

## JOURNAL OF THE CHEMICAL SOCIETY

## Perkin Transactions 2

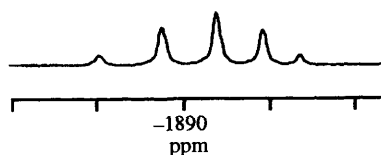
## Physical Organic Chemistry

## CONTENTS

## Perkin Communications

- 639 **Observation of intermolecular ligand exchange in lead(IV) carboxylates by 1- and 2-D  $^{207}\text{Pb}$  NMR spectroscopy**

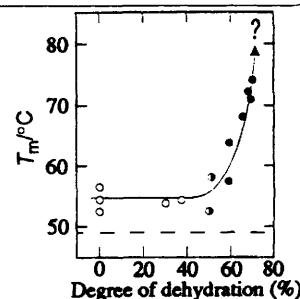
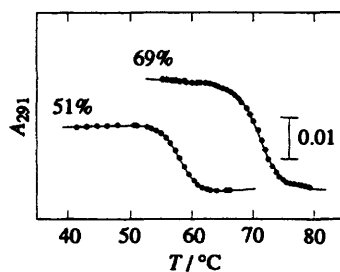
Jonathan E. H. Buston, Tim D. W. Claridge and Mark G. Moloney



On mixing lead(II) acetate and lead(II) benzoate, five distinct species may be observed and are shown to be undergoing intermolecular ligand exchange

- 643 **The effect of gradual dehydration on the thermal stability of a protein entrapped in a polymeric network**

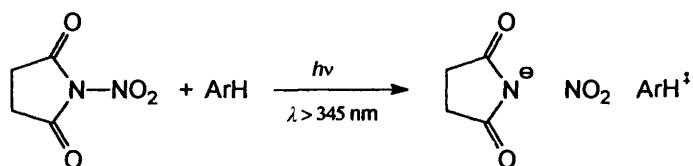
Josefa Nuñez-Olea and Jose M. Sanchez-Ruiz

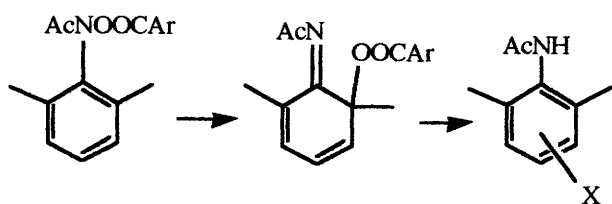
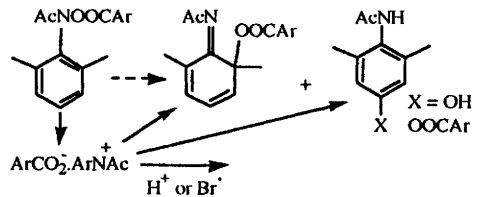
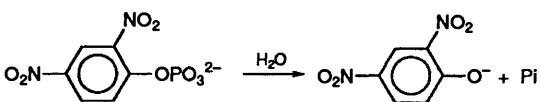
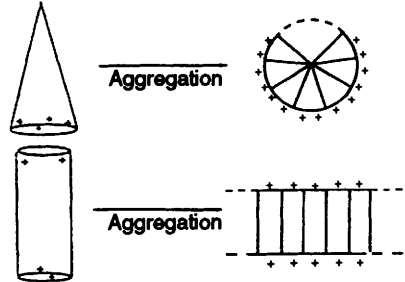
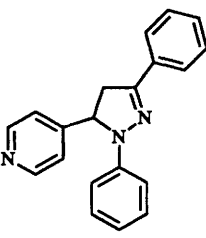


## Articles

- 645 **Succinimidylation and nitration of aromatic compounds by photolysis with *N*-nitrosuccinimide**

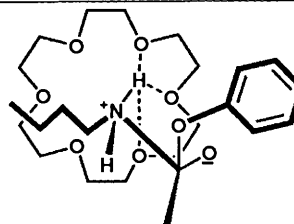
Jane Calvert, Lennart Eberson, Michael P. Hartshorn and Jan O. Svensson



<p>653 Cyclohexadienes from the rearrangement of <i>O</i>-aroyl-<i>N</i>-acetyl-<i>N</i>-(2,6-dimethylphenyl)-hydroxylamines. Reaction in aqueous solution to <i>meta</i>- and <i>para</i>-substituted 2,6-dimethylacetanilides</p> <p>James C. Fishbein and Robert A. McClelland</p>	 <p>Acid-reaction, X = <i>m</i>-OH and <i>m</i>-OOCAr by conjugate addition; neutral reaction, X = <i>p</i>-OH and <i>p</i>-OOCAr by C–O ionization</p>
<p>663 Nature of nitrenium : carboxylate ion pair intermediates in the hydrolysis of <i>O</i>-aroyl-<i>N</i>-acetyl-<i>N</i>-(2,6-dimethylphenyl)hydroxylamines</p> <p>James C. Fishbein and Robert A. McClelland</p>	 <p>Trapping results require three different ion pairs, with lifetimes of 10 ps to 0.5 ns</p>
<p>673 Hydrolysis of 2,4-dinitrophenyl phosphate in normal and reverse micelles</p> <p>Francesca Del Rosso, Antonella Bartoletti, Pietro Di Profio, Raimondo Germani, Gianfranco Savelli, Andrei Blaskó and Clifford A. Bunton</p>	 <p>Spontaneous hydrolysis is catalysed by normal and reverse micelles and by <i>N,N</i>-dimethylhydroxylamine</p>
<p>679 Self-assembly of tetracationic amphiphiles bearing a calix[4]arene core. Correlation between the core structure and the aggregation properties</p> <p>Susumu Arimori, Takeshi Nagasaki and Seiji Shinkai</p>	 <p>The aggregation properties of calix[4]arene-containing amphiphiles can be controlled by the conformational structure difference in the calix[4]arene core</p>
<p>685 Luminescence and charge transfer. Part 4. 'On-off' fluorescent PET (photoinduced electron transfer) sensors with pyridine receptors: 1,3-diaryl-5-pyridyl-4,5-dihydro-pyrazoles</p> <p>A. Prasanna de Silva, H. Q. Nimal Gunaratne and P. L. Mark Lynch</p>	 <p>The fluorescence of <b>1</b> and relatives is switched off upon protonation</p>

- 691 **Complexation catalysis: effective charge development in the aminolysis of phenyl esters in chlorobenzene catalysed by crown ethers**

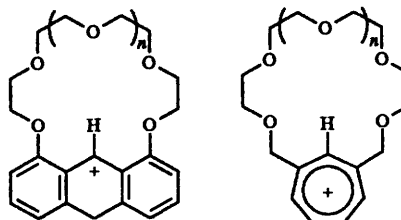
Antony B. Maude and Andrew Williams



Butylaminolysis of substituted phenyl acetates in chlorobenzene possesses a pathway involving rate-limiting complexation of crown ether with the zwitterionic addition intermediate; subsequent leaving group expulsion is not the rate-limiting step

- 697 **Preparation and properties of some crown ethers incorporating stable carbocations**

Owen S. Mills, Nichola J. Mooney, Peter M. Robinson, C. Ian F. Watt and Brian G. Cox



Xanthylum and tropylium based crown ethers ( $n = 3-5$ ) have been prepared

- 707 **Crown ether analogues and their complexes. Solid-state and solution stereochemistry of dibenzo-15-crown-4 ether and its 2:2 complex with sodium iodide as studied by X-ray crystallography and NMR spectroscopic methods**

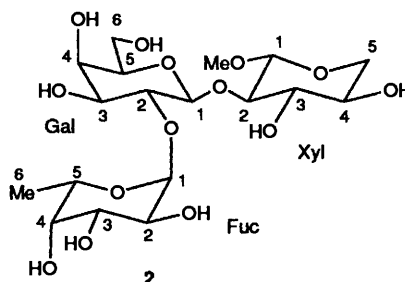
Gerald W. Buchanan, V. Mark Reynolds, Keith Bourque and Corinne Bensimon



The NaI complex of dibenzo-15-crown-4 is a 2:2 dimer with  $C_2$  symmetry. Each sodium cation coordinates to four oxygens of one macrocyclic unit and to one oxygen of the other 15-membered ring of the dimer

- 713 **Conformational studies of a trisaccharide epitope in solution by using NMR spectroscopy and molecular mechanics and dynamics calculations with the MM3\* program**

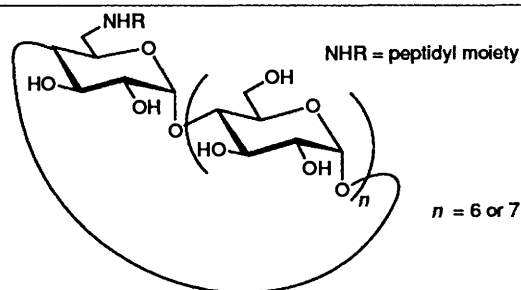
Manuel Martín-Pastor, Juan Luis Asensio, Rosa López and Jesús Jiménez-Barbero



The solution conformation of methyl  $\beta$ -D-galactopyranosyl-(1 $\rightarrow$ 2)-xylopyranoside (1) and methyl L-fucopyranosyl-(1 $\rightarrow$ 2)- $\beta$ -D-galactopyranosyl-(1 $\rightarrow$ 2)-xylopyranoside (2) has been analysed by NMR spectroscopy and molecular mechanics

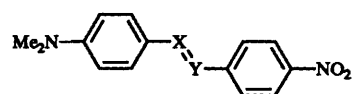
- 723 **Potential formation of intramolecular inclusion complexes in peptido-cyclodextrins as evidenced by NMR spectroscopy**

Florence Djedaïni-Pilard, Nathalie Azaroual-Bellanger, Muriel Gosnat, Delphine Vernet and Bruno Perly



731 **Theoretical investigation of the electronic properties of donor-acceptor *N*-benzylidene-anilines and related molecules**

John O. Morley



X = CH, N

Y = CH, N

735 **Structure and energy spectra of molecules containing anti-aromatic ring systems. Part 2. Energy spectra and stabilization of systems containing the anti-aromatic cycloheptatrienide anion**

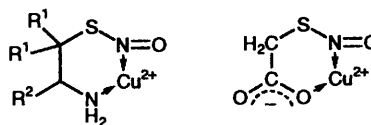
Fritz Dietz, Mordecai Rabinovitz, Alja Tadjer and Nikolai Tyutyulkov



The anti-aromatic character of the cycloheptatrienide anion (CHA), of annelated and substituted CHAs and of model polymers with CHA building blocks has been investigated

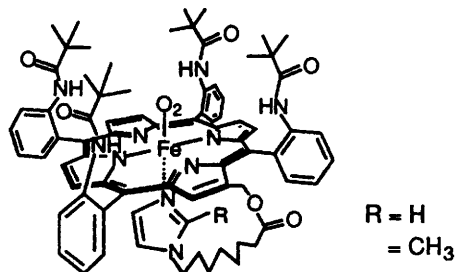
741 **Catalysis by  $\text{Cu}^{2+}$  of nitric oxide release from *S*-nitrosothiols (RSNO)**

Stuart C. Askew, D. Jonathan Barnett, John McAninly and D. Lyn H. Williams



747 **Synthesis and  $\text{O}_2$ -binding properties of tetraphenylporphyrinatoiron(II) derivatives bearing a proximal imidazole covalently bound at the  $\beta$ -pyrrolic position**

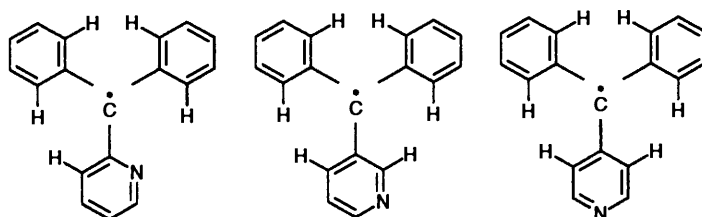
Eishun Tsuchida, Teruyuki Komatsu, Shinichi Kumamoto, Katsutoshi Ando and Hiroyuki Nishide



5,10,15,20-Tetrakis( $\alpha,\alpha,\alpha,\alpha$ -pivalamidophenyl)porphyrinatoiron(II) [Fe(TPVP)] derivatives bearing a proximal imidazole covalently bound at the  $\beta$ -pyrrolic position have been synthesized; the iron(II) complexes were five-coordinated species with intramolecular bound imidazole and reversibly formed stable  $\text{O}_2$  adducts in toluene at 25 °C

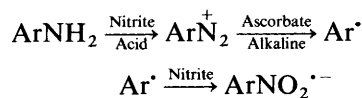
755 **Diphenylpyridylmethyl radicals. Part 1. Synthesis, dimerization and ENDOR spectroscopy of diphenyl(2-, 3- or 4-pyridyl)methyl radicals; bond dissociation enthalpies of their dimers**

Nikolaos I. Tzerpos, Antonios K. Zarkadis, Richard P. Kreher, Liesel Repas and Manfred Lehnig



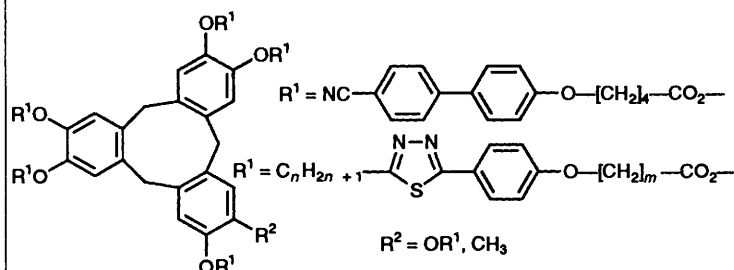
- 763 **EPR study of the aryl nitro anion radicals formed in the reaction between some aminoarenes, sodium nitrite and ascorbate**

Carl Lagercrantz



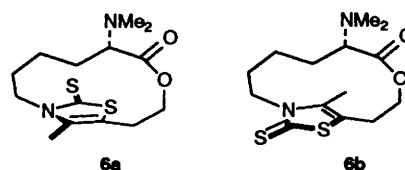
- 767 **Synthesis and investigation of new liquid-crystalline compounds by combination of the pyramidal tribenzocyclononene unit and calamitic structural units**

Hansjörg Budig, Siegmund Diele, Petra Göring, Reinhard Paschke, Christiane Sauer and Carsten Tschierske



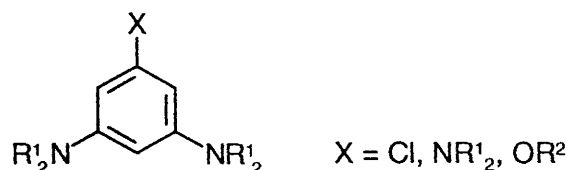
- 777 **Bridged thiazolium salts as models for thiamin: NMR, crystallographic and molecular mechanics studies**

Finian J. Leeper, David H. C. Smith, Michael J. Doyle and Paul R. Raithby



- 785 **4,6-Bis- and 2,4,6-tris-(*N,N*-dialkylamino)-*s*-triazines: synthesis, NMR spectra and restricted rotations**

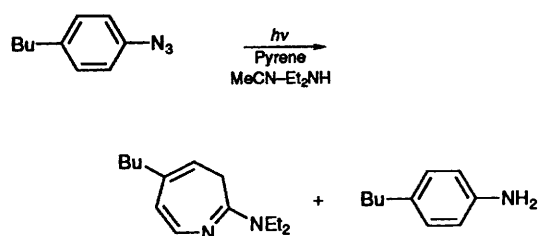
Alan R. Katritzky, Daniela C. Oniciu, Ion Ghiviriga and Richard A. Barcock



Syntheses and variable-temperature NMR spectra of some *s*-triazines are presented

- 793 **Mechanistic studies of pyrene-sensitized decomposition of *p*-butylphenyl azide: generation of nitrene radical anion through a sensitizer-mediated electron transfer from amines to the azide**

Shigeru Murata, Ryuichi Nakatsuji and Hideo Tomioka



- 801 **Conformational studies and pore-forming properties of an  $\alpha$ -aminoisobutyric acid analogue of gramicidin B**

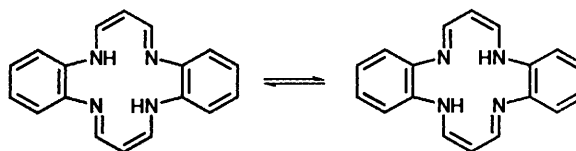
Masood Jelokhani-Niaraki, Hiroaki Kodama, Tsuguhisa Ehara and Michio Kondo

Formyl-L-Val-Gly-L-Ala-Aib-L-Ala<sup>5</sup>-Aib-L-Val-Aib-L-Trp-Aib<sup>10</sup>-L-Phe-Aib-L-Trp-Aib-L-Trp<sup>15</sup>-Glyol

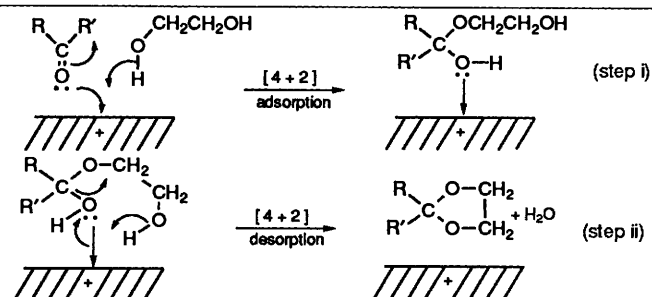
GBA, a short hydrophobic helical peptide, forms multi-conductance pores in membranes

809  $^{13}\text{C}$  CP/MAS NMR studies of tetraazaannulenes: fast proton transfer in the solid state

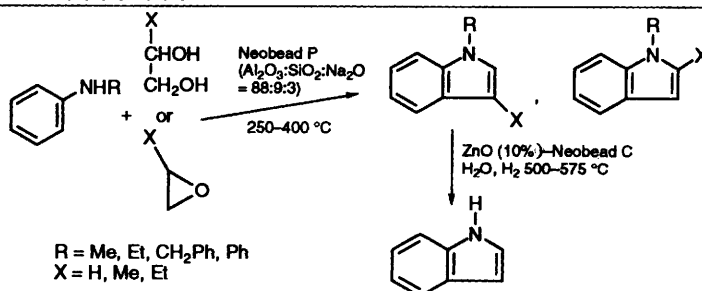
Alan C. McGregor, Peter J. Lukes, Julian R. Osman and Joe A. Crayston

815 Synthesis of 1,3-dioxolanes catalysed by  $\text{AlPO}_4$  and  $\text{AlPO}_4\text{-Al}_2\text{O}_3$ : kinetic and mechanistic studies

Felipa M. Bautista, Juan M. Campelo, Angel García, Josefa León, Diego Luna and José M. Marinas

823 Synthesis of 1-substituted indoles by the vapour phase reaction of *N*-substituted anilines with glycols and epoxides over a solid catalyst and a vapour phase dealkylation of 1-alkylindole

Takuo Nishida, Yoshikazu Tokuda and Michihiro Tsuchiya

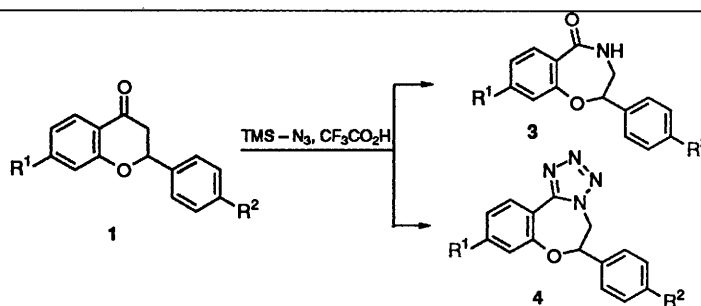
831  $^1\text{H}$  and  $^{13}\text{C}$  NMR and FT-IR studies of the interaction between 1,8-bis(dimethylamino)naphthalene and 3,5-dichlorophenol

Suzanne Toppet, Katrien Platteborze and Thérèse Zeegers-Huyskens

The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of the title complex have been investigated for  $\text{CD}_2\text{Cl}_2$  solutions between  $-70^\circ\text{C}$  and  $30^\circ\text{C}$ . The degree of protonation deduced from NMR and IR techniques are in good agreement

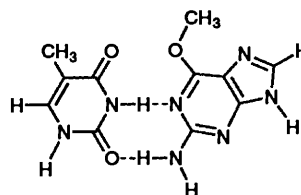
## 835 Benzodiazepine analogues. Part 9. Kinetics and mechanism of the azidotrimethylsilane-mediated Schmidt reaction of flavanones

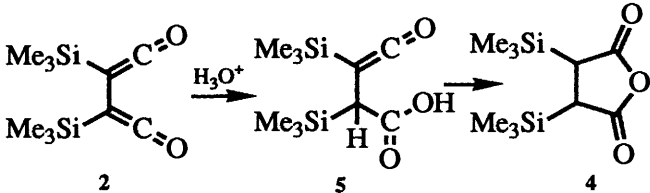
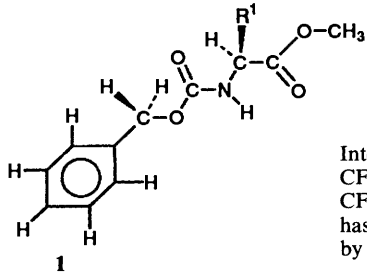
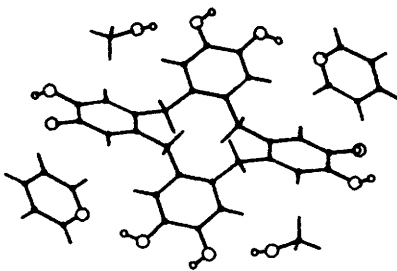
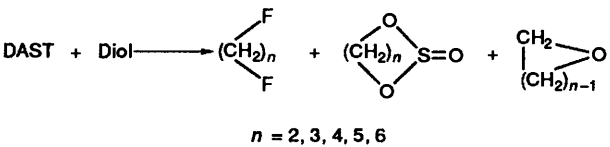
Perry T. Kaye, M. Jack Mphahlele and Michael E. Brown



## 839 Structural, steric and energetic requirements for induction of base substitutional mutations by methylated guanines and thymines

Divi Venkateswarlu and R. H. Duncan Lyngdoh



<p>847 <b>Electrophilic reactivity of bisketenes: an experimental and theoretical study, and photoinduced hydration</b></p> <p>Annette D. Allen, Jihai Ma, Michael A. McAllister, Thomas T. Tidwell and Da-chuan Zhao</p>	
<p>853 <b>Association behaviour of selected amino acid and oligopeptide derivatives with fluorinated alcohols</b></p> <p>Monika Plass, Carola Griehl and Alfred Kolbe</p>	 <p>Interaction between <math>\text{CF}_3\text{-CH(OH)-CF}_3</math> or <math>\text{CF}_3\text{-CH(OH)-Ph}</math> and <b>1</b> has been investigated by vibrational spectroscopy</p>
<p>857 <b>Inclusion chemistry of cyclotetratechylene</b></p> <p>Leonard J. Barbour, Jonathan W. Steed and Jerry L. Atwood</p>	 <p>X-Ray crystal structural investigation of the first inclusion complexes of cyclotetratechylene show that hydrogen-bonded interactions between host and guest(s) play an important role in the molecular structure and, in a particular case a terminated eleven-atom hydrogen bonded chain is observed</p>
<p>861 <b>Reaction of diethylaminosulfur trifluoride with diols</b></p> <p>Dale E. Shellhamer, D. Timothy Anstine, Kelly M. Gallego, Brian R. Ganesh, Aaron A. Hanson, Kelli A. Hanson, Rodney D. Henderson, Jeanie M. Prince and Victor L. Heasley</p>	 <p>Reaction of DAST with diols can give difluorides and sulfite esters or cyclic ethers</p>

## Corrigendum

- 867 **The effective 'size' of the tris(trimethylsilyl)silyl group in several molecular environments** Joseph Frey, Etti Schottland, Zvi Rappoport, Dmitry Bravo-Zhivotovskii, Moshe Nakash, Mark Botoshansky, Menahem Kaftory and Yitzhak Apeloig

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



## Report on the Perkin Journals for 1994

Last year the Editorial Board gained two new members from continental Europe, Professor Reinhard Hoffmann (University of Marburg) and Professor Richard Kellogg (University of Gröningen), together with Dr Philip Taylor (ICI Paints plc) and Professor Tomas Hudlicky as our first North American Associate Editor. We continue to benefit from their expertise and advice, as well as from the prompt and professional services of our panel of referees and the good advice of our newly formed International Advisory Board. To all of them and especially our past Chairman, Professor Stan Roberts, we express our gratitude for their valued cooperation and assistance, which are crucial as we strive for even higher standards and consistency in dealing with further increases in submissions.

We believe that the new Graphical Abstracts format has proved helpful and attractive and welcome the obvious support for inclusion of Communications in both Journals. We have also introduced a series of Keynote Articles, six of which have already appeared; a number of others are projected for 1995. This series is intended to highlight different areas of research in which the introduction is expanded to include a short review of the appropriate field, so that readers, less familiar with the particular topic featured, will be given an update on the current state of affairs before being led on to the new results.

During 1994 *Perkin Transactions 1* received 708 papers, a further increase compared to 1993 (664 papers), and the number of communications rose marginally from 149 to 156. Of this number, 30% of the full papers and 46% of the communications were rejected; of the total number of submissions 75% were received from outside the UK. For *Perkin Transactions 2*, there were 625 full papers and 34 communications (with 34% and 53% rejection rates, respectively), with 80% of the papers non-UK-based, which again provides encouraging evidence of the truly international nature of our *Journal*.

Times from receipt to publication continue to compare very favourably with peer-reviewed, typeset journals, averaging 140–150 days for full papers and 60–90 days for communications. We continue to be committed to a process of development of systems and techniques that will be helpful to authors, both in terms of ease and rapidity of publication: in particular, we strongly encourage authors to submit papers (text and formulae) in disk form, from which the printed form can be directly produced. To date, ChemDraw structure files provided by authors have been used directly by the Royal Society of Chemistry for producing journal illustrations. In future, the RSC will be able to use files produced with the program ChemWindow in the same way. Authors should choose the command Export from the ChemWindow File menu, and save the relevant files to disk as <filename>.chm. The possibility of extending the facility to ISIS Draw files is being investigated.

We are also contributing to the Society's World Wide Web Server on the Internet, scheduled for launch in June. This server will provide information on all the RSC's products and services in chemistry, together with membership information and news of professional activities. From this server, it will be possible to access conference diaries, titles of forthcoming papers in *Perkin 1* and *2*, instructions for authors, and subscription details. Future developments will include the provision of graphical abstracts.

We hope that authors and readers will appreciate the Editorial Board's continued efforts to maintain the quality of Britain's premier organic chemistry journals; comments and suggestions for further improvements would, of course, be welcomed.

Professor Bruce C. Gilbert  
Dr Sheila R. Buxton

## Forthcoming Articles in *Perkin Transactions 2*

- $\pi$ -Complexes incorporating tetrakis(phenylethynyl)ethene **D. Philp, V. Gramlich, P. Seiler and F. Diederich**
- Considerably improved Grunwald–Winstein correlations for solvolyses of several secondary and tertiary benzylic derivatives upon inclusion of a term governed by the aromatic ring parameter (*I*) **D. N. Kevill and M. J. D'Souza**
- The dolastatins 25. Conformational isomerism of *N*-benzyloxycarbonyl-*N*-methylisoleucinol and related substances  
**G. R. Pettit, M. D. Williams, J. K. Srirangam, F. Hogan, N. L. Benoiton and D. Kantoci**
- Regioselectivity in Diels–Alder reactions of benzopyranoquinones **F. Zuloaga, R. Tapia and C. Quintanar**
- Structural and conformational analysis of 2-triphenylphosphoranylidene succinic acid derivatives by <sup>1</sup>H, <sup>13</sup>C and <sup>31</sup>P one and two dimensional NMR spectroscopy and molecular modelling  
**R. Bacaloglu, A. Blaskó, C. A. Bunton, G. Cerichelli, F. Castaneda and E. Rivera**
- Neutral hydrolysis and imidazole-catalysed decomposition of bis(4-nitrophenyl) oxalate. 1,1'-Oxalyldiimidazole as an intermediate  
**H. Neuvonen**
- Hydrogen bonding. Part 40. Factors that influence the distribution of solutes between water and sodium dodecylsulfate micelles  
**M. H. Abraham, H. S. Chadha, J. P. Dixon, C. Rafols and C. Treiner**
- Selective inclusion of phenylenediamine isomers by 1,1-bis(4-hydroxyphenyl)cyclohexane  
**L. R. Nassimbeni, M. R. Caira, A. Horne, K. Okuda and F. Toda**
- EPR studies of the copper-catalysed oxidation of thiols with peroxides **G. Scrivens, B. C. Gilbert and T. C. P. Lee**
- Theoretical study of the cyclization of  $\alpha$ -iminothioaldehydes into dihydrothiazoles **R. Arnaud, N. Pelloux-Léon, J.-L. Ripoll and Y. Vallée**
- EPR spectroscopic studies of *N*-alkyl-*N*-trialkylsilylmethylaminy radicals in solution **B. P. Roberts and A. R. Vazquez-Persaud**
- Linear oligopeptides. Part 329. Synthesis, characterization and solution conformational analysis of C $_{\alpha}$ -ethyl, C $_{\alpha}$ -benzylglycine [( $\alpha$ Et)Phe] containing peptides **F. Formaggio, M. Pantano, M. Crisma, G. M. Bonora, C. Toniolo and J. Kamphuis**
- Synthesis of and metal cation oscillation in ionophoric biscalix[4]arenes **F. Ohseto and S. Shinkai**
- EPR spin-trapping studies of the reaction of radicals derived from hydroperoxide tumour-promoters with nucleic acids and their components **C. Hazlewood and M. J. Davies**
- Conformational analysis by NMR spectroscopy, molecular dynamics simulation in water and X-ray crystallography of glutamic acid analogues: isomers of 1-aminocyclopentane-1,3-dicarboxylic acid (ACPD)  
**V. Larue, J. Gharbi-Benarous, F. Acher, G. Valle, M. Crisma, C. Toniolo, R. Azerad and J.-P. Girault**
- Effects of conformation, substituents and solvent on molecular hyperpolarizabilities of push-pull diaryl-alkenes and -dienes: a computational study **W. M. F. Fabian, R. Dworczak, H. Junek and B. N. Pawar**
- Kinetics and mechanism of the hydrolysis of 1-aryloxyethyl alkanoates **C. D. Hall and C. W. Goulding**
- Amidines. Part 34. <sup>15</sup>N NMR spectra of trisubstituted amidines. Substituent effects  
**J. Oszczapowicz, I. Wawer, M. Dargatz and E. Kleinpeter**
- Pair of pyrene groups as a conformational probe for designed two  $\alpha$ -helix polypeptides  
**H. Mihara, Y. Tanaka, T. Fujimoto and N. Nishino**
- Hyperfluorination of [60]fullerene by krypton difluoride **O. V. Boltalina, A. K. Abdul-Sada and R. Taylor**
- Prediction of planarity and reduction potential of derivatives of tetracyanoquinodimethane using *ab initio* molecular orbital theory  
**P. W. Kenny**
- Design and structure of a novel neurokinin A receptor antagonist cyclo(Met<sup>1</sup>-Asp<sup>2</sup>-Trp<sup>3</sup>-Phe<sup>4</sup>-Dap<sup>5</sup>-Leu<sup>6</sup>)cyclo(2 $\beta$ -5 $\beta$ )  
**V. Pavone, A. Lombardi, F. Nistri, M. Saviano, O. Maglio, G. D'Auria, L. Quartara, C. A. Maggi and C. Pedone**
- Enhanced Eu<sup>III</sup> ion luminescence and efficient energy transfer between lanthanide chelates within polymeric structure in aqueous solutions **M. Latva, H. Takalo, K. Simberg and J. Kankare**
- Proton transfer in the ground and excited electronic states of [2,2'-bipyridyl]-3,3'-diol. A semiempirical study  
**V. Barone, G. Milano, L. Orlandini and C. Adams**