

JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions 2

Physical Organic Chemistry

CONTENTS

Perkin Communications

- 1717 **Accurate prediction of the solvation of nucleotide base pairs using an *ab initio* continuum model**

Phillip E. Young, Ian H. Hillier and Ian R. Gould

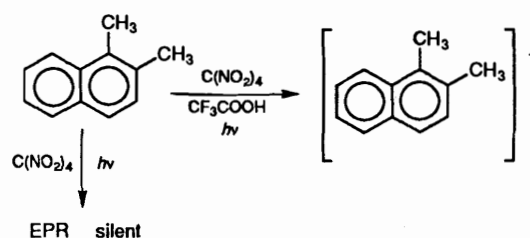
An *ab initio* continuum model successfully predicts the contribution of solvation to the enthalpy of formation of A-T and C-G base pairs in chloroform

Articles

Keynote Article

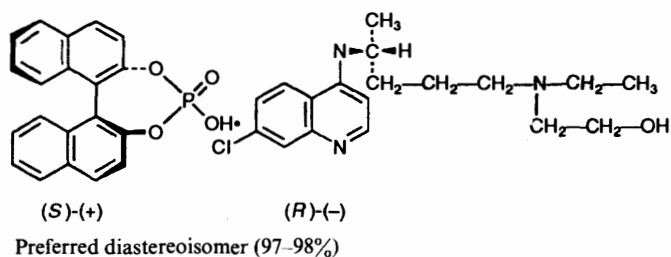
- 1719 **Photochemical nitration by tetranitromethane. Part XIX. The competitive reactions of trinitromethanide and nitrogen dioxide with radical cations and their use for selective nitrations**

Lennart Ebersson, Michael P. Hartshorn, Finn Radner and Jan O. Svensson



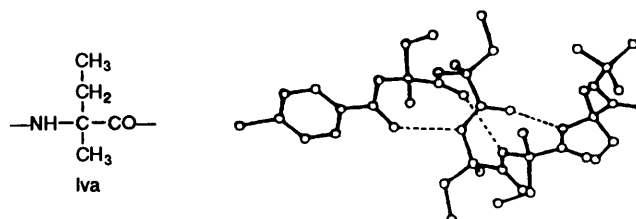
- 1731 **Kinetic resolution of 7-chloro-4-(4-[ethyl-(2-hydroxyethyl)amino]-1-methylbutyl-amino)quinoline (hydroxychloroquine) by an atropisomeric resolving agent**

Aslam M. Ansari and J. Cymerman Craig



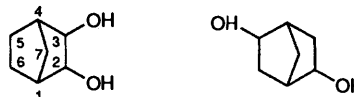
1735 **Linear oligopeptides. Part 316. Conformational characterization of syndiotactic homo-peptides from C $^{\alpha,\alpha}$ -disubstituted glycines**

Marco Crisma, Fernando Formaggio, Monica Pantano, Giovanni Valle, Gian Maria Bonora, Claudio Toniolo, Hans E. Schoemaker and Johan Kamphuis



1743 **Stereochemical differentiation of isomeric trinorbornane-2,3- and trinorbornane-2,5-diols by chemical ionization mass spectrometry**

Tuula Partanen, Mika Pykäläinen, Hannele Hulkkonen, Olli Savolainen and Pirjo Vainiotalo



Di-*exo*, di-*endo* and *trans* (*exo-endo*) isomers were studied using ammonia, isobutane, methane, acetone and trimethyl borate as reagent gas

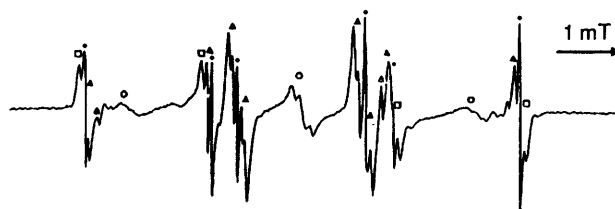
1751 **The use of chemical probes for the characterization of solvent mixtures. Part 2. Aqueous mixtures**

Yizhak Marcus

water water
water water cosolvent
water **probe** water
cosolvent water water
water water water
cosolvent **any** cosolvent
cosolvent **solute** water
water water cosolvent

1759 **Kinetic and structural EPR studies of radical polymerization. Monomer, dimer, trimer and mid-chain radicals formed *via* the initiation of polymerization of acrylic acid and related compounds with electrophilic radicals ($\cdot\text{OH}$, $\text{SO}_4^{\cdot-}$ and $\text{Cl}_2^{\cdot-}$)**

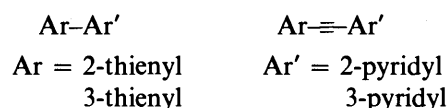
Bruce C. Gilbert, John R. Lindsay Smith, Elizabeth C. Milne, Adrian C. Whitwood and Philip Taylor



EPR spectrum of monomer, dimer, trimer and mid-chain radicals in acrylate-anion polymerisation

1771 **New organic polymer precursors: synthesis and electronic structure of thienylpyridines and thienylethynylpyridines**

Igor Novak, Siu-Choon Ng, Chup-Yew Mok, Hsing-Hua Huang, Jiye Fang and Kevin Kek-Tsong Wang



Isomeric thienylpyridines/thienylethynylpyridines have been synthesized and their electronic structures analysed on the basis of their He I/He II UV photoelectron spectra (UPS)

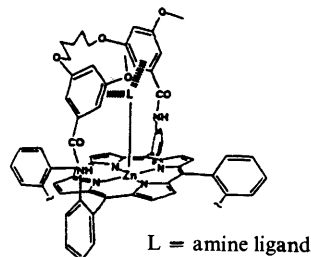
1777 **Hydrogen bonding. Part 34. The factors that influence the solubility of gases and vapours in water at 298 K, and a new method for its determination**

Michael H. Abraham, Jenik Andonian-Haftvan, Gary S. Whiting, Albert Leo and Robert W. Taft

An equation for the solubility of 408 gaseous solutes in water shows that increases in solute dipolarity/polarizability, hydrogen-bond acidity, and hydrogen-bond basicity all lead to an increase in solubility, but that an increase in solute volume leads to a small decrease

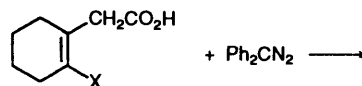
1793 Effects of organization of zinc porphyrin hosts on binding enhancements and recognition of axial ligands

Hiroyasu Imai and Yoshio Uemori



1799 Reactivity of 2-substituted cyclohex-1-enylacetic acids with diazodiphenylmethane in various alcohols

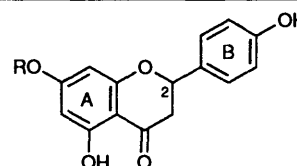
Gordana S. Ušćumlić and Milan D. Muškatirović



The reactivities of 2-substituted cyclohex-1-enylacetic acids with diazodiphenylmethane in 11 alcohols is investigated; the log *k* values for the various acids are correlated by using the appropriate form of the extended Hammett equation

1803 Chiral recognition by cyclodextrins: the interaction of naringin with β-cyclodextrin

Ian J. Colquhoun and Brian J. Goodfellow

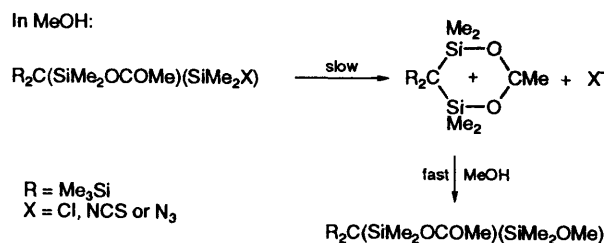


R = α-L-Rha-(1→2)-β-D-Glc

¹H NMR shows differential binding of (2*R*) and (2*S*) isomers to β-cyclodextrin

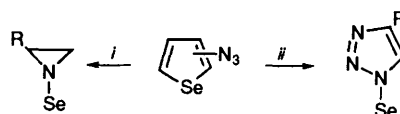
1809 Anchimeric assistance by the acetoxy group in the solvolysis of (Me₃Si)₂C(SiMe₂OCOMe)-(SiMe₂X), X = Cl, NCS or N₃

Colin Eaborn, Paul D. Lickiss and Alan D. Taylor



1815 Preparation, reactivity, NMR properties and semiempirical MNDO/PM3 structural calculations of 2-azido- and 3-azido-selenophene

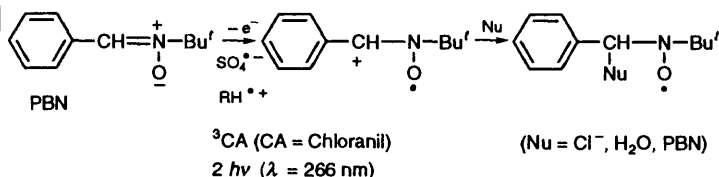
Salo Gronowitz and Paolo Zanirato



i, Trimethyl(vinyl)silane; R = SiMe₃
ii, (Trimethylsilyl)acetylene; Se = selenophen-2- or -3-yl

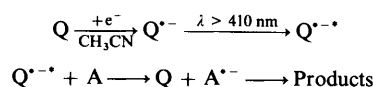
1821 Direct detection of the cation radical of the spin trap α-phenyl-*N*-*tert*-butylnitron

Valentin E. Zubarev and Ortwin Brede



1829 Photoelectrochemistry with quinone radical anions—photoassisted reduction of halobenzenes and carbonyl compounds

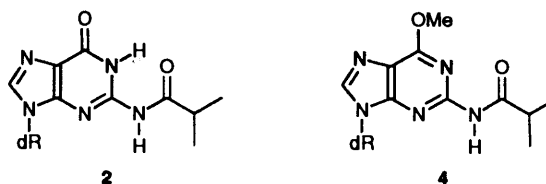
Peter K. J. Robertson and Brian R. Eggins



Q = quinones
A = RX or R¹R²CO

1833 Deacylation of 2-*N*-isobutyryl- and 2-*N*-isobutyryl-6-*O*-methyl-2'-deoxyguanosine in the condensed and gas phase. A kinetic investigation

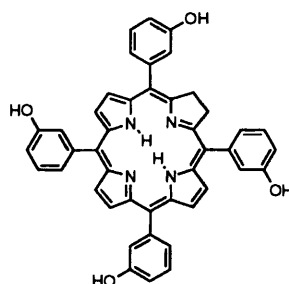
Angelo Liguori, Anna Napoli, Carlo Siciliano and Giovanni Sindona



The ring lactam function affects the deacylation kinetics of **2** and **4** in solution and in the gas phase

1839 Fine structure of 5,10,15,20-tetrakis(*m*-hydroxyphenyl)chlorin (*m*-THPC): a ¹H, ¹³C and ¹⁵N NMR study

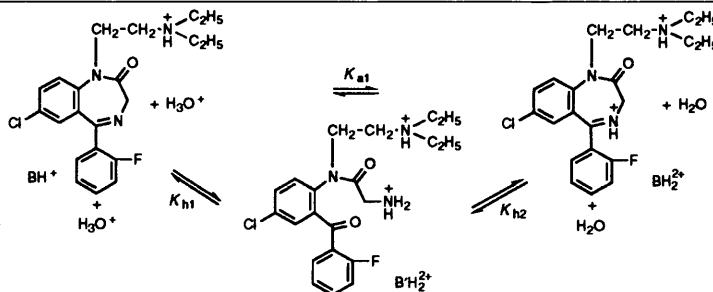
Raymond Bonnett, Birgul D. Djelal, Geoffrey E. Hawkes, Peter Haycock and Francesc Pont



¹H, ¹³C and natural abundance ¹⁵N NMR spectra demonstrate the predominant tautomer shown

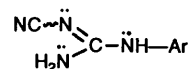
1845 A spectrophotometric method for the determination of equilibrium constants of the reversible 1,4-benzodiazepine ring-opening reaction

Lidija B. Pfendt and Gordana V. Popović



1849 ¹H and ¹⁵N NMR studies of *N*-substituted-*N'*-cyanoguanidines

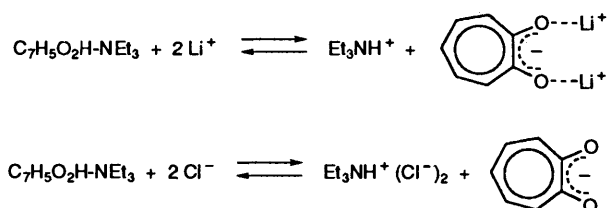
Ian D. Cunningham, Nan Chi Wan and Brian G. Cox



N-Aryl-*N'*-cyanoguanidines in Me₂SO have the C=N conjugated with the cyano group, are monomeric, and show no prototropic tautomerisation on the NMR timescale

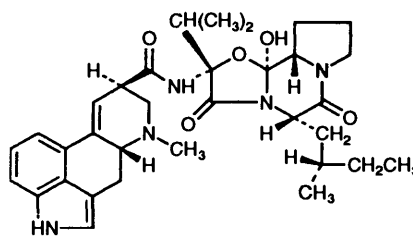
1855 Role of triple ion formation in the acid-base reaction between tropolone and triethylamine in acetonitrile

Masashi Hojo, Hiroshi Hasegawa and Hitoshi Yoneda



1861 **Ergogaline, a new ergot alkaloid, produced by *Claviceps purpurea*: isolation, identification, crystal structure and molecular conformation**

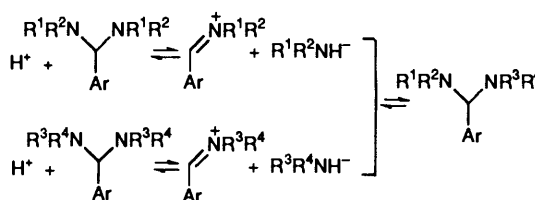
Ladislav Cvak, Alexandr Jegorov, Petr Sedmera, Vladimír Havlíček, Jan Ondráček, Michal Hušák, Svetlana Pakhomova, Bohumil Kratochvíl and Joachim Granzin



Ergogaline

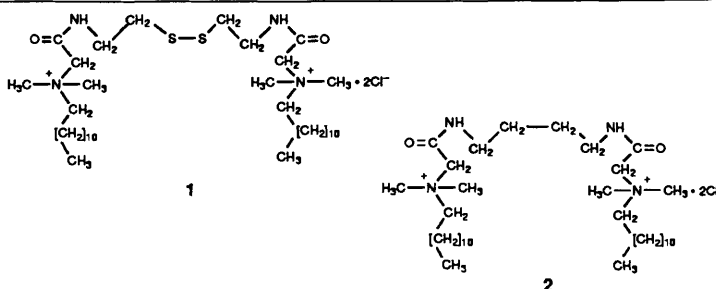
1867 **Aminal exchange**

Alan R. Katritzky, Konstantina Yannakopoulou and Hengyuan Lang



1871 **Synthesis, surface active properties and antimicrobial activity of new bis quaternary ammonium compounds**

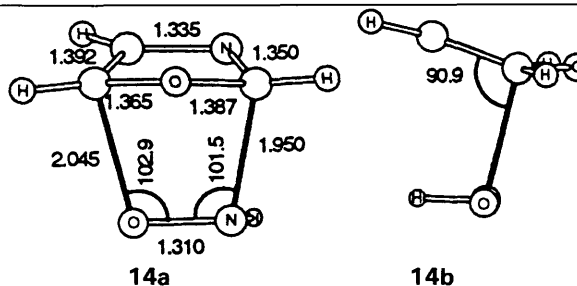
M. Diz, A. Manresa, A. Pinazo, P. Erra and M^aR. Infante



New dimeric cationic surfactants **1** and **2** were prepared from a betaine type amphoteric surfactant and their surface activity and antimicrobial properties are evaluated

1877 ***Ab Initio* Study of heterodienophile addition to oxazole**

Branko S. Jursic and Zoran Zdravkovski



Nitrosyl hydride is the most reactive dienophile of a series studied in the cycloaddition to oxazole

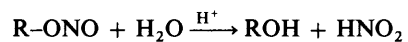
1883 **Racemic compound formation—conglomerate formation. Part 1. Structural and thermoanalytical study of hydrogen malonate, hydrogen phthalate and hydrogen succinate of α -phenylethylamine**

Dávid Kozma, Zsolt Böcskei, Kálmán Simon and Elemér Fogassy

The crystal structures of (*R,S*)- α -phenylethylammonium hydrogen phthalate and (*R,S*)- α -phenylethylammonium hydrogen malonate have been determined and compared with each other and with the known crystal structure of the (*R*)- α -phenylethylammonium hydrogen succinate

1887 **Physicochemical properties of mixed anionic–non-ionic micelles: effects on chemical reactivity**

Luis Freire, Emilia Iglesias, Carlos Bravo,
J. Ramón Leis and M. Elena Peña



Results of the kinetic study of the above reaction in aqueous solution of (i) $\text{C}_{16}\text{E}_{20}$ micelles and (ii) $\text{C}_{16}\text{E}_{20}$ + SDS mixed micelles

Corrigenda

1895 **Allylic mono- and di-hydroxylation of isolated double bonds with selenium dioxide–*tert*-butyl hydroperoxide. NMR characterization of long-chain enols, allylic and saturated 1,4-diols, and enones** Gerhard Knothe, Marvin O. Bagby, David Weisleder and Robert E. Peterson

1895 **Homolytic reactions of ligated boranes. Part 19. Relationships between structure, reactivity and enantioselectivity for hydrogen-atom abstraction by chiral amine–boryl radicals** Hai-Shan Dang, Valérie Diart, Brian P. Roberts and Derek A. Tocher

ix Conference Diary

AUTHOR INDEX

- Abraham, Michael H., 1777
Andonian-Haftvan, Jenik, 1777
Ansari, Aslam M., 1731
Bagby, Marvin O., 1895
Böcskei, Zsolt, 1883
Bonnett, Raymond, 1839
Bonora, Gian Maria, 1735
Bravo, Carlos, 1887
Brede, Ortwin, 1821
Colquhoun, Ian J., 1803
Cox, Brian G., 1849
Craig, J. Cymerman, 1731
Crisma, Marco, 1735
Cunningham, Ian D., 1849
Cvak, Ladislav, 1861
Dang, Hai-Shan, 1895
Dart, Valérie, 1895
Diz, M., 1871
Djelal, Birgul D., 1839
Eaborn, Colin, 1809
Eberson, Lennart, 1719
Eggins, Brian R., 1829
Erra, P., 1871
Fang, Jiye, 1771
Fogassy, Elemér, 1883
Formaggio, Fernando, 1735
Freire, Luis, 1887
Gilbert, Bruce C., 1759
Goodfellow, Brian J., 1803
Gould, Ian R., 1717
Granzin, Joachim, 1861
Gronowitz, Salo, 1815
Hartshorn, Michael P., 1719
Hasegawa, Hiroshi, 1855
Havlíček, Vladimír, 1861
Hawkes, Geoffrey E., 1839
Hawcock, Peter, 1839
Hillier, Ian H., 1717
Hojo, Masashi, 1855
Huang, Hsing-Hua, 1771
Hulkkonen, Hannele, 1743
Hušák, Michal, 1861
Iglesias, Emilia, 1887
Imai, Hiroyasu, 1793
Infante, M^aR., 1871
Jegorov, Alexandr, 1861
Jursic, Branko S., 1877
Kamphuis, Johan, 1735
Katritzky, Alan R., 1867
Knothe, Gerhard, 1895
Kozma, Dávid, 1883
Kratochvíl, Bohumil, 1861
Lang, Hengyuan, 1867
Lindsay Smith, John R., 1759
Leis, J. Ramón, 1887
Leo, Albert, 1777
Lickiss, Paul D., 1809
Liguori, Angelo, 1833
Manresa, A., 1871
Marcus, Yizhak, 1751
Milne, Elizabeth C., 1759
Mok, Chup-Yew, 1771
Muškatirović, Milan D., 1799
Napoli, Anna, 1833
Ng, Siu-Choon, 1771
Novak, Igor, 1771
Ondráček, Jan, 1861
Pakhomova, Svetlana, 1861
Pantano, Monica, 1735
Partanen, Tuula, 1743
Peña, M. Elena, 1887
Peterson, Robert E., 1895
Pfundt, Lidija B., 1845
Pinazo, A., 1871
Pont, Francesc, 1839
Popović, Gordana V., 1845
Pykäläinen, Mika, 1743
Radner, Finn, 1719
Roberts, Brian P., 1895
Robertson, Peter K. J., 1829
Savolainen, Olli, 1743
Schoemaker, Hans E., 1735
Sedmera, Petr, 1861
Siciliano, Carlo, 1833
Simon, Kálmán, 1883
Sindona, Giovanni, 1833
Svensson, Jan O., 1719
Taft, Robert W., 1777
Taylor, Alan D., 1809
Taylor, Philip, 1759
Tocher, Derek A., 1895
Tonio, Claudio, 1735
Uemori, Yoshio, 1793
Ušćumlić, Gordana S., 1799
Vainiotalo, Pirjo, 1743
Valle, Giovanni, 1735
Wan, Nan Chi, 1849
Wang, Kevin Kek-Tsong, 1771
Weisleder, David, 1895
Whiting, Gary S., 1777
Whitwood, Adrian C., 1759
Yannakopoulou, Konstantina, 1867
Yoneda, Hitoshi, 1855
Young, Phillip E., 1717
Zanirato, Paolo, 1815
Zdravkovski, Zoran, 1877
Zubarev, Valentin E., 1821

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

Forthcoming Articles in *Perkin Transactions 2*

The reaction of the OH radical with tetrachloroethene and trichloroacetaldehyde (hydrate) in oxygen-free aqueous solution
R. Mertens and C. von Sonntag

Photoinduced electron transfer reactions of chloranil with benzodioxoles
B.-Z. Yan, Z.-G. Zhang, H.-C. Yuan, L.-C. Wang and J.-H. Xu

Photoinduced reversible *trans*–*cis* isomerisation of azobenzene amphiphile bearing dialkyl side chains in Langmuir–Blodgett membranes
J.-I. Anzai, N. Sugaya and T. Osa

The photolysis of 2,4-dihydroxy-2,4-dimethylpentan-3-one studied by quantitative time-resolved CIDNP and optical spectroscopy
M. Salzmann, Y. P. Tsentalovich and H. Fischer

Predictions of spectral signatures of fullerenes. Second-order Jahn–Teller effects on the structures of C₄₄, C₅₆, C₆₈ and C₉₂
P. W. Fowler and J.P.B. Sandall

1,2-Carbon to nitrogen migrations. Part 2. *Ab Initio* study on the rearrangement of (α -methylazo)alkylisocyanates
R.T. Kroemer, H. Gstach, K.R. Liedl and B.M. Rode

Diquaternized heterocycles with strong electronic coupling between a metal-chelating site and a methylviologen-type redox function: EPR/ENDOR detected coordination of metal ions and complexes by radical cation intermediates
W. Matheis, J. Poppe, W. Kaim and S. Zálaiš

Characterization of the β -cyclodextrin inclusion complexes with bichromophoric 1-benzyloxy-2-pyridone and related compounds
T. Sakurai, E. Saitou, N. Hayashi, Y. Hirasawa and H. Inoue

Acidity of carboxylic acids: resonance delocalization or induction? **T. D. Thomas**

Aromatic nucleophilic substitution reactions of some 2-L-3-nitro-5-X-thiophenes with piperidine and aniline in methanol. Substitution constants for the thiophene system **G. Consiglio, V. Frenna, C. Arnone, E. Mezzina and D. Spinelli**

Synthesis of 9-aryl-6-carbamoyl-1,2-dihydropurines and a study of their tautomerism
M.J. Alves, B.L. Booth, A. Carvalho, P.R. Eastwood, L. Nezhat, R.G. Pritchard and M.F.J.R.P. Proenca

From solvolysis to electron transfer: direct observation of ion-pair dynamics by time-resolved spectroscopy
T.M. Bockman and J.K. Kochi

NMR, crystal structure and FAB mass spectral studies of morpholine *N*-methylenephosphonic acid
M.P. Lowe, J.C. Lockhart, C.J. Matthews, W. Clegg, M.R.J. Elsegood and L. Horsburgh

Eclipsed ground-state conformations from ethoxycyclohexanes with adjacent methyl-group substitution. An NMR criterion and molecular mechanics calculations **J.E. Anderson and A.I. Ijeh**

Structural studies of *N*-chloroaziridine carboxylates by multinuclear NMR spectroscopy
A. Forni, I. Moretti, A. Pironi, F. Prati and L. Schenetti

Gas phase basicities of 1,3-benzazoles: benzimidazole, benzoxazole, benzothiazole, benzoselenazole and benzotellurazole
R. Notario, M. Herreros, E. Ballesteros, M. Essefar, J.-L.M. Abboud, I.D. Sadekov, V.I. Minkin and J. Elguero

The radicals and ions of formic and acetic acids: an *ab initio* study of the structures and gas and solution phase thermochemistry
D. Yu, A. Rauk and D.A. Armstrong

Thermal decomposition of lithium amides: a matrix isolation investigation **R. Withnall, I.R. Dunkin and R. Snaith**

Photochemistry of 1-aryl-4-(pentamethyldisilanyl)buta-1,3-diyne: photoreaction with acetone and dimethyl fumarate
S.C. Shim and S.T. Lee

Effect of hydrogen bonding on the methyl conformation of thioacetamide: an *ab initio* study **F. Ramondo and L. Bencivenni**

Kinetic Analysis of Oxazolopyrroloquinoline formation in the reaction of coenzyme PQQ with amino acids by capillary zone electrophoresis **Y. Esaka, Y. Yamaguchi, M. Goto and K. Kano**

1,10-Dimethyl-1,4,7,10,13,16-hexaazacyclooctadecane (L) and 1,4,7-trimethyl-1,4,7,10,13,16,19-heptaazacyclohencosane (L1): two new macrocyclic receptors for ATP binding. Synthesis, and solution equilibria. The crystal structure of (H₄L)(C10₄)₄.
A. Andrés, C. Bazzicalupi, A. Bencini, A. Bianchi, V. Fusi, E. Garcia-España, C. Giorgi, N. Nardi, P. Paoletti, J.A. Ramirez and B. Valtancoli