

Publications 2003

1. ***Effect of Collisions on One-Color Polarization Spectroscopy of OH A²Σ⁺ - X²Π***
J. Chem. Phys. 2003, 119, 9461-9468
H J Crichton, M L Costen, K G McKendrick
2. ***Techniques for Polymer Organisation and Morphology Characterisation***
John Wiley & Sons, Chichester, UK, 2003, 0-471-49070-9
C Viney, R A Pethrick
3. ***Synthesis of novel macrocyclic peroxides by bis(sym-collidine)iodine (I) hexafluorophosphate-mediated cyclization of unsaturated hydroperoxides and unsaturated alcohols***
Tetrahedron, 2003, 59, 525-536
T Tokuyasu, A Masuyama, M Nojima, K J McCullough, T Ito
4. ***Modelling self assembly of natural silk solutions***
International Journal of Biological Macromolecules, 2003, 32, 59-65
F N Braun, C Viney
5. ***Beyond the icosahedron: Synthesis of the first 13-vertex carborane***
Angew. Chem. Int. Ed., 2003, 42, 225-228
A Burke, D Ellis, B T Giles, B E Hodson, S A Macgregor, G M Rosair, A J Welch
6. ***Regioselective radical cyclization initiated by the reaction of allylic hydroperoxides with iron(II) sulfate***
Tetrahedron, 2003, 59, 353-366
T Sugawara, A Masuyama, M Nojima, K J McCullough
7. ***Antimalarial Activity of Novel 1,2,5,6-Tetraoxacycloalkanes and 1,2,5-Trioxacycloalkanes***
J. Med. Chem., 2003, 46, 1957-1961
H S Kim, H Begum, N Ogura, Y Wataya, Y Nonami, T Ito, A Masuyama, M Nojima, K J McCullough
8. ***Supraicosahedral (metalla)carboranes***
Boron Chemistry at the Beginning of the 21st Century, Yu. N. Bubnov (Ed), URSS, 2003, 218-226
A S F Boyd, D Ellis, S A Macgregor, G M Rosair, A J Welch, A Burke, D Ferrer, B T Giles, M A Laguna, R McIntosh, D L Ormsby, F Schmidt, N M M Wilson
9. ***Synthesis and Reactivity of New Halogenated o-Carborane Derivatives***
Boron Chemistry at the Beginning of the 21st Century, Yu. N. Bubnov (Ed.), URSS, 2003, 192-197
G Barbera, F Teixidor, C Vinas, A J Welch, G M Rosair

10. Creep and low strength of spider dragline subjected to constant loads

Journal of Arachnology, 2003, 31, 421-424
C Viney, C Smith, F I Bell, J Ritchie, I J McEwen

11. Novel gel polymer electrolytes based on a cellulose ester with PEO side chains

Sol. State Ionics, 2003, 156, 155-162
J M G Cowie, I J McEwen, Z Yue

12. New Supraicosahedral Metallacarboranes. The Synthesis and Molecular Structures of 4-dppe-4,1,6-closo-NiC₂B₁₀H₁₂ and [4-(η -C₃H₅)-4-(CO)₂-4,1,6-closo-MoC₂B₁₀H₁₂]

Inorg. Chim. Acta, 2003, 347, 161-167
M A Laguna, D Ellis, G M Rosair, A J Welch

13. The dynamic structure factor in non-entangled polymer melts - Theoretical results for real chains and the stretched exponential approximation

Chem. Phys., 2003, 287, 391-398
F Ganazzoli, G Raffaini, V Arrighi

14. New Interpretation of Local Dynamics of Poly(dimethyl siloxane) Observed by Quasielastic Neutron Scattering

Physical Review Letters, 2003, 90, 058301-1 – 058301-4
V Arrighi, F Ganazzoli, C Zhang, S Gagliardi

15. Effects of Tacticity on the Local Dynamics of Polypropylene Melts

J. Chem. Phys., 2003, 119, 1271-1278
V Arrighi, D B N Coutrot, C Zhang, M T F Telling, R Triolo

16. Quasi elastic neutron scattering characterization of the relaxation processes in a room temperature ionic liquid.

J. Chem. Phys., 2003, 119, 8549-8557
A Triolo, O Russina, V Arrighi, F Juranyi, S Janssen, C M Gordon

17. Local Dynamics of Polyethylene and its Oligomers: A Molecular Dynamics Interpretation of the Incoherent Dynamic Structure Factor

Macromolecules, 2003, 36, 8864-8875
G Arialdi, K Karatasos, J P Ryckaert, V Arrighi, A Triolo, A Desmedt, J Pieper, R E Lechner, F Saggio

18. A unified picture of the local dynamics of poly(dimethyl siloxane) across the melting point

Macromolecules, 2003, 36, 8738-8748
V Arrighi, S Gagliardi, C Zhang, F Ganazzoli, J S Higgins, R Occone, M T F Telling

19. Neutron Scattering

Polymer Characterization: Analytical Techniques, R A Pethrick and C Viney (Editors), John Wiley & Sons Ltd, 2003, Chapter 6
V Arrighi, D G Bucknall, A Triolo

20. Miscibility

Encyclopedia of Polymer Science, 3rd edition, John Wiley & Sons Ltd, 2003
V Arrighi, J M G Cowie

21. Neutron Scattering Studies of Cyclic and Linear Poly(dimethyl siloxane)s

Synthesis and Properties of Silicones and Silicone-Modified Materials,
S J Clarson, J J Fitzgerald, M J Owens, S D Smith and M E van Dyke eds., Symposium Series No 838, 2003, 96-104
A C Dagger, V Arrighi, S Gagliardi, M J Shenton, S J Clarson, J A Semlyen

22. The development of a marine natural product-based antifouling paint

Biofouling, 2003, 19, 197-205
J G Burgess, K G Boyd, E Armstrong, Z Jiang, L Yan, M Berggren, U May, T Pisacane, A Granmo, D R Adams

23. PDE4 cAMP phosphodiesterases: modular enzymes that orchestrate signalling cross-talk, desensitization and compartmentalization

Biochemical Journal, 2003, 370, 1-18
M D Houslay, D R Adams

24. Interaction of caspase-3 with the cyclic GMP binding GMP specific phosphodiesterase (PDE5a1)

European Journal of Biochemistry, 2003, 270, 962-970
M J Frame, R Tate, D R Adams, K M Morgan, M D Houslay, P Vandenabeele, N J Pyne

25. Biofilm-specific cross-species induction of antimicrobial compounds in bacilli

Applied and Environmental Microbiology, 2003, 69, 3719-3727
L Yan, K G Boyd, J G Burgess, D R Adams

26. Occupancy of the catalytic site of PDE4A4 cyclic AMP phosphodiesterase by rolipram triggers the dynamic redistribution of this specific isoform in living cells through a cyclic AMP independent process

Cellular Signalling, 2003, 15, 955-971
R Terry, Y F Cheung, M Praestgaard, G S Baillie, E Huston, I Gall, D R Adams, M D Houslay

27. Macromolecules with electrochemically controllable recognition properties

226th American Chemical Society National Meeting, New York, September 7-11, 2003, G Cooke

28. An Investigation of The Role of the Disparate Redox States of The Tetrathiafulvalene Unit in Modulating Hydrogen Bonding Interactions in Solution

Tet. Lett., 2003, 44, 303-306
A S F Boyd, G Cooke, F M A Duclairoir, V M Rotello

- 29. Ferrocene Incorporating Host-Guest Dyads With Electrochemically Controlled Three-Pole Hydrogen Bonding Properties**
Tetrahedron, 2003, 59, 3341-3347
G Cooke, H A De Cremiers, F M A Duclairoir, J Leonardi, G M Rosair, V M Rotello
- 30. Electrochemically tuneable hydrogen bonding interactions between a phenyl-urea terminated dendrimer and phenanthrenequinone**
Chem. Commun., 2003, 752-753
G Cooke, V Sindelar, V M Rotello
- 31. Triphenylene/Carbazole Mesogens and Their Electrochemistry**
Mol. Cryst. Liq. Cryst., 2003, 397, 399-416
G Cooke, S Kumar, P R Ashton, J A Preece, N Spencer, M Manickam
- 32. Surface Confined Pseudorotaxanes with Electrochemically Controllable Complexation Properties**
J.Mater. Chem., 2003, 13, 2111-2117
M R Bryce, G Cooke, F M A Duclairoir, P John, D F Perepichka, N Polwart, V M Rotello, J F Stoddart, H-R Tseng
- 33. Hydrogen Bonding in Redox-Modulated Molecular Recognition. An Experimental and Theoretical Investigation.**
J. Amer. Chem. Soc., 2003, 125, 7882-7888
M Gray, A O Cuello, G Cooke, V M Rotello
- 34. Electrochemical and Photochemical Control of Host-Guest Complexation at Interfaces.**
Commissioned review article.
Angew. Chem. Int. Ed., 2003, 42, 4860-4870
G Cooke
- 35. Model Systems for Flavoenzyme Activity: Relationships between cofactor structure, binding and redox properties.**
J. Amer. Chem. Soc., 2003, 125, 15789-15795
Y-M Legrand, M Gray, G Cooke, V M Rotello
- 36. C I Pigment Red 266**
Acta. Cryst., 2003, C59, o556-o558
C H Chang, G M Rosair, R M Christie
- 37. Spiro Cyclisations of N-Acyliminium Ions involving an Aromatic Nucleophile**
Tetrahedron, 2003, 59, 3369-3378
K M Morgan, J M Vernon, P D Bailey, D I Smith
- 38. Nucleosides**
Carbohydrate Chemistry (Specialist Periodical Report), 2003, 34, 248-302
R H Wightman
- 39. Carbohydrates in Chiral Organic Synthesis**
Carbohydrate Chemistry (Specialist Periodical Report), 2003, 34, 338-366
R H Wightman

40. Synthesis and Glycosidase Inhibitory Activity of 7-Deoxycasuarine

Helv. Chim. Acta, 2003, 86, 3066-3073

A T Carmona, R H Wightman, I Robina, P Vogel

41. Thiazyl chloride: an experimental and theoretical study of the valence shell HeI photoelectron

Chem. Phys., 2003, 288, 95-104

N Chabert, D Duflot, J-P Flament, J-M Robbe, I C Walker, J H Cameron, A Giuliani, M-J Hubin-Franskin, J Delwiche

42. Core shell excitation of 2-propenal (acrolein) at the O 1s and C 1s edges: An experimental and ab initio study

J. Chem. Phys., 2003, 118, 1137-1145

D Duflot, J-P Flament, I C Walker, J Heinesch, M-J Hubin-Franskin

43. VUV optical absorption and near-threshold electron energy-loss spectra of pyrazole

Chem. Phys. Letters, 2003, 367, 517-522

I C Walker, M H Palmer, M-J Hubin-Franskin, J Delwiche

44. The electronic states of 2-furanmethanol (furfuryl alcohol) studied by photon absorption and electron impact spectroscopies

J. Chem. Phys., 2003, 119, 7282-7288

A Giuliani, I C Walker, J Delwiche, S V Hoffmann, P Limao-Vieira, N J Mason, B Heyne, M Hoobeke, M-J Hubin-Franskin

45. Synthesis of polyamide-based thermoplastic elastomers

Polym. Mater. Sci. Eng., 2003, 88, 163-164

G Rabani, A Kraft

46. Purity control of ester-end-functionalized poly(propylene glycol) telechelics by MALDI-TOF MS

Polym. Mater. Sci. Eng., 2003, 88, 135-136

A Kraft, G Rabani, H Luftmann

47. The determination of the pKa of multiprotic, weak acids by analysing potentiometric acid-base titration data with difference plots

J. Chem. Educ., 2003, 80, 554-559

A Kraft

48. Capsule-like assemblies in polar solvents

J. Org. Chem., 2003, 68, 6511-6521

R Zadmar, M Junkers, T Schrader, T Grawe, A Kraft

49. MALDI-TOF mass spectrometry for detecting impurities in ester-end-functionalized poly(tetrahydrofuran), poly(propylene glycol) and poly(caprolactone) telechelics

Macromolecules, 2003, 36, 6316-6324

H Luftmann, G Rabani, A Kraft

50. Advanced Materials Highlights 1

Chem. Industry, 2003, 3, 25-26
A Kraft

51. Advanced Materials Highlights 2

Chem. Industry, 2003, 7, 25-26
A Kraft

52. Advanced Materials Highlights 3

Chem. Industry, 2003, 11, 27-28
A Kraft

53. Advanced Materials Highlights 4

Chem. Industry, 2003, 15, 25-26
A Kraft

54. Advanced Materials Highlights 5

Chem. Industry, 2003, 19, 34-36
A Kraft

55. Advanced Materials Highlights 6

Chem. Industry, 2003, 23, 30-31
A Kraft

56. Experimental and theoretical studies of the $N_2^+ + O_2$ reaction

Phys. Chem. Chem. Phys., 2003, 5, 3169-3173
M J Frost

57. Rovibrational energy transfer in the $4\nu_{\text{CH}}$ manifold of acetylene, viewed by IR-UV double resonance spectroscopy. I. Foundation studies at low J

J. Phys. Chem., 2003, 107, 10759-10770
M A Payne, A P Milce, M J Frost, B J Orr

58. Non-covalent interactions in the association of aminopyridines

Report for inclusion in UK Computational Chemistry Working Party/EPSRC Annual Report, 2003
M J Frost

59. $[\text{Cr}(\text{C}_6\text{H}_{18}\text{N}_4)][\text{SbS}_3]$, a chromium complex containing an unusual bidentate SbS_3^{3-} ligand

Polyhedron, 2003, 22, 2839-2845
P Vaqueiro, A M Chippendale, A V Powell

60. Templated synthesis of the novel layered silver antimony sulfides, $[\text{H}_3\text{NCH}_2\text{CH}_2\text{NH}_2][\text{Ag}_2\text{SbS}_3]$ and $[\text{H}_3\text{NCH}_2\text{CH}_2\text{NH}_2][\text{Ag}_5\text{Sb}_3\text{S}_8]$

Inorg. Chem., 2003, 42, 7846-7851
P Vaqueiro, A M Chippendale, A R Cowley, A V Powell

- 61. Structure, Reactivity and Computational Studies of a Novel Ruthenium Hydrogen Sulfide Dihydride Complex**
Inorg. Chem., 2003, 42, 7695-7697
S L Chatwin, R A Diggle, R F R Jazzar, S A Macgregor, M F Mahon, M K Whittlesey
- 62. Theoretical study of CO migratory insertion reactions with group 10 metal-alkyl and -alkoxide**
Organometallics, 2003, 22, 4547-4556
S A Macgregor, G W Neave
- 63. Supraicosahedral (metalla)carboranes**
Pure Applied Chem., 2003, 75, 1325-1333
A S F Boyd, A Burke, D Ellis, D Ferrer, B T Giles, M A Laguna, R McIntosh, S A Macgregor, D L Ormsby, G M Rosair, F H Schmidt, N M M Wilson, A J Welch
- 64. Insertion reactions of unsymmetrical ester-activated alkynes with o-benzylamine palladacycles: a regioselectivity study**
Inorg. Chim. Acta, 2003, 352, 79-97
A E Kelly, S A Macgregor, A C Willis, J H Nelson, E Wenger
- 65. Theoretical studies on C-heteroatom bond formation via reductive elimination from group 10 $M(PH_3)_2(CH_3)(X)$ species ($X = CH_3, NH_2, OH, SH$) and the determination of metal-X bond strengths using density functional theory**
Faraday Discussions, 2003, 124, 111-127
S A Macgregor, G W Neave, C Smith
- 66. Synthesis of the four diastereoisomers of 3-thymine-1-(tbutoxycarbonyl)aminocyclopentane-1-carboxylic acid**
Tetrahedron Lett., 2003, 44, 695-698
N M Howarth, L P G Wakelin, D M Walker
- 67. Synthesis of thymine derivatives of 4-hydroxyvaline**
Nucleosides, Nucleotides & Nucleic Acids, 2003, 22, 675-677
A Abraham, N M Howarth
- 68. α -cycloPNA: 1-aminocyclopentane-1-carboxylic acid derived peptide nucleic acid**
Nucleosides, Nucleotides and Nucleic Acids, 2003, 22, 1351-1353
N M Howarth, L P G Wakelin, D M Walker
- 69. Conformationally restricted chiral peptide nucleic acids derived from azetidines**
Nucleosides, Nucleotides and Nucleic Acids, 2003, 22, 1363-1365
L Kovacs, M Hornyak, N M Howarth
- 70. Synthesis and polymerisation of lipophilic peptide nucleic acids derived from stearic acid and pentacosa-10, 12-diynoic acid**
Tetrahedron Lett., 2003, 44, 8089-8092
N M Howarth, W E Lindsell, E Murray, P N Preston

- 71. Synthesis, Structure and Magnetic Characterisation of a New Layered Ammonium Manganese (I) Diphosphate Hydrate ($(NH_4)_2[Mn_3(P_2O_7)_2(H_2O)_2]$)**
J. Mater. Chem., 2003, 13, 1950-1955
A M Chippindale, F O M Gaslain, A D Bond, A V Powell
- 72. Crystal engineering with heteroboranes. II. 1,2-Dicarboxyl-1,2-dicarba-closo-dodecaborane(12) ethanol hemisolvate**
Acta. Cryst., 2003, C59, o559-o561
U Venkatasubramanian, D Ellis, G M Rosair, A J Welch
- 73. Crystal engineering with heteroboranes. III. 2-Carboxyl-1-methoxymethyl-1,2-dicarba-closo-dodecaborane(12), $C_4H_{12}B_{10}O_4$**
Acta. Cryst., 2003, C59, o586-o588
U Venkatasubramanian, D Ellis, G M Rosair, A J Welch
- 74. Synthesis, characterisation and structural studies of $[Zn(phen)_3][Fe(CN)_5(NO)]$ and $[(bipy)_2(H_2O)Zn(\mu\text{-NC})Fe(CN)_4(NO)]$**
Z. Naturforsch., 2003, 58, 916-921
A Datta, N K Karan, S Mitra, G M Rosair
- 75. Nickelation of $[3\text{-Et-7,8-}Ph_2\text{-7,8-nido-}C_2B_9H_8]^{2-}$; Synthesis and characterisation of $1,2 \rightarrow 1,2$ and $1,2 \rightarrow 1,7$ isomerised products**
Appl. Organometal. Chem., 2003, 17, 518-524
S Robertson, D Ellis, G M Rosair, A J Welch
- 76. Platination of $[3\text{-X-7,8-}Ph_2\text{-7,8-nido-}C_2B_9H_8]^{2-}$ ($X=Et, F$); Synthesis and characterisation of slipped and $1,2 \rightarrow 1,7$ isomerised products**
J. Organometal. Chem., 2003, 680, 286-293
S Robertson, D Ellis, G M Rosair, A J Welch
- 77. Dynamics of the gas-liquid interfacial reaction of $O(^3P)$ atoms with hydrocarbons**
J. Chem. Phys., 2003, 119, 9985-9988
H Kelso, S P K Koehler, D A Henderson, K G McKendrick
- 78. Synthesis and characterisation of labelled diphenylcarboranes.**
Polyhedron, 2003, 22, 1293-1301
S Robertson, D Ellis, T D McGrath, G M Rosair, A J Welch
- 79. Synthesis and Structures of Monocyclopentadienylniobium Complexes with Bi and Tridentate Dithiolate Ligands**
J. Chem. Soc., Dalton Trans., 2003, 126-133
W E Lindsell, G M Rosair, H. Jungclas
- 80. The glass transition and interfacial layer in styrene-butadiene rubber containing silica nanofiller**
Polymer, 2003, 44, 6259-6266
V Arrighi, I J McEwen, H Qian, M B Serrano Prieto

81. Order in poly(*di-n-alkyl itaconate*)s revealed by X-ray scattering experiments

Nuclear Instruments and Methods in Physics Research, 2003, 200, 411-415
P Holmes, V Arrighi, I J McEwen, H Qian, N J Terrill

82. The Oxidation of Diamond: The Geometry and Stretching Frequency of Carbonyl on the (100) Surface

J. Amer. Chem. Soc., 2003, 125, 6600-6601
N Polwart, C E Troup, P John, J I B Wilson

83. Nanocrystalline Diamond Films for Nanotechnology Applications

Mat. Sci. and Technol., 2003, 19, 553-556
I S Forbes, J R Rabeau, J I B Wilson, P John

84. Model Systems for Flavoenzyme Activity: Flavin-Functionalised SAMs as Models for Probing Redox Modulation through Hydrogen Bonding

Chem. Commun., 2003, 2468-2469
G Cooke, F M A Duclairoir, P John, N Polwart, V M Rotello

85. New approaches to the synthesis of spiro-perlactones

Org. Biomol. Chem., 2003, 1, 1522-1527
K J McCullough, H Tokuhara, A Masuyama, M Nojima

86. Application of a fib system to nanolithography

Mat. Res. Soc. Symp. Proc., 2003, 379, 63
R M Langford, S O'Reilly, I J McEwen

87. Direct comparison of the effects of vibrational excitation on the reactions $O(^3P) + CH_4(v_3=2)$ and $HCl(v=2)$

XIX Conference on the Dynamics of Molecular Collisions, Lake Tahoe, USA, 2003
H Kelso, F Ausfelder, D A Henderson, K G McKendrick

88. Dynamics of gas-liquid interfacial reactions of oxygen atoms with hydrocarbons

XIX Conference on the Dynamics of Molecular Collisions, Lake Tahoe, USA, 2003
H Kelso, S P K Koehler, D A Henderson, K G McKendrick

89. Collisional Energy Transfer in OH using Polarisation Spectroscopy

XIX Conference on The Dynamics of Molecular Collisions, Lake Tahoe, USA, 2003
H J Crichton, M L Costen, K G McKendrick

90. State-to-State Energy Transfer in Electronically Excited CH Radicals

XIX Conference on The Dynamics of Molecular Collisions, Lake Tahoe, USA, 2003
G Richmond, K G McKendrick

91. Measurement of Relaxation of Orientation and Alignment by Polarisation Spectroscopy

XVII International Conference on Molecular Energy Transfer, San Lorenzo de El Escorial, Spain, 2003,
M L Costen, H J Crichton, K G McKendrick