containing pseudohalide groups, *e.g.* CS_2N_3NCS.[638] *Ab initio* calculations gave vibrational wavenumbers for $S(N_4)_n$, where $n = 1$, 2 or 3.[639]

The UV spectrum of matrix-isolated cyclic–S_2O contained a progression of bands with intervals of about 580 cm^{-1}. This agrees with earlier IR data, which showed $\nu_{as}SO$ at 574.9 cm^{-1}.[640] The radical ClSO was detected by FTIR spectroscopy, with ν_1 (νS=O) centred at 1162.9 cm^{-1}.[641]

A detailed study of line intensities and self-broadening coefficients has been reported for ν_1 of SO_2 (1088 – 1090 cm^{-1}).[642] UV irradiation of $HONO/SO_2/X$, where $X = N_2$ or Ar, has been carried out. In N_2, there was evidence for the $HOSO_2$ radical and $HO(NO)SO_2$. In Ar, only the latter is seen.[643] DFT calculations were carried out to give vibrational wavenumbers for SO_2X_2, where X = F, Cl or Br.[644] *Ab initio* calculations gave vibrational wavenumbers for X–EO_2–NCO, where X = F, Cl, E = S, Se.[645]

IR and Raman spectra were reported and assigned for FSO_2NH_2 and $FSO_2NS(O)F_2$ (using DFT and *ab initio* calculations). Each molecule appears to exist only as single conformer (C_s, C_1 respectively).[646] IR and Raman spectra gave detailed assignments (together with *ab initio* calculations) for CF_3OSO_2Cl *e.g.* $\nu_{as}SO_2$ 1460 cm^{-1}, ν_sSO_2 1224 cm^{-1}, νO–S 787 cm^{-1} (all data from argon matrix).[647] The IR and Raman spectra of $CF_3SO_2OCH_2CF_3$ were assigned using DFT calculations.[648] There have been two high-resolution IR studies of ν_1 (1004.662(24) cm^{-1}), ν_2 (477.50864(5) cm^{-1}), ν_3 (1330.07792(2) cm^{-1}), and ν_4 (502.05565(4) cm^{-1}) for $^{34}S^{18}O^{3}$.[649,650]

An IR and Raman study of hydrogen-bonding has been reported for $M_4LiH_3(EO_4)_4$, where E = S, M = K, Rb, Cs; E = Se, M = K.[651] The IR and Raman spectra of $Rb_{0.33}P_{0.4}S_{2.23}O_x$ suggest the presence of $S_n{}^{2-}$ (n = 3 or 4) anions, and possibly $P_4S_6O^{6+}$ fragments.[652] The Raman spectra of samples in the liquid $Cs_2S_2O_7$–$CsHSO_4$ system were interpreted in terms of a temperature dependent equilibrium between $HSO_4{}^-$, $S_2O_7{}^{2-}$ and H_2O.[653]

A high-resolution FTIR study of the $\nu_2 + \nu_4$ combination band of $^{32}SF_6$ was used to obtain a detailed analysis of this level.[654]

6.3 Selenium.

– Nitrogen-matrix IR spectra were reported for Na_2Se_n clusters. Bands were consistent with selenium chains capped at each end by sodium.[655] Raman spectroscopy was used to characterise hexagonal selenium nanowires.[656] DFT calculations gave vibrational wavenumbers associated with Cl impurities in amorphous selenium.[657]

Ab initio calculations have given vibrational wavenumbers for $SeCF_3{}^-$.[658] There is IR evidence for the formation of surface species [≡SiO–Se(O)OEt] by interaction of $(EtO)_2SeO$ with Aerosil silica, with νSe=O 873 cm^{-1}, νSi–OSe 917, 935 cm^{-1}.[659]

6.4 Tellurium.

– The IR spectra of $RR'TeCl_2$, where R = $PhCOCH_2$, 1-naphthacyl, styrylacyl; R′=*p*-anisyl, *p*-hydroxyphenyl, 3-methyl-4-hydroxyphenol, show bonding of Te to the acyl carbon of the R group and to the *para* carbon (with respect to OH or OMe) of the aryl group.[660]

The IR and Raman spectra of glassy TeO_2 show that the structure approximates to that of the γ-crystalline phase.[661] The Raman spectra of TeO_2–Ga_2O_3 glasses were used to probe the effect of added Ga_2O_3 on the coordination geometry of tellurium.[662] νP–O, νTeO and νTe–O–M were assigned from the IR and Raman spectra of $BaMTeO_4(PO_4$, where M = Nb or Ta.[663]

The IR spectra of $Te[S(CH_2)_nSC(O)OCH_3]_2$, where n = 2, 3 or 4, include νTeS bands in the range 332–353 cm^{-1}.[664] The IR and Raman spectra of tellurium(IV) complexes in CH_2Cl_2 solution gave evidence for equilibria involving $TeCl_5{}^-$ and $TeCl_6{}^{2-}$.[665]

7 Group 17

Neon-matrix IR spectra were reported for $(HF)_2$, $(DF)_2$ and (HF)(DF). Assignments for $(HF)_2$ are shown in Table 15.[666]

The IR spectra of the N_2–HF complex have been reported for neon matrices (in the range 20–8000 cm^{-1}). There was evidence for two distinct sites, *e.g.*

Table 15 *Vibrational assignments for* $(HF)_2$ *(/cm^{-1})*

ν_1	3918.5
ν_2	3848.8
ν_6	409.7
ν_5	182.1
ν_4	141.3

intermolecular bands at 103.0 cm^{-1} (site A) and 81.4/87.1 cm^{-1} (site B).[667] FTIR data (νHF bands) have been reported for the complexes X.HF, where X = Xe, CO_2, CO, HCN, MeCN.[668] Theoretical values of vibrational wavenumbers were reported for $(Ar)_n(HX)_m$, where X = F, Cl.[669] Rotationally-resolved vibrational data have been obtained for $(H_2)_n$–HF and $(D_2)_n$–HF, where n = 2 – 6, in helium droplets (νHF bands).[670] *Ab initio* calculations have been made for vibrational wavenumbers for the hydrogen-bonded species HF–HO_2.[671]

Ab initio calculations also gave vibrational wavenumbers for $HF_2^-.CH_3CH_2OH$.[672] The IR spectrum of $[Rh_3(\mu_3\text{–}OH)_2(COD)_3](HF_2)$ included νFHF of the anion at 1954 cm^{-1}.[673] There is IR and Raman spectroscopic evidence for the formation of $(FH)_xF^-$, where x = 1 – 3, in $Me_4NF.m$HF melts, where m = 3.0 – 5.4.[674]

Ab initio calculations have given vibrational wavenumbers for $Cl^-.H_2/D_2$ complexes,[675] and for $HCl(NH_3)_n$ clusters, where n = 1 – 4.[676] High-resolution far-IR spectroscopy for the OC–$H^{35}Cl$ heterodimer showed that the band origin of the HCl libration band, $\nu_4{}^1$, was 201.20464(27) cm^{-1}.[677] DFT calculations gave vibrational wavenumbers for the adduct $H_2O.ClO$.[678]

A high-resolution IR study of the Kr.HBr complex gave νHBr values of 2557.17899(6) cm^{-1} (^{79}Br) and 2556.79705(8) cm^{-1} (^{81}Br).[679] IR spectra of supersonic jets of $(HBr)_2$ gave assignments to ν_1 and ν_2 bands of $(H^{79}Br)_2$, ($H^{79}Br$-$H^{81}Br$) and $(H^{81}Br)_2$ (2500 – 2600 cm^{-1}).[680]

The Raman spectrum of Me_2dazdt.IBr, where Me_2dazdt = *N,N′*-dimethylperhydrodiazepine-2,3,-dithione, shows ν_3 and ν_1 of the S–I–Br unit at 162, 145 cm^{-1} respectively.[681] Far-IR data were reported for solid I_2 at pressures up to 10 GPa.[682] The Raman spectrum of iodine-doped $I_8Si_{44}I_2$ clathrate gave bands at 75 and 101 cm^{-1} due to guest iodine atoms in host silicon cages.[683] *Ab initio* calculations gave vibrational wavenumbers for isomers of HIO and HIO_2.[684]

8 Group 18

Vibrational wavenumbers were predicted for NeHF and NeDF from *ab initio* calculations.[685] $Ar_nH_3^+$ clusters produced by laser vaporisation showed a characteristic IR band near 350 cm^{-1}.[686] *Ab initio* calculations gave vibrational wavenumbers for HArF.CO and HKrF.CO,[687] as well as for X . . . HKrCl, where X = N_2, OC, HF. All of the latter are predicted to have higher νH–Kr wavenumbers than the parent monomer.[688]

Matrix-IR evidence has been obtained for the formation of HXC_4H, where X = Kr or Xe, with νX–H at 1290 cm^{-1} (X = Kr) or 1532 cm^{-1} (Xe). These assignments were supported by *ab initio* calculations.[689]

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Vibrational Spectra of Transition Element Compounds

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1 Scandium, Yttrium and the Lanthanides

Laser-ablated scandium atoms react with MeOH to form matrix-trapped products, including MeOScH, for which IR assignments are summarised in Table 1 (data referring to an argon matrix).[1]

The IR spectra of endohedral $Li_{3-x}M_xN@C_{80}$, where $0 < x < 3$, M = Sc, Y, Tb, Ho or Er, include vibrations of an encaged trimetal nitride cluster.[2] The Raman spectra of the D_{2d} symmetry species $M_2@C_{84}$, where M = Sc, Y or Dy, show three groups of metal-cage modes in the range 35–200 cm^{-1}. Variable-temperature data for M = Y shows that there is an order/disorder transition near 150 K.[3]

FT Raman (near-IR excitation) and UV-Raman spectra were used to study tetragonal-monoclinic transitions in $(ZrO_2)_{0.98}(M_2O_3)_{0.02}$, where M = Sc or Y. It was found that the temperature of the transition depends on the calcination temperature of the samples.[4] High-pressure Raman spectra of $Sc_2(MoO_4)_3$ gave evidence for two phase transitions, leading to an amorphous state.[5]

IR and Raman spectra gave characteristic bands for the hydrides YH_x, where $2 \leq x \leq 3$.[6] *Ab initio* calculations gave vibrational wavenumbers for solid YH_3.[7]

The tetragonal to monoclinic phase transitions for M_2O_3–ZrO_2, where M = Y or La, were followed by UV Raman spectroscopy.[8] The Raman spectra of

Table 1 *Vibrational mode assignments for Sc + CH_3OH reaction products (/cm^{-1})*

$HScOCH_3$	δCH_2	1167.4
	νSc-H	1482.7
	νCO	1158.5
	νSc–OH	562.2
$OScCH_3$	νScO	912.7
$ScOCH_3$	νCO	1154.3
	νSc–OH	583.5

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Yb^{3+}-doped YAG crystals show Y- and Yb-based modes at wavenumbers below 450 cm^{-1}.[9]

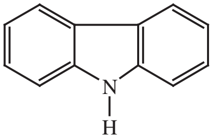
High-pressure Raman spectra show that there is a cubic to orthorhombic phase transition near 10GPa for LaB_6.[10] One report suggests that Raman bands seen at 161, 196 cm^{-1} respectively for $M_2@C_{80}$, where M = La or Ti, can be assigned to movements of the trapped metal in the cage.[11] Another report of the Raman spectrum of $La_2@C_{80}$, however, describes a feature seen at 163 cm^{-1} as a synchronously-coupled mode of the [80]fullerene cage elongation with νLa–La, rather than as a La–C_{80} mode.[12] Characteristic Raman bands were observed and assigned for $LaCrO_3$ for both low-temperature (orthorhombic) and high-temperature (rhombohedral) forms (with the transition between the two forms near 255°C).[13] Bands assignable as νLn–Cl were seen in the range 220–240 cm^{-1} in the IR spectra of $[LnCl_2(OPPh_3)_4]^+$, where Ln = La–Lu, except Pm.[14]

Raman data have been reported for MB_6, where M = Ce, Pr or Yb.[15] The Raman spectrum for thin $Ce@C_{82}$ films includes a band near 160 cm^{-1}, assigned as a Ce–C_{82} cage mode, and consistent with the formal presence of Ce^{3+}.[16]

Raman spectra gave assignments to a feature associated with Ce–O bonds in CeO_2 and mixed Ce/Tb oxides.[17] IR and Raman data for CeO_2–ZrO_2 powders show that the structure is predominantly cubic, but with some evidence for a tetragonal phase.[18] The Raman spectra of molybdenum-containing ceria show features associated with molybdena at high molybdenum coverages.[19]

Raman spectroscopy was used to characterise WO_x/CeO_2 catalysts. There was little evidence for the presence of WO_3.[20] Bands assignable as νM-O features were seen in the Raman spectra of MgO–CeO_2–MnO catalysts.[21]

High-temperature Raman spectra of $Ca_{3-3x}Nd_{2x}(AO_4)_2$, where A = P or V; $0 \leq x \leq 0.14$, gave evidence for reversible phase transitions.[22] The IR and Raman spectra of $[Nd(L)_2Cl_3]_2$, where L = biglycinato, were assigned with the aid of normal coordinate analyses.[23]



(1)

The Raman spectra of $Ln(L)_4$, where Ln = Eu, Yb, HL = (1), include bands due to νLn–L modes, *e.g.* for Ln = Eu, 203, 178, 152 cm^{-1}, Yb, 193, 176, 151, 136, 94 cm^{-1}.[24] The complex GdL, where H_3L = diethylenetriamine-inositol-bi-ester-*N,N',N''*-triacetic acid, has an IR band at 549 cm^{-1}, which may be assignable as νGd–O.[25] *Ab initio* calculations have been reported for vibrational wavenumbers for GdX_3, where X = F or Cl.[26] IR reflectance spectra of $Ln_3Al_5O_{12}$ garnets, where Ln = Dy, Er, gave evidence for νLn–O bands below 200 cm^{-1}.[27] The complex $Ho_2Cl_6(PhCN)_6$ gives IR bands from νHo–N as follows: 270/261, 214, 190, 183 cm^{-1}.[28]

2 Titanium, Zirconium and Hafnium

Previous reference has been made to vibrational studies on $Ti_2@C_{80}$;[11] $(ZrO_3)_{0.98}(M_2O_3)_{0.02}$ (M = Sc, Y);[4] M_2O_3–ZrO_2 (M = Y, La);[8] and CeO_2–ZrO_2 powders.[18]

The resonance Raman spectrum of Ti_2 in argon, krypton and xenon matrices show a decrease in νTiTi from Ar (403.71/405.79 cm^{-1}) to Kr (399.43 cm^{-1}) and Xe (375.9/368.3 cm^{-1}).[29]

Ab initio calculations have been made of vibrational wavenumbers for metallocarbohedrene clusters, M_8C_{12}, where M = Ti or Mo.[30] Similar calculations were reported for isomeric forms of $M@Si_{16}$ clusters, where M = Ti or Zr.[31]

IR and Raman spectra gave skeletal mode assignments for $[Ti(N_3)_n]^{(4-n)-}$, where n = 4, 5 or 6. For example, Raman bands to which νTiN contribute were seen at 472, 454, 391, 371 cm^{-1} (n = 4); 445, 438, 412, 398, 363, 355 cm^{-1} (n = 5) and 398, 316, 307 cm^{-1} (n = 6).[32]

The complex anion $[HPTi(O_2)W_{11}O_{39}]^{4-}$ has IR bands at 630 and 690 cm^{-1}, assigned as ν_s, ν_{as} (respectively) of the $Ti(O_2)$ unit.[33] The Raman spectra of aqueous sulphuric acid solutions containing titanium indicate the presence of $Ti(OH)_2(SO_4)_2(H_2O)_2^{2-}$.[34] The Raman spectrum of a well-characterised TiP_2O_7 catalyst has ν_1 of TiO_6 at 620 cm^{-1}, with ν_6 at 275/240 cm^{-1} (together with PO_3 and P–O–P modes.[35] IR and Raman spectroscopy were used to characterise TiO_2 nanosized powders formed by $TiCl_4$ laser pyrolysis.[36]

Raman spectroscopy was used to characterise densely-assembled TiO_2 nanorods (diameters 150–200 nm).[37] High-temperature Raman spectra of nanocrystalline TiO_2 powders (25–1200°C) were used to monitor temperature-dependent effects on the samples.[38] The effects of UV irradiation on the structure of sol-gel TiO_2 films were followed by IR and Raman spectroscopy.[39]

Pressure-induced phase transformations for anatase-TiO_2 were monitored by Raman spectroscopy.[40] Raman spectroscopy was used to characterise rutile titania nanocrystalline particles with high specific surface areas.[41] Micro-Raman spectra were used to follow surface transformations induced by excimer laser irradiation of TiO_2.[42] There was Raman spectroscopic evidence for modification of a titania surface by attached gold nanoparticles.[43]

Raman spectroscopy was used to characterise mixed oxides CeO_2–MO_2, where M = Ti, Zr, Si.[44] The structures of nanostructurally assembled V_2O_5 doped with titanium, and TiO_2 doped with vanadium, were determined by Raman spectroscopy.[45] IR spectra were able to characterise sol-gel produced quaternary reactive powders in the $MgO.Al_2O_3$–$Al_2O_3.TiO_2$–$3Al_2O_3.2SiO_2$ system.[46] TiO_2/Fe_2TiO_5 composites were characterised using FTIR and Raman spectra.[47]

$CaTiO_3$-based solid solutions, such as $CaTiO_3$–$MM'O_3$, where M = Sr, M' = Ti; M = Ca, M' = Zr; M = Nd, M' = Al; M = La, M' = Ga, were studied by Raman spectroscopy.[48] Hyper-Raman scattering by $SrTi(^{18}O_x{}^{16}O_{1-x})_3$ single crystals led to the observation of the Raman-inactive e_u mode.[49] Raman spectroscopy showed the absence of phase transitions in the range 5–325 K for epitaxial $BaTiO_3$ thin films.[50] Raman data were used to characterise nanometer-sized $BaTiO_3$ crystallites.[51] Structural characterisation of barium titanate thin films deposited by pulsed laser deposition on a (001) MgO substrate was achieved by Raman spectroscopy.[52]

High-pressure Raman spectroscopy on $BaTi_{0.65}Zr_{0.35}O_3$ reveal phase transitions near 5.7 and 15.1 GPa.[53] The effects of irradiation on titanate and niobate glasses were followed by Raman spectroscopy. There was evidence for the formation of Ba_2TiO_4 crystals, $TiO_4{}^{4-}$ anions, $LiNbO_3$ crystals and $NbO_6{}^{7-}$ anions respectively.[54]

The IR spectrum of rhombohedral $Pr(Ti,Zr)O_3$ included characteristic νMO ($M = Ti, Zr$) modes.[55] High-pressure, low-temperature Raman spectra on $PbZr_{0.52}Ti_{0.48}O_3$ were used to follow phase transitions.[56] Strong IR bands near 410 and 600 cm^{-1} for $(Pb,Fe)TiO_3$ and $(Sr,Fe)TiO_3$ ceramics were ascribed to TiO_6 and FeO_6 polyhedra respectively.[57] FT Raman spectra of nanosized $MnTiO_3$ included features due to Ti–O–Mn bonds.[58]

Raman spectroscopy was used to characterise molecular sieves $Na_2Nb_{2-x}M_xO_{6-x}(OH)_x.H_2O$, where $M = Ti$ or Hf, $x \leq 0.2$, and the parent compound $Na_2Nb_2O_6.H_2O$.[59] *Ab initio* calculations were reported on the vibrational wavenumbers for the titanium-containing zeolite titanium affretite.[60] Raman spectra of titanium-aluminophosphate and –silicoaluminophosphates gave evidence on the coordination environment of titanium(IV) centres.[61]

The resonance Raman spectrum of the titanium silicalite-1 catalyst shows significant effects on TiO_4 modes on addition of H_2O, NH_3 or H_2O_2 to the system.[62] An *ab initio* calculation of the vibrational wavenumbers for the titanosilicate ETS-10 (using a one-dimensional chain model) shows that the band at 725 cm^{-1} is due to νTiO, involving only apical oxygen.[63] Variable-temperature Raman spectra of $Bi_4Ti_3O_{12}$ films on SiO_2 substrates showed a phase transition in the range 473–573 K.[64] Characteristic Raman bands were seen at 314 and 464 cm^{-1} for the ferroelectric $Sr_2Bi_4Ti_5O_{18}$.[65]

The complex $Ti_6O_6(O^iPr)_6(OOC^tBu)_6$ shows an IR band at 732 cm^{-1} due to νTi–O of the non-linear $\{[Ti(\mu\text{-}O)]_3\}_2$ cluster. Bending modes of this unit were seen at 317 and 302 cm^{-1}.[66] Raman spectroscopy was used to characterise thin films of $Ca_{1-x}Mg_xCu_3Ti_4O_{12}$.[67] Raman spectra of solid solutions $Ba_{6-3x}Sm_{8+2x}Ti_{18}O_{54}$ included bands due to TiO_6 vibrations at 590 cm^{-1} (symmetric stretch of basal oxygens), 280 and 232 cm^{-1} (symmetric tilting modes of TiO_6).[68]

IR spectroscopy was used to characterise the anions $[TiF_4(SO_4)_2]^{2-}$, $[TiF_2(SO_4)_2]^{2-}$ and $[Ti_3O_2F_2(SO_4)_4]^{4-}$.[69] νTiF was seen in the IR spectrum of $[Ba_8Ti_6F_{30}I_2(Cp^*)_6(hmpa)_6]^{2+}$; the single peak shows the high symmetry of the core of this complex.[70]

IR spectra were used to study the phase transition of $[NH_3(CH_2)_5NH_3]TiCl_5$ at 316K.[71] νTiX modes were assigned for the IR spectra of $TiX_4(L)$, where $X = Cl, Br$; $L = MeC(CH_2EMe)_3$ ($E = S, Se$), *e.g.* νTiCl bands for $E = S$ were seen at 411, 399, 389 and 379 cm^{-1}.[72]

Bands due to νZrO (530–540 cm^{-1}) were assigned from the IR spectra of $(acac)_2ZrL_2$, where $L =$ ON=C(Me)-py-2; ON=C(Me)fu-2; OCH_2CH_2OMe; $OCH_2CH_2O^nBu$, $OSiPh_3$ and related (fu = furan).[73]

The IR spectrum of a new polymorph of ZrO_2 (orthorhombic) indicates the presence of a severely puckered structure.[74] Raman spectroscopy was used characterise ZrO_2 films deposited by RF magnetron sputtering on zircaloy-4 substrates.[75] High-pressure Raman spectroscopy was used to follow pressure-induced phase transitions in nanocrystalline ZrO_2.[76] There is FTIR evidence for the formation of ZrO_2 on phase separation of zirconium silicates.[77] The Raman spectra of tetragonal zirconia nanowires included bands at 120, 461 and 629 cm^{-1}. These were assigned to e_g, e_g and b_{1g} phonon modes respectively.[78] Raman spectroscopy was used to follow the effects of laser-shock compression on yttria-doped tetragonal zirconia – bands due to monoclinic zirconia appeared.[79]

The following assignments were proposed for νMO_6 modes from the Raman spectra of Li_8MO_6 (M = Zr, Hf) and Li_7MO_6 (M = Nb, Ta): (M = Zr) 668 cm^{-1}, (Hf) 677 cm^{-1}, (Nb) 790 cm^{-1}, (Ta) 759 cm^{-1}.[80] The IR spectrum of $Zr_4O_3(OH)_7(OAc)_3$ led to a tentative vibrational assignment.[81]

3. Vanadium, Niobium and Tantalum

Previous reference has been made to vibrational studies on $Ca_{3-3x}Nd_{2x}(VO_4)_2$;[22] Ti-doped V_2O_5;[45] $LiNbO_3$ crystals;[54] $Na_2Nb_{2-x}M_xO_{6-x}(OH)_x.H_2O$ (M = Ti, Hf; $x \leq 0.2$);[59] and Li_7MO_6 (M = Nb, Ta).[80]

The Raman spectra of $Cp_2V(OOCR)_2$, where R = H, CCl_3, CF_3, include a band in the range 275–290 cm^{-1} due to a ring-tilting of Cp in a bent Cp_2V^{2+} fragment.[82]

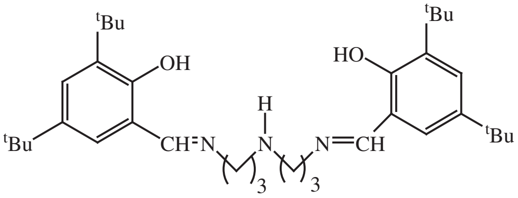
Skeletal mode assignments have been proposed for matrix-isolated $VCl_4.NH_3$ and Cl_3VNH_2 (and related isotopomers), *e.g.* for Cl_3VNH_2, νV–N is at 729 cm^{-1}, and $\nu_{as}VCl_2$ at 453 cm^{-1}.[83] IR bands due to νV–N, νV=O and νV–S were identified for oxovanadium(IV) dithiocarbamate adducts and derivatives with pyridine, $VO(L)_2$.py, where L = cyclohexyl-, di-isobutyl-, dipropyl-dithiocarbamates.[84]

IR bands have been observed and assigned using DFT calculations for gas-phase ions VO_x^+ (x = 1 (νVO 1053 cm^{-1}), 2 (ν_{as} 990 cm^{-1}, ν_s 1017 cm^{-1}) or 3 (1037, 1069 cm^{-1})), together with data on $V_2O_x^+$ (x = 2–6).[85,86]

The IR spectrum of gaseous $V^{III}(O)F$ had νV=O at 1028 cm^{-1}, νV–F at 807 cm^{-1} (the assignments were confirmed by *ab initio* calculations).[87] The species OVCl (formed from $VOCl_3$ over silver wool at 930°C) had νV=O at 1010 cm^{-1}, and νV–Cl at 420 cm^{-1}.[88]

Ab initio and DFT calculations have been made of the vibrational wavenumbers for VOX_3, where X = F, Cl, Br or I.[89] The IR spectra of matrix-isolated 1:1 complexes of $VOCl_3$ with dmso gave the assignments: νV=O 982 cm^{-1}, νV–Cl 434 cm^{-1}. For the CrO_2Cl_2 analogue, νCr=O bands were at 976 and 922 cm^{-1} cm^{-1}, with νCr–Cl 426 cm^{-1}.[90]

An IR band due to νV=O in V(O)L, where L = (2), is at 950 cm^{-1}. This low value suggests six-coordinate vanadium – with the sixth coordination site probably being NH.[91] The complex VO(Cl)[ONNO], where H_2[ONNO] = (3), gives an IR band due to νV=O at 947 cm^{-1}.[92] The IR spectrum of $V^{IV}O(pyr_2en)$, where H_2pyr_2en = *N,N'*-ethylenebis(pyridoxylidene-iminato), has νV=O at 960 cm^{-1}. The equivalent feature for $V^{IV}O(Rpyr_2en)$, where H_2Rpyr_2en = *N,N'*-ethylenebis-(pyridoxylaminato), is at 856 cm^{-1}, *i.e.* there are significant V=O...V=O interactions.[93] Assignments were also made to a νV=O mode for $[V(O)L]_n$, where H_2L = *N*-nicotinyl-*N'*-*p*-hydroxythiobenzhydrazine.[94]



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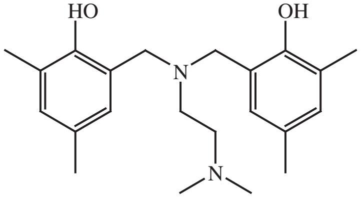

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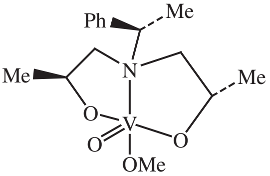


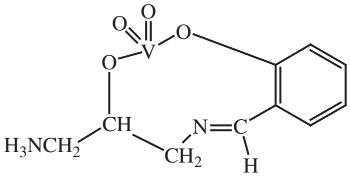
(4)

An IR band at 968 cm^{-1} for (4) was assigned as νV=O.[95] νV=O assignments for $[VO(gluconate)_2]^{n-}$ were at 951 cm^{-1} (n = 2) or 924 cm^{-1} (n = 4). For $[VO(saccharate)_2]^{n-}$, they were at 976 cm^{-1} (n = 2) or 925 cm^{-1} (n = 5).[96] IR bands were assigned to νV=O and νV–O–V modes for VO(sal-ae), where sal-ae = Schiff bases from 2-aminoethanol and salicylaldehde and its derivatives.[97] νV=O mode assignments were also given for Cu(obp)VO(L-L) (obp = oxamidobis(propionato), L–L = phen or 5-Cl- or 5-NO_2-phen);[98] and $VO(L^1)(L^2)(H_2O)$. where HL^1 = 4-benzoyl-3-methyl-1-phenyl-2-pyrazoline-5-one; HL^2 = acetoacetanilide, *o*-acetoacetotoluidide, *o*-acetoanisidide or a range of β-diketones.[99]

The complex anion $[\{Ph_3SiO)\}_2V^VO(O_2)]^-$ has νV=O at 975 cm^{-1}, with ν_s, $\nu_{as}V(O_2)$ at 625, 756 cm^{-1} respectively.[100] The IR spectrum of $[VO(O_2)(CMAA)(H_2O)]^{2-}$, where HCMAA = (*R,S*)-*N*-(carboxymethyl)aspartic acid, shows νV=O at 960 cm^{-1}, νV-(O_2) near 570 cm^{-1}.[101] For $[VO(O_2)(ox)(L)]^-$, where ox = oxalato, L = phen or bipy, νV=O is at 952 cm^{-1} (phen), 957 cm^{-1} (bipy); νV-(O_2) 543, 567 cm^{-1} (phen), 544, 573 cm^{-1} (bipy).[102]

There is Raman evidence for the formation of $[(V^VO)_2O(SO_4)_4]^{4-}$ (νV=O 1046 cm^{-1}; νV–O–V 770 cm^{-1}) on SO_2-oxidation of vanadia/silica catalysts impregnated with Cs_2SO_4.[103] The species $K_8(VO)_2O(SO_4)_6$ has the following IR features: νV=O 983, 1036, 1050 cm^{-1}; νV–O–V 718 cm^{-1}.[104] Skeletal mode assignments have been proposed from the IR spectra of $[(VO)_2(PMTA)L_2]$, where PMTA = tetra-anion of pyromellitic acid, L = bipy, phen.[105]

Raman microscopy was used to follow structural phase transformations of VO_2 thin films.[106,107] An IR band due to νV=O was seen at 1017 cm^{-1} for $Cs_2V^{IV}O_2(SO_4)$.[108] The IR spectrum of *cis*-VO_2(L), where L = salicylaldehyde semicarbazone, has $\nu_{as}VO_2$ at 908 cm^{-1}, ν_sVO_2 at 933 cm^{-1} from the *cis*-VO_2 unit.[109] The equivalent bands in VO_2(L), (5), are at 877, 858 cm^{-1} respectively. The low values are due to hydrogen-bonding to the NH_3 group.[110] νV=O IR bands are seen at 936 and 888 cm^{-1} for $[(L)VO_2K(H_2O)]_\infty$, where H_2L = (6).[111]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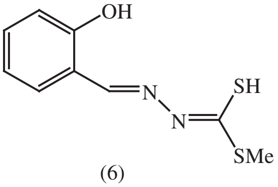
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The IR and Raman spectra of $[(VO_2)_2(4,4'\text{-bipy})_{0.5}(4,4'\text{-Hbipy})(PO_4]\cdot H_2O$ gave the following assignments: νVO_2^+ modes: ν_s 943 cm^{-1} (IR), 939 cm^{-1} (Raman); ν_{as} 919 cm^{-1} (IR), 905 cm^{-1} (Raman); δ 325 cm^{-1} (Raman); νV-O(PO_4) 521 cm^{-1} (IR), 525 cm^{-1} (Raman); νV-N 345 cm^{-1} (IR), 342 cm^{-1} (Raman).[112] νV=O and νV-O (peroxo) bands were observed in the IR spectra of vanadium(v) oxo-peroxo-mandelato complexes.[113]

Raman studies have been reported for VO_x nanotubes – features due to several types of VO group were identified, with a band at 113 cm^{-1} assigned as the radial breathing mode.[114,115] Characteristic VO_4 bands were seen in the Raman spectrum of VO_x/SBA-15 (highly dispersed silica).[116] The Raman spectra of vanadia catalysts supported on TiO_2 or ZrO_2 show that VO_x species are stable at high temperatures.[117] Analysis of the IR and Raman spectra of Yb-doped yttrium orthovanandate crystals shows that VO_4 stretching modes are dominant.[118]

The IR and Raman spectra of $LiCoVO_4$ include bands near 820 cm^{-1} (ν_sVO_4, a_1) and 335 cm^{-1} (δVO_4, e).[119-121] The Raman spectra of $Tb(V_{1-x}P_x)O_4$, where $0 \leq x \leq 0.75$, gave assignments to internal modes of $(V,P)O_4$ tetrahedra.[122] IR and Raman spectra were used to probe the local structure of the vanadate material $LiMoVO_6$, including νV=O 963 cm^{-1} (Raman), 968 cm^{-1} (IR); νMo=O 946 cm^{-1} (Raman), 939 cm^{-1} (IR), ν_{as}VOV 715 cm^{-1}, νV_2O_2 508 cm^{-1}.[123] Similar data were reported for $LiWVO_6$.[124] νV=O (near 980 cm^{-1}) and νV-O(peroxo) (539–585 cm^{-1}) were assigned from IR spectra of $[V_2O_2(O_2)_2(R,S\text{-mand})_2]^{2-}$ and related species (mand = mandelato).[125]

Raman spectroscopy was used to characterise V_2O_5 thin films prepared by vacuum evaporation.[126] DFT calculations gave vibrational wavenumbers for models of vanadia/Al_2O_3 or SiO_2 systems. These were than used to re-assess experimental vibrational spectra for these systems.[127] Similar calculations were also reported for bulk V_2O_5, its (001) surface and thin vanadium oxide films on α-Al_2O_3, giving good agreement with experiment.[128]

The Raman spectra of as-deposited V_2O_5 films with lithium intercalation included the following: νV_3–O, νV_2–O at 520, 650 cm^{-1} respectively, νV^{5+}=O 1027 cm^{-1} and νV^{4+}=O 932 cm^{-1}. The last feature shifted to lower wavenumber on increased lithium concentration.[129] Raman spectroscopy was used to characterise molybdenum-doped vanadium oxide nanotubes, including νV=O 992, 876 cm^{-1}; νV–O 694, 519 cm^{-1}, δ modes 482–96 cm^{-1}.[130] The Raman spectra of nano-V_2O_5/ZrO_2 and nano-WO_3/ZrO_2 gave evidence for surface oxides with M–O–M bridges and almost no M–O bonds.[131]

IR-multiple photon dissociation spectra were reported for $V_2O_5(C_2H_4)^+$ and $V_2O_6(C_2H_4)^+$ and compared to results of DFT calculations for various isomers.[132] There is IR and Raman evidence for the formation of V–O and V=O bonds in V_2O_5–B_2O_3–K_2O glasses.[133] IR and Raman spectra were used to differentiate between δ-, ε– and γ-phases of LiV_2O_5, *e.g.* the δ-phase has Raman bands at 960 and 942 cm^{-1}.[134] The Raman spectra of $Li_xV_2O_5$, where x = 1.0, 1.2, 1.4, show the formation of γ- and δ-LiV_2O_5.[135]

For $Zn(phen)(H_2O)V_2O_6$ and $Ti(bipy)V_2O_7$, IR spectra gave assignments to νV=O and νV–O–V modes.[136,137] The IR spectra of $V_{1.6}Nb_{0.4}O_5$ and $V_{0.3}Nb_{1.7}O_5$ show that the number of V=O bands decreases with increased addition of Nb.[138] The IR spectra of $M_xO_y{}^+$, where M = V, Nb or Ta, x = 3, 4 or 6, show that for M = V, the bands are 20–40 cm^{-1} lower than for M = Nb or Ta (which show very similar wavenumbers).[139]

VCl_4 in an argon matrix shows splitting of the t_2 stretch in the IR spectrum (474, 501 cm^{-1}). This is due to Jahn-Teller effects. Reaction with MeOH forms Cl_3VOCH_3, for which ν_sVCl_3 is at 425 cm^{-1}, $\nu_{as}VCl_3$ 486 cm^{-1} and νVO 668 cm^{-1}.[140]

High-pressure Raman data were reported for $KNbO_3$, $K(Nb,Ta)O_3$ and $NaNbO_3$.[141] The IR spectra of $BaMg_{1/3}Nb_{2/3}O_3$ ceramics include bands due to NbO_6 stretches and O–Nb–O bends.[142] Raman spectra were used to characterise the new photo-catalysts $BaM_{1/3}M'_{2/3}O_3$, where M = Ni or Zn, M' = Nb or Ta.[143] Variable-temperature Raman spectra of $Li_{0.12}Na_{0.88}Ta_{0.2}Nb_{0.8}O_3$ were used to follow the ferroelectric to antiferroelectric phase transition near 350°C.[144]

The Raman spectra of $Li_xNa_{1-x}NbO_3$ solid solutions showed a change in νNbO modes corresponding to formation of a rhombohedral phase at x = 0.12.[145] A Raman band at 825 cm^{-1} in the spectrum of $SrMg_{1/3}Nb_{2/3}O_3$ is consistent with 1:2 long-range ordering of Mg and Nb.[146] IR spectroscopy was used to study highly-ordered $BaMg_{1/3}Nb_{2/3}O_3$ for the first time.[147] νNbO modes were assigned from the IR and Raman spectra of $BaMTeO_4$, where M = Nb or Ta.[148]

FTIR and Raman spectra of Li_2O–Nb_2O_5–CaO–P_2O_5 samples show the presence of NbO_6 octahedra linked to phosphate *via* Nb–O–P bonds.[149] The IR and Raman spectra of potassium lithium niobate show that the deformation mode of $NbO_6{}^{7-}$ is spilt into 3 components as the lithium concentration increases.[150,151] νM-O bands were assigned from the IR and Raman spectra of $Pb_4Te_6M_{10}O_{41}$, where M = Nb or Ta.[152]

The Raman spectra of $NbCl_5$-(LiCl/KCl) show an increase in the intensity of the band at 374 cm^{-1} (due to $NbCl_6^-$) above 200°C. There was a corresponding decrease in the intensity of the $NbCl_5$ monomer band at 394 cm^{-1}.[153]

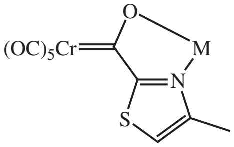
The IR and Raman spectra of $\{(NPN)Ta(\mu\text{-}H)_2(\mu\text{-}\eta^1{:}\eta^2\text{-}N_2)\}$, where NPN = $(PhNSiMe_2CH_2)_2PPh$, include four bands due to the $Ta_2N_2H_2$ core in the range 430–660 cm^{-1}.[154]

Bands assignable to νTaS were seen in the range 429–454 cm^{-1} in the Raman spectrum of $Rb_4Ta_4P_4S_{24}$.[155] νTaS stretching contributes to Raman bands between 120 and 330 cm^{-1} for $Cs_2Ta_2P_2S_{12}$ and $Cs_4Ta_4P_4S_{24}$.[156]

4 Chromium, Molybdenum and Tungsten

Previous reference has been made to vibrational studies on $LaCrO_3$;[13] $CrO_2Cl_2.Me_2SO$;[90] $Sc_2(MoO_4)_3$;[5] $[Ln(PMo_{11}O_{39})_2]^{11-}$ (Ln = Ce, Sm, Dy, Lu);[21] Mo_8C_{12};[30] $LiMoVO_6$;[123] WO_x/CeO_2 catalysts;[20] $[HPTi(O_2)W_{11}O_{39}]^{4-}$;[33] $LiWVO_6$;[124] and nano-WO_3/ZrO_2.[131]

DFT calculations gave vibrational wavenumbers for the clusters MAu_6, where M = Cr, Mo or W.[157] The complexes (7), where M = Cr, Fe or Co, all show νCr=CO IR bands in the region 430–478 cm^{-1}.[158]



(7)

The IR and Raman spectra of $Cr(pic)_3$, where Hpic = 2-picolinic acid, include νCrN at 305 cm^{-1} and νCrO at 379/364 cm^{-1} (IR), 357 cm^{-1} (Raman).[159] The complex $Cr(N)(quin)_2$, where quin = 8-hydroxo-quinolinate, gives an IR band at 1015 cm^{-1}, as expected for $\nu Cr{\equiv}N$ in a five-coordinate complex.[160] Skeletal mode assignments were proposed, from the IR and Raman spectra of $[Cr(ox)(cyclam)]^+$, where ox = oxalate, cyclam = 1,4,8, 11-tetra-azacyclotetradecane. These were consistent with the presence of bidentate oxalate, and a *cis*-V geometry for the cyclam ligand.[161]

Raman spectroscopy was used to follow the effects of chromium substitution on the spinel $LiMn_2O_4$, *i.e.* $LiMn_{2-x}Cr_xO_4$. There was evidence for some tetragonal distortion of the lattice.[162] Vibrational wavenumbers were calculated by DFT methods for CrO_4^{4-}, CrO_4^{2-} and $Cr(OH_2)_6^{3+}$.[163] Raman spectroscopy (νCrO modes) was used to characterise several chromate minerals, *e.g.* Pb_2CrO_4, $PbCrO_4$, $Pb_2Cu(AsO_4)(CrO_4)$ *etc.*[164]

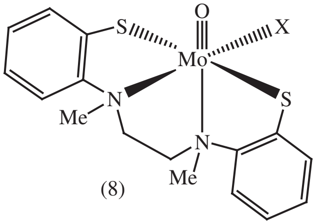
UV Raman spectra were reported for Cr-MCM-41 catalysts during dehydrogenation of propene by CO_2. There was evidence for both $Cr^{VI}O_6$ and $Cr^{III}O_6$ units.[165] The Raman spectrum of CrO_4^{2-} in M_2SO_4 (M = K, Rb or Cs) matrices could be assigned by assuming Fermi-like resonance involving ν_1 of CrO_4^{2-} and a ν_{3a} site-group component.[166]

Raman spectroscopy was used to characterise Cr(VI) oxide species on the surfaces of SiO_2, Al_2O_3, $SiO_2.Al_2O_3$ and TiO_2. Bands were assigned using *ab initio* methods.[167] High-pressure Raman experiments (to 61 GPa) on Cr_2O_3 showed several phase changes in the range 15–30 GPa.[168] An IR study of the low-temperature adsorption of O_2 on calcined chromia showed a decrease in intensity of $\nu Cr^{VI}O$ features, and a growth in bands due to α-Cr_2O_3.[169] Raman spectra showed that the chromium-containing MCM-48 zeolite had chromium present as dichromate, $Cr_2O_7{}^{2-}$.[170]

The complexes $[MFe_4S_4(CO)_{12}]^{2-}$, where M = Cr or Mn, both showed νM-S bands near 336 cm^{-1}. Characteristic νFe–CO bands were also assigned in each case.[171]

Bands due to $\nu M{\equiv}M$ were assigned with the help of *ab initio* calculations for $X_3M{\equiv}MX_3$, where X = alkyl or alkoxide, *e.g.* for x = CH_2SiMe_3, νMoMo was at 369 cm^{-1}, and νWW at 299 cm^{-1}.[172]

The resonance Raman spectra of (8), where X = Cl, SCH_2Ph, SC_6H_4OMe, $SC_6H_4CF_3$, gave the following assignments: νMo–N(ax) 250–256 cm^{-1}, νMo-N (eq) 271–276 cm^{-1}, $\nu Mo{\equiv}O$ 937–961 cm^{-1}, νMo–S 445 cm^{-1}, νMo–Cl 351 cm^{-1}.[173]



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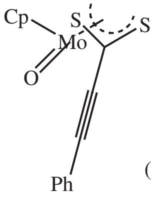

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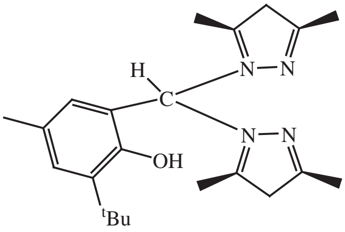


(10)

The IR spectra of $SnMo_{0.6}O_y.nH_2O$ nanolayers on silica gave evidence for the formation of Mo–O–Mo and Sn–O–Mo units on heating to 200°C.[174] νMo=O modes were assigned from the IR spectra of MoO(L)(L′), where L = *O,N,S*-donor ligands, L′ = bipy, phen *etc.*[175] An IR band due to νMo=O is at 975 cm^{-1} in the IR spectrum of (9),[176] and at 942 cm^{-1} for (L10)MoO(OPh)Cl, where L10H = (10).[177] νMo=O was seen at 896 cm^{-1} for $Mo(O)(N^tBu)\{(3,5\text{-}^tBu_2)_2salen\}$.[178]

Fragments with the formula $[Mo^VOS_4]^-$ coordinated to dendritic thiolate ligands show νMo=O near 942 cm^{-1}.[179] The IR spectrum of $[MoO(O_2)(cit)]^{4-}$, where cit = citrate, contains νMoO at 946 cm^{-1}, $\nu_{as}Mo(O_2)$ at 656 cm^{-1} and $\nu_sMo(O_2)$ at 577 cm^{-1}.[180] Characteristic νMo=O and $\nu Mo\text{–}O_2$ bands (920–967 cm^{-1}, 600–650 cm^{-1} respectively) were seen in the IR spectra of $[MoO(O_2)_2(L)]^{2-}$, where L = oxalate, citrate and related.[181]

Skeletal mode assignments were proposed from FTIR spectra of $MoO_2(acac)(OMe)(L)$, where L = Schiff base derivatives ($2\text{-}OC_{10}H_6CH{=}NHR$, R = Ph, Bz).[182] The complexes $MoO_2(L)$,where HL = *O,N,S*-donor Schiff bases of *S*-benzyl- and *S*-methyl-dithiocarbazates and salicylaldehyde, have νMo=O as two bands (979–897 cm^{-1}), *i.e. cis*-MoO_2, with νMoN 634–542 cm^{-1} and νMoS 397–374 cm^{-1}.[183] For $MoO_2(L)(D)$, where L = tridentate Schiff-base ligands, D = MeOH, dmso *etc.*, νMo=O IR bands are seen in the range 894–939 cm^{-1}.[184] Such features lie between 920 and 970 cm^{-1} for $MoO_2Cl[S_2P(OR)_2].OPPh_3$, where R = Me, Et, ^{i}Pr, Ph.[185] For MoO_2(*N*-salicylidene-*D*-glucosamine), ν_sMo=O is at 919 cm^{-1} , and ν_{as}Mo=O at 905 cm^{-1}.[186] Table 2 summarises skeletal mode assignments from the IR spectra of $MoO_2S_2[S_2P(OR)_2]_2$.dmso, where R = Me, Et or ^{i}Pr.[187]

The Raman spectrum of MoO_3 catalysts supported on La_2O_3/ZrO_2 shows characteristic bands at 819 and 997 cm^{-1}.[188] The Raman spectra of MoO_3–Fe_2O_3–P_2O_5 glasses revealed the formation of P–O–Mo units.[189]

Raman bands at 930 and 860 cm^{-1} were assigned to MoO_4 modes of molybdate-substituted akaganéite (β-FeOOH).[190] Variable-temperature IR and Raman spectra of $KAl(MoO_4)_2$ show a second order phase transition near 90 K.[191] Raman bands (νMoO_4) show that $Sc_2(MoO_4)_3$ becomes amorphous in two stages, at about 4 and 12 GPa.[192] The IR spectrum of $NaSbMoO_5$ contains νMoO(t) 926–981 cm^{-1}, and ν_{as}MoOMo 712–753 cm^{-1}.[193]

The complexes $\{Mo_2(O)(X)(\mu\text{-}S)(\eta^2\text{-}S_2)[\eta^2\text{-}S_2C_2Ph(C_2Ph)]\}^{2-}$, where X = O or S, give IR bands as follows: νMo=O 945 cm^{-1}, νMoS 475, 467, 385, 345 cm^{-1}.[194] For $[\{Mo_2^V(\mu\text{-}S)_2O_2\}_6(\mu_3\text{-}SO_3)(\mu\text{-}SO_3)_{12}].7H_2O$, νMoO bands are at 968, 947 cm^{-1}, νMoS 456 cm^{-1}.[195] The IR spectrum of $Mo_2O_4(C_4O_4)py_4$, where $C_4O_4^{2-}$ = squarate, has νMo=O bands at 945 and 928 cm^{-1}.[196]

IR spectroscopy shows that $Mn_3[Zr(H_2O)CoW_9Mo_2O_{39}].21H_2O$ adopts the Keggin structure.[197] Characteristic skeletal bands were assigned from the Raman spectrum of α-$Bi_2Mo_3O_{12}$ nanorods.[198] The Raman spectrum of the triple-cubane $[\{Ru(\eta^6\text{-}C_6H_5Me)\}_4Mo_4O_{16}]$ has ν_sMoO_2 at 940 cm^{-1}, $\nu_{as}MoO_2$ at 905 cm^{-1}. For the 'windmill-like' complex $[\{Ru(\eta^6\text{-}p\text{-}MeC_6H_4{}^iPr)\}_4Mo_4O_{16}$, the Raman spectrum shows a single broad νMo=O(t) band at 920 cm^{-1}, with νMo-O-Mo features at 700 and 850 cm^{-1}.[199]

The IR spectra of oxomolybdenum organoarsenate materials, *e.g.* $[\{Cu(o\text{-}phen)(H_2O)_2\}_2\text{-}Mo_6O_{18}(O_3AsOH)_2]$, contain ν_s and ν_{as}Mo=O 800–925 cm^{-1},

Table 2 *Vibrational mode assignments for $MoO_2S_2[S_2P(OR)_2]_2$.dmso (/cm^{-1})*

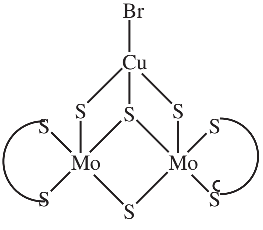
R=	*Me*	*Et*	*^{i}Pr*
ν_{as}Mo=O	970	968	965
ν_sMo=O	950	948	945
ν_{as}Mo–S_2–Mo	458	452	455
ν_sMo–S_2–Mo	420	420	415

Table 3 *Vibrational mode assignments for* $\{[Eu(MeOH)_6(H_2O)_2][PMo_{12}O_{40}]\}$ $(/cm^{-1})$

$\nu_sMo–O_d$	989
$\nu_{as}Mo–O_d$	959, 973
$\nu_{as}Mo–O_b–Mo$	880, 893
$\nu_{as}Mo–O_c–Mo$	800
$\nu_sMo–O_a$	247

with νMo–O–Mo 590–690 cm^{-1}.[200] νMoO contributes to IR bands at 781, 531 and 419 cm^{-1} for $[Mo_6S_6O_6(OH)_4(ox)_3]^{4-}$, where ox = oxalate.[201] The IR spectra of $[Mo_6O_{18}(N_2Ar)]^{3-}$, where Ar = aryl, show that the ν_{as}Mo–O(t) of $Mo_6O_{19}{}^{2-}$ (958 cm^{-1}) is split into two components, separated by about 20 cm^{-1}.[202] The Raman spectra of acidic solutions containing both Mo(VI) and W(VI) include bands due to heptamolybdate (935 cm^{-1}) and heptatungstate (960 cm^{-1}).[203]

The complex $[Ag_6(PMo_{10}V_2O_{40})](CH_3COO).8H_2O$ gives IR bands at 1064, 946, 864 and 785 cm^{-1} – characteristic of the Keggin structure.[204] IR data gave structural information on $(NH_4)_3PM_{12}O_{40}$, where M = Mo or W.[205] Raman spectroscopy (νMO, M=Mo or W) was used to follow the formation of $EW_xMo_{12-x}O_{40}{}^{3-}$, where E = P or As, x = 1–12.[206] Characteristic skeletal modes for the Keggin structure were observed for $[\{Ln(NMP)_6\}(PMo_{12}O_{40})]$.[207] Skeletal mode assignments are summarised in Table 3, from the IR and Raman spectra of the supramolecular compound $\{[Eu(MeOH)_6(H_2O)_2][PMo_{12}O_{40}]\}$(benzo-15-crown-5)$_2$(MeOH)$_2$(MeCN)$_2$.[208] The novel nanoporous materials $[Cu_3(TMA)_2(H_2O)_3]_4[\{(CH_3)_4N\}_2(L)].\sim 40H_2O$, where TMA = 1,3,5-benzenetricarboxylate, L = $H_2SiMo_{12}O_{40}$ or $HPW_{12}O_{40}$, have IR bands as follows: νSiO 908 cm^{-1}, νPO 1074 cm^{-1}, νMo=O 954 cm^{-1}, νW=O 984 cm^{-1}, νOMoO 975–810 cm^{-1}, νOWO 796–827 and 899 cm^{-1} – all consistent with the α-Keggin structure.[209]



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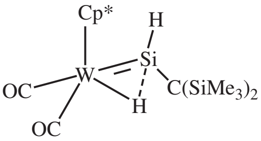


(12)

The complex (11), where S-S = S_2CNEt_2, gives IR bands from the metal/sulfur skeleton at 517 and 465 cm^{-1}.[210] $MoS_4{}^{2-}$ modes were assigned from the IR spectra of diethylenetriammonium tetrathiamolybdate.[211] Far-IR data were reported for $MoS_4Fe_2Cl_4{}^{2-}$ (νMoS(br) 473, 465 cm^{-1} (464, 457 cm^{-1} for ^{34}S), νFeCl 350, 323 cm^{-1}) and $WS_4Fe_2Cl_4{}^{2-}$ (νWS(br) 465, 454 cm^{-1}, νFeCl 348, 324 cm^{-1}).[212] The IR spectra of $[MS_4(CuBp)_4]^{2-}$, where M = Mo or W, Bp = BPz_2^{2-} (Pz = pyrazolyl), have νMS bands at 442 cm^{-1} (M=Mo), 448 cm^{-1} (W).[213]

The complexes $Cp^oMoCl_4(PH_2R)$, where $Cp^o = C_5EtMe_4$, R = ^tBu, 1-adamantyl, Cy, Ph, Mes, 2,4,6-$^iPr_3C_6H_2$, all have ν_sMoCl_4 in the range 282–240 cm^{-1}, $\nu_{as}MoCl_4$ 316–295 cm^{-1}, and δMoCl near 330 cm^{-1} and 215–181 cm^{-1}.[214]

The complex (12) gives an IR band due to νWH at 1589 cm^{-1}.[215] FTIR spectra of thin films of WC include features at 1067, 1144 and 1220 cm^{-1} due to hexagonal and cubic phases.[216] DFT calculations gave vibrational wavenumbers for WAu_{12}.[217]

IR bands were assigned for Tp*W(O)(S)(pyS), where Tp* = hydrotris(3,5-dimethylpyrazol-1-yl)borate, to νW=O (923 cm^{-1}) and νW=S (480 cm^{-1}).[218] There is Raman evidence for a WO_x surface layer on tungstated zirconia, *i.e.* WO_x–ZrO_2.[219]

IR spectroscopy was used to determine the morphology of WO_3 powders formed by thermal decomposition of tungstic acids.[220] IRRAS and Raman data were used to characterise amorphous and crystalline WO_3 thin films.[221] Raman spectroscopy could be used to follow changes to WO_3 electrochromic thin films during electrochemical cycles.[222]

The crystallinity of MWO_4 (M=Ba, Pb) thin films was studied by IR spectroscopy.[223] High-pressure Raman spectra of $Al_2(WO_4)_3$ showed phase transitions at 0.28 ± 0.07 and 2.8 ± 0.1 GPa.[224] The IR spectrum of the double perovskite Sr_2FeWO_6 includes characteristic bands at 143, 227, 377 and 625 cm^{-1}.[225]

Raman microscopy was used to characterise a wide range of tungstate minerals, showing that the ν_{as} and ν_s modes of terminal WO_2 were at 790, 881 cm^{-1} respectively.[226] The IR spectrum of $[W_2O_5(Hcit)_2]^{4-}$, where H_4cit = citric acid, contains νW=O bands at 949 and 911 cm^{-1}, ν_{as}W–O–W 808 cm^{-1} and ν_sW–O–W 698 cm^{-1}. For $[WO_3(cit)]^{4-}$, νW=O bands were at 932, 896, 840 and 821 cm^{-1}.[227] Variable-temperature Raman spectroscopy was used to follow structural phase transitions in $In_2W_3O_{12}$.[228] The IR spectrum of $[Co_3W_4P_4O_{29}]^{6-}$ includes bands due to WO_6 and CoO_6 octahedra and CoO_4 tetrahedra.[229]

Assignments to νWO modes were made from the IR spectra of $[(UO_2)_2(H_2O)_2(EW_9O_{33})_2]^{n-}$ (where E = Sb, n = 14, E = Te, n = 12). For the antimony compound, νWO(t) was at 935 cm^{-1}, with νWO(edge-shared) 881 cm^{-1} and νWO(corner-shared) 773 cm^{-1}.[230] The IR spectrum of $[H_4VW_{11}O_{40}]^{5-}$ showed typical bands from the Keggin structure.[231] IR data for α-$[SiW_{11}O_{39}M\text{-}(H_2PO_4)]^{n-}$, where M = Co(II), Mn(II), Ni(II) or Cr(II), included ν_{as}W=O near 960 cm^{-1}, and νW–O–W 800–700 cm^{-1}.[232]

SERS (νW=O, νW–O–W) was used to study the effects of adsorption of α-$[SiW_{12}O_{40}]^{4-}$ on silver or molybdenum electrode surfaces.[233] The decomposition of $H_3PW_{12}O_{40}$ in aqueous solution or in aqueous/EtOH or aqueous/acetone solutions was followed by IR spectroscopy (νWO).[234] The hybrid organic/inorganic hybrid system $(dmaH_2)_2[Nd(dmf)_4(H_2O)][\alpha\text{-}BW_{12}O_{40}].H_2O$ was characterised by IR spectroscopy (dma = dimethylamine, dmf = dimethylformamide).[235]

5 Manganese, Technetium and Rhenium

Previous reference has been made to vibrational studies on $MgO–CeO_2–MnO$ catalysts;[21] $MnTiO_3$;[58] $LiMn_{2-x}Cr_xO_4$;[162] $[MnFe_4S_4(CO)_{12}]^{2-}$;[171] $Mn_3[Zr(H_2O)CoW_9Mo_2O_{39}].21H_2O$;[197] and α-$[SiW_{11}O_{39}Mn(H_2PO_4]^{n-}$.[232]

The IR spectrum of $Mn_4Br(CH{=}CMe_2)_3(\mu_3\text{-}NPEt_3)_4$ includes νMnC at 565 cm^{-1} and νMn_4N_4 bands at 450 and 482 cm^{-1}.[236] νMnC was observed at 406 cm^{-1}, and νMnP at 257 cm^{-1} in the IR spectrum of $[HC{\equiv}C(dmpe)_2Mn–C{\equiv}C\text{-}]_2$.[237] IR and Raman spectra gave assignments to skeletal modes for $[MBr_2(mMA)_2]_n$, where mMA = *m*-methylaniline, M=Mn, Ni, n = ∞, M=Co, n = 1. The bromine ligands were seen to be bridging for M=Mn or Ni, terminal for M=Co.[238] The complexes $M(4\text{-iaa})_2(H_2O)_2$, where M = Mn or Co, 4-iaa = imidazole-4-acetate, gave the following IR bands: νM–N 318 cm^{-1} (for both), νM–O 362 cm^{-1} (Mn) or 378 cm^{-1} (Co).[239]

Metal-ligand modes were identified by resonance Raman spectroscopy, and assigned after a normal coordinate analysis, for $Mn_2(O)(OAc)_2(bipy)_2(H_2O)_2$.[240] Resonance Raman spectra of MnN(P), where P = a range of porphyrins, included $\nu Mn{\equiv}N$ near 1050 cm^{-1}.[241] The IR spectra of $M^{III}(P)Cl$, $M^{II}(P)$, where M^{III} = Mn, Fe; M^{II} = Co, Ni, Cu, Zn, P = *meso*-tetra-(4-myristyloxy-phenyl)porphyrin, included νMnN (coupled with a porphyrin deformation mode) at 250 cm^{-1}, and $\nu Mn^{III}Cl$ 320 cm^{-1}.[242]

IR spectra included characteristic $(Ni_{1-y}Mn_y)$-O vibrations in the range 600–850 cm^{-1} for $Li_{1-x}Ni_{1-y}Mn_yO_{2-\delta}$, where y = 0.25 or 0.5.[243] IR and Raman spectra were reported for MnO_2 samples, and assigned in terms of MnO_6 modes.[244]

Skeletal mode assignments were made for $(\eta^2\text{-}C_2H_4)MO_2$ in argon matrices, where M = Mn or Fe, *e.g.* $\nu_{as}OMO$ at 1013.7 cm^{-1} (977.6 cm^{-1} for ^{18}O) for M=Mn, 1022.8 cm^{-1} (986.2 cm^{-1}) for M = Fe.[245] For the analogous ethyne complexes, $(\eta^2\text{-}C_2H_2)MO_2$, $\nu_{as}MnO_2$ was seen at 1000.0 cm^{-1}, νFeO_2 at 1011.0 cm^{-1}.[246]

The structural effects of Zn-doping in $LaMn_{1-x}Zn_xO_3$, where $0 \leq x \leq 0.08$, were revealed by shifts in IR and Raman bands from MnO_6 deformations.[247] Polarised Raman and IR reflection spectra were reported and analysed for $HoMnO_3$ single crystals.[248]

The IR spectrum of N_2-matrix-isolated Cs_2MnO_4 includes prominent νMn–O bands at 854.5 and 815.0 cm^{-1}. These figures, together with the results of ^{18}O substitution, are consistent with D_{3d} symmetry.[249] Raman spectroscopy was used to monitor structural changes in elpasolite perovskites Ln_2CoMnO_6 and Ln_2NiMnO_6, where Ln = La, Pr, Nd, Sm or Gd, with changing lanthanide ion radius.[250] The decomposition of Sr_2FeMnO_6 with temperature, and on exposure to oxygen, was followed by Raman spectroscopy.[251]

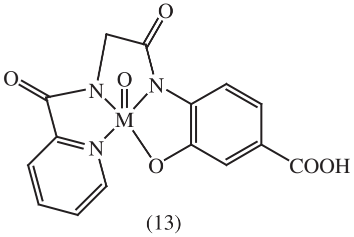
FTIR spectra have been reported for M–O units (M=Mn(III) or Fe(III)) attached to the tripodal ligand tris[*N*-*tert*-butylureaylato)-*N*-ethyl]aminato. For νM–O, the following assignments were made: (Mn) 700 cm^{-1}, (Fe) 671 cm^{-1} (shifting to 645 cm^{-1} for ^{18}O).[252]

The Raman spectrum of the spinel $LiMn_2O_4$ showed characteristic peaks of this species for the first time.[253] Raman spectroscopy was also used to follow structural changes of an $LiMn_2O_4$ electrode on doping with Al and F.[254] The

IR and Raman spectra of $M_2Mn_2O_7$, where M = In or Tl, were analysed using a short-range force constant model.[255]

Cation-ordering in the spinels $Li_2Mn_3MO_8$, where M = Mg, Ti, Co, Ni, Cu, Zn or Ga, was studied using FTIR and Raman spectra.[256] DFT calculations gave vibrational wavenumbers for the single-molecule magnet $Mn_4O_3Cl_4(O_2CEt)_3$-py_3.[257] The IR and Raman spectra of $[Mn_4O_3Cl_4(O_2CEt)_3py_3]_2$ included bands with νMnO contributions at 316, 354, 382, 409, 443, 509, 537 and 608 cm^{-1}.[258]

High-pressure IR reflection measurements for α-MnS show that a phase transformation occurs in the range 23–29 GPa.[259]

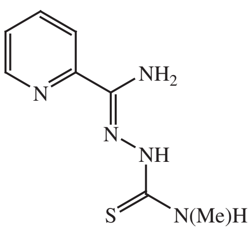


(13)

IR bands due to νM=O were assigned from the IR spectra of (13), where M = ^{99g}Tc (972 cm^{-1}) or Re (981 cm^{-1}).[260]

The complex $[ReH_2(O)(Cyttp)]^+$, where Cyttp = $PhP(CH_2CH_2CH_2PCy_2)_2$, gave the following IR bands: νReH 2030, 1716 cm^{-1}, νReO 923 cm^{-1}, δReH 845, 817 cm^{-1}. These assignments were confirmed by H/D and $^{16}O/^{18}O$ substitutions.[261] IR bands due to νReH were observed at 1827 and 1710 cm^{-1} for $[ReH_2(\eta^2\text{-}SO_3)(Cyttp)]^+$.[262]

The IR spectrum of $(Me_2PhP)_3Cl_2Re{\equiv}N\text{-}IrCl_2Cp^*$ includes νReN at 1028 cm^{-1}, νReCl at 284 cm^{-1}. For $[O_3Os{\equiv}N\text{-}IrCl_2Cp]^-$, νOsN is at 1027 cm^{-1}, νOsO 875, 892 cm^{-1}.[263] Bands due to νReO were assigned from the IR spectra of $ReO(H_4L)Cl^{2+}$, $ReO(H_4L)(Ph_3P)^{3+}$ and related species, where H_4L = 8,17-dimethyl-6,15-dioxo-5,7,14,16-tetrahydrodibenzo[a,h][14]annulene-2,11-dicarboxylic acid.[264] The IR spectrum of *trans*-$[ReO(acac_2en)OReO_3]$, where $acac_2en$ = *N,N'*-ethylene-bis(acetylacetone)imine, includes νRe=O at 908 cm^{-1}, and νRe–O–Re at 694 cm^{-1}.[265] Assignments to νReO modes were also reported for $ReOX_2(OR)(ddpe)$, where X = Cl, Br, R = Me, Et, Pr, Ph, Cy or CH_2CH_2OH;[266] $ReOCl(P\text{–}O)_2$, where P–OH = 2-[bis(ethoxyethyl)phosphino]-phenol;[267] $ReOCl_2(PPh_3)(L)$, where L = 5-nitro-2-furaldehyde semicarbazone;[268] $ReOCl_2(L)$, where HL = (14);[269] and oxo-rhenium(V) mono- and dinuclear species containing annulene-derived ligands.[270]



(14)

A Raman study of thermal phase transitions for $TlReO_4$ showed that the monoclinic form changed to orthorhombic at 170 K, and then to tetragonal at 150 K.[271] Characteristic M–O stretching modes were identified from the IR spectrum of $(NpO_2)(ReO_4)(phen)(H_2O)_2$.[272]

νRe=O bands for $[Re(O)X_2(3,5\text{-}Me_2pzH)_2]_2(\mu\text{-}O)$, where X = Cl or Br, and related complexes appear in the range 950–970 cm^{-1} in the IR spectra (Me_2pzH = dimethylpyrazole). νRe–O–Re gave complex absorptions between 700 and 930 cm^{-1}.[273] For $Cl(Ph_3P)(O)Re(\mu\text{-}O)(\mu\text{-}3,5\text{-}Me_2pz)Re(O)(3,5\text{-}Me_2PzH)Cl$, νRe=O was seen at 962 cm^{-1}.[274]

Bands assignable to νReX in $ReX_2(L)_2$, where L = (*p*-tolyl)N=C(Me)–C(=O)-N(*p*-tolyl) were seen at 317, 304 cm^{-1} (X = Cl), 229, 213 cm^{-1} (Br) – consistent with *cis* geometry.[275]

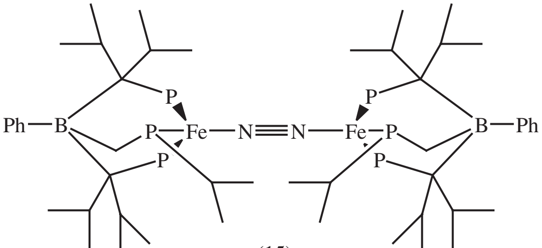
6 Iron, Ruthenium and Osmium

Previous reference has been made to vibrational studies on Fe_2TiO_5/TiO_2 composites;[47] $(M,Fe)TiO_3$ (M=Pb, Sr);[57] $[MFe_4S_4(CO)_{12}]^{2-}$ (M=Cr, Mn);[171] $MoO_3\text{–}Fe_2O_3\text{–}P_2O_5$ glasses;[189] $MS_4Fe_2Cl_4{}^{2-}$ (M = Mo, W);[212] Sr_2FeWO_6;[225] $Fe^{III}(P)Cl$ (P = *meso*-tetra-(4-myristyloxyphenyl)-porphyrin);[242] $(\eta^2\text{-}C_2H_4)FeO_2$;[245] $(\eta^2\text{-}C_2H_2)FeO_2$;[246] Sr_2FeMnO_6;[251] $[Ru(\eta^6\text{-}p\text{-}MeC_6H_4{}^iPr)]_4\text{-}Mo_4O_{16}$;[199] and $O_3Os{\equiv}N\text{-}IrCl_2Cp^*$.[263]

A resonance Raman study has been made of reduced cyano complexes of cytochrome *aa*$_3$ from bovine heart and from *Rhodobacter sphaeroides*, and of cytochrome *ba*$_3$ from *E. coli*. The first two have νFe–CN at 468 cm^{-1}, δFe–C–N at 500 cm^{-1}, the last νFe–CN at 468 cm^{-1}, but δFe–C–N at 491 cm^{-1}.[276]

The resonance Raman spectrum of CO-bound CooA (six-coordinate haem species from *Rhodospirillum rubrium*) includes a characteristic νFe–CO band, whose wavenumber depended on the nature of the haem axial ligands.[277] νFe–CO wavenumbers were used to probe the distal haem pocket conformers on CO-derivatives of *Ascaris* haemoglobin.[278] The CO adduct of ferrous H64V and H64V/K67T mutants of human myoglobin has νFe–CO at 494 cm^{-1} cm^{-1}, with νFe-His at 221 cm^{-1}.[279] Raman studies have been reported for β-$FeSi_2$.[280,281]

A characteristic νFeN band was seen at 1034 cm^{-1} (1007 cm^{-1} for ^{15}N) for the complex (15).[282] Skeletal (νMN, νMO, νMX) modes were assigned from the IR spectra of $M(L)_2X_2$, where M = Fe, Co or Zn, X = Cl, Br or (for Zn only) I, L = 8-hydroxyquinoline, *e.g.* for $Fe(L)_2Cl_2$, νFeN 322, 279 cm^{-1}, νFeO 307 cm^{-1}, νFeCl 264 cm^{-1}.[283]



(15)

The IR spectrum of $Fe^{III}(TPP)(ONO_2)NO$ at low-temperatures has νFe–NO at 548 cm^{-1}.[284] The resonance Raman spectrum of NO-bound ferric derivatives of wild-type and mutated (B10 Tyr → Phe) HbN (a haemoglobin from *Mycobacterium tuberculosis*) showed νFe–NO and δFe–N–O at 591, 579 cm^{-1} respectively.[285] Nuclear resonance vibrational spectroscopy has been used to identify a number of modes involving motion of iron in the plane of the porphyrin in nitrosyl porphyrins, *e.g.* Fe–NO torsion modes at 27 and 54 cm^{-1} in Fe(TPP)NO.[286]

Characteristic differences in skeletal mode wavenumbers in IR spectra were seen for high- and low-spin forms of $[Fe(pybzim)_3](ClO_4)_3.H_2O$, where pybzim = 2-(2'-pyridyl)benzimidazole.[287] The resonance Raman spectra of cross-*trans*-linked iron(II) 'basket-handle' porphyrins gave ν_sFe-Him_2 200–209 cm^{-1}, ν_sFe–py_2 182–205 cm^{-1} (assignments were helped by deuteriation experiments).[288]

A band due to ν_sFe–N(MeIm) was near 190 cm^{-1} for Fe(TpivPP)$(N\text{-MeIm})_2$, where TpivPP = tetrakis(*o*-pivalamidophenyl)porphyrin.[289] Metal-ligand modes were assigned from resonance Raman spectra for the $[Fe(His)_4(Cys)]$ site for the two-iron superoxide reductase from *Desulfovibrio vulgaris*.[290] The resonance Raman spectra of 5 variants of haemoglobin M showed νFe-His at 215 cm^{-1}.[291] TR^3 and time-resolved step-scan (TRS^2) FTIR were reported for nitric oxide reductase from *Paracoccus denitrificans*. The band at 207 cm^{-1} in equilibrium-reduced haem b_3 is assigned as νFe-His.[292] νFe-His modes were also assigned from the resonance Raman spectra of deoxyhaem proteins and their ^{54}Fe isotopically-labelled analogues.[293] The iron-proximal histidine stretch is at 226 cm^{-1} in the haem fragment of aldoxime deydrase (OxdA) – a novel haemoprotein.[294]

The resonance Raman spectra of wild-type, natural-abundance and uniformly ^{15}N-labelled archaeal Rieske-type ferredoxin show significant mixing of νFeN and νFeS for an oxidised biological [2Fe-2S] cluster with partial histidine ligation.[295]

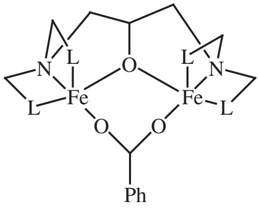
DFT calclations have been reported for the vibrational wavenumbers of $Fe(H_2O)_6^{n+}$, where n = 2 or 3.[296] A normal coordinate analysis has been reported from the IR bands of $Fe(acac)_3$ – giving an unambiguous assignment of experimental data.[297]

The resonance Raman spectra of Fe(IV) complexes $[(L)FeO]^{2+}$, where L = pentadentate pyridylamine ligands, include νFe=O at 752 cm^{-1}.[298] Transient resonance Raman spectra of oxygen intermediates in the non-haem iron enzyme taurine/α-ketoglutarate dioxygenase, include characteristic bands at 812 (^{16}O)/787 (^{18}O) cm^{-1} and 583 (^{16}O)/555 (^{18}O) cm^{-1}.[299] Oxidised intermediates of cytochrome *c* oxidase give resonance Raman bands for νFe=O showing that there are three different forms present.[300]

The resonance Raman spectrum of hydroperoxo-myoglobin at 77 K gave the first observation of νFeO, at 617 cm^{-1} (592 cm^{-1} for ^{18}O).[301] Dioxygen-bound haem oxygenase from *Corynebacterium diphtheriae*, has νFe–O_2 at 565 cm^{-1} and δFe–O–O aat 415 cm^{-1}.[302]

The FTIR spectrum of $SrFeO_{3-\delta}$ contained characteristic stretching and bending modes.[303] The complexes $[(L)Fe\text{-}O\text{-}Fe(X)]^+$, where H_2L = 5{*o*-O-[*N,N*-bis

(2-pyridylmethyl)-2-(6-methoxy)-pyridinemethanamine)phenyl]-10,15-20-tris(2,6-trifluorophenyl)porphin, X = OMe or Cl, have ν_{as}Fe–O–Fe at 844 cm^{-1}.[304] The complex (16) forms an O_2-adduct, with νFeO as a Fermi doublet 453/481 cm^{-1}.[305] The resonance Raman spectrum of $[Fe_2OL_2(MeOH)_2(NO_3)_2]^{2+}$ in MeOH (L = 2,6-bis(*N*-methylbenzimidazol-2-yl)pyridine), shows ν_sFe–O–Fe at 352 cm^{-1}.[306]



(16)

High-pressure Raman spectroscopy gave data on pressure-induced phase transitions for $ZnFe_2O_4$ (transforming to an orthorhombic form in the range 24.6–34.2 GPa).[307] Similar experiments on $CoFe_2O_4$ revealed a phase transition at 32.9 GPa.[308] Raman spectra were used to characterise natural magnetite, Fe_3O_4[309] and the effects on it of oxidation and laser-induced thermal effects.[310] The IR spectrum of Fe^{3+}-substituted yttrium iron garnet, $Y_{3-x}Fe_{5+x}O_{12}$, contained characteristic bands from Fe-O stretches of octahedral and tetrahedral sites.[311]

The resonance Raman spectra of cytochrome P450BM3 and Phe 393 mutants show that νFe–S of five-coordinate, high-spin Fe^{3+} haem is not affected by mutations.[312]

The IR and Raman spectra of $[AH][FeX_4]$, where X = Cl, Br, A = py, quinoline and derivatives, show that the FeX_4^- preserve their tetrahedral structure.[313]

The Raman spectrum of the face-to-face dimer $[(Me_6Et_2Cor)Ru]_2$, where Cor = corrole, includes νRu_2 at 317 cm^{-1}, *i.e.* there is a Ru≡Ru bond present.[314]

The complex $[RuH(CO)(CH_3CN)_2(P^iPr_3)_2]^+$ gives νRuH as an IR band at 2049 cm^{-1}.[315] An analogous feature is seen at 2005 cm^{-1} for RuH(CO)(PPh_3)(L), where L = *N,N'*-bis(salicylidene)-hydrazine.[316] For $[(\eta^6\text{-}C_6Me_6)Ru^{II}(bipy)(H)]^+$, νRuH is at 1908 cm^{-1} (1370 cm^{-1} for Ru-D).[317] The IR spectrum of $Ru_2H_4(\mu\text{-}\eta^2{:}\eta^2{:}\eta^2{:}\eta^2\text{-}SiH_4)(PCy_3)_4$ includes νRuH at 1911 cm^{-1} and νRu–H–Si at 1667 cm^{-1}.[318]

A full-scaled quantum chemical normal coordinate analysis has been reported for the skeletal modes of $Ru(LL')_3$ complexes, where LL' = α-di-imine ligands.[319]

IR data for $[RuCl(dmso\text{-}O)_4(NO)]^{2+}$ show that νRuO bands are at 517 and 501 cm^{-1}, and νRuCl 352 cm^{-1}. For $[RuCl(dmso\text{-}O)_5]^+$, νRuO is at 517 cm^{-1}.[320]

Raman spectroscopy was used to characterise the micro-structure of RuO_2 nanorods.[321] The observation of a single νRuCl (near 350 cm^{-1}) in the IR spectra of $Ru(CO)_2Cl_2$(P–S), where P–S = $Ph_2P(CH_2)_nP(S)Ph_2$, n = 1–4, shows that they contain a *trans* $RuCl_2$ unit.[322]

The IR and Raman spectra of $Os_2(CO)_8(\mu_2\text{-}\eta^1,\eta^1\text{-}C_2H_2)$ showed ν_sOsC at 524 cm^{-1} (Raman), with $\nu_{as}OsC$ 512 cm^{-1} (IR).[323]

Low-temperature luminescence spectra of *trans*-$[OsO_2(NCS)_4]^{2-}$ have vibronic structure involving νO=Os=O (885 cm^{-1}) and ν_sOs–NCS (255 cm^{-1}) modes.[324] Detailed skeletal mode assignments, with normal coordinate analyses, were reported for $[OsCl_4X(SeCN)]^{2-}$ and $OsCl_4X\text{-}(NCSe)]^{2-}$, where X = Cl or I.[325,326]

7. Cobalt, Rhodium and Iridium

Previous reference has been made to vibrational studies on $LiCoVO_4$;[119-121] $Mn_3[Zr(H_2O)CoW_9Mo_2O_{39}].21H_2O$;[197] $[Co_3W_4P_4O_{28}]^{6-}$;[229] α-$[SiW_{11}O_{39}Co(H_2PO_4)]^{n-}$;[232] $CoBr_2$(*m*-methylaniline);[238] $Co(4\text{-iaa})_2(H_2O)_2$ (4-iaa = imidazole-4-acetate);[239] Ln_2CoMnO_6;[250] $CoFe_2O_4$;[308] $(Me_2PhP)_3Cl_2Re{\equiv}N\text{–}IrCl_2Cp$ and $O_3Os{\equiv}N\text{–}IrCl_2Cp^*$.[263]

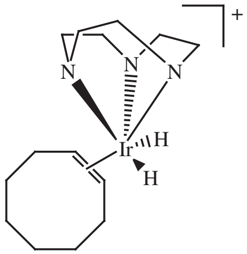
Raman spectroscopy showed the presence of Co_2C and Co_3C units in Co/C_{60} nano-composite materials.[327] The IR and Raman spectra of Co(II), Ni(II) and Cu(II) complexes of 4-imidazoleacetic acid (HIA) have been reported, $M(IA)_2(L)_2$, where L = H_2O, MeOH. There is evidence for extensive mixing of Cu–N and Cu–O modes.[328]

A resonance Raman study of HOO-Co^{III}(bleomycin) shows that νCo-OOH is at 545 cm^{-1} (518 cm^{-1} for ^{18}O).[329] The Raman spectra of alumina-supported Co and Ag/Co catalysts showed the presence of Co_3O_4.[330]

The observation of two IR bands due to νM–Cl confirm the *cis*-MCl_2 geometry in $MCl_2(L)$, where M = Co, Ni, Pd, Pt, L = 1-methyl-lumazine; M = Co, Pt, L = 1,6,7-trimethyl-lumazine.[331]

IR and Raman spectra have been reported for $RhX({=}C{=}CH_2)(P^iPr_3)_2$, where X = F, Cl, Br or I. Isotopic substitution allowed assignments to νRhC modes to be made.[332] SERS data for CO adsorbed on a roughened rhodium electrode showed that νRh–CO was near 450 cm^{-1}.[333] The complex $(OC)_3$(phen)W-*cis*-$Rh(CO)_2Cl$ gave an IR band from νRhCl at 287 cm^{-1}.[334]

The complex $Ir(H)Cl(C{\equiv}CPh)(PPh_3)_3$ gives an IR band at 2168 cm^{-1} from νIrH.[335] Such a feature is at 2184 cm^{-1} in the IR spectrum of IrH(CO)$[\kappa^1\text{-OC(O)OH}]\{C_6H_3{=}2,6\text{-}(CH_2P^tBu_2)_2\}$;[336] and at 2176 cm^{-1} for $[(\eta^4\text{-}C_8H_{12})Ir(H)(\mu\text{-}N{=}CPh_2)2Ir(\eta^4\text{-}C_8H_{12}]^+$.[337] For (17), ν_sIrH_2 is seen at 2209 cm^{-1}, with $\nu_{as}IrH_2$ at 2148 cm^{-1}– both in the IR spectrum.[338]



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The FTIR spectrum of IrO_2 showed a broad band near 550 cm^{-1} due to νIrO.[339] Micro-Raman spectroscopy was used to characterise well-aligned IrO_2 nanotubes.[340]

8 Nickel, Palladium and Platinum

Previous reference has been made to vibrational studies on α-[$SiW_{11}O_{39}Ni(H_2PO_4)]^{n-}$;[232] [$NiBr_2$(*m*-methylaniline)$_2]_\infty$;[238] Ni(P) (P = *meso*-tetra-(4-myristyloxy-phenyl)porphyrin);[242] $Li_{1-x}Ni_{0.75}Mn_{0.25}O_{2-\delta}$;[243] Ln_2NiMnO_6;[250] $Ni(IA)_2(L)_2$ (HIA = 4-imidazoleacetic acid, L = H_2O, MeOH);[328] and $MCl_2(L)$ (M = Ni, Pd, Pt, L = 1-methyl-lumazine).[331]

Ab initio calculations gave vibrational wavenumbers for $NiCH_2$, *cis*- and *trans*-HNiCH and H_2NiC.[341]

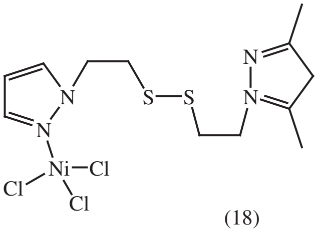

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Table 4 summarises skeletal mode assignments for MI_2(*p*-MA)$_2$, where M = Ni, Zn or Cd; *p*-MA = *p*-methylaniline.[342] The IR spectra of [MCl(med)]$_2$, where M = Ni, Pd or Pt, Hmed = *N*-(2-mercaptoethyl)-3,5-dimethylpyrazole, include νMN 450–513 cm^{-1}, νMS 315–366 cm^{-1} and νMCl 333–388 cm^{-1}. For (18), νNiN is at 484 cm^{-1} and νNiCl at 375 cm^{-1}.[343] *Ab initio* calculations have been made of the vibrational wavenumbers for the onion-like cluster As@-Ni_{12}@As_{20}.[344]

There is Raman evidence for the formation of $Ni_4(OH)_4^{4+}$ (with a characteristic band at 490 cm^{-1}) in aqueous $Ni(NO_2)_3$ solutions.[345] DFT calculations gave values for skeletal (νM–S) modes for $M(H_2timdt)_2$, where M = Ni, Pd or Pt, and H_2timdt = imidazoline-2,4,5-trithione.[346]

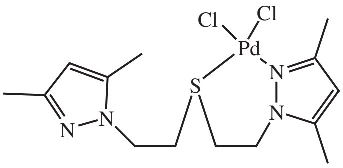
A band at 119 cm^{-1} in the Raman spectrum of $[Pd_2(dmb)_2(PPh_3)_2]^{2+}$ is assigned to νPdPd, with νPdP at 180 cm^{-1} (dmb = 1,8-di-isocyano-*p*-menthone).[347] The IR and Raman spectra of $[M(SnB_{11}H_{11})_4]^{x-}$, where M = Pd, Pt, x = 6; M=Au, x = 5, contain νM–Sn bands at 191 cm^{-1} (Pd), 170 cm^{-1} (Pt) and 159 cm^{-1} (Au).[348] The complex (19) gives IR bands at 456 cm^{-1} (νPdN),

Table 4 *Skeletal mode assignments for $MI_2(pMA)_2$ (/cm^{-1})*

M=	*Ni*	*Zn*	*Cd*
νMN	408	426	393
	387	377	387
νMI	142	161	150
		141	130

367, 336 cm^{-1} (νPdCl) and 280 cm^{-1} (νPdS).[349] Skeletal mode assignments have been made from far IR spectra for $ML_2M'X_2$, where L = tetrakis(pyridine-2-thiolato), M = Pd, $M'X_2$ = $PtCl_2$, $CdCl_2$, $HgCl_2$; M = Pt, $M'X_2$ = $HgCl_2$; L = bis(1-oxypyridine-2-thione), M = Pd, $M'X_2$ = $CdCl_2$, HgX_2 (X = Cl, Br or I), $PtCl_2$; M = Pt, $M'X_2$ = $HgBr_2$, HgI_2.[350]

DFT calculations gave vibrational wavenumbers for $Pd(PR_3)_2X^-$, where R = H, Me, vinyl, Ph; X=Cl, Br, I, OAc or TFA, and $[Pd\{Ph_2P(CH_2)_nPPh_2\}X]^-$, where n = 3–6, X =Cl or OAc.[351] νM–S bands are seen in the range 346–379 cm^{-1} for $[M(C_2N_2S_2)_2]^{2-}$, where M = Pd or Pt.[352]



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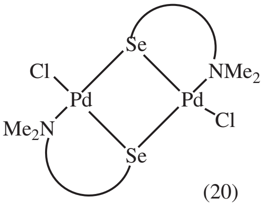

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Bands at 323 and 295 cm^{-1} in the IR spectrum of $PdCl_2\{Pd[2\text{-}FC_6H_3C(Me)=N–N=C(S)NHEt](Ph_2PCH_2PPh_2)\text{-}P,S\}$ were assigned to νPdCl.[353] The complex $PdCl_2L_2$, where L = $As(CH_2–CMe=CH_2)_3$, has νPdCl at 354 cm^{-1}.[354] Complex (20), where $(Me_2N–Se)_2$ = $[Me_2N(CH_2)_3Se]_2$, has such a band at 291 cm^{-1}.[355]

Laser-ablated Pt atoms react with C_2H_4 to form matrix-isolated $HPt(CH=CH_2)$, with νPtH at 2317.7 cm^{-1}.[356] νPtH is at 2066 cm^{-1} in the IR spectrum of $PtH\{(Ph_2SCH_2)_2Si(CH_3)\}(PPh_3)_2$.[357] DFT calculations gave vibrational wavenumbers for MH_2, where M = Pt, Au, species in a silicon matrix.[358] The terminal hydrogens in $[Pt_2(dcype)_2H_3]^+$, where dcype = 1,2-bis(dicyclohexyl-(phosphanyl)ethane, give an IR band due to νPtH at 1980 cm^{-1}.[359] Raman and inelastic neutron scattering (INS) spectra of Rb_2PtH_6 and Rb_2PtD_6 gave assignments to νPtH(D) – Table 5.[360]

IR and Raman spectra gave skeletal mode assignments for *trans*-$[Pt(CN)_4X_2]^{2-}$, where X = Cl, Br or I – Table 6.[361] The IR and Raman spectra of $(Cy_3P)_2Pt=SiMe_2$, together with a normal coordinate analysis, show that νPt=Si contributes to features at 465 and 612 cm^{-1}.[362]

IR bands due to νPtN were assigned for *cis*- and *trans*-$Pt(amine)_2I_2$, where amine = RNH_2 (R = Me, Et, ^{n}Bu, ^{i}Pr, ^{i}Bu, ^{sec}Bu), Me_2NH, *e.g.* for R = Me, IR bands are at 470, 420 cm^{-1} (*trans*), 465 cm^{-1} (*trans*).[363] Skeletal (νPtN, νPtO) assignments have been proposed from IR spectra for *cis*- and *trans*-$Pt(amine)_2$

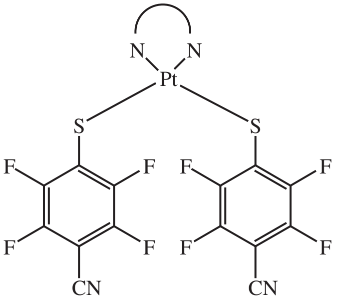
Table 5 *Vibrational assignments for Rb_2PtH_6 and Rb_2PtD_6 (/cm^{-1})*

	H	*D*
ν_2 (e_g) (Raman)	2074	1487
ν_1 (a_{1g}) (Raman)	2044	1466
ν_3 (t_{1u}) (I.N.S.)	1743	–

Table 6 *Skeletal mode assignments for trans-*$[Pt(CN)_4X_2]^{2-}$ *(/cm*$^{-1}$*)*

X=	*Cl*	*Br*	*I*
δPt–C–N	495, 472	494,474	491, 473
νPtC	411	410	408
νPtX	328	201	141

$(NO_3)_2$, where amine = RNH_2 (R = Me, Et, ^nBu, ^iPr, ^iBu, ^{sec}Bu), Me_2NH.[364] Skeletal modes (νPtN, νPtS, νPtCl) were also assigned for $Pt(R_2SO)$(pyrazine)Cl_2, e.g. for the dmso complex νPtN is at 517 cm^{-1}, νPtS 444 cm^{-1} and νPtCl 350 cm^{-1}.[365]



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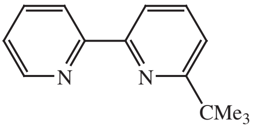

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The resonance Raman spectra of (21), where N–N = bipy or phen, contain νPtS bands at 405 cm^{-1} (bipy) or 414 cm^{-1} (phen).[366] Pt(Cl)(L)(dmso), where HL = (21), give νPtCl in the IR spectrum at 276 cm^{-1}, *i.e.* the chlorine atom is *trans* to a ligand with a high *trans*-influence.[367] The all-*trans* geometry for *trans,trans*-$Pr(R_2SO)Cl_2$(μ-pyrazine)$Pt(R_2SO)Cl_2$, where R = Me, Pr, Bu, Bz, Ph; $R_2 = (CH_2)_4$, is confirmed by the observation of a single νPtCl IR band in all cases.[368] The complex $PtCl_2(Ph_2PNHNHpy\text{-}P)_2$ has νPtCl at 307 and 288 cm^{-1} – showing *cis*-$PtCl_2$.[369]

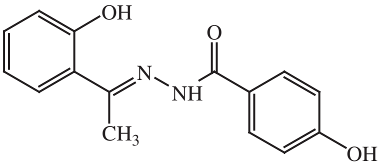
9 Copper, Silver and Gold

Previous reference has been made to vibrational studies on $Ca_{1-x}Mg_xCu_3Ti_4O_{12}$;[67] Cu(obp)VO(L–L) (obp = oxamidobisphosphonato, L–L = phen or substituted phen);[98] $Pb_2Cu(AsO_4)(CrO_4)(OH)$;[164] $[Cu(o\text{-phen})(H_2O)_2]_2Mo_6O_{18}(O_3AsOH)_2$;[200] $[Cu_3(TMA)_2(H_2O)_3]_4[\{(CH_3)_4N\}_2(L)]$ (TMA = 1,3,5-benzenetricarboxylate, L = polymolybdate, -tungstate);[209] $[MS_4(CuBp)_4]^{2-}$ (M = Mo, W, Bp = BPz_2^{2-}, Pz = pyrazolyl);[213] $Cu(IA)_2L_2$ (HIA = 4-imidazoleacetic acid, L = H_2O, MeOH);[328] $[Ag_6(PMo_{10}V_2O_{40})](CH_3COO).8H_2O$;[204] and $[Au(SnB_{11}H_{11})_4]^{5-}$.[348]

IR spectroscopy was used to identify Cu_x clusters in Cu/ZnO nanocomposites.[370] The resonance Raman spectrum of $[\{Cu^{II}(PYAN)\}_2(O_2)]^{2+}$ includes a band at 278 cm^{-1}, which was assigned as νCu . . . Cu.[371]

Laser-ablated M (=Cu, Ag or Au) atoms react with H_2 to give matrix-trapped MH, $(H_2)MH$ as major, and MH_2^- and AuH_4^- as minor products. Assignments included (MH) ν 1879.8 cm^{-1} (Cu), 1717.0 cm^{-1} (Ag), 2226.6 cm^{-1} (Au); $(H_2)MH$ νMH 1862.5 cm^{-1} (Cu), 1746.5 cm^{-1} (Ag), 2173.6/2170.6 cm^{-1} (Au) (all data for an argon matrix).[372,373] Matrix-IR data were assigned (using isotopic shifts and *ab initio* calculations) for MH_2^-: M = Cu (1517.8 cm^{-1}), Ag (1442.4 cm^{-1}), Au (1636.0 cm^{-1}), and for AuH_4^- (1676.4 cm^{-1}).[374]

Raman spectroscopy was used to characterise Cu–C composite films deposited on Si substrates.[375] IR and Raman spectra were reported for $[Cu(NH_3)_5](ClO_4)_2$, with νCuN bands at 430 cm^{-1} , 312 cm^{-1}, 287 cm^{-1} (Raman), 395 cm^{-1} (IR).[376] IR spectra of CuL(L'), where H_2L = (23), L' = bipy, phen, gave assignments to νCuN(heterocyclic base), νCuN (L) and νCuO.[377] IR spectra gave assignments to νCuN for (24), where R = R' = ^{i}Pr, n = 3; R = R' = ^{t}Bu, n = 4; R = ^{t}Bu, R' = ^{i}Pr, n = 4 (509–519 cm^{-1}).[378] The IR spectrum of $[Cu(imi)_2(H_2O)_4][(Himi)_2(imi)_2Mo_8O_{26}]$, where imi = imidazole, gave skeletal mode assignments.[379]



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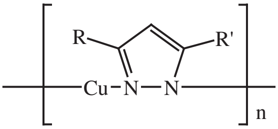


(24)

Micro-Raman scattering was used to characterise CuO nanorods.[380] DFT calculations have been made of vibrational wavenumbers for CuO_x, where x = 1–3, 6, and related anions.[381,382] IR and Raman spectra of Cu/O samples formed by A.C electrolysis from aqueous copper(II) acetate included features due to Cu_2O.[383]

The complex $Cu(L)_2$, where L = 1-phenyl-3-methyl-4-benzoyl-5-pyrazolone, gives IR bands due to νCuO at 425 and 495 cm^{-1}.[384] Aeration of the two-electron reduced cytochrome *c* oxidase leads to characteristic Raman bands at 804 and 356 cm^{-1}, due to νOO, νCuO respectively.[385] Skeletal (νCuO) modes were assigned from IR and Raman spectra of $[Cu_2(TAA)_4]_n$, where HTAA = 2-thiophene acetic acid, using $^{63}Cu/^{65}Cu$ isotopic shifts.[386]

The resonance Raman spectrum of $[\{Cu(L)\}_2(O_2)]^{2+}$, where L = tris(*N*-benzylaminoethyl)-amine, contains νCuO features at 556 and 539 cm^{-1}, suggesting the presence of two peroxo species in solution.[387] There is resonance Raman evidence for the formation of peroxo and bis(μ-oxo) species (from characteristic νCuO_2 and νCuOCu bands) on treatment of Cu^I_2 or Cu^{II}_2 complexes of polyamine ligands with O_2 or H_2O_2.[388]

Metastable species derived from $(L)Cu(O_2)$, where L^- = 2,4-di-*tert*-butyl-phenolate linked to 1,4-di-*iso*-propyl-1,4,7-triazacyclononane, show multiple νCuO bands in the wavenumber range 500–550 cm^{-1}.[389] The resonance Raman spectrum of $[Cu_2(\mu\text{-}O)_2(d_4\text{-}Me_2\text{-}etpy)_2]^{2+}$ has a νCu–O–Cu band at 579 cm^{-1} (551 cm^{-1} for ^{18}O).[390] Selective catalytic reduction of NO by NH_3/O_2 on copper-faujasite catalysts gave rise to IR bands showing changes in copper oxidation states (using the $\nu_{as}[Cu\text{–}O\text{–}Cu]^+$ band near 900 cm^{-1}).[391]

νCu–OH, νCu–OH_2 and νCu–Cl modes were identified from Raman spectra of copper chloride minerals (nantokite, eriocalchite and clasingbullite).[392] Raman-active modes were observed for superconductor thin films of $Cu_{1-x}Tl_xBa_2CaCu_2O_{8-y}$, *e.g.* Tl–$O_A$–Cu(2) and Cu(1)–$O_A$–Cu(2) modes at 530, 600 cm^{-1} respectively.[393] Low-wavenumber, oxygen-sensitive modes of $YBa_2Cu_3{}^{16,18}O_{6.9}$ show anomalous isotope effects.[394] There is IR and Raman spectroscopic evidence for the formation of P–O–Cu units in glasses in the system Na_2O–CuO–P_2O_5.[395,396]

Metal-ligand stretching modes were assigned from the resonance Raman spectrum of aa_3-quinol oxidase of *Acidianus ambivalens*.[397]

The complex $[Cu_2(tu)_6]Cl_2.2H_2O$, where tu = thiourea, shows a Raman band at 203 cm^{-1} due to νCu–S.[398] Characteristic Raman bands were seen at 292, 305, 340 and 472 cm^{-1} for $CuInS_2$ powder.[399] The Raman spectrum of a thin film of $CuInSe_2$ included a feature at 260 cm^{-1} which was sensitive to copper concentration.[400] Raman bands in the range 160–175 cm^{-1} for $Cu(In_{1-x}Ga_x)_3Se_5$ were related to copper motions.[401]

The Raman spectra of the complexes $CuBr_2(L)_2$, where L = *m*- or *p*-methylaniline (mMA or pMA) show νCuBr bands at 202 cm^{-1} (mMA) or 207 cm^{-1} (pMA).[402]

SERS data for glycine adsorbed on silver colloidal particles include a band at 238 cm^{-1} due to νAg–N.[403] νAgN modes were assigned from the IR spectra of [bis(1,2,4-triazol-1-yl)methane]silver(I) complexes AgX:$tz_2(CH_2)$:ER_3:MeCN, where X = NO_3, R = Ph, E = P, As, Sb, and related systems.[404]

IR and Raman spectra of Ag_2S–B_2S_3–GeS_2 glasses gave evidence for the presence of $AgSGeS_{3/2}$ and $Ag_3B_3S_3S_{3/2}$ units.[405,406] Raman spectra of samples in the Ag–Se–I system showed bands from νAgSe and νAgI.[407]

Laser-ablated gold atoms and H_2 gave AuH_2 trapped in an H_2 matrix, with δHAuH at 638.1 cm^{-1} (570.6 cm^{-1} for AuHD, 457.0 cm^{-1} for AuD_2).[408]

SERS data for CN^- adsorbed on a gold surface gave evidence for νAu-CN and δAu-C-N features (near 370, 300 cm^{-1} respectively).[409,410] *Ab initio* calculations gave νAuC and νAuX wavenumbers for $Au(CN)_4{}^-$ and *trans*-$Au(CN)_2X_2{}^-$, where X = F, Cl, Br or I.[411]

Raman data were reported for $[(F_3As)AuXe]^+$, including νAuAs at 190.7 cm^{-1} and νAuXe at 138.5 cm^{-1}.[412] The complexes $[AuCl(L)]^+$, where HL = 2-pyridine formamide thiosemicarbazones, gave νAuCl IR bands in the range 352–364 cm^{-1}.[413]

10 Zinc, Cadmium and Mercury

Previous reference has been made to vibrational studies on $Zn(phen)(H_2O)V_2O_6$;[136] Zn(P), where P = *meso*-tetra-(4-myristyloxyphenyl)porphyrin;[242] $LaMn_{1-x}Zn_xO_3$ ($0.01 \leq x \leq 0.08$);[247] $ZnFe_2O_4$;[307] MI_2(*p*MA) (M = Zn, Cd, *p*MA = *p*-methylaniline);[342] and PdL_2MCl_2 (L = tetrakis(pyridine-2-thiolato, M = Cd, Hg).[350]

νM–H bands were seen in the IR spectra of matrix-isolated $HM(SiH_3)$, where M = Zn, Cd or Hg, *i.e.* 1846.6–1821.6 cm^{-1} (Zn), 1745.9–1704.2 cm^{-1} (Cd), 1886.7–1855.9 cm^{-1} (Hg).[414] The IR and Raman spectra of ML_nI_2, where M = Ni, n = 4; M = Zn, Cd, n = 2; L = *m*-methylaniline, gave the following assignments: νM–N 408 cm^{-1} (Ni), 413 cm^{-1} (Zn), 416 cm^{-1} (Cd); νM–I 206 cm^{-1} (Ni), 201 cm^{-1} (Zn), 209 cm^{-1} (Cd).[415]

The IR spectra of $[\{N(PPh_2NR)_2\}M(OAc)]$ and $[\{N(PPh_2NR_2)_2\}_2M]$, where M = Zn, Cd or Hg, R = Ph or $SiMe_3$, gave evidence for trigonal planar and tetrahedral geometry around the metal atoms.[416] DFT calculations gave metal-ligand vibrational wavenumbers for polymeric $[ZnCl(IA)(HIA)]_n$, where HIA = 4-imidazoleacetic acid.[417]

IR and Raman spectra gave skeletal mode assignments for ZnX_2PR_3 and $ZnX_2(PR_3)_2$, where X = Cl, Br or I, R = Ph, *p*-ClC_6H_4; X = Cl or Br, R = *p*-Me- or *p*-$MeOC_6H_4$. For example, for X = Cl, R = Ph, νZnCl bands were at 334, 244, 230 cm^{-1} (IR); 340, 270 cm^{-1} (Raman); νZnP 167 cm^{-1} (IR), 172 cm^{-1} (Raman); δZnCl 122 cm^{-1} (Raman).[418]

Far-IR spectra of $M(H_2O)_6{}^{2+}$, where M = Zn, Cd or Hg, together with earlier Raman data, gave a full assignments of MO_6 fundamentals for the first time.[419] *In situ* Raman spectra of zinc nanoparticles formed at the anode of a Zn/MnO_2 battery gave evidence for the formation of Zn/O species.[420] Raman spectroscopy was used to characterise ZnO nanowires and nanorods – showing the presence of wurtzite structural units.[421] Raman data for ZnO films deposited on a Si(111) surface showed a low density of oxygen vacancies in films grown at low temperatures.[422] The complex $[L_3Zn(OClO_3)]ClO_4$ (where L = 5-^{t}butylpyrazole) has νZnO at 232 cm^{-1} in the IR spectrum.[423] The Raman spectrum of Zn_2L_4, where L = *O,O*-di(cyclohexyl)dithiophosphate, has νZnS at 307 cm^{-1}.[424] Force constant model calculations were used to assign vibrational spectra for AGa_2X_4, where A = Zn, Cd, X = S, Se.[425] Raman spectra were reported for ZnSe and samples doped with P and P/Ga.[426] The high-pressure Raman spectrum of $ZnGa_2Se_4$ (at 300 K, up to 18.9 GPa) gave evidence for an order-disorder phase transition in the cation sublattice.[427]

IR bands due to νZnCl (315–355 cm^{-1}, 280–300 cm^{-1}) were assigned for Zn(RaaiR')Cl_2, where RaaiR' = 1-alkyl-2-(arylazo)imidazole, *p*-R-C_6H_4–N=N–C_3H_2-NNR' , R = H, Me or Cl, R' = Me, Et, CH_2Ph.[428]

Analysis of the molecular emission spectrum of Cd_2 gave the vibrational parameters which are listed in Table 7.[429] The complex $[Cd(O_2CMe)(O_2CPh)(H_2O)_2]_n$ gives νCdO bands at 286, 277, 255, 244, 222 and 201 cm^{-1}. The last two are probably νCd–OH_2.[430] The IR and Raman spectra of glasses in the Na_2O–CdO–PbO–P_2O_5 system gave evidence for the formation of P–O–Cd units.[431,432]

Raman spectra gave evidence for quantum size effects in CdS clusters confined in zeolite pores.[433] The Raman spectra of nanocrystals of $CdS_{1-x}Se_x$

Table 7 *Vibrational parameters for Cd_2 (/cm^{-1})*

State	ω_e	$\omega_e x_e$
R_10^+	87.9 ± 0.4	2.53 ± 0.03
$R_{2u}{}^u$	88.7 ± 0.4	2.37 ± 0.08
$1g(5^3P_1)$	142.9 ± 0.09	0.56 ± 0.02

embedded in a borosilicate glass matrix showed confinement-, surface and disorder-related effects.[434] The Raman spectrum of the CdSe/BeTe interface contained bands at 170 and 220 cm^{-1}.[435] Micro-Raman spectra of $Hg_{1-x}Cd_xTe$ epitaxial films show bands at 120, 138 cm^{-1} (Hg–Te), 155 cm^{-1} (Cd–Te) and 261 cm^{-1} (combination of Hg-Te modes).[436]

The far-IR and Raman spectra of $Cd_2X_4(tpa)_2$, where tpa = tris(2-pyridyl) amine, X = Cl, Br or I, yielded assignments to terminal and bridging Cu–X stretching modes.[437]

Raman spectra gave values for νHgHg for solvated $[Hg_2]^{2+}$ in H_2O, MeOH, dmso, *N,N*-dimethylpropylene-urea, MeCN or py solutions. Solid Hg(I) trifluoromethanesulfonate gave a very high value for νHgHg (198 cm^{-1}) despite the bond length not being particularly short.[438] The IR spectrum of MeHg $[(SeP^iPr_2)_2N]$ includes νHgC at 541 cm^{-1}.[439] Anharmonic ro-vibrational spectra were calculated for HgXO, where X = Cl or Br.[440]

11 Actinides

Previous reference has been made to vibrational studies on $[(UO_2)_2(H_2O)_2(SbW_9O_{33})_2]^{14-}$;[230] and $(NpO_2)(ReO_4)(phen)(H_2O)_2$.[272]

It was possible to record a Raman spectrum of crystalline $U(COT)_2$ under liquid nitrogen at 77 K. Bands due to ring-U-ring stretching and tilting were seen at 212, 236 cm^{-1} respectively.[441] There have been several reports of matrix-IR studies of noble-gas (Ng) complexes of CUO, *i.e.* $CUO(Ng)_n$. Table 8 summarises the data obtained for Ng = Ar, n = 1–4.[442–444]

The IR spectrum of $UO_2(PhCONHNH_2)_2$ included νU–N at 438 cm^{-1}, νU–O at 540 cm^{-1} and νU=O at 943 and 908 cm^{-1}.[445] Matrix-IR data were

Table 8 *Vibrational assignments for $CUO(Ar)_n$ (/cm^{-1})*

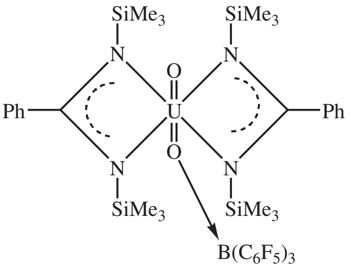
n	*νUO*
1	866.6
2	861.9, 858.8
3	857.2
4	854.3

Table 9 *Vibrational assignments ($\nu_{as}UO_2$) for $UO_2(X)_n$ (/cm^{-1})*

$\nu_{as}UO_2$	*X*
980.1	Ne
952.3	Ar
940.6	Kr
929.0	Xe

obtained for $UO_2(X)_n$, where X = Ne, n = 6, X = Ar, Kr, Xe, n = 5. Table 9 summarises the values of $\nu_{as}UO_2$.[446]

The Raman spectrum of andersonite, a uranyl tricarbonate mineral, showed ν_sUO_2 at 832 cm^{-1}.[447] The complex $UO_2(NCN)_2(thf)$, where NCN = {(SiMe$_3$N)(CPh)(NSiMe$_3$)}, has $\nu_sO{=}U{=}O$ at 803 cm^{-1}. This decreases to 780 cm^{-1} on formation of (25). This is the lowest recorded value for such a mode in a mononuclear uranyl(VI) complex.[448] ν_{as} and $\nu_sO{=}U{=}O$ modes were assigned for (26) (X = CH, ν_{as} 908 cm^{-1}, ν_s 825 cm^{-1}; N , 909 cm^{-1}, 829 cm^{-1}) and (27) (X = CH, 924 cm^{-1}, 836 cm^{-1}; N, 924 cm^{-1}, 846 cm^{-1}).[449]



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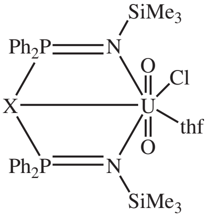

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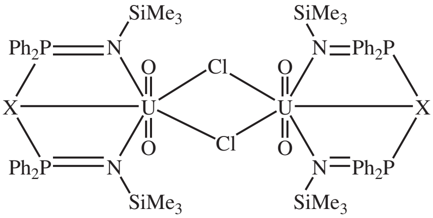

(27)

νUO_2 assignments were proposed from the IR spectra of UO_2^{2+} complexes of dianionic tetradentate Schiff base ligands, from $RCH{=}N(CH_2)_nN{=}CHR$ (R = 2-hydroxy-1-naphthyl, n = 2–10) and bis(2-hydroxy-1-naphthylmethylene)-2-hydroxy-1,3-propane diamine.[450] FTIR and Raman spectra of aqueous UO_2^{2+}/citrate solutions gave evidence for the formation of $[(UO_2)_2Cit_2]^{2-}$, $[(UO_2)_3Cit_3]^{3-}$ and $(UO_2)_3Cit_2$.[451] Raman spectra were obtained at 77 K, together with IR data, for $M(UO_2)_2(XO_4)_2.8\text{-}12H_2O$, where M = Mg, Ca, Ba, Mn, Fe or Cu, X = P, As. Assignments were made to ν_sUO_2 (820 cm^{-1}), $\nu_{as}UO_2$ (913 cm^{-1}) and δUO_2 (295, 222 cm^{-1}).[452,453]

The resonance Raman spectrum of $UO_2(OOCH)_2$ in dmso solution revealed the excitation profile for ν_sUO_2 at 831 cm^{-1}.[454] The observation of $\nu_{as}UO_2$ at 908 cm^{-1} for $(LH)_2(UO_2)_2(OH)_2$, where H_2L = *S,S'*-bis[2(2'-ferrocenemethylaminobenzyl)]dithioglyoxime, is consistent with the dimeric structure.[455] Other uranyl(VI) species for which νUO_2 assignments were proposed were: $UO_2(L)(D)$ (H_2L = acetyl pyridine benzoylhydrazones, D = dmso, thf, py;[456] UO_2^{2+}complexes of furohydroxamic acid and derivatives;[457] and $UO_2L_2(NO_3)_2$, where L = $(CH_2)_{11}CONC_4H_9$ or $(CH_2)_3CONC_8H_{17}$.[458] Raman data were obtained for stoichiometric and hyperstoichiometric UO_2. There was evidence of U_3O_8 modes in UO_x, where x $\geq$ 2.09.[459]

Ab initio calculations have been made of vibrational wavenumbers for UF_4X_2, where X = H, F, Cl, CN, NC, NCO, OCN, NCS or SCN.[460] DFT calculations gave vibrational wavenumbers for UF_5 and UF_6.[461]

The complex $[NpO_2(TPPO)_4][ReO_3]$ has ν_sNpO_2 at 776 cm^{-1} in the Raman spectrum, and $\nu_{as}NpO_2$ at 826 cm^{-1} in the IR spectrum.[462] FTIR spectroscopy gave assignments to NpO_2 modes for $[(NpO_2)_2(CrO_4)_3(H_2O)]^{2-}$.[463] *Ab initio* and DFT calculations have been reported for the wavenumbers of PuO_3 and PuO_3^+.[464]

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Vibrational Spectra of Some Co-ordinated Ligands

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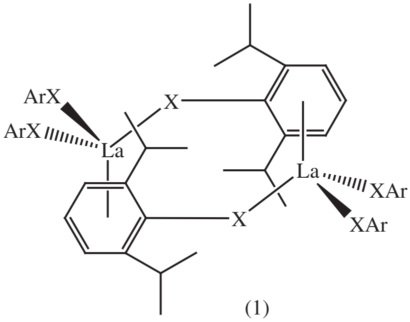
1 Carbon, Silicon, Germanium and Tin Donors

There is IR evidence for the formation of $Li_2(C_2)$ ($\nu C{\equiv}C$ at 1845 cm^{-1}) by laser irradiation of lithium films containing carbonate groups.[1]

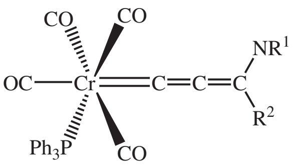
Laser-ablated beryllium atoms react with MeOH to give matrix-trapped MeBe(OH) (δCH_3 modes at 685.4 and 683.4 cm^{-1}), together with (MeO)BeH (δCH_3 1485.6 cm^{-1}).[2] IR laser spectroscopy gave assignments to νCH modes for the species $Mg_2(HCCCN)$.[3]

The IR and Raman spectra of (1) show characteristic bands of terminal and π-bonded, bridging aryl groups, both in the solid state and in solution.[4] The Raman spectrum of uranocene, $U(COT)_2$, at 77 K, gave ligand mode assignments, *e.g.* νCH at 3042 cm^{-1} and νCC at 1500 cm^{-1}.[5]

Matrix-IR spectroscopy was used to study the reaction products of $OVCl_3$ or $CrCl_2O_2$ with C_2H_2. Evidence was found for η^1-ketene complexes, which isomerised to the more stable η^2–C=C 'side-on' complexes.[6] The IR spectra of (2), where R^1 = Me, R^2 = NMe_2, OMe or Ph; R^1 = Ph, R^2 = OMe, all contain a band assigned as $\nu_{as}CCC$, in the range 1956–1971 cm^{-1}.[7] The complex (3) has νC=O of the ketone fragment at 1718 cm^{-1}.[8] Gas-phase IR spectra of the complexes $Cr^+(aniline)_n$, where n = 1 or 2, were consistent with metal-to-ring bonding (characteristic peaks near 1300 cm^{-1}).[9]



(1)



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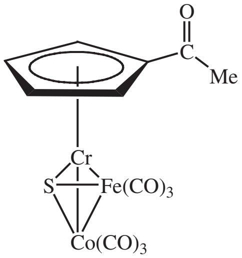
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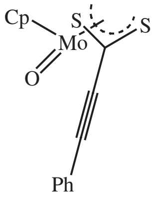
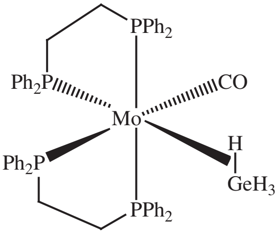

(4)

The complex (4) gives IR bands due to νCS_2 at 1060 and 745 cm^{-1}.[10] The species *cis*-(η^5-RC_5H_4)$_2$$Mo_2$($\mu$-Te)($\mu$-TePh)$_2$, where R = MeCO, PhCO, $MeCO_2$ or $EtCO_2$, all show $\nu C{=}O$ from the ketone or ester carbonyl group in the range 1630–1709 cm^{-1}.[11] *Mer*-[(η^2-C_{60})M(CO)$_3${(-)-DIOP}] and *mer*-[(η^2-C_{60})M(CO)$_3${(+)-DIOP}], where M = Mo or W; DIOP = 2,3-*O,O′*-isopropylidene-2,3-dihydroxy-1,4-bis(diphenylphosphanyl)butane, all show 4 characteristic C_{60} bands in the range 1434–525 cm^{-1}.[12] The coordinated GeH_4 in (5) gives IR bands due to νGeH at 1969, 1938 and 1922 cm^{-1}, with νMo–H–Ge at 1756 cm^{-1}.[13]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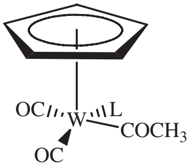
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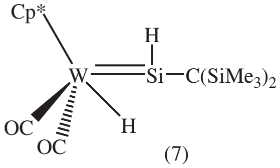
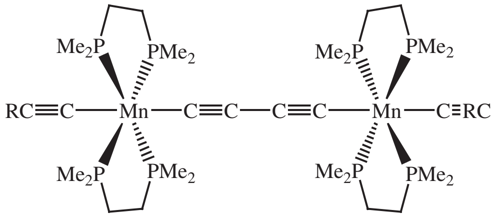

(7)

The complex (6), where L = P(C_6H_4F–*p*)$_3$, has an IR band from $\nu C{=}O$ (acyl) at 1629 cm^{-1}.[14] The IR spectrum of Tp*WCl(η^2-$HOCH_2C{\equiv}CCH_2OH$), where Tp* = hydrotris(3,5-dimethylpyrazol-1-yl)borate, includes $\nu C{\equiv}C$ at 1640 cm^{-1}, with νOH at 3379 cm^{-1}.[15] For (7), the coordinated silane has νSiH at 2052 cm^{-1}.[16]

Bands due to νCCO were assigned for the metalloketene complexes M(H)CCO isolated in argon matrices. For M = Mn, this is at 2082.2 cm^{-1}, while for M = Fe it is at 2087.2 cm^{-1}.[17] The IR spectrum of $Mn_4Br(CH{=}CMe_2)_3(\mu_3\text{-}NPEt_3)_4$ shows that $\nu C{=}C$ is at 1568 cm^{-1}, with $\nu{=}CH$ at 2805 cm^{-1}.[18] The Raman spectra of (8) have ν_sC_4 (a_{1g}) at 1931 cm^{-1} (R = H) or 2006 cm^{-1} ($SiMe_3$). For the one-electron oxidation species the corresponding wavenumbers are 1800 cm^{-1} and 1799 cm^{-1} respectively. Analogous bands are near 2000 cm^{-1} for the two-electron oxidation complexes.[19] The matrix-IR spectra of $(\eta^2\text{-}C_2H_4)MO_2$, where M = Mn or Fe, gave assignments to ethane modes, backed by DFT calculations.[20]



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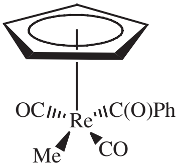

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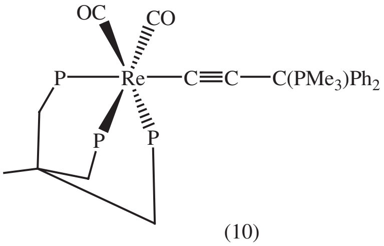

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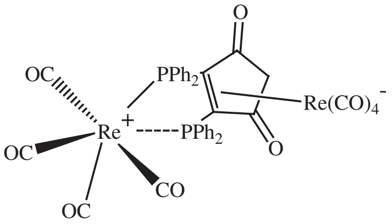

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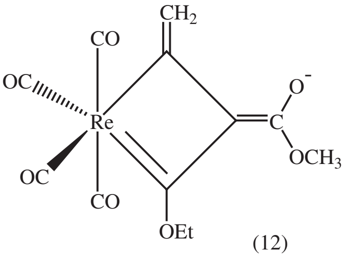

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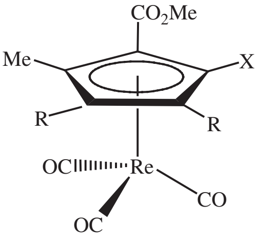
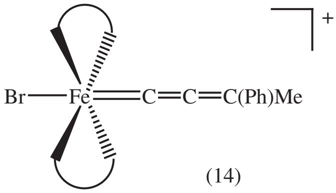


(13)

The complex (9) shows an IR band at 1603 cm^{-1} due to $\nu C{=}O$(acyl).[21] For (10) $\nu C{\equiv}C$ is seen in the IR spectrum at 2074 cm^{-1}.[22] The η^2-coordinated 2,3-bis(diphenylphosphino)maleic anhydride ligand in (11) gives bands at 1781 and 1723 cm^{-1} from $\nu C{=}O$ modes.[23] The carboxylate νCO band at 1630 cm^{-1} for $Li[(OC)Re\{\eta^2\text{-}C(=CH_2)C(CO_2Me)C(OEt)\}]$ shows that there is a contribution from the resonance form (12).[24] The complexes (13), where X = OEt, R = Me, Ph, CO_2Me; X = NEt_2, R = CO_2Me, have an IR band from carboxylate νCO in the range 1720–1745 cm^{-1}.[25]

The IR spectra of $(OC)_3Fe(\mu\text{-}Me_2NCO)Fe(CO)_2(dppm)$ and related species all contain a band near 1500 cm^{-1} from the bridging carbamoyl ligand.[26] (14), where the chelating ligand is depe, $Et_2PCH_2CH_2PEt_2$, has an IR band from νC=C=C of the allenylidene unit at 1893 cm^{-1}.[27] For (15), νC≡C is at 2033 cm^{-1} for the Fe–bound unit, 2052 cm^{-1} from the Ru–bound. The one-electron oxidation product has equivalent bands at 1980 cm^{-1} and 2085 cm^{-1} respectively, showing that the ruthenium is acting as a donor, the iron as an acceptor.[28] The IR and Raman spectra (νC≡C) were able to differentiate between *anti*- and *gauche*-conformations of Cp*(dppe)Fe–$(C{\equiv}C)_n$–Fe(dppe)Cp*, where n = 1 or 2.[29]



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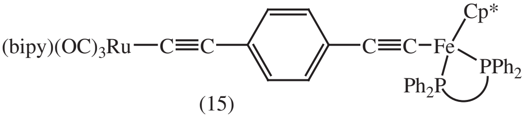

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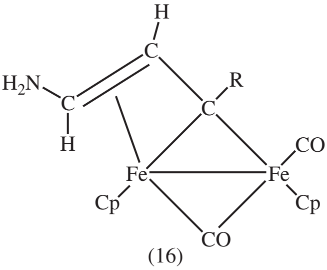

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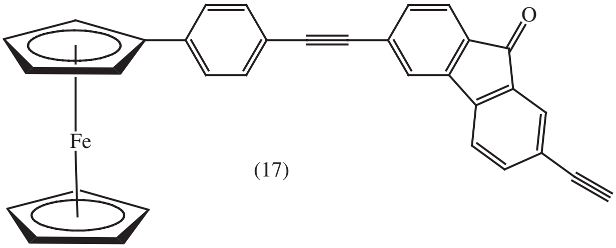

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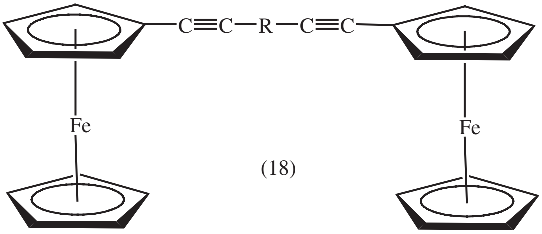

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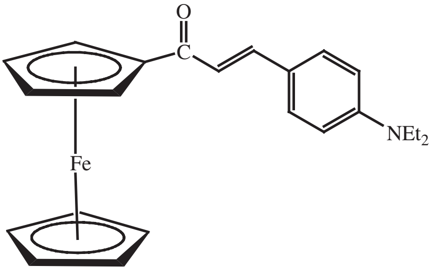

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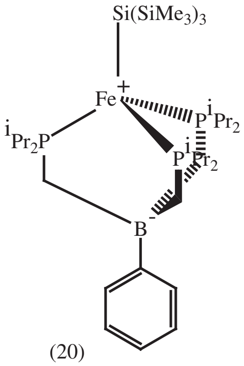


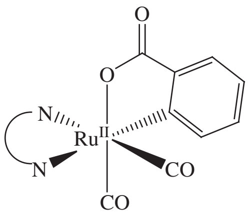
(20)

The IR spectra of matrix-trapped reaction products of iron atoms and ethane show the formation of $Fe(C_2H_4)$ at low, and $Fe(C_2H_4)_2$ at high ethane concentrations.[30] The complex (16), where R = tolyl, gives characteristic terminal and bridging νCO bands.[31] The IR spectrum of $(CpCo)_2[Fe(CO)(CN\text{-}Me)_2(\mu_3\text{-}S)(\mu_3\text{-}C_2S_3)]$ includes νCS of the bridging (*C,S*-bonded) C_2S_3 units at 1019, 1012 cm^{-1}.[32]

IR bands due to the fluorenone νC=O at 1720 cm^{-1} and ν≡C–H at 3302 cm^{-1} were observed for (17).[33] The complexes (18), where R is an aromatic linking group, all have a characteristic ferrocene-ethynyl νC≡C band at about 2210 cm^{-1}.[34] (19) has a νC=O (acyl) band at low wavenumbers, due to conjugation with the π-system $–CH{=}CHC_6H_4–$.[35] There is IR and Raman spectroscopic evidence for the formation of 'improper' hydrogen bonds by Cp_2Fe^+ with PF_6^- and BF_4^- (*i.e.* increased νCH) and of 'proper' hydrogen bonds (decreased νCH) with $FeCl_4^-$ and I_3^-.[36]

The complex (20) gives IR bands from the $Si(SiMe_3)_3$ ligand at 831, 671 and 622 cm^{-1}.[37]

DFT calculations gave vibrational wavenumbers for chemisorbed formyl species (HCO) on a Ru(001) surface.[38] (21), where N–N = bipy, phen, give IR bands from the *O,C*–coordinate benzoate, with $\nu_{as} - \nu_s$ for CO_2 stretches about 300 cm^{-1}.[39] An IR band due to νC=C=C was seen at 1884 cm^{-1} for (22) – a very low value for ruthenium-vinylidene complexes.[40] One-electron oxidation of (23) causes a shift in νCO from 1962 cm^{-1} to 1901 cm^{-1}, and for νC=N from 1494 cm^{-1} to 1542 cm^{-1}.[41] A characteristic νC=C band (1636 cm^{-1}) was observed in the IR spectrum of $(^tBuHC{=}C{=})(dcypb)Ru(\mu\text{-}Cl)_3Ru(dcypb)({=}C{=}CH^tBu)$, where dcypb = $Cy_2P(CH_2)_4PCy_2$.[42]



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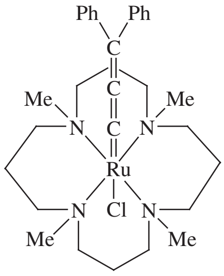

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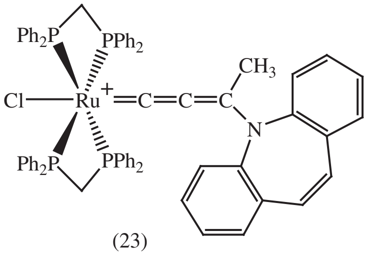

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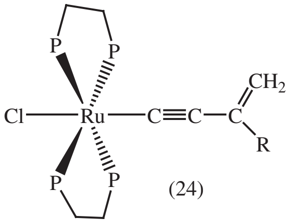

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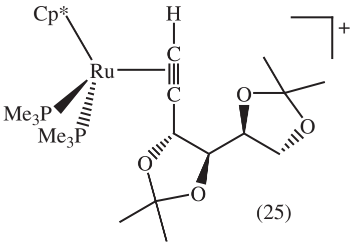


(25)

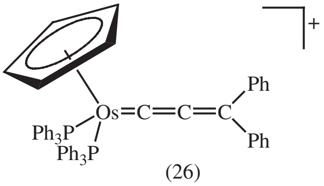
The complexes (24), where R = Me or Ph, have νC≡C at 2049 cm^{-1} (Me), 2041 cm^{-1} (Ph) and νC=C at 1586 cm^{-1} (Me) and 1557 cm^{-1} (Ph).[43] For Ru(Me$_2$bipy)(PPh$_3$)$_2$Cl(C≡CR), where R = ^{t}Bu, *p*-C$_6$H$_4$Me or Ph, νC≡C bands lie in the range 2040–2080 cm^{-1}.[44] All of the species Ru$_2$(R–DMBA)$_4$(C≡C-C$_6$H$_4$Y)$_2$, where R-DMBA = *N*,*N*′-dimethylbenzamidinate or *N*,*N*′-dimethyl-*m*-methoxybenzamidinate; Y = H, 4-NO$_2$, 4-CN, 3-CN or 4-NMe$_2$, give νC≡C near 2070 cm^{-1}.[45] The η^2-alkyne ligand in (25) shows an IR band at 1828 cm^{-1}.[46] The IR spectra of CpRu(L)$_2$SnX$_2$Y, where L = PPh$_3$ or 1/2(dppe), X,

Table 1 *Ligand mode assignments for $CpRu(PPh_3)_2SnX_2Y$ (/cm^{-1})*

X	*Y*	*νSnF*	*νSnCl*	*νSnBr*
F	F	490		
Cl	Cl		290, 272	
Br	Br			256, 263
F	Cl	498	279, 267	
F	Br	487		263
Cl	Br		275	264
Br	Cl		273	265

Y = F, Cl, Br, gave assignments to νSnX and νSnY for the tin-ligands – Table 1.[47]

The complex (26) shows νCCC as a strong IR band at 1924 cm^{-1}.[48] Ligand mode assignments were proposed from the IR spectrum of $Os_2(CO)_8(\mu_2\text{–}\eta^1,\eta^1\text{-}C_2H_2)$, including ν_{as}CH 3025 cm^{-1} (b_1), ν_sCH 2962 cm^{-1} (a_1) and ν_sCC 1519 cm^{-1} (a_1).[49]



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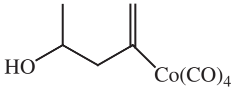

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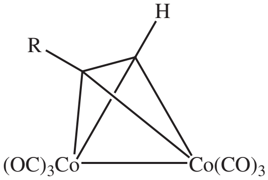

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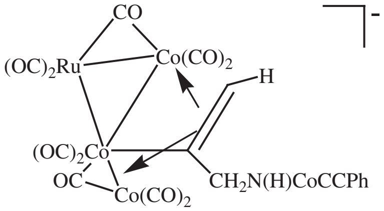

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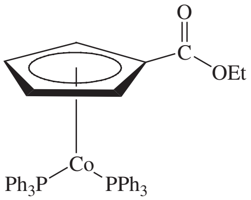

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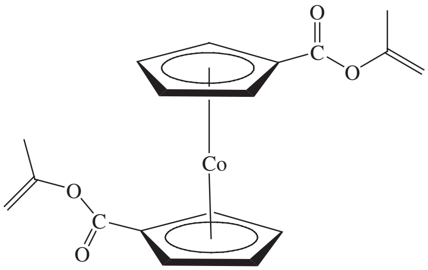
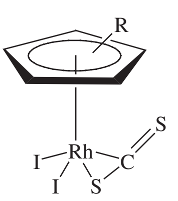


(31)

ATR-IR spectra of (27) showed that the acyl νC=O stretch was at 1710 cm^{-1}, with νC≡O at 2107, 2041, 2022 and 2003 cm^{-1}.[50] The IR band due to νCC was seen near 1560 cm^{-1} for (28, R = imidazolyl-alkyl group), compared to about 2120 cm^{-1} for the free ligand, consistent with the η^2-coordination shown.[51] The complex (29) has νC=O (amide) at 1646 cm^{-1}.[52] IR spectroscopy gave ligand mode assignments for $Co_3(CO)_6[\mu_2{:}\eta^2,\eta^1\text{-}C(Ph)C{=}C(PPh_2)C(O)S\text{-}C(O)](\mu_2\text{-}PPh_2)$.[53] The ester νC=O mode for (30) gave an IR band at 1686 cm^{-1}.[54] An analogous feature for (31) was at 1688 cm^{-1}.[55]

The complex (32), where R = $COOCH_2CH{=}CH_2$, has νCS of the η^2-CS_2 ligand at 1026 cm^{-1}. For (33), characteristic modes of cyclo–octadiene (COD) were seen at 2875, 2827, 1323, 968, 867 and 804 cm^{-1}. The free C=C has νC=C at 1649 cm^{-1}, with the ester νC=O at 1692 cm^{-1} (lowered by conjugation with the cyclopentadienyl ring).[56] (34), where L = P^iPr_3 has νC≡C at 2073 cm^{-1} from the coordinated alkyne.[57] The complexes $Rh_2Co_2(CO)_8(\mu\text{-}CO)_2(\mu_4\text{-}\eta^2\text{–}HC{\equiv}CCH_2O)_2R$, where R = 1,4-$[C(O)]_2$, $[C(O)CH_2]_2$, $[C(O)CH]_2$, $[C(O)_2]_2CH_2$, all have νC=O from the ester unit in the range 1715–1764 cm^{-1}, with bridging νC≡O 1856–1877 cm^{-1}.[58]



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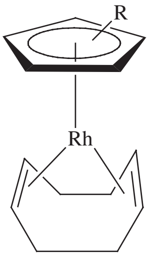

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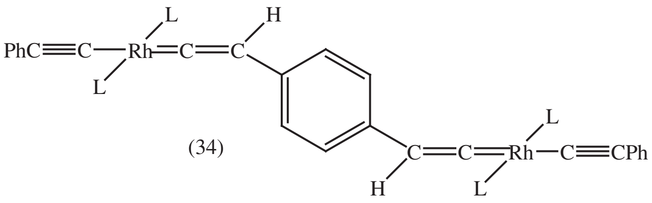

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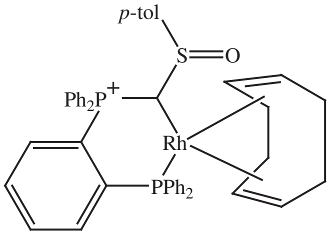

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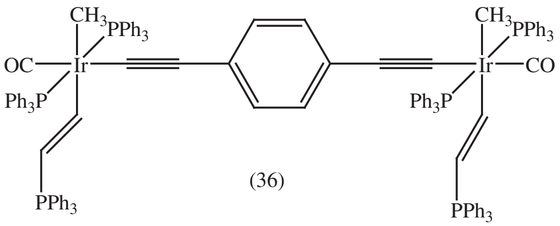

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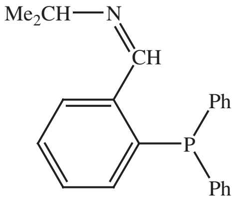


(37)

The IR spectrum of (35) contains a band at 1034 cm^{-1} due to νS=O, confirming the absence of a RhO bond.[59] The complex $IrH(Cl)(C{\equiv}CPh)(PPh_3)_3$ gives an IR band at 2098 cm^{-1} from νC≡C.[60] Such a mode was seen near 2121 cm^{-1} in the IR spectra of (36) and related species.[61]

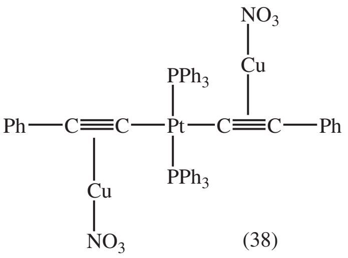
The complexes $Pd[C(O)Me](OTf)(L\text{-}\kappa^2\text{-}P,N)$, where L = $PR_2(N_2C_7H_5)$, R = Ph or NC_4H_4, *i.e.* 7-aza-*N*-indolyl phosphines, have νC=O of the acyl ligand in the region 1697–1729 cm^{-1}.[62] νC=O for the *C*–bound CO_2Ph group in $Pd(Cl)(CO_2Ph)(PPh_3)_2$ is seen as an IR band at 1686 cm^{-1}.[63] $Pd(C{\equiv}CPh)(SnBu_3)(P–N)$, where P–N = (37), has νC≡C at 2088 cm^{-1}.[64]

Matrix-IR spectra of the products of reaction of laser-ablated M (= Pd, Pt) atoms with C_2H_4 gave the π-complex $Pd(C_2H_4)$, but an insertion product $HPt(CHCH_2)$. Vibrational assignments are summarised in Tables 2 ($Pd(C_2H_4)$) and 3 ($HPt(CHCH_2)$).[65] IR data were used to characterise the fullerene complexes $Pd(\eta^2\text{-}C_{60})L_2$, where L = range of phosphines.[66]

Laser-ablated Pt atoms and C_2H_2 reacted to give the matrix-trapped products $PtCCH_2$, HPtCCH and the metallocyclopropane, $Pt(\eta^2C_2H_2)$. All gave characteristic ligand mode assignments from IR spectra.[67] DFT calculations gave vibrational wavenumbers for the aminocarbynes CNH_2, CNHMe and $CNMe_2$ attached to Pt, Pt_7H_6, Pt_2, Pt_9H_{14} and Pt_4 clusters. The results were used to help understand the experimental spectra measured on a Pt(111) surface.[68]

Table 2 *Ligand mode assignments for $Pd(C_2H_4)$ (/cm^{-1})*

ν_2	a_1	νCC + δCH_2	1505.1, 11502.4
ν_3	a_1	δCH_2 + νCC	1216.4, 1208.7
ν_4	a_1	CH_2 rock	933.9
ν_{10}	b_1	CH_2 rock	769.5
ν_{11}	b_1	PdCH bend	585
ν_{13}	b_2	CH_2 sciss.	1420.1, 1417.1
ν_{14}	b_2	CH_2 wag	930.1, 926.8



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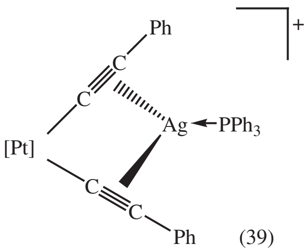

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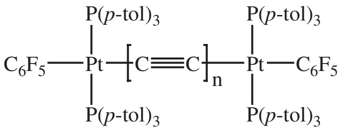

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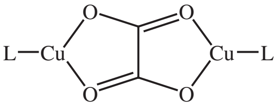


(41)

The IR spectrum of (38) includes $\nu C\equiv C$ bands at 1993 and 1954 cm^{-1}, together with features from η^2-*O,O*-nitrato ligands.[69] $\nu C\equiv C$ was observed at 2090 cm^{-1} for (39), where [Pt] = Pt(4,4'-dimethyl-2,2'-bipyridyl, compared to 2124 and 2114 cm^{-1} in the precursor platinum complex.[70] The following $\nu C\equiv C$ values were assigned for (40), where n = 4 (2152, 2011 cm^{-1}), 6 (2127, 2088, 1992 cm^{-1}) and 8 (2154, 2088, 2054, 1984 cm^{-1}).[71] IR bands from $Pt(C\equiv CR)_4^{2-}$, where R = Ph, 4-Me-, 4-OMe-, 4-CN-, 3-OMe–C_6H_4 *etc.*, give $\nu C\equiv C$ bands in the range 2039–2086 cm^{-1}.[72]

The complex (41), where L = norbornene, has $\nu C{=}C$ at 1473 cm^{-1}, compared to 1567 cm^{-1} for the free ligand. $\nu_{as}CO_2$ of bridging oxalate was seen at 1644 cm^{-1}.[73] IR and Raman spectra of $NaCu_5(C_2)_3$ show νCC of the C_2 unit coordinated to two copper and two sodium atoms in the range 1899–1722 cm^{-1}.[74]

IR data of $(Ph_3PAu)_2(\mu\text{-dec})$, where dec = 1,12-bis(ethynyl)-1,12-dicarba-*closo*-dodeca-borane, 1,12-$(HC\equiv C)_2$-1,12-$C_2B_{10}H_{10}$, include $\nu C\equiv C$ of the Au–C≡C–C unit at 2146 cm^{-1}, with νBH at 2666 and 2614 cm^{-1}.[75] SERS data for C_{60} adsorbed on an aqueous gold colloid show band splitting and the presence of many formally forbidden bands due to lowered symmetry.[76] For C_{60} and C_{70} adsorbed on gold nanoparticles similar data are consistent with metal coordination *via* pentagonal faces.[77]

The IR spectra of $Zn(OTf)_2$ with terminal alkynes in the presence of amine bases show that zinc alkynylides are formed.[78] νCH and $\nu C\equiv C$ values were reported from Raman spectra of $M(C_2H)_4^{2-}$, where M = Zn or Cd. For example, the Rb^+ salts show νCH at 3260 cm^{-1} (Zn or Cd), νCC at 1939 cm^{-1} (Zn) or 1935 cm^{-1} (Cd).[79] Bands due to δSiH_3 were seen in the matrix-IR spectra of $HMSiH_3$, where M = Zn, Cd or Hg, *i.e.* 855–860 cm^{-1} (Zn), 850–860 cm^{-1} (Cd), and 862–871 cm^{-1} (Hg).[80]

Ligand mode assignments were reported for $HAl(Cl)CH_3$, see Table 4 – confirmed by H/D and $^{12}C/^{13}C$ substitution.[81] The complexes (L)Al(C≡CPh), where L = salen or related, include $\nu C\equiv C$ near 2120 cm^{-1}.[82]

Table 3 *Ligand mode assignments for* $HPt(CHCH_2)$ *(/cm^{-1})*

ν_5	C=C str.	1559.7
ν_6	CH_2 sciss.	1365.6
ν_7	CCH i.p. bend	1242.1
ν_9	HCCH o.o.p.bend	928.0
ν_{10}	CH_2 wag	868.5

Table 4 *Ligand mode assignments for* $HAl(Cl)CH_3$ *(/cm^{-1})*

$\nu_{as}CH_3$	3015.2
ν_sCH_3	2984.4
δ_sCH_3	1199.7
ρCH_3	743.7

Ab initio and DFT calculations have been made for vibrational wavenumbers of $CH_3Si(C{\equiv}CH)_3$.[83] Assignments and intensity measurements have been made for νC≡C modes for $Me_3MC{\equiv}CX$, where M = Si, Ge or Sn, X = organic and inorganic substituents.[84]

IR bands due to νC=C were assigned (range 1636–1656 cm^{-1}) for the complexes (p-R-$C_6H_4COCH_2)_2TeX_2$, and (p-R-$C_6H_4COCH_2)_2Te$, where R = Me or MeO, X = Cl, Br or I.[85]

2 Dihydrogen Complexes

FTIR spectra and DFT calculations have been reported for matrix-isolated $(H_2)MH$, where M = Cu or Ag, showing νH–H bands at 3805.9 cm^{-1} (M=Cu) or 3566.6 cm^{-1} (Ag).[86]

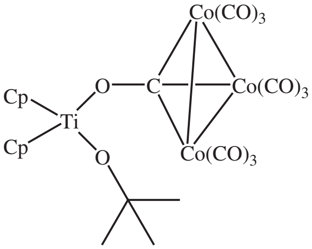
3 Boron Donors

Well-resolved terminal νBH bands were seen in the IR spectra of 2,2',4,4'-$(Me_3Si)_4$-3,5',6'-[$(\mu\text{-H})_3Na(X)_n(Y)_m$]-1,1'-*commo*-Ln($\eta^5$-2,4-$C_2B_4H_4)_2$, where Ln = Nd, X = thf, n = 2, Y = none, *etc.* (2270–2590 cm^{-1}).[87] The IR spectra of $(thf)_4Eu\{(\mu\text{-H})_2BC_8H_{14}\}_2$ and related, include νCH at 2760 cm^{-1} due to agostic interaction of Eu with the α-C–H of the organohydroborate, together with νEu-H–B 2012–2075 cm^{-1}.[88]

The complex RuH[7,8-$(PPh_3)_2$-7,8-$C_2B_9H_{10}$]$(PPh_3)_2$ shows IR bands due to νBH at 2609, 2578, 2561 and 2534 cm^{-1}.[89] The complex *nido*-(η^5-$C_5H_4I)Co(2,3\text{-}Et_2C_2B_3H_5)$ gives IR bands of νBH(t) 2535.3 cm^{-1}, and νB–H–B 1867.5 cm^{-1}.[90] For (Tp*)$NiBH_4$, where Tp* = hydrotris(3,5-dimethylpyrazolyl)borate, the η^3-BH_4 ligand has νBH(t) near 2500 cm^{-1} and νBH(br) 2110 and 2063 cm^{-1}.[91]

4 Carbonyl and Thiocarbonyl Complexes

The adsorption of CO on Li–ZSM-5 showed the presence of two lithium sites. Thus Li^+–CO has νCO at 2193 and 2187 cm^{-1} for these two. There was also some evidence (a weak band at 2100–2120 cm^{-1}) for formation of Li^+–OC.[92] An FTIR study (νCO) has been reported for carbonyl species formed by CO adsorption on polycrystalline and single-crystal MgO.[93]



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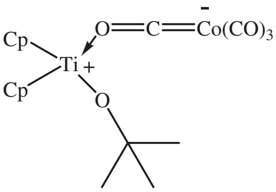


(43)

The complex (42) gives an IR band due to multiply-bridged carbonyl at 1472 cm^{-1}, while for (43) the bridging carbonyl group has νCO at 1741 cm^{-1}.[94] The adsorption of CO on $Pd/WO_3{-}ZrO_2$ at 85K gives νCO from Zr^{4+}–CO at 2212 cm^{-1}, together with νCO due to Pd^{n+} surface carbonyls (n = 0–3).[95] IRAS data of νCO adsorbed on alumina-supported vanadium nanoparticles show the formation of $V(CO)_x$, where x = 1–3.[96]

IR spectroscopy shows that CO adsorption on $Mo_3N/\gamma\text{-}Al_2O_3$ catalysts gives νCO bands at 2045 and 2200 cm^{-1} due to linearly-adsorbed CO on Mo and N sites respectively.[97] Similar data for CO on $MoP/\gamma\text{-}Al_2O_3$ includes νCO at 2037 cm^{-1} from linearly-coordinated CO,[98] while for CO adsorption on silica-supported Mo_2C catalysts they are at 2089 and 2032 cm^{-1}.[99] CO adsorption on silica-supported molybdenum forms a Mo(II) carbonyl, with νCO near 2170 cm^{-1}.[100]

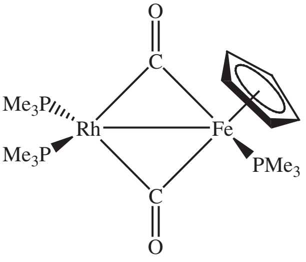
Temperature-dependent TRIR spectra were used to probe the mechanism of anchoring and decarbonylation processes for $Mo(CO)_6$ in dehydrated NaY zeolite.[101] Resonance Raman spectroscopic methods have been developed to obtain spectra of photolabile transition metal carbonyls including $Cp_2Mo_2(CO)_6$ and $Cp_2Fe_2(CO)_4$.[102]

TRIR data were used to follow ligand substitution reactions of photocatalytically-generated intermediates $CpMn(CO)_2(CyH)$, where CyH = cyclohexane, with L = cyclopentene, thf, furan or pyrrolidine, to form $CpMn(CO)_2(L)$.[103] Picosecond to microsecond time-scale TRIR was used to follow the photoinduced dynamics of $[\eta^5\text{-}C_5H_4C(O)R]Mn(CO)_3$, where R = $CH(SMe)_2$ or $C(SMe)_3$.[104]

DFT calculations and TRIR data have been reported for a range of *fac*-$Re(CO)_3$ complexes containing bipy or dipyridophenazine derivatives.[105] Ultrafast two-dimensional transient IR spectroscopy was used to follow photoinduced charge transfer processes in $Re(CO)_3(dmbpy)$, where dmbpy = 4,4'-dimethyl-2,2'-bipyridine. νCO bands showed significant shifts to higher wavenumbers due to MLCT.[106]

A review has appeared on the use of TRIR to probe excited states and reaction intermediates, *e.g.* for *fac*-$[Re(CO)_3(dppz\text{-}Cl_2)(R)]^{n+}$, where dppz-$Cl_2$ = 11,12-dichloropyrido[3,2-a:2',3'-c]phenazine, R = Cl^- (n = 0), py (n = 1).[107] DFT calculations of νCO bands have been reported for the ground and MLCT-excited states for *fac*-$[Re(4,4'\text{-}Xbipy)(CO)_3(4\text{-}Etpy)]PF_6$, where X = CH_3, H or CO_2Et.[108] Resonance Raman data for *fac*-$[Re(Cl)(CO)_3(bopy)_2]$, where bopy = 4-benzoylpyridine, show increased νC≡O and decreased νC=O on the first allowed electronic transition, confirming the Re → bipy MLCT character of this transition.[109] Low-temperature TRIR (νCO) was used to probe the transient mixed-valence character of $Re_4{}^{I}(CO)_{12}(4,4'\text{-}bipy)_4Cl_4$ during the ^{3}MLCT transition.[110]

The 6-coordinate complex $[Fe(TpivPP)(NO_2)(CO)]^-$ has νCO at 1974 cm^{-1} – only slightly higher than in 6-coordinate complexes with neutral N-donors (rather than $NO_2{}^-$) *trans* to CO.[111] There is IR (νCO) evidence for the formation of a range of carbonyl species by adsorption of CO on a silica-supported Fe–Ru alloy.[112] The bridging carbonyls in (44) have νCO bands at 1673 and 1712 cm^{-1}.[113]



(44)

DFT calculations have been reported for νCO and νCN wavenumbers in $[Fe(CN)_x(CO)_y]^q$, where x = 0–6, y = 0–5.[114] The FTIR spectra of matrix-isolated products of electron bombardment of $Fe(CO)_5$ gave evidence for $Fe(CO)_n$, where n = 2, 3 or 4, $Fe(CO)_m{}^-$, where m = 3 or 4.[115] A detailed analysis has been given of νCO modes in planar clusters containing $M(CO)_4$ groups, *e.g.* $\{[Fe(CO)_4]_4Au\}^-$, $\{[Fe(CO)_4]_4Pt\}^{2-}$ and $M_3(CO)_{12}$, where M = Ru or Os.[116] FTIR spectra and DFT calculations have been used to probe D_{3h}, C_{2v} and C_{4v} conformers of $Fe(CO)_5$ in solution.[117]

IR and resonance Raman studies have been reported for a large number of CO-bound biologically important systems. These include haemoglobin;[118] myoglobin;[119–121] a range of cytochrome systems;[122–125] and microperoxidase.[126]

CO adsorbed on a Ru(0001) electrode gave IR bands from linear (1970–2040 cm^{-1}) and three-fold bridging (1770–1820 cm^{-1}) carbonyl systems.[127] The IR spectrum of CO adsorbed on a ruthenium-modified Pt(100) surface includes a feature due to terminal Ru–CO at 2092 cm^{-1}.[128] IR data (νCO) were given for selenido–carbonyl ruthenium clusters anchored to functionalised silica gels.[129]

The complex $Ru(CO)_2(sq)_2$, where sq = 3,5-di-*tert*-butyl-1,2-benzosemiquinone, shows shifts of 53–99 cm^{-1} to lower wavenumber for νCO on two-electron reduction.[130] Oxidation of $Ru(PPh_3)_2(CO)_2(L)$, where H_2L = 7,8-hydroxy-6-methoxycoumarin, to the monocation shifted νCO from 1978 and 2042 cm^{-1} to 2018 and 2072 cm^{-1}.[131] IR spectroelectrochemistry and resonance Raman spectroscopy were used to probe the photo- and electrochemistry of the clusters $Ru_3(CO)_8(\mu\text{-}CO)_2$(α-di–imine), where α-di–imine = bipy, 4,4-Me_2bipy or 2,2'-bipyrimidine.[132]

IR spectroelectrochemical studies on $Os_3(CO)_n(\mu_m\text{-}\eta^2\text{-L–H})(\mu\text{-H})$, where L = quinoline-4-carboxaldehyde, n = 10, m = 2, n = 9, m = 3 (N–C(S) bound), *etc*., show characteristic decreases in νCO on reduction.[133]

Adsorption of CO on Co–Pd bimetallic particles gives νCO bands which enable the surface to be characterised.[134] FTIR spectra of CO adsorbed on cobalt-exchanged mordenites show the presence of two types of Co(II) carbonyls at the surface.[135]

The IR spectrum of jet-cooled $Co(CO)_3(NO)$ shows that ν_1 (νCO) is centred at 2111.7457(9) cm^{-1}.[136] A detailed IR study (νCO) has been made for $XCo(CO)_4$, where X = H, D, EtC(O), EtOC(O) or $EtOC(O)CH_2$, including data for ^{13}CO-substituted analogues. The reported results of an energy-factored normal coordinate analysis gave good agreement with esperiment.[137]

SERS data for CO adsorbed on roughened rhodium electrodes gave νCO of Rh–CO at about 2000 cm^{-1}.[138] νCO data were used to quantify the *cis*-effects of phosphine, arsine and stibine (= L) ligands in *trans*-$RhCl(CO)L_2$.[139]

IR bands due to νCO for $[Rh(CO)_2(L)]^+$, where L = bis[2-(3,5-dimethyl-1-pyrazolyl)ethyl]-ether, showed that two isomers were present in solution (four bands seen).[140] Fast TRIR data were used to follow the reactions of $(\eta^5\text{-}C_5R_5)Rh(CO)_2$ (R = H or Me) in supercritical noble gases (Xe, Kr). Evidence was found for the formation of CpRh(CO)(L), where Cp = C_5H_5 or C_5Me_5, L = Xe or Kr, at room temperature.[141]

Adsorption of CO on Rh–ZSM-5 leads to the formation of $Rh^+(CO)_3$ (νCO 2181, 2118, 2084 cm^{-1}) – converted to *gem*-$Rh^+(CO)_2$ (2115, 2048 cm^{-1}) on decreasing the CO pressure. A short evacuation at 673–783K, followed by quenching, led to the appearance of a band at 2101 cm^{-1} from linear Rh^+–CO.[142] Adsorption of CO on Rh_n clusters (n = 3–15) was studied in the gas phase. A range of anionic, neutral and cationic species was formed, with νCO IR bands in the region 1650–2200 cm^{-1}. Assignments were assisted by DFT calculations.[143]

Time-resolved FTIR spectra of $Rh_4(CO)_{12}$ subjected to 266 nm. irradiation in heptane gave evidence for the formation of two isomeric forms of $Rh_4(CO)_{11}$(solv).[144] Vibrational assignments were made to νCO modes for gas-phase rhodium cluster carbonyls using IR multiphoton depletion spectroscopy. For $Rh_n(CO)$, νCO was at 1950 ± 2 cm^{-1} (n = 6), 1960–1965 cm^{-1} (n = 7–11; 13–20).[145] TRIR data (νCO) were used to follow the formation of intrinsically chiral clusters $Rh_6(CO)_{14}(\mu,\kappa^2\text{-PX})$, where PX = bidentate bridging ligands diphenyl(benzothienyl)phosphine and related systems.[146]

TRIR spectra (νCO) gave evidence on the photolysis of Vaska's complex, *trans*-$(Ph_3P)_3Ir(CO)Cl$ – suggesting the formation of a dimeric intermediate species.[147] IR spectroscopy (νCO) was used to probe the binding of CO to carbon monoxidedehydrogenase/acetyl-CoA synthase. A band at 1996 cm^{-1} was assigned to a terminally-bound Ni^I–CO unit.[148]

IR (νCO) studies of CO adsorbed on Ni_2P/SiO_2 showed the formation of $Ni^{\delta+}(CO)$ (terminal) (2083–2089 cm^{-1}), $Ni^{\delta+}(CO)$ (bridged) (1914 cm^{-1}), $Ni(CO)_4$ (2056 cm^{-1}) and P–CO (near 2200 cm^{-1}).[149] IR photodissociation spectra have been reported for the ion-molecule clusters $NiO_2{}^+(CO)_m$ (m = 2–6) and $Ni^+(CO_2)_n$ (n = 3–7).[150]

IR data (νCO) for CO adsorbed on Pd/Pt on Mg/Al mixed oxides showed the formation of 'on-top' coordinated M(CO) (M = Pd, Pt), with a feature below 2000 cm^{-1} from a Pd^0 bridging species.[151] The nature of the surfaces of 5.0 wt. % Pt/γ-Al_2O_3 catalysts was studied by CO adsorption and FTIR (νCO) spectroscopy.[152] The effects of the presence of tin on the Pt(111) surface were studied similarly,[153] as were the effects of laser heating on the Pt(111) surface.[154]

SERS data were used to study the adsorption and electro-oxidation of CO at a platinum-formic acid interface.[155] *In situ* microscopic FTIRS studies were reported for the carbonyl species formed by CO adsorption on nanostructured platinum micro-electrodes.[156] The nature of the surfaces of Pt_n nanoparticles and their aggregates were probed by examining νCO bands of the carbonyl species formed on CO adsorption.[157]

The FTIR spectra (νCO) of CO adsorbed at low-temperature (85K) on CuMgAl–hydrotalcite gave evidence for the formation of $Cu^I(CO)_2$ species, which convert to $Cu^I(CO)$ on evacuation.[158] A resonance Raman study (νCO) has been made of the electron distribution in mixed-valence cytochrome *c* oxidase.[159]

IRAS data (νCO) were reported for CO adsorbed on gold clusters (1.8–3.1 nm) supported on TiO_2. νCO was approximately 4 cm^{-1} higher than for adsorption on to bulk gold.[160]

Laser-ablated M (=Ag, Au) atoms react with CS_2 to form matrix-trapped species including M(CS), $M(CS)_2$ and $M_2(CS)$ – the first observed binary silver and gold thiocarbonyl complexes – assignments are listed in Table 5. There was also evidence for SM(CS), with νCS 1362.2 cm^{-1} (Ag) or 1382.2 cm^{-1} (Au), together with M(SCS), with characteristic bands at 1507.1 cm^{-1} (Ag) or 1485.9 cm^{-1} (Au).[161,162]

FTIR spectra of CO adsorbed on high-surface-area SnO_2 gave evidence for $Sn^{IV}(CO)$ coordination (νCO 2201 cm^{-1}).[163]

Table 5 *νCS assignments for the products of Ag or Au + CS_2 reactions (/cm^{-1})*

AgCS	1176.1
$Ag(CS)_2$	1232.3
Ag_2CS	1308.2
AuCS	1239.5
$Au(CS)_2$	1317.6
Au_2CS	1366.8

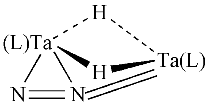
5 Nitrogen Donors

5.1 Molecular Nitrogen, Azido- and Related Groups. – DRIFT data for N_2 adsorbed on sodium mordenites gave evidence for both end-on and perpendicular coordination of the N_2 to Na^+.[164] Ultrafast polarisation IR spectra were reported for ν_3 (ν_{as}) for azide in NaN_3, $MgN_3{}^+$ and $CaN_3{}^+$ ion-pairs in dmso solutions.[165]

IR bands from bridging $N_3{}^-$ ligands were assigned for $[Be_4X_4(\mu\text{-}N_3)_6]^{2-}$, where X = Cl ($\nu_{as}$ 2142 cm^{-1}, ν_s 1297 cm^{-1}, δ 649 cm^{-1}) or Br (2132, 1299, 644 cm^{-1}).[166]

IR and Raman spectra gave assignments to azido-ligand modes for the Ti–NNN bonded complexes $[Ti(N_3)_n]^{(4-n)-}$, where n = 4, 5 or 6, *e.g.* for n = 5, ν_{as} modes were seen at 2100, 2070, 2058 cm^{-1} (IR), 2133, 2110, 2083, 2070 cm^{-1} (Raman).[167] Coupled νN=N and νC=N modes were observed in the range 1380–1390 cm^{-1} in the IR spectra of $Zr(L)Cl_2$, where L = p-C_6H_4–N=N–C_3H_2NNR' (R = H, Me, Cl; R′ = Me, Et, CH_2Ph).[168]

DFT calculations gave vibrational wavenumbers for the complexes ML_n, where M = V, Cr, Mn, Fe, Co, Ni; L = pentazolato; n = 1 or 2.[169] An IR band due to νNN for (45), where L = $(PhNSiMe_2CH_2)_2PPh$, is seen at 1165 cm^{-1} (1108 cm^{-1} for the ^{15}N analogue).[170] Assignments were made as follows for the modes of $N_3{}^-$ ligands in $[Cp^*Ta(N_3)_3(\mu\text{-}N_3)]_2$: ν_{as} 2134 cm^{-1} (bridging), 2110, 2090 cm^{-1}(terminal); ν_s 1232 cm^{-1} (bridging), 1280 cm^{-1} (terminal).[171]



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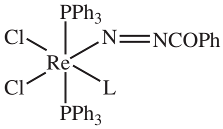


(46)

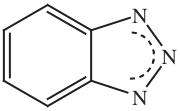
The complexes (46), where L = py, $C_3N_2H_4$, give IR bands from coupled νN=N, νC=N and νC=O modes in the range 1550–1650 cm^{-1}.[172]

An IR band at 2037 cm^{-1} was assigned as $\nu_{as}N_3$ for $Fe(bpga)(N_3)(OMe)$, where bpga = bis(6-pivalamido-2-pyridymethyl)(carboxymethyl)amine.[173] The complexes [Ru]–N≡N–Ar, where [Ru]=RuTp(L)(L′), where Tp = hydrotris(pyrazolyl)borate, L = $P(OEt)_3$, $PPh(OEt)_2$, L′ = PPh_3, or L = L′ = $P(OEt)_3$; Ar = Ph, 4-MeC_6H_4, all give νN_2 in the range 2095–2073 cm^{-1}, consistent with the presence of a linear ArN_2 group.[174]

IR spectroscopy gave azido ligand mode assignments for $Co(trenb)(N_3)^+$ and $Co(dienb)(N_3)_2(OAc)$, where trenb = tris[2-(benzyamine)ethyl]amine; dienb = 1,9-dibenzyl-2,5,8-triazanonane.[175] The $\nu_{as}N_3$ modes for the bridging and terminal azido ligands for $Co_2(immepy)_2(N_3)_4$, where immepy = 4,4,5,5-tetramethyl-2(6′-methyl-2′-pyridyl)imidazoline-1-oxyl, were seen at 2067 cm^{-1}, 2047 cm^{-1} respectuvely.[176]

Adsorption of N_2 on Cu–ZSM-5 zeolite produced an IR feature due to a surface complex at 2295 cm^{-1}.[177] The complex $Cu_2L_2(N_3)_2$, where

L = 1-(N-salicylideneamino)-2-aminoethane, shows $\nu_{as}N_3$ at 2036 cm^{-1}.[178] IR bands due to $\nu_{as}N_3$ for $[Cu(L)(N_3)_2]_n$ and $[Cu(Me\text{–}L)(N_3)_4]_n$, where L = 2-(pyrazol-1-ylmethyl)pyridine, Me–L = 2-(3-methylpyrazol-1-ylmethyl)pyridine, show the presence of both 'end-on' and 'end-to-end' bridging azido groups.[179] SERS data for benzotriazole, (47), in an aqueous silver sol show coordination to Ag *via* nitrogen atoms of the benzotriazole ring.[180]



(47)

The mercury(I) complex $Hg_2(N_3)_2$ gives IR bands due to $\nu_{as}N_3$ (2080 cm^{-1}) and ν_sN_3 (1268, 1317 cm^{-1}).[181] The Raman spectrum of $^tBu_2Ga(N_3)$ includes ν_sN_3 at 1406 cm^{-1}.[182] The first report has been made of vibrational data for pure solid $E(N_3)_3$, where E = As or Sb. Assignments are summarised in Table 6.[183] The IR spectrum of $(C_6F_5)_3As(I)(N_3)$ includes $\nu_{as}N_3$ at 2133 cm^{-1}, ν_sN_3 at 1282 cm^{-1} and δN_3 at 663 cm^{-1}.[184]

5.2 Amines and Related Ligands. – The IR and Raman spectra of $LiX.NH_3$, where X = Br or I, show νNH of the coordinated ammonia at 3362, 3277 cm^{-1} (Br) or 3366, 3276 cm^{-1} (I).[185] The complexes $Cp_2Mg(NHRR')$, where R = H, $R' = CH[CH(CH_3)_2]_2$, $CH(CH_3)_2$, $C(CH_3)_3$, $CH_2C_6H_5$, C_6H_{11}, $R = R' = CH_2CH_3$, $CH_2C_6H_5$, C_6H_{11}, $R = CH(CH_3)_2$, $R' = CH_2C_6H_5$, all show νNH in the range 3313–3164 cm^{-1}. The low values arise from hydrogen–bonding interactions.[186]

Table 7 summarises the assignments made from matrix-IR data for the 1:1 adduct $VCl_4.NH_3$ (all figures relate to the $^{14}NH_3$ form). For Cl_2VNH_2, ν_sNH_2 is at 3317 cm^{-1}, δNH_2 at 1419 cm^{-1} and τNH_2 at 581 cm^{-1}.[187]

Table 6 *Ligand mode assignments for $E(N_3)_3$ (/cm^{-1})*

	E=	*As*	*Sb*
a	$\nu_{as}N_3$ in-phase	2128	2121
	ν_sN_3 in-phase	1251	1243
e	$\nu_{as}N_3$ out-of-phase	2092	2085
	ν_sN_3 out-of-phase	1231	1243

Table 7 *Ligand mode assignments for $VCl_4.^{14}NH_3$ (/cm^{-1})*

$\nu_{as}NH_3$	3395
ν_sNH_3	3296
$\delta_{as}NH_3$	1598
δ_sNH_3	1197
ρNH_3	696

Variable-temperature IR data (20–295K) for $[Cr(NH_3)_6](BF_4)_3$ showed no changes due to phase transitions in this range.[188] IR and Raman spectra gave detailed assignments of ligand modes for $[MBr_2(mMA)_2]_n$, where M = Mn or Ni, mMA = m-methylaniline.[189] IR and Raman data for $[Mn_4O_3Cl_4(O_2CEt)_3py_3]_2$ included characteristic pyridine ligand bands at 647, 1017, 1075, 1160, 1222, 1541, 1570 and 1609 cm^{-1}.[190]

TRIR and TR^3 spectra were used to study the dynamics and mechanism of metal-to-ligand and interligand electron transfer in *fac*-$[Re(MQ^+)(CO)_3(dmb)]^{2+}$, where MQ^+ = *N*-methyl-4,4′-bipyridinium, dmb = 4,4′-dimethyl-2,2′-bipyridine.[191,192]

TR^3 spectra were used to obtain data on the ligand modes of both high- and low-spin isomers of $[Fe(L)]^{2+}$, where L = *N,N,N′,N′*-tetrakis(2-pyridylmethyl)-6,6′-bis(aminomethyl)-2,2′-bipyridine or *N,N′*-bis(benzyl)-*N,N′*-bis(2-pyridylmethyl)-6,6′-bis(aminomethyl)-2,2′-bipyridine.[193] Resonance Raman and TR^3 data were used to obtain detailed ligand mode information for $Ru(bipy)_2(dpp)^{2+}$ and $(bipy)_2Ru(dpp)Ru(bipy)_2{}^{4+}$, where dpp = 2,3-bis(2-pyridyl)pyazine, and their bipy-d_8 analogues.[194] A resonance Raman study has been carried out on electronic communication and delocalisation in complexes involving two Ru_3 clusters linked by a pyrazine ligand.[195]

A temperature-dependent Raman analysis was performed on the MLCT excited states of the complexes $[Os(bipy)_{3-0.5n}(py)_n]^{2+}$, where n = 0, 2 or 4.[196]

The IR and Raman spectra of ML_nI_2, where M = Ni, n = 4; M = Zn or Cd, n = 2, L = m-methylaniline, gave quite detailed ligand mode vibrational assignments.[197] The IR spectra of platinum(II) complexes in carbamide and carbamide-halide melts show the formation of $Pt(NH_3)_4{}^{2+}$ on dissolution of $(NH_4)_2[PtCl_4]$, as well as $Pt(NH_3)X_3{}^-$ in the presence of $NH_4{}^+X^-$, where X = Cl or Br.[198] Picosecond-scale TRIR spectroscopy was used to probe the dynamics of the lowest excited state of $Pt(bipy)(4\text{-}CN\text{–}C_6F_4\text{–}S)_2$.[199]

IR and Raman spectra gave ligand mode assignments for crystalline $[Cu(NH_3)_5](ClO_4)_2$.[200] The IR and Raman spectra of $[Cu(phen)(PPh_3)_2]^+$ and its phen-d_8 analogue were observed and assigned using DFT calculations. TR^3 studies gave evidence for $phen^{\bullet -}$ and d_8-$phen^{\bullet -}$ species.[201] *Ab initio* and DFT calculations have been reported for vibrational wavenumbers and Raman intensities for $(py)M_n$ clusters, where M = Cu, Ag or Au, n = 2–4.[202,203]

IR ligand mode assignments (νC=O, νNH) have been proposed for $[(L)Zn](ClO_4)_2$ and $[(L)Zn(H_2O)(NCCH_3)](ClO_4)_2$, where L = 6-R-2-pyridylmethyl)-R, where R = $NHCO^tBu$ and related.[204] ATR-FTIR spectroscopy was used to characterise the coordination of Cd^{2+} to pyridine terminal groups of self-assembled bilayers.[205]

The IR and Raman spectra of $SnX_4(DMPP)$ and $R_2SnX_2(DMPP)$, where X = Cl, Br or I; R = Me, Et, Bu or Ph; DMPP = 3,5-dimethyl-1-(2′-pyridyl)pyrazole, were all consistent with the presence of an *N,N*–bidentate ligand.[206]

5.3 Ligands Containing >C=N– Groups. – The Raman spectrum of chlorophyll *d* from *Acaryochloris marina* has been reported, and ligand modes assigned using DFT calculations.[207]

The IR spectra of $M(Pc)_2$, $M(Pc^*)_2$, where M = Y, La–Lu (except Pm), H_2Pc = phthalocyanine, H_2Pc^* = 2,3,9,10,16,17,24,25-octakis(octyloxy)phthalocyanine, show that the $Pc^{-\bullet}$ marker band (1312–1323 cm^{-1}) and the isoindole stretching band (1439–1454 cm^{-1}) are dependent on the ionic radius of M.[208] Ligand mode assignments were proposed for M^{III}(OEP)(2,3-Nc), where M = Y, La–Lu, except Ce, Pm, OEP = octaethylporphyrinato; Nc = naphthalocyaninato, and for the intermediate valence species Ce(OEP)(Nc).[209] Ligand mode assignments for (Pc)M(OOPc)M(OOPc), where Pc = phthalocyaninato, M = Eu, Gd, Tb, Dy, Ho, Er, Yb, Lu or Y, H_2OOPc = 2,3,9,10,16,17,24,25-octakis(octyloxy)phthalocyanine, show weaker π–π interactions in these triple-decker sandwich species by comparison with double–decker complexes.[210]

The resonance Raman spectrum of a 1:1 complex of Cm^{III} with 6-methyl-2-(2-pyridyl)-benzimidazole, includes a band due to the heterocyclic ring breathing mode at 1023 cm^{-1}, compared to 1003 cm^{-1} for the free ligand. This is consistent with a strong Cm^{3+}-ligand interaction.[211]

The complex $(OC)_4Cr(\mu\text{-}C{=}NR)(\mu\text{-dppm})Pt(PPh_3)$, where R = CH_2SO_2-*p*-tolyl, gives an IR band from νC=N of the bridging isocyanide at 1667 cm^{-1}.[212] Resonance Raman data were reported for $Mo(CO)_4L$, where L = 2,3-di(2-pridyl)-quinoxaline (dpq) or 5-methyl-2,3-di(2-pyridyl)-quinoxaline (5mdpq), for oxidised and reduced species. The latter showed bands from dpq^-, $5mdpq^-$ respectively.[213]

The FTIR spectra of $M(L)_2{}^{2+}$, where M = Mn, Co, Ni, Cd; L = 2-aminopyrimidine, show that L is coordinated *via* the pyrimidine ring nitrogen atom only.[214] The resonance Raman spectrum of Mn^{III}(TPP)Cl encapsulated in Ti–MCM-41 was used to probe the electron-accepting ability of the MCM-41 framework.[215] Resonance Raman data gave assignments to ligand marker bands for cytochrome *c* peroxidase and a number of variants with an engineered Mn(II) binding site.[216]

TR^3 and TRIR spectra gave data on the picosecond relaxation of ^{3}MLCT excited states of $[Re(Etpy)(Cl)(dmb)]^+$ and $Re(CO)_3(bipy)$, where dmb = 4,4′-dimethyl-2,2′-bipyridine.[217]

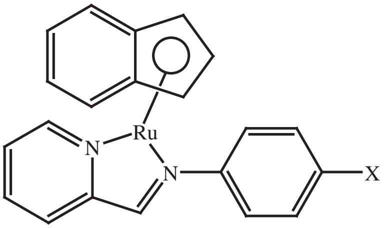
The bis(base) (where base = *N*-methylimidazole, 1,5-dicyclohexylimidazole, pyridine) complexes of Fe^{II}(TpivPP), where TpivPP = tetrakis(*o*-pivalamidophenyl)porphyrin, give characteristic porphyrinate ligand bands.[218] Resonance Raman spectra were used to obtain excitation profiles for two a_{2g} ligand modes for a range of iron(II) porphyrins.[219] Ligand modes in the resonance Raman spectra of *trans*-cross-linked ‘basket-handle’ iron(II) porphyrins were used to characterise the ruffled, six-coordinated low-spin iron(II) porphyrin complexes.[220]

Resonance Raman spectra show that *E. coli* flavoHb coordinates fatty acids to give a six-coordinate high-spin haem iron.[221] TR^3 studies were used to study the allosteric pathway of haemoglobin.[222,223] The resonance Raman spectra of the H64V mutant of human neuroglobin show that it is 6-coordinate, high-spin in the Fe(III) state, 5-coordinate high-spin in the Fe(II) state.[224] TRIR studies have been reported for the dynamic behaviour of myoglobin and its mutants.[225,226]

There have been several IR and resonance Raman studies of cytochrome species.[227–234] The out-of-plane haem modes give characteristic patterns due to haem distortions in inducible nitric oxide synthase.[235] Resonance Raman data for Fe(AcMP8), where AcMP8 = *N*-acetylmicro-peroxidase, were used to follow HS/LS equilibria in iron (II) and (III) species.[236,237]

Resonance Raman data were used to study the change of iron spin state in horseradish peroxidase *c* – induced by the removal of calcium.[238] Ligand modes for spin-state cycling of photosystem II from a cyanobacterium are very similar to those for related systems from spinach.[239]

Full scaled quantum chemical normal coordinate analyses have been reported for ligand modes of $Ru(LL')_3^{2+}$, where LL′ = an α-di-imine.[240] The complexes (48), where X = H, Me, OMe, NO_2 or Cl, all have an IR band due to νC=N in the range 1589–1598 cm^{-1}.[241]



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A resonance Raman study has been reported for MLCT and intraligand (IL) transition states of $Ru(phen)_2(qdppz)^{2+}$, where qdppz = naphtha[2,3-α]dipyrido[3,2-*h*:2′,3′-*f*]phenazine-5,18-dione.[242] IR bands due to νBH of the hydridotrispyrazol-1-ylborate (Tp) in $Ru(\kappa^2\text{-}Tp^{PhCl})(CO)_2$ lie in the range 2445–2476 cm^{-1}.[243]

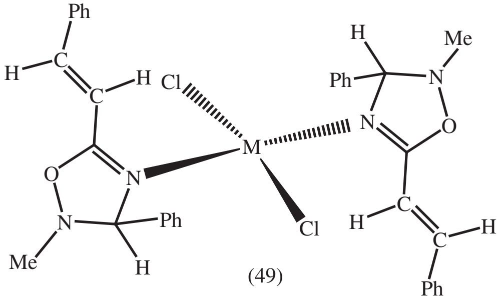
The resonance Raman spectra of Co(TMPyP(4)), with cobalt in the oxidation states +2 or +3, where TMPyP(4) = tetrakis(*N*-methyl-4-pyridinyl)porphyrin, were obtained. Oxidation state marker bands were identified, which suggested that the effects of axial coordination by solvent molecules are greater for the Co(III) than for the Co(II) species.[244]

The IR spectra of $LMCl_2$, $[L_2Cu(H_2O)_2]^{2+}$ and $[L_2M]^{2+}$, where M = Co or Cu, L = 2-acetylpyridine(5,6-diphenyl-[1,2,4]-triazin-3-yl)hydrazone, show that L is tridentate *via* triazine N, azomethine N and pyridine N atoms[245] The resonance Raman spectrum of RhCl(CO)($^iPr_2$Ph–bian), where $^iPr_2$Ph–bian = 1,2-bis[(2,6-diisopropylphenyl)imino)acenaphthene, revealed the predominantly Rh → bian (MLCT) character of the visible electronic absorption.[246]

The IR spectra of $[Ni(R_2Me_4[18]aneN_{10})]^{2+}$, where R = Me, Et, Pr, benzyl, confirm that all 4 α-di-imine nitrogen atoms are coordinated to Ni.[247] SERRS data have been obtained for Ni(P), where P = OEP, TPP, adsorbed on electrochemical interfaces. For Ni(OEP), adsorption appeared to be edge-on, with *meso*-carbons closest to the surface.[248] Raman spectroscopy was used to follow pH-influenced metal-ion coordination changes in NiHb.[249] The complexes (49), where M = Pd, Pt, have νC=N at 1647 cm^{-1} (Pd) or 1639 cm^{-1} (Pt).[250]

IR and Raman spectra of copper(II) complexes of histamine gave evidence for the formation of $[Cu_2(L\text{–}H)_2]^{2+}$, CuL^{2-} and CuL_2^{+} at high pH, $Cu(LH)^{2-}$, CuL^{2-} and CuL_2^{+} at lower pH– all with coordination through the imidazole moiety.[251] Time-resolved step-scan FTIR spectroscopy was used to probe the dynamics of the haem–Cu_B binuclear centre in haem–copper oxidases.[252] The IR spectrum of *ba*$_3$-type cytochrome *c* oxidase of *Thermus thermophilus* showed νC=O (amide I) bands indicative of strong redox-induced perturbation of the predominantly β-sheet-type structure.[253]

The complex $[Ag(NH{=}CMe_2)_2]^+$, together with related species, have IR bands from νC=N at 1662 cm^{-1}, and νNH at 3294 cm^{-1}.[254] SERS data for 5,10,15,20-tetrakis(1-decylpyridinium-4-yl)-21*H*,23-porphin tetrabromide on silver hydrosols gave evidence for silver porphyrin complex formation.[255]



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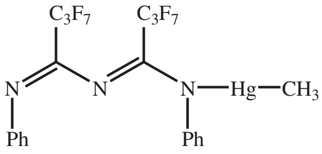
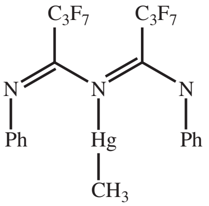




(50) (51)

The photophysics of a three-dimensional zinc(II) porphyrin box, $(PyZZ)_4$, was followed by resonance Raman spectroscopy – giving evidence for perturbation of the ring planarity.[256] DFT calculations have been reported for the vibrational wavenumbers of Zn(2-NO_2–TPP).[257] The IR spectra of two isomers (50, νCN 1640 cm^{-1}) and (51, νCN 1610, 1587 cm^{-1}) were both seen in solution (in $C_2D_2Cl_4$).[258]

5.4 Cyanides, Isocyanides and Related Complexes. – IR data (νCN) were used to study the effects of heating $La[Co(CN)_6].5H_2O$. A band at 2141 cm^{-1} was assigned to a bridging Co–CN–La or Co–NC–La unit.[259] The IR spectrum of $Sm(H_2O)_5[W(CN)_8]$ suggests the presence of 4 terminal and 4 bridging cyano groups.[260]

νCN IR data were reported for $Cp_2(OC)Ti(TCNX)$, where Cp = C_5H_5, C_5Me_5; TCNX = TCNE or TCNQ, and their stepwise redox products.[261]

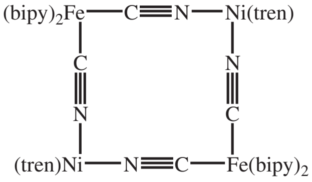
IR multiphoton dissociation spectra were reported for the clusters $[Nb.nCH_3CN]^+$, where n = 4 or 5. For n = 5, there was evidence for $\{Nb^{III}(NCCH_3)_3[N{=}C(CH_3)C(CH_3){=}N]\}^+$.[262]

IR spectra (νCN) have been given for complexes of the 'ligands' $(OC)_5M(CN)^-$ (M = Cr, Mo or W), Cp(dppe)Fe(CN), $Cp(Ph_3P)_2Ru(CN)$ with $Ru_2(OAc)_4{}^+$, $Co_3(dpa)_4{}^{2+}$, $Ni_5(tdpa)_4{}^{2+}$, where dpa, tdpa = amine-bridged poly(pyridyls), showing that these are bridged cyano-complexes, where the Ru_2, Co_3 or Ni_5 units withdraw electron density from the external organometallic units.[263] Picosecond TRIR and resonance Raman spectra were used to probe the nature of the ^{3}MLCT (pyCN) excited state for $W(CO)_5(pyCN)$, where pyCN = 4-cyanopyridine.[264]

IR spectra were used to characterise $Mn(NO)_2(CN)_2(L)$, where L = one of a range of imidazole or thiazole ligands.[265] The complex $[Mn(CN^tBu)_2(NO)(\eta^5\text{-}C_5H_4Me]^+$ gives IR bands at 2192, 2173 cm^{-1} from νCN, with νNO at 1786 cm^{-1}.[266] IR bands for $[Mn(L)(MeOH)(\mu\text{-}L)(\mu\text{-}2,2'\text{-bpm})_{0.5}]_n$, where L = X-phenylcyanamide, X = H, 3-Cl, 3-F; bpm = bipyrimidine, show terminal (near 2130 cm^{-1}) and $\mu_{1,3}$ (near 2160 cm^{-1}) νCN bands.[267]

IR bands due to νCN were assigned for complexes such as *cis,cis*-$[Fe(CN)_2(CO)_2(CS_3\text{-}S,S)]^{2-}$ (2102, 2111 cm^{-1}).[268] The IR spectra (νCN) of $[KCpFe(CN)_2]_2\text{-}\mu\text{-}(Ph_2P)_2\text{–}(CH_2)_n$, where n = 2–4, show that replacing CO in $CpFe(CN)_2CO^-$ by phosphanes leads to enhanced withdrawal of electron-density from the iron centres.[269]

The complex $\{[(o\text{-}C_6F_4Hg)_3]_2[Fe(CN)_5NO]\}^{2-}$ has νCN at 2124 cm^{-1}, νNO at 1883 cm^{-1}, *i.e.* respectively lower and higher than for free $[Fe(CN)_5NO]^{2-}$.[270] The bridging cyano-groups in $[CpFe(PPh)_2(\mu\text{-}CN)_2ZnI(thf)]_2$ give νCN at 2092 and 2082 cm^{-1}.[271] Bands due to νCN were assigned from IR spectra for several cyanide-bridged tetranuclear complexes such as (52) (2081 cm^{-1}).[272]



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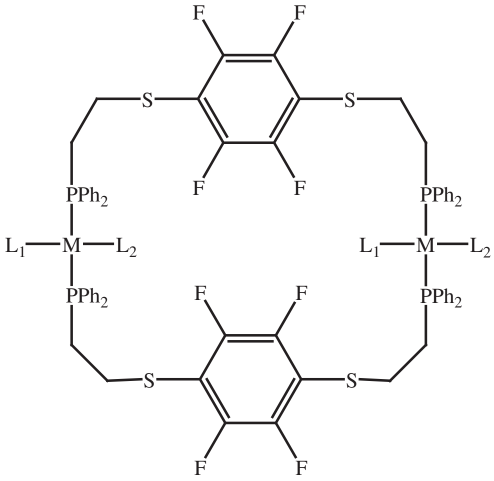


(53)

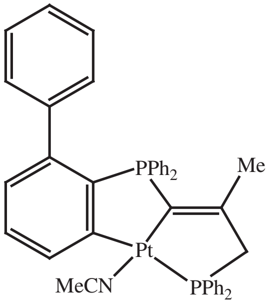
The complex $[Ru(NCC{\equiv}CPh)(PPh_3)_2Cp]^+$ gives an IR band from $\nu C{\equiv}C$ at 2141 cm^{-1}.[273] νCN IR bands have been reported for the *ttt* and *cct* isomers of $RuCl_2(RNC)_2(PPh_3)_2$, *e.g.* for R = ^tBu, the *ttt* isomer has νCN at 2126 cm^{-1}, while the *cct* form has νCN at 2112 and 2154 cm^{-1}.[274]

Femtosecond TRIR spectroscopy was used to probe vibrational mode coupling to ultrafast electron transfer in $[(NC)_5OsCNRu(NH_3)_5]^-$.[275] The IR spectrum of $(\eta^2\text{-}C_{60})Os(CO)(^tBuNC)(PPh_3)_2$ includes νCN at 2153 cm^{-1}, with νCO at 1953 cm^{-1}.[276]

The IR spectra gave assignments to νCN modes for $[Co(CNCH_2Ph)_4\{OAs(C_6H_4Me\text{-}p)_3\}_2]^{3+}$ and related complexes.[277] Assignments to νCN modes have been proposed for (53), where M = Rh or Ir, L_1 = MeCN, L_2 = ^tBuNC.[278]

The bridging ligand in $\{(L)Ni[NCC(CN)CN]_2Ni(L)\}^{2+}$, where L = triethylene tetramine, gave νCN IR bands at 2243, 2211 and 2185 cm^{-1}.[279] The complexes $[Ni_2(\mu\text{-}CNR)(CNR)_2(\mu\text{-}dppm)_2]^{2+}$, where R = Me, ^nBu, Bz, ^iPr, Cy, ^tBu, $p\text{-}C_6H_4$, 2,6-$Me_2C_6H_3$, all show two terminal νCN bands (2130–2200 cm^{-1}) and one from semi-bridging νCN (2000–2100 cm^{-1}).[280]

Characteristic νNCN IR bands were seen for Pd(en)(3,4-NCNsq). where 3,4-$NCNsq^{2-}$ = 3,4-bis(dicyanamido)squarate. These were at 2187 and 2151 cm^{-1}, *i.e.* increased compared to the free ligand.[281] An ATR-IR study of aryl isocyanides adsorbed on palladium or gold surfaces show that the former gives two species, a strongly σ-bound and a σ/π synergically bound species. For the latter, only a (relatively weak) σ-bound complex is seen.[282]



(54)

The complex (54) shows νCN of the isocyanide ligand at 2323 cm^{-1}.[283] IR and Raman spectra of *trans*-$[Pt(CN)_4X_2]^{2-}$, where X = Cl, Br or I, gave the νCN mode assignments shown in Table 8.[284] DFT calculations gave vibrational

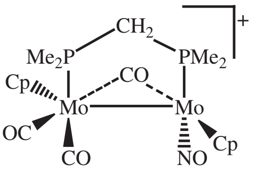
Table 8 *νCN assignments for trans-$[Pt(CN)_4X_2]^{2-}$ (/cm^{-1})*

X=	*Cl*	*Br*	*I*
(IR)	2176	2171	2162
(Raman)	2199	2195	2185
	2187	2182	2174

wavenumbers (νCN) for $Au(CN)_4^-$ and *trans*-$Au(CN)_2X_2^-$, where X = F, Cl, Br and I.[285]

5.5 Nitrosyl Complexes. – DRIFT spectra of the products of NO_2 adsorption on BaO gave evidence for coordinated NO_x (x = 1, 2 or 3) species.[286]

The IR spectrum of NO adsorbed on Cr/ZrO_2 and Cr/TiO_2 samples gave evidence for the formation of $Cr^{n+}(NO)$ ($n > 3$), with smaller amounts of $Cr^{3+}(NO)_2$ (νNO 1908, 1782 cm^{-1}).[287,288] The complex *trans*-$Mo(dmpe)_2(NO)[NPh(CH_2Ph)]$, where dmpe = bis(dimethylphosphino)ethane, has νNO at 1538 cm^{-1}.[289] The complex (55) has νNO at 1651 cm^{-1}.[290]



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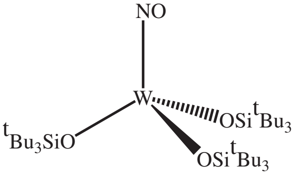


(56)

The observation of νNO at 1574 cm^{-1} in the IR spectrum of (56) is consistent with considerable W(II) → NO back donation.[291]

IR bands due to νNO were assigned for a range of (por)Mn(NO)(L) complexes, where por = T(*p*-MeO)PP, L = piperidine, methanol *etc*., e.g. for L = piperidine, 1746 cm^{-1}.[292] The observed νNO band for $[Mn(PaPy_3)(NO)]ClO_4$, where $HPaPy_3$ = *N*,*N*-bis(2-pyridinylmethyl)amine-*N*-ethyl-2-pyridine-2-carboxamide, at 1745 cm^{-1} is consistent with a {low-spin-Mn(II)-NO•} formulation.[293]

Adsorption of NO on Fe-BEA zeolite catalysts gives νNO at 1874 cm^{-1}, assigned to NO coordinated to Fe_xO_y units in zeolite channels.[294] The IR bands due to νNO for *cis*- and *trans*-isomers of $[(cyclam)Fe(NO)Cl]^+$, where cyclam = 1,4,8,11-tetraazacyclotetradecane, are observed at 1720 cm^{-1} (*cis*), 1605 cm^{-1} (*trans*). These values suggest an approximately linear Fe–N–O unit for the former, but bent for the latter.[295]

The νNO mode for $[Fe(L)(NO)]^{2+}$, where HL = *N,N*-bis(2-pyridylmethyl)amine-*N*–ethyl-2-pyridine-2-carboxamide, is at 1937 cm^{-1} – as expected for an $\{Fe–NO\}^6$ complex. Reduction to $[Fe(L)(NO)]^+$ shifts νNO to about 1615 cm^{-1}, *i.e.* bent Fe–N–O, typical of $\{Fe–NO\}^7$ complexes.[296] There is matrix-IR evidence for conversion of $(TPP)Fe(NO)(NO_2)$ to the (TPP)Fe(ON)(ONO) species (νON 1699 cm^{-1}), *i.e.* an unprecedented example of double linkage isomerism.[297]

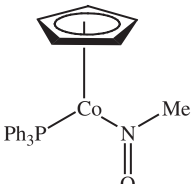
Nitric oxide reacts with Fe^{II}(M4PyTPP), where M4PyTPP = *meso*-4-pyridyltriphenyl-porphyrinate, to form two nitrosyl complexes, identified by IR spectroscopy.[298] The resonance Raman spectrum of the NO-bound ferric derivative of HbN (a haemoglobin from *Mycobacterium tuberculosis*) showed a shift of νNO from 1914 cm^{-1} to 1908 cm^{-1} on forming the B10 Tyr → Phe mutant.[299] The resonance Raman spectrum of the iron(II)–NO complex of the haem-regulated eukaryotic initiation factor 2α kinase (HRI) is consistent with a

5-coordinate NO-haem.[300] FTIR spectra show νNO bands (confirmed by ^{15}N substitution) suggestive of $\{Fe(NO)_2\}^9$ (S = 1/2) and $\{Fe(NO)_2\}^8$ (S = 0) species in iron-substituted ferric uptake regulation (FUR) protein.[301]

IR bands due to νNO were assigned for the complexes *cis*-$Ru(NO)(X)(pyca)_2$, where X = OMe (1861 cm^{-1}), Cl (1864 cm^{-1}); pyca = 2-pyridine carboxylato.[302] The species (bpb)Ru(NO)Cl, where H_2bpB = 1,2-bis(pyridine-2-carboxamido)benzene, and related complexes, all show νNO in the range 1830–1870 cm^{-1}, *i.e.* $\{Ru–NO\}^6$.[303] A spectroelectrochemical study (νNO) has been reported for the redox properties of *cis*-$[RuCl(cyclen)(NO)]^{2+}$, where cyclen = 1,4,7,10-tetraazacyclododecane.[304]

The complex $[Ru(PaPy_3)(NO)](BF_4)_2$, where $HPaPy_3$ = *N,N*-bis(2-pyridinylmethyl)amine-*N*-ethyl-2-pyridine-2-carboxamide, shows νNO at 1899 cm^{-1}, *i.e.* $\{Ru–NO\}^6$ configuration.[305] The IR spectrum of Ru(TTP)(HNO)(1-MeIm), where TTP = tetratolylporphyrinato, 1-MeIm = 1-methylimidazole, includes νNO at 1380 cm^{-1} (1348 cm^{-1} for $H^{15}NO$).[306] The nitrosoarene complexes $(por)Ru(ArNO)_2$, where por = TPP, TTP, Ar = aryl group, have νNO in the range 1346–1350 cm^{-1}. Replacing ArNO by py led to a lowering of νNO.[307]

The complex (57) shows νN=O of the nitrosoaryl ligand at 1301 cm^{-1}.[308] IR spectroelectrochemistry (νNO) reveals that reduction of $Cl_5Ir(NO)^-$ is reversible, and predominantly NO-centred, *i.e.* νNO is at 1952 cm^{-1} for original complexes, 1677 cm^{-1} for the one-electron reduction product.[309] NO adsorbed on supported iridium catalysts (Ir/SiO_2, Ir/Al_2O_3) gives νNO at 1870 cm^{-1} from $Ir^{\delta+}(NO)$ species.[310]



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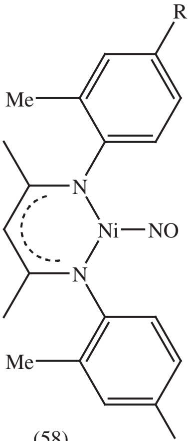
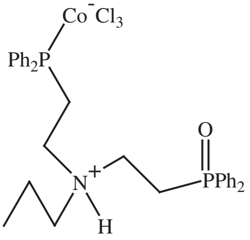


(58)

The complexes (58), where R = H or Me, have νNO at 1792 cm^{-1} (R = H), 1785 cm^{-1} (Me) – at the low end of the wavenumber range for neutral pyrazolato–nickel complexes.[311] DRIFTS studies of NO adsorbed on Au–TiO_2 surfaces reveal the formation of bridging species with νNO in the range 1696–1690 cm^{-1}.[312]

6 Phosphorus and Arsenic Donors

IR assignments have been proposed for $(\eta^5\text{-}RC_5H_4)_2Mo_2(CO)_4(\mu\text{-}\eta^2\text{-}P_2)$.[313] The complexes $Cp^0MoCl_4(PH_2R)$, where $Cp^0 = C_5EtMe_4$, R = ^tBu, 1-adamantyl, Cy, Ph, Mes, 2,4,6-$^iPr_3C_6H_2$, all show νPH_2 modes in the range 2380–2455 cm^{-1}, *i.e.* all higher than in the free ligands.[314]



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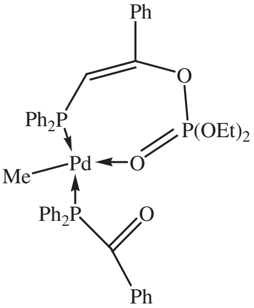


(60)

The free P=O group in the complex (59) shows νP=O at 1158 cm^{-1}.[315] The complex $PdCl_2(L)$, where L = $As(CH_2CMe{=}CH_2)_3$, gives a νC=C band from the allylarsine ligand at 1633 cm^{-1}.[316] The complex (60) has νP=O (coordinated) at 1223 cm^{-1}, νC=O (free) 1672 cm^{-1}.[317] The $PHCy_2$ ligand in $PtCl(PHCy_2)\{(PCy_2O)_2H\}$ gives νPH at 2343 cm^{-1}.[318] The following AsF_3 ligand mode assignments were made from the Raman spectrum of $[(F_3As)AuXe]^+Sb_2F_{11}^-$: ν_s 764.4 cm^{-1} cm^{-1}, ν_{as} 752.6 cm^{-1}, δ_s 354.9 cm^{-1}, δ_{as} 260.0 cm^{-1}.[319]

7 Oxygen Donors

7.1 Molecular Oxygen, Peroxo, Aquo and Related Complexes.

– *Ab initio* calculations have been reported for vibrational wavenumbers for $M^+(H_2O)_n$, where M = Li, Na, K, Rb or Cs; n = 1–6.[320] νOH mode assignments were proposed from the IR photodissociation spectra of gaseous $Mg(H_2O)_4^+$ and $[Mg(H_2O)_4Ar]^+$ (3000–3450 cm^{-1}).[321]

There is Raman evidence (νOO 840 cm^{-1}, $^{18/16}O$ shifts) for the formation of lanthanum peroxide species by oxidation of a La_2O_3 surface by O_2.[322]

In situ spectroscopy at a TiO_2(rutile)/aqueous solution interface on UV irradiation shows bands at 838 and 812 cm^{-1}, due (respectively) to νO–O of surface Ti–O–O–H, Ti–O–O–Ti.[323]

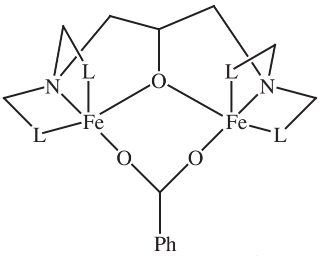
Mass-selected IR photodissociation spectra of $V^+(H_2O)Ar_n$ and $V^+(D_2O)Ar_n$ clusters show νOH bands shifted by 50–80 cm^{-1} to lower wavenumbers compared to free H_2O.[324] The peroxo group in $[\{Ph_3SiO\}_2V^VO(O_2)]^-$ shows νOO at 872 cm^{-1}.[325] A similar feature was seen at about 920 cm^{-1} in the IR spectrum of $[VO(O_2)(CMAA)(H_2O)]^{2-}$, from the η^1-peroxo ligand.[326] IR and Raman bands for $[VO(O_2)(oxalate)(L)]^-$, where L = bipy or phen, contain νOO at 927 cm^{-1} (bipy), 935 cm^{-1} (phen).[327]

The complex $[V_2O_2(O_2)_2(R,S\text{-mand})_2]^{2-}$, where mand = mandelato, gives an IR band from νOO at 920 cm^{-1}, with νCO_2 bands of unidentate carboxylates.[328] νOO bands in the IR spectra of $V_2O_2(O_2)_3(L)_3$, where L = amino acid ligands, gave evidence for terminal and bridging peroxo ligands.[329]

IR bands due to νOO were seen at 945 and 888 cm^{-1} for $(Tp^{iPr2})Cr(O_2)_2$, where Tp^{iPr2} = hydrotris(3,5-diisopropylpyrazolyl)borato.[330] The IR spectrum of $MoO(O_2)(cit)^{4-}$, where cit = citrate, includes νOO of the η^2-O_2 ligand at 853 cm^{-1}.[331] νOO (peroxo) bands are seen in the range 849–874 cm^{-1} for $[MoO(O_2)_2(H_xL)]^{2-}$, where H_xL = oxalate, citrate, tartrate, glycolate, malate.[332]

The bridging OH group in the complex $\{[(bipy)Re(CO)_3]_2(\mu\text{-}OH)\}^+$ has been shown to give an IR band from νOH at 3456 cm^{-1}.[333]

IR and Raman bands due to νOH from Fe–OH and Al–OH units were seen for the minerals cacoxenite and gormanite.[334] Dioxygen reacted with recombinant human serum albumin incorporating $Fe^{II}(TPP)$ to give νO_2 at 1158 cm^{-1} due to coordinated O_2.[335] The complex (61) forms an O_2 adduct with νOO as a Fermi doublet at 877, 893 cm^{-1}.[336]



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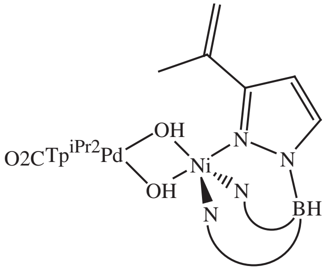


(62)

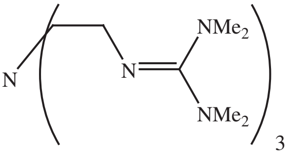
The complex $Os_6(CO)_{16}(\mu_4\text{-}O)(\mu\text{-}OH)_2(\mu\text{-}CO)_2$ gives IR bands from the bridging hydroxyl groups at 3689 and 3675 cm^{-1}.[337]

The resonance Raman spectrum of HOO–Co^{III}(bleomycin) includes νO–OH at 828/784 cm^{-1} ($^{16}O/^{18}O$).[338] Matrix-isolated Co(MPyTPP), where MPyTPP = *meso*-triphenyl(4-pyridyl)-porphyrinato, and O_2 form an unstable 5-coordinate O_2-adduct (νO_2 1286 cm^{-1}) and a more stable 6-coordinate species (additional coordination by a py group of adjacent Co(MPyTPP)) with νO_2 at 1160 cm^{-1} (1103 cm^{-1} for ^{18}O).[339]

The IR spectra of O_2 adducts of $Rh(Q)(PR_3)_2$, Rh(Q)(dppp), where HQ = 1-phenyl-3-methyl-4-R-prazol-5-one, R = 2-thenoyl, 2-furanoyl, show νOO of η^2-peroxo near 890 cm^{-1}.[340]

The complex (62) has νOH of the bridging hydroxyls as an IR band at 3591 cm^{-1}.[341] The adsorption of O_2 on a Pt(111) surface leads to the formation of peroxo and superoxo species, with IR bands near 700 and 870 cm^{-1} respectively.[342]

The resonance Raman spectrum of (L)CuOOH, where L = *N*-{(2-bis(2-pyridylmethyl)-aminoethyl)methylamino]ethyl}-2,2-dimethylpropionamide, includes νOO at 853 cm^{-1} (807 cm^{-1} for the ^{18}O analogue).[343] The coordinated superoxide ligand in (L)Cu(O_2), where L^- = 2,4-di-*tert*-butylphenolate linked to 1,4-di-*iso*-propyl-1,4,7-triazacyclononane, gives νOO at 1120 cm^{-1}, ($^{16}O_2$), 1093 cm^{-1} ($^{16}O^{18}O$), 1058 cm^{-1} ($^{18}O_2$).[344] The Raman spectrum of the superoxo adduct of Cu(TMG$_3$tren), where TMG$_3$tren = (63), has $\nu^{16}O^{16}O$ at 1117 cm^{-1} ($\nu^{18}O^{18}O$) 1059 cm^{-1}).[345]



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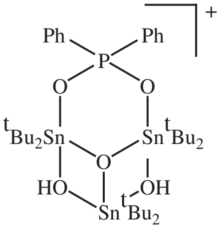


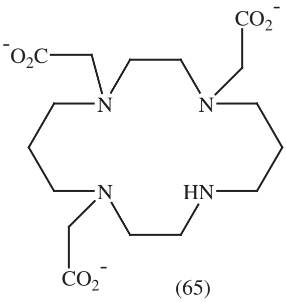
(64)

The IR spectrum of $[HO–Al–H]^+$ has νOH at 3714 cm^{-1}. νOH features were also reported for $M(H_2O)_n{}^+$, where M = Mg, Al, n = 1 or 2.[346] The bridging hydroxyl group in (64) gives an IR band due to νOH at 3328 cm^{-1}.[347]

7.2 Carboxylate and Related Complexes. – The FTIR spectrum of M(Nap)$_3$ (phen), where M = Y, La, Eu, Tb or Dy; HNap = α-naphthoic acid, includes bands from bidentate carboxylates.[348] IR and Raman data for $[Ln(2,6\text{-}dhb)_5(H_2O)_2]^{2-}$, where Ln = Sm, Tb; Hdhb = 2,6-dihydroxybenzoic acid, also reveal νCO_2 bands from bidentate carboxylates.[349] νC=O bands for homobinuclear Ln^{3+} complexes of (65) linked by *p*-xylyl groups are seen in the range 1580–1600 cm^{-1}, compared to 1690 cm^{-1} for the free ligand (Ln = Eu, Tb, Yb).[350]

The IR and Raman spectra of Ln(Hnico)$_2$(μ-Hnico)(H_2O), where Ln = Eu, Gd, Tb, Er or Tm, H$_2$nico = 2-hydroxynicotinic acid, show coordination by a unidentate carboxylate and phenolate oxygen atoms.[351] The bridging bidentate carboxylate groups in $[Tb_2Zn_2L_{10}(bipy)(H_2O)_2]_2$, where HL = α-methylacrylic acid, have $\nu_{as}CO_2$ at 1557 cm^{-1}, and ν_sCO_2 at 1431 cm^{-1}.[352]

There is IR evidence for the formation of surface formato species by the adsorption of formaldehyde on a UO_2(111) surface.[353]



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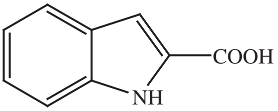


(66)

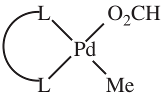
The IR bands from νCO_2 for $Cp_2V(OOCR)_2$, where R = H, CCl_3, CF_3, are consistent with the presence of two unidentate carboxylates.[354] Toluene partial oxidation on V_2O_5 in vanadia–titania catalysts leads to the formation of benzoate species, detected by DRIFTS.[355]

The ν_s and $\nu_{as}CO_2$ bands of $Mn(O_2CCF_3)_2[(py)CHNOH]_2$ are separated by only 220 cm^{-1}, despite being unidentate. This was explained by hydrogen-bonding of the 'free' oxygens to oxime groups, *i.e.* the carboxylate is pseudo-bridging.[356] The observation of ν_sCO_2 and $\nu_{as}CO_2$ at 1414 cm^{-1} and 1535 cm^{-1} respectively show that the carboxylates in $Mn(2\text{-}IC)(H_2O)_2$, where 2-HIC = (66), are bidentate.[357] The complexes $M(4\text{-}iaa)_2(H_2O)_2$, where M = Mn or Co, H-4-iaa = imidazole-4-acetic acid, have νCO_2 modes showing unidentate carboxylates, involved in hydrogen–bonding with H_2O.[358] The complexes LnL^+, FeL and GdL, where H_3L = diethylenetriamine-inositol-biester-*N,N,'N''*-triacetic acid, have IR spectra suggesting unidentate carboxylates.[359] νCO_2 modes for $Mn_2(Me_2phen)(2,6\text{-}dmb)_4(H_2O)_2$, where dmb = dimethoxybenzoate, gave evidence for the presence of both bridging and terminal carboxylates, but with the wavenumbers affected by hydrogen-bonding.[360]

The bidentate formato ligand in $[ReH(CO)(Cyttp)(\eta^2\text{-}CO_2H)]^+$, where Cyttp = $PhP(CH_2CH_2CH_2PCy_2)_2$, has νCO_2 bands at 1545 and 1364 cm^{-1} (1500, 1340 cm^{-1} for the ^{13}C analogue).[361] The IR spectrum of $[ReO(H_3L)Cl_3Fe(OH_2)_3]^{2+}$, where H_4L = 8,17-dimethyl-6,15-dioxo-5,7,14,16-tetrahydrodibenzo[a,h][14]-annulene-2,11-dicarboxylic acid, shows the presence of unidentate carboxylates.[362]

The IR spectra show characteristic bands of a tetradentate, bridging oxalate (= ox) group in $(acac)_2Fe(\mu\text{-}ox)Fe(acac)_2$ ($\nu_{as}CO$, 1672 cm^{-1}, δCO_2 802 cm^{-1}, *etc.*).[363] IR bands due to ν_{as}, ν_sCO_2 for unidentate carboxylates were seen at 1624 and 1380 cm^{-1} respectively for $Ru(PhCOO)_2(dppf)(CH_3CN)(H_2O)$, where dppf = 1,1′-bis(diphenylphosphino)ferrocene. Modes from bidentate carboxylates were, however, observed for $Ru(EtCOO)_2(dppf)$.[364]

The IR spectrum of $Co_3(O_2CC_{12}H_8CO_2)_{2.5}(OH)(H_2O)_2$ has $\Delta\nu_{as-s}$ of 135 cm^{-1}, consistent with a bridging bidentate coordination mode.[365] Similar data for $Rh_2(\mu\text{-}OOCH)_4(dmf)_2$ and related complexes all show that the formato ligands are bridging.[366]



(67)

The complex (67), where L–L = tmeda, has an IR band at 1621 cm^{-1} from the bicarbonate ligand.[367] There is IR evidence for the formation of a CO_2 surface complex as a result of CO oxidation at a Pt{100} surface.[368]

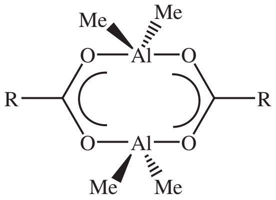
The unidentate carboxylato groups in $Na_2Cu(OAc)_4(H_2O)$ give IR bands at 1607, 1583 cm^{-1} ($\nu_{as}CO_2$), 1405, 1344 cm^{-1} (ν_sCO_2).[369] The IR spectra of Cu(L), $Cu(HL)_2$ and $Cu(HL)_2(L')_2$, where H_2L = pyrazine-2,3-dicarboxylic acid, L′ = 3-pyridylmethanol, show that the carboxylates are unidentate.[370] Similar results were obtained for $Cu_2(3,5\text{-}Cl_2sal)_4.H_2O$ and related species (where sal = salicylate).[371]

IR bands for ν_{as}/ν_sCO_2 for $Ag_2(R_fCOO)_2(dppm)$, where R_f = CF_3, C_3F_7, C_4F_9, C_6F_{15}, C_9F_{19}, all lie in the range expected for bridging carboxylates.[372] The IR spectra of Au(ppy)X, where ppy = 2-phenylpyridine, X = OAc, OOCPh, have νCO_2 bands typical of unidentate carboxylates.[373]

The complex [Tpms^{tBu}]Zn(OAc), where Tpms^{tBu} = tris(3-*tert*-butylpyrazolyl)methane-sulfonate, has $\nu_{as}CO_2$ at 1592 cm^{-1}, ν_sCO_2 at 1331 cm^{-1}, *i.e.* η^1-OAc. The bridging acetate ligand in [(Tpms^{tBu})Zn]$_2$(μ-OAc)(μ-OH), on the other hand, has $\nu_{as}CO_2$ at 1573 cm^{-1}, ν_sCO_2 at 1437 cm^{-1}.[374] IR bands from unidentate and *syn,syn*-bridging carboxylates were seen in the IR spectrum of $Zn_3(benz)_6(nia)_2$, where benz = benzoate, nia = nicotinamide.[375] The IR spectra of $Na_6Zn(L)PtX_2$ and $Zn(L)(PtX_2)_4$, where $H_{10}L$ = tetra-4,5-dicarboxyphthalocyanine, X = NH_2 or dmso, show coordination by carboxylate oxygen atoms to form a 7-atom metallochelate ring.[376]

The polymeric complex $[Cd(O_2CMe)(O_2CPh)(H_2O)_2]_n$ shows νCO_2 bands in both IR and Raman spectra which are consistent with both sets of carboxylates being bidentate.[377]

IR photodissociation spectra were reported for the clusters $Al^+(CO_2)_n$ and $Al^+(CO_2)_n$.Ar, and compared with the results of *ab initio* calculations (all in the region of $\nu_{as}CO_2$ modes).[378] The complex (68), where R = 2,4,6-$Ph_3C_6H_2$, has νCO at 1624 cm^{-1}, compared to 1696 cm^{-1} in the free ligand, confirming the coordination shown.[379] There is IR evidence for the formation of bi- and polydentate carbonato complexes by the adsorption of gaseous CO_2 on to β-Ga_2O_3.[380]



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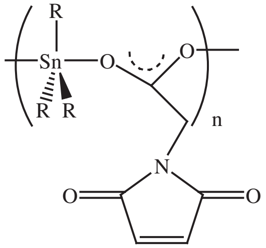


(69)

Assignments to νCO bands confirm the coordination shown for polymeric (69), where R = Ph, C_6H_{11}.[381] The IR spectra of $[^nBu_2Sn(L)]_2O$ and $^nBu_2Sn(L)_2$, where HL = 4′/2′-dinitrophenyl-2-carboxylic acids, show that the carboxylates are anisobidentate.[382] The IR and Raman spectra of $Bu_2Sn(IV)^{2+}$ and $Ph_3Sn(IV)^+$ complexes with a range of organic carboxylic acids show that all contain bidentate chelated carboxylates.[383]

The IR spectra of $(Ph_3SnCl)_4[\mu_4\text{-}\{Y(CO_2)_2\}]$, where Y = CH_2, CH_2CH_2 or (Z)-CH=CH, are consistent with tetradentate dicarboxylate ligands.[384] The IR spectrum of [dibenzyl(2-furanylcarboxylato)tin(IV)]oxide shows the presence of bridging carboxylates.[385]

The observed values for ν_s and $\nu_{as}CO_2$ modes for $[Pb(phen)_2(OAc)]^+$ confirm the bidentate bonding of the acetate group.[386]

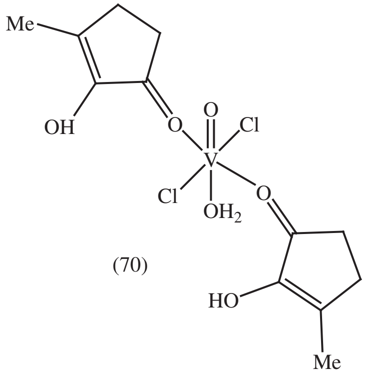
The species (Fc)C(Me)=CH$(COO)_2SbAr_3$, where Fc = ferrocenyl, Ar = Ph, 4-Me-, 4-Cl–, 4-F–C_6H_4, give $\nu_{as,}$ ν_s for unidentate carboxylates, *e.g.* for Ar = Ph, 1624, 1358 cm^{-1} respectively.[387] Bidentate carboxylates were indicated by the IR spectra ($\Delta\nu CO_2$) for $Ar_3Bi(O_2CCHR^1CHR^2\text{–}GePh_3)_2$, where R^1 = H, CH_3, R^2 = H, Ph, Ar = Ph, 4-Me-, 4-F-, 4-Cl-, 4-Br–C_6H_4.[388]

7.3 Keto-, Alkoxy-, Ether and Related Complexes. – Raman spectra of (diglyme)$_n$LiClO$_4$ samples revealed that the Li$^+$ is coordinated by 6 ether oxygens in the solid state (diglyme = MeO(CH$_2$CH$_2$O)$_2$Me).[389] Similar results were obtained for LiSbF$_6$(diglyme)$_2$.[390]

Laser-ablated magnesium atoms react with MeOH to form matrix-trapped Mg(MeOH), with the assignments listed in Table 9.[391] IR photodissociation spectra of gaseous Mg(MeOH)$_n$$^+$, where n = 1–4, gave assignments to νOH (assigned using DFT calculations).[392]

Laser-ablated scandium atoms react with MeOH to form (MeO)ScH. Matrix-IR data for this species gave the following assignments: δCH$_3$ 1167.4 cm^{-1}, νC–O 1158.5 cm^{-1}.[393]

Table 10 summarises assignments for Cl$_3$V(OCH$_3$), formed by the reaction of VCl$_4$ with MeOH in an argon matrix. The assignments were based on H/D and ^{12}C/^{13}C substitutions.[394] The IR spectrum of (70) shows νC=O at 1591 cm^{-1}, compared to 1650 cm^{-1} in the free ligand, confirming C=O–V coordination.[395]



(70)

The Raman spectra of [Mn^{II}(SQ)$_3$]$^{2-}$, where SQ = *o*-semiquinone of L-dopa or dopamine, show that the ligands are present in *o*-semiquinone radical anion form.[396]

Table 9 *Ligand mode assignments for matrix-trapped Mg(MeOH) (/cm^{-1})*

νOH	3602.4
δCH$_3$	1439.9
δCH$_3$OH	1060.4
νC–O	989.0

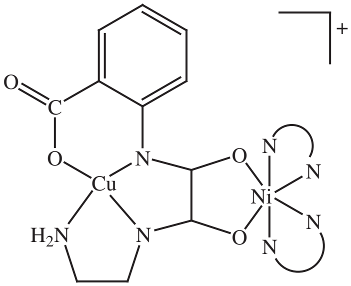
Table 10 *Ligand mode assignments for matrix-trapped Cl$_3$V(OCH$_3$) (/cm^{-1})*

ν$_{as}$CH$_3$	2944
δ$_{as}$CH$_3$	1444
δ$_s$CH$_3$	1423

IR photodissociation spectra were reported for gaseous $Fe(CH_3OCH_3)_2^+$ and $Fe(CH_3OCH_2CH_2OCH_3)_n^+$. Assignments to uni- and bidentate ether ligands were based on *ab initio* calculations.[397] The complex $[(L)Fe(acac)]^+$, where L = tridentate bis(imino)carbazolide ligand, gives νCO/νCC for $acac^-$ at 1557 and 1527 cm^{-1} – showing symmetrical bidentate coordination.[398]

Assignments were made to νCO/νCC modes from the IR spectra of $[Co_2(tpmc)(dik)]^{3+}$, where tpmc = *N,N′,N″,N‴*-tetrakis(2-pyridylmethyl)-1,4,8,11-tetraazacyclotetradecane; dik = acac, dibzac, hfac *etc*. The wavenumbers decrease in the sequence hfac > dibzac > acac.[399] The IR spectra of $[Co(Rac)(cyclam)]^{2+}$, where cyclam = 1,4,8,11-tetraazacyclotetradecane., Rac^- = range of β-diketonates – all show *O,O′*-bidentate coordination by Rac^-.[400] νC=O for $[Rh_2(O_2CCF_3)_4].2(\eta^1\text{-}OCMe_2)$ is at 1686 cm^{-1} from the *O*-bound acetone (1716 cm^{-1} for the free ligand).[401]

IR spectroscopy gave characteristic ligand modes for the bridging unit in (71).[402] νCO bands in $Cu(hfac)_2({}^tBuNH_2)$ in benzene solution shift to lower wavenumber compared to the solid. This is due to increased Cu → O back-donation (hfacac = $CF_3C(O)CHC(O)CF_3^-$).[403]



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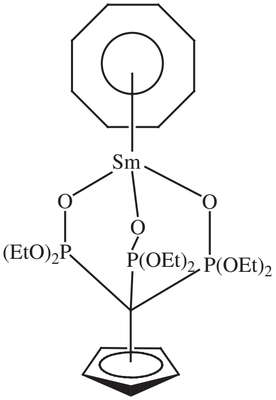


(72)

IR and Raman spectra (with DFT calculations) gave assignments to ligand modes for a 1 : 1 Al^{III}/caffeic acid complex, $Al(H_2O)_5L^+$. This shows that aluminium is coordinated to a deprotonated catechol site.[404] IR data for argon-matrix isolated $Cl_3Si(OEt)$ include νCH 2941 cm^{-1}, νCO 1172, 1103 cm^{-1}, νCC 985 cm^{-1}.[405]

7.4 Ligands Containing O–N, O–P or O–As Bonds. – IR bands due to νP=O of *O*-coordinated $OPPh_3$ in $[LnCl_2(OPPh_3)_4]^+$, where Ln = La–Lu, except Pm, were all seen in the range 1139–1150 cm^{-1}, compared to 1195 cm^{-1} for the free ligand.[406] The complex (72) shows νP=O from the Sm–O=P unit at 1144 cm^{-1}.[407] The IR spectra of $[Ln(L)(NO_3)_2(H_2O)_2]^+$, where Ln = Tb, Dy, L = range of substituted 2,6-diphenylpiperidin-4-ones, showed that the nitrato ligands were bidentate, while L is coordinated only *via* the ring nitrogen atom.[408]

The IR spectrum of $Fe^{III}(TPP)(ONO_2)(NO)$ at low temperatures gave the following assignments: $\nu_{as}NO_2$ 1505 cm^{-1}, ν_sNO_2 1266 cm^{-1}, νN–O 978 cm^{-1}, together with νN≡O at 1901 cm^{-1}.[409] The complex $[Fe_2OL_2(MeOH)_2(NO_3)_2](NO_3)_2$ gave IR bands from both free and unidentate coordinated nitrates, where L = 2,6-bis(*N*-methylbenzimidazol-2-yl)pyridine.[410] The FTIR spectrum of arsenate in an iron hydroxide sludge gave evidence for $AsO_4{}^{3-}$ coordinated to iron.[411]

The complexes $Ru(CO)_2Cl_2(Ph_3PX)_n$, where X = O, S or Se, n = 1 or 2, show νP=X bands 19–41 cm^{-1} to lower wavenumber than for the free ligand, showing Ru-X=P coordination. The νCO values suggest that the electron-donor abilities are in the order X = Se > S > O.[412]

The IR spectra of $LiNi_yCo_{1-y}PO_4$ samples, y = 0–1, gave assignments to PO_4 bands.[413] The electronic properties of the fragments (*p*-XPCP)Ir, where *p*-XPCP = η^3-5-*X*-$C_6H_2[OP^tBu_2]_2$-1,3; X = Me, MeO, H, F, C_6F_5, were probed by shifts in νCO for (*p*-XPCPO)Ir(CO).[414]

The IR spectrum of $[Ni(H_2L)(NO_3)](NO_3)$, where H_2L = ethylenediamine dioxime derivative of 3-carene, shows that the nitrato ligand is bidentate, with H_2L coordinated as an N_4 ligand.[415] IR bands due to nitrato ligands in *cis*- and *trans*-$Pt(amine)_2(NO_3)_2$, where amine = RNH_2 (R = Me, Et, ^nPr, ^nBu, ^iPr, ^iBu, ^{sec}Bu, ^tBu) or Me_2NH, were all consistent with unidentate coordination.[416]

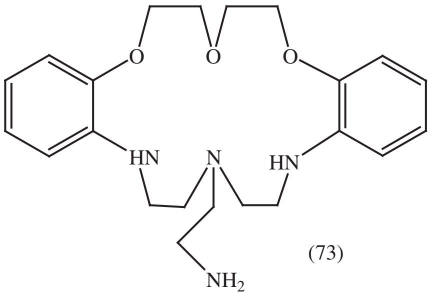
The IR spectra of $R_3Sn(DNP)$ and *n*-$Bu_2SnCl_{2-x}(DNP)_x$, where R = Ph or Me, x = 1 or 2, DNP = 2,4-dinitrophenolate, show bidentate coordination *via* the two nitro groups of the ligand.[417] IR and Raman spectra gave assignments to modes of coordinated phosphato groups for $[Me_2Sn(HTDP)(H_2O)]Cl$, where H_2TDPCl = thiaminediphosphate hydrochloride.[418]

7.5 Ligands Containing O–S or O–Te Bonds. – There is FTIR evidence for the formation of the ion-pair $Li^+[N(CF_3SO_2)_2]^-$ in propylene carbonate/poly(methyl methacrylate) systems.[419] The Raman spectrum of aqueous $MgSO_4$ includes νSO_4 bands from a unidentate $Mg(OSO_3)$ unit,[420] as well as a triple-ion $Mg_2SO_4{}^{2+}$.[421]

The IR spectrum of $K_8(VO)_2O(SO_4)_6$ includes bands from both unidentate and bridging sulfato ligands.[422]

IR data for $[Me_2Sn(OPPh_2)_2(O_3SCF_3)](O_3SCF_3)$ include $\nu_{as}SO_3$ at 1326 and 1206 cm^{-1} from bidentate (C_s) coordinated triflate (1788 cm^{-1} from free triflate), and ν_sSO_3 as a single band at 1032 cm^{-1}.[423] The IR spectra of $R_nSn(OSO_2C_6H_4CH_3\text{-}4)_{4-n}$, where n = 2 or 3, R = Et, ^nPr or ^nBu, show bidentate bridging *p*-toluenesulfonate ligands.[424] The complexes $Me_2Sn(Cl)(OTeF_5)$ and $Me_3Sn(OTeF_5)$ both give IR and Raman bands near 860 cm^{-1}, due to νTeO.[425]

7.6 Ligands Containing O–Cl or O–I Bonds. – The IR spectra of $M(L)(ClO_4)_2$, where M = Ca, Sr or Ba, L = (73), include bands showing the presence of coordinated perchlorato groups.[426]



(73)

The IR spectra of $M(ClO_4)_3(L)_5$, where M = La, Pr, Nd, Sm, Eu, L = phenyl phenacyl sulfoxide, suggest that two of the perchlorate ions are coordinated to M.[427] IR data for $[Fe(AA)_2(ClO_4)](ClO_4)_2$ show the presence of a bidentate coordinated perchlorato ligand (AA = 4-*N*-(4'-antipyrylmethylidene)aminoantipyrine).[428]

IR spectroscopy has confirmed the presence of a unidentate coordinated perchlorato ligand in $Ni_2(L)_2(OClO_3)_2$, where L = 2-[(4-methylpyridin-2-ylimino)methyl]phenol.[429] The expected bands for an η^1-$OClO_3$ perchlorato ligand were observed in the IR spectrum of $Cu(OClO_3)_2(DMU)_4$, where DMU = dimethylurea.[430] $Cu(L)(IO_3)$, where HL = pyridine-2-carbaldehyde thiosemicarbazone, shows νIO bands at 808 and 735 cm^{-1}.[431] Typical bands of unidentate perchlorato were also seen in the IR and Raman spectra of $[L_3Zn(OClO_3)](ClO_4)$ (1121, 1032, 1026 cm^{-1}).[432]

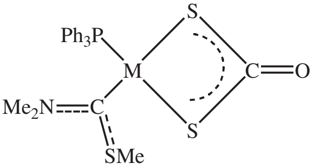
8 Sulfur and Selenium Donors

The complexes $\{Mo_2(O)(X)(\mu\text{-}S)(\eta^2\text{-}S_2)[\eta^2\text{-}S_2C_2Ph(C_2Ph)]\}^{2-}$, where X = O or S, show νSS at 520 cm^{-1}.[433]

FTIR spectra for *fac*-$[Re(CO)_3Br\{R_2P(S)P(S)R_2\}]$, where R = Me, Et, ^nPr, ^nBu, Ph, show that the ligands are *cis*-chelated. For $Re_2(CO)_8Br_2\{$*cis*-μ-$R_2P(S)P(S)PR_2\}$, the data indicate *cis*-bridging bidentate coordination.[434] The IR spectrum of $Rh_2(OAc)_4(tu)_2$, where tu = thiourea, is consistent with *S*-coordination of the thiourea.[435]

For $[Ni(C_2N_2S_{2.2}Se_{0.8})_2]^{2-}$, νC=C is seen at the low value of 1311 cm^{-1} – consistent with the long CC bond found crystallographically.[436] The νCS bands for $Ni(dnpdtc)(PPh_3)(X)$, where X = NCS, CN, dnpdtc = *N,N*-di-*n*-propyldithiocarbamate, are consistent with bidentate *S,S*-dithiocarbamate coordination.[437] For $[Ni(dnpdtc)L_2]^+$, where L = PPh_3, 1/2dppe, the IR spectra show isobidentate coordination by the dithiocarbamate fragment (thioureide stretch at 1536, 1526 cm^{-1} respectively).[438] The IR spectra of $[Ni^{II}(ER)\{P(o\text{-}C_6H_4S)_2\}(o\text{-}C_6H_4SH)]^-$, where ER = SePh, 2-*S*-C_4H_3S, include νSH bands at 2273 cm^{-1}, 2263 cm^{-1} respectively. These values are consistent with intramolecular Ni-S . . . H-SR/Ni . . . H-SR interactions.[439]

The IR spectra of (74), where M = Pd or Pt, include νC=O at 1675, 1603 cm^{-1} (Pd), 1681, 1605 cm^{-1} (Pt); $\nu_{as}CS$ 832 cm^{-1} (Pd), 832 cm^{-1} (Pt).[440] IR data for $[M(ESDT)Cl]_n$. M(ESDT)(Am)Cl, where M = Pd, Pt, ESDT = $EtO_2CCH_2(CH_3)NCS_2Me$, Am = chiral amino-alcohols, show that the dithiocarbamate is coordinated *via* two sulfur atoms.[441]



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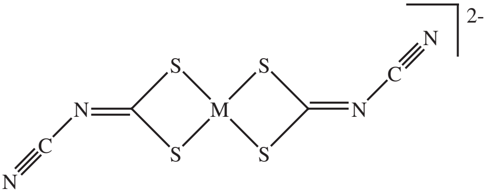

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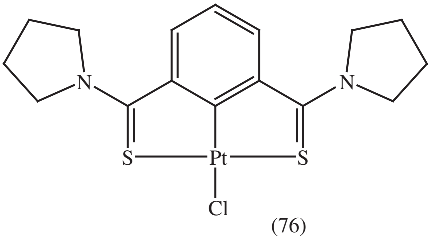


(76)

The IR spectra of (75), where M = Pd or Pt, include νC=N at 1435 cm^{-1}, *i.e.* there has been a significant increase compared to the free ligand, showing changes in delocalisation patterns.[442] IR bands for (76) indicate shifts in ligand modes showing *S*-coordination of the thioamide groups.[443]

The complex $[Cu_2(tu)_6]Cl_2.2H_2O$, gives νC=S of bridging and terminal thiourea (tu) ligands in the Raman spectrum at 705, 718 cm^{-1} respectively.[444]

An IR band at 1002 cm^{-1} for $Zn(meadtc)_2(2,2'\text{-bipy})$, where meadtc = ethanoldithio-carbamate, shows that the dithiocarbamate is unidentate.[445] The Raman spectrum of $Zn_2[di(cyclohexyl)dithiophosphate]_4$ shows a phase change in the range 40–55°C, involving ring conformational change.[446] The IR spectrum of the complex $S_4N_3Cl.ZnO$ suggests the presence of *S,S*-bidentate S=NS(Cl)=NSN=S=O coordinated to Zn^{2+}.[447]

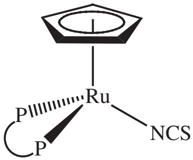
The IR spectra of $Cd(tsac)_2(Im)_2$, $[Cd(tsac)_3(H_2O)]^-$, where tsac = anion of thiosaccharin, Im = imidazole, are consistent with *S*-coordination of $tsac^-$.[448] IR data for $C_6H_5Hg[(EP^iPr_2)_2N]$, where E = S or Se, include νPNP at 1251, 1222 cm^{-1} (Se), 1259, 1224 cm^{-1} (S).[449]

The IR spectra of organotin-iron trinuclear complexes containing xanthate or dithiocarbamate show unidentate *S*-coordination.[450] Ligand modes were observed (IR) and assigned (using *ab initio* calculations) for $[Bi(dmit)_2]^-$, where H_2dmit = 4,5-dimercapto-1,3-dithiol-2-thione.[451]

9 Potentially Ambident Ligands

9.1 Cyanates, Thio– and Selenocyanates and their Iso–analogues. – The IR spectrum of $[In(dmso)_4(H_2O)_2][Cr(NH_3)_2(NCS)_4]$ show that the NCS^- is *N*-bonded and the dmso *O*-bonded.[452]

Characteristic differences were seen in IR and Raman bands due to ν_{as}NCS and ν_sNCS in *cis*- and *trans*-[Fe(NCS)$_2$(*rac*-prP$_4$), where prP$_4$ = 1,1,4,8,11,11-hexaphenyl-1,4,8,11-tetraphosphaundecane. Thus, ν_{as} bands were seen at 2112, 2105 cm^{-1} for the *cis*-isomer, 2099 cm^{-1} for the *trans*-isomer. For the ν_s modes, the wavenumbers are 845 cm^{-1}, 818 cm^{-1} respectively.[453]



(77)

The complex (77), where P–P = 1,1'-bis(diphenylphosphino)ferrocene, shows IR bands at 2105 cm^{-1} (ν_{as}NCS) and 697 cm^{-1} (ν_sNCS).[454] An IR band at 2109 cm^{-1} (ν_{as}NCS) was assigned to *N*-bonded NCS$^-$ in *trans*-[Ru^{II}(NCS)(NH$_3$)$_4$(MeQ$^+$)](PF$_6$)$_2$, where MeQ$^+$ = *N*-methyl-4,4'-bipyridinium.[455] The complexes (L)$_2$Ru(NCS)$_2$, where L = 4,4'- or 5,5'-diethyl ester of phosphonate-2,2'-bipyridine, show ν_{as}NCS IR bands at 2114 cm^{-1} (4,4'-) and 2118 cm^{-1} (5,5'-), confirming Ru–N coordination.[456]

Ligand modes have been assigned from IR and Raman spectra and normal coordinate analyses for [OsCl$_5$(L)]$^{2-}$ and *trans*-[OsCl$_4$I(L)]$^{2-}$, where L = NCSe or SeCN.[457,458] The complex [CpOs(PPh$_3$)$_2$(NCS)] gives ν_{as}NCS as an IR band at 2108 cm^{-1}.[459]

The complexes M(NCS)$_2$L$_2$, where M = Ni, L = PMe$_3$; M = Pd, L = PMe$_3$, PEt$_3$, PMe$_2$Ph, M = Pt, L = PEt$_3$, all show ν_{as}NCS in the range 2077–2098 cm^{-1}.[460] Characteristic IR bands for ligand modes were reported and assigned for Ni(SCN)$_2$(fp)$_4$, Ni(SCN)$_2$(mfp)$_4$ and Ni(SCN)$_2$(dmfp)$_3$, where fp = fural[3,2-*c*]pyridine, mfp = 2-methyl-fural[3,2-*c*]pyridine, dmfp = 2,3-dimethyl-fural[3,2-*c*]pyridine.[461] Table 11 summarises ligand mode assignments from the IR spectra of Ni(SCN)$_2$(HSCN)$_2$(4-Mepy)$_2$, where 4-Mepy = 4-methylpyridine.[462]

The IR spectra of Pd(*N,C*-dmba)(NCO)(L), where dmba = C$_6$H$_4$CH$_2$NMe$_2$-2, L = 2,3- or 3,4-lutidine, are consistent with the presence of *N*-bonded cyanato ligands.[463] The thiocyanate-bridged polymeric complex {[Cu$^{II}_2$(L)(NCS)][Cu$^{II}_2$(L)(SCN)](ClO$_4$)$_2$}$_x$, where H$_2$L = triazole-containing Schiff base macrocyclic ligand, shows ν_{as}NCS at 2135 cm^{-1}.[464] The observation of an IR band at 2116 cm^{-1} for [Cu(dadpm)(SCN)$_2$]$_n$ shows the presence of bridging thiocyanato ligands.[465] IR data for [Cu(*N*-Et-en)$_3$][Cr(NCS)$_6$]$_2$, where *N*-Et-en = *N*-ethyl-ethylenediamine, and related species show bands from Cr–NCS–Cu bridges.[466]

Table 11 *Ligand mode assignments for Ni(SCN)$_2$(HSCN)$_2$(4-Mepy)$_2$ (/cm^{-1})*

νCN	2117, 2128
νCS	788, 773
δSCN	468, 476

DRIFTS data show the formation of surface NCO^- species on catalytic reduction of NO by C_3H_6 on an Ag–Pd/Al_2O_3 surface.[467] The IR spectrum of $[Ag_4Fe_2(SCN)_{12}(H_2O)_2]^{2-}$ includes bands from the 32-membered $Ag_4Fe_4(SCN)_8$ rings, including bands from Fe–NCS–Ag units.[468] NO and CO co-adsorption on gold catalysts leads to the observation of IR bands due to ν_{as}NCO for adsorbed cyanate species: 2212 cm^{-1} (Au/TiO_2), 2220–2230 cm^{-1} (Au/MgO), 2256 cm^{-1} (Au/Al_2O_3), 2305 cm^{-1} (Au/SiO_2).[469]

The complex $Hg(L)(SCN)_2$, where L = *N*-(2-pyridyl)carbonylaniline, shows ν_{as}SCN at 2030 cm^{-1}, from Hg–S bonded ligands.[470] *Ab initio* calculations gave vibrational wavenumbers for the species $Me_{3-n}H_nM(NCX)$, where M = Ge, Sn or Pb, X = O or S.[471]

9.2 Ligands Containing N and O, N and P or P and O Donor Atoms. – IR studies of the binding of Sr^{2+}, Ba^{2+}, Cd^{2+} and Hg^{2+} to caffeine and theophylline, show that caffeine is coordinated *via* O(6) and N(9), theophylline *via* O(6), N(9) and N(7).[472] The νC=O of the dmf ligand in $\{[Ba_2(dmf)_5(H_2O)_5]SiW_{12}O_{40}.dmf.H_2O\}_n$ (1640 cm^{-1}) shows coordination of dmf *via* the carbonyl oxygen.[473]

The IR spectra of $Ln(TFA)_3(MMNO)_3$, where Ln = Y, Eu, Dy, Ho, Er or Yb, TFA = trifluoroacetate, MMNO = 4-methylmorpholine-*N*-oxide, show that the MMNO is coordinated *via* oxide O.[474] IR data for $Ln(N_2H_3COO)_3$ (Ln = La, Ce, Pr, Nd, Sm), and $Ln(N_2H_3COO)_3(H_2O)_3$ (Ln = La, Nd) show that all have hydrazinecarboxylate coordinated in bidentate fashion (*N,O*), with νNN 980–1000 cm^{-1}.[475]

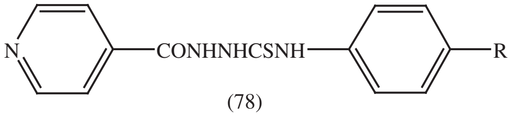
The complexes $Ln(L)(NO_3)(H_2O)_n$, where H_2L = 2,6-diacetylpyridine-bis-(benzoyl-hydrazone), Ln = La, Sm, Y, n = 1; Ln = Er, n = 2, all give IR spectra showing coordination of L^{2-} through azomethine N and hydrazone O atoms.[476] Similar data for $M(NO_3)_3(L)$, where M = La, Nd, Eu, Tb, Y; L = tris{2-[*N*-(2-pyridylcarbonyl)amine]ethyl}amine, show that L is coordinated *via* carbonyl O and pyridyl N atoms. [477] *N,O*-ligand coordination was also inferred from the IR spectra of $[Ln_2(H_4L)_3(NO_3)]^{2+}$, where Ln = La, Ce, Pr, Nd, Sm, Gd, Dy, Er, Yb, Y; H_5L = 2,6-bis-(salicylaldehyde-hydrazone)-4-chlorophenol.[478]

IR spectra of the La(III) and Ce(III) complexes of Schiff bases from the condensation of 2-hydroxy-1-naphthaldehyde with α-aminoacids show ONO-tridentate coordination (except for the L–glutamine derivative, which is OONO–tetradentate.[479] The IR spectra of Pr(III), Eu(III), Gd(III), Dy(III) and Yb(III) complexes of furohydroxamic acid show that the ligands are *N,O*–bidentate.[480] Raman and IR spectra of $[Er(pic)_4]^-$, where Hpic = picolinic acid, reveal that the complex is 8-coordinate, with each ligand coordinated through a (unidentate) carboxylate O and a ring N atom.[481]

Ligand mode assignments were proposed and conformed by a normal coordinate analysis for $UO_2(PhCONHNH_2)_2$ – extensive mixing of modes was seen for all modes except νNH and νCH.[482] IR data for $UO_2(NO_3)_2(NCP)_2$, where NCP = *N*-cyclohexyl-2-pyrrolidone, show that the ligand is coordinated through the carbonyl oxygen alone.[483]

The IR spectra of VO_2L, NiL_2 and MnL_2, where HL = *N*-phenyl-picoloylhydrazide, show that νC=O and νCN are both decreased in wavenumbers compared to the free ligand, *i.e.* *N,O*-coordination.[484] The complex $V^{III}(Hcys)_3$, where H_2cys = L-cysteine, has IR bands showing that the $Hcys^-$ ligands are coordinated to V(III) through amine N and carboxylate O atoms.[485] The IR spectra of $V^{IV}(L)_2$, where H_2L = tridentate bis(phenol) O_2N ligand with methyl or *t*-butyl substituents, contain characteristic νCH bands from the ligand.[486] The IR spectra have been reported and assigned for VO(acac)(L), $VOCl_2(L)$ and $VOCl(L)_2$, where HL = acyclic phosphazene ligands $HN(PPh_2NR)_2$ (R = Ph, $SiMe_3$). All data were consistent with the presence of bidentate L^- ligands.[487]

IR bands were reported and assigned for $Cr(pic)_3$ (Hpic = picolinic acid) – showing unidentate carboxylates.[488] The IR spectra of $M_2O_4L_2(H_2O)_2$, where M = Mo(V), W(V), HL = (78), R = H, Me, OMe, Cl, show bidentate ligands.[489]



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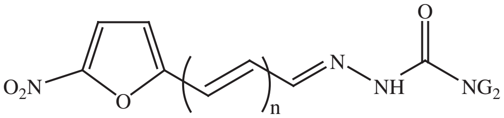


(79)

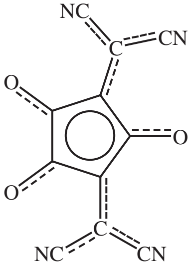
IR spectra are consistent with *N,O*-coordination of the ligands in the following: ML_2 (M = Mn, Ni; HL = *N*-propionylpicoloylhydrazide);[490] 2-pyridylethanol complexes of M(II) (M = Mn, Fe, Co, Ni, Cu, Zn);[491] and $ML(H_2O)_3$ (M = Mn, Co, Ni, Cu, Zn; L = *o*-vanillin-L-histidine).[492] The IR spectra of M(II) (M = Mn, Fe, Co, Ni, Cu, Zn, or Cd) complexes of a Schiff base from 2-hydroxy-5-methylacetophenone and *S*-methyldithiocarbazate, show coordination *via* phenolic O, azomethine N and thio–enolic S atoms.[493]

The IR spectra of complexes of $M(CO)_3{}^+$ (M = Tc, Re) with [(5-amino-pentyl)-pyridin-2-ylmethylamino]acetic acid show that the ligand coordinates through carboxylate O, tertiary N and pyridine N atoms.[494] Shifts of νC=O and νC=N on coordination in $ReOCl_2(PPh_3)_2(L)$, where L = (79, n = 0 or 1) are consistent with coordination of azomethine N and carbonyl O atoms.[495]

IR spectra gave detailed assignments to ligand modes for ML_2X_2, where M = Fe, Co, Zn; X = Cl, Br, I; L = 8-hydroxyquinoline.[496] IR spectra of $FeLCl_2$, $MLCl(H_2O)$ (M = Co, Ni, Cu, Zn) and $ML(OAc)(H_2O)$ (M = Co, Cu), where HL = 2-(2-hydroxyphenyl)-4-(phenylmethylene)-5-oxazolone, are all consistent with coordination of L^- *via* N and O atoms.[497] Similar data for $Fe_2(aphz)_2(\mu\text{-}MeOH)_2Cl_2$ and $Fe(phphz)Cl_2$, where Haphz = *N*-acetylpicoloylhydrazide, Hphphz = *N*-phenylpicoloylhydrazide, show coordination *via* 2N + O ligand atoms.[498]

FTIR data gave ligand mode assignments for M(II) (=Fe, Co, Ni, Cu, Zn) complexes of 3-carboxyacetonehydroxamic acid.[499] The IR spectrum of

{[Fe(2,2'-bipy)L(H_2O)$_2$].H_2O}$_2$, where L^{2-} = (80), includes νCO 1679 cm^{-1}, νCN(coord.) 2230 cm^{-1}, νCN (free) 2192 cm^{-1}.[500] The IR spectra of [Fe(HL)(H_2O)$_3$]$^{2+}$, where H_2L = salicylidene-2-aminobenzimidazole, and related species, show that the ligand is coordinated *via* azomethine N, benzimidazole N3 and phenolic O atoms.[501]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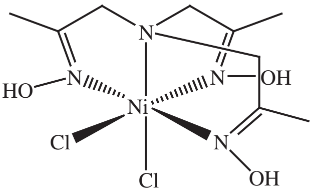
The IR spectra of Ru(TTP)(NO)(L), where TTP = tetra-*p*-tolylporphyrin, L = ONO, NO_2, gave the following assignments: (ONO) νNO 1842 cm^{-1}, νNO_2 1512, 928 cm^{-1}; (NO_2) νNO 1852 cm^{-1}, νNO_3 1515, 1269, 950 cm^{-1}.[502] Os(P)(NO)(ONO), where P = range of porphyrins, show ν_{as}ONO in the range 1495–1531 cm^{-1}, with ν_sONO 913–962 cm^{-1}, from the *O*–bound nitrito ligand.[503]

Low-pressure NO_2 and layers of Co^{II}(TPP) react to form the 5-coordinate nitro-complex Co^{III}(TPP)(NO_2). This in turn adds py to form the 6-coordinate complex (py)Co^{III}(TPP)(NO_2). Both of these show the expected bands for *N*-bound nitro ligand.[504] Detailed ligand mode assignments have been given from IR and Raman spectra for Co(PGO)$_2$, where PGO = piperazine glyoxime.[505] The IR spectra of MCl_2(L), where M = Co, Ni, Pd, Pt, L = 1-methyllumazine; M = Co, Pt, L = 1,6,7-trimethyllumazine, are all consistent with *N,O*-chelation.[506]

The IR spectra of Co(II), Ni(II) and Cu(II) complexes of Schiff bases derived from condensation of 2-pyridine-carboxaldehyde with DL–alanine, DL–valine and DL–phenylalanine, show that all act as uninegative, bidentate ligands.[507] Similar data for complexes of the heterocyclic Schiff base LH_2 derived from 1-amino-5-benzoyl-4-phenyl-1*H*-pyrimidin-2-one and 3-hydroxy-salicylaldehyde show that the ligand is tridentate (*O,N,O*) in M(LH)$_2$ (M = Co, Cu, Zn), but bidentate (*N,O*) in Ni(LH_2)$_2$$Cl_2$.[508]

The complexes ML_2, where M = Co, Cu, Ni, Zn; HL = 2-hydroxy-5-(chloro/nitro)-benzaldehyde[4-(3-methyl-3-mesitylcyclobutyl)-1,3-thiazol-2-yl]hydrazone, give IR spectra indicating chelation of L^- through azomethine N and phenolate O atoms.[509] Coordination of the 5-(2'-carboxyphenylazo)-8-hydroxyquinoline to Co, Ni, Cu or UO_2^{2+} *via* CN, N=N, COOH and OH was shown by IR spectroscopy.[510] IR data for M(II) (=Co, Ni, Cu, Zn) complexes of *N*-salicyloyl-*N'*-*p*-hydroxythiobenzohydrazide and related ligands show coordination by thiolato S, enolic O and two hydrazine N atoms.[511]

IR and Raman spectra, together with DFT calculations, gave assignments to ligand modes for (81).[512] Ligand mode assignments were also made for M(iso)$_2$Ni(CN)$_4$, Cd(iso)$_2$$X_2$, where M = Ni, Cu, Zn, Cd, iso = isonicotinamide, X = Cl, Br or I.[513]



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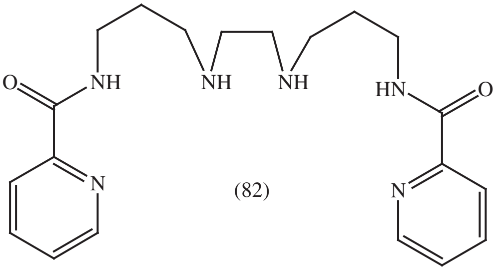
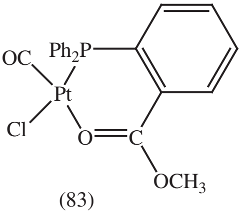


(82)

IR data show that the Ni(II), Cu(II) and Zn(II) complexes of the Schiff base derived from 1,2-bis(*o*-aminophenoxy)ethane and salicylaldehyde involve ONNO tetradentate coordination.[514] The ligand (82) (=HL) coordinates *via* amido O and 2N atoms in $M(HL)^{2+}$ (M = Ni, Cu), but *via* amido N and two other N atoms in NiL^{+}.[515] The IR spectrum of $Ni_2(L)(3,5\text{-prz})$, where L = 1,3-bis(2-hydroxy-5-bromosalicylideneamino)propan-2-ol, 3,5-prz = 3,5-dimethylpyrazolate, is consistent with coordination of L through O and imino N atoms.[516]

Ligand mode assignments have been proposed from the IR spectra of Pt(dach)(L), where dach = *trans*-(±)-1,2-diaminocyclohexane, H_2L = *N*-substituted L-glutaric or L-aspartic acids.[517] Similar data were given for $[Pt_4(\mu_2\text{-isonic})_4(dppf)_4]^{4+}$, where isonic = isonicotinate, dppf = 1,1'-bis(diphenylphosphine)ferrocene.[518] The IR spectrum of (83) includes νCOO of the *P,O*-ligand at 1638 cm^{-1}.[519]



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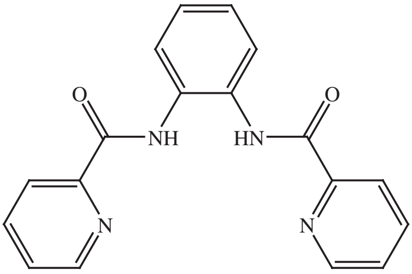

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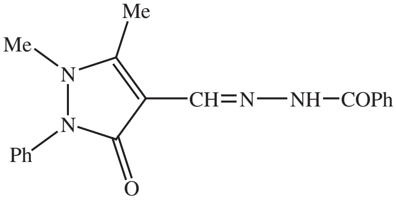

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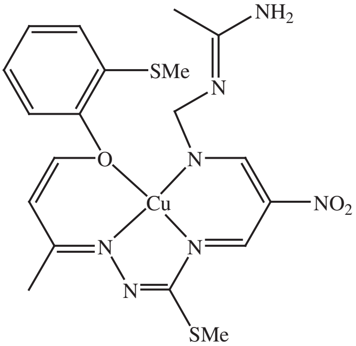


(86)

The IR spectrum of Cu(L), where H_2L = (84), is consistent with coordination by all 4 N atoms, with free C=O groups.[520] FTIR data for Cu(II) complexes of (85) (=L), *i.e.* $CuL_2{}^{2+}$, $Cu(L)Cl_2$, $Cu(L)_2Br_2$, show that L is acting as a neutral bidentate ligand *via* azomethine and carbonyl (of pyrazolone) O atoms.[521] The adsorption of (*S*)-histidine on Cu(110) gave RAIRS data consistent with coordination by bidentate carboxylate O atoms and the dehydrogenated N of the imidazole group.[522]

The IR spectrum of $[Cu(NPTLH)_2]^{2-}$, where NPTLH = 2-hydroxy-1-naphthylidene-*o*-toluidine Schiff base, includes bands indicating coordination by azomethine N and phenolic O atoms.[523] The complex (86) gives IR bands due to νNH_2 at 3344.9 and 3434.8 cm^{-1}.[524] IR and Raman spectra gave ligand mode assignments for the *p*-nitrocatecholate (NCat) adduct of $[Cu_2(L66)]^4$, where L66 = α,α'-bis{bis[2-(1'-methyl-2'-benzimidazolyl)ethyl]amino}-*m*-xylene, and related species.[525] DFT calculations of vibrational wavenumbers for $[Cu(HL)L]^-$, where HL = 2-hydroxyiminopropanoic acid, were used to assign experimental data (IR and Raman) for the *N,O*-ligands.[526]

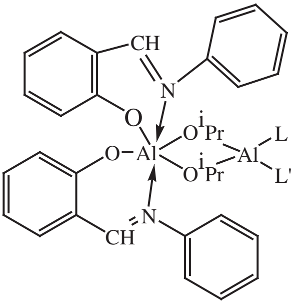
The IR spectrum of asparagine adsorbed on a gold electrode shows that it is coordinated *via* oxygen atoms of COO^- and through the amide carbonyl.[527]

IR data for $[ZnL_2]_n$, where L = catena-poly[bis(benzoato)-bis(3-pyridine)methanol], show coordination *via* 2 unidentate benzoate groups, 2 methanolic O atoms, and two N atoms.[528] A decrease in νNH from the free ligand L (=(87)) (3440 cm^{-1}) to 3330 cm^{-1} in the complex $(L)ZnCl_2$ was ascribed to N–H . . . Cl-Zn hydrogen bonding.[529] The IR and Raman spectra of $(Me_3Si)_2Zn[Ph_2PNSiMe_3]_2$ were assigned using DFT calculations.[530] IR spectra of CdL^- and $CdL_2{}^{4-}$, where H_3L = *N*-(phosphonomethyl)glycine, were consistent with unidentate coordination of carboxylates to Cd.[531]

Significant differences were found in the IR spectra of two isomers of $Al(Q)_3$, where Q = quinolin-8-olate, *i.e.* α- and δ-$Al(Q)_3$.[532] FTIR and Raman spectra, with DFT calculations, gave assignments to ligand modes for $[Al(Ser)(H_2O)_4]^{2+}$, where Ser = serine.[533] Characteristic ligand modes were assigned from IR data for (88), where L = L' = RR'C=NOH (R = Me, R' = Me, C_4H_3S-2 *etc.*, or L = O^iPr, L' = RR'C=NOH.[534]

6-NHCO^{t}Bu-2-pyridylmethyl-$N(CH_2CH_2)_2O$

(87)



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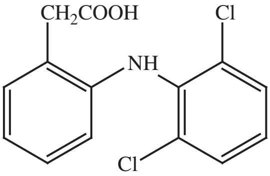

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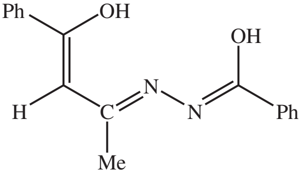

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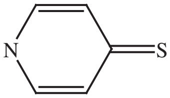


(91)

Co-adsorption of NO, CH_4 and O_2 on In-ZSM-5 catalyst gives an IR band at 1622 cm^{-1} due to $InO^+(ONO)$, and one at 1575 cm^{-1} from $InO^+(NO_3)$.[535]

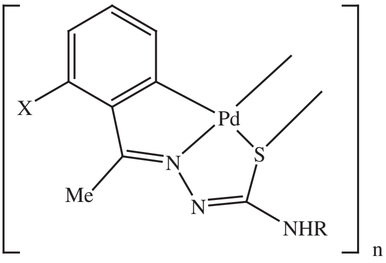
The complex $[^nBu_2Sn(picolinate)_2]_n$ gives IR bands due to νCO_2, showing the presence of both uni- and bidentate carboxylates.[536] Such modes for $^nBu_2Sn(L)$, where L = esters of salicylidene-*L*-tryptophan and salicylidene-*L*-valine, however, showed that only unidentate carboxylates were present.[537] For $Me_2Sn(L)O(L)SnMe_2$, where HL = (89), νCO_2 modes were consistent with anisobidentate carboxylato coordination.[538] An IR band assigned as ν(C=N–N=C) was seen at 1592 cm^{-1} in the IR spectrum of $R_2Sn(L)$, where H_2L = (90).[539] Ligand mode assignments were proposed from the IR and Raman spectra of $[SnR_2(MePN–H)]I$, where R = Me, Et, Bu, Ph, MePN = *N*-methylpyridoxine.[540]

9.3 Ligands containing N and S, N and Se or P and S Donor Atoms. – SERS data were reported for $[Fe(CN)_5(pyS)]^{4-}$, where pyS = (91), adsorbed on a gold electrode, including a νCS band at 1096 cm^{-1}.[541] The value of νP=S in $Ru(CO)_2Cl_2$(P-S), where P–S = $Ph_2P(CH_2)_nP(S)Ph_2$, n = 1, shows chelate coordination. For n = 2–4, νP=S is almost unshifted compared to the free ligand, *i.e.* unidentate *P*-coordination.[542]

The IR spectrum of $[Co(MPz3Hex)_2]^+$, where HMPz3Hex = 5-methyl-3-formyl-pyrazole 3-hexamethyleneiminylthiosemicarbazone, is consistent with

N,N,S-coordination, *via* pyrazolyl N, azomethine N and thiol S.[543] The IR spectra of CoL_3, NiL_2, $Cu_2L_2Cl_2$ and ZnL_2, where HL = furan-2-aldehyde thiosemicarbazone, show coordination of L^- involving azomethhine N and thiolate S.[544] The IR spectra of dto (=dithio-oxamide) complexes M(terpy)$(dto)_2{}^{2+}$ (M = Co, Ni); Cu(terpy)(dto)Cl^{2+}, and tsc (=thiosemicarbazide) complexes Co(terpy)$(tsc)_2{}^{2+}$ and Cu(terpy)(tsc)Cl^{2+}, show that tsc is *N,S*-coordinated, and the dto *S*-coordinated.[545]

The complex $[Ni(HMPz4MCy)_2]^{2+}$, where HMPz4MCy = 5-methyl-3-formylpyrazole-*N*(4)-methyl-*N*(4)-cyclohexylthiosemicarbazone, has an IR spectrum consistent with *N,N,S*-tridentate coordination.[546] Similar conclusions were drawn from an IR study of $NiX_2(L)(H_2O)$ and $Ni(L)_2{}^{2+}$, where L = 4-[*N*-(2'-hydroxy-1'-naphthalidene)amino]antipyrine thiosemicarbazone.[547] The complexes $\{Ni^{II}(ER)[P(o\text{-}C_6H_4S)_2(o\text{-}C_6H_4SH)]\}^-$, where ER = SePh or C_4H_3S-*S*-2, gave IR evidence for [Ni–S . . . H-SR]/[Ni . . . H-SR] interactions (νSH near 2280 cm^{-1}).[548]



(92)

IR spectra were consistent with the structure shown for (92), where X = F, Cl, R = Me, Et.[549] The IR spectra of square-planar-coordinated dimers $LPtCl_2PtL$, where L = range of thiosemicarbazone ligands, show that L is *N,S*-bidentate.[550] IR data for Pt(II) complexes of bioactive thiosemicarbazones derived from 4-amino-antipyrine show that they are coordinated as *N,N,S*-donors.[551]

A SERS study of the coordination of *n*-butylethoxycarbonylthiourea at copper surfaces revealed *S,N*-coordination.[552] The IR spectrum of Cu(pysme)(sac)(CH_3OH), where sac = saccharinate, pysme = anion of pyridine-2-carboxaldehyde Schiff base of *S*-methyldithiocarbazate, shows *N,N,S*-chelation by the Schiff base ligand.[553]

The wavenumbers associated with νCSe of selenourea (Seu) decrease on formation of the complexes $[(R_3P)Au(Seu)]^+$, where R = Me, Et, Ph, Cy *etc.*, showing Au–Se coordination.[554]

Vibrational assignments for $[M(SNNNS)]_n$, where H_2SNNNS = 2,6-diacetylpyridinebis(*S*-benzyldithiocarbazate), M = Zn, n = 2, M = Cd, n = 1, were as follows: νNN 1131, 1030 cm^{-1} (Zn), 1134, 1006 cm^{-1} (Cd); νCSS 1005 cm^{-1} (Zn), 1028 cm^{-1} (Cd).[555] The IR spectrum of $Hg(L)_2(OH)_2$, where L = sulfathiazole, show that L is coordinated *via* the thiazole N atom.[556]

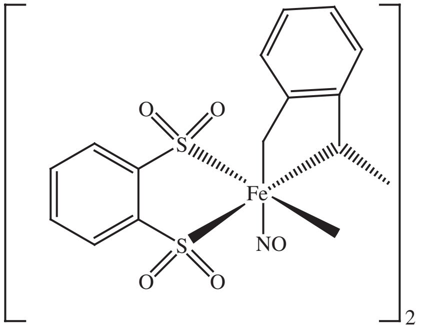
IR data for $Me_2Sn(aptsc)X$, where X = Cl, Br, Haptsc = acetone *N*(4)-phenylthiosemicarbazone, were consistent with *N,S*-coordination of the ligand.[557] Values of ν_{as}, ν_sCS_2 bands for $SnBr_2[S_2CN(CH_2CH_2)_2O]_2$ and related species were all consistent with anisobidentate coordination by the dithiomorpholincarbamato groups.[558]

9.4 Ligands Containing S and O Donor Atoms. – The IR spectra of $ML_2(HL')$, where M = Mg, Ca, Sr or Ba; L = deprotonated 1-nitroso-2-naphthol, 8-hydroxyquinoline, *o*-nitrophenol and 2,4-dinitrophenol, HL' = thiosalicylic acid, show that HL' is coordinated through the S atom of the SH group and carboxylate O.[559]

The IR spectra of Sm(III), UO_2^{2+} and M(II) (M = Co, Ni, Cu, Zn) complexes containing bipy and sulfamerazine, show coordination by the azomethine N atom of the sulfonamide ligand.[560] The IR spectra of $UO_2(L)_2(L')$, where L = thenoyltrifluoroacetone and related species, L'=$PhSOCH_2SOPh$, show that L' is *O*-unidentate. In $[UO_2(L)_2]_2L'$, bridging L' is present.[561]

There is matrix-IR evidence for the formation of a sulfene complex, $Cl_2Cr(O)(O_2SMe_2)$, from the reaction of CrO_2Cl_2 and dmso.[562] A band assigned as $\nu S{=}O$ was seen in the range 1050–1060 cm^{-1} for the dmso ligand in $Mo_2O_2(\mu\text{-}S_2)[S_2P(OR)_2]_2$.dmso, where R = Me, Et or ^iPr, showing *O*-coordination.[563]

The complex (93) gives IR bands due to νSO_2 at 1212, 1067 and 1057 cm^{-1} from the coordinated bis(sulfinate) groups.[564] The complex RuCl(dmso-*O*)$_4$(NO)$^{2+}$ has νSO bands at 896 and 878 cm^{-1}. For Ru(dmso-*O*)$_5$(NO)$^{3+}$, νSO is at 870 cm^{-1}.[565] $Ru(ma)_2(tmso)_2$, where ma = maltolato, tmso = tetramethylenesulfoxide, gives $\nu S{=}O$ bands at 1056 and 1117 cm^{-1}, showing Ru–S coordination.[566] $\nu S{=}O$ is at 1071 cm^{-1} for the *O*-coordinated ligand in *trans*-Ru(L)Cl_2, where L = (94).[567]



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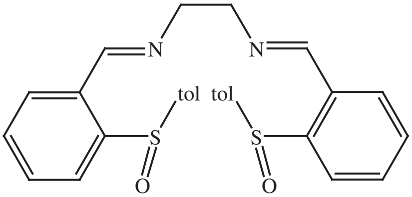

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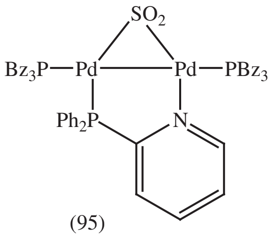

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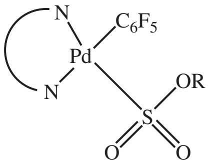

(96)

The IR spectrum of *cis*-Ru(acac)(dmso)$_2$ and Ru(acac)$_2$(*meso*-BESE), where BESE = EtS(O)(CH$_2$)$_n$S(O)Et, n = 4, all show *S*-coordinated sulfoxide groups.[568] Similar conclusions were drawn from the IR spectra of [RuCl$_2$(*p*-cymene)]$_2$(μ-L), where L = EtS(O)(CH$_2$)$_n$S(O)Et, n = 2 or 3.[569]

The complex (95) shows IR bands assigned to the bridging SO$_2$ group at 1092, 1070 and 1028 cm^{-1}.[570] The complexes (96), where N–N = bipy, Me$_2$bipy, tmeda; R = Me, Et, Pr, all show ν_{as}, ν_sSO$_2$ of the *S*-coordinated alkyl sulfite near 1230 cm^{-1} and 1095 cm^{-1} respectively.[571]

The IR and Raman spectra of Au(PPh$_3$)(Hfspa), where H$_2$fspa = 3-(2-furyl)-2-sulfanylprop-enoic acid, are consistent with *S*-coordination of the Hfspa$^-$ ligand.[572]

A band assigned as ν_{as}P$_2$N was seen at 1290–1200 cm^{-1} in the IR spectra of PhHg[(XPR$_2$)(YPPh$_2$)N], where X = O, Y = S, R = Me, Ph or OEt; X = Y = O, R = OEt.[573] The IR spectrum of [2-(Me$_2$NCH$_2$)C$_6$H$_4$]Hg[S(O)PPh$_2$] contains νP=O is at 1165 cm^{-1}, νP=S 575 cm^{-1}, consistent with η^1-*S*-coordination.[574]

The IR spectrum of [(SnN^{t}Bu)$_4$(μ-OSO$_2$)].thf, gives sulfito ligand modes at 1023, 919 and 591 cm^{-1}.[575] The FTIR and Raman spectra of R$_2$Sn(cap), where H$_2$cap = *N*-[(*S*)-3-mercapto-2-methyl-propanyl]-*L*-proline, R = Me, Et, ^{n}Bu, ^{t}Bu, show coordination *via* the S atom, together with carboxylate and amide carbonyl groups.[576]

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Gas-phase Molecular Structures Determined by Electron Diffraction

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1 Introduction

Last year we wrote an introduction to our review of gas-phase structures, in which we declared that modern technology had made such reviews redundant, and that chapter would be our last. The editors decided otherwise. Their red pen excised the offending material, and our arms were duly twisted. So here we are again, with the same positive view of the scientific benefits of the data given by electron diffraction studies; and with the same reluctance to spend time providing a summary of data that can be found on-line, and which is not widely read. So this year we will give fewer numbers and instead will concentrate on critical discussion of the significant results. Such an approach must of course be subjective.

Where we do present geometrical parameters, we follow our usual practice of quoting them for the structural type (r_e, r_α, r_g, r_a, *etc.*) reported in the original papers and with the same uncertainties, quoted in parentheses after numerical values. Such uncertainties may be estimated standard deviations, or multiplied by two or three to reflect supposed inadequacies in the modelling of the structures, or with additions for possible systematic errors. It is our view that systematic errors should be largely avoidable, that models should not be inadequate, and that an estimated standard deviation is a perfectly good and well understood quantity, and therefore that it should be left to readers to multiply it by whatever number they choose.

The following compounds are included in this report.

Section 2, Groups 2 and 13: $Mg(acac)_2$, 1-Br-B_5H_8, 2-Br-B_5H_8, *closo*-2,3-$C_2B_9H_{11}$, *nido*-2,9-$C_2B_9H_{13}$, $Hf(BH_4)_4$.

Section 3, Group 14: CFI(O), $C_{60}F_{48}$, $CH_2{=}CHSiF(CH_3)_2$, 1,1,2,2-Si_2H_2-Bu^t_4, *cyclo*-$Bu^t_2Si(NH)_2(CH_2)_2$, $HSi(OCH_2CH_2)_3N$ (silatrane), $F_3SiN(Me)NMe_2$, $F_3SiN(SiMe_3)NMe_2$, $Cl_2HSiONMe_2$, $Me_2Ge(C{\equiv}COMe)_2$, $SnBr_2$, $Me_3SnC{\equiv}CH$.

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Section 4, Group 15: *N*,*N*-dimethyldiaziridine, 6,6'-*bis*-(1,5-diazabicyclo-[3.1.0]-hexane, 1,3-$C_6H_4F(NO_2)$, 1,4-$C_6H_4F(NO_2)$, $PCl(SCH_3)_2$, $P(CH_3)_2(C_6H_5)$, all-*cis*-1,4,7-trimethyl-3,6,9-trioxa-10-phosphatricyclo[5,2,1,$0^{4,10}$]decane-2,5,8-trione, $OPBu^t_3$, $HNPBu^t_3$, $P_2Bu^t_4$, $P[N(SiMe_3)_2](NPr^i_2)$, 1,2-thiaarsol.

Section 5, Group 16: CH_2FOCH_2F, CHF_2OCHF_2, CF_3OCHF_2, 1,4-$C_6H_4F(OCF_3)$, $CF_3C(O)OC(O)CF_3$, $ClC(O)OCF_3$, $CH_3C(O)SCH_3$, $CF_3OC(O)C(O)OCF_3$, $FC(O)OSO_2CF_3$, SF_5OSO_2F.

Section 6, Transition metals and lanthanides: $LaCl_3$, $LaBr_3$, $PrBr_3$, $HoBr_3$, $Lu(dpm)_3$ (dpm=$Bu^tCOCHCOBu^t$).

2 Compounds of Elements in Group 2 and 13

Magnesium bis-acetylacetonate has been studied in the gas phase at 630 K.[1] The two ligands lie in perpendicular planes, giving the molecule overall D_{2d} symmetry. The Mg–O bond length is given as 196.6(4) pm, of type r_α. However, the vibrational corrections were determined using the programme SHRINK, which allows for curvilinear atomic motions, so the structural type should be given as r_{h1}. There are now several different ways in which vibrational corrections are calculated, and it would be good to distinguish between distances determined experimentally with the various methods. The structure with average nuclear positions at 0 K is then $r_\alpha{}^0$. If it should be required at any other temperature (it is difficult to see when that would be of value), then it should be given as $r_\alpha{}^T$. Experimentally determined values, historically given as r_α, should be r_{h0} if rectilinear atomic motions were used, and r_{h1} for curvilinear motions. There is not yet any convention for those cases when an anharmonic force field is used, but one should be introduced. The level of anharmonicity used needs to be specified.

Not much is known about the structural consequences of replacing hydrogen atoms in cage boranes by other atoms or groups, and particularly by halogen atoms. There are quite a few cages that are completely halogenated, but they are usually of the form B_nH_n, and lack bridging atoms. A study of derivatives of pentaborane(9) in which terminal hydrogens atoms at B(1) (apical) and B(2) (basal) have been replaced by bromine shows that the structural effects are minimal.[2] Calculations have also been done for molecules with other halogen substituents. The biggest effects are lengthening of the B(base)-B(apex) bonds adjacent to the halogen in the 2-isomers, with an associated shortening of the other two base-apex bonds, shortening of the base-apex bonds in the 1-fluoro compound, and widening of the B(apex)-B(base)-F angle in the 2-fluoro derivative. Otherwise there is remarkably little change, even due to steric effects in the 1,2-dibromo compound.

The 11-vertex carbaboranes are important synthetically, being precursors to a wide range of metallacarbaboranes and to many heteroboranes. The structures of two of the parent compounds have now been determined.[3] *Closo*-2,3-$C_2B_9H_{11}$ has C_{2v} symmetry and the carbon atoms are not adjacent to one another, so there are three different C-B and six B-B distances, all lying within the range 158 to 167 pm. It was therefore necessary to apply flexible restraints to many of the differences between similar distances, although eight parameters were refined without restraints. This is a good example of the work that can now be done, making the most of both experimental and computational methods. A few years ago any attempt to study the structure of such a molecule would have been much less satisfactory.

Nido-2,9-$C_2B_9H_{13}$ has C_s symmetry, so there are even more distances, five C-B and nine B-B, although they cover a wider range, from 160 to 196 pm. The open CB_4 face of the *nido* structure has two B-H-B bridges, as well as the five terminal hydrogen atoms. The B-B distances associated with the bridges are long [178.8(3) pm], but the bond between the two bridges is even longer, at 196.1(2) pm. The hydrogen bridges are distinctly asymmetric, with B-H distances of 134.2(6) and 139.5(12) pm. An attempt to study the isomer *nido*-7,8- $C_2B_9H_{13}$ was not successful, because the compound was not sufficiently thermally stable.

Hafnium tetrakis(tetrahydroborate), $Hf(BH_4)_4$, has T symmetry in its ground state, with the four triply-bridged BH_4 groups all twisted 14(1)° from the perfectly staggered positions, at which the molecule has T_d symmetry.[4] The bridging Hf-H distance, 221.5(7) pm, is not much shorter than the Hf…B distance, 231.4(2) pm, but the most remarkable feature of the structure is the exceptional magnitude of the anharmonicity parameters for both the Hf . . . B and Hf-B(bridge) atom pairs, which is attributed to the fluxional hydrogen atom exchange process.

3 Compounds of Elements in Group 14

The structure of fluorocarbonyl iodide, CFI(O), has been determined by electron diffraction, and by calculations at levels up to CCSD(T)-aug-cc-pVQZ.[5] The FCO and ICO angles are not very different, at 123.8(14) and 125.1(16)° (r_α structure), respectively, but are much greater than the FCI angle, 111.1(21)°.

The problems in determining cage structures, where there are often many similar inter-atomic distances, were discussed in the last section. They were frustratingly present in a study of a particularly interesting molecule, $C_{60}F_{48}$.[6] This is the fullerene derivative with the largest number of attached atoms or groups, and it has been shown by NMR spectroscopy to belong to a point group of order 6, *i.e.* S_6 or D_3. Thirty parameters are therefore required to define the positions of ten unique carbon atoms, and a further 17 parameters are needed for fluorine atom positions, even with the assumption that all C–F bond distances are equal. Not surprisingly, these parameters could not be refined simultaneously. Our approach in such circumstances would be to apply restraints to such parameters as differences between some C–C or C=C distances. What was actually done was series of successive refinements of small groups of four or five parameters – dozens of them, all giving satisfactory fits to the observed diffraction data. Values of individual parameters differed substantially over the many refinements, but what was clear was that C–C distances between two sp^3-hybridised carbon atoms were long, averaging over 158 pm, whereas those between sp^3 and sp^2 carbon atoms averaged only a little over 150 pm, while the C=C distances averaged just below 133 pm. The structure reported is of type r_a. It is possible that the vibrational corrections, albeit individually small, that would be applied in converting to an r_{h1} structure could make a significant difference when there is such strong correlation between so many similar distances.

A study of vinyl dimethylfluorosilane, $CH_2{=}CHSiF(CH_3)_2$, focuses on the conformational properties.[7] The refinement of the structure assumed that the *gauche* conformer, with the CCSiF dihedral angle close to 120°, was more stable than the *syn* form by 0.59 kJ mol^{-1}, in accord with an earlier study by infra-red spectroscopy. A Fourier cosine potential function representing the large-amplitude torsional motion about the =C–Si bond was used. However, most *ab initio* calculations indicated that the *syn* form was the more stable, only MP2/6-31G(d) favouring the *gauche* conformer, by 0.67 kJ mol^{-1}.

It is almost axiomatic that staggered conformations are more stable than eclipsed ones, and that the energy difference is greatest when large substituents are present. It was therefore a great surprise when we found that two of the *tert*-butyl groups in 1,1,2,2-tetra-*tert*-butyldisilane were almost eclipsed, in the C_2-symmetry *anticlinal* structure.[8] Of course, if we had read the literature properly, we would not have been quite so surprised. When there are four butyl groups present, it is possible for two of them to be substantially bent away from one another, aided by the flexibility of the silicon atoms. Two SiSiC angles are as wide as 117.0(5)°, whereas the other two are just 110.7(6)°. (In fact, the computed angles differ even more dramatically, being 120.5 and 107.7°.) It is predicted that in pentabutyldisilane the butyl groups will not be able to avoid one another so easily, so wide SiSiC angles are expected, while in hexabutyldisilane the steric strain should lead to an extremely long Si–Si bond, or possibly even spontaneous dissociation to give tributylsilyl radicals.

Two conformers, both twisted, with C_2 symmetry, of 2,2-di-*tert*-butyl-1,3-diaza-2-silacyclopentane coexist in the gas phase.[9] At 305 K 76(6)% of the molecules are in the form in which the N–H bonds are staggered with respect to the adjacent CH_2 groups, while in the remaining molecules the N–H and C–H bonds are eclipsed. However, B3LYP calculations indicate that the eclipsed form should predominate, contributing 65% under the conditions of the experiment. This reminds us to be careful of computed relative energies. Quite a small error can lead to a major difference in the relative abundances of conformers, and when the energies are finely balanced, the experimental data may well not be in good agreement with what is computed – and what is computed by different methods is very likely to be inconsistent.

In silatranes, the nitrogen atom is placed so that it can donate its lone pair of electrons to silicon, making the latter atom five-coordinate. The strength of this interaction varies considerably, depending on the substituent on silicon, but there are also very big differences between the Si–N distances for the same compound in gaseous and crystalline phases. The only compounds studied in the gas phase were the N-methyl and N-fluoro derivatives, but now the parent silatrane, with an Si–H bond, has been added.[10] The refined Si–N distance (perhaps better described as Si . . . N) is 240.6(27) pm, compared with 231.8(9) pm for fluorosilatrane in the gas phase and 204.2(1) pm in the crystalline phase, and 245.3(47) (gas) and 217.5(4) pm (crystal) for methylsilatrane. With such sensitivity to substituents and environment, it is perhaps not surprising that computational methods do not perform well in predicting the Si–N distance. With the 6-311 ++ G** basis set, the MP2 method gives 235.1 pm, too short by 5 pm, while B3LYP gives 254.2 pm, nearly 14 pm too long, and HF is even worse, at 268.0 pm. It should be noted that the NSiO angles are less than 90° [refining to 78.8(21)°], but that the SiNC angles are more than 90°, refining to 105.4(14)°, although the computed values are 6 to 8° more than this.

Compounds exhibiting intramolecular secondary Si . . . N and Si . . . O bonds continue to confound expectations, and to provide challenges for theory. A study of $F_3SiN(Me)NMe_2$ and $F_3SiN(SiMe_3)NMe_2$, in which the fluorine atoms greatly enhance the acceptor strength of the silyl groups, has provided the first experimental proof for the existence of strong β-donor-acceptor bonds in silylhydrazines.[11] However, the replacement of a methyl group by a trimethylsilyl group in the α position has an enormous effect on the structure: in the first of these compounds, the (F_3)SiNN angle is 106.5(4)° in the gas phase [104.2(1)° in the crystal], whereas the corresponding angle in the trimethylsilyl compound is 84.9(4)° [83.6(1)° in the crystal]. In the latter case the contrast with the (Me_3)SiNN angle of 139.8(5)° is particularly striking. As is often the case for molecules of this type, computational methods are way off the mark. This last SiNN angle is underestimated by more than 11° at the MP2/6-311+G** level.

Silicon . . . nitrogen secondary bonding, this time with an intermediate oxygen atom, is shown in *O*-dichlorosilyl-*N*,*N*-dimethylhydroxylamine, $Cl_2HSiONMe_2$.[12] In the gas phase it exists as 40% of the conformer in which the Si–H bond is *anti* with respect to the O–N bond, with the remaining 60% adopting the *gauche* conformation. The strengths of the N . . . Si interactions in these two forms are remarkably different, as demonstrated by the SiON angles, 111.1(20)° in the *anti* conformation but 98.8(12)° in the *gauche*. The critical factor giving rise to this very large difference in angles is the presence of a chlorine atom *anti* to the O–N bond in the *gauche* conformer. The OSiCl angle is also much smaller for a chlorine atom in the *anti* position, 101.9(8)° compared to 111.8(5)° for one in a *gauche* position. Of course, there are other factors contributing to the structures, including repulsive van der Waals and attractive weak hydrogen-bond interactions, so it is unwise to focus too much on a single type of interaction.

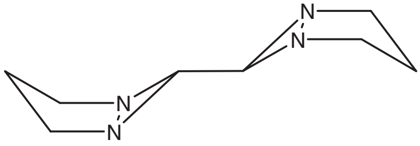
The benefits of taking curvilinear motions of atoms into account when calculating vibrational corrections having already been referred to in this review. The program SHRINK makes this almost routine, by using the so-called first order approximation, which uses the second derivatives of atomic positions, calculated at the equilibrium positions. The r_{h1} structures obtained in this way are a great improvement on their predecessors – but it is always possible to come up with a situation that calls for an even higher level of approximation. In dimethyl-bis(methoxyethynyl)germanium, $Me_2Ge(C\equiv COMe)_2$, there is very little to restrict the torsional motions of the methoxy groups.[13] In consequence, there are some enormous amplitudes of vibration – over 100 pm for the distance between the two carbon atoms of the methoxy groups and also for another long C . . . C distance. The perpendicular correction coefficients calculated using the first-order approximation (k_{h1}) are likewise extremely large, up to 133 pm for the distance between the pair of methoxy carbon atoms. And that, of course, is impossible. The motions of these atoms arising from the torsions about the O–C≡C–C axes are essentially circular, and will not be well described by taking any number of derivatives of atomic positions at the origin. It would be better than nothing to determine an r_{h2} or r_{h3} structure, but a different approach is needed for systems such as this – which fortunately are not common.

In a study of tin dibromide, it was prudent to allow for the presence of the dimer, Sn_2Br_2, although in the end the refined amount of dimer was just 1.4(5)%.[14] The Sn-Br distance (r_g) refined to 251.5(5) pm and the BrSnBr angle to 97.9(4)°. The structure proved to be rather difficult to reproduce theoretically, requiring a very large basis set (quadruple zeta quality).

Existing data for trimethylstannyl acetylene have been reanalysed to give an r_{h1} structure.[15] The Sn–C bond to the ethynyl group, at 209.6(17) pm, is 5 pm shorter than those to the methyl groups. Parameters are very similar to those of bis(trimethylstannyl)acetylene, and the C≡C bond is about 1 pm longer than those in $Sn(C\equiv CH)_4$ and about 2 pm longer than in $Sn(C\equiv CCF_3)_4$.

4 Compounds of Elements in Group 15

Although the C–C bond length in cyclopropane is short, N–N distances in diaziridines have been found to be much longer than in analogous acyclic compounds. Measuring such distances by electron diffraction is rarely easy, because overlap with similar distances in the radial distribution curve leads to strong correlation of distance parameters. Two studies, backed by quantum chemical calculations, have now provided further evidence for this phenomenon. In *N*,*N*-dimethyldiaziridine the N–N bond length refined to 151.4(6) pm,[16,17] which should be compared to 142.7(7) pm in the corresponding molecule with a four-membered ring, 1,2-dimethyl-1,2-diazetidine, and 141.9(11) pm in 1,2-dimethylhydrazine. In 6,6'-*bis*-(1,5-diazabicyclo[3.1.0]hexane), **1**, the N–N bonds are 151.1(2) pm long, and similar distances have also been reported in two crystal structures. In the dimethyldiaziridine the two methyl groups are on opposite sides of the ring, in accord with calculations at the B3LYP/6-311 ++ G** level, which indicate that the *trans* form is 38 kJ mol^{-1} lower in energy than the *cis* form. In the bis(bicyclohexane) derivative the six-membered rings adopt boat conformations (*i.e.* the three-membered rings are in *endo* positions relative to the folded five-membered rings), and the conformation about the central C–C bond is *anti*.

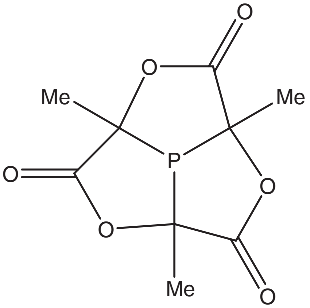


1

Many structures of nitrobenzenes have been reported in these reviews. They are permitted to masquerade as inorganic molecules by virtue of their N–O bonds. This year it is the turn of the *meta* and *para*-fluoronitrobenzenes.[18] The carbon-halogen bond lengths in all monohalonitrobenzenes have been computed and analysed. In general they are all shorter than in the parent halobenzenes, with the shortening greatest for the *ortho* isomers and least for the *meta* isomers. These patterns are largely obscured by the random noise in the experimentally determined bond lengths.

Five conformers of chloro(dimethyldithio)phosphite, $PCl(SCH_3)_2$, have been identified by Density Functional Theory (B3PW91/6-311+G*) and *ab initio* (MP2/6-31+G*) calculations.[19] The DFT method makes the *gauche*+, *gauche*-conformation with C_s symmetry the most stable, whereas MP2 favours an *anti*, *gauche*+ conformation. In each case there is a second form close in energy, so that a mixture would be expected in the gas phase. In practice, only the *anti*, *gauche*+ conformer was found in the analysis of the experimental data, although the possibility of the presence of up to 10% of the *anti*, *gauche*− form could not be excluded. The conformational preference is attributed to anomeric effects, involving donation of σ or π lone pairs of electrons on sulfur into antibonding orbitals of the opposite P–S or P–Cl bonds.

We have already alluded to the problems of dealing with very large-amplitude vibrations, which are modelled poorly by conventional methods, even allowing for curvilinear atomic motions. One way forward in such cases is to model these motions explicitly, and this has been done in a study of dimethylphenylphosphine.[20] The potential for internal rotation about the P–C(phenyl) bond was described by the function $V(\varphi) = 0.5V_2(1–\cos 2\varphi)$, where φ is the angle between the MePMe bisector and the ring plane. The constant V_2 refined to 1.6(16) kJ mol^{-1}, which tells us that the barrier to rotation is small, but not much else. However, a published plot of the potential, V, as a function of the angle φ rises to a maximum of well over 6 kJ mol^{-1}, so it is not clear what the situation really is.



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It is not often that one finds a name as long as all-*cis*-1,4,7-trimethyl-3,6,9-trioxa-10-phosphatricyclo[5,2,1,$0^{4,10}$]decane-2,5,8-trione in the world of electron diffraction, but the structure of this molecule has been determined.[21] It is more pithily described as the trilactone of phospha-tris(2-hydroxy-2-methylacetic acid), or more frequently in the paper itself as tris-γ-lactone **2**. It has C_3 symmetry, which makes its structure determination no more difficult than an equivalent molecule with just one ring, and it has sufficient vapour pressure to allow data collection at just 100°C. With many parameters to refine, a good fit to the experimental data should be expected (after all, they say that with enough parameters you can fit an elephant), but the authors make things appear worse than they really are, by (unusually) presenting the radial distribution curve as $r.f(r)$, which has the effect of enlarging the outer regions – and the associated difference curve. The most significant structural features are the near planarity of the three rings, and the small angles of 89.5° at the phosphorus atom.

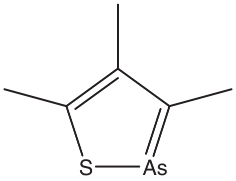
Two papers describe a new method for refining the structures of molecules containing bulky groups, for which assumptions about local symmetry may not be justified. The DYNAMic Interaction of Theory and Experiment (DYNAMITE) method was first applied to $OPBu^t_3$.[22] The principle is that the fine details of part of the structure are provided by a computational method (in this case molecular mechanics), and that they are continually updated during the course of the refinement, which is based on electron diffraction or other experimental data, backed as always by computed parameters. In this example, the *tert*-butyl groups were modelled by molecular mechanics, although the average C–H distance, CCH angle and torsional angles for the three symmetry-unrelated methyl groups were allowed to refine as normal. The remaining parameters describing the butyl groups (differences between C–H distances and between CCH angles, and between torsion angles within the methyl groups) were updated continually – not just between cycles of refinement, but during the calculation of derivatives for the least-squares refinement. In this way the asymmetry of the butyl groups is modelled more accurately, and consequential effects on parameters relating to the heavy atoms are eliminated. The outcome of the study was a structure in which the P=O distance was 149.5(6) pm, compared with 159.0(12) pm in an earlier study based on the same set of experimental data.

Having established the principles of the DYNAMITE method, it was then applied to a similar molecule, but one where the symmetry is lower, $HNPBu^t_3$.[23] In the original study it was assumed that the structure would be like that of $OPBu^t_3$, with three-fold local symmetry for the methyl groups, the *tert*-butyl groups, and the PBu^t_3 fragment. Such assumptions were no longer required, and it became clear that the hydrogen atom bonded to nitrogen has dramatic effects on the structure. The three different NPC angles were shown to cover a range of more than 12°, with values of 99.2(9)°, 110.9(7)° and 111.5(11)°, while the CPC angles ranged from 109.8 to 113.9°. Reflecting the consequences for the $OPBu^t_3$ structure, here the P=N distance refined to

158.7(4) pm, down from 165.2(11) pm in the original study, and again indicating the presence of a double bond, which can therefore be regarded as covalent rather than the ionic P^+–N^-.

Earlier in this review we described the structure of 1,1,2,2-tetra-*tert*-butyldisilane, which adopts a conformation in which two butyl groups are almost eclipsed. A similar circumstance has been observed for tetra-*tert*-butyldiphosphine,[24] but the presence of lone pairs of electrons on the phosphorus atoms, instead of hydrogen atoms on the silicon atoms, makes them much more flexible. In consequence the two different PPC angles at each of the phosphorus atoms differ by an enormous 20°, refining to 118.8(6) and 98.9(6)°. The third angle at phosphorus, CPC, sits nicely between these values, at 110.3(8)°. The P–P bond is a little long, at 226.4(8) pm, and the dissociation energy was computed to be correspondingly small, 150.6 kJ mol^{-1}. However, detailed calculations on the dissociation process revealed that the intrinsic P–P bond energy, 258.2 kJ mol^{-1}, is normal for a diphosphine. The DYNAMITE method was used in this analysis, and made it possible to allow for the large deformations within the *tert*-butyl groups.

The standard dissociation enthalpy of diphosphines can be reduced even more dramatically if the fragments formed on dissociation have large reorganisation energies. This is the case for $\{P[N(SiMe_3)_2](NPr^i{}_2)\}_2$, for which the intrinsic P–P bond energy has been calculated to be 286 kJ mol^{-1}, but the enthalpy for dissociation into $P[N(SiMe_3)_2](NPr^i{}_2)$ radicals is only 54 kJ mol^{-1}.[25] The highly disordered structure of the diphosphine has been determined by X-ray crystallography, and the structure of the radical in the gas phase by electron diffraction. It is a tricky subject for both computational and experimental methods. The radial distribution curve has a huge, broad peak stretching from 350 to 800 pm, with rather few distinctive features, representing hundreds of different interatomic distances. In the theoretical study conformations that were minima on the potential energy curve were first identified at the low HF/3-21G* level. Geometry optimisations followed at B3LYP/3-21G* and B3LYP/6-31+G* levels, and finally at MP2/6-31+G*, with only the valence orbitals active. Eventually it was shown that there was probably only one conformer significantly present in the gas phase, with the next one more than 13 kJ mol^{-1} higher in energy. The structure could then be refined. Most computed parameters agreed well with experiment, including the NPN angle [99(2)°, calculated 102.1°], but the mean P–N bond length refined to 162(3) pm, much less than the calculated value of 173.8 pm. There was so satisfactory explanation for this discrepancy, but it was quite clear that any larger value resulted in a poor fit to the experimental data. The reorganisation on dissociation involved (i) narrowing of the NPN angle by more than 10°, (ii) a large decrease in the difference between the two PNSi angles, from 20 to 4°, (iii) a decrease in the average NSiC angle, and (iv) conformational changes, most notably rotation of the CNC plane by almost 90°, from perpendicular to the NPN plane to coplanar with it. Together, these substantial changes make possible the cleavage of the P–P bond, which is of itself just as strong as normal for a diphosphine.



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The equilibrium structure of 1,2-thiaarsol, **3**, has been determined.[26] Eight parameters were refined, the five ring bond lengths, two ring angles, and the mean C–H distance. Vibrational corrections were taken from *ab initio* calculations, and it was shown that, although geometrical parameters may vary substantially with the level of theory and size of basis set, the differences in the vibrational corrections are small and insignificant. Final equilibrium parameters included S-As 219.3(1), As–C 182.0(3) and S–C 170.2(3) pm. The standard deviation for the S–As distance is six times smaller than the difference between the r_e and r_a distances. At this level of precision, vibrational corrections are important.

5 Compounds of Elements in Group 16

The structures and conformations of three fluorinated derivatives of dimethyl ether, CH_2FOCH_2F, CHF_2OCHF_2 and CF_3OCHF_2, have been determined.[27] The most stable conformer of CH_2FOCH_2F has C_2 symmetry, with the COCF dihedral angles 70(2)°, *i.e.* with the CH_2F groups both having *synclinal* orientation. It is possible that there could also be up to 14% of the other conformer with two *synclinal* CH_2F groups, *i.e.* the one in which the two fluorine atoms are on the same side of the COC plane, and with molecular C_s symmetry. In the case of CHF_2OCHF_2 the terms used to describe the conformers relate to the C–H bonds, so one needs the think carefully about the positions of the fluorine atoms. The most abundant [82(8)%] conformer is *antiperiplanar, synperiplanar*, with one C–H bond almost eclipsing the further O–C bond [dihedral angle COCH 18(2)°] and one in exactly the opposite position. In CF_3OCHF_2 the one CHF_2 group is oriented *antiperiplanar*, with the dihedral angle COCH 19(3)°. The eclipsed conformations of some groups may be seen as counter-intuitive, but natural bond orbital analysis shows that anomeric effects may stabilise some eclipsed conformers, although steric effects counter the anomeric stabilisation in some situations.

The structure of 4-fluoro(trifluoromethoxy)benzene has been determined independently in two laboratories.[28] They agree that the dominant conformer has the O–C bond to the trifluoro group perpendicular to the ring plane, and that there may be a little of the conformer in which this bond lies in the ring plane. How little is more debatable: one study gives an upper limit of 13%, whereas the limit is 25% in the other study. A matrix-isolation infra-red experiment indicates that only one conformer is present in the neon matrix at 15 K, while computational methods indicate that the planar conformation is either a transition state, or at most a very shallow minimum.

A single conformer of trifluoroacetic anhydride, $CF_3C(O)OC(O)CF_3$, is indicated by the analysis of gas electron diffraction data, but there is some doubt about the precise structure of this conformer.[29] The two C=O bonds have the *synperiplanar* orientation, but it is not possible to say whether the equilibrium structure is planar, with C_{2v} symmetry, or distorted to C_2 symmetry. The refined effective dihedral angle C–O–C=O is 18(4)°, reasonably consistent with values of 16.5 and 13.9° given by MP2 and B3LYP calculations with the 6-31G* basis set.

Trifluoromethyl chloroformate, $ClC(O)OCF_3$, exists in the conformation in which the O–CF_3 bond is *synperiplanar* with respect to the C=O bond, with C_s symmetry,[30] but neither calculated nor experimental OCOC dihedral angles are given in the paper. Although the *anti* form can be observed in infra-red spectra of the compound isolated from heated samples into frozen matrices, it is estimated that there is less than 1% of this form in the gas at room temperature.

The *syn* conformation, *i.e.* with the S–CH_3 bond eclipsing C=O, has also been observed for *S*-methyl thioacetate, $CH_3C(O)SCH_3$.[31] The *anti* conformer is also a minimum on the computed potential-energy curve, but at about 20 kJ mol^{-1} higher in energy than the *syn* form, its abundance is negligible at room temperature, and it has not been observed, even by sensitive methods such as infra-red spectroscopy of matrix-isolated samples. Factors affecting the relative stabilities of the conformers of this and related compounds are discussed. In the present case there both steric and electronic factors working in favour of the *syn* form.

In perfluorodimethyloxalate, $CF_3OC(O)C(O)OCF_3$, the conformation about three bonds must be considered. B3LYP/6-31++G(2df) calculations showed that the CF_3 groups are *synperiplanar* with respect to the C=O bonds, with an *antiperiplanar* form more than 35 kJ mol^{-1} higher in energy.[32] That reduces the conformational problem to the central C–C bond. Calculations indicated that two conformations are possible, with the O=C–C=O dihedral angle equal to 0° (*syn*, C_{2v} symmetry) or 180° (*anti*, C_{2h} symmetry). The energy difference was given as 2.8 kJ mol^{-1} by the B3LYP method, and 1.8 kJ mol^{-1} using MP2/6-31G*. The experimental distribution of 58(12)% *antiperiplanar* to 42% *synperiplanar* corresponds to $\Delta G^0 = 0.8(16)$ kJ mol^{-1}. Note the '*periplanar*' part of the descriptions of the experimental structures. Neither of them is exactly planar. The refined O=C–C=O dihedral angles are 144(5) and 26(8)°, substantial deviations from the computed planar arrangements. In the crystalline phase there are four independent molecules, all *antiperiplanar*, but the dihedral angles are not given.

Conformations about two bonds must be considered for fluorocarbonyl trifluoromethanesulfonate, $FC(O)OSO_2CF_3$.[33] There are two different arrangements of the FC(O) groups relative to the CF_3 group, *trans* [67(8%)] and *gauche*, with the CSOC dihedral angle 72(6)°. In both of these the C=O bond is orientated *synperiplanar* with respect to the O–S single bond. This distribution corresponds to $\Delta G^0 = 2.1$ kJ mol^{-1}, rather less than calculated (between 3.1 and 3.9 kJ mol^{-1}, depending on the computational method). In the crystalline phase the molecules are exclusively *trans*. The predominance of the *trans* form, confirmed by infra-red spectroscopy, has thus been recorded for the first time in a sulfonate. A natural bond orbital analysis does not provide a straightforward rationalisation of this observation, and it is thought that (unquantified) steric factors may be responsible.

With pentafluorosulfur fluorosulfonate, SF_5OSO_2F, there is only one significant conformational question. Where is the SF_5 group relative to the other S–F bond? *Gauche*.[34] Mainly. Maybe with just a little *trans*. Calculations indicate that ΔG^0 for the *gauche*-*trans* change is 8–9 kJ mol^{-1}. They also show that in the *gauche* form the SF_5 group is staggered with respect to the O–SO_2F bond, whereas it is eclipsed in the *trans* conformation. The experimental data are consistent with this, but do not prove it. The experiments put an upper limit of 10% on the abundance of the *trans* conformer, consistent with the computed abundance of 4%.

6 Compounds of Transition Elements and Lanthanides

Lanthanide trihalides always seem to feature in these reviews. There are a lot of them, and they have been the subjects of repeated study. A new paper has 18 references describing computational and/or experimental work on lanthanum trichloride and 11 relating to lanthanum tribromide.[35] The problem is that the potentials for out-of-plane bending are extremely flat. One consequence of this is that some computational methods place the minimum at the perfectly planar position (D_{3h} symmetry), whereas others lead to slightly non-planar equilibrium structures (C_{3v} symmetry), albeit often with the ground vibrational level lying above the potential maximum corresponding to the planar structure. The second consequence is that the vibrationally averaged structure determined by electron diffraction is substantially pyramidal, typically with angles between two lanthanum-halogen bonds of about 115°. In the latest work, for which new experimental data were collected (at two different temperatures in the case of $LaBr_3$), the thermal-average ClLaCl angle in $LaCl_3$ at 1295 K refined to 116.7(12)°, while the BrLaBr angle in $LaBr_3$ was 115.7(11)° at 1095 K and 114.8(11)° at 1180 K. However, after applying shrinkage corrections, the $<_\alpha$ values were 120° in each case.

Despite the impressive list of references to the structures of $LaCl_3$ and $LaBr_3$, praseodymium and holmium tribromides have not until now been the subjects of electron diffraction studies. That has now been put right, using data collected at 1100 and 991 K respectively.[36] The thermal average BrPrBr and BrHoBr angles are 114.7(10) and 115.3(11)° respectively. It is said that 'given the low deformation vibration frequencies of lanthanide tribromide molecules, the insignificant pyramidality of the r_g configuration may correspond to the planar equilibrium geometry of D_{3h} symmetry for the molecules'. That can be paraphrased as 'We think it is flat.' With the angles roughly midway between those of planar and regular tetrahedral structures, the pyramidality perhaps has more significance than it is credited with. It is indeed possible that the equilibrium structures are planar, but a more objective demonstration of this would have been welcome. There is also reference to equilibrium Pr–Br and Ho–Br bond lengths in a table, but the values do not appear in that table, or anywhere else. However, it is noted that the experimental distances are 7 pm greater than those calculated by a multiconfiguration interaction technique with effective core potentials, and that more effective quantum mechanical methods to describe lanthanide halide structures are needed.

Metal β-diketonates have also been featured in these reviews for many years, and this year it is the turn of tris(dipivaloylmethanato)lutetium,[37] where the ligand is also known as 2,2,6,6-tetramethyl-heptane-3,5-dionato), or less precisely, but more comprehensibly, as acetylacetonato with the methyl groups replaced by *tert*-butyl groups. The molecule has D_3 symmetry, with the ligand rings planar, *i.e.* not folded along the O . . . O axes. The ligands therefore have C_{2v} local symmetry, and they are twisted 22.1(22)° away from the positions in which the molecule has a trigonal prismatic structure, with D_{3h} symmetry. DFT methods consistently overestimate the Lu–O bond length, which refined to 219.7(6) pm (r_{h1}), by about 4 pm, but there is excellent agreement between bond length parameters in the gas phase and those measured in the crystalline phase, although the molecules in the crystal have the trigonal prismatic structure. Computational methods all give the D_3 structure, with the twist angle of the ligands close to the experimental value. The gas-phase molecule, and probably all other lanthanide β-diketonate complexes, are thus consistent with a model proposed by Kepert, in which ligands distribute themselves on a unit sphere, so that interactions between adjacent ligands are minimised.

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