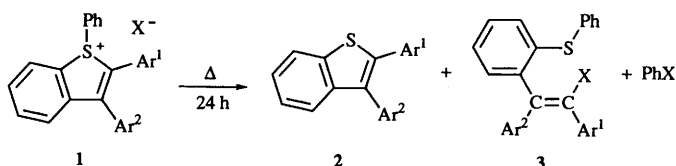


## Perkin Communications

- 473 **A drastic effect of halide anions on the nucleophilic substitution of 1-phenylbenzo[*b*]thiophenium salts**

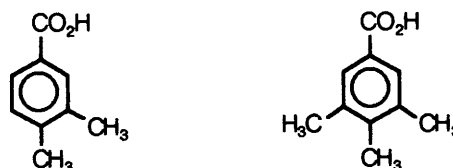
Tsugio Kitamura, Shin-ichi Soda, Kunihiro Morizane, Yuzo Fujiwara and Hiroshi Taniguchi



## Articles

- 475 **Non-classical buttressing effect: gas-phase ionization of some methyl-substituted benzoic acids**

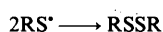
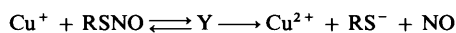
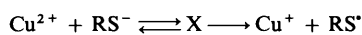
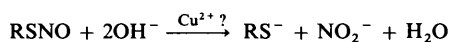
Michèle Decouzon, Otto Exner, Jean-François Gal and Pierre-Charles Maria



The effect of methyl groups on the enthalpy of formation or on the gas-phase acidity is stronger than anticipated from monomethyl derivatives

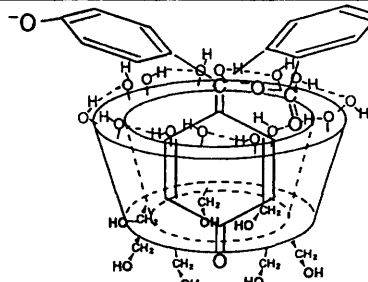
- 481 **Identification of Cu<sup>+</sup> as the effective reagent in nitric oxide formation from *S*-nitrosothiols (RSNO)**

Andrew P. Dicks, Helen R. Swift, D. Lyn H. Williams, Anthony R. Butler, Haitham H. Al-Sa'doni and Brian G. Cox



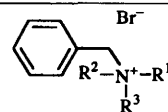
489 Hydroxypropyl- $\beta$ -cyclodextrins: induced circular dichroism spectra of included phenolphthalein as a function of the degree of substitution

Ágnes Buvári-Barcza, Judit Kajtár, Lajos Sente and Lajos Barcza



493 Intramolecular motions in a series of crystalline benzylammonium bromides and dibenzylamines studied by CP/MAS NMR

Frank G. Riddell and Martin Rogerson



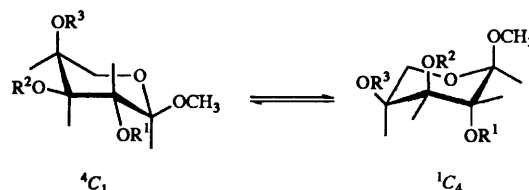
$R^1 = Pr^i, Bu^t, Am^f$

$R^2, R^3 = H, Me, CH_2Ph$

Molecular motions in a series of solid benzylamines and benzylammonium salts have been investigated by CP/MAS NMR methods. The results show a remarkable variety of conformational processes present in a simple series of solids

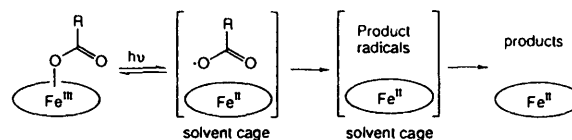
505 Conformational equilibria of methyl  $\alpha$ -L-arabinopyranosides in solution

Rosa Lanzetta, Michelangelo Parrilli, Carmine Garzillo, Andrea di Matteo and Giuseppe del Re



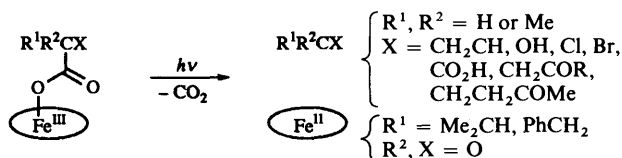
511 Reactions of carboxyl radicals generated by the photocleavage of complexes of iron(III) tetra(2-N-methylpyridyl)porphyrin with unsaturated and aromatic carboxylic acids in aqueous solution

Bruce C. Gilbert, John R. Lindsay Smith, Philip MacFaul and Philip Taylor



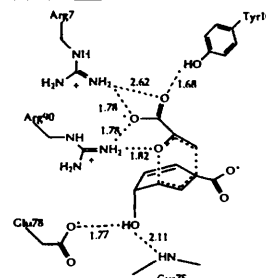
519 Photo-decarboxylation of substituted alkylcarboxylic acids brought about by visible light and iron(III) tetra(2-N-methylpyridyl)porphyrin in aqueous solution

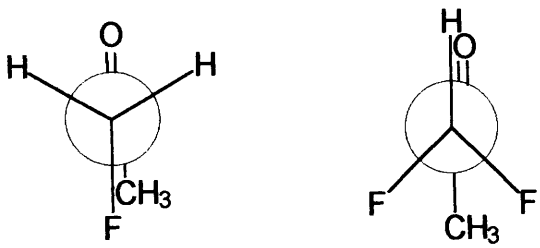
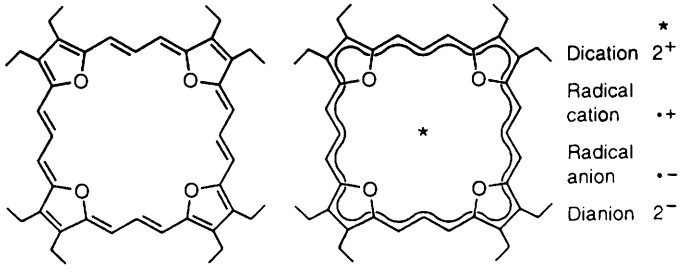
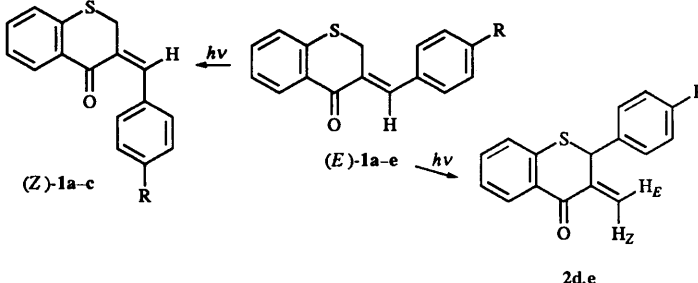
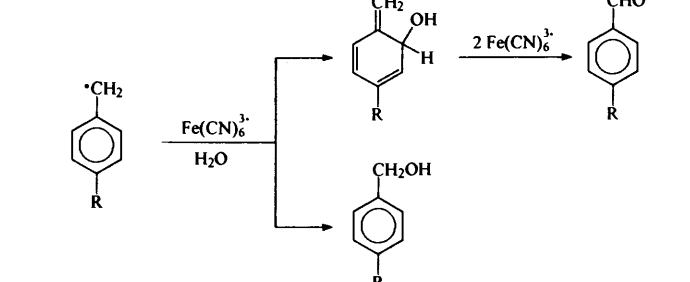
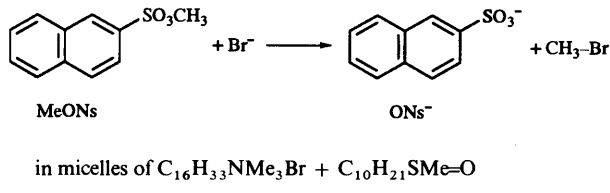
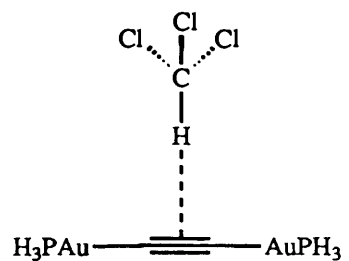
Bruce C. Gilbert, George R. Hodges, John R. Lindsay Smith, Philip MacFaul and Philip Taylor



525 The mechanism of the catalysis of the Claisen rearrangement of chorismate to prephenate by the chorismate mutase from *Bacillus subtilis*. A molecular mechanics and hybrid quantum mechanical/molecular mechanical study

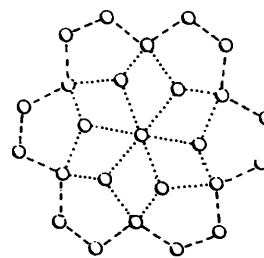
Mark M. Davidson, Ian R. Gould and Ian H. Hillier



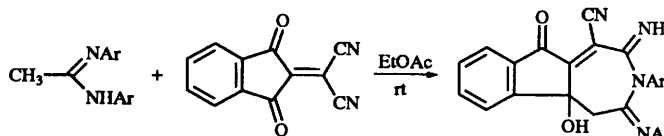
<p>533 <b>Conformational analysis. Part 27. NMR, solvation and theoretical investigation of conformational isomerism in fluoro- and 1,1-difluoro-acetone</b></p> <p>Raymond J. Abraham, Andrew D. Jones, Mark A. Warne, Roberto Rittner and Claudio F. Tormena</p>	
<p>541 <b>UV-VIS-Near-IR, MO and EPR studies of five redox stages of an octaethyltetraoxa-[26]porphyrin</b></p> <p>Rainer Bachmann, Fabian Gerson, Claudia Pütz and Emanuel Vogel</p>	
<p>547 <b>UV-induced isomerisation and ring transformation of (<i>E</i>)-3-arylidene-1-thiochromanones and -1-thioflavanones</b></p> <p>Gábor Tóth, Judit Halász, Albert Lévai, Csaba Nemes and Tamás Patonay</p>	
<p>551 <b>Oxidation of benzyl radicals by <math>\text{Fe}(\text{CN})_6^{3-}</math></b></p> <p>Getahun Merga, Heinz-Peter Schuchmann, B. S. Madhava Rao and Clemens von Sonntag</p>	
<p>557 <b>Nucleophilicity of bromide ion in mixed cationic/sulfoxide micelles</b></p> <p>Houshang J. Foroudian, Clifford A. Bunton, Paul M. Holland and Faruk Nome</p>	
<p>563 <b>Novel intermolecular C-H...<math>\pi</math> interactions: an <i>ab initio</i> and density functional theory study</b></p> <p>Man-Fai Fan, Zhenyang Lin, John E. McGrady and D. Michael P. Mingos</p>	

## 569 High-symmetry inclusion compounds with mixed guests

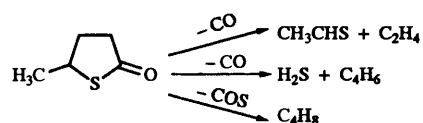
Mino R. Caira, Anita Coetzee, Klaus R. Koch, Luigi R. Nassimbeni and Fumio Toda

573 Reaction of  $N^1, N^2$ -diarylamidines with dicyanomethylene compounds

Dietrich Döpp, Mohsen A. Gomaa, Gerald Henkel and Ahmed M. Nour El-Din

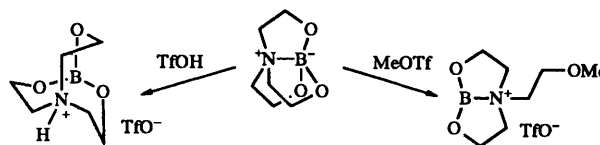
577 Thermal decomposition of methylated  $\gamma$ -thiobutyrolactones: a photoelectron spectroscopic study

Yek Tann Chua, Chup Yew Mok, Hsing Hua Huang, Igor Novak and Siu Choon Ng



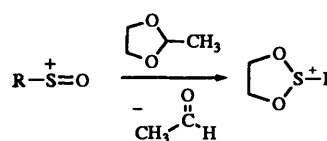
## 583 Methylation and protonation of 1-aza-5-bora-4,6,11-trioxabicyclo[3.3.3]undecane and 1-aza-5-borabicyclo[3.3.3]undecane

Roger W. Alder and Zhao Jin



## 587 The generation, stability, dissociation and ion/molecule chemistry of sulfinyl cations in the gas phase

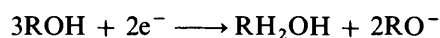
Fábio Cesar Gozzo, Ana Elisa P. M. Sorrilha and Marcos N. Eberlin

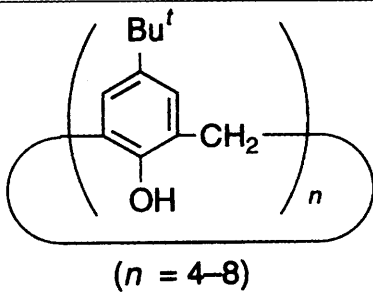
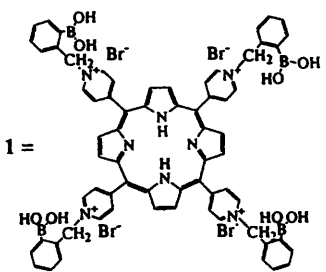
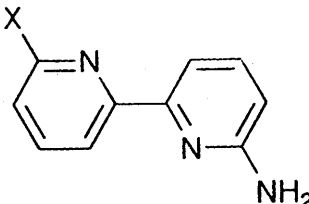
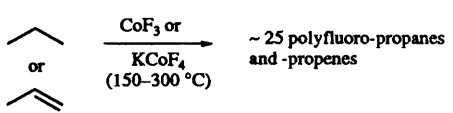
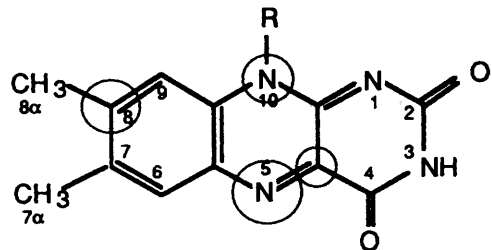


Sulfinyl cations are stable and easily accessible gas phase species, and undergo a structurally diagnostic ion/molecule reaction with 2-methyl-1,3-dioxolane

## 597 Self-protonation mechanism in the electroreduction of hydroxyimines

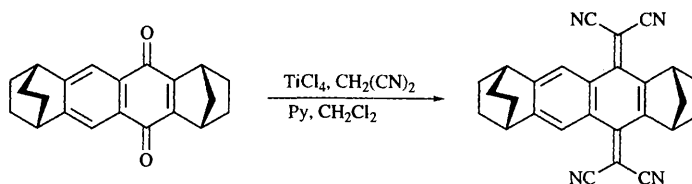
Abdirisak Ahmed Isse, Ahmed Maye Abdurahman and Elio Vianello


 $\text{ROH} = p\text{-HO-C}_6\text{H}_4\text{CH=NC}_6\text{H}_5$  or  $p\text{-HO-C}_6\text{H}_4\text{N=CHC}_6\text{H}_5$   
 $\text{RH}_2\text{OH} = p\text{-HO-C}_6\text{H}_4\text{CH}_2\text{NHC}_6\text{H}_5$  or  $p\text{-HO-C}_6\text{H}_4\text{NHCH}_2\text{C}_6\text{H}_5$

<p>601 <b>Do calix[<i>n</i>]arenes really exist as discrete monomers in solution? Comments based on mass spectrometry</b></p> <p>Fumiaki Inokuchi and Seiji Shinkai</p>	 <p style="text-align: center;"><math>(n = 4-8)</math></p>
<p>607 <b>Sugar-controlled association–dissociation equilibria between DNA and boronic acid-appended porphyrin</b></p> <p>Hikaru Suenaga, Susumu Arimori and Seiji Shinkai</p>	<p>DNA + 1 + Sugar</p> <p style="text-align: center;">⇌</p> <p>DNA + 1·Sugar</p> 
<p>613 <b>6-Amino-2,2'-bipyridine as a new fluorescent organic compound</b></p> <p>Koji Araki, Toshiki Mutai, Yasuhiro Shigemitsu, Masaki Yamada, Takayoshi Nakajima, Shigeyasu Kuroda and Ichiro Shimao</p>	 <p style="text-align: right;"><math>X = \begin{matrix} \text{NH}_2 \\ \text{H} \\ \text{Cl} \end{matrix}</math></p> <p>6-Aminobipyridines were found to exhibit a strong emission in the near-UV region</p>
<p>619 <b>Solvent effects on nitrogen NMR shieldings in thiazole and thiadiazole systems</b></p> <p>Michal Witanowski, Wanda Sicinska, Zenobia Biedrzycka, Zbigniew Grabowski and Graham A. Webb</p>	<p>Solvent polarity and hydrogen bonding interactions can lead to an increase or decrease in the nitrogen shielding of solute molecules</p>
<p>625 <b>Fluorination of propane and propene over cobalt(III) trifluoride and potassium tetrafluorocobaltate(III)</b></p> <p>James Burdon, Laurent Garnier and Richard L. Powell</p>	 <p>Mechanism: carbocations, radicals, allyl radicals and cations, rearrangements and eliminations are all involved</p>
<p>633 <b>Flavoproteins involved in photosynthetic electron transport in the cyanobacterium <i>Anabaena</i> sp PCC 7119. Electron spin-echo envelope modulation spectroscopic studies</b></p> <p>Milagros Medina and Richard Cammack</p>	

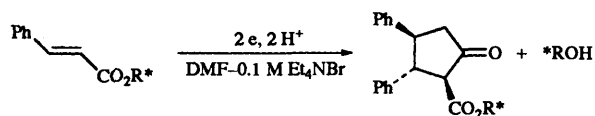
- 639 **Synthesis, electrochemistry and *ab initio* molecular orbital calculations on some norbornane- and bicyclo[2.2.2]octane-fused 5,12-bis(dicyanomethylidene)-naphthalene systems**

Daniel F. Rothenfluh, Anna M. Oliver and Michael N. Paddon-Row



- 649 **Stereoselectivity and mechanism in the electrohydrodimerisation of esters of cinnamic acid**

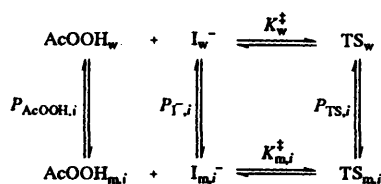
Ingrid Fussing, Mustafa Güllü, Ole Hammerich, Abid Hussain, Merete Folmer Nielsen and James H. P. Utley



R\* = Me, Et, Bu', (-)-menthyl, (-)-bornyl, (+)-*N*-Bu-ephedrine, (+)-*N*-tosylephedrine, phenyl, 4-MeO-C<sub>6</sub>H<sub>4</sub>, 4-CN-C<sub>6</sub>H<sub>4</sub>

- 659 **Catalysis and inhibition of the iodide reduction of peracids by surfactants: partitioning of reactants, product and transition state between aqueous and micellar pseudophases**

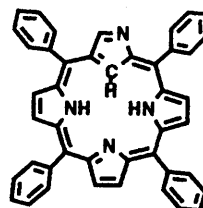
D. Martin Davies, Nicholas D. Gillitt and Paul M. Paradis



Subscripts w and m, i represent, respectively the bulk water and *i*th micellar pseudophases

- 667 **Specific binding of iodide ion to *N*-confused tetraphenylporphyrin (NC-TPP) at the air-water interface**

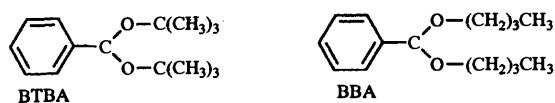
Katsuhiko Ariga, Toyoki Kunitake and Hiroyuki Furuta



NC-TPP

- 673 **Micellar-mediated general acid catalysed acetal hydrolysis. Reactions in comicelles**

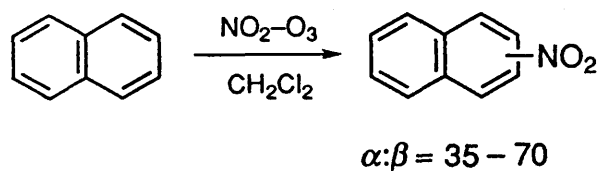
Sandro José Froehner, Faruk Nome, Dino Zanette and Clifford A. Bunton



The reaction of BTBA is general acid catalysed in comicelles of sodium dodecyl sulfate and sodium decyl hydrogen phosphate, while BBA exhibits only hydrogen ion catalysed hydrolysis

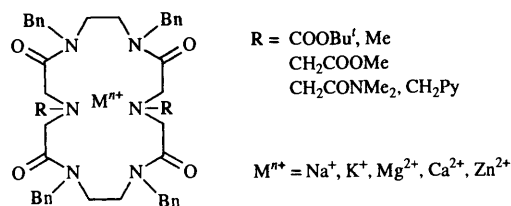
- 677 **Ozone-mediated nitration of naphthalene and some methyl derivatives with nitrogen dioxide. Remarkable enhancement of the 1-nitro/2-nitro isomer ratio and mechanistic implications**

Hitomi Suzuki and Tadashi Mori



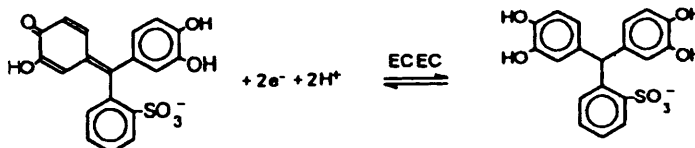
685 **Bibracchial diazatetralactams. Side-chain effects on cation binding and ionophoric properties**

Bernard Cathala, Claude Picard, Louis Cazaux, Pierre Tisnès and Claudius D'Silva



691 **Electrochemical studies on sulfonephthaleins. Part 2. Electrochemical reduction mechanism of catechol violet in aqueous solutions on a mercury electrode**

Refat Abdel-Hamid



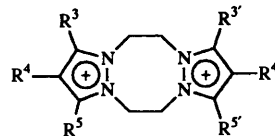
697 **Computation of ionization potential of conjugated radicals by hybrid density functional theory methods**

Branko S. Jursic

The suitability of hybrid DFT methods for computing IPs for conjugated radicals is presented

701 **Synthesis, structure (NMR and mass spectrometry) and conformational analysis of heterocyclic analogues of dibenzo[*a,e*]cycloocta-1,5-diene: 5,6,12,13-tetrahydrobispyrazolo[1,2-*a*:1',2'-*e*][1,2,5,6]tetraazocinediium dihalides**

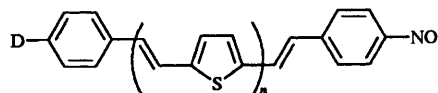
Pilar Cabildo, Rosa M. Claramunt, Pilar Cornago, José Luis Lavandera, Dionisia Sanz, Nadine Jagerovic, María Luisa Jimeno, José Elguero, Isabelle Gilles and Jean-Louis Aubagnac



The structural characterization of several 5,6,12,13-tetrahydrobispyrazolo[1,2-*a*:1',2'-*e*][1,2,5,6]tetraazocinediium dihalides is achieved by NMR and mass spectrometry: dynamic NMR spectroscopy allowed the barrier (about 13 kcal mol<sup>-1</sup>) for the chair-chair interconversion for two of the compounds to be measured

713 **Synthesis and characterization of end-functionalized oligo(vinylthiophenes) with liquid crystal properties**

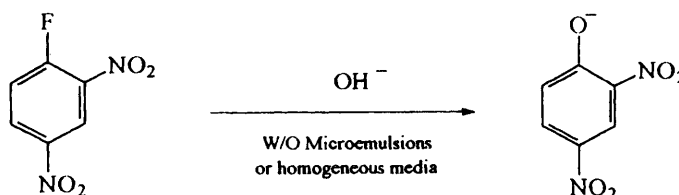
Christophe Maertens, Jian-Xin Zhang, Philippe Dubois and Robert Jérôme



D is an alkylamino or an alkoxy group; n = 1, 2

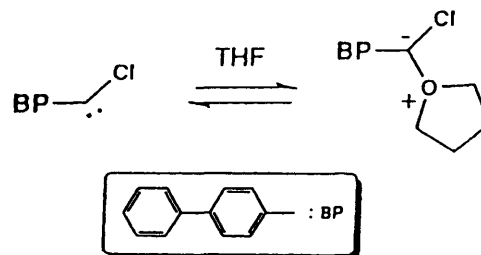
719 **Kinetics and mechanism of the reaction of 1-fluoro-2,4-dinitrobenzene with hydroxide ion in 'water in oil' microemulsions**

Edgardo N. Durantini and Claudio D. Borsarelli



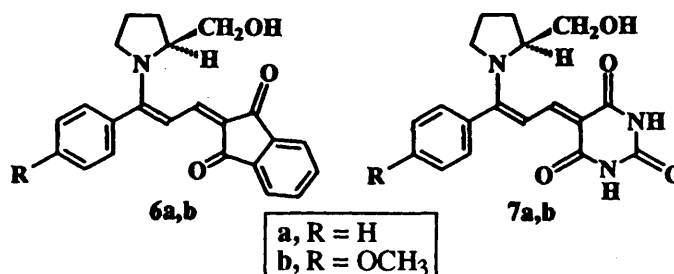
## 725 Formation of oxonium ylide evidenced by the laser flash photolysis of (biphenyl-4-yl)chlorodiazirine in ethers

Ikuo Naito, Akira Oku, Naoaki Otani, Yoshihisa Fujiwara and Yoshifumi Tanimoto



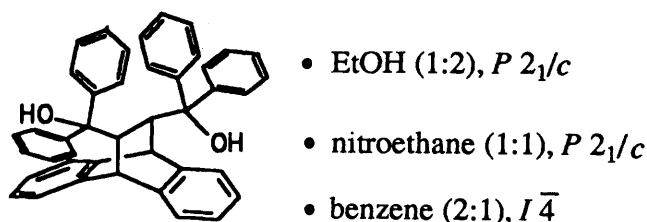
## 731 Synthesis and characterisation of some donor-acceptor substituted butadienes for second harmonic generation

Suresh Das, Mathew George, Thomas Mathew and C. V. Asokan



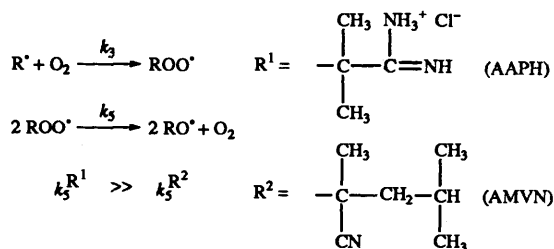
## 737 Roof-shaped hydroxy hosts: synthesis, complex formation and X-ray crystal structures of inclusion compounds with EtOH, nitroethane and benzene

Edwin Weber, Thomas Hens, Olga Gallardo and Ingeborg Csöreg



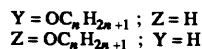
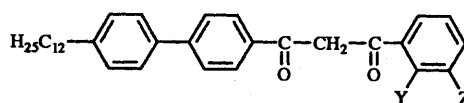
## 747 Comparison of 2,2'-azobis(2-amidinopropane) hydrochloride (AAPH) and 2,2'-azobis(2,4-dimethylvaleronitrile) (AMVN) as free radical initiators: a spin-trapping study

Arkadi G. Krainev and Diana J. Bigelow

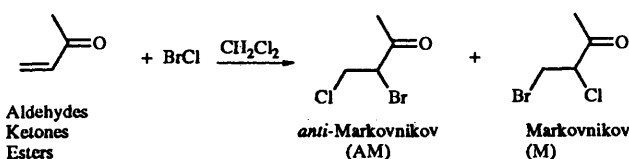


## 755 Mesomorphic properties of 1-(4'-dodecylbiphenyl-4-yl)-3-(2 or 3-alkoxyphenyl)propane-1,3-diones: the influence of alkoxy-substituent position

Bukkinakere K. Sadashiva and Veena Prasad

761 Effect of pyridine on the regio- and stereo-chemistry in the addition of bromine chloride to  $\alpha,\beta$ -unsaturated aldehydes and ketones

Victor L. Heasley, Daniel S. Elias, Paul E. Erdman, David Van Horn, Paul M. Whitelaw and Dale F. Shellhamer



Acid scavengers (pyridine) increase M regioisomers and erythro

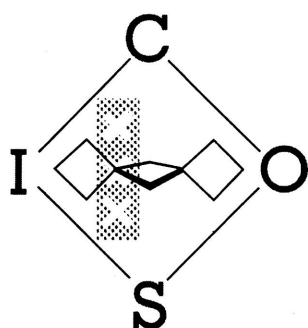


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NOTE: An asterisk in the heading of each paper indicates the author who is to receive any correspondence.



# 11th

## INTERNATIONAL CONFERENCE ON ORGANIC SYNTHESIS (ICOS-11)

organized by the Stichting Chemische Congressen V under the auspices of

the International Union of Pure and Applied Chemistry and  
the Royal Netherlands Chemical Society

Amsterdam, The Netherlands, June 30 - July 4, 1996

### The conference program will include:

- Plenary Lectures
- Section Lectures
- Oral Communications
- Poster Presentations

### The following topics will be highlighted:

- New Synthetic Methods
- Stereoselective Synthesis
- Metal-mediated Synthesis
- Target-oriented Synthesis

### Plenary Lectures

A.G.M. Barrett  
C.A.A. van Boeckel  
F.N. Diederich

M. Isobe  
A.S. Kende  
G. Mehta

K.C. Nicolaou  
W.C. Still  
C-H. Wong

### Lectures in the Mini Symposium on Synthesis Directed towards Complex Medicinal Agents

J.P. Kutney  
A. De Mesmaeker

M. Neya  
J. Nuss

I. Shinkai  
P. Sinaÿ

### Section Lectures

Atta-Ur-Rahman  
C.J. Easton  
M. Hirama  
A.M. Lobo  
J.P. Michael  
B-J. Uang

J. Becher  
A.G. Fallis  
A.B. Holmes  
X. Lu  
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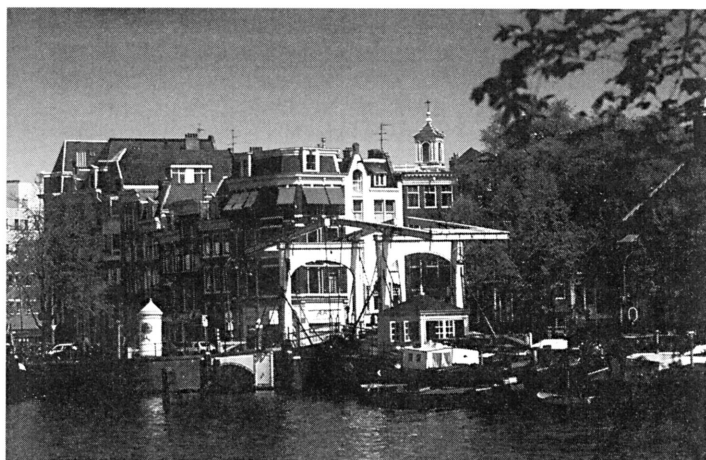
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### Thieme-IUPAC Prize 1996 in Synthetic Organic Chemistry

The Thieme-IUPAC Prize is awarded every two years to a scientist under 40 years of age, whose research has had a major impact on the field of synthetic organic chemistry. The third Thieme-IUPAC Prize will be presented at an Award Talk on 2 July 1996 during the ICOS-11 in Amsterdam.



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Organic Synthesis