

## Chemistry Publications 2006

1. Christiansen, O; Kongsted, J; **Paterson, MJ**; Luis, JM.  
Linear response functions for a vibrational configuration interaction state  
*JOURNAL OF CHEMICAL PHYSICS*, *125*, 214309 (2006)
2. Mazurkiewicz, K; Bachorz, RA; **Gutowski M**; Rak, J.  
On the unusual stability of valence anions of thymine based on very rare tautomers: A computational study  
*JOURNAL OF PHYSICAL CHEMISTRY B*, *110*, 24696-24707 (2006)
3. **Paterson, MJ**; Kongsted, J; Christiansen, O; Mikkelsen, KV; Nielsen, CB.  
Two-photon absorption cross sections: An investigation of solvent effects. Theoretical studies on formaldehyde and water  
*JOURNAL OF CHEMICAL PHYSICS*, *125*, 184501 (2006)
4. Ling, SL; Yu, WB; Huang, ZJ; Lin, J; **Gutowski M**.  
Gaseous arginine conformers and their unique intramolecular interactions  
*JOURNAL OF PHYSICAL CHEMISTRY A*, *110*, 12282-12291 (2006)
5. **Ferguson, R; Arrighi, V; McEwen, IJ**; Gagliardi, S; Triolo, A.  
An improved algorithm for the Fourier integral of the KWW function and its application to neutron scattering and dielectric data  
*JOURNAL OF MACROMOLECULAR SCIENCE PART B-PHYSICS*, *45*, 1065-1081 (2006)
6. Chakraborty, J; Samanta, B; **Rosair, GM**; Gramlich, V; El Fallah, MS; Ribas, J; Matsusita, T; Mitra, S.  
Two new hydrothermally synthesised L-M-L type cobalt(II) hydrogen bonded co-ordination complexes with mixed ligands: Characterisation and magneto-structural correlation  
*POLYHEDRON*, *25*, 3006-3016 (2006)
7. Padar, P; Bokros, A; Paragi, G; Forgo, P; Kele, Z; **Howarth, NM**; Kovacs, L.  
Single diastereomers of polyhydroxylated 9-oxa-1-azabicyclo[4.2.1] nonanes from intramolecular 1,3-dipolar cycloaddition of omega-unsaturated nitrones  
*JOURNAL OF ORGANIC CHEMISTRY*, *71*, 8669-8672 (2006)
8. Majumder, A; Gramlich, V; **Rosair, GM**; Batten, SR; Masuda, JD; El Fallah, MS; Ribas, J; Sutter, JP; Desplanches, C; Mitra, S.  
Five new cobalt(II) and copper(II)-1,2,4,5-benzenetetracarboxylate supramolecular architectures: Syntheses, structures, and magnetic properties  
*CRYSTAL GROWTH & DESIGN*, *6*, 2355-2368 (2006)
9. Zhang, CH; **Arrighi, V**; Gagliardi, S; **McEwen, IJ**; Tanchawanich, J; Telling, MTF; Zanotti, JM.  
Quasielastic neutron scattering measurements of fast process and methyl group dynamics in glassy poly(vinyl acetate)  
*CHEMICAL PHYSICS*, *328*, 53-63 (2006)
10. **Howarth, NM**.  
Recent advances in the field of peptide nucleic acids  
*LETTERS IN ORGANIC CHEMISTRY*, *3*, 495-503 (2006)

11. Al-Duaij, O; Davies, DL; **Macgregor, SA**; Donald, SMA.  
Acetate-assisted cyclometalation, an experimental and computational study of the mechanism  
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 231, 653-INOR (2006)
12. Shaw, DA; Holland, DMP; **Walker, IC**  
Ion-pair formation mechanisms in chloromethane, bromomethane and dichlorodifluoromethane  
JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS, 39, 3549-3560 (2006)
13. Lee, JK; Anderson, MW; Gray, FA; **John, P.**  
Explosive oxidation of HPHT diamond particles  
DIAMOND AND RELATED MATERIALS, 15, 1206-1209 (2006)
14. Bolger, GB; Baillie, GS; Li, X; Lynch, MJ; Herzyk, P; Mohamed, A; Mitchell, LH; McCahill, A; Hundsucker, C; Klussmann, E; **Adams, DR**, Houslay, MD.  
Scanning peptide array analyses identify overlapping binding sites for the signalling scaffold proteins, beta-arrestin and RACK1, in cAMP-specific phosphodiesterase PDE4D5  
BIOCHEMICAL JOURNAL, 398, 23-36 (2006)
15. Hornyak, M; Kele, Z; Kovacs, L; Forgo, P; **Howarth, NM.**  
Investigation of 1,3-dipolar cycloaddition reactions of unsaturated nitrones in ionic liquids  
NUCLEOSIDES NUCLEOTIDES & NUCLEIC ACIDS, 25, 867-870 (2006)
16. McIntosh, RD; Ellis, D; Giles, BT; **Macgregor, SA**; **Rosair, GM**; **Welch, AJ.**  
Mapping the pathway of heteroborane isomerisation: Two parallel "1,2 → 1,7" isomerisations of a crowded molybdacarborane and the isolation of isomerisation intermediates  
INORGANICA CHIMICA ACTA, 359, 3745-3753 (2006)
17. Rabani, G; Luftmann, H; **Kraft, A.**  
Synthesis and characterization of two shape-memory polymers containing short aramid hard segments and poly( $\epsilon$ -caprolactone) soft segments  
POLYMER, 47, 4251-4260 (2006)
18. **Vaqueiro, P.**  
3-[4-(3-aminopropyl)piperazin-1-yl]propan-1-aminium chloride  
ACTA CRYSTALLOGRAPHICA SECTION E-STRUCTURE REPORTS ONLINE, 62, o2632-o2633 (2006)
19. **Vaqueiro, P**; Sobany, GG; **Powell, AV**; Knight, KS.  
Structure and thermoelectric properties of the ordered skutterudite CoGe<sub>1.5</sub>Te<sub>1.5</sub>  
JOURNAL OF SOLID STATE CHEMISTRY, 179, 2047-2053 (2006)
20. McIntosh, RD; Ellis, D; **Rosair, GM**; **Welch, AJ.**  
A 15-vertex heteroborane  
ANGEWANDTE CHEMIE-INTERNATIONAL EDITION, 45, 4313-4316 (2006)
21. **Arrighi, V**; **Cowie, JMG**; **Ferguson, R**; **McEwen, IJ**; McGonigle, EA; Pethrick, RA; Princi, E.  
Physical ageing in poly(4-hydroxy styrene)/poly(vinyl methyl ether) blends

POLYMER INTERNATIONAL, 55, 749-756 (2006)

22. Kohler, SPK; Reed, SK; Westacott, RE; **McKendrick, KG**.  
Molecular dynamics study to identify the reactive sites of a liquid squalane surface  
JOURNAL OF PHYSICAL CHEMISTRY B, 110, 11717-11724 (2006)
23. Ampt, KAM; Burling, S; Donald, SMA; Douglas, S; Duckett, SB; **Macgregor, SA**; Perutz, RN; Whittlesey, MK.  
Photochemical isomerization of N-heterocyclic carbene ruthenium hydride complexes:  
In situ photolysis, parahydrogen, and computational studies  
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 128, 7452-7453 (2006)
24. Tominey, A; Andrew, D; Oliphant, L; **Rosair, GM**; Dupré, J; **Kraft, A**.  
Supramolecular binding of protonated amines to a receptor microgel in aqueous medium  
CHEMICAL COMMUNICATIONS, 2492-2494 (2006)
25. Majumder, A; **Rosair, GM**; Mallick, A; Chattopadhyay, N; Mitra, S.  
Synthesis, structures and fluorescence of nickel, zinc and cadmium complexes with the  
N,N,O-tridentate Schiff base N-2-pyridylmethylidene-2-hydroxy-phenylamine  
POLYHEDRON, 25, 1753-1762 (2006)
26. Jones, RVH; **Lindsell, WE**; Paddon-Jones, GC; Palmer, DD; **Preston, PN**; **Rosair, GM**; Whitton, AJ.  
Studies of reactions of *o*-xylylene- $\alpha,\alpha'$ -dihalides with palladium complexes and the  
catalytic synthesis of 3-isochromanone  
JOURNAL OF ORGANOMETALLIC CHEMISTRY, 691, 2378-2385 (2006)
27. **Vaqueiro, P.**  
From one-dimensional chains to three-dimensional networks: Solvothermal synthesis of  
thiogallates in ethylenediamine  
INORGANIC CHEMISTRY, 45, 4150-4156 (2006)
28. **Powell, AV**; Lees, RJE; Chippindale, AM  
Macroyclic amines as structure-directing agents for the synthesis of three-dimensional  
antimony-sulfide frameworks  
INORGANIC CHEMISTRY, 45, 4261-4267 (2006)
29. Das, A; **Rosair, GM**; El Fallah, MS; Ribas, J; Mitra, S.  
Weak metamagnetic-like 1D manganese(II) complex with a double  $\mu_{1,1}$ -azido bridge: A  
structure and magnetic study  
INORGANIC CHEMISTRY, 45, 3301-3306 (2006)
30. Griesbaum, K; Frank, A; **McCullough, KJ**.  
syn- and anti-isomers of a O-methyloxime-substituted tricyclic ozonide  
EUROPEAN JOURNAL OF ORGANIC CHEMISTRY, 1978-1980 (2006)
31. Alagappan, A; **Costen, ML**; **McKendrick, KG**.  
Frequency modulated spectroscopy as a probe of molecular collision dynamics  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR  
SPECTROSCOPY, 63, 910-922, (2006)
32. Davies, DL; Donald, SMA; Al-Duaij, O; **Macgregor, SA**; Polleth, M.  
Electrophilic C-H activation at {Cp\*Ir}: Ancillary-ligand control of the mechanism of  
C-H activation  
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 128, 4210-4211 (2006)

33. Tominey, AF; Docherty, PH; **Rosair, GM**; Quenardelle, R; **Kraft, A.**  
Unusually weak binding interactions in tetrazole-amidine complexes  
ORGANIC LETTERS, 8, 1279-1282 (2006)
34. Cooke, G; Woisel, P; Bria, M; Delattre, F; Garety, JF; Hewage, SG; Rabani, G; **Rosair, GM.**  
A tuneable self-complexing molecular switch  
ORGANIC LETTERS, 8, 1423-1426 (2006)
35. Sen, S; Talukder, P; Dey, SK; Mitra, S; **Rosair, GM**; Hughes, DL; Yap, GPA; Pilet, G;  
Gramlich, V; Matsushita, T.  
Ligating properties of a potentially tetradeinate Schiff base  
[(CH<sub>3</sub>)<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>N=CHC<sub>6</sub>H<sub>3</sub>(OH)(OMe)] with zinc(II), cadmium(II), cobalt(II),  
cobalt(III) and manganese(III) ions: synthesis and structural studies  
DALTON TRANSACTIONS, 1758-1767 (2006)
36. Ellis, D; Garrioch, RM; **Rosair, GM**; **Welch, AJ.**  
Isomerisation following the platination of [7,8-Ph<sub>2</sub>-9,11-I<sub>2</sub>-7,8-*nido*-C<sub>2</sub>B<sub>9</sub>H<sub>7</sub>]<sup>2-</sup>  
POLYHEDRON, 25, 915-922 (2006)
37. Kohler, SPK; Allan, M; **Costen, ML**; **McKendrick, GM.**  
Direct gas-liquid interfacial dynamics: The reaction between O(P-3) and a liquid  
hydrocarbon  
JOURNAL OF PHYSICAL CHEMISTRY B, 110, 2771-2776 (2006)
38. Jazzar, RFR; Varrone, M; Burrows, AD; **Macgregor, SA**; Mahon, MF; Whittlesey, MK.  
Synthesis and isomerisation of two metallated N,O-complexes of ruthenium: Models for  
the Murai reaction  
INORGANICA CHIMICA ACTA, 359, 815-820 (2006)
39. Christie, RM; Hill, JM; **Rosair, GM.**  
The crystal structure of CI Pigment Yellow 97, a superior performance Hansa yellow  
pigment  
DYES AND PIGMENTS, 71, 194-198 (2006)
40. **Vaqueiro, P.**  
Solvothermal synthesis and characterisation of new one-dimensional indium and gallium  
sulphides: [C<sub>10</sub>N<sub>4</sub>H<sub>26</sub>]<sub>0.5</sub>[InS<sub>2</sub>] and [C<sub>10</sub>N<sub>4</sub>H<sub>26</sub>]<sub>0.5</sub>[GaS<sub>2</sub>]  
JOURNAL OF SOLID STATE CHEMISTRY, 179, 302-307 (2006)
41. Chatwin, SL; Davidson, MG; Doherty, C; Donald, SM, Jazzar, RFR; **Macgregor, SA**;  
McIntyre, GJ; Mahon, MF; Whittlesey, MK.  
H-X bond activation via hydrogen transfer to hydride in ruthenium N-heterocyclic  
carbene complexes: Density functional and synthetic studies  
ORGANOMETALLICS, 25, 99-110 (2006)
42. **Paterson, MJ**; Christiansen, O; Jensen, F; Ogilby, PR.  
Invited review - Overview of theoretical and computational methods applied to the  
oxygen-organic molecule photosystem  
PHOTOCHEMISTRY AND PHOTOBIOLOGY, 82, 1136-1160, (2006)
43. Pinna, R; Jamme, F; Rutten, FJM; Smith, EF; Willis, MR; Briggs, D; **McCoustra, MRS.**

Towards a fully optimised organic LED device: Analysis of surface synthesis using coupling reactions by ToF-SIMS  
APPLIED SURFACE SCIENCE, 252, 6672-6675, (2006)

44. **Gutowski M**; Bachorz, RA; Li, J; Schenter, GK; Kathmann, SM.  
Understanding of hydrogen storage in the NBH<sub>x</sub> materials through computational studies  
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 231, 252-IEC, (2006)
45. **Gutowski M**; Dabkowska, I; Haranczyk, M; Bachorz, RA; Golebiowska, M; Storoniak, P; Rak, J.  
Proton transfer driven by excess charge as a trigger of chemical transformations  
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 231, 91-PHYS, (2006)
46. **Gutowski M**; Autrey, T.  
On-board Hydrogen Storage, Bottleneck to the Hydrogen Economy?  
CHEMISTRY WORLD, 3, 44-48, (2006)
47. Bearpark, MJ; Blancafort, L; **Paterson, MJ**.  
Mapping the intersection space of the ground and first excited states of fulvene  
MOLECULAR PHYSICS, 104, 1033-1038, (2006)
48. Worth, GA; Welch, G; **Paterson, MJ**.  
Wavepacket dynamics study of Cr(CO)<sub>5</sub> after formation by photodissociation: relaxation through an (E ⊕ A) ⊗ e Jahn-Teller conical intersection  
MOLECULAR PHYSICS, 104, 1095-1105, (2006)
49. **Paterson, MJ**; Christiansen, O; Pawlowski, F; Jørgensen, P; Hättig, C; Helgaker, T; Salek, P.  
Benchmarking two-photon absorption with CC3 quadratic response theory, and comparison with density-functional response theory  
JOURNAL OF CHEMICAL PHYSICS, 124, 054322, (2006)
50. Palumbo, ME; Baratta, GA; Collings, MP; **McCoustra, MRS**.  
The profile of the 2140 cm<sup>-1</sup> solid CO band on different substrates  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 8, 279-284, (2006)
51. Davies, DL; Donald, SMA; Al-Duaij, O; Fawcett, J; Little, C; **Macgregor, SAM**.  
N-H versus C-H activation of a pyrrole imine at {Cp\*Ir}: A computational and experimental study  
ORGANOMETALLICS, 25, 5976-5978 (2006)
52. Turner, DR; **Paterson, MJ**; Steed, JW.  
A conformationally flexible, urea-based tripodal anion receptor: Solid-state, solution and theoretical studies  
JOURNAL OF ORGANIC CHEMISTRY, 71, 1598-1608, (2006)
53. **John, P**; Lee, J-K; Anderson, M; Gray, F; Wilson, JIB.  
The fabrication of diamond microshells  
CHEMICAL VAPOUR DEPOSITION, 12, 714-717 (2006)
54. **Kraft, A**; Tominey, A; Andrew, D; Dupré, J; McIver, A; Oliphant, L; **Rosair, GM**; Otto, S.

Supramolecular binding of protonated amines to functionalized microgel particles  
POLYMER PREPRINTS, 4, 937-938, (2006)

55. **Kraft, A.**  
Advanced Materials Highlights  
CHEMISTRY & INDUSTRY, (3) 32-33 (2006)
56. **Kraft, A.**  
Advanced Materials Highlights  
CHEMISTRY & INDUSTRY, (7) 30-31 (2006)
57. **Kraft, A.**  
Advanced Materials Highlights  
CHEMISTRY & INDUSTRY, (11) 26-27 (2006)
58. **Kraft, A.**  
Advanced Materials Highlights  
CHEMISTRY & INDUSTRY, (15) 28-29 (2006)
59. **Kraft, A.**  
Advanced Materials Highlights  
CHEMISTRY & INDUSTRY, (19) 30-31 (2006)
60. **Kraft, A.**  
Advanced Materials Highlights  
CHEMISTRY & INDUSTRY, (23) 26-27 (2006)
61. **Vaqueiro, P.**  
Solvothermal synthesis and thermoelectric properties on new complex tellurides  
PROCEEDINGS OF 4<sup>TH</sup> EUROPEAN CONFERENCE ON THERMOELECTRICS, 30 (2006)
62. Cooper, IE; **McCoustra, MRS**; Chesters, MA.  
Dynamical studies of the dissociation of some primary alkanes on Pt(111)  
CIENCIA, 14, 96-103 (2006)
63. Green, S; Collings, MP; El-Shall, S; Mautner, M; **McCoustra, MRS**.  
Silicate Nanoparticles as Laboratory Models for the Interstellar Silicate Grain Population: Synthesis and Characterisation.  
FARADAY DISCUSS. CHEM. SOC., 133, 103-112 (2006)
64. **McCoustra, MRS**.  
Questions in the general discussion  
FARADAY DISCUSS. CHEM. SOC., 133, 90 (2006)  
FARADAY DISCUSS. CHEM. SOC., 133, 348 (2006)
65. **McCoustra, MRS**.  
Comments in the general discussion  
FARADAY DISCUSS. CHEM. SOC., 133, 97 (2006)  
FARADAY DISCUSS. CHEM. SOC., 133, 191-195 (2006)  
FARADAY DISCUSS. CHEM. SOC., 133, 208-211 (2006)  
FARADAY DISCUSS. CHEM. SOC., 133, 367 (2006)  
FARADAY DISCUSS. CHEM. SOC., 133, 373 (2006)

66. Mei, D; **Gutowski M**; Neurock, N; Yang, Y; Disselkamp, R; Campbell, CT. Development of microkinetic models for water-gas shift, methanol decomposition, and preferential oxidation of CO in the presence of H<sub>2</sub> reactions PREP. PAP. - AM. CHEM. SOC., DIV. FUEL CHEM., 51, 559 (2006)
67. Li, J; Kathmann, VSM; Schenter, GK; Linehan, JC; Autrey, T; **Gutowski M**. Computational modeling of H(BH<sub>2</sub>NH<sub>2</sub>)<sub>n</sub>H oligomers: Understanding the electronic structures of boron-nitrogen hydrides as potential hydrogen storage materials PREP. PAP. - AM. CHEM. SOC., DIV. FUEL CHEM., 51, 577 (2006)
68. Stowe, AC; **Gutowski M**; Hess, NJ; Autrey, T; Hartl, MA; Daemen, LL. Contributions of neutron scattering to the chemistry of ammonia borane PREP. PAP. - AM. CHEM. SOC., DIV. FUEL CHEM., 51, 582 (2006)
69. **Gutowski M**; Li, J; Schenter, GK; Autrey, T; Linehan, JC. Thermodynamics of hydrogen release from the molecular BNC compounds: A computational study PREP. PAP. - AM. CHEM. SOC., DIV. FUEL CHEM., 51, 586 (2006)
70. **Gutowski, M**; Ge, Q; Yakovkin, I; Bachorz, RA. Theoretical studies of planar model transition metal oxide catalysts ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 232, 116-PHYS (2006)
71. Haranczyk, M; **Gutowski, M**. Quantum mechanical energy-based screening of combinatorially generated library of tautomers ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 232, 64-CINF (2006)
72. Stowe, AC; **Gutowski, M**; Autrey, T; Hess, NJ; Schmid, BA; Daemen, LL; Hartl, M; Proffen, T; Brown, CM; Mamantov, E; Udovic, TJ. Neutron scattering studies of the hydrogen storage material ammonia borane ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 232, 62-Fuel (2006)
73. Heldebrant, DJ; Stowe, AC; Karkamkar, A; Hess, NJ; **Gutowski M**; Linehan, JC; Autrey, T. Spectroscopic investigations of ammonium borohydride and diammoniate of diborane: Evaluating the potential of a hydrogen storage material ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 232, 63-Fuel (2006)
74. Paravanov, V; Camaioni, DM; Li, J; Kathmann, SM; Schenter, GK; **Gutowski M**. Computational studies of materials for hydrogen storage based on boron and nitrogen ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 232, 65-Fuel (2006)