

Chemistry Publications 2004

- 1. Structural investigation of polymers by neutron scattering**
Arrighi V, Higgins JS
PLASTICS RUBBERS AND COMPOSITES **33** 313-329 (2004)
- 2. Computational studies on intramolecular C-H and C-C bond activation in ruthenium N-heterocyclic carbene complexes**
Macgregor SA, Whittlesey MK, Diggle RA
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY **228** U839-U840 (2004)
- 3. Redox modulated molecular recognition in phenanthrenequinone-thiourea based systems**
Carroll JB, Gray M, Wouters KL, Cooke G, MacDonnell FM, Rotello V
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY **228** U63-U63 (2004)
- 4. Ferromagnetic resonance and magnetic properties of single-domain particles of $Y_3Fe_5O_{12}$ prepared by sol-gel method**
Sanchez RD, Ramos CA, Rivas J, Vaqueiro P, Lopez-Quintela MA
PHYSICA B-CONDENSED MATTER **354** 104-107 (2004)
- 5. $[Co(en)_3][Sb_{12}S_{19}]$: A new antimony sulfide with a zeolite-like structure containing one-dimensional channels**
Vaqueiro P, Chippindale AM, Powell AV
INORGANIC CHEMISTRY **43** 7963-7965 (2004)
- 6. Determining log P of ionisable pharmaceutical drugs by acid-base titrations**
Kraft A, Howarth NM, Barzanti C, Levet E, Kean G
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY **227** U151-U151 (2004)
- 7. Thermally induced shape-memory effect in segmented copolymers containing polycaprolactone soft segments and aramid hard segments**
Kraft A, Rabani G
POLYMERIC MATERIALS SCIENCE & ENGINEERING **90**, 41-42 (2004)
- 8. End-to-end single cyanato and thiocyanato bridged Cu(II) polymers with a new tridentate Schiff base ligand: Crystal structure and magnetic properties**
Talukder P, Datta A, Mitra S, Rosair GM, El Fallah MS, Ribas J
DALTON TRANSACTIONS 4161-4167 (2004)
- 9. The electrochemically tuneable recognition properties of an electropolymerised flavin derivative**
Cooke G, Garety J, Mabruk S, Rotello V, Surpateanu G, Woisel P
CHEMICAL COMMUNICATIONS 2722-2723 (2004)
- 10. Structure-property relationships in ordered-defect sulphides**

Powell AV, Vaqueiro P, McDowall A
SOLID STATE IONICS **172** 469-475 (2004)

11. **Solvothermal synthesis of novel antimony sulphides containing [Sb₄S₇]²⁻ units**
Vaqueiro P, Darlow DP, Powell AV, Chippindale AM
SOLID STATE IONICS **172** 601-605 (2004)
12. **The role of C₂ in nanocrystalline diamond growth**
Rabeau JR, **John P**, Wilson JIB, Fan Y
JOURNAL OF APPLIED PHYSICS **96** 6724-6732 (2004)
13. **The influence of intralayer structural distortions on the electrical and magnetic properties of V_{1+x}Mo_{2-x}S₄ (0 < x < 2)**
Powell AV, McDowall A, Vaqueiro P, Smith RI, Ohtani T, Okuya Y
JOURNAL OF MATERIALS CHEMISTRY **14** 3051-3057 (2004)
14. **Nanophase-separated regions and side-chain relaxation in dialkyl itaconate copolymers**
Arrighi V, Holmes PF, McEwen IJ, Terrill NJ, Qian H
JOURNAL OF MATERIALS CHEMISTRY **14** 3306-3307 (2004)
15. **Kinetics of phase separation of poly(styrene-co-methyl methacrylate) and poly(styrene-co-acrylonitrile) blends**
Tang P, **Arrighi V, Higgins JS, Li GX**
POLYMER INTERNATIONAL **53** 1686-1692 (2004)
16. **Order in amorphous di-n-alkyl itaconate polymers, copolymers, and blends**
Arrighi V, Holmes PF, McEwen IJ, Qian H, Terrill NJ
JOURNAL OF POLYMER SCIENCE PART B-POLYMER PHYSICS **42** 4000-4016 (2004)
17. **Conformation of cyclics and linear chain polymers in bulk by SANS**
Arrighi V, Gagliardi S, Dagger AC, Semlyen JA, Higgins JS, Shenton MJ
MACROMOLECULES **37** 8057-8065 (2004)
18. **Relative binding affinities of molecular capsules investigated by ESI-mass spectrometry**
Zadmard R, **Kraft A, Schrader T, Linne U**
CHEMISTRY-A EUROPEAN JOURNAL **10** 4233-4239 (2004)
19. **C-C bond formation at ozonide rings by substitution of chlorinated ozonides**
Griesbaum K, Quinkert RO, **McCullough KJ**
EUROPEAN JOURNAL OF ORGANIC CHEMISTRY 3657-3662 (2004)
20. **Self-assembly as a route to fibrous materials: concepts, opportunities and challenges**
Viney C
CURRENT OPINION IN SOLID STATE & MATERIALS SCIENCE **8** 95-101 (2004)
21. **Supramolecular self-assembly of fibres**
Pasini D, **Kraft A**
CURRENT OPINION IN SOLID STATE & MATERIALS SCIENCE **8** 157-163 (2004)

22. **Inspiration versus duplication with biomolecular fibrous materials: learning nature's lessons without copying nature's limitations**
Viney C, Bell FI
CURRENT OPINION IN SOLID STATE & MATERIALS SCIENCE **8** 165-171 (2004)
23. **Dielectric relaxations in poly(di-n-alkyl itaconate)s**
Arrighi V, McEwen IJ, Holmes PF
MACROMOLECULES **37** 6210-6218 (2004)
24. **Synthesis, optical properties, crystal structures and phase behaviour of selectively fluorinated 1,4-bis(4'-pyridylethynyl)benzenes, 4-(phenylethynyl)pyridines and 9,10-bis(4'-pyridylethynyl)anthracene, and a Zn(NO₃)₂ coordination polymer**
Fasina TM, Collings JC, Lydon DP, Albesa-Jove D, Batsanov AS, Howard JAK, Nguyen P, Bruce M, Scott AJ, Clegg W, Watt SW, Viney C, Marder TB
JOURNAL OF MATERIALS CHEMISTRY **14** 2395-2404 (2004)
25. **Structure and magnetism in synthetic pyrrhotite Fe₇S₈: A powder neutron-diffraction study**
Powell AV, Vaqueiro P, Knight KS, Chapon LC, Sanchez RD
PHYSICAL REVIEW B **70** 014415 (2004)
26. **Square planar complexes of Cu(II) with an N₂O donor set of a new Schiff base ligand: Synthesis and structural aspects**
Talukder P, Datta A, Mitra S, Rosair GM
ZEITSCHRIFT FUR NATURFORSCHUNG SECTION B-A JOURNAL OF CHEMICAL SCIENCES **59** 655-660 (2004)
27. **Synthesis of diamond spheres**
Lee JK, Baik YJ, Eun KY, Lee JY, Park JW, John P
CHEMICAL VAPOR DEPOSITION **10** 133-136 (2004)
28. **Expression, intracellular distribution and basis for lack of catalytic activity of the PDE4A7 isoform encoded by the human PDE4A cAMP-specific phosphodiesterase gene**
Johnston LA, Erdogan S, Cheung YF, Sullivan M, Barber R, Lynch MJ, Baillie GS, Van Heeke G, Adams DR, Huston E, Houslay MD
BIOCHEMICAL JOURNAL **380** 371-384 (2004)
29. **Structure and phase behavior of a 2:1 complex between arene- and fluoroarene-based conjugated rigid rods**
Watt SW, Dai C, Scott AJ, Burke JM, Thomas RL, Collings JC, Viney C, Clegg W, Marder TB
ANGEWANDTE CHEMIE-INTERNATIONAL EDITION **43** 3061-3063 (2004)
30. **On the valence shell electronic spectroscopy of 2-vinyl furan**
Giuliani A, Walker IC, Delwiche J, Hoffmann SV, Kech C, Limao-Vieira P, Mason NJ, Hubin-Franskin MJ
JOURNAL OF CHEMICAL PHYSICS **120** 10972-10982 (2004)
31. **Oxidation of CVD diamond powders**

Lee JK, Anderson MW, Gray FA, **John P**, Lee JY, Baik YJ, Eun KY
DIAMOND AND RELATED MATERIALS **13** 1070-1074 (2004)

32. **Model systems for flavoenzyme activity: an electrochemically tuneable model of roseoflavin**
Cooke G, Legrand YM, Rotello VM
CHEMICAL COMMUNICATIONS 1088-1089 (2004)
33. **A heterometallic polymeric complex: $[\text{Cu}_2(\text{N}_3)_2(\text{medpt})_2\{\text{Ni}(\text{CN})_4\}]_n$ [medpt is bis(3-aminopropyl)methylamine]**
Ghoshal D, Maji TK, **Rosair GM**, Mostafa G
ACTA CRYSTALLOGRAPHICA SECTION C-CRYSTAL STRUCTURE COMMUNICATIONS **60** M212-M214 (2004)
34. **Measurement of orientation and alignment moment relaxation by polarization spectroscopy: Theory and experiment**
Costen ML, Crichton HJ, **McKendrick KG**
JOURNAL OF CHEMICAL PHYSICS **120** 7910-7926 (2004)
35. **Ability of N-heterocyclic carbene ligands to promote intermolecular oxidative addition reactions at unsaturated ruthenium centers**
Diggle RA, **Macgregor SA**, Whittlesey MK
ORGANOMETALLICS **23** 1857-1865 (2004)
36. **Proton transfer versus redox modulation in thiourea-phenanthrenequinone molecular and polymeric complexes**
Carroll JB, Gray M, **Cooke G**, Rotello VM
CHEMICAL COMMUNICATIONS 442-443 (2004)
37. **Low-temperature route to thermoplastic polyamide elastomers**
Rabani G, **Rosair GM**, **Kraft A**
JOURNAL OF POLYMER SCIENCE PART A-POLYMER CHEMISTRY **42** 1449-1460 (2004)
38. **The synthesis and molecular and crystal structures of 1-methyl-2-carboxy-1,2-dicarba-closo-dodecaborane(12), 1-phenyl-2-carboxy-1,2-dicarba-closo-dodecaborane(12) and 1-phenyl-2-benzoyl-1,2-dicarba-closo-dodecaborane(12)**
Venkatasubramanian U, Donohoe DJ, Ellis D, Giles BT, **Macgregor SA**, Robertson S, **Rosair GM**, **Welch AJ**, Batsanov AS, Boyd LA, Copley RCB, Fox MA, Howard JAK, Wade K
POLYHEDRON **23** 629-636 (2004)
39. **Theoretical study of the CO migratory insertion reactions of Pt(Me)(OMe)(dppe) and Ni(Me)(OR)(bpy) (R = Me, O-*p*-C₆H₄CN): Comparison of group 10 metal-alkyl, -alkoxide, and -aryloxide bonds**
Macgregor SA, Neave GW
ORGANOMETALLICS **23** 891-899 (2004)
40. **Model systems for flavoenzyme activity: Interplay of hydrogen bonding and aromatic stacking in cofactor redox modulation**
Gray M, Goodman AJ, Carroll JB, Bardon K, Markey M, **Cooke G**, Rotello VM

ORGANIC LETTERS **6** 385-388 (2004)

41. **The electronic states of isoxazole studied by VUV absorption, electron energy-loss spectroscopies and *ab initio* multi-reference configuration interaction calculations**
Walker IC, Palmer MH, Delwiche J, Hoffmann SV, Limao-Vieira P, Mason NJ, Guest MF, Hubin-Franskin MJ, Heinesch J, Giuliani A
CHEMICAL PHYSICS **297** 289-306 (2004)
42. **Arene-perfluoroarene interactions in crystal engineering: structural preferences in polyfluorinated tolans**
Smith CE, Smith PS, Thomas RL, Robins EG, Collings JC, Dai CY, Scott AJ, Borwick S, Batsanov AS, Watt SW, Clark SJ, Viney C, Howard JAK, Clegg W, Marder TB
JOURNAL OF MATERIALS CHEMISTRY **14** 413-420 (2004)
43. **Pronounced stabilisation of the ferrocenium state of ferrocenecarboxylic acid by salt bridge formation with a benzamidine**
Cooke G, Duclairoir FMA, Kraft A, Rosair G, Rotello VM
TETRAHEDRON LETTERS **45** 557-560 (2004)
44. **Simplified synthesis, H-1, C-13, N-15, Sn-119 NMR spectra and X-ray structures of diorganotin(IV) complexes containing the 4-phenyl-2,4-butanedionebenzoylhydrazone(2-) ligand**
Dey DK, Lycka A, Mitra S, Rosair GM
JOURNAL OF ORGANOMETALLIC CHEMISTRY **689** 88-95 (2004)
45. **Experimental and *ab initio* computational studies of self-association: 2-aminopyridine and 3-aminopyridine**
Boyd ASF, Frost MJ, Howarth NM
JOURNAL OF MOLECULAR STRUCTURE **688** 149-158 (2004)
46. **Advanced Materials Highlights**
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CHEMISTRY & INDUSTRY (3) 30-32 (2004)
47. **Advanced Materials Highlights**
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CHEMISTRY & INDUSTRY (7) 26-27 (2004)
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50. **Advanced Materials Highlights**
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CHEMISTRY & INDUSTRY (19) 26-27 (2004)
51. **Advanced Materials Highlights**

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52. **Synthesis, structure and electrochemical properties of some oxime complexes of rhodium**
R. Acharyya R, Basuli F, **Rosair GM**, Bhattacharya S
NEW JOURNAL OF CHEMISTRY 28 115-119 (2004)
53. **A study of the valence shell spectroscopic and thermodynamic properties of thiophene by photoabsorption and photoion spectroscopy**
Rennie EE, Holland DMP, Shaw DA, **Johnson CAF**, **Parker JE**
CHEMICAL PHYSICS 306 295-308 (2004)
54. **Optical studies of ion–molecule reactions**
Frost MJ
ANNUAL REPORTS PROG. CHEMISTRY SECT. C 100 29-72 (2004)