

## JOURNAL OF THE CHEMICAL SOCIETY

## Perkin Transactions 2

## Physical Organic Chemistry

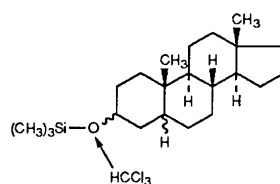
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- ix Instructions for authors (1994)  
 xxviii Refereeing procedure and policy

## Perkin Communications

- 1 **Steric effects on NMR chemical shifts controlled by the solvent's accessible surface**

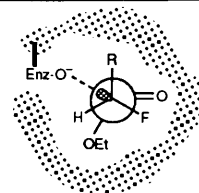
Jan Schraml, Marie Jakoubková, Magdalena Kvičalová and Alexander Kasal



Hydrogen bond effects on steric shifts in  $^{29}\text{Si}$  NMR are discussed

- 3 **Stereoelectronic influence of fluorine in enzyme resolutions of  $\alpha$ -fluoroesters**

David O'Hagan and Henry S. Rzepa

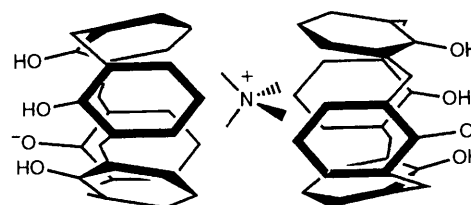


The efficient resolution of  $\alpha$ -fluoroesters by lipase enzymes is shown to arise from an Ahn-Eisenstein type  $n-\sigma^*$  stabilisation in the transition state

## Articles

- 5 **Alkylammonium cation interactions with calixarene anions. Part 2. Structural characterisation of a salt of 2:3 cation:calixarene stoichiometry**

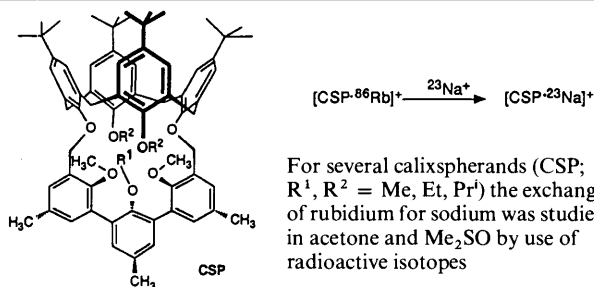
Jack M. Harrowfield, William R. Richmond, Alexander N. Sobolev and Allan H. White



An ion triplet in the tetramethylammonium salt of calix[4]arene

- 11 **A general method for the determination of the kinetic stability of macrocyclic alkali-metal complexes with rates of decomplexation below  $10^{-3} \text{ s}^{-1}$**

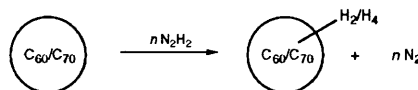
Wouter I. Iwema Bakker, Marijke Haas, Herman J. den Hertog, Jr., Willem Verboom, Dick de Zeeuw and David N. Reinhoudt



For several calixspherands (CSP;  $\text{R}^1, \text{R}^2 = \text{Me, Et, Pr}^i$ ) the exchange of rubidium for sodium was studied in acetone and  $\text{Me}_2\text{SO}$  by use of radioactive isotopes

- 15 **Formation of hydrides of fullerene- $\text{C}_{60}$  and fullerene- $\text{C}_{70}$**

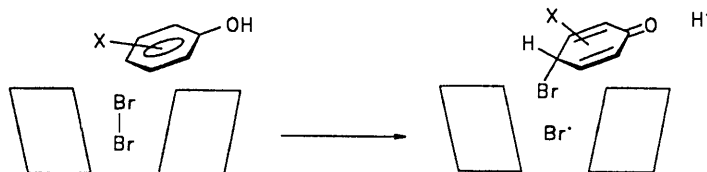
Anthony G. Avent, Adam D. Darwish, Dirk K. Heimbach, Harold W. Kroto, Mohamed F. Meidine, Jonathan P. Parsons, Christelle Remars, Rolf Roers, Osamu Ohashi, Roger Taylor and David R. M. Walton



Reaction of diimide with either  $\text{C}_{60}$  or  $\text{C}_{70}$  produces all of the di- and tetra-hydro derivatives that can arise from addition across interpentagonal bonds

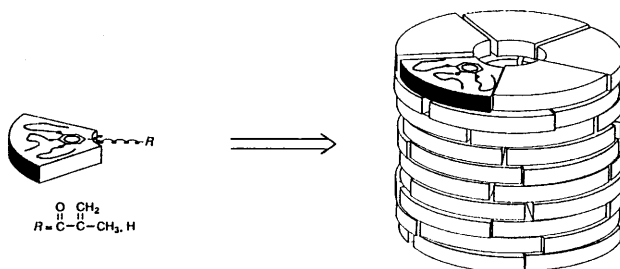
- 23 **Catalysis of electrophilic bromine attack by  $\alpha$ -cyclodextrin**

Oswald S. Tee and Bushra C. Javed



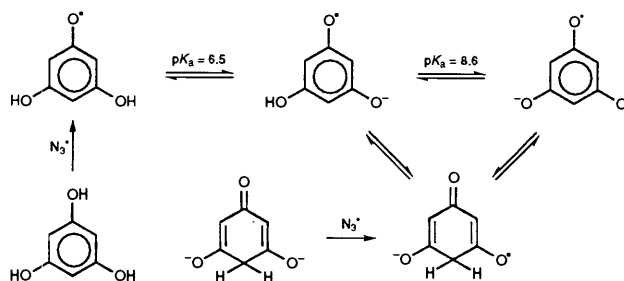
- 31 **Self-assembly of taper-shaped monoesters of oligo(ethylene oxide) with 3,4,5-tris(*n*-dodecan-1-yloxy)benzoic acid and of their polymethacrylates into tubular supramolecular architectures displaying a columnar hexagonal mesophase**

Virgil Percec, Dimitris Tomazos, James Heck, Helen Blackwell and Goran Ungar



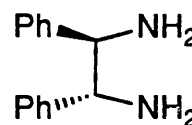
- 45 **Free radical induced oxidation of phloroglucinol. A pulse radiolysis and EPR study**

Degui Wang, Istvan György, Knut Hildenbrand and Clemens von Sonntag



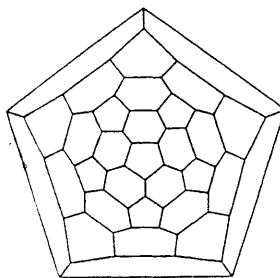
- 57 **1,2-Diphenylethane-1,2-diamine: an effective NMR chiral solvating agent for chiral carboxylic acids**

Russell Fulwood and David Parker



65 **Aromatic character of typical C<sub>60</sub> derivatives**

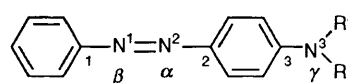
Jun-ichi Aihara and Shigetoshi Takata



The topological resonance energy (TRE) method revealed that typical derivatives of C<sub>60</sub> are moderately aromatic like the parent molecule C<sub>60</sub>. In general, addition and insertion reactions with C<sub>60</sub> proceed in such a manner that the reaction products become as aromatic as possible

71 **A theoretical study of protonation and tautomerization of N-substituted aminoazobenzenes**

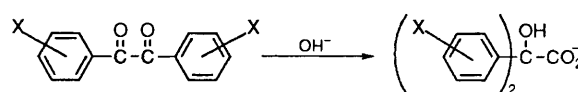
Adam Liwo, Anna Tempczyk, Teresa Widernik, Teresa Klentak and Jurand Czermański



The proton affinities of the amino and azo nitrogens of aminoazobenzene (AAB) and its *N*-methyl (MAAB), *N,N*-dimethyl (DMAAB), and *N*-phenyl (PhAAB) derivatives in the gas phase and in water were calculated using the AM1 and *ab initio* STO-3G method

77 **Reactions of carbonyl compounds in basic solutions. Part 20. Mechanism of the base-catalysed rearrangement of symmetrically substituted benzils**

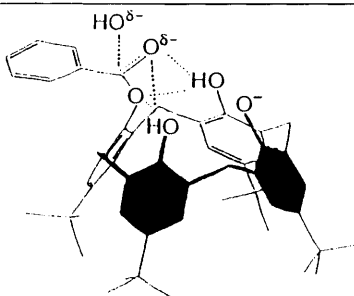
Keith Bowden and Karl D. Williams



Hammett  $\rho$  is 5.70; with  $\rho$  for migration and non-migration being 3.85 and 1.85, respectively

83 **Enhanced alkaline hydrolysis of monoesterified 4-*tert*-butylcalix[4]arenes involving intramolecular electrophilic catalysis by the phenolic hydroxy group**

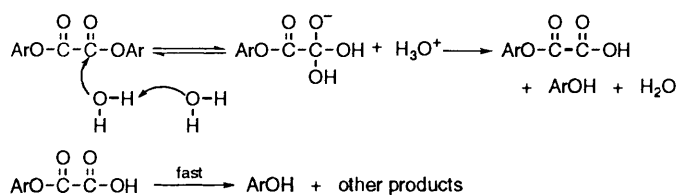
Kevin B. Ray, Richard H. Weatherhead, Necmettin Pirincioglu and Andrew Williams



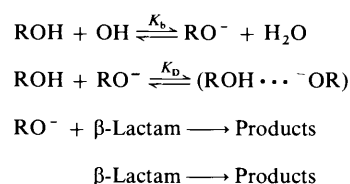
Intramolecular hydrogen bonding increases the alkaline hydrolysis rates for monoanionic calixarene esters over 1600-fold; the kinetically equivalent mechanism involving attack of water on the dianion is unambiguously excluded

89 **Kinetics of the decomposition of a chemiluminescent reagent bis(2,4-dinitrophenyl) oxalate in aqueous acetonitrile**

Helmi Neuvonen

97 **The carbohydrate-catalysed hydrolysis of cephalosporins**

John Burgess, Maria de Jesus Perry, Eduarda Rosa and Jim Iley



- 103 **Amidines. Part 32. Influence of substitution at the amino nitrogen atom on the sensitivity to substitution at the imino nitrogen atom.  $pK_a$  Values of  $N^1$ -methyl- $N^1$ -phenylformamidines in water-ethanol solutions**

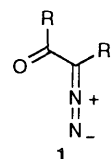
Janusz Oszczapowicz and Mariola Kumińska



The influence of substitution at any site on the  $pK_a$  values of amidines depends on the substituents at the other two sites

- 109 **MM2 Force field parameters for compounds containing the diazoketone function**

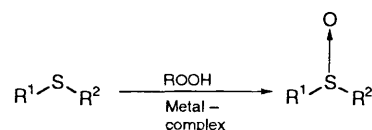
Jonathan M. Goodman, Jeffrey J. James and Andrew Whiting



MM2 force field parameters for structures of type 1 are reported

- 117 **Mechanistic study of the oxidation of sulfides to sulfoxides and asymmetric sulfoxides catalysed by transition metal peroxide complexes**

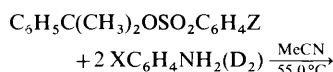
Karl Anker Jørgensen



A mechanistic study of the oxidation and asymmetric oxidation of sulfides to sulfoxides by transition metal complexes is presented

- 125 **Nucleophilic substitution reaction of cumyl arenesulfonates with anilines**

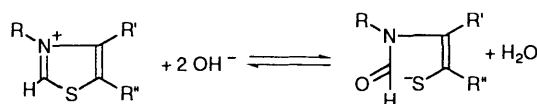
Han Joong Koh, Hai Whang Lee and Ikchoon Lee



The  $S_N2$  mechanism with frontside nucleophilic attack in MeCN

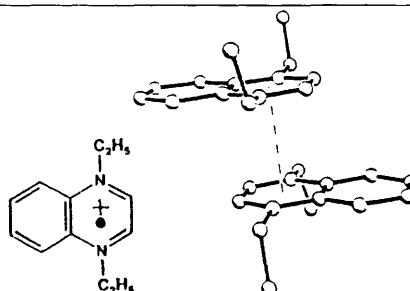
- 131 **Kinetic study on the hydrolysis of thiazolium cations**

Susanne Barrabass, Irmgard Heiber-Langer and Wilhelm Knoche



- 135 **Electronic absorption spectroscopy of some exceptionally stable 1,4-dialkyl-1,4-dihydro-1,4-diazinium radical cations: assignment of transitions, vibrational structure and effects of  $\pi$ - $\pi$  dimerization**

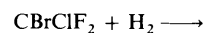
Frank Hilgers, Wolfgang Kaim, Andreas Schulz and Stanislav Zális



The different  $\pi$  molecular orbital situation of structurally characterized radical cations is studied with the help of UV-VIS absorption spectra in solution and INDO/CI calculations

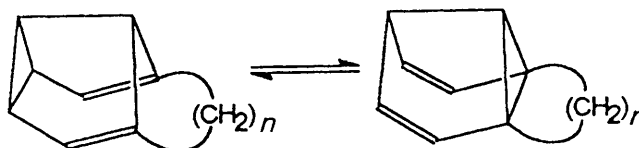
## 139 Thermal gas phase hydrodehalogenation of bromochlorodifluoromethane

Huub J. P. de Lijser, Robert Louw and Peter Mulder

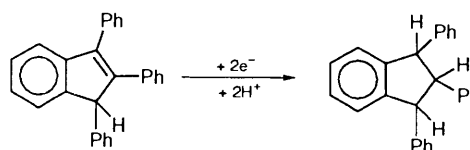
Products, kinetics and mechanisms of the high temperature (400–900 °C) decomposition of CBrClF<sub>2</sub> (Halon-1211)

## 147 A theoretical investigation of through-space interactions. Part 3. A semiempirical study of the Cope rearrangement in singly annellated semibullvalenes

Richard V. Williams and Henry A. Kurtz

151 Reactivity of unsaturated substrates under reductive electron transfer conditions. Part 1. Reduction of 1,2,3-triphenyl-1*H*-indene with sodium metal in various solvents

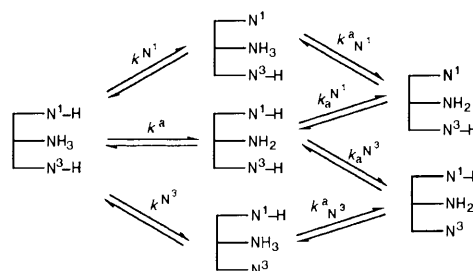
Stefano Gotta, Mauro Marchetti, Mario Branca and Giovanni Melloni



Results of the reduction with Na under different conditions are compared with the results of the cathodic reduction in DMF

## 157 Multinuclear NMR and potentiometric study on tautomerism during protonation and zinc(II) complex formation of some imidazole-containing peptide derivatives

Tamas Gajda, Bernard Henry and Jean-Jacques Delpuech



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

## Forthcoming Articles in *Perkin Transactions 2*

Charge-transfer activation of aromatic EDA complexes with *N*-nitrosopyridinium. Direct comparison with the *N*-nitropyridinium acceptor **K.Y. Lee and J.K. Kochi**

A mechanistic study of quinoxaline formation **A.R. Butler and L.M. Anderson**

Inverted spin trapping. Part 3. Further studies on the chemical and photochemical oxidation of spin traps in the presence of nucleophiles **L. Ebersson**

The influence of arene substituent on the mode and regiochemistry of the photocycloaddition of furan to the benzene ring **H. Garcia, A. Gilbert and O. Griffiths**

Mechanism of dediazonation of arenediazonium salts with triphenylphosphine and trialkyl phosphites. Generation of cation radicals from trivalent phosphorus compounds and their reactions **S. Yasui, M. Fujii, C. Kawano, Y. Nishimura, K. Shioji and A. Ohno**

Bimolecular nucleophilic substitution ( $S_N2$ ) reactions of neopentyl arenesulfonates with anilines and benzylamines in methanol **H.J. Koh, H.W. Lee and I. Lee**

A crystallographic and PM3-COSMO SCF-MO study of the structure and properties of aryl thiazinone derivatives **M. Hilton, P. Fisk, B. Odell, H.S. Rzepa, D.J. Williams and M.Y. Yi**

Alkali-metal ion catalysis and inhibition of acetyl transfer from *p*-nitroaryl acetates to hexanoate ion **R. Cacciapaglia, L. Mandolini and A. Tomei**

The thermal decomposition of 2,3-dihydro-1,4-benzodioxin and 1,2-dimethoxybenzene **G.J. Schraa, I.W.C.E. Arends and P. Mulder**

Formation of *N*-carbamoylaspartic acid and its cyclisation to orotic acid **M.J. Bruce, A.R. Butler and K.V. Russell**

The prediction of hydrogen bond basicity from computed molecular electrostatic properties: implications for comparative molecular field analysis **P.W. Kenny**

Protonation sequence of linear aliphatic polyamines by  $^{13}\text{C}$  nuclear magnetic resonance spectroscopy **D.N. Hague and A.D. Moreton**

Molecular and crystal structure of 1,3-bisdiphenylene-2-(*p*-chlorophenyl)allyl radical: an organic antiferromagnet with  $T_N = 3.25\text{ K}$  **N. Azuma, T. Ozawa and J. Yamauchi**

Selective recognition of carboxylate anions by polyammonium receptors in aqueous solution. Criteria for selectivity in molecular recognition **A. Bencini, A. Bianchi, M.I. Burguete, P. Dapporto, A. Doménech, E. García-España, S.V. Luis, P. Paoli and J.A. Ramírez**

The mechanism of acid catalysis in the cyclisation of 5-aminolevulinic acid and acetylacetone to 3-acetyl-4-(2-carboxyethyl)-2-methylpyrrole **A.R. Butler and S.D. George**

Iminophosphorane-substituted proton sponges. Part 5. Structures in the solid state. Correlation between solid state  $^{31}\text{P}$  MAS NMR spectra and crystal structures **A.L. Llamas-Saiz, C. Foces-Foces, J. Elguero, F. Aguilar-Parrilla, H.-H. Limbach, P. Molina, M. Alajarín, A. Vidal, R. Ma. Claramunt and C. López**

A quantum chemical AM1 study of a Diels-Alder and retro-Diels-Alder tandem reaction **M. Ventura, C. Segura and M. Sola**

A  $^{31}\text{P}$  NMR investigation of the comparative hydrolytic breakdown of nickel(II) - and cadmium(II) versus zinc(II) - bis (*O,O*-diethyl dithiophosphates) in an aqueous medium **A.J. Burn, S.K. Dewan, I. Gosney, K.G. McKendrick, C.P. Warrens, J.P. Wastle and C.W. Watson**

Relationships between nitro group reduction potentials and torsion angles in di-*ortho*-substituted nitrobenzenes; a crystallographic and oxygen-17 NMR study **M. Boyd, H.H. Lee, R.F. Anderson and W.A. Denny**

Tautomerism in some acetamido aza-containing heterocycles: X-ray structural analysis of 2-amino and 2-imino forms of benzothiazole derivatives **M. Annese, A.B. Corradi, L. Forlani, C. Rizzoli and P. Sgarabotto**

Kinetics and mechanism of the oxidation of diols by ethyl *N*-chlorocarbamate **A. Grover, S. Varshney and K.K. Banerji**

