

## JOURNAL OF THE CHEMICAL SOCIETY

**Perkin Transactions 2**

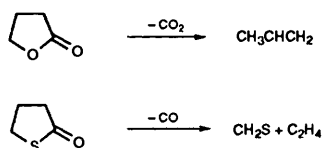
## Physical Organic Chemistry

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## Perkin Communications

**1249 Gas phase pyrolysis of  $\gamma$ -butyrolactone and  $\gamma$ -thiobutyrolactone**

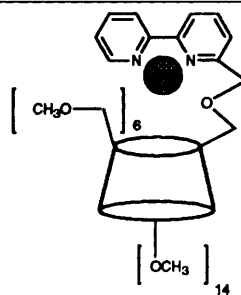
Anjana Rai-Chaudhuri, Wee Shong Chin,  
Devinder Kaur, Chup Yew Mok and Hsing  
Hua Huang



## Articles

**1251 Synthesis and a high field NMR study of a 2,2'-bipyridyl substituted  $\beta$ -cyclodextrin and its luminescent  $\text{Re}^I$  metal complex**

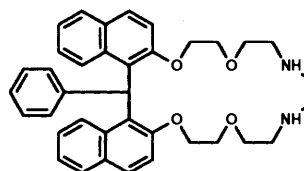
Robert Deschenaux, Margaret M. Harding  
and Thomas Ruch



The synthesis, characterization, and  
solution conformation of the title  
compounds are reported

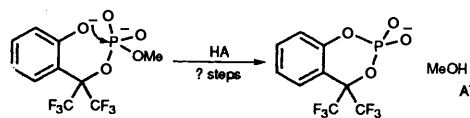
**1259 Two series of aza macrocycles containing the phenyldinaphthomethane subunit (a three bladed propeller); crystal structures and dynamic NMR spectroscopy**

William Clegg, Paul J. Cooper, Kenneth I.  
Kinnear, David J. Rushton and Joyce C.  
Lockhart



1269 **Models for nuclease catalysis: mechanisms for general acid catalysis of the rapid intramolecular displacement of methoxide from a phosphate diester**

Kevin N. Dalby, Anthony J. Kirby and (in part) Florian Hollfelder



This phosphate diester has a half-life of 2 min at 50 °C

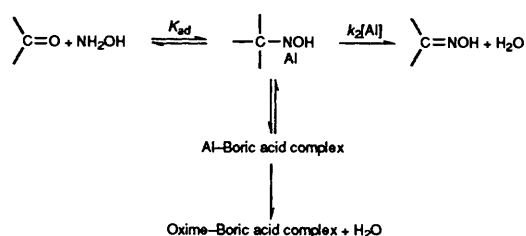
1283 **Solvation and steric effects on electrophilic reactivity of ethylenic compounds. Part 4. Bromination of oct-1-ene in anionic microemulsions**

Marie-Françoise Ruasse, Iva B. Blagoeva, Sophie Krysz and Maria-Angela Sebastian-Gambaro

The microenvironment for the bromination of the lipophilic oct-1-ene is aqueous in anionic water-rich microemulsions but not in pure water, since bromohydrins are the main product ( $\geq 75\%$ ) in the former and dibromo adducts ( $\geq 90\%$ ) in the latter

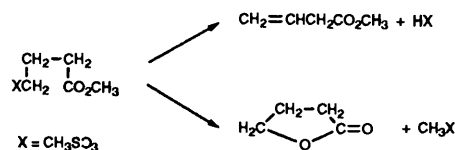
1291 **The effect of boric acid on the dehydration step in the formation of oxime from salicylaldehyde**

Edesio L. Simionatto, Pablo R. Yunes and Rosendo A. Yunes



1295 **Anchimeric assistance of the  $\text{CO}_2\text{CH}_3$  substituent in the elimination kinetics of 3-(methoxycarbonyl)propyl methanesulfonate in the gas phase**

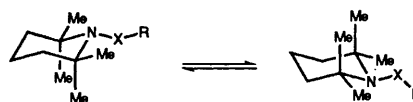
Gabriel Chuchani and Rosa M. Domínguez



The homogeneous unimolecular reaction of 3-(methoxycarbonyl)-propyl methanesulfonate in the gas phase leads mostly to the formation of  $\gamma$ -butyrolactone and small amounts of methylbut-3-enoates

1299 **The measurement of the one-fold rotational barrier of eclipsed bonds. A dynamic NMR determination of N-O or N- $\text{CH}_2$  bond rotation in N-alkoxy- or N-alkyl-2,2,6,6-tetramethylpiperidines**

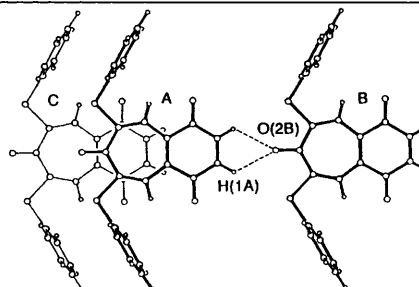
J. Edgar Anderson, Daniele Casarini, John E. T. Corrie and Lodovico Lunazzi



The rate of interconversion ( $R \neq H$ ) is determined by the rate of rotation about the eclipsed N-X bond, and leads to a measure of the one-fold rotational barrier

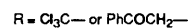
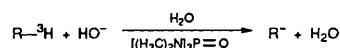
1305 **Syntheses, physical properties and X-ray structures of benzocycloheptene-1,4,7-trione and its 6-phenylthio- and 6,8-bis(phenylthio)-derivatives. Novel A, A-D and D-A-D molecular units aiming at organic conductors**

Hitoshi Tada, Yasuyo Takeuchi, Yoshimasa Amatatsu, Kimiaki Furuichi, Masahiko Kato, Shuji Matsumoto and Masao Hashimoto



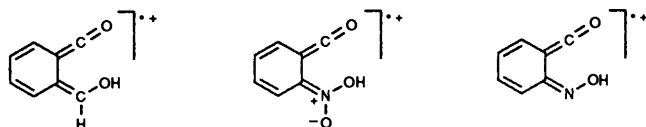
- 1317 **Kinetic acidity of carbon acids: the hydroxide ion-catalysed ionization of chloroform and acetophenone in aqueous hexamethylphosphoric triamide**

Markku Lahti, Alpo Kankaanperä and Pasi Virtanen



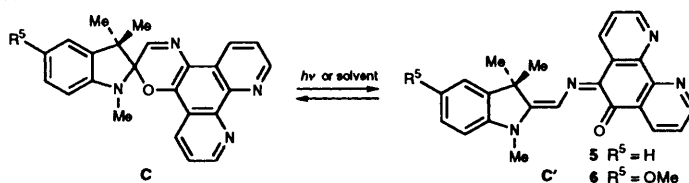
- 1321 **Radiation induced transformations of benzaldehydes carrying formyl-, nitro- or nitroso-substituents in the *ortho* position**

Jacek Michalak, Jerzy Gębicki and Thomas Bally



- 1327 **Solvatochromic and photochromic characteristics of new 1,3-dihydrospiro[2*H*-indole-2,2'-[2*H*]-bipyrido[3,2-*f*][2,3-*h*][1,4]benzoxazines]**

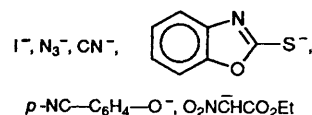
Jean-Luc Pozzo, André Samat, Robert Guglielmetti and Denis De Keukeleire



The equilibrium between closed colourless form C and open coloured form C' of spiro[indole-oxazines] 5 and 6 has been studied *versus* solvent with or without flash photolysis

- 1333 **Oxidation potential as a measure of the effect of environment on the reactivity of anionic nucleophiles**

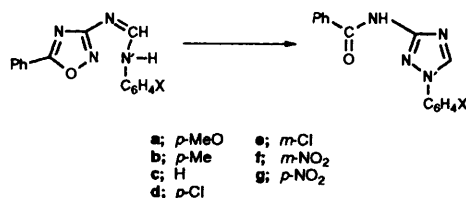
Murat E. Niyazymbetov and Dennis H. Evans



The irreversible anodic peak potential of anionic nucleophiles has been shown to be linearly correlated with various measures of their nucleophilic reactivity, including rates of  $S_N2$  and  $S_NAr$  reactions as well as addition to Michael acceptors

- 1339 **Mononuclear heterocyclic rearrangements. Effect of the structure of the side chain on the reactivity. Part 2. Rearrangement of some *N*-(5-phenyl-1,2,4-oxadiazol-3-yl)-*N'*-arylformamidines into 1-aryl-3-benzoylamino-1,2,4-triazoles in dioxane-water at various  $pS^+$**

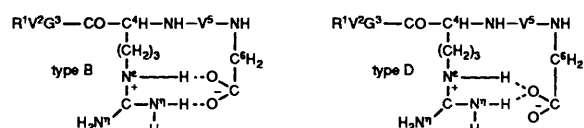
Vincenzo Frenna, Nicolò Vivona, Giovanni Consiglio, Domenico Spinelli and Elisabetta Mezzina



A kinetic study of the title reaction has shown the occurrence of an uncatalysed ( $pS^+$ -independent) and of a catalysed ( $pS^+$ -dependent and then  $pS^+$ -independent) range

- 1345  **$^1\text{H}$  NMR Studies on the preferred interactions of guanidinium and C-terminal carboxylate groups in arginine-containing peptides**

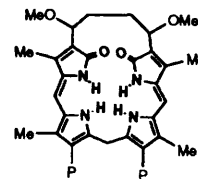
Vassilios Tsikaris, Mahn Thong Cung, Eugenia Panou-Pomonis, Constantinos Sakarellos and Maria Sakarellos-Daitsiotis



The  $R^4$ -side chain preferentially interacts with the  $G^6$ -carboxylate group, in contrast to the  $R^1$ -side chain

1351 **Helically fixed chiral bilirubins and biliverdins: a new insight into the conformational, associative and dynamic features of linear tetrapyrrols**

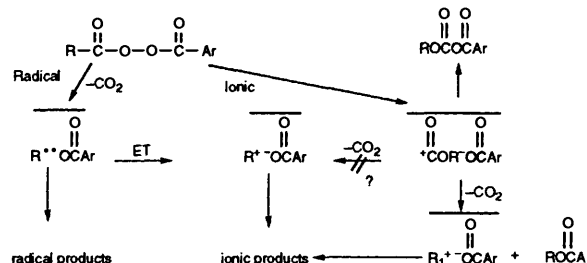
Daniel Krois and Harald Lehner



Due to the differences in the hydrogen-bond pattern between bilirubins and biliverdins helical and non-helical conformers of non-bridged members occur under quite different conditions

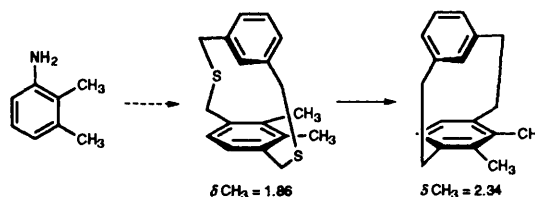
1361 **Evidence for electron transfer, radical and ionic pathways in the decomposition of diacyl peroxide**

Sueg-Geun Lee



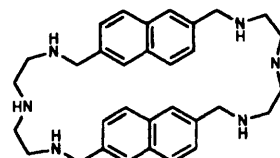
1373 **Synthesis and rigid conformers of 14,15-dimethyl-2,11-dithia[3.3](1,3)(1,4)cyclophane and 12,13-dimethyl[2.2](1,3)(1,4)cyclophane**

Yee-Hing Lai and Angeline Hui-Tin Yap



1379 **Molecular recognition of nucleosides, nucleotides and anionic planar substrates by a water-soluble bis-intercaland-type receptor molecule**

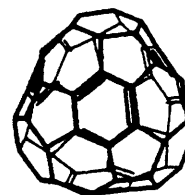
Michel Dhaenens, Jean-Marie Lehn and Jean-Pierre Vigneron



Selective binding of planar molecular anionic substrates

1383 **A prediction of the structure of C<sub>60</sub>H<sub>36</sub>**

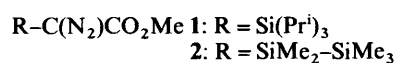
Sarah J. Austin, Robin C. Batten, Patrick W. Fowler, David B. Redmond and Roger Taylor



A chiral structure with *T* symmetry is a promising candidate for C<sub>60</sub>H<sub>36</sub>

1387 **Silyl-substituted diazoacetic esters in superacid media—a stable ion and solvolysis study**

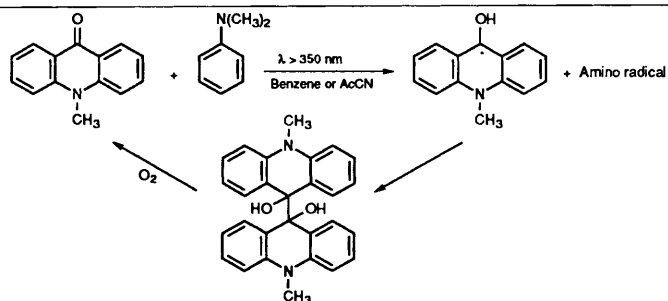
Kenneth K. Laali, Gerhard Maas and Monika Gimmy



Protonation and subsequent chemistry of 1 and 2 in superacid media [FSO<sub>3</sub>H·SbF<sub>5</sub>(1:1), FSO<sub>3</sub>H, CF<sub>3</sub>SO<sub>3</sub>H, HF] have been studied

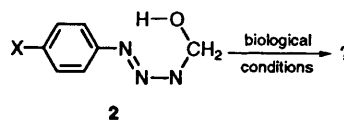
- 1395 **Mechanism of photodimerization reaction of 10-methylacridone in polar and non-polar solvents**

Hiroki Kawata, Kazuaki Shimada, Tsutomu Kumagai and Shigeya Niizuma



- 1399 **The geometry of *N*-hydroxymethyl compounds. Part 4. Studies on ground-state geometry and decomposition of *N*-(hydroxymethyl)triazenes using MNDO calculations and kinetic studies**

Richard J. Simmonds, Wickramaratna Mallawaarachchi, Padma A. Mallawaarachchi and David E. Parry



*N*-(Hydroxymethyl)triazenes are too unstable in water at pH 7.4 ( $t_{1/2}$  43 s for **2d** (X = NO<sub>2</sub>)) to have antitumour activity of their own. MNDO calculations found O-protonation and loss of water giving an iminium ion to be the favoured acid-catalysed decomposition route

## Corrigendum

- 1405 **The mechanism of propene elimination from the immonium ions  $\text{CH}_2=\text{N}^+(\text{CH}_3)\text{CH}(\text{CH}_3)_2$  and  $\text{CH}_2=\text{N}^+(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$**   
R. D. Bowen, A. W. Colburn and P. J. Derrick

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