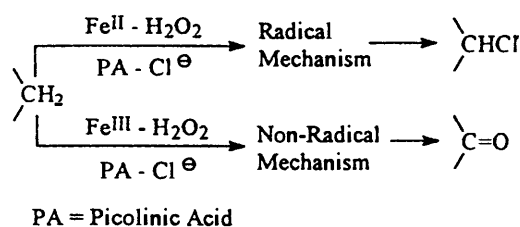




Keynote Article

1031 **The selective functionalization of saturated hydrocarbons. Part 32. Distinction between the Fe^{II}-Fe^{IV} and Fe^{III}-Fe^V manifolds in Gif chemistry. The importance of carboxylic acids for alkane activation. Evidence for a dimeric iron species involved in Gif-type chemistry**

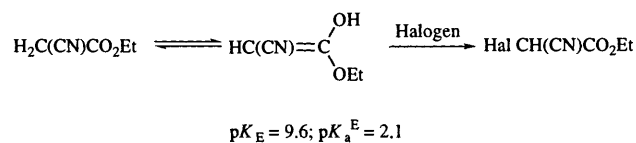
Derek H. R. Barton, Bin Hu, Dennis K. Taylor and Roy U. Rojas Wahl



Articles

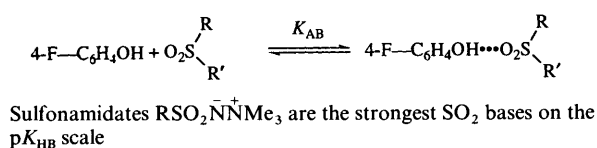
1043 **Halogenation and deuterium exchange in ethyl cyanoacetate. Enolisation mechanism and enol reactivity**

Alex R. Eberlin and D. Lyn H. Williams



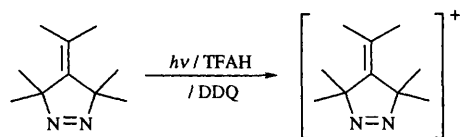
1047 **Hydrogen-bond basicity of the sulfonyl group. The case of strongly basic sulfonamidates RSO₂⁻NNMe₃⁺**

Aurélie Chardin, Christian Laurence, Michel Berthelot and David G. Morris



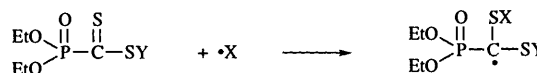
- 1053 EPR studies of pyrazoline radical ions that are potential precursors to non-Kekulé polyene radical ions

Richard J. Bushby and Kai M. Ng



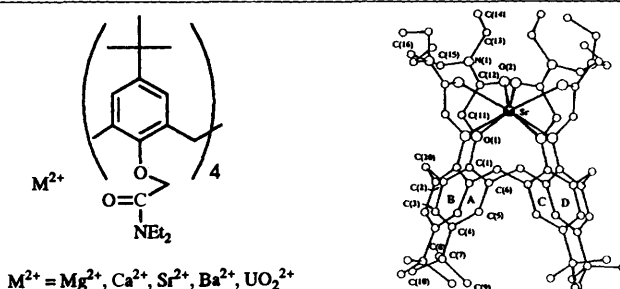
- 1057 EPR studies on phosphoryldithioformates. Part 2

Angelo Alberti, Massimo Benaglia, Maria Antonietta Della Bona, Dante Macciantelli, Bénédicte Heuzé, Serge Masson and Andrew Hudson



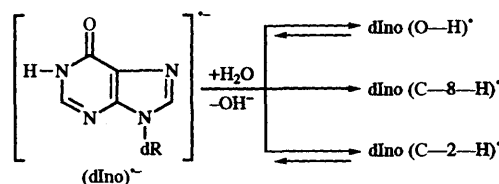
- 1065 Alkaline earth and uranyl cation complexes of a calix[4]arene-tetraamide: MD and FEP simulations in aqueous and acetonitrile solutions and X-ray structure of its Sr(Picrate)₂ complex

Nicolas Muzet, Georges Wipff, Alessandro Casnati, Laura Domiano, Rocco Ungaro and Franco Ugozzoli



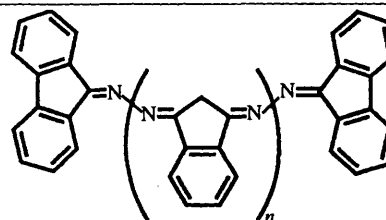
- 1077 Kinetics and spectral properties of electron adducts of 2'-deoxyinosine: a comparison with other purine nucleosides

Raghavendra R. Rao, C. T. Aravindakumar, B. S. Madhava Rao, Hari Mohan and Jai P. Mittal



- 1081 Oligomeric bis(1,3-indandiyliidene)azines: preparation, electrochemical and spectroscopic properties, and implications for the use of polyazines as conducting materials

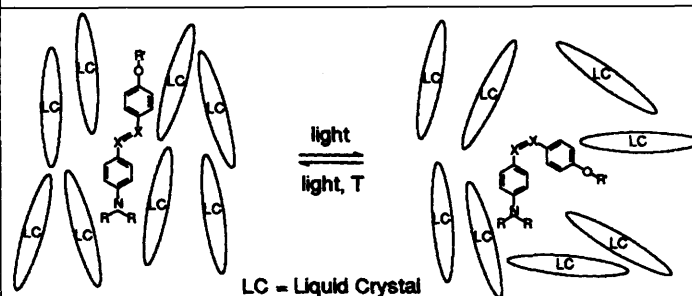
Donald Bethell, Dong-Hyo Kang and Giuseppe Zerbi



Vibrational spectra of oligomers with $n = 0-4$ suggest that the p_z electrons are localised within each repeat unit; polyazines may thus prove to be poor electrical conductors

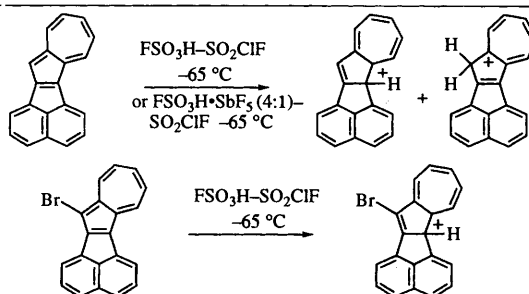
- 1087 Photochemically induced structure transfer from analogous azobenzenes and stilbenes onto a liquid crystalline phase

Thorsten Fischer, Ralf Ruhmann and Arno Seeboth



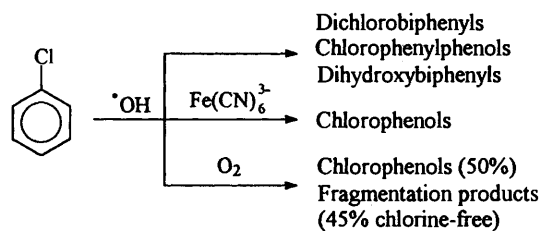
- 1091 **Protonation of azuleno[1,2-*a*]acenaphthylene and 7-bromoazuleno[1,2-*a*]acenaphthylene in superacids: azulonium, acenaphthenium or naphthalenium cations?**

Kenneth K. Laali, Simon Bolvig, Shigeyasu Kuroda, Mitsunori Oda, Masaru Mouri, Ichiro Shimao, Takanori Kajioka and Masfumi Yasunami



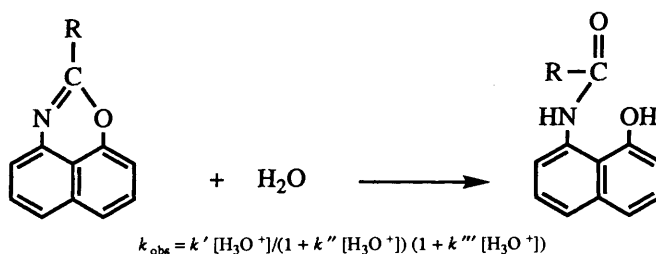
- 1097 **$\cdot\text{OH}$ Radical-induced oxidation of chlorobenzene in aqueous solution in the absence and presence of oxygen**

Getahun Merga, H.-P. Schuchmann, B. S. Madhava Rao and Clemens von Sonntag



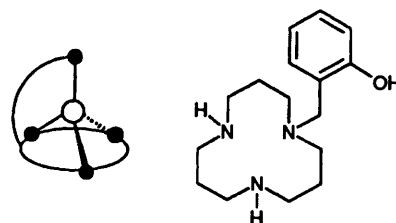
- 1105 **Substituent and solvent isotope effects on the reaction of 2-alkylnaphth[1,8-*de*]-1,3-oxazines to 1-hydroxy-8-acylaminonaphthalenes through reversible formation of a cyclic tetrahedral addition intermediate**

Andrew S. Baynham, Wendy J. Dixon, Frank Hibbert and Jagvi R. Patel



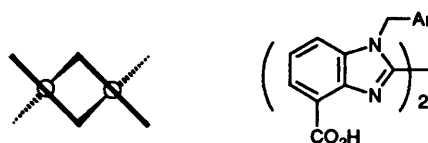
- 1109 **Complexation behaviour of C- and N-functionalized tetradentate ligands based on 1,5,9-triazacyclododecane**

George B. Bates and David Parker



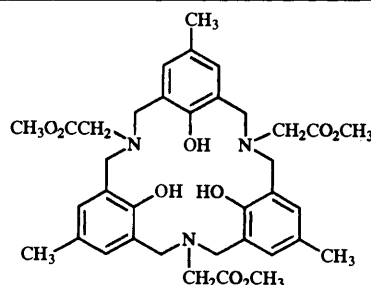
- 1117 **Synthesis and solution complexation behaviour of dimeric zinc-selective bis(benzimidazole) derivatives**

George B. Bates, David Parker and Peter A. Tasker



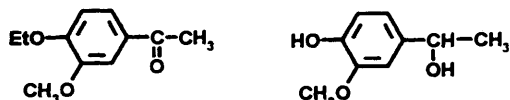
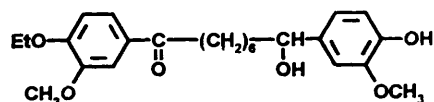
- 1127 **Synthesis, X-ray structure and alkali-metal binding properties of a new hexahomotriazacalix[3]arene**

Philip D. Hampton, Weidong Tong, Si Wu and Eileen N. Duesler



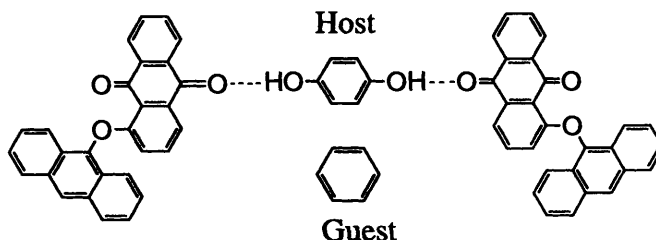
- 1131 **Photophysics and photochemistry of a lignin model molecule containing α -carbonyl guaiacyl and 4-hydroxy-3-methoxybenzyl alcohol moieties**

Alain Castellan, Stéphane Grelier,
Larbi Kessab, Aziz Nourmamode and
Yacine Hannachi



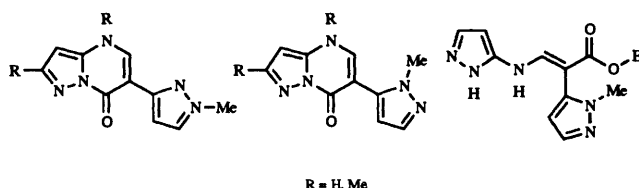
- 1139 **Crystalline inclusion compounds of 1-(9-anthryloxy)anthraquinone as a host compound: X-ray structural characterization and π - π interaction modes in the crystal enclathrating benzene as a guest**

Kazunori Ochiai, Yasuhiro Mazaki, Shin-ichi
Nishikiori, Keiji Kobayashi and Shigenobu
Hayashi



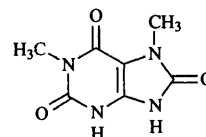
- 1147 **Chemistry of substituted pyrazolo[1,5-*a*]-pyrimidines. Part 5. 7-Oxo-6-[pyrazol-3'(5')-yl]-4,7-dihydropyrazolo[1,5-*a*]pyrimidines from 6-ethoxycarbonyl-7-(2-dimethylaminovinyl)pyrazolo[1,5-*a*]pyrimidines: elucidation of the reaction mechanism through NMR spectroscopy and X-ray diffraction analysis**

Stefano Chimichi, Fabrizio Bruni, Barbara
Cosimelli, Silvia Selleri and Giovanni Valle



- 1153 **Electrochemical and peroxidase catalysed oxidation of 1,7-dimethyluric acid and effect of methyl groups on the oxidation mechanism**

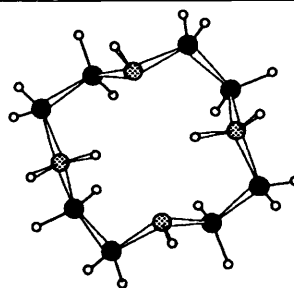
Rajendra N. Goyal, Ajay K. Jain and
Neena Jain



Electrochemical and enzymic oxidations of 1,7-dimethyluric acid proceed by an identical pathway

- 1161 ***Ab initio* SCF MO calculations on triaza and tetraaza cyclic amines**

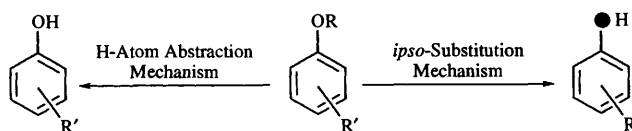
Paulo J. A. Ribeiro-Claro, Ana M. Amado,
M. Paula M. Marques and José J. C.
Teixeira-Dias



Two main factors governing conformational preferences of tri- and tetraaza macrocycles in different protonation states: intramolecular N-H...N bonds, N:...N and NH...HN repulsions

- 1169 **Substrate-dependent changes of the oxidative *O*-dealkylation mechanism of several chemical and biological oxidizing systems**

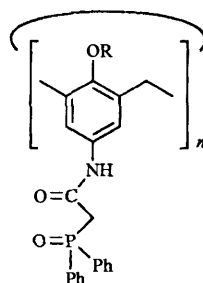
Yasuteru Urano, Tsunehiko Higuchi and
Masaaki Hirobe



In every chemical and biological oxidizing system examined, *e.g.* the cytochrome P450-dependent monooxygenase system, the *O*-dealkylation mechanisms changed dramatically depending on the nature of the substrates (in the reaction scheme, ● indicates the oxygen atom originating from the active oxidizing intermediate)

1175 **Calixarenes with diphenylphosphoryl oxide acetamide functions at the upper rim. A new class of highly efficient extractants for lanthanides and actinides**

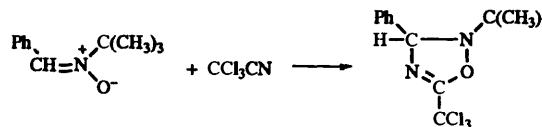
Françoise Arnaud-Neu, Volker Böhmer, Jean-François Dozol, Cordula Grüttner, Ralf A. Jakobi, Dagmar Kraft, Olivier Mauprivez, Hélène Rouquette, Marie-José Schwing-Weill, Nicole Simon and Walter Vogt



Calixarenes bearing CMPO-like functions show drastically increased efficiency in extraction and transport experiments in comparison to (*N,N*-diisobutylcarbamoylmethyl)octylphenylphosphine oxide

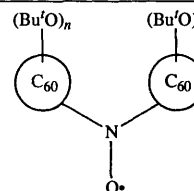
1183 **Spontaneous free radical/spin adduct formation and 1,3-dipolar molecular addition in reactions of cyanohalocarbons and C-phenyl *N*-*tert*-butyl nitrene (PBN)**

Hong Sang, Edward G. Janzen and J. Lee Poyer



1191 **Stabilities and reactivities of buckminsterfullerene radicals, $(Bu'O)_n C_{60}^{\bullet}$, towards dioxygen, nitric oxide and spin trapping agents**

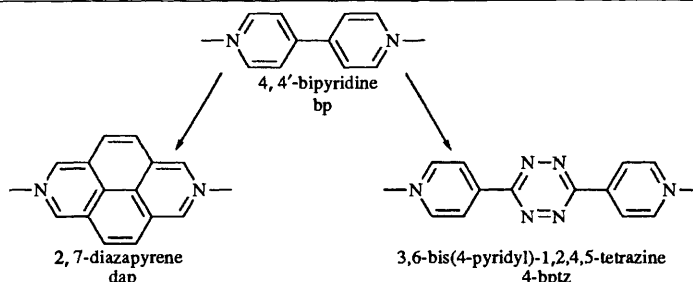
Yong-Kang Zhang, Edward G. Janzen and Yashige Kotake



Reaction of $(Bu'O)_n C_{60}^{\bullet}$ with $^{\bullet}NO$ takes place within several minutes; stable dibuckminsterfullerene aminoxyl radicals have been discovered for the first time

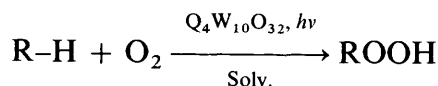
1197 **Coordination-induced switch between the singly occupied and the lowest unoccupied molecular orbitals in two methylviologen-derived chromophores**

Eberhard Waldhör, Mthembeni M. Zulu, Stanislav Zalis and Wolfgang Kaim



1205 **Aerobic photocatalysed oxidation of alkanes in the presence of decatungstates: products and effects of solvent and counter-ion of the catalyst**

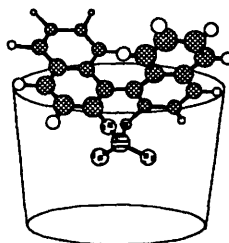
Ludmila P. Ermolenko and Charles Giannotti



$R-H$ = alkane; Q = Na, Me_4N , Pr_4N , Bu_4N ; Solv. = MeCN, EtCN, Pr^iCn

1211 **Mechanism for chiral recognition of binaphthyl derivatives by cyclodextrins**

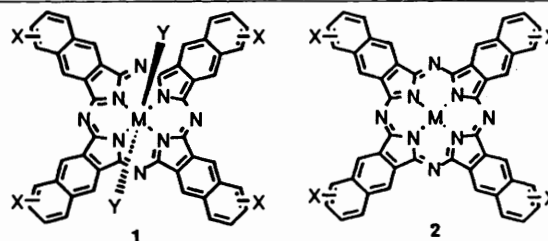
Koji Kano, Yoshihiko Kato and Masahito Kodera



The mechanism for chiral recognition of binaphthyl derivatives by heptakis-(2,3,6-tri-*O*-methyl)- β -cyclodextrin has been studied

1219 **Unique reflection properties of thin films of organic soluble naphthalocyanines**

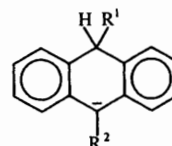
Takeo Tomiyama, Seiji Tai, Mitsuo Katayose, Masanobu Habiro and Nobuyuki Hayashi



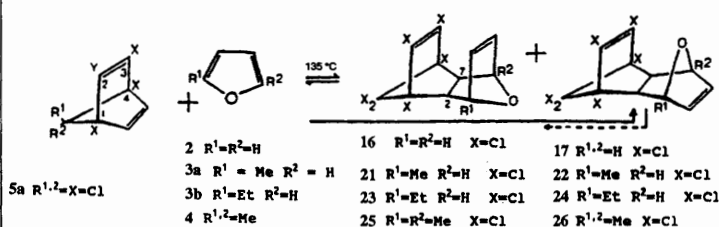
Reflection properties of thin films of organic-soluble naphthalocyanines (1 and 2) were analysed using their complex dielectric constants (relative permittivities)

1225 **Acidity of dibasic carbon acids. Part 3. Ion solvation state of monometallic salts of 9,10-dihydroanthracene and its derivatives in THF**

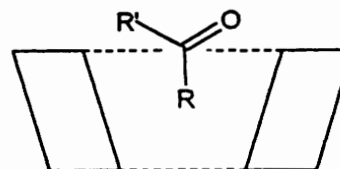
Roy E. Hoffman, Malka Nir, Israel O. Shapiro and Mordecai Rabinovitz

1233 **Kinetic and thermodynamic control in the formation of stereoisomeric 1:1 (4π + 2π) thermal cycloadducts of furans with hexachloronorbordienes**

Kenneth Mackenzie, Edward C. Gravett, Judith A. K. Howard, K. Brian Astin and Andrew M. Tomlins

1243 **Binding of aliphatic ketones to cyclodextrins in aqueous solution**

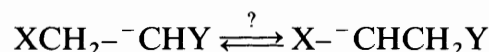
Oswald S. Tee, Alexei A. Fedortchenko, Paul G. Loncke and Timothy A. Gadosy



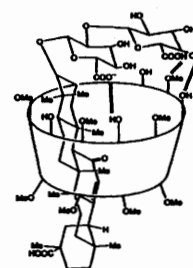
The binding of unsymmetrical ketones RCOR' is mainly, but not solely, determined by the larger group, R

1251 **Do carbanions undergo 1,2 hydrogen transfers in the gas phase?**

Suresh Dua, Gregory W. Adams, John C. Sheldon and John H. Bowie

1257 **Inhibitory effects of cyclodextrins by inclusion on the catalytic activity of glycyrrhizinate for the hydrolysis of a nonionic ester surfactant**

Seizo Tamagaki, Misao Koide, Masahiko Takahashi, Takao Mizushima, Junta Ukawa and Waichiro Tagaki



AUTHOR INDEX

- Adams, Gregory W., 1251
 Alberti, Angelo, 1057
 Amado, Ana M., 1161
 Aravindakumar, C. T., 1077
 Arnaud-Neu, Françoise, 1175
 Astin, K. Brian, 1233
 Barton, Derek H. R., 1031
 Bates, George B., 1109, 1117
 Baynham, Andrew S., 1105
 Benaglia, Massimo, 1057
 Berthelot, Michel, 1047
 Bethell, Donald, 1081
 Böhmer, Volker, 1175
 Bolvig, Simon, 1091
 Bona, Maria Antonietta Della, 1057
 Bowie, John H., 1251
 Bruni, Fabrizio, 1147
 Bushby, Richard J., 1053
 Casnati, Alessandro, 1065
 Castellán, Alain, 1131
 Chardin, Aurélie, 1047
 Chimichi, Stefano, 1147
 Cosimelli, Barbara, 1147
 Dixon, Wendy J., 1105
 Domiano, Laura, 1065
 Dozol, Jean-François, 1175
 Dua, Suresh, 1251
 Duesler, Eileen N., 1127
 Eberlin, Alex R., 1043
 Ermolenko, Ludmila P., 1205
 Fedortchenko, Alexei A., 1243
 Fischer, Thorsten, 1087
 Gadosy, Timothy A., 1243
 Giannotti, Charles, 1205
 Goyal, Rajendra N., 1153
 Gravett, Edward C., 1233
 Grelier, Stéphane, 1131
 Grüttner, Cordula, 1175
 Habiro, Masanobu, 1219
 Hampton, Philip D., 1127
 Hannachi, Yacine, 1131
 Hayashi, Nobuyuki, 1219
 Hayashi, Shigenobu, 1139
 Heuzé, Bénédicte, 1057
 Hibbert, Frank, 1105
 Higuchi, Tsunehiko, 1169
 Hirobe, Masaaki, 1169
 Hoffman, Roy E., 1225
 Howard, Judith A. K., 1233
 Hu, Bin, 1031
 Hudson, Andrew, 1057
 Jain, Ajay K., 1153
 Jain, Neena, 1153
 Jakobi, Ralf A., 1175
 Janzen, Edward G., 1183, 1191
 Kaim, Wolfgang, 1197
 Kajjoka, Takanori, 1091
 Kang, Dong-Hyo, 1081
 Kano, Koji, 1211
 Katayose, Mitsuo, 1219
 Kato, Yoshihiko, 1211
 Kessab, Larbi, 1131
 Kobayashi, Keiji, 1139
 Kodera, Masahito, 1211
 Koide, Misao, 1257
 Kotake, Yashige, 1191
 Kraft, Dagmar, 1175
 Kuroda, Shigeyasu, 1091
 Laali, Kenneth K., 1091
 Laurence, Christian, 1047
 Loncke, Paul G., 1243
 Macciantelli, Dante, 1057
 Mackenzie, Kenneth, 1233
 Marques, M. Paula M., 1161
 Masson, Serge, 1057
 Mauprivez, Olivier, 1175
 Mazaki, Yasuhiro, 1139
 Merga, Getahun, 1097
 Mittal, Jai P., 1077
 Mizushima, Takao, 1257
 Mohan, Hari, 1077
 Morris, David G., 1047
 Mouri, Masaru, 1091
 Muzet, Nicolas, 1065
 Ng, Kai M., 1053
 Nir, Malka, 1225
 Nishikiori, Shin-ichi, 1139
 Nourmamode, Aziz, 1131
 Ochiai, Kazunori, 1139
 Oda, Mitsunori, 1091
 Parker, David, 1109, 1117
 Patel, Jagvi R., 1105
 Poyer, J. Lee, 1183
 Rabinovitz, Mordecai, 1225
 Rao, B. S. Madhava., 1077, 1097
 Rao, Raghavendra R., 1077
 Ribeiro-Claro, Paulo J. A., 1161
 Rouquette, Hélène, 1175
 Ruhmann, Ralf, 1087
 Sang, Hong, 1183
 Schuchmann, H.-P., 1097
 Schwing-Weill, Marie-José, 1175
 Seeboth, Arno, 1087
 Selleri, Silvia, 1147
 Shapiro, Israel O., 1225
 Sheldon, John C., 1251
 Shimao, Ichiro, 1091
 Simon, Nicole, 1175
 Tagaki, Waichiro, 1257
 Tai, Seiji, 1219
 Takahashi, Masahiko, 1257
 Tamagaki, Seizo, 1257
 Tasker, Peter A., 1117
 Taylor, Dennis K., 1031
 Tee, Oswald S., 1243
 Teixeira-Dias, José J. C., 1161
 Tomiyama, Takeo, 1219
 Tomlins, Andrew M., 1233
 Tong, Weidong, 1127
 Ugozzoli, Franco, 1065
 Ukawa, Jinta, 1257
 Ungaro, Rocco, 1065
 Urano, Yasuteru, 1169
 Valle, Giovanni, 1147
 Vogt, Walter, 1175
 von Sonntag, Clemens, 1097
 Wahl, Roy U. Rojas, 1031
 Waldhör, Eberhard, 1197
 Williams, D. Lyn H., 1043
 Wipff, Georges, 1065
 Wu, Si, 1127
 Yasunami, Masfumi, 1091
 Zalis, Stanislav, 1197
 Zerbi, Giuseppe, 1081
 Zhang, Yong-Kang, 1191
 Zulu, Mthembeni M., 1197

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

Journal of Chemical Research

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 5, is reproduced below.

Contents

- 211 1,3- σ -Adducts in the Reactions of 1-Dialkylamino-substituted 2,4,6-Trinitrobenzenes with Amines in Dimethyl Sulfoxide **Yoshinori Hasegawa and Shizen Sekiguchi**
(M 1201)
- 212 X-Ray Structure of 4-[5-Amino-1-(4-tolyl)-1*H*-imidazol-4-yl]-5-imino-2,2-dimethyl-2,5-dihydrooxazole and the Synthesis of a Related *N*³-Acetyl Analogue **M. José Alves, Brian L. Booth, Alice Carvalho, Alice M. Dias, Robin G. Pritchard and M. Fernanda J. R. P. Proença**
(M 1101)
- 214 Rupture and Formation of a C—N Bond in a Stable Tetrahedral Intermediate
Larry Angulo and Oswaldo Núñez
(M 0979)
- 216 Complexation Thermodynamics of Crown Ethers. Part 5. Substitution and Lariat Effects upon Cation Complexation with Azacrown Ethers **Yu Liu, Yumei Li, Lijuan Zhang, Yunti Chen, Mikio Ouchi and Yoshihisa Inoue**
(M 1147)
- 218 The Probable Absence of Intramolecular General Base Catalysis in the Hydrolysis of Ethyl 6-Ethyl-4-hydroxycinnoline-3-carboxylate **Richard G. Button and Peter J. Taylor**
(M 1162)
- 220 Stereochemistry of Biscycloadducts of Benzonitrile Oxide with 1,2- and 1,3-Diazines **Giovanni Grassi, Francesco Risitano, Giuseppe Bruno and Francesco Nicolò**
(M 1173)
- 222 Crystal Structure and Absolute Configuration of (1*R*,2*S*,5*R*)-Menthyl (2*S*)-2-(Diphenylphosphinoyl)propanoate: Attempted Resolution and Chiral Synthesis of 2-(Diphenylphosphinoyl)propanoic Acid **Ronald J. Cross, Louis J. Farrugia, Paul D. Newman, Robert D. Peacock and Diane Stirling**
(M 1227)
- 224 Asymmetric Synthesis. Part 1. Enantioselective Conjugate Additions of Grignard Reagents to Cinnamamides derived from *N*-Methyl, *N*-Butyl and *N*-Benzyl Derivatives of (*R*)-(-)-2-Aminobutan-1-ol **Joël Touet, Sylvie Baudouin and Eric Brown**
(M 1251)
- 226 Competitive 5-*Exo* vs. 6-*Exo* Ring Closure in Intramolecular Electrophile-induced Etherification Reactions **C. V. Ramana, R. Murali, K. Ravikumar and M. Nagarajan**
(M 1267)
- 228 Kinetics and Mechanism of the Oxidation of Formic and Oxalic Acids by Pyridinium Hydrobromide Perbromide **Deepa Suri, Seema Kothari and Kalyan K. Banerji**
(M 1301)
- 230 Kinetics and Mechanism of the Oxidation of Primary Aliphatic Alcohols by Benzyltrimethylammonium Tribromide **Shruti Goel, Seema Kothari and Kalyan K. Banerji**
(M 1318)
- 232 A Facile Synthetic Approach to Symmetrical 3,3'-Difunctionalised-2,2'-bithiophenes from 3,3'-Dibromo-2,2'-bithiophene **Siu-Choon Ng, Hardy Sze-On Chan, Hsing-Hua Huang and Richard Swee-How Seow**
(M 1285)
- 234 Synthesis and Characterization of Some 1-Aryl-3-hydroxypyridin-4(1*H*)-ones. Solubilities and their Solvation in Methanol–Water Mixtures **John Burgess, Baltazar de Castro, Celeste Oliveira and Maria Rangel**
(M 1338)
- 236 Sulfuration Reactions of Pyrrolidine Polycarbonyl Derivatives with Lawesson's Reagent **K. Ostrowska, W. Żankowska-Jasińska, M. Ciechanowicz-Rutkowska and T. Pilati**
(M 1352)
- 238 Molybdovanadophosphate Heteropolyanion Catalysed Oxidation of 2,3,6-Trimethylphenol by Dioxygen in a Two-phase System **Ivan V. Kozhevnikov, Anton Sinnema and Herman van Bekkum**
(—)
- 240 Friedel–Crafts Arylmethylation of Aromatics with Bis(chloromethyl)benzenes Catalysed by Zinc Chloride Supported on Silica Gel **Mitsuo Kodomari and Shinkichi Taguchi**
(—)
- 242 A Clean One-step Synthesis of 2-Hydroxythiophene [Thiophen-2(5*H*)-one] by a Fenton-like [Copper(II)–Hydrogen Peroxide] Oxidation of Thiophene under Aqueous Conditions **David W. Allen, Malcolm R. Clench, Alan T. Hewson and Munevver Sokmen**
(—)
- 244 Ozone-mediated Nitration of Pyrazole, Imidazole and Uracil with Nitrogen Dioxide
(—) **Hitomi Suzuki and Nobuaki Nonoyama**
- 246 Synthesis and Characterisation of Palladium(II) and Platinum(II) Complexes Containing Substituted Hydrazines **Anshu Singhal and Vimal K. Jain**
(—)
- 248 A Route to 4-Hydroxy-2-quinolone involving an α,α' -Dioxoketene. A Structural Proof **Halina Borowiec, Jacek Grochowski and Pawel Serda**
(—)
- 250 Structural Elucidation of 6,7,8,9-Tetrasubstituted Cyclooctapyrimidines by Nuclear Magnetic Resonance Spectroscopy **Augusto C. Tomé, Artur M. S. Silva, José A. S. Cavaleiro and Richard C. Storr**
(—)
- 252 Intramolecular Photocyclization of Naphthalene Derivatives with an Anilino Group linked by a —[CH₂]₆— or —[CH₂]₂—O—[CH₂]₃— Chain **Akira Sugimoto, Noriyuki Fukada, Tomohiro Adachi and Hiroo Inoue**
(—)
- 254 Microwave-induced Syntheses of 6-(Substituted aryl)-3-[(5-methyl-1,3,4-thiadiazol-2-ylsulfanyl)methyl]-1,2,4-triazolo[3,4-*b*][1,3,4]thiadiazoles **Mozaahir Kidwai and Parven Kumar**
(—)
- 256 Synthesis of 2-Phenyl-4,5,6,7-tetrahydroindol-5-one, -tetrahydrobenzo[*b*]thiophen-5-one and -tetrahydrobenzo[*b*]furan-5-one **Paul W. Groundwater and Munawar Ali Munawar**
(—)
- 258 Reaction of (*Z,Z*)-Cycloocta-1,5-diene under Modified Woodward–Prevost Conditions: A Simple Synthesis of Functionalised *cis*-Bicyclo[3.3.0]octanes **Pradeep T. Deota and Vishwakarma Singh**
(M 1220)

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*

Antitumour benzothiazoles. Part 4. An NMR study of the sites of protonation of 2-(4-aminophenyl)benzothiazoles
R.T. Wheelhouse, D-F. Shi, D.E.V. Wilman and M.F.G. Stevens

Enhancement of luminescence of europium(III) ions in water by use of synergistic chelation. Part 1. 1:1 and 2:1 complexes
J. Coates, P.G. Sammes and R.M. West

Enhancement of luminescence of europium(III) ions in water by use of synergistic chelation. Part 2. 1:1:1 complexes
J. Coates, P.G. Sammes and R.M. West

EPR spectra and redox properties of radical cations of dibenzofuran, methylated dibenzofurans and bidibenzofurans; relation to the chemistry of the dibenzofuran radical cation **L. Ebersson, M.P. Hartshorn, O. Persson, F. Radner and C.J. Rhodes**

New insights on *N-tert*-butyl- α -phenylnitron (PBN) as a spin trap. Part 1. Reaction between PBN and *N*-chlorobenzotriazole
P. Carloni, L. Ebersson, L. Greci, P. Sgarabotto and P. Stipa

Ground state charge transfer complex of [84]fullerene and *N,N*-diethylaniline
C.E. Bunker, H.W. Rollins and Y-P. Sun

Nitration of styrenes by dinitrogen pentoxide in dichloromethane **R.J. Lewis and R.B. Moodie**

Thermal decomposition of arylnitramines **D.L. Naud**

Solution and solid state proton transfer from phenols to triphenylphosphine oxide studied by ^1H , ^{13}C and ^{31}P NMR spectroscopy
C.M. Lagier, U. Scheler, G. McGeorge, M.G. Sierra, A.C. Olivieri and R.K. Harris

Structure determination of reaction products of PQQ with L-tryptophan *in vitro* and their effects for microbacterial growth
E. Kawamoto, T. Amano, J. Kanayama, Y. In, M. Doi, T. Ishida, T. Iwashita and K. Nomoto

Conformational analysis by NMR spectroscopy and molecular simulation in water of methylated glutamic acids, agonists at glutamate receptors **N. Todeschi, J. Gharbi-Benarours, F. Acher, V. Larue, R. Azerad and J-P. Girault**

Kinetics and mechanism of aminolysis of phenyl acetates and phenyl trimethylacetates in dimethyl sulfoxide
H.J. Koh, S.I. Kim, B.C. Lee and I. Lee

Rearrangement of *N*-acyl-3,4-dihydro-2,1-benzoxazines to 2-substituted-4*H*-3,1-benzoxazines through a retro-Diels–Alder extrusion of formaldehyde **S.A. Glover, K.M. Jones I.R. McNee and C.A. Rowbottom**

Chalcogenes as electron donors for selected NLO phores
M. Blenkle, P. Boldt, C. Bräuchle, W. Grahn, I. Ledoux, H. Nerenz, S. Stadler, J. Wichern and J. Zyss

Formation of bicyclo[3.2.1]oct-2-en-8-ones and 1-hydroxy dihydrosemibullvalenes from the *meta* photocycloaddition of cyclopentene to phenols **A. Gilbert and D.T. Jones**

How does the alkoxy group at the benzylic carbon affect the transition state of the hydrogen-atom abstraction reaction? Dual-parameter correlation analysis of relative rates measured by a rigorous methodology for 14 *p*-Y-substituted α,α -ethylenedioxytoluenes
X-K. Jiang, Y-H. Zhang and W.F-X. Ding

Structure of Velutinol A is (15*R*,16*R*,20*S*)-14,16:15,20:16,21-triepoxy-15,16-seco-14 β ,17 α -pregn-5-ene-3 β ,15-diol. A combined quantitative Overhauser effect and molecular modelling study
E.S. Bento, J.B. Calixto, G.E. Hawkes, A.E.G. Sant'Ana and R.A. Yunes

Study of electron densities of methyl acetate, *N*-methylacetamide and *N,N'*-dimethylurea by quantum mechanical investigations. Part 1. Gas phase **B. Kallies and R. Mitzner**

Study of electron densities of methyl acetate, *N*-methylacetamide and *N,N'*-dimethylurea by quantum mechanical investigations. Part 2. Solvent models **B. Kallies and R. Mitzner**

Oxidation of phosphines containing two or three TTF or *o*-dimethyl-TTF moieties. Evidence for formation of radical polycations
F. Gerson, A. Lamprecht and M. Fourmigué

Hydrogenation of [76]-, [78]- and [84]-fullerenes: cage degradation **R. Taylor, A.D. Darwish, H.W. Kroto and D.R.M. Walton**

Characterization of lactate–guanidinium and lactate–lactate interactions in aqueous solution by spectropolarimetry
P. Horváth, A. Gergely and B. Noszál

Allene and fluoroallens as dienophiles in Diels–Alder reactions: an AM1 and PM3 study
M. Manoharan and P. Venuvanalingam

Synthesis and high field NMR study of a new cyclodipeptide- β -cyclodextrin derivative
G. Impellizzeri, G. Pappalardo, E. Rizzarelli and C. Tringali

Synthesis and spectroscopic studies of novel photochromic benzodithiacrown ethers and their complexes
M.V. Alfimov, Y.V. Fedorov, O.A. Fedorova, S.S. Gromov, R.E. Hester, I.K. Lednev, J.N. Moore, V.P. Oleshko and A.I. Vedernikov

X-Ray crystal structure analysis and ^{13}C NMR investigation of estriol 16- and 17-monoglucuronide derivatives
W. Yinju, J.M. Waters and L.F. Blackwell

Reaction of phosphorus-stabilized carbanions with cyclic enones. Aromatization of the substitution and addition products
M.J. Mphahlele, A. Pienaar and T.A. Modro

EPR spectroscopy study of the radical oxidation of hydroxypurines in aqueous solution. Acid–base properties of the derived radicals
S.R. Langman, M.C.B.L. Shohoji, J.P. Telo, A.J.S.C. Vieira and H.M. Novais

Picosecond radical kinetics. Rate constants for ring openings of (2-alkoxy-3-phenylcyclopropyl)methyl radicals
M-H. Le Tadic-Biadatti and M. Newcomb

Studies in crystal engineering: effect of fluorine substitution in crystal packing and topological photodimerization of styryl coumarins in the solid state
K. Vishnumurthy, T.N. Guru Row and K. Venkatesan

Nitrogen inversion and N–O bond rotation processes in di- and tri-substituted hydroxylamines. A dynamic NMR study
Sk.A. Ali, A. Hassan and M.I.M. Wazeen

Intermolecular hydrogen bonds in monosaccharides in dimethyl sulfoxide solution
S.J. Angyal and J.C. Christofides

Chromatographic enantiomer separation and circular dichroism spectra of chiral rhodanines
K. Rang, R. Isaksson and J. Sandström

Solute–solvent and solvent–solvent interactions in binary solvent mixtures. Part 3. The $E_T(30)$ polarity of binary mixtures of hydroxylic solvents
J. Ortega, C. Ràfols, E. Bosch and M. Rosés

Cyclisation and decarboxylation in Zwitterionic micelles. Effects of head group structure
P.D. Profio, R. Germani, G. Savelli, G. Cerichelli, N. Spreti and C.A. Bunton

Racemic compound formation–conglomerate formation. Part 3. Investigation of the acidic salts of α -phenylethylamine by achiral dicarboxylic acids. Optical resolution by preferential crystallization and a structural study of (*R*)- α -phenylethylammonium hydrogen itaconate
D. Kozma, Z. Böcskei, C. Kassai, K. Simon and E. Fogassy

Proton and charge transfer in the intercalating antitumor drug pazelliptine
M.P. Fontaine-Aupart, H. Laguitton-Pasquier, R. Pansu, L. Brian, E. Renault, M.C. Marden, C. Rivalle and E. Bisagni

Comparative conformational and dynamical study of some *N*-quaternarized UV-filters: structure–activity relationships
C. Anselmi, M. Centini, M. Francioli and A. Sega

Flash photolysis study of a Friedel–Crafts alkylation. Reaction of the photogenerated 9-fluorenyl cation with aromatic compounds
R.A. McClelland, F.L. Cozens, J. Li and S. Steenken

Halide anion recognition by new acyclic quaternary polybipyridinium and polypyridinium receptors
P.D. Beer, N.C. Fletcher, A. Grieve, J.W. Wheeler, C.P. Moore and T. Wear

Polypeptides with supersecondary structures as templates in rational catalyst design. Catalysis of self-functionalization by designed helix–loop–helix motifs
L. Baltzer, A-C. Lundh, K. Broo, S. Olofsson and P. Ahlberg

Conformational analysis for a series of polymorphs of a disperse azobenzene dyestuff
G. McGeorge, R.K. Harris, A.M. Chippendale and J.F. Bullock

Halide anion recognition by new acyclic quaternary polybipyridinium and polypyridinium receptors
P.D. Beer, N.C. Fletcher, A. Grieve, J.W. Wheeler, C.P. Moore and T. Wear

Photoinduced electron transfer from enol silyl ethers to quinone. I. Pronounced effects of solvent polarity and added salt on the formation of enone
T.M. Bockman, D. Shukla and J.K. Kochi

Photoinduced electron transfer from enol silyl ethers to quinone. II. Direct observation of ion-pair dynamics by time-resolved spectroscopy
T.M. Bockmann and J.K. Kochi