

## Chemistry Publications 2007

1. Palmer, MH; Walker, IC  
The electronic states of but-2-yne studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio configuration interaction methods  
CHEMICAL PHYSICS, **2007**, *340*, 158-170
2. Leyva-Bailen, P; Powell, AV; Vaqueiro, P  
Ethylenediammonium tetraaquabis(sulfato)cobaltate(II)  
ACTA CRYSTALLOGRAPHICA SECTION E-STRUCTURE REPORTS ONLINE , **2007**, *63*, M2643-M178
3. Li, X; Bowen, KH; Haranczyk, M; Bachorz, RA; Mazurkiewicz, K; Rak, J; Gutowski, M  
Photoelectron spectroscopy of adiabatically bound valence anions of rare tautomers of the nucleic acid bases  
JOURNAL OF CHEMICAL PHYSICS, **2007**, *127*, 174309
4. Smith, KJ; Baillie, GS; Hyde, EI; Li, X; Houslay, TM; McCahill, A; Dunlop, AJ; Bolger, GB; Klusmann, E; Adams, DR; Houslay, MD  
H-1 NMR structural and functional characterisation of a cAMP-specific phosphodiesterase-4D5 (PDE4D5) N-terminal region peptide that disrupts PDE4D5 interaction with the signalling scaffold proteins, arrestin and RACK1  
CELLULAR SIGNALLING, **2007**, *19*, 2612-2624
5. Adebambo, KF; Zanolli, S; Thomas, MG; Cancio, R; Howarth, NM; Maga, G  
N-2-Benzyloxycarbonylguan-9-yl acetic acid derivatives as HIV-1 reverse transcriptase non-nucleoside inhibitors with decreased loss of potency against common drug-resistance mutations  
CHEMMEDCHEM, **2007**, *2*, 1405-1409
6. Allan, M; Bagot, PAJ; Costen, ML; McKendrick, KG  
Temperature dependence of OH yield, translational energy, and vibrational branching in the reaction of O(<sup>3</sup>P)(g) with liquid squalane  
JOURNAL OF PHYSICAL CHEMISTRY C, **2007**, *111*, 14833-14842
7. Devereux, M; O'Shea, D; O'Connor, M; Grehan, H; Connor, G; McCann, M; Rosair, G; Lyng, F; Kellett, A; Walsh, M; Egan, D; Thati, B  
Synthesis, catalase, superoxide dismutase and antitumour activities of copper(II) carboxylate complexes incorporating benzimidazole, 1,10-phenanthroline and bipyridine ligands: X-ray crystal structures of [Cu(BZA)<sub>2</sub>(bipy)(H<sub>2</sub>O)], [Cu(SalH)<sub>2</sub>(BZDH)<sub>2</sub>] and [Cu(CH<sub>3</sub>COO)<sub>2</sub>(5,6-DMBZDH)<sub>2</sub>] (SalH<sub>2</sub> = salicylic acid; BZAH = benzoic acid; BZDH = benzimidazole and 5,6-DMBZDH=5,6-dimethylbenzimidazole)  
POLYHEDRON, **2007**, *26*, 4073-4084
8. Powell, AV; McDowall, A; Szkoda, I; Knight, KS; Kennedy, BJ; Vogt, T  
Cation substitution in defect thiospinels: Structural and magnetic properties of GaV<sub>4-x</sub>Mo<sub>x</sub>S<sub>8</sub> (0 ≤ x ≤ 4)  
CHEMISTRY OF MATERIALS, **2007**, *19*, 5035-5044
9. Haranczyk, M; Miller, JH; Gutowski, M  
Differences in electrostatic potential around DNA fragments containing adenine and 8-oxo-adenine  
An analysis based on regular cylindrical projection  
JOURNAL OF MOLECULAR GRAPHICS & MODELLING, **2007**, *26*, 282-289

10. Allan, M; Bagot, PAJ; Kohler, SPK; Reed, SK; Westacott, RE; Costen, ML; McKendrick, KG  
Dynamics of interfacial reactions between O(<sup>3</sup>P) atoms and long-chain liquid hydrocarbons  
PHYSICA SCRIPTA, **2007**, 76, C42-C47
11. Zlatogorsky, S; Edie, MJ; Ellis, D; Erhardt, S; Lopez, ME; Macgregor, SA; Rosair, GM; Welch, AJ  
The mechanism of reduction and metalation of para carboranes: The missing 13-Vertex MC<sub>2</sub>B<sub>10</sub>  
isomer  
ANGEWANDTE CHEMIE-INTERNATIONAL EDITION, **2007**, 46, 6706-6709
12. Marinakis, S; Paterson, G; Klos, J; Costen, ML; McKendrick, KG  
Inelastic scattering of OH(X<sup>2</sup>Π) with Ar and He: a combined polarization spectroscopy and quantum  
scattering study  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **2007**, 9, 4414-4424
13. Mazurkiewicz, K; Haranczyk, M; Gutowski, M; Rak, J  
Can an excess electron localize on a purine moiety in the adenine-thymine Watson-Crick base pair? A  
computational study  
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, **2007**, 107, 2224-2232
14. Li, G; Mong, S; Jiang, S; Ragupathy, L; Cowie, JMG; Ferguson, R; Arrighi, V  
Miscibility of blends of bisphenol-a-polycarbonate and poly(styrene-co-acrylonitrile-co-  
hydroxystyrene) terpolymer  
JOURNAL OF APPLIED POLYMER SCIENCE, **2007**, 106, 944-949
15. Mal, D; Koner, S; Tuchagues, JP; Rosair, GM  
Encapsulation of [Mn(bpy)<sub>3</sub>]<sup>2+</sup> cations in 2D [Mn(dca)<sub>3</sub>]<sup>-</sup> sheet: Synthesis, X-ray structure and EPR  
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INORGANICA CHIMICA ACTA, **2007**, 360, 3575-3580
16. Vaqueiro, P; Romero, ML  
[Ga<sub>10</sub>S<sub>16</sub>(NC<sub>7</sub>H<sub>9</sub>)<sub>4</sub>]<sup>2-</sup>: a hybrid supertetrahedral nanocluster  
CHEMICAL COMMUNICATIONS, **2007**, 3282-3284
17. Vaqueiro, P; Romero, ML  
catena-Poly[piperazinium di-μ-sulfido-gallium]  
ACTA CRYSTALLOGRAPHICA SECTION E-STRUCTURE REPORTS ONLINE, **2007**, 63,  
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18. Wagner, T; Powell, AV; Zima, V  
7th International Conference of Solid State Chemistry 2006 (SSC) – Preface  
JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS, **2007**, 68, 673-674
19. Powell, AV; Engin, TE; Vaqueiro, P; Hull, S  
Simultaneous diffraction and resistance measurements of metal sulphides  
JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS, **2007**, 68, 1052-1056
20. Lees, RJE; Powell, AV; Chippindale, AM  
The synthesis and characterisation of four new antimony sulphides incorporating transition-metal  
complexes  
JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS, **2007**, 68, 1215-1219
21. Vaqueiro, P; Romero, ML  
Three-dimensional gallium sulphide open frameworks  
JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS, **2007**, 68, 1239-1243

22. Devereux, M; Shea, DO; Kellett, A; McCann, M; Walsh, M; Egan, D; Deegan, C; Kgdziora, K; Rosair, G; Muller-Bunz, H  
Synthesis, X-ray crystal structures and biomimetic and anticancer activities of novel copper(II)benzoate complexes incorporating 2-(4'-thiazolyl)benzimidazole (thiabendazole), 2-(2-pyridyl)benzimidazole and 1,10-phenanthroline as chelating nitrogen donor ligands  
JOURNAL OF INORGANIC BIOCHEMISTRY, **2007**, *101*, 881-892
23. Arnbjerg, J; Paterson, MJ; Nielsen, CB; Jorgensen, M; Christiansen, O; Ogilby, PR  
One- and two-photon photosensitized singlet oxygen production: Characterization of aromatic ketones as sensitizer standards  
JOURNAL OF PHYSICAL CHEMISTRY A, **2007**, *111*, 5756-5767
24. Macgregor, SA; Vadivelu, P  
Computational studies on the stabilities of trans-[Ir(OMe)(CO)(PPh<sub>3</sub>)<sub>2</sub>] and trans-[Ir(CH<sub>2</sub>Me)(CO)(PPh<sub>3</sub>)<sub>2</sub>] toward beta-H elimination  
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25. Jana, AD; Manna, SC; Rosair, GM; Drew, MGB; Mostafa, G; Chaudhuri, NR  
4,4'-Dipyridyl-N,N'-dioxide complexes of metal-thiocyanate/selenocyanate:  $\pi$ -stacked molecular rods as three-dimensional support for two-dimensional polymeric sheets and intra/interchain S $\cdots$ S interaction dependent architecture of the R-2(2)(8) synthon driven assembly of one-dimensional polymeric chains  
CRYSTAL GROWTH & DESIGN, **2007**, *7*, 1365-1372
26. Jaffe, JE; Bachorz, RA; Gutowski, M  
Band offset and magnetic property engineering for epitaxial interfaces: A monolayer of M<sub>2</sub>O<sub>3</sub> (M=Al,Ga,Sc,Ti,Ni) at the  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>/ $\alpha$ -Cr<sub>2</sub>O<sub>3</sub> (0001) interface  
PHYSICAL REVIEW B, **2007**, *75*, 205323
27. Lopez, ME; Edie, MJ; Ellis, D; Horneber, A; Macgregor, SA; Rosair, GM; Welch, AJ  
Symmetric and asymmetric 13-vertex bimetalliccarboranes by polyhedral expansion  
CHEMICAL COMMUNICATIONS, **2007**, 2243-2245
28. Alexander, AM; Bria, M; Brunklaus, G; Caldwell, S; Cooke, G; Garety, JF; Hewage, SG; Hocquel, Y; McDonald, N; Rabani, G; Rosair, G; Smith, BO; Spiess, HW; Rotello, VM; Woisel, P  
Probing the solvent-induced tautomerism of a redox-active ureidopyrimidinone  
CHEMICAL COMMUNICATIONS, **2007**, 2246-2248
29. Barzanti, C; Evans, R; Fouquet, J; Gouzin, L; Howarth, NM; Kean, G; Levet, E; Wang, D; Wayemberg, E; Yeboah, AA; Kraft, A  
Potentiometric determination of octanol-water and liposome-water partition coefficients (log *P*) of ionizable organic compounds  
TETRAHEDRON LETTERS, **2007**, *48*, 3337-3341
30. Walker, IC; Holland, DMP; Shaw, DA; McEwen, IJ; Guest, MF  
The electronic states of cyclopropane studied by VUV absorption and ab initio multireference configuration interaction calculations  
JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS, **2007**, *40*, 1875-1888
31. Lee, JK; Anderson, MW; Gray, FA; John, P  
Fabrication of spherical diamond microshells  
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32. Palmer, MH; Ganzenmuller, G; Walker, IC  
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33. Baillie, GS; Adams, DR; Bhari, N; Houslay, TM; Vadrevu, S; Meng, D; Li, X; Dunlop, A; Milligan, G; Bolger, GB; Klusmann, E; Houslay, MD  
Mapping binding sites for the PDE4D5 cAMP-specific phosphodiesterase to the N- and C-domains of beta-arrestin using spot-immobilized peptide arrays  
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34. Sen, S; Mitra, S; Hughes, DL; Rosair, G; Desplanches, C  
Two new pseudohalide bridged di- and poly-nuclear copper(II) complexes: Synthesis, crystal structures and magnetic studies  
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35. Zlatogorsky, S; Ellis, D; Rosair, GM; Welch, AJ  
Unexpectedly facile isomerisation of  $[7,10\text{-Ph}_2\text{-}7,10\text{-nido-C}_2\text{B}_{10}\text{H}_{10}]^{2-}$  to  $[7,9\text{-Ph}_2\text{-}7,9\text{-nido-C}_2\text{B}_{10}\text{H}_{10}]^{2-}$   
CHEMICAL COMMUNICATIONS, **2007**, 2178-2180
36. Arnbjerg, J; Jimenez-Banzo, A; Paterson, MJ; Nonell, S; Borrell, JI; Christiansen, O; Ogilby, PR  
Two-photon absorption in tetraphenylporphycenes: Are porphycenes better candidates than porphyrins for providing optimal optical properties for two-photon photodynamic therapy?  
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **2007**, *129*, 5188-5199
37. Yakovkin, IN; Gutowski, M  
Driving force for the  $\text{WO}_3(001)$  surface relaxation  
SURFACE SCIENCE, **2007**, *601*, 1481-1488
38. Richmond, G; Costen, ML; McKendrick, KG  
The effects of energy-level resonance on collision-induced electronic energy transfer:  $\text{CD}(A^2\Delta \leftrightarrow B^2\Sigma^-)$  coupling  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **2007**, *9*, 1568-1578
39. Haranczyk, M; Gutowski, M; Li, X; Bowen, KH  
Bound anionic states of adenine  
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Quantum mechanical energy-based screening of combinatorially generated library of tautomers. TauTGen: A tautomer generator program  
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41. Dalby, KJ; Ellis, D; Erhardt, S; McIntosh, RD; Macgregor, SA; Rae, K; Rosair, GM; Settels, V; Welch, AJ; Hodson, BE; McGrath, TD; Stone, FGA  
The conformations of 13-vertex  $\text{ML}_2\text{C}_2\text{B}_{10}$  metallocarboranes: Experimental and computational studies  
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **2007**, *129*, 3302-3314

42. Li, J; Kathmann, SM; Schenter, GK; Gutowski, M  
Isomers and conformers of  $H(NH_2BH_2)_nH$  oligomers: Understanding the geometries and electronic structure of boron-nitrogen-hydrogen compounds as potential hydrogen storage materials  
JOURNAL OF PHYSICAL CHEMISTRY C, **2007**, *111*, 3294-3299
43. Bachorz, RA; Klopper, W; Gutowski, M  
Coupled-cluster and explicitly correlated perturbation-theory calculations of the uracil anion  
JOURNAL OF CHEMICAL PHYSICS, **2007**, *126*, 085101
44. Macgregor, SA; Wondimagegn, T  
Mechanism of the  $[RhF(PPh_3)_3]$  to  $cis-[RhPh(PPh_3)_2(PFPh_2)]$  interconversion: P-C activation and F/Ph exchange via a metallophosphorane pathway  
ORGANOMETALLICS, **2007**, *26*, 1143-1149
45. Ragupathy, L; Arrighi, V; Cowie, JMG; Ferguson, R; McEwen, IJ; Shenoy, SL  
Miscibility study of stereoregular poly(methyl methacrylate) blends. Experimental determination of phase diagrams and predictions  
MACROMOLECULES, **2007**, *40*, 1667-1674
46. Biswas, M; Rosair, GM; Pilet, G; Mitra, S  
Syntheses, structures and magnetic properties of  $[M^{II}(dca)_2(CH_3OH)_2]_n$ , where  $M = Co$  or  $Cu$  and  $dca^- = dicyanamide, N(CN)_2^-$   
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47. Alagappan, A; Ballingall, I; Costen, ML; McKendrick, KG; Paterson, G  
Efficiencies of state and velocity-changing collisions of superthermal  $CN A^2\Pi$  with He, Ar,  $N_2$  and  $O_2$   
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48. Haranczyk, M; Gutowski, M  
Differences in electrostatic potential around DNA fragments containing guanine and 8-oxo-guanine  
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51. Macgregor, SA  
Transition metal-mediated P-C/X exchange at bound phosphine ligands (X = aryl, alkyl,  $NR_2$ , OR and F): scope and mechanisms  
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53. Biswas, M; Rosair, GM; Pilet, G; El Fallah, MS; Ribas, J; Mitra, S  
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POLYHEDRON, **2007**, *26*, 123-132

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Variance in molecular and crystalline architectures with pseudohalides  
INORGANIC CHEMISTRY COMMUNICATIONS, **2007**, *10*, 61-65
55. Danopoulos, AA; Tsoureas, N; Macgregor, SA; Smith, C  
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ORGANOMETALLICS, **2007**, *26*, 253-263
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**2007**, *63*, M27-M29
57. Costen, ML; Hall, GE  
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64. Tao SW; Irvine JTS  
Conductivity studies of dense yttrium-doped BaZrO<sub>3</sub> sintered at 1325 C  
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645. Power, NP; Dalgarno, SJ; Atwood, JL  
Guest and ligand behavior in zinc-seamed pyrogallol[4]arene molecular capsules  
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