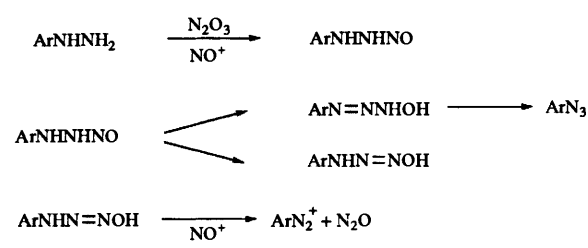
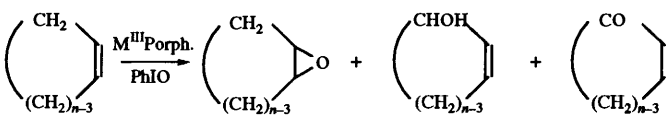
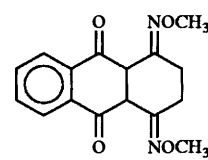
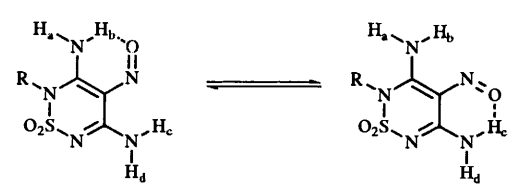
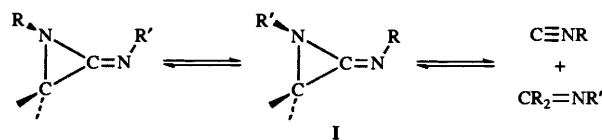


Articles

<p>275 Kinetics and mechanism of the reaction of nitrous acid with 2,4-dinitrophenylhydrazine</p> <p>Pierre Bernheim, Agnes Dobos, Anne M. M. Doherty, Neil Haine and Geoffrey Stedman</p>	
<p>281 Allylic oxidation and epoxidation of cycloalkenes by iodosylbenzene catalysed by iron(III) and manganese(III) tetra(dichlorophenyl)porphyrin: the marked influence of ring size on the rate of allylic oxidation</p> <p>Amanda J. Appleton, Steven Evans and John R. Lindsay Smith</p>	
<p>287 Experimental and theoretical study of tautomerism in 1,4-bis[methoxyamino]anthracene-9,10-diones and their reduced forms</p> <p>John O. Morley, A. Paul Krapcho and Douglas S. Cummings</p>	 <p>Preparation, calculated structure with the 3-21G basis set</p>
<p>293 Synthesis, hydrolysis reactions and conformational study of 2-substituted 3,5-diamino-4-nitroso-2H-1,2,6-thiadiazine 1,1-dioxides</p> <p>Ibon Alkorta, Concepción García-Gómez, Jose Luis G. de Paz, María Luisa Jimeno and Vicente J. Arán</p>	

299 **Opening the aziridinimine ring: a theoretical study**

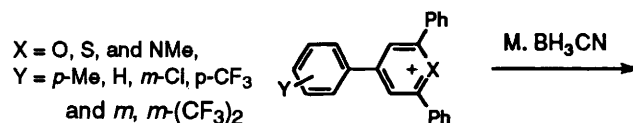
Minh Tho Nguyen, Annik Van Keer and Luc G. Vanquickenborne



Ab initio MO studies have been performed on the aziridinimine molecule I

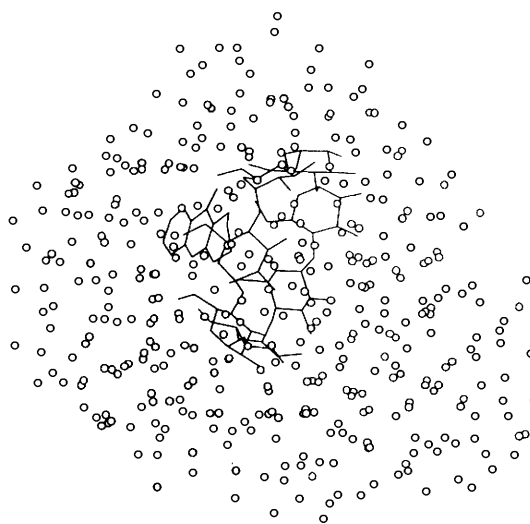
307 **Substituent effects in cyanoborohydride reductions of heterocyclic aromatic cations**

Roy Beddoes (in part), David Heyes, Ramesh S. Menon and C. Ian. F. Watt



321 **NMR spectroscopic evidence 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)**

Maria E. Amato, Kenny B. Lipkowitz, Giuseppe M. Lombardo and Giuseppe C. Pappalardo



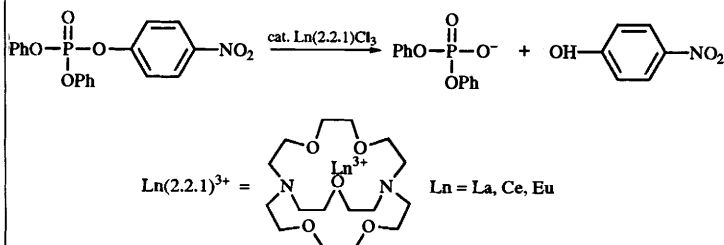
327 **Comments on the utility of aromatic ring parameters in the correlation analysis of solvolytic reactivities for benzylic substrates**


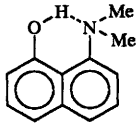
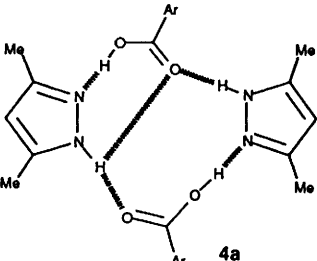
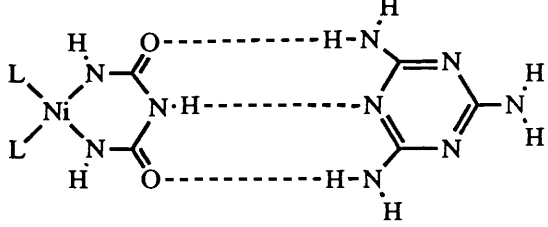
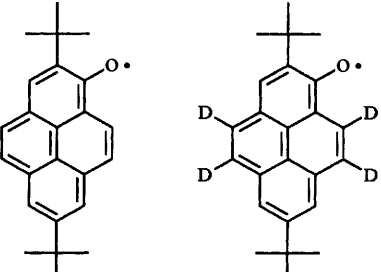
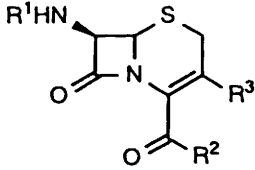
Kwang-Ting Liu

The disadvantage of using $\log(k/k_0) = mY + hI$ in correlation analysis has been discussed

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

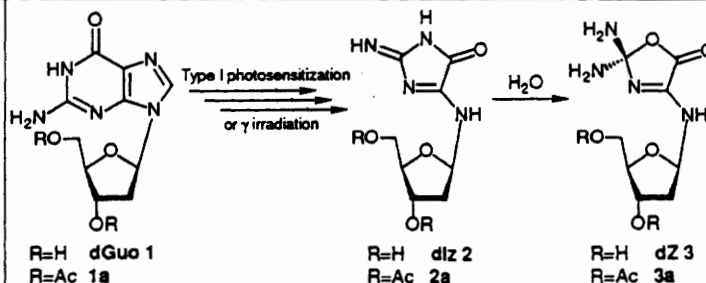
Soon Jin Oh, Chang Won Yoon and Joon Won Park



<p>333 Substituent chemical shifts in NMR spectroscopy. Part 6. A model for the calculation of proton chemical shifts in substituted alkanes</p> <p>Raymond J. Abraham, Mark Edgar, Robert P. Glover, Mark A. Warne and Lee Griffiths</p>	
<p>343 An IR, NMR, dipole moment and X-ray study on intramolecular O–H ··· N hydrogen bonding in 8-hydroxy-<i>N,N</i>-dimethyl-1-naphthylamine</p> <p>E. Grech, J. Nowicka-Scheibe, Z. Olejnik, T. Lis, Z. Pawełka, Z. Malarski and L. Sobczyk</p>	 <p>Structure, dipole moment and IR and NMR spectroscopic behaviour</p>
<p>349 Mixed crystals of pyrazoles and benzoic acids. Part 1. The molecular structure of 3,5-dimethylpyrazole-2,4,6-trimethylbenzoic acid co-crystals</p> <p>Concepción Foces-Foces, Lourdes Infantes, Francisco Aguilar-Parrilla, Nicolai S. Golubev, Hans-Heinrich Limbach and José Elguero</p>	 <p>Two pyrazoles and two benzoic acids form a tetramer unit through N–H ··· O and O–H ··· N hydrogen bonds</p>
<p>355 The role of transition metal ions in hydrogen bonded networks: a density functional molecular orbital theory study</p> <p>John E. McGrady and D. Michael P. Mingos</p>	
<p>359 Exceptionally persistent and oxygen-insensitive 2,7-di-<i>tert</i>-butylpyren-1-oxyl radical: synthesis, dimerization, EPR and ENDOR spectra</p> <p>Yozo Miura, Eiji Yamano, Akira Miyazawa and Masashi Tashiro</p>	 <p>EPR and ENDOR spectra are measured and the corresponding dimers of these radicals give very low ΔH and negative ΔS values in the equilibrium with these radicals</p>
<p>365 Carbon–hydrogen and carbon–carbon coupling patterns in the cephalosporin series</p> <p>Jarosław Jaźwiński, Jacek Pankowski and Jerzy Winiarski</p>	 <p>The C–C and C–H coupling constants and the method of unambiguous assignment of <i>E</i> or <i>Z</i> geometry of 2-(2-aminothiazol-4-yl)-2-alkoxyiminoacetyl substituent R^1 are given</p>

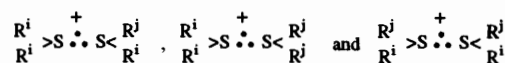
- 371 ^1H , ^{13}C and ^{15}N Nuclear magnetic resonance analysis and chemical features of the two main radical oxidation products of 2'-deoxy-guanosine: oxazolone and imidazolone nucleosides

Sébastien Raoul, Maurice Berger, Garry W. Buchko, Prakash C. Joshi, Bénédicte Morin, Michael Weinfeld and Jean Cadet



- 383 Three-electron bonded σ/σ^* radical cations from mixedly substituted dialkyl sulfides in aqueous solution studied by pulse radiolysis

Shamim A. Chaudhri, Hari Mohan, Elke Anklam and Klaus-Dieter Asmus



Radical cations in aqueous solution

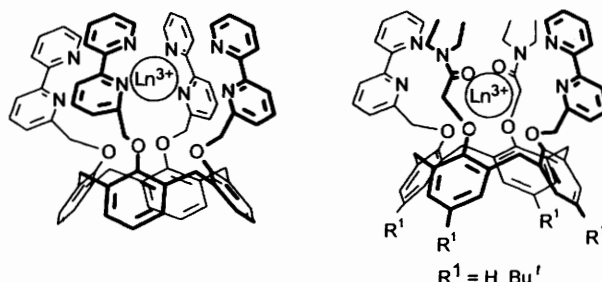
- 391 Factors controlling reactivity in hydrogen abstractions by free radicals

Andreas A. Zavitsas

In identity hydrogen abstractions by radicals, $\text{X-H} + \cdot\text{X} \longrightarrow \text{X}^* + \text{H-X}$, the energy of activation is determined primarily by the molecular properties of molecule X-X

- 395 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^{3+} and Tb^{3+} complexes

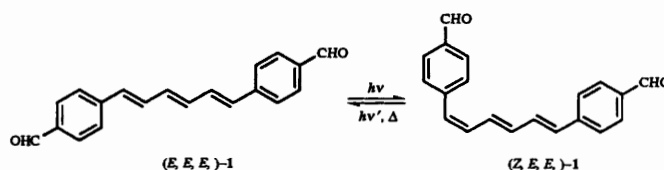
A. Casnati, C. Fischer, M. Guardigli, A. Isernia, I. Manet, N. Sabbatini and R. Ungaro



Ligands incorporating bipyridine groups of calix[4]arenes give Eu^{3+} and Tb^{3+} complexes with interesting photophysical properties

- 401 Stereoselective *Z,E*-photoisomerization of formyl-substituted (*E,E,E*)-1,6-diphenylhexa-1,3,5-triene in solution

Yoriko Sonoda and Yasuzo Suzuki

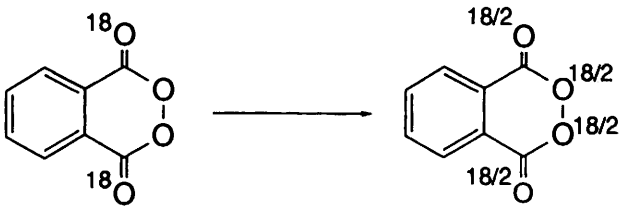
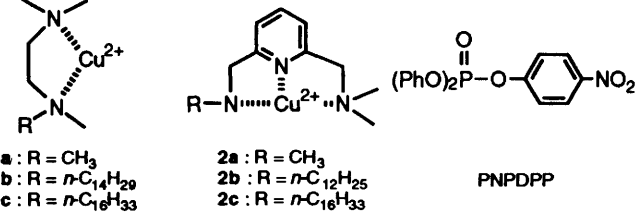
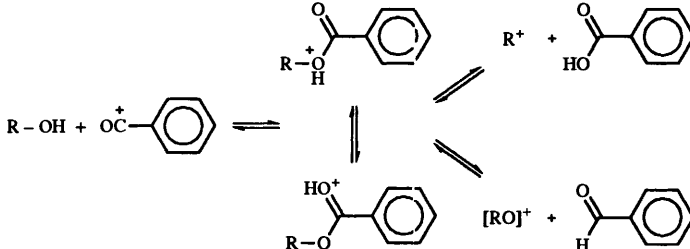
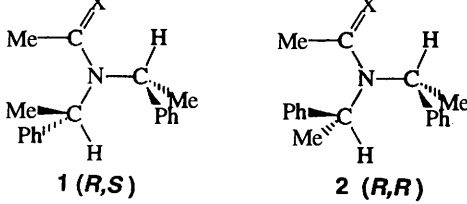
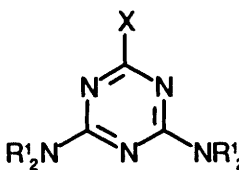
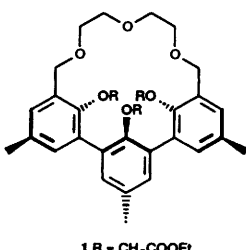


- 405 Thermal decomposition of diacyl peroxide. Part 10. Evidence for acyloxyl radical pair mechanism for ^{18}O -scrambling of ^{18}O -labelled cyclopropanecarbonyl peroxide

Ken Fujimori, Yoshikazu Hirose and Shigeru Oae

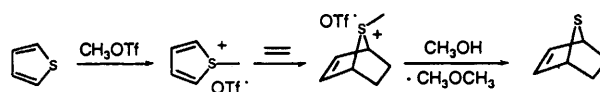


Kinetics and mechanism

<p>413 Thermal decomposition of diacyl peroxide. Part 11. ^{18}O-Scrambling in carbonyl-^{18}O-labelled phthaloyl peroxide, a cyclic Case III diacyl peroxide. Extremely large return of unescapable acyloxyl radical pair</p> <p>Ken Fujimori, Yoshihiro Oshibe, Yoshikazu Hirose and Shigeru Oae</p>	 <p style="text-align: center;">Kinetics and mechanism</p>
<p>419 Source of catalysis of dephosphorylation of <i>p</i>-nitrophenyldiphenylphosphate by metallomicelles</p> <p>Clifford A. Bunton, Paolo Scrimin and Paolo Tecilla</p>	 <p style="text-align: center;">PNPDPP</p> <p>Quantitative evaluation of the source of rate acceleration in dephosphorylation of PNPDPP by metallomicelles 1b, c and 2b, c is reported</p>
<p>427 Ion-molecule reactions of benzoyl ions in a quadrupole ion trap mass spectrometer</p> <p>Colin S. Creaser and Brian L. Williamson</p>	
<p>435 Conformational analysis of (<i>R,R</i>)- and (<i>R,S</i>)-<i>N,N</i>-bis(1-phenylethyl)-acetamide and -thioacetamide. A study by NMR spectroscopy and by empirical force-field and AM1 calculations</p> <p>Morten Langgård and Jan Sandström</p>	 <p style="text-align: center;">1 (<i>R,S</i>) 2 (<i>R,R</i>)</p> <p style="text-align: center;">a, X = O b, X = S</p> <p>The conformations of 1 and 2 have been studied by ^1HNMR spectroscopy and by MM2 and AM1 calculations</p>
<p>443 Restricted rotations in 4,6-bis- and 2,4,6-tris-(<i>N,N</i>-dialkylamino)-<i>s</i>-triazines</p> <p>Alan R. Katritzky, Ion Ghiviriga, Peter J. Steel and Daniela C. Oniciu</p>	 <p style="text-align: center;">X = Cl, NR¹₂, OR²</p> <p>X-Ray crystal structures and barriers to rotation of some <i>s</i>-triazines are reported</p>
<p>449 Solid-state structure, dynamical properties in solution and computational studies of a new sodium hemispherand complex</p> <p>Frank C. J. M. van Veggel, John P. M. van Duynhoven, Sybolt Harkema, Manon P. Oude Wolbers and David N. Reinhoudt</p>	 <p style="text-align: center;">1 R = CH₂COOEt</p> <p>In methanol a fast interconversion takes place in which one of the two outer carbonyl groups is coordinated to the Na⁺, resulting in a structure that resembles the solid-state structure</p>

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

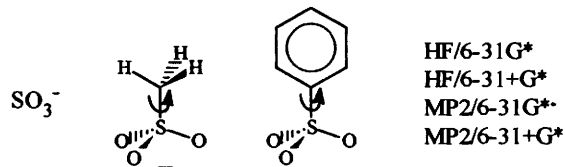
Branko S. Jursic, Zoran Zdravkovski and Scott L. Whittenburg



Ab initio theoretical study of the *S*-methylthiophenium cation as a diene for cycloaddition reactions is presented

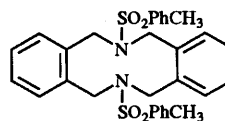
461 ***Ab initio* study of the methylsulfonate and phenylsulfonate anions**

Isabel Rozas and Donald F. Weaver



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

Silke Lehmann, Gerald W. Buchanan, Corinne Bensimon, Jens Hartmann and Werner Schroth



Restricted rotation about the exocyclic N–S bond was found ($\Delta G^\ddagger = 43.5 \pm 0.5 \text{ kJ mol}^{-1}$)

Corrigendum

471 **UV and ¹⁵N NMR integrated study of the protonation of aminoazoles** Adele Garrone, Roberta Fruttero, Carla Tironi and Alberto Gasco

AUTHOR INDEX

- Abraham, Raymond J., 333
Aguilar-Parrilla, Francisco, 349
Alkorta, Ibon, 293
Amato, Maria E., 321
Anklam, Elke, 383
Appleton, Amanda J., 281
Arán, Vicente J., 293
Asmus, Klaus-Dieter, 383
Beddoes, Roy, 307
Bensimon, Corinne, 467
Berger, Maurice, 371
Bernheim, Pierre, 275
Buchanan, Gerald W., 467
Buchko, Garry W., 371
Bunton, Clifford A., 419
Cadet, Jean, 371
Casnati, A., 395
Chaudhri, Shamim A., 383
Creaser, Colin S., 427
Cummings, Douglas S., 287
de Paz, Jose Luis G., 293
Dobos, Agnes, 275
Doherty, Anne M. M., 275
Edgar, Mark, 333
Elguero, José, 349
Evans, Steven, 281
Fischer, C., 395
Foces-Foces, Concepción, 349
Fruttero, Roberto, 471
Fujimori, Ken, 405, 413
García-Gómez, Concepción, 293
Garrone, Adele, 471
Gasco, Alberto, 471
Ghiviriga, Ion, 443
Glover, Robert P., 333
Golubev, Nicolai S., 349
Grech, E., 343
Griffiths, Lee, 333
Guardigli, M., 395
Haine, Neil, 275
Harkema, Sybolt, 449
Hartmann, Jens, 467
Heyes, David, 307
Hirose, Yoshikazu, 405, 413
Infantes, Lourdes, 349
Isernia, A., 395
Jaźwiński, Jarosław, 365
Jimeno, María Luisa, 293
Joshi, Prakash C., 371
Jursic, Branko S., 455
Katritzky, Alan R., 443
Krapcho, A. Paul, 287
Langgård, Morten, 435
Lehmann, Silke, 467
Limbach, Hans-Heinrich, 349
Lipkowitz, Kenny B., 321
Lis, T., 343
Liu, Kwang-Ting, 327
Lombardo, Giuseppe M., 321
Malarski, Z., 343
Manet, I., 395
McGrady, John E., 355
Menon, Ramesh S., 307
Mingos, D. Michael P., 355
Miura, Yozo, 359
Miyazawa, Akira, 359
Mohan, Hari, 383
Morin, Bénédicte, 371
Morley, John O., 287
Nguyen, Minh Tho, 299
Nowicka-Scheibe, J., 343
Oae, Shigeru, 405, 413
Oh, Soon Jin, 329
Olejnik, Z., 343
Oniciu, Daniela C., 443
Oshibe, Yoshihiro, 413
Pankowski, Jacek, 365
Pappalardo, Giuseppe C., 321
Park, Joon Won, 329
Pawelka, Z., 343
Raoul, Sébastien, 371
Reinhoudt, David N., 449
Rozas, Isabel, 461
Sabbatini, N., 395
Sandström, Jan, 435
Schroth, Werner, 467
Scrimin, Paolo, 419
Smith, John R. Lindsay, 281
Sobczyk, L., 343
Sonoda, Yoriko, 401
Stedman, Geoffrey, 275
Steel, Peter J., 443
Suzuki, Yasuzo, 401
Tashiro, Masashi, 359
Tecilla, Paolo, 419
Tironi, Carla, 471
Ungaro, R., 395
van Duynhoven, John P. M., 449
Van Keer, Annik, 299
van Veggel, Frank C. J. M., 449
Vanquickenborne, Luc G., 299
Warne, Mark A., 333
Watt, C. Ian F., 307
Weaver, Donald F., 461
Weinfeld, Michael, 371
Whittenburg, Scott L., 455
Williamson, Brian L., 427
Winiarski, Jerzy, 365
Wolbers, Manon P. Oude, 449
Yamano, Eiji, 359
Yoon, Chang Won, 329
Zavitsas, Andreas A., 391
Zdravkovski, Zoran, 455

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

Forthcoming Articles in *Perkin Transactions 2*

Synthesis and characterization of end functionalized oligo(vinylthiophenes) with liquid crystal properties
C. Maertens, J.-X. Zhang, P. Dubois and R. Jerome

Kinetics and mechanism of the reaction of 1-fluoro-2,4-dinitrobenzene with hydroxide ion in W/O microemulsions
E.N. Durantini and C.D. Borsarelli

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**

Non-classical buttressing effect: gas-phase ionization of some methyl substituted benzoic acids
M. Decouzon, O. Exner, J.F. Gal and P.C. Maria

Hydroxypropyl- β -cyclodextrins: induced circular dichroism spectra of included phenolphthalein as a function of the degree of substitution **A. Buvári-Barcza, J. Kajtar, L. Szente and L. Barcza**

Intramolecular motions in a series of crystalline benzylammonium bromides and dibenzylamines studied by CP/MAS NMR
F.G. Riddell and M. Rogerson

Conformational equilibria of methyl α -L-arabinopyranosides in solution
R. Lanzetta, M. Parrilli, C. Garzillo, A. di Matteo and G. Del Re

Photo-decarboxylation of substituted alkylcarboxylic acids brought about by visible light and iron(III) tetra(2-N-methylpyridyl)porphyrin in aqueous solution **B.C. Gilbert, G.R. Hodges, J.R. Lindsay Smith, P. MacFaul and P. Taylor**

Conformational analysis. Part 27. An NMR solvation and theoretical investigation of conformational isomerism in fluoro- and 1,1-difluoro-acetone **R.J. Abraham, A.D. Jones, M.A. Warne, R. Rittner and C.F. Tormena**

UV-Visible-near-IR, MO and EPR studies of five redox stages of an octaethyltetraoxa[26]porphyrin
R. Bachmann, F. Gerson, C. Pütz and E. Vogel

UV-Induced isomerisation and ring transformation of (*E*)-3-arylidene-1-thiochromanones and -1-thioflavanones
G. Toth, J. Halász, A. Lévai, C. Nemes and T. Patonay

Oxidation of benzyl radicals by $\text{Fe}(\text{CN})_6^{3-}$ **G. Merga, H.-P. Schuchmann, B.S.M. Rao and C. von Sonntag**

Nucleophilicity of bromide ion in mixed cationic sulfoxide micelles **H.J. Foroudian, C.A. Bunton, P.M. Holland and F. Nome**

^1H - ^1H long range couplings in fused cyclopropanes. NMR spectral assignment and conformation of 17,18-cyclosteroids
E.M. Sproviero, A. Ferrara, R.H. Contreras and G. Burton

Novel intermolecular C-H \cdots π interactions: a combined *ab initio* and density functional theory study
M.F. Fan, Z. Lin, J.E. McGrady and D.M.P. Mingos

Reaction of *N*¹,*N*²-diarylamidines with dicyanomethylene compounds **D. Döpp, M.A. Gomaa, G. Henkel and A.M.N. El-Din**

Photo-Michael reaction of silyl enol ethers with β -nitro and β,β -dicyano styrenes **D. Ramkumar and S. Sankararaman**

Thermal decomposition of methylated α -thiobutyrolactones. A photoelectron spectroscopic study
Y.T. Chua, C.Y. Mok, H.H. Huang, I. Novak and S.C. Ng

Methylation and protonation of 1-aza-5-bora-4,6,11-trioxabicyclo[3.3.3]undecane and 1-aza-5-borabicyclo[3.3.3]undecane
R.W. Alder and Z. Jin

Generation, stability, dissociation and ion-molecule chemistry of sulfinyl cations in the gas phase
F.C. Gozzo, A.E.P.M. Sorrilha and M.N. Eberlin

Self-protonation mechanism in the electroreduction of hydroxyimines **A.A. Isse, A.M. Abdurahman and E. Vianello**

Sugar-controlled association-dissociation equilibria between DNA and boronic-acid-appended porphyrin
H. Suenaga, S. Arimori and S. Shinkai

Solvent effects on nitrogen NMR shieldings in thiazole and thiadiazole systems
M. Witanowski, W. Sicinska, Z. Biedrzycka, Z. Grabowski and G.A. Webb

The Hammett equation and Snyder theory as a criterion for adsorption of a functional group under liquid-solid chromatography
M. Palamareva and S. Chorbadjiev

Journal of Chemical Research, Issue 1, 1996

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 1, is reproduced below.

- 1 Synthesis of Ethyl (2*S*,3*S*)-2,3-Dihydroxy-2-methylbutanoate (the Chiral Part of Phomozin) in Enantiopure Form **Miguel Carda, Eva Falomir, Juan Murga and J. Alberto Marco** (M 0201)
- 2 Isolation of 2',3',6-Trihydroxy-4'-methoxy-7-*O*-neohesperidoside, a Novel Flavone Glycoside from *Cassia siamea* **Shafiullah, Mohammad Sohrab Khan, Mehtab Parveen, Mohammad Kamil and Mohammad Ilyas** (M 0101)
- 4 Synthesis and Reactions of 3-Aminothiazolo[3,2-*a*]benzimidazole-2-carbonitrile **Abd El-Wareth Abd El-Haleem Osman Sarhan, Hasan Ahmed Hasan El-Sherief and Abdalla Mohamed Mahamoud** (M 0116)
- 6 Preparation of Polydeuterated Phenylpropanoic Acids by the Desulfurization of Halogenated Benzo[*b*]thiophenecarboxylic Acids with Nickel- and Cobalt-Aluminium Alloys in Alkaline D₂O **Mamoru Mukumoto, Hirohisa Tsuzuki, Shuntaro Mataka, Masashi Tashiro, Takehito Tsukinoki, Yoshiaki Nagano and Iwao Hashimoto** (M 0136)
- 8 *o*-Pleiadienequinones. Part 5. 1,3-Dipolar Cycloaddition of *o*-Pleiadienequinone and Acenaphthylene-1,2-quinone with Benzonitrile Sulfide: Formation of a Bi(pleiadienyldiene)dione and a Bi(acenaphthylidene)dione **Takashi Aida, Akira Nagasawa and Josuke Tsunetsugu** (M 0169)
- 10 A New Synthesis of the 1,4-Dihydroindeno[1,2-*b*]pyrrole Heterocycle **Fiona M. Murphy and Mary J. Meegan** (M 0301)
- 12 Antitumour Heterocycles. Part 12. The Synthesis of New Hydroxypyrrrolocarbazoles and Hydroxypyridocarbazoles **Priyanthi Dharmasena, Ana-M. F. Oliveira-Campos, Maria-Joao R. P. Queiroz and Patrick V. R. Shannon** (M 0316)
- 14 Methanobenzoannulenes. Part 2. Synthesis of 5,8- and 5,9-Methanobenzo[7]annulene-10-amines **Duncan R. Rae and John Strachan** (M 0401)
- 16 Kinetic Studies of Ground State Atomic Caesium, Cs(6 ²S_{1/2}), with Bromine-containing Molecules by Time-resolved Laser-induced Fluorescence [Cs(7 ²P_{3/2}-6 ²S_{1/2}), λ = 455.5 nm] following Pulsed Irradiation **Ernesto Martinez, José Albaladejo, Alberto Notario and David Husain** (M 0364)
- 18 Carbon 13 and Proton NMR, Spin Density Distributions and Solid-state Structures of some Manganese *meso*-Tetraphenylporphyrin Complexes bearing Neutral Axial Ligands **Peter Turner, Maxwell J. Gunter, Brian W. Skelton, Allan H. White and Trevor W. Hambley** (M 0220)
- 20 Synthesis and Physicochemical Studies of New Lithium Alkoxocobaltate(II) Complexes **Mostafa El-Behairy, Aisha I. Ibrahim, Adel A. A. Emara and Tarik A. Tawfic** (—)
- 22 Synthesis, Physicochemical Studies and Solvatochromism of Some New Lithium μ-(Tetraaryloxo)cobaltate(II) and Allied Complexes **Mostafa El-Behairy, Aisha I. Ibrahim, Adel A. A. Emara and Tarik A. Tawfic** (M 0206)
- 23 Thermally-induced Electron Transfer Reaction of a Heterometallic Dinuclear Complex in the Solid State **Parimal Kundu, Manas Kumar Saha, Sutapa Sen, Samiran Mitra, Sanjay Kumar, Dilip Banerjee and Ranga Lal Bhattacharya** (M 0149)
- 24 A Convenient *in situ* Generation and Mild Oxidizing Ability of Triaryl(bismuthane Tosylimides **Hitomi Suzuki and Tohru Ikegami** (—)
- 26 Benzodiazepine Analogues. Part 11. A Kinetic-Mechanistic Study of the Formation of 1,5-Benzodioxepin-2-ones *via* Baeyer-Villiger Oxidation of Flavanones **Aifheli C. Gelebe and Perry T. Kaye** (—)
- 28 SnCl₂·2H₂O-Mg-H₂O: a Mild Reagent System for the Regioselective Transformation of Conjugated Nitroalkenes to Carbonyl Compounds **Nalin B. Das, Chintamani Sarangi, Bhagabat Nanda, Amalendu Nayak and Ram P. Sharma** (—)
- 30 Stereochemical and NMR Reassignment of 6-Norlysergic Acid Diethylamide and 6-Nor-6-allyllysergic Acid Diethylamide **Andrew V. Stachulski, David E. Nichols and Feodor Scheinmann** (—)
- 32 An Unexpected Acid-catalysed Rearrangement of the Tricyclic System of Vinigrol to the Fusoxysporone Skeleton **Jean-François Devaux, Issam Hanna, Jean-Yves Lallemand and Thierry Prangé** (—)
- 34 The Role of Silicon-Oxygen Interactions in Determining the Stereochemical Outcome of the Peterson Reaction **Alan R. Bassindale, Richard J. Ellis and Peter G. Taylor** (—)
- 36 Phase-transfer Catalysis: a Convenient Tool for the Functionalization of Benzocyclobutene-1-carbonitrile **Michał Fedoryński, Marek Zieliński and Andrzej Jończyk** (—)
- 38 A Novel Approach to the Prediction of Binding Constants for the Inclusion Complexation of α-Cyclodextrin with Benzene Derivatives by Artificial Neural Networks **Qing-Xiang Guo, Shuang-Hui Luo, Hong Wang, Mao-Sen Zhang and You-Cheng Liu** (—)
- 40 Binding of Oxovanadium(IV) to Imidazole, Pyrazole and Thiazole Ligands **Daniele Sanna, Giovanni Micera, Liliana Strinna Erre, Marcia Giovanna Molinu and Eugenio Garribba** (—)
- 42 An Electron Paramagnetic Resonance Study on the Binding of Oxovanadium(IV) to L-Histidine and L-Carnosine **Daniele Sanna, Giovanni Micera and Maria Giovanna Molinu** (—)
- 44 A Novel and Efficient Method for the Synthesis of Pyrazolo[3,4-*d*]pyrimidine Nucleosides **Pulak J. Bhuyan and Jagir S. Sandhu** (—)
- 46 Mild Azide-mediated Palladium-catalysed Cleavage of Allyloxycarbonyl Protected Alcohols in Aqueous Media **Silvana Sigismondi and Denis Sinou** (—)
- 48 Electron Paramagnetic Resonance Characterization of High Spin States of Tribenzoylenebenzene Radical Anions **M. Celina R. L. R. Lazana, M. Luisa T. M. B. Franco and M. Cândida B. L. Shohoji** (—)
- 50 A Novel Dimeric Dipeptide from the Indian Ocean Starfish *Pentacaster regulus* **Ammanamanchi S. R. Anjaneyulu, Mukku J. R. V. Venu Gopal and Nidasanametla S. K. Rao** (—)

- 52 Semiempirical AM1 Calculations on the Competing 1- and 4-Alkylation of 2-Methylbuta-1,3-diene With Primary Allylic Cations
(—) **Ivar Martin** and **Elvi Muks**
- 54 A Tellurium-125 and Proton Nuclear Magnetic Resonance Spectroscopic Study of Disubstituted Vinylic Telluride Dichlorides and of their Corresponding Tellurides **Hélio A. Stefani, Ivan P. de Arruda Campos, Luiz C. Roque, Marcel A. Montoro** and **Antônio L. Braga**
- 56 Kinetics and Mechanism of the Oxidation of Hydroxylamine by Bromine in Aqueous Sulfuric Acid **Ivan Valent** and **L'ubica Adamčíková**
(—)
- 58 Solvent Effect on the Aquation of *trans*-Tetraamminedichlorocobalt(III) Ion
(—) **Ol'ga Grančičová** and **Vladislav Holba**
- 60 Binding of Benzenehexacarboxylic Anion by Protonated Diethanolamine and Ethylenediamine, in Aqueous Solution
(—) **Alessandro De Robertis, Concetta De Stefano, Claudia Foti, Ottavia Giuffrè** and **Silvio Sammartano**
- 62 Regioselective Catalytic Halogenation of Arenes, mimicking Vanadium Haloperoxidase Reactions **Vishnumurthy R. Hegde, Godwin C. G. Pais, Rajiv Kumar, Pradeep Kumar** and **Bipin Pandey**
(—)
- 64 An Inadvertent Synthesis of Cyclic and Acyclic Trithiocarbonates under Phase-transfer Conditions **Vishnu J. Ram, Sunil K. Singh, Mahendra Nath** and **Pratibha Srivastava**
(—)
- 66 Raney Co–Al Alloy, an Efficient Catalyst for the Selective Incorporation of Deuterium Atoms at the Benzylic Position of Aromatic Compounds **Takehito Tsukinoki, Keiko Ishimoto, Mamoru Mukumoto, Michio Suzuki, Takatoshi Kawaji, Yoshiaki Nagano, Hirohisa Tsuzuki, Shuntaro Mataka** and **Masashi Tashiro**
(—)
- 68 Sulfated Zirconia: an Efficient Catalyst for the Synthesis of 1,1-Diacetates from Aldehydes and Ketones
(—) Satya V. N. Raju

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