

JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions 2

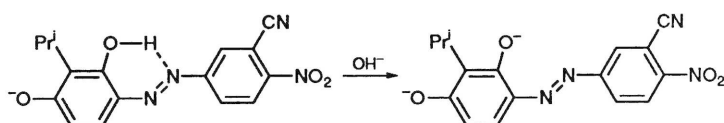
Physical Organic Chemistry

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Perkin Communications

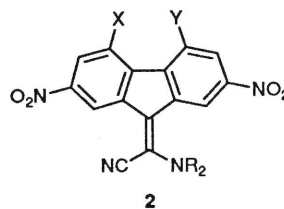
- 1 **Substituent effects leading to ultra-slow proton removal from an intramolecular hydrogen bond**



In 90% (v/v) Me₂SO-H₂O the half-life for deprotonation is in the minutes range

Alex Coker and Frank Hibbert

- 3 **Fluorene derivatives with intramolecular charge-transfer: exceptionally easy rotation around the double C(9)=C(α) bond in nitro-substituted 9-aminomethylenefluorenes**

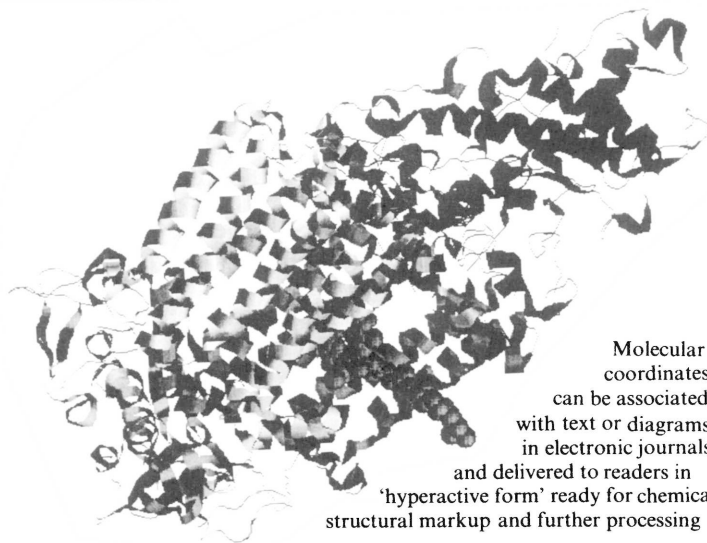


New push-pull fluorenes, *e.g.* **2** have been studied: solution NMR and UV spectra and an X-ray crystal structure are reported

Igor F. Perepichka, Anatolii F. Popov, Tatyana V. Artyomova, Alexander N. Vdovichenko, Martin R. Bryce, Andrei S. Batsanov, Judith A. K. Howard and (in part) Joanne L. Megson

Articles

- 7 **Hyperactive molecules and the World-Wide-Web information system**

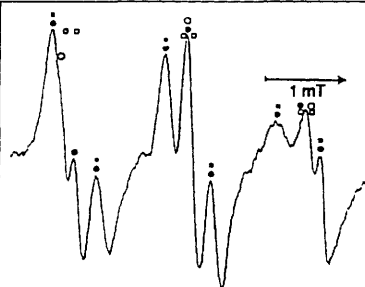


Molecular coordinates can be associated with text or diagrams in electronic journals and delivered to readers in 'hyperactive form' ready for chemical structural markup and further processing

Omer Casher, Gudge K. Chandramohan, Martin J. Hargreaves, Christopher Leach, Peter Murray-Rust, Henry S. Rzepa, Roger Sayle and Benjamin J. Whitaker

13 **EPR spin-trapping studies of radical damage to DNA**

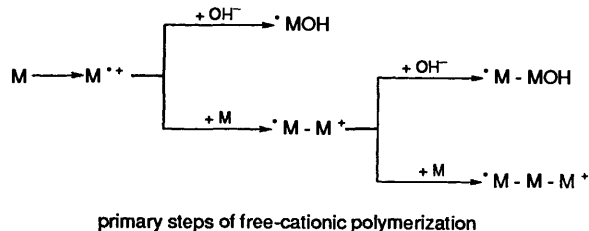
Michael J. Davies, Bruce C. Gilbert, Clare Hazlewood and Natalie P. Polack



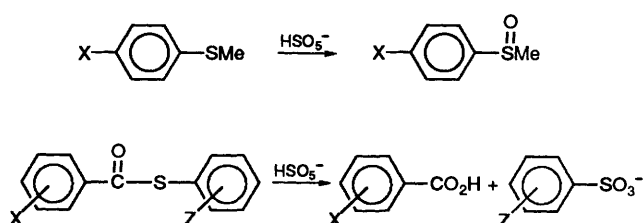
EPR spectrum of spin-trapped radical adducts of thymidine and deoxycytidine obtained from radical attack upon DNA

23 **Photo- and radiation-induced chemical generation and reactions of styrene radical cations in polar and non-polar solvents**

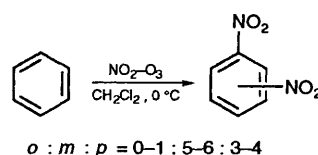
Ortwin Brede, Frank David and Steen Steenken

33 **Sulfide oxidation and oxidative hydrolysis of thioesters by peroxydisulfate ion**

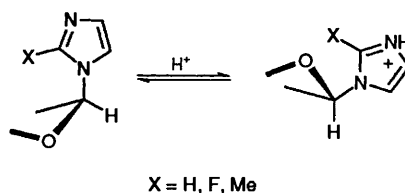
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41 **Unusual isomer distribution of dinitrobenzenes and nitrophenols formed as side products during the ozone-mediated nitration of benzene with nitrogen dioxide. Further evidence for the alternative mechanism of electrophilic nitration of arenes**

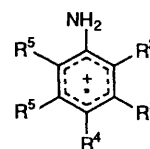
Hitomi Suzuki and Tadashi Mori

45 **The reverse anomeric effect in *N*-pyrano-sylimidazolides: a molecular orbital study**

Stewart S. C. Chan, Walter A. Szarek and Gregory R. J. Thatcher

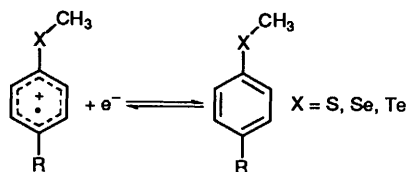
61 **N-H Bond dissociation energies, reduction potentials and pK_a s of multisubstituted anilines and aniline radical cations**

Mats Jonsson, Johan Lind, Gábor Merényi and Trygve E. Eriksen

The one-electron reduction potentials and pK_a s of substituted aniline radical cations have been determined by pulse radiolysis

67 Redox properties of 4-substituted aryl methyl chalcogenides in water

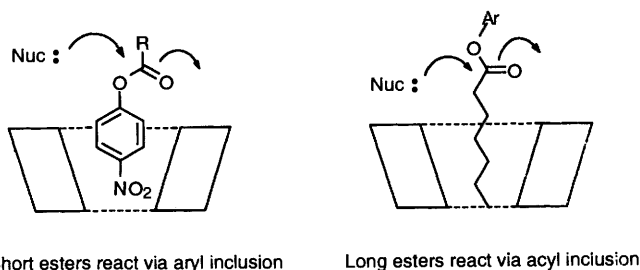
Mats Jonsson, Johan Lind, Gábor Merényi and Trygve E. Eriksen



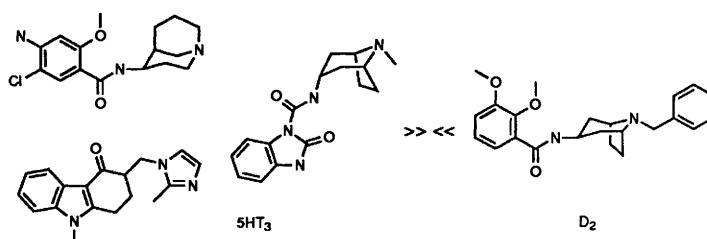
By means of pulse radiolysis the one-electron reduction potentials of 14 4-substituted aryl methyl chalcogenide radical cations have been measured

71 Acyl transfer reactions mediated by cyclodextrins. The reaction of external nucleophiles with encapsulated alkanolate esters of varying chain length

Timothy A. Gadosy and Oswald S. Tee

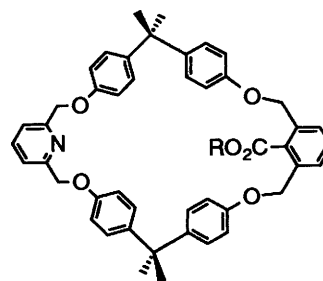
77 Stereoelectronic requirements of benzamide 5HT₃ antagonists. Comparison with D₂ antipaminergic analogues

Sonia Collin, Florence Moureau, Mirna Gil Quintero, Daniel P. Vercauteren, Guy Evrard and François Durant



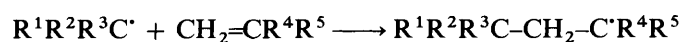
85 Towards structurally responsive synthetic macrocyclic receptors for acetylcholine

David Parker and Mark Rosser



91 Separation of polar and enthalpic effects on radical addition reactions using principal component analysis

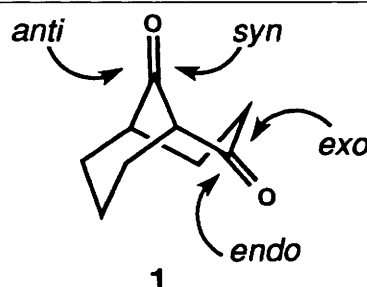
Károly Héberger and Antal Lopata



Where $R^1R^2R^3C^\cdot = Bu^\cdot, PhCH_2^\cdot, 2\text{-cyanoprop-2-yl}, Bu^\cdot OCOCH_2^\cdot,$
etc. $CH_2=CR^4R^5 = \text{acrylonitrile, styrene, 1,1-dichloroethylene, vinyl acetate, vinyl ethyl ether, etc.}$

97 Stereochemistry of the reduction of bicyclo[3.3.1]nonane-2,9-dione by complex hydrides

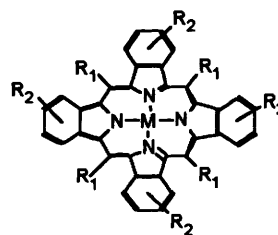
Ulf Berg, Eugenius Butkus and Arvydas Stoncius



The regio- and diastereoselectivity upon reduction of **1** by complex hydrides have been studied experimentally and computationally

- 103 **Metallotetrabenzoporphyrins. New phosphorescent probes for oxygen measurements**

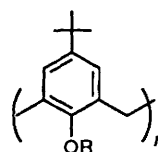
Sergei A. Vinogradov and David F. Wilson



$R_1 = \text{Ph, H}$
 $R_2 = \text{Ph, H}$

- 113 **Cation complexation by chemically modified calixarenes. Part 7. Transport of alkali cations by *p*-*tert*-butylcalix[*n*]arene esters and amides**

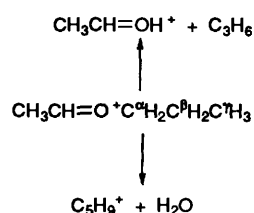
Françoise Arnaud-Neu, Stefano Fanni, Lourdes Guerra, William McGregor, Khadija Ziat, Marie-José Schwing-Weill, Geraldine Barrett, M. Anthony McKervey, Deborah Marrs and Eileen M. Seward



$n = 4, 5, 6, 8$
 $R = \text{ester, amide}$

- 119 **Mechanism of propene and water elimination from the oxonium ion $\text{CH}_3\text{CH}=\text{O}^+\text{CH}_2\text{CH}_2\text{CH}_3$**

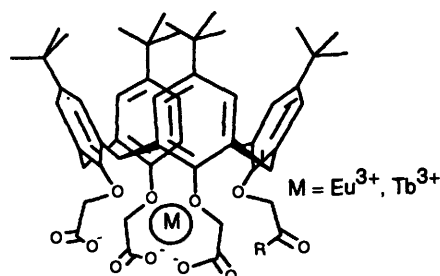
Richard D. Bowen, Dennis Suh and Johan K. Terlouw



Elimination of propene and water in the slow unimolecular dissociation of the oxonium ion $\text{CH}_3\text{CH}=\text{O}^+\text{CH}_2\text{CH}_2\text{CH}_3$ is shown by ^2H -labelling experiments to involve hydrogen transfer primarily from the α - and γ -positions of the propyl substituent, as would be expected if irreversible rearrangement of the incipient propyl group to its isopropyl isomer precedes hydrogen transfer

- 131 **Calix[4]arene-triacids as receptors for lanthanides; synthesis and luminescence of neutral Eu^{3+} and Tb^{3+} complexes**

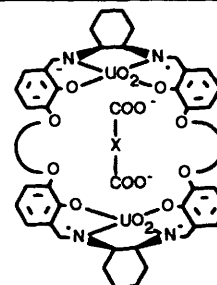
Dmitry M. Rudkevich, Willem Verboom, Erik van der Tol, Catherina J. van Staveren, Frans M. Kaspersen, Jan W. Verhoeven and David N. Reinhoudt



$M = \text{Eu}^{3+}, \text{Tb}^{3+}$

- 135 **Dinuclear, diuranyl-containing metallomacrocycles: neutral receptors for dicarboxylates**

Stephen M. Lacy, Dmitry M. Rudkevich, Willem Verboom and David N. Reinhoudt



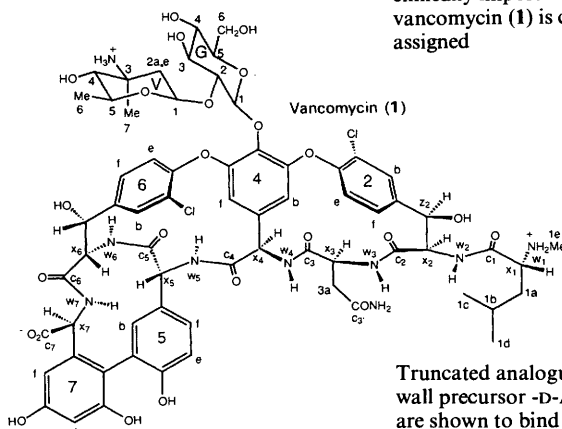
141 **Application of a generalised enthalpy–entropy relationship to binding co-operativity and weak associations in solution**

Mark S. Searle, Martin S. Westwell and Dudley H. Williams

We present a generalised enthalpy–entropy relationship for weak interactions (derived from experimental data on gas-phase associations); the utility of this curved plot in analysing co-operativity and binding phenomena in solution is illustrated

153 **Complete assignment of the ¹³C NMR spectrum of vancomycin**

Clive M. Pearce and Dudley H. Williams



The ¹³C NMR spectrum of the clinically important antibiotic vancomycin (1) is completely assigned

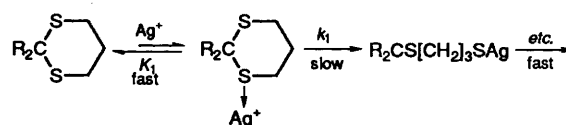
159 **Ligands which bind weakly to vancomycin: studies by ¹³C NMR spectroscopy**

Clive M. Pearce, Ute Gerhard and Dudley H. Williams

Truncated analogues of the cell wall precursor -D-Ala-D-Ala are shown to bind to vancomycin in the anticipated manner, *i.e.* to the right-hand side of the molecule (1)

163 **Kinetics of the silver ion-promoted hydrolysis of 2-methyl-2-(substituted phenyl)-1,3-dithianes in 10% dioxane–water mixtures. Implications for cyclic acetal hydrolysis catalysed by hydrogen ions**

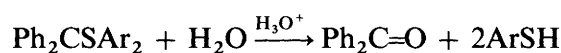
Tasneem F. Mohiuddin, Derek P. N. Satchell and Rosemary S. Satchell



Both K_1 and k_1 are much smaller than for open-chain analogues; relevance to H_3O^+ catalysed hydrolysis of acetals is discussed

167 **Kinetics and mechanism of hydrolysis of open-chain thioacetals derived from benzophenone and the reactivity of α -thiophenyl carbocations**

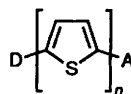
Muhammad Ali and Derek P. N. Satchell



Kinetics over a wide acidity range and reactivity of $\text{Ph}_2\text{C}^+\text{Ar}$ ions

171 **Quadratic non-linear optical properties of some donor-acceptor substituted thiophenes**

Michael G. Hutchings, Ian Ferguson, David J. McGeen, John O. Morley, Joseph Zyss and Isabelle Ledoux

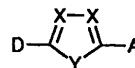


D = Me₂N, Me₂NN=CH
A = NO₂, CH=C(CN)₂
n = 1, 2

EFISH measurements have shown the hydrazone group to be an efficient electron donor for non-linear optics

177 **Non-linear optical properties of organic molecules. Part 20. Calculation of the structure, electronic properties and hyperpolarizabilities of donor-acceptor heterocycles containing sulfur, oxygen and nitrogen**

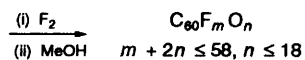
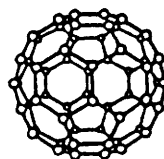
John O. Morley



Structures and electronic properties of donor-acceptor heterocycles

181 **Oxygenated species in the products of fluorination of [60]- and [70]-fullerene by fluorine gas**

Roger Taylor, G. John Langley, John H. Holloway, Eric G. Hope, Alan K. Brisdon, Harold W. Kroto and David R. M. Walton



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

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- A photoelectron spectroscopic study of the thermal decomposition of 2-pyrrolidinone and 2-pyrrolidinethione
W. S. Chin, C. Y. Mok, H. H. Huang and H. S. Rzepa
- Studies of imidazole and pyrazole protonation using electrostatically trained neural networks
H. B. Broughton, S. M. Green and H. S. Rzepa
- Synthesis and characterisation of selectively fluorinated stearic acids and their tristearins: the effect of introducing one and two fluorine atoms into a hydrocarbon chain
L. Dasaradhi, D. O'Hagan, M. C. Petty and C. Pearson
- Quantitative measurement of proton dissociation and tautomeric constants of apigeninidin
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- On the solvatochromic reversal of merocyanines. Part 1. The behaviour of vinylogous γ -pyridones
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- Radical cations of alkylazulenes: an EPR and ENDOR study
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- Alkene epoxidation by iodobenzene catalysed by iron(III) 5,10,15,20-tetra(2,6-dichlorophenyl)porphyrin coordinated by pyridine-modified silica
C. Gilmartin and J. R. Lindsay Smith
- A kinetic study of the reaction of *tert*-butyl hydroperoxide with iron(III) 5,10,15,20-tetra(4-sulfonatophenyl)porphyrin and related compounds in aqueous solution
N. Colclough and J. R. Lindsay Smith
- Phosphorus-31 NMR investigation of the heterogeneous hydrolytic decomposition of zinc(II) bis(*O,O*-dialkyl dithiophosphate) lubricant additives
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- Basicity properties of a novel azaparacyclophane receptor and its acyclic precursor: a thermodynamic and structural approach
C. Bazzicalupi, A. Bencini, A. Bianchi, V. Fusi, C. Giorgi, P. Paoletti, A. Stefani and B. Valtancoli
- Complexation with diol host compounds. Part 20. Kinetics of desolvation of inclusion compounds of 2,2'-bis(2,7-dichloro-9-hydroxy-9-fluorenyl)biphenyl with 1,4-dioxane and 1,3-dioxolane
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- Interaction between metal ions and NAD(P) coenzymes. ^1H , ^{13}C and ^{59}Co NMR spectroscopy and conformational analysis
S. Mazzini, R. Mondelli, E. Ragg and L. Scaglioni
- Decay of the hydroperoxide spin adduct of 5-diethoxyphosphoryl-5-methyl-1-pyrroline-*N*-oxide (DEPMPO): an EPR kinetic study
B. Tuccio, R. Lauricella, C. Frejaville, J.-C. Bouteiller and P. Tordo
- Photocycloaddition of fumaronitrile to adamantan-2-ones and modification of face selectivity by inclusion in β -cyclodextrin and its derivatives
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- Organophosphorus compounds. Part 93. Aromaticity of thia- and seleno-phospholes: a photoelectron spectroscopic and quantum chemical study
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- ^{17}O and ^{13}C NMR spectra of stable simple enols
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- Iron chelators of the pyridoxal 2-pyridyl hydrazone class. Part 4. pK_a values of the chelators and their relevance to biological properties
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- Intramolecular Michael-type addition in the solid state
B. S. Goud, K. Panneerselvam, D. E. Zacharias and G. R. Desiraju
- Kinetics and mechanisms of the oxidation reactions of some 2,3-dialkylindole derivatives by peroxodisulfate and peroxomonosulfate anions
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- 1,12-Digermacyclodocosanes. Synthesis, structure and anion transport capability
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