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| **BrNa**<br>NaBr | **Sodium bromide**<br>Structure by ED and ab initio calculations<br><br>*J. K. Dewhurst, P. D. McCaffrey, R. J. Mawhorter and D. W. H. Rankin*<br>Manuscript in preparation. |
| **$Br_2Na_2$**<br>$Na_2Br_2$ | **Sodium bromide dimer**<br>Structure by ED and ab initio calculations<br><br>*J. K. Dewhurst, P. D. McCaffrey, R. J. Mawhorter and D. W. H. Rankin*<br>Manuscript in preparation. |
| **FNa**<br>NaF | **Sodium fluoride**<br>Structure by ED and ab initio calculations<br><br>*J. K. Dewhurst, P. D. McCaffrey, R. J. Mawhorter and D. W. H. Rankin*<br>Manuscript in preparation. |
| **$F_2Na_2$**<br>$Na_2F_2$ | **Sodium fluoride dimer**<br>Structure by ED and ab initio calculations<br><br>*J. K. Dewhurst, P. D. McCaffrey, R. J. Mawhorter and D. W. H. Rankin*<br>Manuscript in preparation. |
| **INa**<br>NaI | **Sodium iodide**<br>Structure by ED and ab initio calculations<br><br>*J. K. Dewhurst, P. D. McCaffrey, R. J. Mawhorter and D. W. H. Rankin*<br>Manuscript in preparation. |
| **$I_2Na_2$**<br>$Na_2I_2$ | **Sodium iodide dimer**<br>Structure by ED and ab initio calculations<br><br>*J. K. Dewhurst, P. D. McCaffrey, R. J. Mawhorter and D. W. H. Rankin*<br>Manuscript in preparation. |
| **$H_{10}O_{15}Si_{10}$**<br>$Si_{10}O_{15}H_{10}$ | **Decasilsesquioxane**<br>Structure by ED and ab initio calculations<br>*D. A. Wann, F. Rataboul, A. M. Reilly, H. E. Robertson, P. D. Lickiss and D. W. H. Rankin*<br>Dalton Trans. (2009) 6843-6848 |
| **$CH_4ClP$**<br>$ClCH_2PH_2$ | **Chloromethylphosphine**<br>Structure by ED, MW and ab initio calculations<br>*R. Noble-Eddy, S. L. Masters (née Hinchley), D. W. H. Rankin, D. A. Wann, H. E. Robertson, B. Khater and J.-C. Guillemin*<br>Inorg. Chem. **48** (2009) 8603-8612 |
| **$CH_8BN$** | **Methylaminoborane**<br>Structure by X-ray, ED and ab initio calculations |

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| $(CH_3)H_2NBH_3$ | *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*<br>J. Am. Chem. Soc. **131** (2009) 2231-2243 |
| **$C_2Cl_2N_2S$**<br>$C_2Cl_2N_2S$ | **3,4-Dichloro-1,2,5-thiadiazole**<br>Structure by ED and computational methods<br>*J. T. Schirlin, D. A. Wann, S. F. Bone, H. E. Robertson and D. W. H. Rankin*<br>J. Mol. Struct. **922** (2009) 103-108 |
| **$C_2H_3AsCl_2$**<br>$CH_2CHAsCl_2$ | **Vinyldichloroarsine**<br>Structure by ED and computational methods<br>*R. Noble-Eddy, S. L. Masters, D. W. H. Rankin, H. E. Robertson and J.-C. Guillemin*<br>J. Mol. Struct., in press. |
| **$C_2H_3P$**<br>$HC{\equiv}CPH_2$ | **Ethynylphosphine**<br>Structure by ED, MW and ab initio calculations<br>*R. Noble-Eddy, S. L. Masters (née Hinchley), D. W. H. Rankin, D. A. Wann, H. E. Robertson, B. Khater and J.-C. Guillemin*<br>Inorg. Chem., **48** (2009) 8603-8612 |
| **$C_2H_4O_4S_2$**<br>$O_2$-cyclo-$S(CH_2)_2S$-$O_2$ | **1,3-Dithietane-1,1,3,3-tetraoxide**<br>Structure by ED and ab initio calculations<br>*D. A. Wann, D.W. H. Rankin et al.*<br>Manuscript in preparation. |
| **$C_2H_5P$**<br>$CH_2{=}CHPH_2$ | **Vinylphosphine**<br>Structure by ED, MW and ab initio calculations<br>*R. Noble-Eddy, S. L. Masters (née Hinchley), D. W. H. Rankin, D. A. Wann, H. E. Robertson, B. Khater and J.-C. Guillemin*<br>Inorg. Chem. **48** (2009) 8603-8612 |
| **$C_2H_{10}BN$**<br>$(CH_3)_2HNBH_3$ | **Dimethylaminoborane**<br>Structure by X-ray, ED and ab initio calculations<br>*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*<br>J. Am. Chem. Soc. **131** (2009) 2231-2243 |
| **$C_3Cl_3N_3$**<br>$C_3N_3Cl_3$ | **2,4,6-Trichloro-1,3,5-triazine**<br>Equilibrium structure by ED with vibration corrections from molecular dynamics<br>*D. A. Wann, A. V. Zakharov, A. M. Reilly, P. D. McCaffrey and D. W. H. Rankin*<br>J. Phys. Chem. A **113** (2009) 9511-9520 |
| **$C_3H_3F_3O_2$**<br>$CF_3COOCH_3$ | **Methyl trifluoroacetate**<br>Structure by ED and ab initio calculations<br>*M. E. Defonsi Lestard, M. E. Tuttolomondo, E. L. Varetti, D. A. Wann, H. E. Robertson, D. W. H. Rankin and A. Ben Altabef*<br>J. Raman Spectrosc. **40** (2009) 2053-2062 |
| **$C_3H_5P$**<br>$HC{\equiv}CCH_2PH_2$ | **Propargyl phosphine**<br>Structure by ED, MW and ab initio calculations<br>*R. Noble-Eddy, S. L. Masters (née Hinchley), D. W. H. Rankin, D. A. Wann, H. E. Robertson, B. Khater and J.-C. Guillemin*<br>Inorg. Chem. **48** (2009) 8603-8612 |
| **$C_3H_5P$**<br>$CH_2{=}C{=}CHPH_2$ | **Allenyl phosphine**<br>Structure by ED and ab initio calculations<br>*R. Noble-Eddy, S. L. Masters (née Hinchley), D. W. H. Rankin, D. A. Wann, H. E. Robertson, B. Khater and J.-C. Guillemin*<br>Inorg. Chem. (2009) 8603-8612 |
| **$C_3H_6Cl_3N$**<br>$N(CH_2Cl)_3$ | **Tris(chloromethyl)amine**<br>Structure by ED and computational methods<br>*N. W. Mitzel, J. T. Schirlin, S. L. Masters, D. W. H. Rankin et al.* |

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| | Manuscript in preparation. |
| **$C_3H_7P$**<br>$CH_2$=$CHCH_2PH_2$ | **Allylphosphine**<br>Structure by ED and ab initio calculations<br>*R. Noble-Eddy, S. L. Masters (née Hinchley), D. W. H. Rankin, D. A. Wann, H. E. Robertson, B. Khater and J.-C. Guillemin*<br>Inorg. Chem. **48** (2009) 8603-8612 |
| **$C_3H_{10}Ge$**<br>$Me_3GeH$ | **Trimethylgermane**<br>Vibrational spectra and structure by ED and computational methods<br>*M. L. Roldán, S. A. Brandán, S. L. Masters (née Hinchley), D. A. Wann, H. E. Robertson, D. W. H. Rankin and A. Ben Altabef*<br>J. Phys. Chem. A **113** (2009) 5195-5204 |
| **$C_4H_2Cl_2S$**<br>$C_4H_2Cl_2S$ | **2,5-Dichlorothiophene**<br>Structure by ED and computational methods<br>*J. T. Schirlin, D. A. Wann, S. F. Bone, H. E. Robertson and D. W. H. Rankin*<br>J. Mol. Struct. **922** (2009)103-108 |
| **$C_4H_2F_6O_2$**<br>$CF_3CO_2CH_2CF_3$ | **Trifluoroethyl trifluoroacetate**<br>Structure by ED and ab initio calculations<br>*M. E. D. Lestard, M. E. Tuttolomondo, E. L. Varetti, D. A. Wann, H. E. Robertson, D. W. H. Rankin and A. Ben Altabef*<br>J. Mol. Struct. **917** (2009) 183-192 |
| **$C_4H_3BrS$**<br>2-Br-$C_4H_3S$ | **2-Bromothiophene**<br>Structure by ED and computational methods<br>*J. T. Schirlin, D. A. Wann, S. F. Bone, H. E. Robertson and D. W. H. Rankin*<br>J. Mol. Struct. **922** (2009) 103-108 |
| **$C_4H_3ClS$**<br>$C_4H_3ClS$ | **2-Chlorothiophene**<br>Structure by ED and computational methods<br>*J. T. Schirlin, D. A. Wann, S. F. Bone, H. E. Robertson and D. W. H. Rankin*<br>J. Mol. Struct. **922** (2009) 103-108 |
| **$C_4H_5F_3OS$**<br>$CF_3COSCH_2CH_3$ | **Ethyl trifluorothioacetate**<br>Structure and conformation by ED, ab initio calculations and vibrational spectroscopy<br>*M. E. Defonsi Lestard, M. E. Tuttolomondo, D. A. Wann, H. E. Robertson, D. W. H. Rankin and A. Ben Altabef*<br>J. Chem. Phys. **131** (2009) 214303 |
| **$C_4H_5F_3O_2$**<br>$CF_3COOCH_2CH_3$ | **Ethyl trifluoroacetate**<br>Structure by ED and ab initio calculations<br>*M. E. Defonsi Lestard, M. E. Tuttolomondo, E. L. Varetti, D. A. Wann, H. E. Robertson, D. W. H. Rankin and A. Ben Altabef*<br>J. Chem. Phys. **131** (2009) 214303 |
| **$C_4H_9F_3O_2Si$**<br>$(CH_3)_3SiOC(O)CF_3$ | **Trimethylsilyl trifluoroacetate**<br>Vibrational spectra and structure by ED and ab initio calculations<br>*D. A. Wann, A. Ben Altabef et al.*<br>Manuscript submitted for publication. |
| **$C_4H_9F_3O_3SSi$**<br>$(CH_3)_3SiSO_2OCF_3$ | **Trimethylsilyl trifluoromethanesulfonate**<br>Vibrational spectra and structure by ED and ab initio calculations<br>*D. A. Wann, A. Ben Altabef et al.*<br>Manuscript in preparation. |
| **$C_4H_{10}Cl_2Si$**<br>$Si(CH_2CH_3)_2Cl_2$ | **Diethyldichlorosilane**<br>Structure and conformations by ED, IR and Raman spectroscopies and quantum chemical calculations<br>*M. Montejo, D. A. Wann, P. G. Rodríguez Ortega, H. E. Robertson, F. Márquez, D. W. H. Rankin and J. J. López González*<br>J. Raman Spectrosc., 2009, early view. |

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| **$C_6HCl_5$**<br>$C_6HCl_5$ | **Pentachlorobenzene**<br>Structure by ED and liquid crystal NMR spectroscopy<br>*R. Blom, D. A. Wann, D. W. H. Rankin et al.*<br>Manuscript in preparation. |
| **$C_6H_2Cl_4$**<br>1,2,3,4-$C_6H_2Cl_4$ | **1,2,3,4-Tetrachlorobenzene**<br>Structure by ED and liquid crystal NMR spectroscopy<br>*R. Blom, D. A. Wann, D. W. H. Rankin et al.*<br>Manuscript in preparation. |
| **$C_6H_4BrF$**<br>$C_6H_4BrF$ | **1-Bromo-4-fluorobenzene**<br>Structure by ED, liquid crystal NMR spectroscopy, ab initio calculations and X-ray diffraction<br>*S. L. Masters, I. D. Mackie, D. W. H. Rankin, H. E. Robertson and S. Parsons*<br>Manuscript complete. |
| **$C_6H_4ClF$**<br>$C_6H_4ClF$ | **1-Chloro-4-fluorobenzene**<br>Structure by ED, liquid crystal NMR spectroscopy, ab initio calculations and X-ray diffraction<br>*S. L. Masters, I. D. Mackie, D. W. H. Rankin, H. E. Robertson and S. Parsons*<br>Manuscript complete. |
| **$C_6H_4F_2$**<br>1,2-$C_6H_4F_2$ | **1,2-Difluorobenzene**<br>Structure by ED and liquid crystal NMR spectroscopy<br>*E. M. Brown, P. D. McCaffrey, D. A. Wann and D. W. H. Rankin*<br>Manuscript complete. |
| **$C_6H_4F_2$**<br>$C_6H_4F_2$ | **1,3-Difluorobenzene**<br>Structure by ED and liquid crystal NMR spectroscopy<br>*E. M. Brown, P. D. McCaffrey, D. A. Wann and D. W. H. Rankin*<br>Manuscript complete. |
| **$C_6H_7P$**<br>$C_6H_5PH_2$ | **Phenylphosphine**<br>Structure by ED and ab initio calculations<br>*R. Noble-Eddy, S. L. Masters (née Hinchley), D. W. H. Rankin, D. A. Wann, H. E. Robertson, B. Khater and J.-C. Guillemin*<br>Inorg. Chem. **48** (2009) 8603-8612 |
| **$C_6H_{11}NSSi$**<br>$SiMe_3$-cyclo-CNCCS | **2-(Trimethylsilyl)-1,3-thiazole**<br>Structure by ED and computational methods<br>*T. Foerster, D. A. Wann, H. E. Robertson and D. W. H. Rankin*<br>Dalton Trans. (2009) 3026-3033 |
| **$C_6H_{12}F_6Si_2$**<br>$CF_3Me_2SiSiMe_2CF_3$ | **1,2-Trifluoromethyl-1,1,2,2-tetramethyldisilane**<br>Structure by ED, X-ray diffraction and ab initio calculations, interpretation of Raman spectra<br>*S. L. Masters, D. A. Wann, H. E. Robertson, F. Lennox, D. W. H. Rankin, I. Arnason, K. Hassler et al.*<br>Manuscript in preparation. |
| **$C_7F_{14}$**<br>$C_6F_{11}CF_3$ | **Perfluoromethylcyclohexane**<br>Structure by ED and ab initio calculations<br>*G. R. Kafka, S. L. Masters, D. W. H. Rankin et al.*<br>Manuscript in preparation. |
| **$C_7H_9N$**<br>$C_6H_4MeNH_2$ | **2-Methylaniline**<br>Structure by ED and ab initio calculations<br>*D. A. Wann, C. K. Spanswick, H. E. Robertson et al.*<br>Manuscript in preparation. |
| **$C_7H_9P$**<br>$C_6H_5CH_2PH_2$ | **Benzylphosphine**<br>Structure by ED and ab initio calculations<br>*R. Noble-Eddy, S. L. Masters (née Hinchley), D. W. H. Rankin, D. A. Wann, H. E. Robertson, B. Khater and J.-C. Guillemin* |

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| | Inorg. Chem. **48** (2009) 8603-8612 |
| **$C_7H_{16}Cl_3PSi$**<br>$(tBu)(iPr)PSiCl_3$ | **(tert-Butyl)(iso-propyl)(trichlorosilyl)phosphine**<br>Structure by ED and ab initio calculations<br>*E. Seppälä, W.-W. du Mont, S. L. Masters, D. W. H. Rankin and H. E. Robertson*<br>Manuscript in preparation. |
| **$C_8H_{24}B_4N_4S_2$**<br>$B_4S_2(NMe_2)_4$ | **Tetrakis(dimethylamino)-1,4-dithiatetraborinane**<br>Structure by ED and ab initio calculations<br>*D. A. Wann, H. E. Robertson, G. Bramham, A. E. A. Bull, N. C. Norman, C. A. Russell and D. W. H. Rankin*<br>Dalton Trans. (2009) 1446-1449 |
| **$C_9H_{13}N_3Si$**<br>$SiMe_3$-$NN(C_6H_4)N$ | **1-(Trimethylsilyl)-1H-benzotriazole**<br>Structure by ED and computational methods<br>*T. Foerster, D. A. Wann, H. E. Robertson and D. W. H. Rankin*<br>Dalton Trans. (2009) 3026-3033 |
| **$C_9H_{24}Br_4Si_4$**<br>$C(SiMe_2Br)_4$ | **Tetrakis(bromodimethylsilyl)methane**<br>Structure by ED and computational methods<br>*K. Batz, G. R. Kafka, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin*<br>Manuscript in preparation. |
| **$C_9H_{24}Cl_4Si_4$**<br>$C(SiMe_2Cl)_4$ | **Tetrakis(chlorodimethylsilyl)methane**<br>Structure by ED and computational methods<br>*K. Batz, G. R. Kafka, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin*<br>Manuscript in preparation. |
| **$C_9H_{24}F_4Si_4$**<br>$C(SiMe_2F)_4$ | **Tetrakis(fluorodimethylsilyl)methane**<br>Structure by ED and computational methods<br>*K. Batz, G. R. Kafka, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin*<br>Manuscript in preparation. |
| **$C_9H_{28}Si_4$**<br>$C(SiMe_2H)_4$ | **Tetrakis(dimethylsilyl)methane**<br>Structure by ED and computational methods<br>*K. Batz, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin*<br>Manuscript in preparation. |
| **$C_{10}H_{17}P$**<br>$C_{10}H_{15}PH_2$ | **Adamantylphosphine**<br>Structure by ED and ab initio calculations<br>*J. R. Goerlich, D. A. Wann, R. Schmutzler, D. W. H. Rankin, H. E. Robertson and A. R. Turner*<br>Manuscript in preparation. |
| **$C_{10}H_{20}N_2$**<br>ButN=CHCH=NBut | **N,N'-Di-tert-butyl-1,4-diaza-1,3-butadiene**<br>Structure by ED and computational methods<br>*C. Jones, D. A. Wann, H. E. Robertson and D. W. H. Rankin*<br>Manuscript in preparation. |
| **$C_{10}H_{26}Ga_2O_4$**<br>$[Me_2Ga(OCH_2CH_2OMe)]_2$ | **Di-μ-ethoxydiethoxydimethyldigallium**<br>Structure by ED and ab initio calculations<br>*D. A. Wann, C. E. Knapp, C. J. Carmalt, H. E. Robertson, D. W. H. Rankin et al.*<br>Manuscript in preparation. |
| **$C_{10}H_{30}Si_4$**<br>$(Me_3Si)_3CSiH_3$ | **(Silyl)tris(trimethylsilyl)methane**<br>Structure by ED and computational methods<br>*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*<br>Manuscript submitted to Dalton Trans. |
| **$C_{11}H_{30}Br_2Si_4$** | **Bis(bromodimethylsilyl)bis(trimethylsilyl)methane**<br>Structure by ED and computational methods |

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| $C(SiMe_3)_2(SiMe_2Br)_2$ | *K. Batz, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin*<br>Manuscript in preparation. |
| **$C_{11}H_{30}Cl_2Si_4$**<br>$(Me_3Si)_2C(SiClMe_2)_2$ | **Bis(chlorodimethylsilyl)bis(trimethylsilyl)methane**<br>Structure by ED and computational methods<br>*K. Batz, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin*<br>Manuscript in preparation. |
| **$C_{11}H_{32}Si_4$**<br>$C(SiMe_3)_2(SiMe_2H)_2$ | **Bis(dimethylsilyl)bis(trimethylsilyl)methane**<br>Structure by ED and computational methods<br>*K. Batz, P. D. Lickiss, S. L. Masters, H. E. Robertson and D. W. H. Rankin*<br>Manuscript in preparation. |
| **$C_{12}Fe_3O_{12}$**<br>$Fe_3(CO)_{12}$ | **Dodecacarbonyltriiron**<br>Structure by ED and ab initio calculations<br>*G. R. Kafka, S. L. Masters, D. W. H. Rankin et al.*<br>Manuscript in preparation. |
| **$C_{12}H_{30}Ga_2O_2$**<br>$[Me_2GaOtBu]_2$ | **Di-μ-tert-butoxytetramethyldigallium**<br>Structure by ED and ab initio calculations<br>*D. A. Wann, C. E. Knapp, C. J. Carmalt, H. E. Robertson, D. W. H. Rankin et al.*<br>Manuscript in preparation. |
| **$C_{12}H_{32}Ga_2N_2O_2$**<br>$[Me_2Ga(OCH_2CH_2NMe_2)]_2$ | **[Me2Ga(OCH2CH2NMe2)]2**<br>Structure by ED and ab initio calculations<br>*C. E. Knapp, C. J. Carmalt, P. F. McMillan, D. A. Wann, H. E. Robertson and D. W. H. Rankin*<br>Dalton Trans. (2008) 6880-6882 |
| **$C_{16}H_{38}N_4W$**<br>$W(NHBut)_2(NBut)_2$ | **Bis(tert-butylamino)bis(t-butylimido)tungsten**<br>Structure by ED and ab initio calculations<br>*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*<br>Inorg. Chem. **48** (2009) 2289-2299 |
| **$C_{18}H_{54}O_{15}Si_{12}$**<br>$Si_6O_9(OSiMe_3)_6$ | **Hexa(trimethylsiloxy)silsesquioxane**<br>Equilibrium structure by GED with vibrational corrections from molecular dynamics<br>*D. A. Wann, A. M. Reilly, F. Rataboul, P. D. Lickiss and D. W. H. Rankin*<br>Z. Naturforsch. B **64** (2009) 1269-1275 |