

Prof. Dr. David W. H. Rankin
School of Chemistry
University of Edinburgh
West Mains Road
Edinburgh EH9 3JJ, Scotland

Telephone: (+0)(131) 650 4728

Telefax: (+0)(131) 650 6452

E-Mail: D.W.H.Rankin@ed.ac.uk

BrNa NaBr	Sodium bromide J. K. Dewhurst, P. D. McCaffrey, R. J. Mawhorter and D. W. H. Rankin Structure by ED and <i>ab initio</i> calculations Manuscript in preparation.
Br₂Na₂ Na ₂ Br ₂	Sodium bromide dimer J. K. Dewhurst, P. D. McCaffrey, R. J. Mawhorter and D. W. H. Rankin Structure by ED and <i>ab initio</i> calculations Manuscript in preparation.
CH₅P CH ₃ PH ₂	Methylphosphine R. Noble-Eddy, S. L. Masters (née Hinchley), D. W. H. Rankin, D. A. Wann, B. Khater and J.-C. Guillemin Structure by ED, MW and <i>ab initio</i> calculations Dalton Trans. (2008), 5041-5047
CH₈BN (CH ₃)H ₂ NBH ₃	Methylaminoborane S. Aldridge, A. J. Downs, C. Y. Tang, S. Parsons, M. C. Clarke, R. D. L. Johnstone, H. E. Robertson, D. W. H. Rankin and D. A. Wann Structure by X-ray, ED and <i>ab initio</i> calculations J.Am.Chem.Soc., accepted subject to corrections.
CH₈BP CH ₃ PH ₂ BH ₃	Methyl phosphine borane adduct R. Noble-Eddy, S. L. Masters (née Hinchley), D. W. H. Rankin, D. A. Wann, B. Khater and J.-C. Guillemin Structure by ED, MW and <i>ab initio</i> calculations Dalton Trans. (2008), 5041-5047
C₂Cl₂N₂S C ₂ Cl ₂ N ₂ S	3,4-Dichloro-1,2,5-thiadiazole J. T. Schirlin, D. A. Wann, S. F. Bone, H. E. Robertson and D. W. H. Rankin

	Structure by ED and computational methods Manuscript submitted.
C₂H₁₀BN (CH ₃) ₂ HNBH ₃	Dimethylaminoborane S. Aldridge, A. J. Downs, C. Y. Tang, S. Parsons, M. C. Clarke, R. D. L. Johnstone, H. E. Robertson, D. W. H. Rankin and D. A. Wann Structure by X-ray, ED and <i>ab initio</i> calculations J. Am. Chem. Soc., accepted subject to corrections.
C₃Cl₃N₃ C ₃ N ₃ Cl ₃	2,4,6-Trichloro-1,3,5-triazine D. A. Wann, A. M. Reilly, P. D. McCaffrey and D. W. H. Rankin. Structure by ED and <i>ab initio</i> calculations Manuscript submitted.
C₃H₃F₃O₂ CF ₃ COOCH ₃	Methyl trifluoroacetate M. E. Defonsi Lestard, M. E. Tuttolomondo, E. L. Varetti, D. A. Wann, H. E. Robertson, D. W. H. Rankin and A. Ben Altabef Structure by ED and <i>ab initio</i> calculations Manuscript complete.
C₃H₆Cl₃N N(CH ₂ Cl) ₃	Tris(chloromethyl)amine N. W. Mitzel, J. T. Schirlin, S. L. Masters, D. W. H. Rankin et al. Structure by ED and computational methods Manuscript in preparation.
C₃H₁₀Ge Me ₃ GeH	Trimethylgermane M. L. Roldán, S. A. Brandán, S. L. Masters, D. A. Wann, H. E. Robertson, D. W. H. Rankin and A. Ben Altabef Vibrational spectra and structure by ED and computational methods Manuscript submitted to J. Phys. Chem. A
C₄HCl₃N₂ C ₄ N ₂ Cl ₃	2,4,6-Trichloropyrimidine S. L. Masters, D. A. Wann and D. W. H. Rankin Structure by ED and computational methods Manuscript in preparation.
C₄H₂Cl₂S C ₄ H ₂ Cl ₂ S	2,5-Dichlorothiophene J. T. Schirlin, D. A. Wann, S. F. Bone, H. E. Robertson and

	<p>D. W. H. Rankin Structure by ED and computational methods Manuscript submitted.</p>
<p>C₄H₂F₆O₂ CF₃CO₂CH₂CF₃</p>	<p>Trifluoroethyltrifluoroacetate M. E. Defonsi Lestard, M. E. Tuttolomondo, E. L. Varetti, D. A. Wann, H. E. Robertson, D. W. H. Rankin and A. Ben Altabef Structure by ED and <i>ab initio</i> calculations J. Mol. Struct. in press</p>
<p>C₄H₃BrS 2-Br-C₄H₃S</p>	<p>2-Bromothiophene J. T. Schirlin, D. A. Wann, S. F. Bone, H. E. Robertson and D. W. H. Rankin Structure by ED and computational methods Manuscript submitted.</p>
<p>C₄H₃ClS C₄H₃ClS</p>	<p>2-Chlorothiophene J. T. Schirlin, D. A. Wann, S. F. Bone, H. E. Robertson and D. W. H. Rankin Structure by ED and computational methods Manuscript submitted.</p>
<p>C₄H₅F₃OS CF₃COSCH₂CH₃</p>	<p>Ethyl trifluorothioacetate M. E. Defonsi Lestard, M. E. Tuttolomondo, E. L. Varetti, D. A. Wann, H. E. Robertson, D. W. H. Rankin and A. Ben Altabef Structure by ED and <i>ab initio</i> calculations Manuscript in preparation.</p>
<p>C₄H₅F₃O₂ CF₃COOCH₂CH₃</p>	<p>Ethyl trifluoroacetate M. E. Defonsi Lestard, M. E. Tuttolomondo, E. L. Varetti, D. A. Wann, H. E. Robertson, D. W. H. Rankin and A. Ben Altabef Structure by ED and <i>ab initio</i> calculations Manuscript in preparation.</p>
<p>C₄H₁₀N₄Si (N₄CH)SiMe₃</p>	<p>1-Trimethylsilyltetrazole D. A. Wann, I. Gronde, T. Foerster, S. A. Hayes, S. L. Masters, H. E. Robertson, N. W. Mitzel and D. W. H. Rankin Structure by ED, X-ray and computational methods Dalton Trans. (2008), 3817-3823</p>

<p>C₅H₁₁N₃Si SiMe₃-NNCNC</p>	<p>1-(Trimethylsilyl)-1,2,4-triazole D. A. Wann, I. Gronde, T. Foerster, S. A. Hayes, S. L. Masters, H. E. Robertson, N. W. Mitzel and D. W. H. Rankin Structure by ED and computational methods Dalton Trans. (2008), 3817-3823</p>
<p>C₆HCl₅ C₆HCl₅</p>	<p>Pentachlorobenzene R. Blom, D. A. Wann, D. W. H. Rankin et al. Structure by ED and liquid crystal NMR spectroscopy Manuscript in preparation.</p>
<p>C₆H₂Cl₄ 1,2,3,4-C₆H₂Cl₄</p>	<p>1,2,3,4-Tetrachlorobenzene R. Blom, D. A. Wann, D. W. H. Rankin et al. Structure by ED and liquid crystal NMR spectroscopy Manuscript in preparation.</p>
<p>C₆H₄BrF C₆H₄BrF</p>	<p>1-Bromo-4-fluorobenzene S. L. Masters, I. D. Mackie, D. W. H. Rankin, H. E. Robertson and S. Parsons Structure by ED, liquid crystal NMR spectroscopy, <i>ab initio</i> calculations and X-ray diffraction Manuscript complete.</p>
<p>C₆H₄ClF C₆H₄ClF</p>	<p>1-Chloro-4-fluorobenzene S. L. Masters, I. D. Mackie, D. W. H. Rankin, H. E. Robertson and S. Parsons Structure by ED, liquid crystal NMR spectroscopy, <i>ab initio</i> calculations and X-ray diffraction Manuscript complete.</p>
<p>C₆H₄F₂ C₆H₄F₂</p>	<p>1,4-Difluorobenzene E. M. Brown, P. D. McCaffrey, D. A. Wann and D. W. H. Rankin Structure by ED and liquid crystal NMR spectroscopy Manuscript in preparation.</p>
<p>C₆H₄F₂ 1,2-C₆H₄F₂</p>	<p>1,2-Difluorobenzene E. M. Brown, P. D. McCaffrey, D. A. Wann and D. W. H. Rankin Structure by ED and liquid crystal NMR spectroscopy Manuscript in preparation.</p>

<p>C₆H₆ClN C₆H₄ClNH₂</p>	<p>2-Chloroaniline D. A. Wann, C. K. Spanswick, H. E. Robertson et al. Structure by ED and <i>ab initio</i> calculations Manuscript in preparation.</p>
<p>C₆H₁₁NSSi SiMe₃-cyclo-CNCCS</p>	<p>2-(Trimethylsilyl)-1,3-thiazole T. Foerster, D. A. Wann, H. E. Robertson and D. W. H. Rankin Structure by ED and computational methods Manuscript in preparation.</p>
<p>C₆H₁₂F₆Si₂ CF₃Me₂SiSiMe₂CF₃</p>	<p>1,2-Trifluoromethyl-1,1,2,2-tetramethyldisilane S. L. Masters, D. A. Wann, H. E. Robertson, F. Lennox, D. W. H. Rankin, I. Arnason, K. Hassler et al. Structure by ED and <i>ab initio</i> calculations, interpretation of Raman spectra Manuscript in preparation.</p>
<p>C₇F₁₄ C₆F₁₁CF₃</p>	<p>Perfluoromethylcyclohexane G. R. Kafka, S. L. Masters, D. W. H. Rankin et al. Structure by ED and <i>ab initio</i> calculations Manuscript in preparation.</p>
<p>C₇H₉N C₆H₄MeNH₂</p>	<p>2-Methylaniline D. A. Wann, C. K. Spanswick, H. E. Robertson et al. Structure by ED and <i>ab initio</i> calculations Manuscript in preparation.</p>
<p>C₇H₁₆Cl₃PSi (tBu)(iPr)PSiCl₃</p>	<p>(tert-butyl)(iso-propyl)(trichlorosilyl)phosphine E. Seppälä, W.-W. du Mont, S. L. Masters, D. W. H. Rankin and H. E. Robertson Structure by ED and <i>ab initio</i> calculations Manuscript in preparation.</p>
<p>C₈H₂₄B₄N₄S₂ B₄S₂(NMe₂)₄</p>	<p>Tetrakis(dimethylamino)-1,4-dithiatetaborinane D. A. Wann, H. E. Robertson, G. Bramham, A. E. A. Bull, N. C. Norman, C. A. Russell and D. W. H. Rankin Structure by ED and <i>ab initio</i> calculations Dalton Trans., accepted subject to minor corrections.</p>
<p>C₈H₂₄O₁₂Si₈ Si₈O₁₂Me₈</p>	<p>Octamethylsilsesquioxane D. A. Wann, R. J. Less, F. Rataboul, P. D. McCaffrey, A. M. Reilly, H. E. Robertson, P. D. Lickiss and D. W. H.</p>

	<p>Rankin Structure by ED and <i>ab initio</i> calculations Organometallics 27 (2008), 4183-4187</p>
<p>C₉H₁₃N₃Si SiMe₃-NN(C₆H₄)N</p>	<p>1-(Trimethylsilyl)-1H-benzotriazole T. Foerster, D. A. Wann, H. E. Robertson and D. W. H. Rankin Structure by ED and computational methods Manuscript in preparation.</p>
<p>C₉H₂₄Br₄Si₄ C(SiMe₂Br)₄</p>	<p>Tetrakis(bromodimethylsilyl)methane K. Batz, G. R. Kafka, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin Structure by ED and computational methods Manuscript in preparation.</p>
<p>C₉H₂₄Cl₄Si₄ C(SiMe₂Cl)₄</p>	<p>Tetrakis(chlorodimethylsilyl)methane K. Batz, G. R. Kafka, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin Structure by ED and computational methods Manuscript in preparation.</p>
<p>C₉H₂₄F₄Si₄ C(SiMe₂F)₄</p>	<p>Tetrakis(fluorodimethylsilyl)methane K. Batz, G. R. Kafka, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin Structure by ED and computational methods Manuscript in preparation.</p>
<p>C₉H₂₈Si₄ C(SiMe₂H)₄</p>	<p>Tetrakis(dimethylsilyl)methane K. Batz, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin Structure by ED and computational methods Manuscript in preparation.</p>
<p>C₁₀H₁₇P C₁₀H₁₅PH₂</p>	<p>Adamantylphosphine J. R. Goerlich, D. A. Wann, R. Schmutzler, D. W. H. Rankin, H. E. Robertson and A. R. Turner Structure by ED and <i>ab initio</i> calculations Manuscript in preparation.</p>
<p>C₁₀H₁₈CIP₃ P₂C(t-Bu)₂PCl</p>	<p>Tricyclo-CIP₃C₂(t-Bu)₂ D. A. Wann, C. A. Russell, H. E. Robertson and D. W. H. Rankin</p>

	Structure by ED and computational methods Manuscript in preparation.
C₁₀H₂₀N₂ ButN=CHCH=NBut	N,N'-Di-<i>tert</i>-butyl-1,4-diaza-1,3-butadiene C. Jones, D. A. Wann, H. E. Robertson and D. W. H. Rankin Structure by ED and computational methods Manuscript in preparation.
C₁₀H₂₆Ga₂O₄ [Me ₂ Ga(OCH ₂ CH ₂ OMe)] ₂	bis[μ-(2-methoxyethanolato-κO:κO)](tetramethyl)digallium D. A. Wann, C. E. Knapp, C. J. Carmalt, H. E. Robertson, D. W. H. Rankin et al. Structure by ED and <i>ab initio</i> calculations Manuscript in preparation.
C₁₀H₃₀Si₄ (Me ₃ Si) ₃ CSiH ₃	(Silyl)tris(trimethylsilyl)methane K. Batz, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin Structure by ED and computational methods Manuscript in preparation.
C₁₁H₃₀Br₂Si₄ C(SiMe ₃) ₂ (SiMe ₂ Br) ₂	Bis(bromodimethylsilyl)bis(trimethylsilyl)methane K. Batz, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin Structure by ED and computational methods Manuscript in preparation.
C₁₁H₃₀Cl₂Si₄ (Me ₃ Si) ₂ C(SiClMe ₂) ₂	Bis(chlorodimethylsilyl)-bis(trimethylsilyl)methane K. Batz, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin Structure by ED and computational methods Manuscript in preparation.
C₁₁H₃₂Si₄ C(SiMe ₃) ₂ (SiMe ₂ H) ₂	Bis(dimethylsilyl)bis(trimethylsilyl)methane K. Batz, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin Structure by ED and computational methods Manuscript in preparation.
C₁₂Fe₃O₁₂ Fe ₃ (CO) ₁₂	Dodecacarbonyltriiron G. R. Kafka, S. L. Masters, D. W. H. Rankin et al. Structure by ED and <i>ab initio</i> calculations

	Manuscript in preparation.
$C_{12}H_{32}Ga_2N_2O_2$ $[Me_2Ga(OCH_2CH_2NMe_2)]_2$	bis{μ-[$_2$-(dimethylamino)ethanolato-$\kappa O:\kappa O$]}(tetramethyl)digallium C. E. Knapp, C. J. Carmalt, P. F. McMillan, D. A. Wann, H. E. Robertson and D. W. H. Rankin Structure by ED and <i>ab initio</i> calculations Dalton Trans., in press
$C_{16}H_{38}N_4W$ $W(NHBut)_2(NBut)_2$	Bis(tert-butylamino)-bis(tert-butylimido)tungsten H. Choujaa, S. D. Cosham, A. L. Johnson, G. R. Kafka, M. F. Mahon, S. L. Masters, K. C. Molloy, D. W. H. Rankin, H. E. Robertson and D. A. Wann Structure by ED and <i>ab initio</i> calculations Inorg. Chem., accepted subject to minor revisions
FNa NaF	Sodium fluoride J. K. Dewhurst, P. D. McCaffrey, R. J. Mawhorter and D. W. H. Rankin Structure by ED and <i>ab initio</i> calculations Manuscript in preparation.
F_2Na_2 Na_2F_2	Sodium fluoride dimer J. K. Dewhurst, P. D. McCaffrey, R. J. Mawhorter and D. W. H. Rankin Structure by ED and <i>ab initio</i> calculations Manuscript in preparation.
F_4P_2S $S(PF_2)_2$	Bis(difluorophosphino) sulfide A. M. Reilly, D. A. Wann and D. W. H. Rankin Structure by ED and <i>ab initio</i> calculations, and explanation of NMR spectra J. Phys. Chem. A, in press.
$H_8O_{12}Si_8$ $H_8Si_8O_{12}$	Octa-silsesquioxane D. A. Wann, R. J. Less, F. Rataboul, P. D. McCaffrey, A. M. Reilly, H. E. Robertson, P. D. Lickiss and D. W. H. Rankin Structure by ED and <i>ab initio</i> calculations Organometallics 27 (2008), 4183-4187
$H_{10}O_{15}Si_{10}$ $Si_{10}O_{15}H_{10}$	Decasilsesquioxane D. A. Wann, F. Rataboul, A. M. Reilly, H. E. Robertson, P.

	<p>D. Lickiss and D. W. H. Rankin Structure by ED and <i>ab initio</i> calculations Manuscript in preparation.</p>
<p>INa NaI</p>	<p>Sodium iodide J. K. Dewhurst, P. D. McCaffrey, R. J. Mawhorter and D. W. H. Rankin Structure by ED and <i>ab initio</i> calculations Manuscript in preparation.</p>
<p>I₂Na₂ Na₂I₂</p>	<p>Sodium iodide dimer J. K. Dewhurst, P. D. McCaffrey, R. J. Mawhorter and D. W. H. Rankin Structure by ED and <i>ab initio</i> calculations Manuscript in preparation.</p>
	<p>Gas-phase molecular structures determined by electron diffraction D. W. H. Rankin and H. E. Robertson Review of structure of inorganic molecules published in 2005 Royal Society of Chemistry Specialist Periodical Reports, "Spectroscopic Properties of Inorganic and Organometallic Compounds" 39 (2007), 355-367</p>
	<p>Gas-phase molecular structures determined by electron diffraction D. W. H. Rankin and H. E. Robertson Review of structure of inorganic molecules published in 2006 - 2007 Royal Society of Chemistry Specialist Periodical Reports, "Spectroscopic Properties of Inorganic and Organometallic Compounds", in press</p>
	<p>Stereochemistry of free boranes and heteroboranes from electron scattering and model chemistries D. Hnyk and D. W. H. Rankin Dalton Trans. (2009), in press.</p>