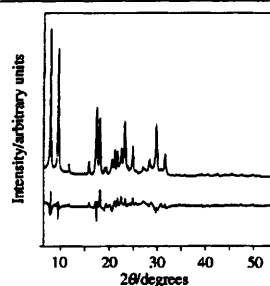


### Communications

1527 **X-Form metal-free phthalocyanine: crystal structure determination using a combination of high-resolution X-ray powder diffraction and molecular modelling techniques**

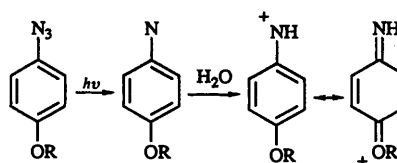
Robert B. Hammond, Kevin J. Roberts, Robert Docherty, Michael Edmondson and Ray Gairns



X-Ray powder diffraction data and final Rietveld plot for X-form metal-free phthalocyanine

1529 **Direct observation of 4-alkoxyphenylnitrenium ions upon irradiation of 4-alkoxyphenyl azides in aqueous solution**

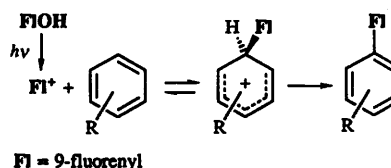
Pratima Sukhai and Robert A. McClelland



### Keynote Article

1531 **Flash photolysis study of a Friedel-Crafts alkylation. Reaction of the photogenerated 9-fluorenyl cation with aromatic compounds**

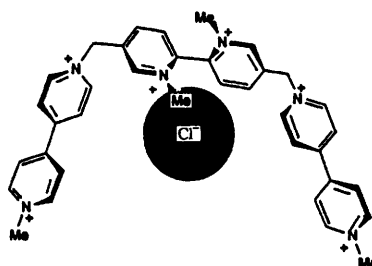
Robert A. McClelland, Frances L. Cozens, Jianhui Li and Steen Steenken



## Articles

## 1545 Halide anion recognition by new acyclic quaternary polybipyridinium and polypyridinium receptors

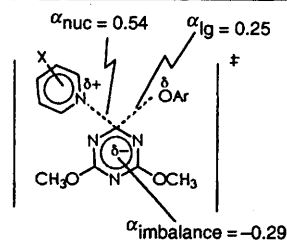
Paul D. Beer, Nicholas C. Fletcher, Alan Grieve, John W. Wheeler, Christopher P. Moore and Trevor Wear



New acyclic quaternary polybipyridinium receptors complex and electrochemically sense chloride anions

## 1553 Concerted displacement mechanisms at trigonal carbon: the aminolysis of 4-aryloxy-2,6-dimethoxy-1,3,5-triazines

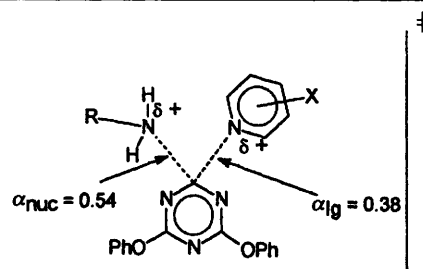
Janice Shakes, Christel Raymond, Donatella Rettura and Andrew Williams



Transition structure exhibits charge imbalance

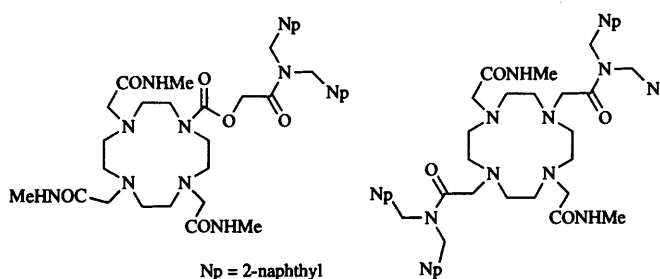
1559 The aminolysis and hydrolysis of *N*-(4,6-diphenoxy-1,3,5-triazin-2-yl) substituted pyridinium salts: concerted displacement mechanism

Neil R. Cullum, Donatella Rettura, James M. J. Whitmore and Andrew Williams



## 1565 Photochemical investigations of functionalised 1,4,7,10-tetraazacyclododecane ligands incorporating naphthyl chromophores

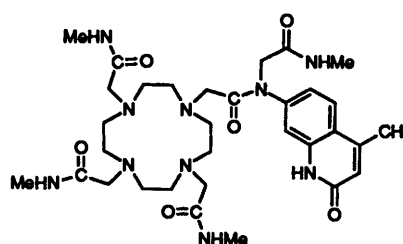
Andrew Beeby, David Parker and J. A. Gareth Williams



Metal complexation with these ligands is rapid in aqueous solution and both the total luminescence intensity and the ratio of excimer to monomer intensity are affected both sensitively and distinctively by different metal ions, allowing the selective signalling of their presence in solution

## 1581 Modest effectiveness of carbostyryl 124 as a sensitising chromophore in europium and terbium amide complexes based on 1,4,7,10-tetraazacyclododecane

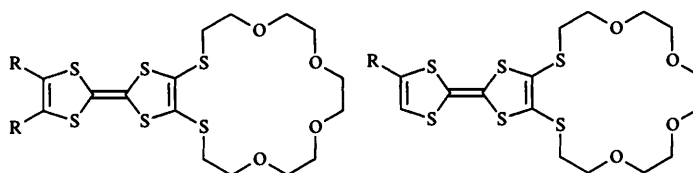
David Parker and J. A. Gareth Williams



In the terbium complex of 1, the intensity and lifetime of metal-based emission are limited by a thermally activated back energy transfer process

1587 **Crown-annulated tetrathiafulvalenes: synthesis of new functionalised derivatives and spectroscopic and electrochemical studies of metal complexation**

Reinhold Dieing, Vincent Morisson, Adrian J. Moore, Leonid M. Goldenberg, Martin R. Bryce, Jean-Michel Raoul, Michael C. Petty, Javier Garin, María Savirón, Igor K. Lednev, Ronald E. Hester and John N. Moore



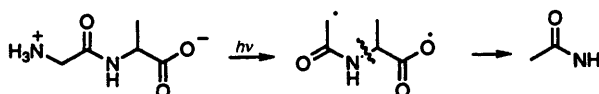
R = SC<sub>18</sub>H<sub>37</sub>; CO<sub>2</sub>Me

R = H; CHO; CO<sub>2</sub>Me; CH<sub>2</sub>OH; CO<sub>2</sub>H; CH<sub>2</sub>OC(O)C<sub>17</sub>H<sub>35</sub>

Syntheses and metal complexation studies are reported

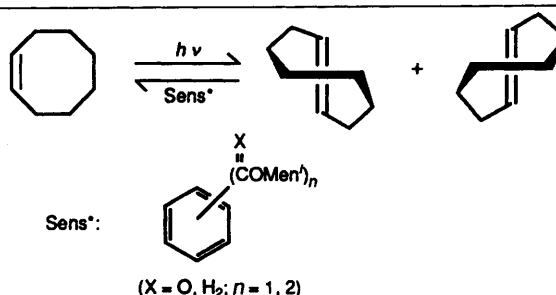
1595 **Photo-induced electron transfer in small peptides: glycylalanine**

Roger R. Hill, Graham E. Jeffs, Frank Banaghan, Tony McNally and Alan R. Werninck



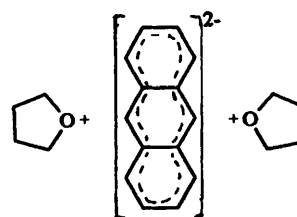
1601 **Singlet- versus triplet-sensitized enantiodifferentiating photoisomerization of cyclooctene: remarkable effects of spin multiplicity upon optical yield**

Hiroshi Tsuneishi, Tadao Hakushi and Yoshihisa Inoue



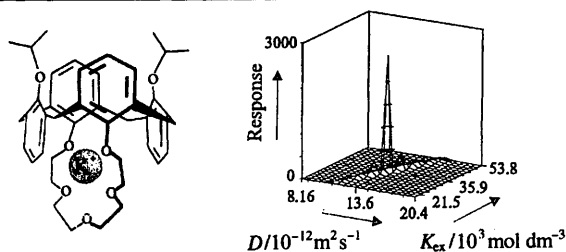
1607 **Acidity of dibasic carbon acids. Part 4. Structure and ion solvation state of dimetallic salts of 9,10-dihydroanthracene and its derivatives in tetrahydrofuran**

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



1617 **Carrier mediated transport through supported liquid membranes; determination of transport parameters from a single transport experiment**

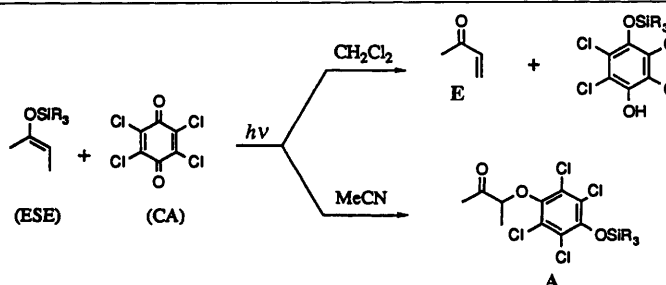
Lysander A. J. Chrisstoffels, Wilhelmina Struijk, Feike de Jong and David N. Reinhoudt



A new method has been developed to determine transport parameters for cations in supported liquid membrane transport

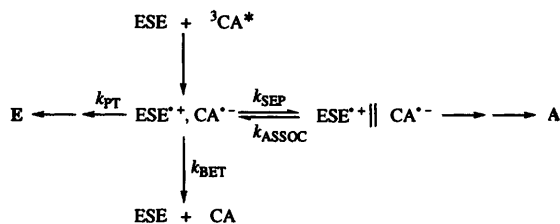
1623 **Photoinduced electron transfer from enol silyl ethers to quinone. Part 1. Pronounced effects of solvent polarity and added salt on the formation of  $\alpha$ -enones**

T. Michael Bockman, D. Shukla and Jay K. Kochi



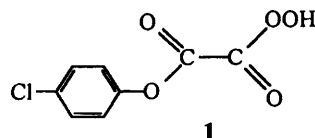
1633 Photoinduced electron transfer from enol silyl ethers to quinone. Part 2. Direct observation of ion-pair dynamics by time-resolved spectroscopy

T. Michael Bockman and Jay K. Kochi



1645 Synthesis and characterisation of an intermediate in the peroxyoxalate chemiluminescence: 4-chlorophenyl *O,O*-hydrogen monoperoxyoxalate

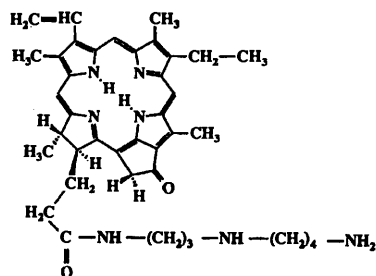
Cassius V. Stevani, Ivan P. de Arruda Campos and Wilhelm J. Baader



Peracid **1** is synthesised and characterised by  $^{13}\text{C}$  NMR, IR and mass spectrometry; studies on its chemiluminescence properties unequivocally confirm that **1** is not a reactive intermediate in the peroxyoxalate reaction

1649 Organization processes of a pyropheophorbide-spermidine conjugate in the presence or absence of DNA

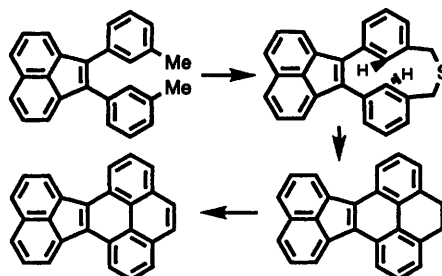
Souad Mansouri, Suzanne Fery-Forgues, Bernard Meunier and Nicole Paillous



Molecular aggregation and DNA interactions of this new chemical photonuclase have been determined by spectroscopy

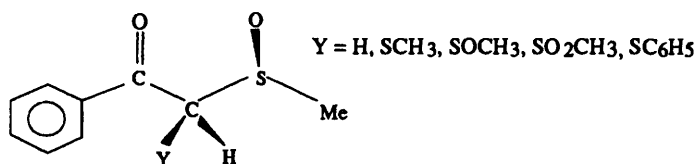
1655 A cyclophane route to acenaphthylene[1,2-*e*]-pyrene. Relative bathochromic shifts (colour changes) in a series of 1,2-diaryl-acenaphthylenes

Yee-Hing Lai, Pu Chen and Yu Xin Cui



1661 Experimental and theoretical study of the intramolecular interactions determining the conformation of  $\beta$ -carbonyl sulfoxides

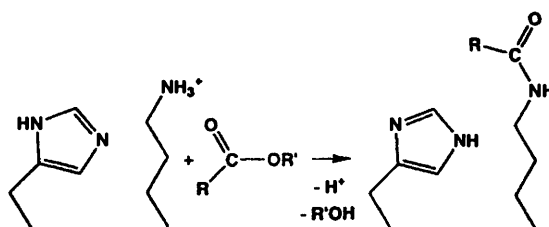
Giuseppe Distefano, Maurizio Dal Colle, Marcello de Palo, Derek Jones, Gabriella Bombieri, Antonio Del Pra, Paulo R. Olivato and Mirta G. Mondino



The electronic and geometric structure of  $\beta$ -carbonyl sulfoxides is determined by X-ray diffraction, PE spectroscopy and *ab initio* calculations

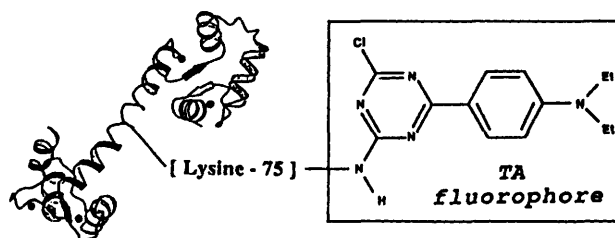
1671 Polypeptides with supersecondary structures as templates in rational catalyst design. Catalysis of self functionalization by designed helix-loop-helix motifs

Lars Baltzer, Ann-Christin Lundh, Klas Broo, Susanne Olofsson and Per Ahlberg



1677 **Triazinylaniline derivatives as fluorescence probes. Part 3. Effects of calcium and other metal ions on the steady-state and time-resolved fluorescence of bovine brain calmodulin labelled at lysine-75**

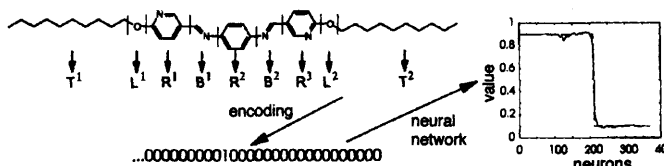
David J. Cowley and James P. McCormick



Hydrophobic interactions in calmodulin on calcium ion binding induce dramatic responses in the probe fluorescence

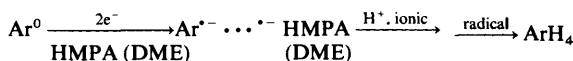
1685 **Predicting the transition temperature of smectic liquid crystalline compounds from their structure using artificial neural networks**

Rachel Schröder, Helge Kränz, Volkmar Vill and Bernd Meyer



1691 **Unexpected electrochemical reduction of fluoranthene in the solvents DME and HMPA: new light onto the mechanism of hydrogenation to produce tetrahydrofluoranthene**

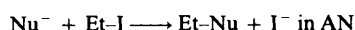
Stéphane G. Boué, Céline G. Jung, José Castillo and Emile Vander Donckt



The 2e<sup>-</sup> reduction of fluoranthene Ar<sup>0</sup> in DME and in HMPA produces an aromatic-solvent complex which on addition of H<sup>+</sup>-H<sub>2</sub>O undergoes first a protonation step followed by H radical abstractions from the solvent, to yield 1,2,3,10b-tetrahydrofluoranthene

1699 **Single-ion enthalpies of transfer as a scale of nucleophilic reactivity towards ethyl iodide in acetonitrile**

Yasuhiko Kondo, Tamio Tsukamoto and Chika Moriguchi

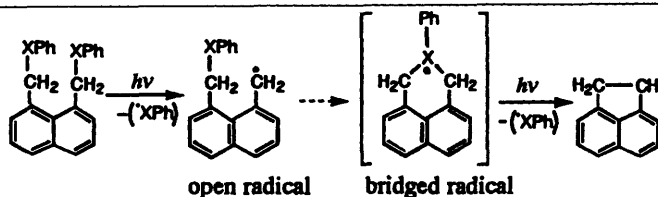


Nu<sup>-</sup>, carboxylate ions  
 $3 + \log k = -1.53 - 8.76 \times 10^{-2} \times \Delta_1 H_{\text{SI}}^{\text{AN-MeOH}}$

Nu<sup>-</sup>, imidide ions  
 $3 + \log k = -0.42 - 7.23 \times 10^{-2} \times \Delta_1 H_{\text{SI}}^{\text{AN-MeOH}}$

1705 **Laser flash photolysis of 1,8-bis(substituted methyl)naphthalenes**

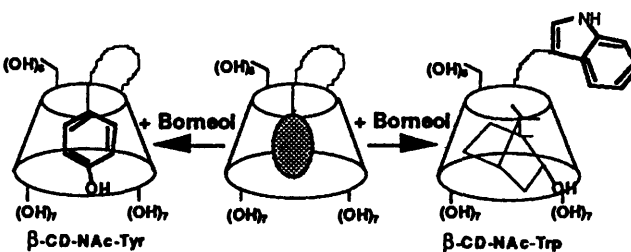
Akihiko Ouchi, Yoshinori Koga, Maksudul M. Alam and Osamu Ito



Laser flash photolysis: X = O (triplet state)  
 S (open radical)  
 Se (bridged radical)

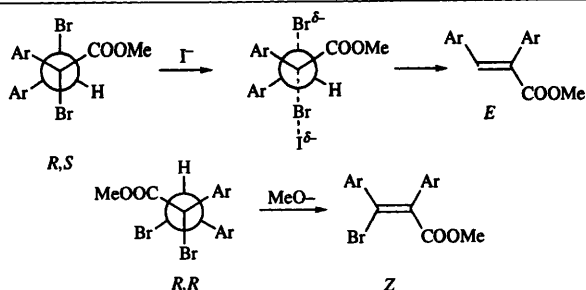
1711 **Fluorescent amino acids as reporter systems in peptido-cyclodextrin inclusion compounds**

Mohamed Eddaoudi, Helene Parrot-Lopez, Sophie Frizon de Lamotte, Damien Ficheux, Patrice Prognon and Anthony W. Coleman

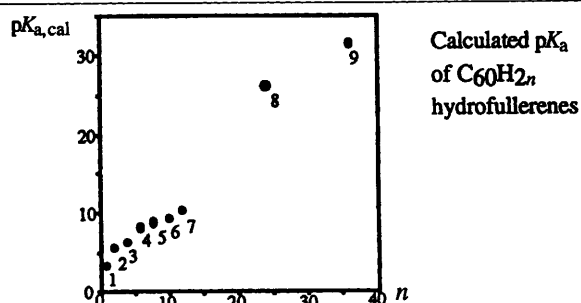


1717 **Methyl 2,3-dibromo-2,3-diarylpropanoates. Debromination and dehydrobromination reactions**

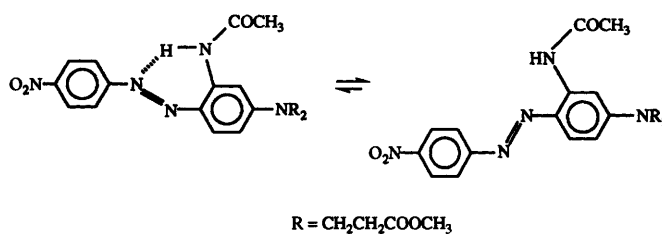
Mercedes A. Badajoz, Rosana S. Montani and Mercedes C. Cabaleiro

1723 **Acidity of hydrofullerenes: a quantum chemical study**

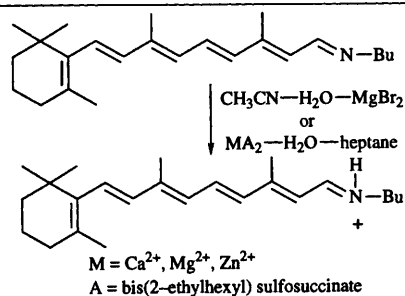
K. Choho, G. Van Lier, G. Van de Woude and P. Geerlings

1733 **Conformational analysis by magic-angle spinning NMR spectroscopy for a series of polymorphs of a disperse azobenzene dyestuff**

Gary McGeorge, Robin K. Harris, A. Margaret Chippendale and James F. Bullock

1739 **Metal cation assisted protonation of retinylidene Schiff base in aqueous acetonitrile and in reverse micelles**

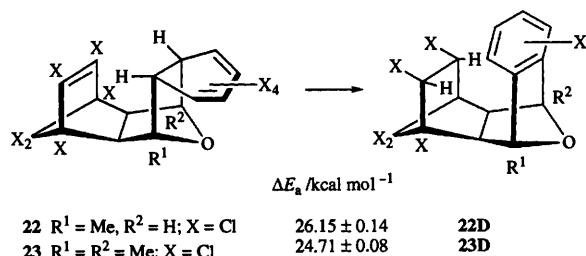
Anil K. Singh and Joydip Das

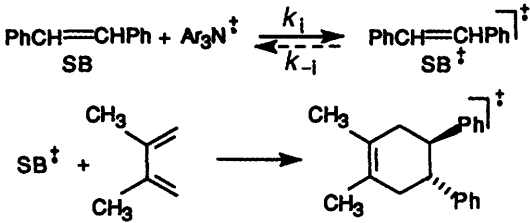
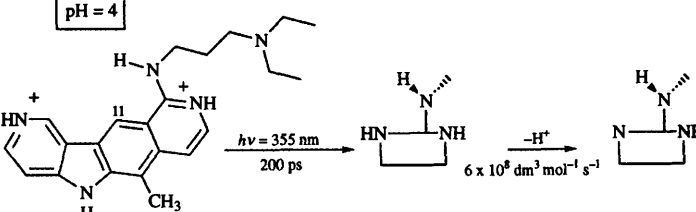
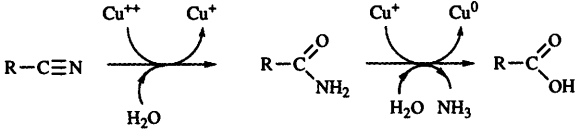
1743 **Structure and gas-phase acidity of oxalic acid and its disila derivative. A theoretical study by means of the DFT quantum theoretical method**

Milan Remko, Klaus R. Liedl and Bernd M. Rode

 $M = C, Si$ 1749 **On intramolecular dyotropy: structural effects on reaction rates and crystal structure-molecular mechanics correlations for some new examples**

Kenneth Mackenzie, Judith A. K. Howard, Renata Siedlecka, K. Brian Astin, Edward C. Gravett, Claire Wilson, Jason Cole, Robert G. Gregory and Andrew S. Tomlins



<p>1761 <b>Characterization of cation radical reactions. Aminium salt-catalysed Diels–Alder reactions</b></p> <p>Wang Yueh and Nathan L. Bauld</p>	
<p>1767 <b>Proton and charge transfer in the intercalating antitumour drug pazelliptine</b></p> <p>Marie P. Fontaine-Aupart, Hélène Laguitton-Pasquier, Robert Pansu, Laurence Brian, Eric Renault, Mike C. Marden, Christian Rivalle and Emile Bisagni</p>	 <p>Whatever the pH, a twist and a proton transfer occur leading to the excited, non-fluorescence 9N protonated form of PZE</p>
<p>1775 <b>Absolute rate constants for abstraction of chlorine from three chlorinating agents by alkyl radicals</b></p> <p>James M. Tanko and Joseph F. Blackert</p>	$R\cdot + Z-Cl \xrightarrow{k_{z-cl}} R-Cl + Z\cdot$ <p>Z = Cl, Bu'O, imidyl</p> <p>Using the cyclopropylcarbonyl free radical clock, absolute rate constants for Cl atom abstraction from Cl<sub>2</sub>, Bu'OCl and <i>N</i>-chloro-3,3-dimethylglutarimide have been determined</p>
<p>1781 <b>'Dry' hydrolysis of nitriles by sodium perborate and copper salts in heterogeneous media</b></p> <p>Farid Chemat, Martine Poux and Jacques Berlan</p>	 <p>Dry hydrolysis of nitrile by copper chloride</p>

## AUTHOR INDEX

- Ahlberg, Per, 1671  
 Alam, Maksudul M., 1705  
 Astin, K. Brian, 1749  
 Baader, Wilhelm J., 1645  
 Badajoz, Mercedes A., 1717  
 Baltzer, Lars, 1671  
 Banaghan, Frank, 1595  
 Bauld, Nathan L., 1761  
 Beeby, Andrew, 1565  
 Beer, Paul D., 1545  
 Berlan, Jacques, 1781  
 Bisagni, Emile, 1767  
 Blackert, Joseph F., 1775  
 Bockman, T. Michael, 1623, 1633  
 Bombieri, Gabriella, 1661  
 Boué, Stéphane G., 1691  
 Brian, Laurence, 1767  
 Broo, Klas, 1671  
 Bryce, Martin R., 1587  
 Bullock, James F., 1733  
 Cabaleiro, Mercedes C., 1717  
 Castillo, José, 1691  
 Chemat, Farid, 1781  
 Chen, Pu, 1655  
 Chippendale, A. Margaret, 1733  
 Choho, K., 1723  
 Christoffels, Lysander A. J., 1617  
 Cole, Jason, 1749  
 Coleman, Anthony W., 1711  
 Colle, Maurizio Dal, 1661  
 Cowley, David J., 1677  
 Cozens, Frances L., 1531  
 Cui, Yu Xin, 1655  
 Cullum, Neil R., 1559  
 Das, Joydip, 1739  
 de Arruda Campos, Ivan P., 1645  
 de Jong, Feike, 1617  
 de Lamotte, Sophie Frizon, 1711  
 de Palo, Marcello, 1661  
 Del Pra, Antonio, 1661  
 Dieing, Reinhold, 1587  
 Distefano, Giuseppe, 1661  
 Docherty, Robert, 1527  
 Donckt, Emile Vander, 1691  
 Eddaoudi, Mohamed, 1711  
 Edmondson, Michael, 1527  
 Fery-Forgues, Suzanne, 1649  
 Ficheux, Damien, 1711  
 Fletcher, Nicholas C., 1545  
 Fontaine-Aupart, Marie P., 1767  
 Gairns, Ray, 1527  
 Garin, Javier, 1587  
 Geerlings, P., 1723  
 Goldenberg, Leonid M., 1587  
 Gravett, Edward C., 1749  
 Gregory, Robert G., 1749  
 Grieve, Alan, 1545  
 Hakushi, Tadao, 1601  
 Hammond, Robert B., 1527  
 Harris, Robin K., 1733  
 Hester, Ronald E., 1587  
 Hill, Roger R., 1595  
 Hoffman, Roy E., 1607  
 Howard, Judith A. K., 1749  
 Inoue, Yoshihisa, 1601  
 Ito, Osamu, 1705  
 Jeffs, Graham E., 1595  
 Jones, Derek, 1661  
 Jung, Céline G., 1691  
 Kochi, Jay K., 1623, 1633  
 Koga, Yoshinori, 1705  
 Kondo, Yasuhiko, 1699  
 Kränz, Helge, 1685  
 Laguitton-Pasquier, Hélène, 1767  
 Lai, Yee-Hing, 1655  
 Lednev, Igor K., 1587  
 Li, Jianhui, 1531  
 Liedl, Klaus R., 1743  
 Lundh, Ann-Christin, 1671  
 Mackenzie, Kenneth, 1749  
 Mansouri, Souad, 1649  
 Marden, Mike C., 1767  
 McClelland, Robert A., 1529, 1531  
 McCormick, James P., 1677  
 McGeorge, Gary, 1733  
 McNally, Tony, 1595  
 Meunier, Bernard, 1649  
 Meyer, Bernd, 1685  
 Mondino, Mirta G., 1661  
 Montani, Rosana S., 1717  
 Moore, Adrian J., 1587  
 Moore, Christopher P., 1545  
 Moore, John N., 1587  
 Moriguchi, Chika, 1699  
 Morisson, Vincent, 1587  
 Nir, Malka, 1607  
 Olivato, Paulo R., 1661  
 Olofsson, Susanne, 1671  
 Ouchi, Akihiko, 1705  
 Paillous, Nicole, 1649  
 Pansu, Robert, 1767  
 Parker, David, 1565, 1581  
 Parrot-Lopez, Helene, 1711  
 Petty, Michael C., 1587  
 Poux, Martine, 1781  
 Prognon, Patrice, 1711  
 Rabinovitz, Mordecai, 1607  
 Raoul, Jean-Michel, 1587  
 Raymond, Christel, 1553  
 Reinhoudt, David N., 1617  
 Remko, Milan, 1743  
 Renault, Eric, 1767  
 Rettura, Donatella, 1553, 1559  
 Rivalle, Christian, 1767  
 Roberts, Kevin J., 1527  
 Rode, Bernd M., 1743  
 Savirón, Maria, 1587  
 Schröder, Rachel, 1685  
 Shakes, Janice, 1553  
 Shapiro, Israel O., 1607  
 Shukla, D., 1623  
 Siedlecka, Renata, 1749  
 Singh, Anil K., 1739  
 Steenken, Steen, 1531  
 Stevani, Cassius V., 1645  
 Struijk, Wilhelmina, 1617  
 Sukhai, Pratima, 1529  
 Tanko, James M., 1775  
 Tomlins, Andrew S., 1749  
 Tsukamoto, Tamio, 1699  
 Tsuneishi, Hiroshi, 1601  
 Van de Woude, G., 1723  
 Van Lier, G., 1723  
 Vill, Volkmar, 1685  
 Wear, Trevor, 1545  
 Werninck, Alan R., 1595  
 Wheeler, John W., 1545  
 Whitmore, James M. J., 1559  
 Williams, Andrew, 1553, 1559  
 Williams, J. A. Gareth, 1565, 1581  
 Wilson, Claire, 1749  
 Yueh, Wang, 1761

---

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



## **Correction to 'Instructions for Authors (1996)'**

The e-mail address for the Cambridge Crystallographic Data Centre given on p. xxi of the 'Instructions for Authors (1996)' in Issue 1 is no longer valid.

The correct address is: [deposit@chemcrys.cam.ac.uk](mailto:deposit@chemcrys.cam.ac.uk)

# 9th International Symposium on Molecular Recognition and Inclusion

Lyon, France      7-12 September 1996

## International advisory board

J L Atwood	Y Murikami	S Shinkai
T Bein	D Reinhoudt	J F Stoddart
G Gokel	J Ripmeester	J Szejtli
J-M Lehn	E Rizzarelli	T Osa
J Lipkowski	H-J Schneider	

\* Supramolecular Science \* Inclusion Phenomena \* Molecular Recognition \*  
\* Chemistry \* Physics \* Biology \*

## Plenary lecturers

Yasuhiro Aoyama  
A Dwek  
Felix Franks  
H-J Güntherodt  
George W Gokel  
Olivier Kahn  
Tetsuo Osa  
G A Ozin  
Colin Raston  
David N Reinhoudt  
Akihiko Ueno

## Invited lecturers

Patrick Batail  
Jan Becher  
Paul D Beer  
Anthony Davis  
J-M Garcia Fernandez  
Michael Harmata  
Waiss Hosseini  
Angel Kaifer  
Jun-Ichi Kikuchi  
Klaus Müllen

Eric Monflier  
Luigi R Nassimbeni  
Shin-Ichiro Nishimura  
Dermot O'Hare  
Dr Rolf Saalfrank  
Paolo Scrimin  
Alain Vandorsselaer  
Jacques Vicens  
André Collet  
Janusz Jurczak

Symposium organiser Dr A W Coleman

For details including the second circular and registration form contact

Mr M Munoz (Committee Secretary), IBCP, CNRS UPR 412,  
7 passage du Vercors, Lyon cedex 07, F69367 FRANCE  
Fax +33 72 72 26 01 or +33 72 76 90 50. Email awc@ibcp.fr