

## CONTENTS

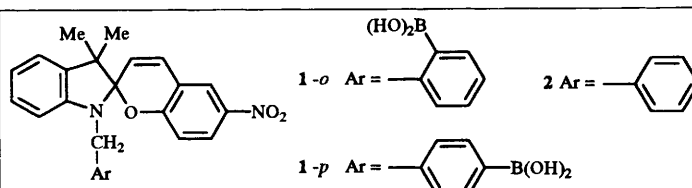
ix Instructions for authors (1996)

xxxi Refereeing procedure and policy

## Perkin Communications

- 1 **Spectroscopic detection of diols and sugars by a colour change in boronic acid-appended spirobenzopyrans**

Hideyuki Shinmori, Masayuki Takeuchi and Seiji Shinkai

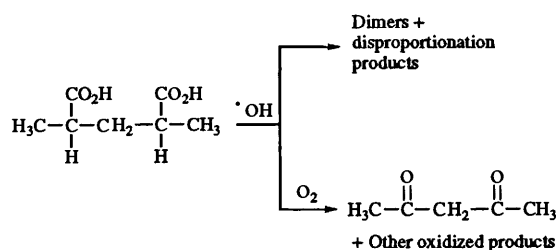


When the boron atom could intramolecularly interact with the tertiary amine in the spiropyran moiety, added diols and sugars changed the colour which was induced by the shift of the spiropyran-merocyanine equilibrium

## Articles

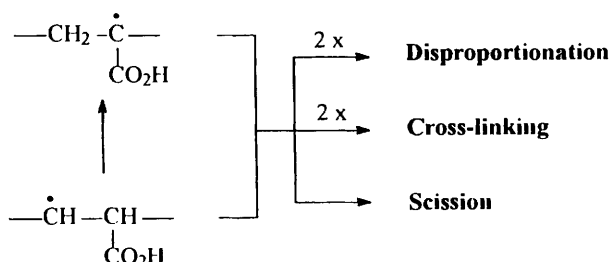
- 5 **Radiolysis of the poly(acrylic acid) model 2,4-dimethylglutaric acid: a pulse radiolysis and product study**

Piotr Ulanski, Eberhard Bothe, Janusz M. Rosiak and Clemens von Sonntag



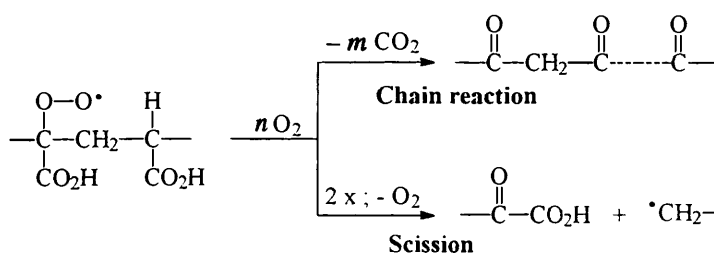
- 13 **Hydroxyl-radical-induced reactions of poly(acrylic acid); a pulse radiolysis, EPR and product study. Part I. Deoxygenated aqueous solutions**

Piotr Ulanski, Eberhard Bothe, Knut Hildenbrand, Janusz M. Rosiak and Clemens von Sonntag



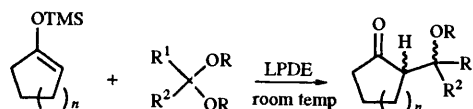
- 23 **Hydroxyl-radical-induced reactions of poly(acrylic acid); a pulse radiolysis, EPR and product study. Part II. Oxygenated aqueous solutions**

Piotr Ulanski, Eberhard Bothe, Knut Hildenbrand, Janusz M. Rosiak and Clemens von Sonntag



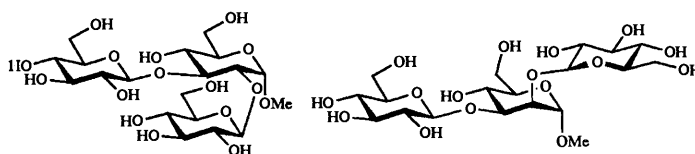
- 29 **Chemoselective aldol type condensation of silyl enol ethers and acetals in 5 mol dm<sup>-3</sup> lithium perchlorate–diethyl ether**

V. Geetha Saraswathy and S. Sankararaman



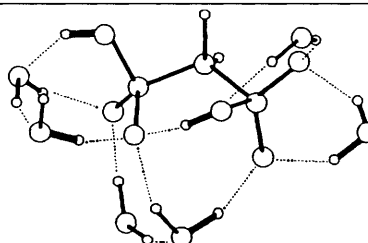
- 33 **Synthesis, NMR spectroscopy and conformational studies of two vicinally disubstituted trisaccharides**

Per-Erik Jansson, Alexandra Kjellberg, Torgny Rundlöf and Göran Widmalm



- 39 **Ab initio studies on organophosphorus compounds. Part 4. Intramolecular hydrogen bonding and water interactions of bisphosphonates**

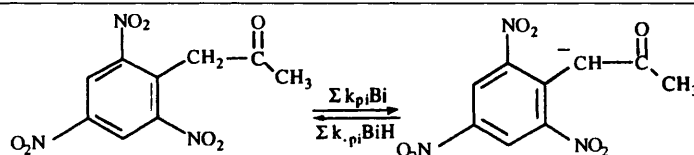
Jari P. Räsänen, Esko Pohjala and Tapani A. Pakkanen



The bisphosphonate–water complex

- 49 **The low intrinsic reactivity of picrylacetone: an index for the  $\pi$ -acceptor capability of a 2,4,6-trinitrophenyl structure**

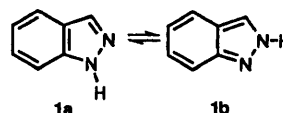
Gilles Moutiers, Bouchaïb El Fahid, Anne-Gaëlle Collot and François Terrier



In accord with the observation that the conjugate anionic species undergoes initial protonation at an NO<sub>2</sub> group at low pH, the reactivity of picrylacetone is typical for the formation of a strongly resonance-stabilized 2,4,6-trinitrobenzyl-type carbanion

- 57 **Importance of aromaticity on the relative stabilities of indazole annular tautomers: an *ab initio* study**

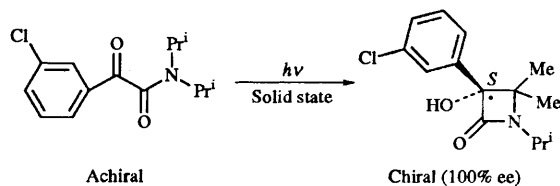
Javier Catalán, José Luis G. de Paz and José Elguero



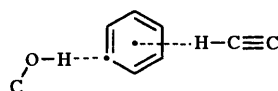
MP2-6-31G\*\* calculations on the two indazole annular tautomers, 1H **1a** and 2H **1b**, show that **1a** is more stable than **1b** by 3.6 kcal mol<sup>-1</sup>; in the case of 1H-indazole, the MP2-6-31G\*\* calculations reproduce with great accuracy the microwave rotational constants

61 Mechanism of asymmetric photocyclization of  $\alpha$ -oxoamides

Daisuke Hashizume, Hidenori Kogo, Akiko Sekine, Yuji Ohashi, Hisakazu Miyamoto and Fumio Toda

67 Weak hydrogen bonding. Part 3. A benzyl group accepting equally strong hydrogen bonds from O-H and C-H donors: 5-ethynyl-5H-dibenzo[*a,d*]cyclohepten-5-ol

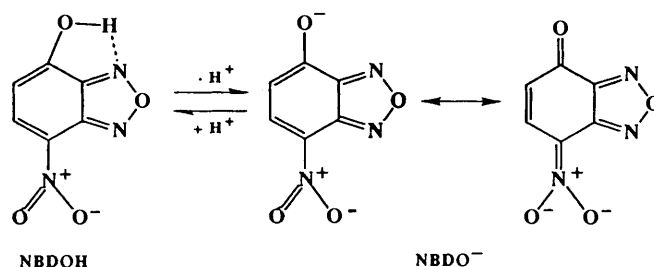
Thomas Steiner, Evgeni B. Starikov and Matthias Tamm



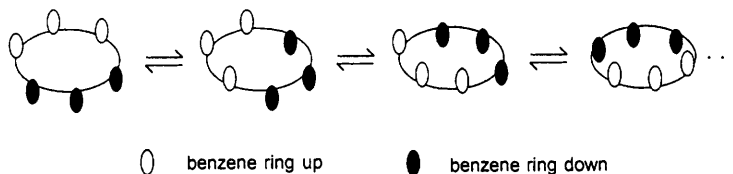
Hydrogen bonds of similar strength

## 73 Unusual solvatochromic behaviour of the 4-hydroxy-7-nitrobenzofurazan conjugated anion in protic solvents

Suzanne Fery-Forgues, Christiane Vidal and Dominique Lavabre

79 Conformational behaviour of methyl *p*-*tert*-butylcalix[6]arene ester: interconversions among 1,2,3-alternate conformations

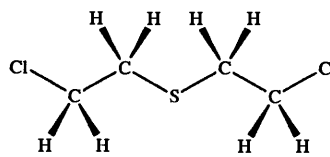
Sangdoon Ahn, Jo Woong Lee and Suk-Kyu Chang



Thermodynamic parameters were obtained for conformational interconversions in methyl *p*-*tert*-butylcalix[6]arene ester **1**

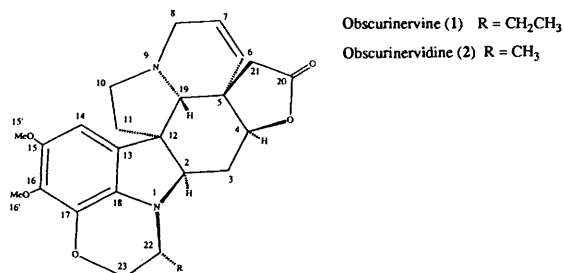
## 83 Using theoretical descriptions in structure activity relationships: retention indices of sulfur vesicants and related compounds

William H. Donovan and George R. Famini

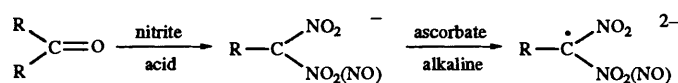


## 91 NMR characterization of obscurinervine and obscurinervidine using novel computerized analysis techniques

James K. Harper, Reinhard Dunkel, Steven G. Wood, Noel L. Owen, Du Li, Rex G. Cates and David M. Grant

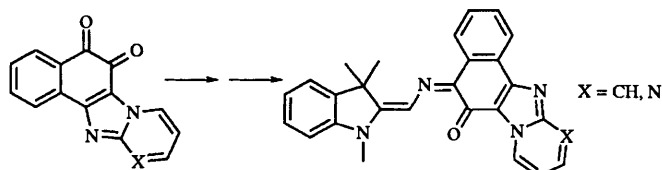


- 101 *gem*-Dinitro and *gem*-nitronitroso dianion radicals formed in the reaction between sodium nitrite–ascorbate and carbonyl compounds such as aldehydes, alicyclic ketones, lactams and peptides. An EPR study



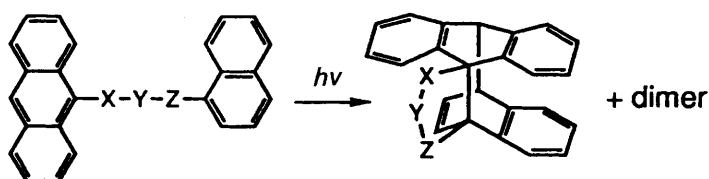
Carl Lagercrantz

- 107 First permanent opened forms in spiro[indoline-oxazine] series: synthesis and structural elucidation



Pierre Laréginie, Vladimir Lokshin, André Samat, Robert Guglielmetti and Gérard Pèpe

- 113 Photochemical reactions of anthracene–naphthalene bichromophoric systems linked by a three-carbon chain



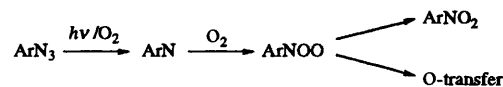
Yukie Mori and Koko Maeda

- 121 Mechanism of the chemiluminescence of bisoquinolinium salts

A plausible reaction pathway for the chemiluminescence of the  $\text{BIQ}-\text{H}_2\text{O}_2-\text{OH}^-$  system is as follows:  $\text{BIQ}^{2+}$  is reduced by electron donors such as  $\text{OH}^-$  and  $\text{OOH}^-$  to BIQ, which reacted with molecular oxygen to give a 1,2-dioxetane

Koko Maeda, Yoko Matsuyama, Kumiko Isozaki, Sachiko Yamada and Yukie Mori

- 127 Reactivity of nitroso oxides: effect of polar substituents and reaction mechanism



Shinji Ishikawa, Takayuki Nojima and Yasuhiko Sawaki

## AUTHOR INDEX

- Ahn, Sangdoo, 79  
Bothe, Eberhard, 5, 13, 23  
Catalán, Javier, 57  
Cates, Rex G., 91  
Chang, Suk-Kyu, 79  
Collot, Anne-Gaelle, 49  
de Paz, José Luis G., 57  
Donovan, William H., 83  
Dunkel, Reinhard, 91  
El Fahid, Bouchaïb, 49  
Elguero, José, 57  
Famini, George R., 83  
Fery-Forgues, Suzanne, 73  
Geetha Saraswathy, V., 29  
Grant, David M., 91  
Guglielmetti, Robert, 107
- Harper, James K., 91  
Hashizume, Daisuke, 61  
Hildenbrand, Knut, 13, 23  
Ishikawa, Shinji, 127  
Isozaki, Kumiko, 121  
Jansson, Per-Erik, 33  
Kjellberg, Alexandra, 33  
Kogo, Hidenori, 61  
Lagercrantz, Carl, 101  
Laréginie, Pierre, 107  
Lavabre, Dominique, 73  
Lee, Jo Woong, 79  
Li, Du, 91  
Lokshin, Vladimir, 107  
Maeda, Koko, 113, 121  
Matsuyama, Yoko, 121
- Miyamoto, Hisakazu, 61  
Mori, Yukie, 113, 121  
Moutiers, Gilles, 49  
Nojima, Takayuki, 127  
Ohashi, Yuji, 61  
Owen, Noel L., 91  
Pakkanen, Tapani A., 39  
Pépe, Gérard, 107  
Pohjala, Esko, 39  
Räsänen, Jari P., 39  
Rosiak, Janusz M., 5, 13, 23  
Rundlöf, Torgny, 33  
Samat, André, 107  
Sankararaman, S., 29  
Sawaki, Yasuhiko, 127  
Sekine, Akiko, 61
- Shinkai, Seiji, 1  
Shinmori, Hideyuki, 1  
Starikov, Evgeni B., 67  
Steiner, Thomas, 67  
Takeuchi, Masayuki, 1  
Tamm, Matthias, 67  
Terrier, François, 49  
Toda, Fumio, 61  
Ulanski, Piotr, 5, 13, 23  
Vidal, Christiane, 73  
von Sonntag, Clemens, 5,  
13, 23  
Widmalm, Göran, 33  
Wood, Steven G., 91  
Yamada, Sachiko, 121

---

NOTE: An asterisk in the heading of each paper indicates the author who is to receive any correspondence.

## Journal of Chemical Research, Issue 12, 1995

Other papers in the subject areas covered by *J. Chem. Soc.* are published in synopsis/microform format in *J. Chem. Research*. For the benefit of readers of *J. Chem. Soc.*, the contents list of *J. Chem. Research (S)*, Issue 12, is reproduced below.

- 483 Carbon-13 NMR Spectroscopic Studies of Some Triacylglycerols of Type AAA containing Conjugated Diacetylenic and Allenic Acyl Groups **Marcel S. F. Lie Ken Jie** and **C. C. Lam**  
(M 2901)
- 484 Theoretical Study of Anthracycline Antibiotic Analogues. Part 2. Conformational Analysis on Different 2,3,6-Trideoxy-3-amino- $\alpha$ -L-hexopyranoses **Redouan El Bergmi** and **José Molina Molina**  
(M 2947)
- 485 FT-IR and  $^1\text{H}$  and  $^{13}\text{C}$  NMR Studies of the Proton Acceptor Ability of 1,8-Bis(dimethylaminomethyl)naphthalene **Suzanne Toppet**, **Katherine Platteborze**, **Nathalie Leroux**, **Ilse Lambrechts** and **Thérèse Zeegers-Huyskens**  
(M 3018)
- 486 A Comparative Study on the Conformation of Derivatives of Furanoses, 4-Thiofuranoses and C-, N- and S-Furanosides **Patricia A. Zunszain** and **Oscar Varela**  
(M 2910)
- 488 Alkyl(oxo)pyridazinecarbonitriles as Building Blocks in Heterocyclic Synthesis: Novel Syntheses of Pyrido[3,4-c]pyridazines, Pyrido[3,4-d]pyridazines, Thiopyrano[3,4-c]pyridazines and 1,3,4-Thiadiazacacenaphthylenes **Fathi A. Abu-Shanab**, **Basil Wakefield**, **Fatima Al-Omran**, **Mervat M. Abdel Khalek** and **Mohamed Hilmy Elnagdi**  
(M 2924)
- 490 The Formation of Polyheterocyclic Systems by the Reaction of 2-Oxo-2H-1-benzopyran-3-carboxamide and Related Compounds with Active Methylene Compounds **Conor N. O'Callaghan**, **T. Brian H. McMurry** and **John E. O'Brien**  
(M 3001)
- 492 Reactions with Hydrazonoyl Halides. Part 11. Synthesis and Reactions of 1-Bromo-2-(4-cyano-5-phenyl-1-p-tolylpyrazol-3-yl)-ethanedione 1-Phenylhydrazone **Abdou O. Abdelhamid**, **Fouad F. Abd-el-Mageid**, **Nabil M. Hassan** and **Hussein F. Zohdi**  
(M 3036)
- 494 Condensation of Salicylaldehyde with 2-(5-Amino-3,4-dicyano-2H-pyrrol-2-ylidene)-1,1,2-tricyanoethanide. Synthesis and Characterization of the Corresponding Salicylideneiminat and X-Ray Crystal Structure of its Tetraphenylarsonium Salt **Vincenzo Fares**, **Alberto Flamini** and **Nicola Poli**  
(M 3054)
- 496 Pathways to the Higher Products in Lewis Acid Catalysed Additions of Allylic Chlorides to Isoalkenes and Isoprene  
(—) **Elvi Muks**
- 498 N-Arylisoindolines: Charge-transfer Complexation and Novel Synthesis of 2'-Arylspiro[1,3-benzodioxole-2,1'-isoindolin]-3'-ones  
(—) **Alaa A. Hassan**
- 500 Hydrolysis, Alcoholysis and Aminolysis of 12H-Benzoxazolo[2,3-b]quinazolin-12-imines **Plamen Atanassov** and **Krum Davidkov**  
(—)
- 502 Synthesis of 14-Alkyl-14H-Dibenzo[a,j]xanthenes  
(—) **Okan Sirkecioğlu**, **Naciye Talinlı** and **Ahmet Akar**
- 503 Synthesis of Diaryloxymethanes using Poly(ethylene glycol) as a Phase-transfer Catalyst **Manikrao M. Salunkhe**, **Bhanudas P. Kavitate**, **Sucheta V. Patil** and **Prakash P. Wadgaonkar**  
(—)
- 504 Palladium-catalysed Cyclisation of a 1-Acetoxyoct-2-yn-7-ene and of One of its Homologues **Jaume Castro**, **Geneviève Balme** and **Jacques Goré**  
(—)
- 506 Chlorotrimethylsilane-Sodium Nitrite or Nitrate in Synthesis: Efficient Regeneration of Aldehydes and Ketones from their Semicarbazones **Rahat H. Khan**, **Raj K. Mathur** and **Anil C. Ghosh**  
(—)
- 508 Ethanolysis of 3-Bromo-4-[N-bromo-N-(3,4-dimethylisoxazol-5-yl)amino]-1,2-naphthoquinone **Viviana G. Dabbene**, **Margarita C. Briñón** and **María M. de Bertorello**  
(—)
- 510 Solvent Effect on the Cleavage Rate Constant of Chloroanthracene Radical Anions formed at a Mercury Electrode **Jan S. Jaworski**, **Piotr Leszczyński** and **Janusz Tykarski**  
(—)
- 512 Preparation of 1,2,4-Trichlorobenzene by Regioselective Chlorination of 1,2-Dichlorobenzene in the Presence of Catalytic Amounts of Zeolites **Anand P. Singh**, **Sahida Sharma** and **Supada R. Rojatkar**  
(—)
- 514 Disulfenamides as Precursors of Aminyl Radicals  
(—) **W. Russell Bowman**, **David N. Clark** and **Robert J. Marmon**

N.B. The numbers in parentheses, prefaced by *M*, indicate the first frame occupied by the *full-text version* of the paper in *J. Chem. Research (M)*. Where no such number is given, the paper as published in *J. Chem. Research (S)* is complete in itself, and there is no extra material in Part *M*.

## Forthcoming Articles in *Perkin Transactions 2*

Tertiary:secondary:primary C–H bond relative reactivity in the one-electron oxidation of alkylbenzenes. A tool to distinguish electron transfer from hydrogen atom transfer mechanisms **E. Baciocchi, F. D'Acunzo, C. Galli and O. Lanzalunga**

3-Acetoxyaminoquinazolin-4(3*H*)-ones as aziridinating agents: relative rate of inversion at the exocyclic nitrogen **R.S. Atkinson and P.J. Williams**

Role of nitrogen atom in the complex metal hydride reduction of unhindered  $\gamma$ -azacyclohexanones **Y. Senda, M. Morita and H. Itoh**

Inverted spin trapping. Part V. 1,1,1,3,3,3-Hexafluoropropan-2-ol as a solvent for the discrimination between proper and inverted spin trapping **L. Ebersson, M.P. Hartshorn and O. Persson**

On the existence of quinone radical cations. A study in 1,1,1,3,3,3-hexafluoropropan-2-ol **L. Ebersson and M.P. Hartshorn**

Stability and IR spectra of isomers of C<sub>60</sub>F<sub>48</sub> **S.J. Austin, P.W. Fowler and J.P.B. Sandall**

Kinetic study of the stability of (NH<sub>2</sub>)<sub>2</sub>CSSC(NH<sub>2</sub>)<sub>2</sub><sup>2+</sup> **L.G. Rio, C.G. Munkley and G. Stedman**

EPR spectra of tris(trimethylsilyl)methyl(hydroxy)silyl radicals, (Me<sub>3</sub>Si)<sub>3</sub>CSi(R)OH and of tris(trimethylsilyl)methylsilanone radical anions, (Me<sub>3</sub>Si)<sub>3</sub>CSi(R)=O<sup>•-</sup> (R=H, Me, Et, Bu, Ph, F) **A.G. Davies, C. Eaborn, P.D. Lickiss and A.G. Neville**

Kinetic constraints on possible reaction pathways for the osmium catalysed asymmetric dihydroxylation (AD) **P.O. Norrby and K.P. Gable**

Geometric and electronic structure of dicyanofuroxan by experiment and theory **T. Pasinszki, G. Ferguson and N.P.C. Westwood**

Synthesis and studies on surface and self-assembly properties of polyphenylsulfonates in aqueous solution. Part 2. Sodium 2'-methyl-5'-phenyl-1,1':3',1''-terphenyl-4-sulfonate **J. Czapkiewicz and P. Milart**

Synthesis of 1,4-phenylene-bridged linear porphyrin arrays **A. Osuka, N. Tanabe, S. Nakajima and K. Maruyama**

4-Iodonitrosobenzene. Structural and spectroscopic studies of the monomeric solid and of previously unreported dimers **D.A. Fletcher, B.G. Gowenlock, K.G. Orrell, V. Sik, D.E. Hibbs, M.B. Hursthouse and K.M. Abdul Malik**

Mixed crystals of pyrazoles and benzoic acids. 1. Molecular structure of 3,5-dimethylpyrazole-2,4,6-trimethylbenzoic acid co-crystals **C. Foces-Foces, L. Infantes, F. Aguilar-Parrilla, N.S. Golubev, H-H. Limbach and J. Elguero**

Gas-phase generation of trifluoromethyl cyclopentadienides **M.C. Baschky, J.R. Sowa, Jr., P.G. Gassman and S.R. Kass**

Thermal decomposition of diacyl peroxide. Part 10. Evidences for acyloxy radical pair mechanism for <sup>18</sup>O-scrambling of carbonyl-<sup>18</sup>O-labelled cyclopropanecarbonyl peroxide **K. Fujimori, Y. Hirose and S. Oae**

Thermal decomposition of diacyl peroxide. Part 11. <sup>18</sup>O-Scrambling in carbonyl-<sup>18</sup>O-labelled phthaloyl peroxide, a cyclic case III diacyl peroxide. Extremely large return of unescapable acyloxy radical pair **K. Fujimori, Y. Oshibe, Y. Hirose and S. Oae**

Influence of magnesium(II) ions on cathodic reactions in aprotic solvents: the carboxylation of methyl aryl ketones **D. Pletcher and L. Slevin**

Source of catalysis of dephosphorylation of *p*-nitrophenyldiphenylphosphate by metallomicelles **C.A. Bunton, P. Scrimin and P. Tecilla**

Photochromism of double-bridged viologen in polar polymer matrix **S. Xuehwei and Y. Yu-kun**

Tetraalkoxybenzo-1,4-quinones and structurally related tetraalkoxybenzene derivatives: synthesis, properties and solid-state packing motifs **E.M.D. Keegstra, B-H. Huisman, E.M. Paardekooper, F.J. Hoogesteger, J.W. Zwikker and L.W. Jenneskens**

Solid-state structure, dynamical properties in solution and computational studies of a new sodium hemispherand complex **F.C.J.M. van Veggel, J.P.M. van Duynhoven, S. Harkema, M.P.O. Wolbers and D.N. Reinhoudt**

*Ab initio* study of the methylsulfonate and phenylsulfonate anions **I. Rozas and D.F. Weaver**

Photoisomerization of ammonium  $\alpha,\beta$ -unsaturated carboxylates in the solid state: effect of the hydrogen-bond network on the reactivity **K. Kinbara, A. Kai, Y. Maekawa, Y. Hashimoto, S. Naruse, M. Hasegawa and K. Saigo**

Redox-initiated radical decomposition of triazenes and their platinum complexes (cyclic voltammetry, EPR)

**P.Rapta, L. Omelka, A. Stasko, J. Dauth, B. Deubzer and J. Weis**

Laser flash photolysis study of dithiobis-2,2'-benzoxazole and dithiobis-2,2'-benzothiazole; reactivities of benzoxazole-2-thiyl radical and benzothiazole-2-thiyl radical **M.M. Alam, H. Konami, A. Watanabe and O. Ito**

Ring closing and photooxidation in *N*-analogues of 3-hydroxyflavone **F. Gao, K.F. Johnson and J.B. Schlenoff**

Stereoselectivity and mechanism in the electrohydrodimerisation of esters of cinnamic acid

**I. Fussing, M. Güllü, O. Hammerich, A. Hussain, M.F. Neilsen and J.H.P. Utley**

Conformational analysis of (*R,R*)- and (*R,S*)-*N,N*-bis(1-phenylethyl)-acetamide and -thioacetamide. A study by NMR spectroscopy and by empirical force-field and AM1 calculations **M. Langgard and J. Sandstrom**

Theoretical study of Diels–Alder reaction between the *S*-methylthiophenium ion and ethene

**B.S. Jursic, Z. Zdravkovski and S.L. Whittenburg**

<sup>1</sup>H Dynamic NMR and X-ray crystal structure studies of conformational preferences in dibenzo[*c,h*][1,6]diazecines

**S. Lehmann, G.W. Buchanan, C. Bensimon, J. Hartmann and W. Schroth**

Synthesis, hydrolysis reactions and conformational study of 2-substituted 3,5-diamino-4-nitroso-2*H*-1,2,6-thiadiazine 1,1-dioxides

**I. Alkorta, C. Garcia-Gomez, J.L.G. de Paz, M.L. Jimeno and V.J. Aran**

Catalytic hydrolysis of phosphate triesters by lanthanide(III) cryptate (2.2.1) complexes

**S.J. Oh, C.W. Yoon and J.W. Park**

An IR, NMR, dipole moment and X-ray study on intramolecular O–H...N hydrogen bonding in 8-hydroxy-*N,N*-dimethyl-1-naphthylamine **E. Grech, J.Nowicka-scheibe, Z. Olejnik, T. Lis, Z. Pawelka, Z. Malarski and L. Sobczyk**

Exceptionally persistent and oxygen-insensitive 2,7-di-*tert*-butyl-1-pyrenoxyl radical: synthesis, dimerization, EPR and ENDOR spectra **Y. Miura, E. Yamano, A. Miyazawa and M. Tashiro**

Carbon–hydrogen and carbon–carbon coupling patterns in the cephalosporin series **J. Jazwinski, J. Pankowski and J. Winiarski**

Experimental and theoretical study of tautomerism in 1,4-bis(methoxyamino)anthracene-9,10-diones and their reduced forms

**J.O. Morley, A.P. Krapcho and D.S. Cummings**

Factors controlling reactivity in hydrogen abstractions by free radicals **A.A. Zavitsas**

Synthesis of calix[4]arene receptors incorporating (2,2'-bipyridin-6-yl)methyl and (9-methyl-1,10-phenanthrolin-2-yl)methyl chromophores and luminescence of their Eu<sup>3+</sup> and Tb<sup>3+</sup> complexes

**A. Casnati, C. Fischer, M. Guardigli, A. Isernia, I. Manet, N. Sabbatini and R. Ungaro**

Stereoselective *cis,trans*-photoisomerization of formyl-substituted *trans,trans,trans*-1,6-diphenylhexa-1,3,5-triene in solution

**Y. Sonoda and Y. Suzuki**

Ion–molecule reactions of benzoyl ions in a quadrupole ion trap mass spectrometer **C.S. Creaser and B.L. Williamson**

Synthesis and characterization of end-functional oligo-vinylthiophenes with liquid crystal properties

**C. Maertens, J.-X. Zhang, P. Dubois and R. Jerome**

One electron oxidation of 2,3-dihydro-5,6-dihydroxyindole: the influence of Zn<sup>2+</sup>

**A.T. Al-Kazwini, P. O'Neill, G.E. Adams, R.B. Cundall, J. Maignan and A. Junino**

Roof-shaped hydroxy hosts: synthesis, complex formation and X-ray crystal structures of inclusion compounds with EtOH, nitroethane and benzene **E. Weber, T. Hens, O. Gallardo and I. Csöreg**

Opening the aziridinimine ring: cycloreversion *versus* isomerization **M.T. Nguyen, A. Van Keer and L.G. Vanquickenborne**

NMR spectroscopic evidences and molecular dynamics studies on inclusion and non-inclusion phenomena between β-cyclodextrin and new anti-alzheimer's drugs tacrine (CI-970), velnacrine (HP-029) and suronacrine (HP-128)

**M.E. Amato, K.B. Lipkowitz, G.M. Lombardo and G.C. Pappalardo**

Comments on the utility of aromatic ring parameters in the correlation analysis of solvolytic reactivities for benzylic substrates

**K-T. Liu**

Role of transition metal ions in hydrogen bonded networks: a density functional molecular orbital theory study

**J.E. McGrady and D.M.P. Mingos**