

Dr. Derek A. Wann  
 University of Edinburgh  
 School of Chemistry  
 West Mains Road  
 Edinburgh EH9 3JJ  
 U. K.

Telephone: (+44) 131 650 4817  
 Telefax: (+44) 131 650 6453  
 E-Mail: derek.wann@ed.ac.uk  
 Homepage: <http://www.ged.chem.ed.ac.uk/>

BrNa NaBr	<b>Sodium bromide</b> 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.
Br <sub>2</sub> Na <sub>2</sub> Na <sub>2</sub> Br <sub>2</sub>	<b>Sodium bromide dimer</b> 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.
C <sub>2</sub> H <sub>3</sub> AsCl <sub>2</sub> CH <sub>2</sub> CHAsCl <sub>2</sub>	<b>Vinyl dichloroarsine</b> Structure by ED and computational methods R. Noble-Eddy, S. L. Masters, D. W. H. Rankin, H. E. Robertson and J.-C. Guillemin J. Mol. Struct. <b>978</b> (2010), 36
C <sub>2</sub> H <sub>4</sub> O <sub>4</sub> S <sub>2</sub> O <sub>2</sub> -cyclo-S(CH <sub>2</sub> ) <sub>2</sub> S-O <sub>2</sub>	<b>1,3-Dithietane-1,1,3,3-tetraoxide</b> 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.
C <sub>2</sub> H <sub>5</sub> As CH <sub>2</sub> CHAsH <sub>2</sub>	<b>Vinylarsine</b> Structure by ED and computational methods R. Noble-Eddy, S. L. Masters, D. W. H. Rankin, H. E. Robertson and J.-C. Guillemin J. Mol. Struct. <b>978</b> (2010), 36
C <sub>3</sub> H <sub>6</sub> Cl <sub>3</sub> N N(CH <sub>2</sub> Cl) <sub>3</sub>	<b>Tris(chloromethyl)amine</b> Structure by ED and computational methods N. W. Mitzel, J. T. Schirlin, S. L. Masters, D. W. H. Rankin et al. Manuscript in preparation.
C <sub>4</sub> H <sub>5</sub> F <sub>3</sub> OS CF <sub>3</sub> COSCH <sub>2</sub> CH <sub>3</sub>	<b>Ethyl trifluorothioacetate</b> 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 J. Chem. Phys. <b>131</b> (2010), 214303
C <sub>4</sub> H <sub>9</sub> F <sub>3</sub> O <sub>2</sub> Si (CH <sub>3</sub> ) <sub>3</sub> SiOC(O)CF <sub>3</sub>	<b>Trimethylsilyl trifluoroacetate</b> Vibrational spectra and structure by ED and <i>ab initio</i> calculations M. E. Defonsi Lestard, M. E. Tuttolomondo, E. L. Varetta, D. A. Wann, H. E. Robertson, D. W. H. Rankin and A. Ben Altabef J. Mol. Struct. <b>978</b> (2010), 114
C <sub>4</sub> H <sub>9</sub> F <sub>3</sub> O <sub>3</sub> SSi (CH <sub>3</sub> ) <sub>3</sub> SiSO <sub>2</sub> OCF <sub>3</sub>	<b>Trimethylsilyl trifluoromethanesulfonate</b> Vibrational spectra and structure by ED and <i>ab initio</i> calculations M. E. Defonsi Lestard, M. E. Tuttolomondo, E. L. Varetta, D. A. Wann, H. E. Robertson, D. W. H. Rankin and A. Ben Altabef J. Mol. Struct. <b>984</b> (2010), 376
C <sub>4</sub> H <sub>10</sub> Cl <sub>2</sub> Si	<b>Diethyldichlorosilane</b> Structure and conformations by ED, IR and Raman spectroscopies and quantum chemical calculations

$\text{Si}(\text{CH}_2\text{CH}_3)_2\text{Cl}_2$	M. Montejo, D. A. Wann, P. G. Rodríguez Ortega, H. E. Robertson, F. Márquez, D. W. H. Rankin and J. J. López González J. Raman Spectrosc. <b>41</b> (2010), 1323
$\text{C}_5\text{H}_9\text{P}$ ButCP	<b>tert-Butylphosphaethyne</b> 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.
$\text{C}_6\text{HCl}_5$ $\text{C}_6\text{HCl}_5$	<b>Pentachlorobenzene</b> Structure by ED and liquid crystal NMR spectroscopy R. Blom, D. A. Wann, D. W. H. Rankin et al. Manuscript in preparation.
$\text{C}_6\text{H}_2\text{Cl}_4$ 1,2,3,4- $\text{C}_6\text{H}_2\text{Cl}_4$	<b>1,2,3,4-Tetrachlorobenzene</b> Structure by ED and liquid crystal NMR spectroscopy R. Blom, D. A. Wann, D. W. H. Rankin et al. Manuscript in preparation.
$\text{C}_6\text{H}_4\text{BrF}$ $\text{C}_6\text{H}_4\text{BrF}$	<b>1-Bromo-4-fluorobenzene</b> 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 Struct. Chem., in press.
$\text{C}_6\text{H}_4\text{ClF}$ $\text{C}_6\text{H}_4\text{ClF}$	<b>1-Chloro-4-fluorobenzene</b> 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 Struct. Chem., in press.
$\text{C}_6\text{H}_4\text{F}_2$ 1,2- $\text{C}_6\text{H}_4\text{F}_2$	<b>1,2-Difluorobenzene</b> Structure by ED and liquid crystal NMR spectroscopy E. M. Brown, D. A. Wann and D. W. H. Rankin J. Mol. Struct. <b>984</b> (2010), 102
$\text{C}_6\text{H}_4\text{F}_2$ $\text{C}_6\text{H}_4\text{F}_2$	<b>1,3-Difluorobenzene</b> Structure by ED and liquid crystal NMR spectroscopy E. M. Brown, D. A. Wann and D. W. H. Rankin J. Mol. Struct. <b>984</b> (2010), 102
$\text{C}_6\text{H}_{12}\text{F}_6\text{Si}_2$ $\text{CF}_3\text{Me}_2\text{SiSiMe}_2\text{CF}_3$	<b>1,2-Trifluoromethyl-1,1,2,2-tetramethyldisilane</b> 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.
$\text{C}_7\text{F}_{14}$ $\text{C}_6\text{F}_{11}\text{CF}_3$	<b>Perfluoromethylcyclohexane</b> 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 J. Phys. Chem. A <b>114</b> (2010), 11022
$\text{C}_7\text{H}_{16}\text{Cl}_3\text{PSi}$ (tBu)(iPr)PSiCl <sub>3</sub>	<b>(tert-Butyl)(iso-propyl)(trichlorosilyl)phosphine</b> 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.
$\text{C}_9\text{H}_{24}\text{Br}_4\text{Si}_4$ $\text{C}(\text{SiMe}_2\text{Br})_4$	<b>Tetrakis(bromodimethylsilyl)methane</b> 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.
$C_9H_{24}Cl_4Si_4$ $C(SiMe_2Cl)_4$	<b>Tetrakis(chlorodimethylsilyl)methane</b> 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.
$C_9H_{24}F_4Si_4$ $C(SiMe_2F)_4$	<b>Tetrakis(fluorodimethylsilyl)methane</b> 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.
$C_9H_{28}Si_4$ $C(SiMe_2H)_4$	<b>Tetrakis(dimethylsilyl)methane</b> 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.
$C_{10}H_{17}P$ $C_{10}H_{15}PH_2$	<b>Adamantylphosphine</b> 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	<b>N,N'-Di-tert-butyl-1,4-diaza-1,3-butadiene</b> Structure by ED and computational methods C. Jones, D. A. Wann, H. E. Robertson and D. W. H. Rankin Manuscript in preparation.
$C_{10}H_{26}Ga_2O_4$ $[Me_2Ga(OCH_2CH_2OMe)]_2$	<b>Di-<math>\mu</math>-ethoxydiethoxydimethyldigallium</b> 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.
$C_{10}H_{30}Si_4$ $(Me_3Si)_3CSiH_3$	<b>(Silyl)tris(trimethylsilyl)methane</b> 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. <b>39</b> (2010), 9353
$C_{11}H_{30}Br_2Si_4$ $C(SiMe_3)_2(SiMe_2Br)_2$	<b>Bis(bromodimethylsilyl)bis(trimethylsilyl)methane</b> 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.
$C_{11}H_{30}Cl_2Si_4$ $(Me_3Si)_2C(SiClMe_2)_2$	<b>Bis(chlorodimethylsilyl)-bis(trimethylsilyl)methane</b> 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.
$C_{11}H_{32}Si_4$ $C(SiMe_3)_2(SiMe_2H)_2$	<b>Bis(dimethylsilyl)bis(trimethylsilyl)methane</b> 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.
$C_{12}Fe_3O_{12}$ $Fe_3(CO)_{12}$	<b>Dodecacarbonyltriiron</b> Structure by ED and <i>ab initio</i> calculations G. R. Kafka, S. L. Masters, D. W. H. Rankin et al. Manuscript in preparation.
$C_{12}H_{30}Ga_2O_2$	<b>Di-<math>\mu</math>-tert-butoxymethyldigallium</b> Structure by ED and <i>ab initio</i> calculations

$[\text{Me}_2\text{GaOtBu}]_2$	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.
$\text{C}_{16}\text{H}_{24}\text{O}_{12}\text{Si}_8$ $\text{Si}_8\text{O}_{12}(\text{CH}=\text{CH}_2)_8$	<b>Octavinyl silsesquioxane</b> 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.
$\text{C}_{24}\text{H}_{72}\text{O}_{20}\text{Si}_{16}$ $\text{Si}_8\text{O}_{12}(\text{OSiMe}_3)_8$	<b>Octakis(trimethylsiloxy)octasilsesquioxane</b> 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.
$\text{C}_{48}\text{H}_{40}\text{O}_{12}\text{Si}_8$ $\text{Si}_8\text{O}_{12}(\text{C}_6\text{H}_5)_8$	<b>Octa-phenyl-silsesquioxane</b> 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. <b>39</b> (2010), 6960
<b>FNa</b> NaF	<b>Sodium fluoride</b> 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.
$\text{F}_2\text{Na}_2$ $\text{Na}_2\text{F}_2$	<b>Sodium fluoride dimer</b> 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.
<b>INa</b> NaI	<b>Sodium iodide</b> 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.
$\text{I}_2\text{Na}_2$ $\text{Na}_2\text{I}_2$	<b>Sodium iodide dimer</b> 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.