

## Chemistry Publications 2005

1. **Two new octahedral Cd(II) complexes  $[Cd(L)_2]$  and  $\{[Cd(LH)_2(SCN)_2]H_2O\}$  [ $L = C_6H_5C(OH)NN = C(CH_3)C_5H_4N$ ]: Synthesis and structural studies**  
Sen S, Talukder P, **Rosair GM**, Mitra S  
STRUCTURAL CHEMISTRY **16** 605-610 (2005)
2. **Two new 1-D dicyanamide bridged polymeric complexes  $[Mn(\mu_{1,5}-dca)_2(salicyh)_2]_n$  and  $\{[Ni(\mu_{1,5}-dca)(TTA)](ClO_4)\}_n$  ( $dca =$  dicyanamide,  $N(CN)_2^-$ ;  $salicyh =$  salicylic hydrazide; TTA = triethylenetetramine): Synthesis, structures and magnetic studies**  
Sen S, Talukder P, Mitra S, **Rosair GM**, Yap G, Gramlich V, Kim J, Matsushita T, Desplanches U, Sutter JP  
INORGANICA CHIMICA ACTA **358** 4534-4540 (2005)
3. **Directing the structures of silver-antimony sulphides: A new topological variant of the  $[Ag_5Sb_3S_8]^{2-}$  double layer**  
**Powell AV**, Thun J, Chippindale AM  
JOURNAL OF SOLID STATE CHEMISTRY **178** 3414-3419 (2005)
4. **Methylammonium antimony sulfide**  
Lees RJE, **Powell AV**, Chippindale AM  
ACTA CRYSTALLOGRAPHICA SECTION C-CRYSTAL STRUCTURE COMMUNICATIONS **61** M516-M518 (2005)
5. **Probing dipeptide trans/cis stereochemistry using pH control of thiopeptide analogues, and application to the PepT1 transporter**  
Bailey PD, Boyd CAR, Collier ID, Kellett GL, Meredith D, **Morgan KM**, Pettecrew R, Price RA  
ORGANIC & BIOMOLECULAR CHEMISTRY **3** 4038-4039 (2005)
6. **Palladium-catalyzed carbonylation of arylmethyl halides: efficient synthesis of arylacetic acid and esters**  
Jones RVH, **Lindsell WE**, Palmer DD, **Preston PN**, Whitton AJ  
TETRAHEDRON LETTERS **46** 8695-8697 (2005)
7. **The synthesis and characterisation of two new iron thioantimonates:  $[Fe(en)_3]_2Sb_2S_5 \cdot 0.55H_2O$  and  $[Fe(en)_3]_2Sb_4S_8$**   
Lees RJE, **Powell AV**, Chippindale AM  
POLYHEDRON **24** 1941-1948 (2005)
8. **The F/Ph rearrangement reaction of  $[(Ph_3P)_3RhF]$ , the fluoride congener of Wilkinson's catalyst**  
**Macgregor SA**, Roe DC, Marshall WJ, Bloch KM, Bakhmutov VI, Grushin VV  
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **127** 15304-15321 (2005)
9. **Conformational and spacial preferences for substrates of PepT1**  
Bailey PD, Boyd CAR, Collier ID, George JG, Kellett GL, Meredith D, **Morgan KM**, Pettecrew R, Price RA, Pritchard RG  
CHEMICAL COMMUNICATIONS 5352-5354 (2005)

10. An intramolecular 1,3-dipolar cycloaddition reaction towards the synthesis of chiral azetidine nucleoside analogues: The D-gluco case  
Padar P, Forgo P, Kele Z, **Howarth NM**, Kovacs L  
NUCLEOSIDES NUCLEOTIDES & NUCLEIC ACIDS **24** 743-745 (2005)
11. Computational study of the mechanism of cyclometalation by palladium acetate  
Davies DL, Donald SMA, **Macgregor SA**  
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **127** 13754-13755 (2005)
12. A new Cu(II) bridging-carboxylate helical chain polymer: synthesis and structural aspects  
Datta A, Dey DK, Hwang WS, Matsushita T, **Rosair GM**  
JOURNAL OF CHEMICAL RESEARCH-S 502-504 (2005)
13. New polymeric materials for paper and textile conservation. I. Synthesis and characterization of acrylic copolymers  
Princi E, Vicini S, Pedemonte E, **Arrighi V**, McEwen IJM  
JOURNAL OF APPLIED POLYMER SCIENCE **98** 1157-1164 (2005)
14. Lipophilic peptide nucleic acids containing a 1,3-diyne function: synthesis, characterization and production of derived polydiacetylene liposomes  
**Howarth NM**, Lindsell WE, Murray E, Preston PN  
TETRAHEDRON **61** 8875-8887 (2005)
15. A study of the valence shell photoelectron and photoabsorption spectra of  $\text{CF}_3\text{SF}_5$   
Holland DMP, Shaw DA, **Walker IC**, McEwen IJ, Apra E, Guest MF  
JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS **38** 2047-2067 (2005)
16. Muon spin rotation study of magnetism in electron-doped chromium sulfide  
Brooks ML, Blundell SJ, Steer CA, Lancaster T, Pratt FL, **Vaqueiro P**, Powell AV  
PHYSICAL REVIEW B **72** 012419 (2005)
17. The electrochemically-tunable interactions between flavin-functionalised C-60 derivatives and 2,6-diethylamidopyridine  
Carroll JB, **Cooke G**, Garety JF, Jordan BJ, Mabruk S, Rotello VM  
CHEMICAL COMMUNICATIONS 3838-3840 (2005)
18. Photochromic protein substrates  
Shah MRB, Christie RM, **Morgan KM**, Shamey R  
MOLECULAR CRYSTALS AND LIQUID CRYSTALS **431** 535-539 (2005)
19. Intramolecular 1,3-dipolar cycloaddition of unsaturated nitrones derived from methyl alpha-D-glucopyranoside  
Padar P, Hornyak M, Forgo M, Kele Z, Paragi G, **Howarth NM**, Kovacs L  
TETRAHEDRON B 6816-6823 (2005)
20. Model systems for flavoenzyme activity: Site-isolated redox behavior in flavin-functionalized random polystyrene copolymers  
Carroll JB, Jordan BJ, Xu H, Erdogan B, Lee L, Cheng L, Tiernan C, **Cooke G**, Rotello VM

21. **Topotactic oxidation of TiGaPO-1, a pyridine-templated titanium gallophosphate with a new octahedral-tetrahedral 3-D framework structure containing Ti<sup>III</sup>/Ti<sup>IV</sup>**  
Chippindale AM, Grimshaw MR, Powell AV, Cowley AR  
INORGANIC CHEMISTRY **44** 4121-4123 (2005)
22. **Reactions of amines with CVD diamond nanopowders**  
Lee JK, Anderson MW, Gray FA, John P, Lee JY  
DIAMOND AND RELATED MATERIALS **14** 675-678 (2005)
23. **Solvothermal syntheses, crystal structures and properties of five new thloantimonates(III) containing the [Sb<sub>4</sub>S<sub>7</sub>]<sup>2-</sup> anion**  
Puls A, Schaefer M, Nather C, Bensch W, Powell AV, Boissiere S, Chippindale AM  
JOURNAL OF SOLID STATE CHEMISTRY **178** 1171-1181 (2005)
24. **Orientation and alignment moments in two-color polarization spectroscopy**  
Costen ML, McKendrick KG  
JOURNAL OF CHEMICAL PHYSICS **122** 164309 (2005)
25. **Model systems for flavoenzyme activity: a tuneable intramolecularly hydrogen bonded flavin-diamidopyridine complex**  
Boyd ASF, Carroll JB, Cooke G, Garety JF, Jordan BJ, Mabruk S, Rosair G, Rotello VM  
CHEMICAL COMMUNICATIONS 2468-2470 (2005)
26. **Thermopower across the insulator-metal divide in NiCr<sub>2-x</sub>V<sub>x</sub>S<sub>4</sub> (0 < x < 2)**  
Powell AV, Vaqueiro P, Ohtani T  
PHYSICAL REVIEW B **71** 125120 (2005)
27. **Thermal characterisation of cellulose based materials - Investigation of water content**  
Princi E, Vicini S, Pedemonte E, Arrighi V, McEwen IJM  
JOURNAL OF THERMAL ANALYSIS AND CALORIMETRY **80** 369-373 (2005)
28. **Enthalpy relaxation and free volume changes in aged styrene copolymers containing a hydrogen bonding co-monomer**  
McGonigle EA, Cowie JMG, Arrighi V, Pethrick RA  
JOURNAL OF MATERIALS SCIENCE **40** 1869-1881 (2005)
29. **The synthesis and characterisation of 4,1,2-MC<sub>2</sub>B<sub>10</sub> metallacarboranes**  
McIntosh R, Ellis D, Gil-Lostes J, Dalby KJ, Rosair GM, Welch AJ  
DALTON TRANSACTIONS 1842-1846 (2005)
30. **Investigations of benzyl and aryl palladium complexes with pendant hydroxy substituents and their transformation into benzolactones on carbonylation**  
Lindsell WE, Palmer DD, Preston PN, Rosair GM, Jones RVH, Whitton AJ  
ORGANOMETALLICS **24** 1119-1133 (2005)
31. **Towards the mechanism of heteroborane isomerisation: 1,2 → 1,2 and 1,2 → 1,7 low-temperature isomerisations from metallations of [5-I-7,8-Ph<sub>2</sub>-7,8-nido-C<sub>2</sub>B<sub>9</sub>H<sub>8</sub>]<sup>2-</sup>**  
Robertson S, Garrioch RM, Ellis D, McGrath TD, Hodson BE, Rosair GM, Welch AJ  
INORGANICA CHIMICA ACTA **358** 1485-1493 (2005)

32. **Synthetic, spectroscopic, computational and structural studies of some 13-vertex ruthenacarboranes**  
Burke A, Ellis D, Ferrer D, Ormsby DL, **Rosair GM**, Welch AJ  
DALTON TRANSACTIONS 1716-1721 (2005)
33. **Synthesis of C-disaccharide analogues of the alpha-D-arabinofuranosyl-(1 → 5)-alpha-D-arabinofuranosyl motif of mycobacterial cell walls via alkynyl intermediates**  
Aslam T, Fuchs MGG, Le Formal A, **Wightman RH**  
TETRAHEDRON LETTERS **46** 3249-3252 (2005)
34. **Synthesis, structure and luminescence behaviour of complexes of type [Cd(dpa)<sub>2</sub>X<sub>2</sub>]**  
(dpa=2,2'-dipyridylamine; X = N<sub>3</sub><sup>-</sup>, NCS<sup>-</sup>, NCO<sup>-</sup>)  
Chowdhury H, Ghosh R, Rahaman SH, **Rosair GM**, Ghosh BK  
INDIAN JOURNAL OF CHEMISTRY SECTION A-INORGANIC BIO-INORGANIC PHYSICAL THEORETICAL & ANALYTICAL CHEMISTRY **44** 687-692 (2005)
35. **Isolation of a new two-dimensional honeycomb carbonato-bridged copper(II) complex exhibiting long-range ferromagnetic ordering**  
Majumder A, Choudhury CR, Mitra S, **Rosair GM**, El Fallah MS, Ribas J  
CHEMICAL COMMUNICATIONS 2158-2160 (2005)
36. **Enthalpy relaxation in poly(4-hydroxy styrene)/poly(methyl methacrylate) blends**  
Cowie JMG, Arrighi V, McGonigle EA  
MACROMOLECULAR CHEMISTRY AND PHYSICS **206** 767-776 (2005)
37. **Rhodium and iridium complexes of N-(2'-hydroxyphenyl)pyrrole-2-aldimine: Synthesis, structure, and spectral and electrochemical properties**  
Basu S, Pal I, Butcher RJ, **Rosair GM**, Bhattacharya S  
JOURNAL OF CHEMICAL SCIENCES **117** 167-173 (2005)
38. **Fourteen-vertex homo- and heterobimetallic metallacarboranes**  
Ellis D, Lopez ME, McIntosh R, **Rosair GM**, Welch AJ  
CHEMICAL COMMUNICATIONS 1917-1919 (2005)
39. **(η<sup>5</sup>-Cyclopentadienyl)(N,N-dimethyldithiocarbamato-κ S<sub>2</sub>,S'') [η<sup>4</sup>-tetrakis(trifluoromethyl)cyclobutadienyl]-molybdenum(IV)**  
Davidson JL, Jarvie A, Muir KW  
ACTA CRYSTALLOGRAPHICA SECTION C-CRYSTAL STRUCTURE COMMUNICATIONS **61** M209-M210 (2005)
40. **A new one-dimensional coordination polymer [Co(CCl<sub>3</sub>COO)<sub>2</sub>(CH<sub>3</sub>OH)<sub>2</sub>(μ<sub>4,4</sub>-bipy)]<sub>n</sub>:**  
**Synthesis and structural aspects**  
Talukder P, Datta A, Mitra S, **Rosair GM**  
ZEITSCHRIFT FUR NATURFORSCHUNG SECTION B-A JOURNAL OF CHEMICAL SCIENCES **60** 33-36 (2005)
41. **The first 4,1,10-MC<sub>2</sub>B<sub>10</sub> supraicosahedral metallacarboranes and a route to previously inaccessible 4,1,12-ruthenium arene species**  
Ellis D, Lopez ME, McIntosh R, **Rosair GM**, Welch AJ, Quenardelle R  
CHEMICAL COMMUNICATIONS 1348-1350 (2005)

42. **On the difference in scattering behavior of cyclic and linear polymers in bulk**  
Gagliardi S, Arrighi V, Ferguson R, Dagger AC, Semlyen JA, Higgins JS  
JOURNAL OF CHEMICAL PHYSICS **122** 064904 (2005)
43. **Synthesis, optical properties, crystal structures and phase behaviour of symmetric, conjugated ethynylarene-based rigid rods with terminal carboxylate groups**  
Fasina TM, Collings JC, Burke JM, Batsanov AS, Ward RM, Albesa-Jove D, Porres L, Beeby A, Howard JAK, Scott AJ, Clegg W, Watt SW, Viney C, Marder TB  
JOURNAL OF MATERIALS CHEMISTRY **15** 690-697 (2005)
44. **The effects of surface temperature on the gas-liquid interfacial reaction dynamics of O<sup>3</sup>P plus squalane**  
Kohler SPK, Allan M, Kelso H, Henderson DA, McKendrick KG  
JOURNAL OF CHEMICAL PHYSICS **122** 024712 (2005)
45. **Benzyl 2-amino-6-chloro-9H-purine-9-carboxylate**  
Adebambo KF, Howarth NM, Rosair GM  
ACTA CRYSTALLOGRAPHICA SECTION E-STRUCTURE REPORTS ONLINE **61** O486-O488 (2005)
46. **Collision-partner dependence of energy transfer between the CH A<sup>2</sup>Δ and B<sup>2</sup>Σ states**  
Richmond G, Costen ML, McKendrick KG  
JOURNAL OF PHYSICAL CHEMISTRY A **109** 542-553 (2005)
47. **Synthesis of cyclic peroxides by chemo- and regioselective peroxidation of dienes with Co(II)/O<sup>2</sup>/Et<sub>3</sub>SiH**  
Tokuyasu T, Kunikawa S, McCullough KJ, Masuyama A, Nojima M  
JOURNAL OF ORGANIC CHEMISTRY **70** 251-260 (2005)
48. **Synthesis and properties of segmented copolymers containing short aramid hard segments and aliphatic polyester or polycarbonate soft segments**  
Rabani G, Luftmann H, Kraft A  
POLYMER **46** 27-35 (2005)
49. **Reactions of α,ω-dithiolate ligands with bis(cyclopentadienyl)molybdenum dichloride; crystal structures of Mo(η-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>{S(CH<sub>2</sub>)<sub>n</sub>S}{(n=2, 3) and a layered hydrate, Mo(η-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>(SCH<sub>2</sub>CH<sub>2</sub>O)<sub>4.5</sub>H<sub>2</sub>O**  
Lindsell WE, Rosair GM, Rothmann MM  
JOURNAL OF ORGANOMETALLIC CHEMISTRY **690** 126-133 (2005)
50. **The application of molecular modelling techniques in the prediction of the photochromic behaviour of spiroindolinonaphthoxazines**  
Christie RM, Chi LJ, Spark RA, Morgan KM, Boyd ASF, Lycka A  
JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY **169** 37-45 (2005)
51. **Shape-memory polymers containing aramid hard segments and polycaprolactone soft segments**  
Kraft A, Rabani G, Schuh C, Müller K, Lechmann MC

POLYMERIC MATERIALS SCIENCE & ENGINEERING **93** 935-936 (2005)

52. **Advanced Materials Highlights**  
**Kraft A**  
CHEMISTRY & INDUSTRY **(3)** 26-27 (2005)
53. **Advanced Materials Highlights**  
**Kraft A**  
CHEMISTRY & INDUSTRY **(7)** 22-23 (2005)
54. **Advanced Materials Highlights**  
**Kraft A**  
CHEMISTRY & INDUSTRY **(11)** 30-31 (2005)
55. **Advanced Materials Highlights**  
**Kraft A**  
CHEMISTRY & INDUSTRY **(15)** 26-27 (2005)
56. **Advanced Materials Highlights**  
**Kraft A**  
CHEMISTRY & INDUSTRY **(19)** 34-35 (2005)
57. **Advanced Materials Highlights**  
**Kraft A**  
CHEMISTRY & INDUSTRY **(23)** 22-23 (2005)
58. **Hyperfine quantum beats from photolytic orientation and alignment**  
**Costen ML, Hall GE**  
PHYS. CHEM. CHEM. PHYS. **7** 1408-1413 (2005)
59. **Rovibrational energy transfer in the 4v(CH) manifold of acetylene viewed by IR-UV double resonance spectroscopy. 2. Perturbed states with J = 17 and 18**  
Payne MA, Milce AP, Frost MJ, Orr BJ  
JOURNAL OF PHYSICAL CHEMISTRY B **109** 8332-8343 (2005)
60. **Rovibrational energy transfer in the 4v(CH) manifold of acetylene, viewed by IR-UV double resonance spectroscopy. 3. State-to-state J-resolved kinetics**  
Payne MA, Milce AP, Frost MJ, Orr BJ  
ZEITSCHRIFT FUR PHYSIKALISCHE CHEMIE-INTERNATIONAL JOURNAL OF RESEARCH IN PHYSICAL CHEMISTRY & CHEMICAL PHYSICS **219** 601-633 (2005)