

Prof. Dr. David W. H. Rankin

University of Edinburgh

School of Chemistry

West Mains Road

Edinburgh EH9 3JJ

U. K.

Telephone: (+44) 131 650 4728

Telefax: (+44) 131 650 6453

E-Mail: d.w.h.rankin@ed.ac.uk

Homepage: <http://www.ged.chem.ed.ac.uk/>

BrNa NaBr	Sodium bromide Structure by ED and <i>ab initio</i> calculations P. D. McCaffrey, D. A. Wann, R. J. Mawhorter and D. W. H. Rankin Manuscript in preparation.
Br₂Na₂ Na ₂ Br ₂	Sodium bromide dimer Structure by ED and <i>ab initio</i> calculations P. D. McCaffrey, D. A. Wann, R. J. Mawhorter and D. W. H. Rankin Manuscript in preparation.
C₂H₃AsCl₂ CH ₂ CHAsCl ₂	Vinyldichloroarsine Structure by ED and computational methods R. Noble-Eddy, S. L. Masters, D. W. H. Rankin, H. E. Robertson and J.-C. Guillemin <i>J. Mol. Struct.</i> 978 (2010), 36
C₂H₄O₄S₂ O ₂ -cyclo-S(CH ₂) ₂ S-O ₂	1,3-Dithietane-1,1,3,3-tetraoxide Structure by ED and <i>ab initio</i> calculations D. A. Wann, H. E. Robertson, E. Block and D. W. H. Rankin Manuscript in preparation.
C₂H₅As CH ₂ CHAsH ₂	Vinylarsine Structure by ED and computational methods R. Noble-Eddy, S. L. Masters, D. W. H. Rankin, H. E. Robertson and J.-C. Guillemin <i>J. Mol. Struct.</i> 978 (2010), 36
C₃H₆Cl₃N N(CH ₂ Cl) ₃	Tris(chloromethyl)amine Structure by ED and computational methods N. W. Mitzel, J. T. Schirlin, S. L. Masters, D. W. H. Rankin et al. Manuscript in preparation.
C₄H₅F₃OS CF ₃ COSCH ₂ CH ₃	Ethyl trifluorothioacetate Structure and conformation by ED, <i>ab initio</i> calculations and vibrational spectroscopy M. E. Defonsi Lestard, M. E. Tuttolomondo, D. A. Wann, H. E. Robertson, D. W. H. Rankin and A. Ben Altabef <i>J. Chem. Phys.</i> 131 (2010), 214303
C₄H₉F₃O₂Si (CH ₃) ₃ SiOC(O)CF ₃	Trimethylsilyl trifluoroacetate Vibrational spectra and structure by ED and <i>ab initio</i> calculations M. E. Defonsi Lestard, M. E. Tuttolomondo, E. L. Varetti, D. A. Wann, H. E. Robertson, D. W. H. Rankin and A. Ben Altabef <i>J. Mol. Struct.</i> 978 (2010), 114
C₄H₉F₃O₃SSI (CH ₃) ₃ SiSO ₂ OCF ₃	Trimethylsilyl trifluoromethanesulfonate Vibrational spectra and structure by ED and <i>ab initio</i> calculations M. E. Defonsi Lestard, M. E. Tuttolomondo, E. L. Varetti, D. A. Wann, H. E. Robertson, D. W. H. Rankin and A. Ben Altabef <i>J. Mol. Struct.</i> 984 (2010), 376
C₄H₁₀Cl₂Si	Diethyldichlorosilane Structure and conformations by ED, IR and Raman spectroscopies and quantum chemical calculations

<chem>Si(CH2CH3)2Cl2</chem>	M. Montejo, D. A. Wann, P. G. Rodríguez Ortega, H. E. Robertson, F. Márquez, D. W. H. Rankin and J. J. López González <i>J. Raman Spectrosc.</i> 41 (2010), 1323
<chem>C5H9P</chem> ButCP	tert-Butylphosphaethyne Structure by ED and <i>ab initio</i> calculations D. A. Wann, S. L. Masters, H. E. Robertson, M. Green, R. J. Kilby, C. A. Russell, C. Jones and D. W. H. Rankin Manuscript submitted.
<chem>C6HCl5</chem> <chem>C6HCl5</chem>	Pentachlorobenzene Structure by ED and liquid crystal NMR spectroscopy R. Blom, D. A. Wann, D. W. H. Rankin et al. Manuscript in preparation.
<chem>C6H2Cl4</chem> <chem>1,2,3,4-C6H2Cl4</chem>	1,2,3,4-Tetrachlorobenzene Structure by ED and liquid crystal NMR spectroscopy R. Blom, D. A. Wann, D. W. H. Rankin et al. Manuscript in preparation.
<chem>C6H4BrF</chem> <chem>C6H4BrF</chem>	1-Bromo-4-fluorobenzene Structure by ED, liquid crystal NMR spectroscopy and <i>ab initio</i> calculations S. L. Masters, I. D. Mackie, D. A. Wann, H. E. Robertson, D. W. H. Rankin and S. Parsons <i>Struct. Chem.</i> , in press.
<chem>C6H4ClF</chem> <chem>C6H4ClF</chem>	1-Chloro-4-fluorobenzene Structure by ED, liquid crystal NMR spectroscopy, <i>ab initio</i> calculations and X-ray diffraction S. L. Masters, I. D. Mackie, D. A. Wann, H. E. Robertson, D. W. H. Rankin and S. Parsons <i>Struct. Chem.</i> , in press.
<chem>C6H4F2</chem> <chem>1,2-C6H4F2</chem>	1,2-Difluorobenzene Structure by ED and liquid crystal NMR spectroscopy E. M. Brown, D. A. Wann and D. W. H. Rankin <i>J. Mol. Struct.</i> 984 (2010), 102
<chem>C6H4F2</chem> <chem>C6H4F2</chem>	1,3-Difluorobenzene Structure by ED and liquid crystal NMR spectroscopy E. M. Brown, D. A. Wann and D. W. H. Rankin <i>J. Mol. Struct.</i> 984 (2010), 102
<chem>C6H12F6Si2</chem> <chem>CF3Me2SiSiMe2CF3</chem>	1,2-Trifluoromethyl-1,1,2,2-tetramethylsilane Structure by ED, X-ray diffraction and <i>ab initio</i> calculations, interpretation of Raman spectra S. L. Masters, D. A. Wann, H. E. Robertson, F. Lennox, D. W. H. Rankin, I. Arnason, K. Hassler et al. Manuscript in preparation.
<chem>C7F14</chem> <chem>C6F11CF3</chem>	Perfluoromethylcyclohexane Structure by ED and <i>ab initio</i> calculations G. R. Kafka, S. L. Masters, D. A. Wann, H. E. Robertson and D. W. H. Rankin <i>J. Phys. Chem. A</i> 114 (2010), 11022
<chem>C7H16Cl3PSi</chem> <chem>(tBu)(iPr)PSiCl3</chem>	(tert-Butyl)(iso-propyl)(trichlorosilyl)phosphine Structure by ED and <i>ab initio</i> calculations E. Seppälä, W.-W. du Mont, S. L. Masters, D. W. H. Rankin and H. E. Robertson Manuscript in preparation.
<chem>C9H24Br4Si4</chem> <chem>C(SiMe2Br)4</chem>	Tetrakis(bromodimethylsilyl)methane Structure by ED and computational methods K. Bätz, G. R. Kafka, D. A. Wann, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin

	Manuscript in preparation.
$C_9H_{24}Cl_4Si_4$ $C(SiMe_2Cl)_4$	Tetrakis(chlorodimethylsilyl)methane Structure by ED and computational methods K. Bätz, G. R. Kafka, D. A. Wann, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin Manuscript in preparation.
$C_9H_{24}F_4Si_4$ $C(SiMe_2F)_4$	Tetrakis(fluorodimethylsilyl)methane Structure by ED and computational methods K. Bätz, G. R. Kafka, D. A. Wann, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin Manuscript in preparation.
$C_9H_{28}Si_4$ $C(SiMe_2H)_4$	Tetrakis(dimethylsilyl)methane Structure by ED and computational methods K. Bätz, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin Manuscript in preparation.
$C_{10}H_{17}P$ $C_{10}H_{15}PH_2$	Adamantylphosphine Structure by ED and <i>ab initio</i> calculations D. A. Wann, A. R. Turner, J. R. Goerlich, L. J. Kettle, R. Schmutzler and D. W. H. Rankin Struct. Chem., in press.
$C_{10}H_{20}N_2$ ButN=CHCH=NBut	N,N'-Di-tert-butyl-1,4-diaza-1,3-butadiene Structure by ED and computational methods C. Jones, D. A. Wann, H. E. Robertson and D. W. H. Rankin Manuscript in preparation.
$C_{10}H_{26}Ga_2O_4$ [Me ₂ Ga(OCH ₂ CH ₂ OMe)] ₂	Di-μ-ethoxydiethoxydimethyldigallium Structure by ED and <i>ab initio</i> calculations D. A. Wann, C. E. Knapp, J. T. Schirlin, H. E. Robertson, S. L. Masters, C. J. Carmalt and D. W. H. Rankin Manuscript in preparation.
$C_{10}H_{30}Si_4$ (Me ₃ Si) ₃ CSiH ₃	(Silyl)tris(trimethylsilyl)methane Structure by ED and computational methods S. L. Masters, D. W. H. Rankin, D. B. Cordes, K. Bätz, P. D. Lickiss, N. M. Boag, A. D. Redhouse and S. M. Whittaker Dalton Trans. 39 (2010), 9353
$C_{11}H_{30}Br_2Si_4$ $C(SiMe_3)_2(SiMe_2Br)_2$	Bis(bromodimethylsilyl)bis(trimethylsilyl)methane Structure by ED and computational methods K. Bätz, D. A. Wann, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin Manuscript in preparation.
$C_{11}H_{30}Cl_2Si_4$ (Me ₃ Si) ₂ C(SiClMe ₂) ₂	Bis(chlorodimethylsilyl)-bis(trimethylsilyl)methane Structure by ED and computational methods K. Bätz, D. A. Wann, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin Manuscript in preparation.
$C_{11}H_{32}Si_4$ $C(SiMe_3)_2(SiMe_2H)_2$	Bis(dimethylsilyl)bis(trimethylsilyl)methane Structure by ED and computational methods K. Bätz, D. A. Wann, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin Manuscript in preparation.
$C_{12}Fe_3O_{12}$ $Fe_3(CO)_{12}$	Dodecacarbonyltriiron Structure by ED and <i>ab initio</i> calculations G. R. Kafka, S. L. Masters, D. W. H. Rankin et al. Manuscript in preparation.
$C_{12}H_{30}Ga_2O_2$	Di-μ-tert-butoxymethyldigallium Structure by ED and <i>ab initio</i> calculations

<chem>[Me2GaOtBu]2</chem>	D. A. Wann, C. E. Knapp, J. T. Schirlin, H. E. Robertson, S. L. Masters, C. J. Carmalt and D. W. H. Rankin Manuscript in preparation.
<chem>C16H24O12Si8</chem> <chem>Si8O12(CH=CH2)8</chem>	Octavinylsilsesquioxane Structure by ED and <i>ab initio</i> calculations D. A. Wann, C. N. Dickson, P. D. Lickiss, H. E. Robertson and D. W. H. Rankin Manuscript submitted.
<chem>C24H72O20Si16</chem> <chem>Si8O12(OSiMe3)8</chem>	Octakis(trimethylsiloxy)octasilsesquioxane Structure by ED and <i>ab initio</i> calculations D. A. Wann, C. N. Dickson, P. D. Lickiss, H. E. Robertson and D. W. H. Rankin Manuscript submitted.
<chem>C48H40O12Si8</chem> <chem>Si8O12(C6H5)8</chem>	Octaphenylsilsesquioxane Structure by ED and computational methods A. V. Zakharov, S. L. Masters, D. A. Wann, S. A. Shlykov, G. V. Girichev, S. Arrowsmith, D. B. Cordes, P. D. Lickiss and A. J. P. White Dalton Trans. 39 (2010), 6960
FNa <chem>NaF</chem>	Sodium fluoride Structure by ED and <i>ab initio</i> calculations P. D. McCaffrey, D. A. Wann, R. J. Mawhorter and D. W. H. Rankin Manuscript in preparation.
F2Na2 <chem>Na2F2</chem>	Sodium fluoride dimer Structure by ED and <i>ab initio</i> calculations P. D. McCaffrey, D. A. Wann, R. J. Mawhorter and D. W. H. Rankin Manuscript in preparation.
INa <chem>Nal</chem>	Sodium iodide Structure by ED and <i>ab initio</i> calculations P. D. McCaffrey, D. A. Wann, R. J. Mawhorter and D. W. H. Rankin Manuscript in preparation.
I2Na2 <chem>Na2I2</chem>	Sodium iodide dimer Structure by ED and <i>ab initio</i> calculations P. D. McCaffrey, D. A. Wann, R. J. Mawhorter and D. W. H. Rankin Manuscript in preparation.