

PUBLICATIONS: W. CLEGG 1997

- 510.** Crystal structure determination and *ab initio* molecular structure prediction for *exo,exo*- α -P₄Se₃(CN)₂, the first phosphorus selenide cyanide
 B. W. Tattershall, E. L. Sandham and W. Clegg.
J. Chem. Soc. Dalton Trans. 1997, 81–87.
- 511.** Macropolyhedral boron-containing cluster chemistry: isolation and characterization of twenty-one-vertex [(PM₂Ph)₃HReB₂₀H₁₅Ph(PHMe₂)]
 P. Kaur, S. D. Perera, T. Jelínek, B. Štíbir, J. D. Kennedy, W. Clegg and M. Thornton-Pett.
Chem. Commun. 1997, 217–218.
- 512.** Facilitation of displacements at the 6-position of purines by the use of 1,4-diazabicyclo[2.2.2]octane as leaving group
 N. K. Lembicz, S. Grant, W. Clegg, R. J. Griffin, S. L. Heath and B. T. Golding.
J. Chem. Soc. Perkin Trans. 1 1997, 185–186.
- 513.** Effects of metal-centre orbital control on cluster character and electron distribution between borane and hydrocarbon ligands; significance of the structures of [μ -9, 10-(SMe)-8, 8-(PPh₃)₂-*nido*-8, 7-IrSB₉H₉] and μ -9, 10-(SMe)-8-(η^4 -C₅Me₅H)-*nido*-8, 7-RhSB₉H₉]
 R. Macías, J. Holub, J. D. Kennedy, B. Štíbir, M. Thornton-Pett and W. Clegg.
J. Chem. Soc. Dalton Trans. 1997, 149–151.
- 514.** Synthesis and characterization of rhodium(I) boryl and rhodium(III) tris(boryl) compounds: molecular structures of [(PM₃)₄Rh(B(cat))] and *fac*-[(PM₃)₃Rh(B(cat))₃] (cat = 1, 2-O₂C₆H₄)
 C. Dai, G. Stringer, T. B. Marder, A. J. Scott, W. Clegg and N. C. Norman.
Inorg. Chem. 1997, **36**, 272–273.
- 515.** Unexpected structure of 1,3-diphenyl-2-azaallylpotassium-*N,N,N',N''*-pentamethyldiethylene-triamine: infinite, zigzag chains of alternating cations and two distinct types of anion, one azaallyl bonded, the other allyl bonded
 P. C. Andrews, D. R. Armstrong, W. Clegg, F. J. Craig, L. Dunbar and R. E. Mulvey.
Chem. Commun. 1997, 319–320.
- 516.** New reaction pathways for μ - η^1 , η^2 -allenyl ligands: on–off allenyl coordination and CO insertion into the hydrocarbyl bridge in Ru₂(CO)₆(μ -PPh₂) $\{\mu$ - η^1 , $\eta^2_{\alpha,\beta}$ -C(Ph)=C=CPh₂ $\}$
 P. Blenkiron, J. F. Corrigan, N. J. Taylor, A. J. Carty, S. Doherty, M. R. J. Elsegood and W. Clegg.
Organometallics 1997, **16**, 297–300.
- 517.** Lewis-base adducts of the diborane(4) compounds B₂(1, 2-E₂C₆H₄)₂ (E = O or S)
 W. Clegg, C. Dai, F. J. Lawlor, T. B. Marder, P. Nguyen, N. C. Norman, N. L. Pickett, W. P. Power and A. J. Scott.
J. Chem. Soc. Dalton Trans. 1997, 839–846.
- 518.** Nucleophilic addition of alcohols to [Fe₂(CO)₆(μ -PPh₂) $\{\mu$ - η^1 : $\eta^2_{\alpha\beta}$ -(R)C _{α} =C _{β} =C _{γ} H₂ $\}$] (R = H, Ph): generation of the binuclear β , γ -unsaturated esters [Fe₂(CO)₅(μ -PPh₂) $(\mu$ - η^1 (O): η^1 (C): η^2 (C)-{R¹O(O)CCH₂}C=CH₂]⁺ (R¹ = Me, Et, ⁱPr)
 S. Doherty, M. R. J. Elsegood, W. Clegg and D. Mampe.
Organometallics 1997, **16**, 1186–1192.
- 519.** A tetracyclic benzimidazole derivative of Kemp's triacid
 C. J. Matthews, S. L. Heath, W. Clegg and J. C. Lockhart.
J. Chem. Soc. Perkin Trans. 2 1997, 665–666.

- 520.** Lithiated amidines: syntheses and structural characterisations
 J. Barker, D. Barr, N. D. R. Barnett, W. Clegg, I. Cragg-Hine, M. G. Davidson, R. P. Davies, S. M. Hodgson, J. A. K. Howard, M. Kilner, C. W. Lehmann, I. Lopez-Solera, R. E. Mulvey, P. R. Raithby and R. Snaith.
J. Chem. Soc. Dalton Trans. 1997, 951–955.
- 521.** Neutral [2]catenanes from oxidative coupling of π -stacked components
 D. G. Hamilton, J. K. M. Sanders, J. E. Davies, W. Clegg and S. J. Teat.
Chem. Commun. 1997, 897–898.
- 522.** Isolation and structural characterization of novel compounds containing B_4O_2 rings
 C. J. Carmalt, W. Clegg, A. H. Cowley, F. J. Lawlor, T. B. Marder, N. C. Norman, C. R. Rice, O. J. Sandoval and A. J. Scott.
Polyhedron 1997, **13**, 2325–2328.
- 523.** “Potassium potassates” based on dihydrotriazinide ligands: syntheses, crystal structures, and comparison with other alkali metal dihydrotriazinide compounds
 W. Clegg, M. R. J. Elsegood, L. Horsburgh, R. E. Mulvey and M. J. Ross.
Chem. Ber. 1997, **130**, 621–631.
- 524.** Preparation, structure and properties of trinuclear $[M_3Se_4(CN)_9]^{5-}$ ($M = Mo$ or W) complexes obtained from M_3Se_7 core compounds and related studies
 V. P. Fedin, G. J. Lamprecht, T. Kohzuma, W. Clegg, M. R. J. Elsegood and A. G. Sykes.
J. Chem. Soc. Dalton Trans. 1997, 1747–1751.
- 525.** Diborane(4) compounds and transition metal catalysed diboration reactions
 W. Clegg, C. Dai, F. J. Lawlor, G. Lesley, T. B. Marder, P. Nguyen, N. C. Norman, N. L. Pickett, C. R. Rice, E. G. Robins, A. J. Scott and N. J. Taylor.
Advances in Boron Chemistry, ed. W. Siebert, Royal Society of Chemistry, Cambridge 1997, 389–392.
- 526.** Benzyltrimethylammonium tetramethoxoborate
 W. Clegg, R. J. Errington and C. J. Carmalt.
Acta Cryst. 1997, **C53**, 751–753.
- 527.** *N*-(2,3,5,6-Tetrachloropyrid-4-yl)cinnamide
 W. Clegg, M. R. J. Elsegood, R. F. W. Jackson, J. L. Fraser and L. J. Emsden.
Acta Cryst. 1997, **C53**, 797–799.
- 528.** Macropolyhedral boron-containing cluster chemistry. Assessment of the possibilities of thermolytic mixed-cluster fusion, and of the use of synchrotron X-radiation for the examination of small single crystals of metallaboranes. Isolation and structure of eighteen-vertex $[7-(CO)-7,7-(PMMe_3)_2-syn-7-IrB_{17}H_{20}]$
 J. Bould, W. Clegg, J. D. Kennedy, S. J. Teat and M. Thornton-Pett.
J. Chem. Soc. Dalton Trans. 1997, 2005–2007.
- 529.** Preparation, structure and reactivity of the di- μ -disulfido Nb^{IV}_2 aqua ion $[Nb_2(\mu-S_2)_2(H_2O)_8]^{4+}$, the structure of $[Nb_2(\mu-S_2)_2(NCS)_8]^{4-}$, and properties of the related $(\mu-S)_2$ aqua ion
 M. N. Sokolov, R. Hernandez-Molina, M. R. J. Elsegood, S. L. Heath, W. Clegg and A. G. Sykes.
J. Chem. Soc. Dalton Trans. 1997, 2059–2065.
- 530.** Mixed aggregation between lithium diisopropylamide and lithium chloride: NMR, solid-state structure and *ab initio* calculations
 W. Clegg, J. C. Greer, J. M. Hayes, F. S. Mair, P. M. Nolan and P. A. O’Neil.
Inorg. Chim. Acta 1997, **258**, 1–9.

- 531.** Synthesis and structural characterization of some novel metallocboroxides bearing boron-bound mesityl and fluoromesityl substituents: the molecular structure of the first metallaboroxane complex
 V. C. Gibson, C. Redshaw, W. Clegg and M. R. J. Elsegood.
Polyhedron 1997, **16**, 2637–2641.
- 532.** Exploiting a substituted dihydrotriazinide as a novel bulky ligand: synthesis and crystal structure of a rubidium complex with an unprecedented tetrameric cyclic core
 W. Clegg, A. M. Drummond, R. E. Mulvey and P. O'Shaughnessy.
Chem. Commun. 1997, 1301–1302.
- 533.** Addition of organolithium nucleophiles to the diiron allenyl complex $[\text{Fe}_2(\text{CO})_6(\mu\text{-PPPh}_2)\{\mu\text{-}\eta^1\text{:}\eta^2_{\alpha,\beta}\text{-(H)C}_\alpha=\text{C}_\beta=\text{C}_\gamma\text{H}_2\}]$: synthesis and characterization of organodiiron-coordinated β, γ -unsaturated ketones
 S. Doherty, M. R. J. Elsegood, W. Clegg, N. H. Rees, T. H. Scanlan and M. Waugh.
Organometallics 1997, **16**, 3221–3228.
- 534.** Can alkali-metal ions influence the coordination and reactivity of calix[4]arenes at transition-metal centres?
 V. C. Gibson, C. Redshaw, W. Clegg and M. R. J. Elsegood.
Chem. Commun. 1997, 1605–1606.
- 535.** Evidence for directed metalation: a structural intermediate in the formation of a novel C-bound adenine complex of ruthenium
 C. Price, M. R. J. Elsegood, W. Clegg, N. H. Rees and A. Houlton.
Angew. Chem. Internat. Edit. Engl. 1997, **36**, 1762–1764.
- 536.** 5-(*o*-Chlorophenyl)-1,3-dithia-2,4-diazolylium hexafluoroarsenate
 W. Clegg, M. R. J. Elsegood, A. J. Banister and T. G. Hibbert.
Acta Cryst. 1997, **C53**, 1208–1211.
- 537.** A new high-flux chemical and materials crystallography station at the SRS Daresbury. 1. Design, construction and test results.
 R. J. Cernik, W. Clegg, C. R. A. Catlow, G. Bushnell-Wye, J. V. Flaherty, G. N. Greaves, I. Burrows, D. J. Taylor, S. J. Teat and M. Hamichi.
J. Synchrotron Rad. 1997, **4**, 279–286.
- 538.** Practical aspects of structure refinement
 W. Clegg.
B. C. A. Intensive School, Durham University 1997, unnumbered pages.
- 539.** Synthesis and characterisation of molybdenum complexes bearing highly functionalised imido substituents
 V. C. Gibson, C. Redshaw, W. Clegg and M. R. J. Elsegood.
J. Chem. Soc. Dalton Trans. 1997, 3207–3212.
- 540.** Pentamethylcyclopentadienyl tungsten complexes containing imido, hydrazido and amino acid derived N—O chelate ligands
 C. Redshaw, V. C. Gibson, W. Clegg, A. J. Edwards and B. Miles.
J. Chem. Soc. Dalton Trans. 1997, 3343–3347.
- 541.** Reaction of phosphites with the electrophilic allenyl complex $[\text{Fe}_2(\text{CO})_6(\mu\text{-PPPh}_2)\{\mu\text{-}\eta^1\text{:}\eta^2\text{-(H)C}_\alpha=\text{C}_\beta=\text{C}_\gamma\text{H}_2\}]$: stepwise transformation of a $\mu\text{-}\eta^1\text{:}\eta^2$ -allenyl into a $\mu\text{-}\eta^1\text{:}\eta^2$ -acetylide *vs* phosphite activation
 S. Doherty, M. R. J. Elsegood, W. Clegg, M. F. Ward and M. Waugh.
Organometallics 1997, **16**, 4251–4253.

- 542.** Reaction of thiophenol with glucal epoxides: X-ray structure of 3,4,6-tri-O-tert-butyldimethylsilyl-1-S-phenyl-1-thio- α -D-glucopyranoside
 C. Walford, R. F. W. Jackson, N. H. Rees, W. Clegg and S. L. Heath.
Chem. Commun. 1997, 1855–1856.
- 543.** Organometallic compounds of the alkali metals with phenylsilyl substituents at the carbanionic center. Crystal structures of $\text{LiC}(\text{SiMe}_3)_2(\text{SiMe}_2\text{Ph})\cdot\text{Et}_2\text{O}$, $\text{NaC}(\text{SiMe}_3)_2(\text{SiMe}_2\text{Ph})\cdot\text{TMEDA}$, $\text{NaC}(\text{SiMe}_3)(\text{SiMe}_2\text{Ph})_2\cdot\text{TMEDA}$, $\text{RbC}(\text{SiMe}_2\text{Ph})_3$, and $\text{CsC}(\text{SiMe}_2\text{Ph})_3$ (TMEDA = tetramethylethylenediamine)
 C. Eaborn, W. Clegg, P. B. Hitchcock, M. Hopman, K. Izod, P. O'Shaughnessy and J. D. Smith.
Organometallics 1997, **16**, 4728–4736.
- 544.** Synthesis and structure of bis(methylaluminium.NCCH₃)-*p*-tert-butylcalix[4]arene
 V. C. Gibson, C. Redshaw, W. Clegg and M. R. J. Elsegood.
Polyhedron 1997, **16**, 4385–4387.
- 545.** Theoretical, structural and NMR studies of fluxionality in thiolato-bridged platinum(II)-platinum(IV) dinuclear complexes
 N. Duran, P. González-Duarte, A. Lledós, T. Tarella, J. Sola, G. Ujaque, W. Clegg and K. A. Fraser.
Inorg. Chim. Acta 1997, **265**, 89–102.
- 546.** 4,4'-Dimethoxytrityl and 4,4',4''-trimethoxytrityl as protecting groups for amino functions; selectivity for primary amino groups and application in ¹⁵N-labelling
 A. P. Henderson, J. Riseborough, C. Bleasdale, W. Clegg, M. R. J. Elsegood and B. T. Golding.
J. Chem. Soc. Perkin Trans. 1 1997, 3407–3413.
- 547.** An unusual rearrangement of isoxazoles to 2-alkenoylpyrroles or 1-azafulvenes
 A. R. Al Dulayymi, M. S. Baird and W. Clegg.
Tet. Letters 1997, **38**, 8271–8274.
- 548.** Mercury(II) halide adducts of esters of 2-pyridinecarboxylic acid. Crystal structures and structural variations within the series [HgCl₂(C₅H₄NCOOR)], R = Me, Et, Prⁿ, Prⁱ
 A. Álvarez-Larena, W. Clegg, L. Cucurull-Sánchez, P. González-Duarte, R. March, J. F. Piniella, J. Pons and X. Solans.
Inorg. Chim. Acta 1997, **266**, 81–90.
- 549.** The first structurally authenticated σ -bonded organosamarium(II) derivative and its reaction with benzophenone
 W. Clegg, C. Eaborn, K. Izod, P. O'Shaughnessy and J. D. Smith.
Angew. Chem. Internat. Edit. Engl. 1997, **36**, 2815–2817.
- 550.** Solid state structures and dynamic solution equilibria of bis(dibenzylamido)magnesium complexes: aggregation dependence on stoichiometry and denticity of donor solvent
 W. Clegg, F. J. Craig, K. W. Henderson, A. R. Kennedy, R. E. Mulvey, P. A. O'Neil and D. Reed.
Inorg. Chem. 1997, **36**, 6238–6246.
- 551.** Modelling the dioldehydratase reaction
 B. Köhler, M. Knauer, W. Clegg, M. R. J. Elsegood, B. T. Golding and J. Rétey.
Bioinorganic Chemistry: Transition Metals in Biology and their Coordination Chemistry, ed. A. X. Trautwein, Wiley-VCH, Weinheim 1997, 505–519.