

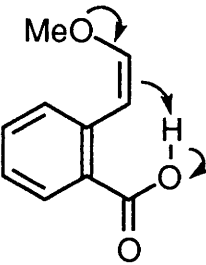
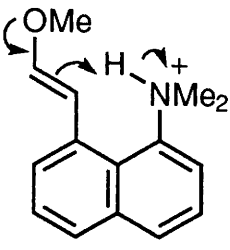
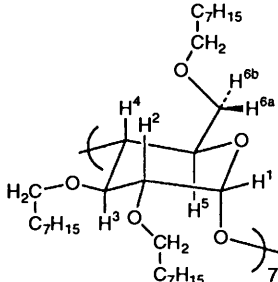
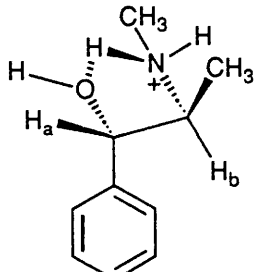
JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions 2

Physical Organic Chemistry

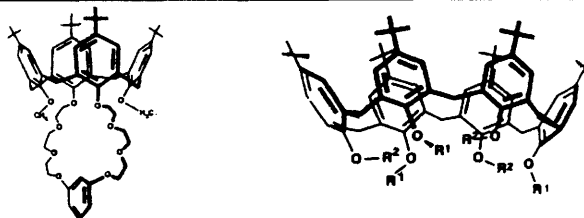
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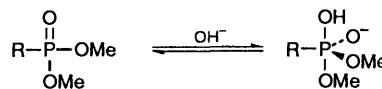
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Novel *p*-*tert*-butyl-calix[4]arenes and -calix[6]arenes used as guanidinium ionophores on CHEMFETs

- 683 Stereoelectronic effects in pentacoordinate intermediates and acceleration of nucleophilic substitution at phosphorus

Gregory R. J. Thatcher, E. S. Krol and Dale R. Cameron

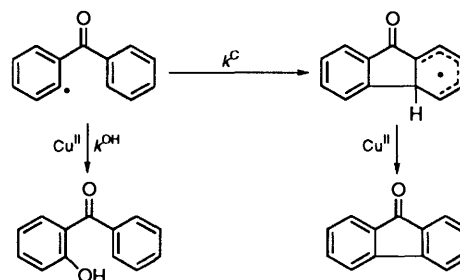


R = CH₃, CF₂H, CHO, CO₂H

Comparison of stereoelectronic effects from an *ab initio* MO study (HF/6-31G*) with experimental data for hydrolysis

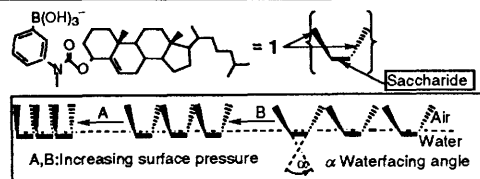
- 691 Sandmeyer reactions. Part 2. Estimation of absolute rate constants for some hydrogen-transfer reactions and for the transfer of water ligands on Cu^{II} to aryl radicals by use of a Pschorr radical clock

Peter Hanson, Roger C. Hammond, Paul R. Goodacre, Juliet Purcell and Allan W. Timms



- 697 Chiral discrimination of monosaccharides by monolayers of a steroidal boronic acid

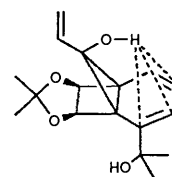
Rainer Ludwig, Takaaki Harada, Keiko Ueda, Tony D. James and Seiji Shinkai



The structure of the chiral complexes between **1** and monosaccharides at the air-water interface is correlated with physical properties of their monolayers

- 703 A crystallographic, AM1 and PM3 SCF-MO investigation of strong OH... π -alkene and alkyne hydrogen bonding interactions

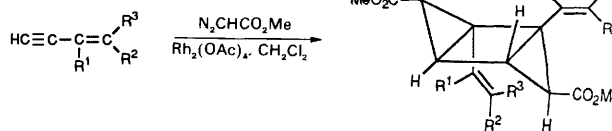
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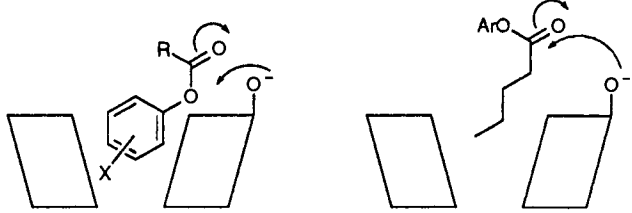

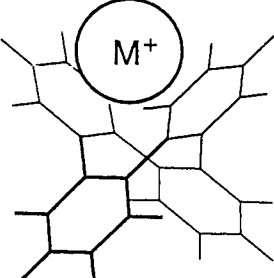
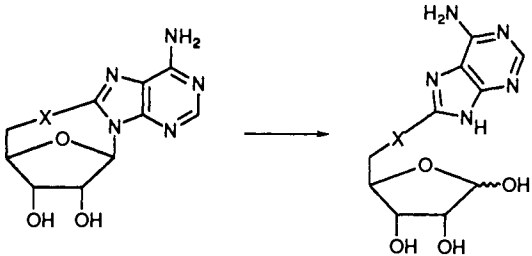
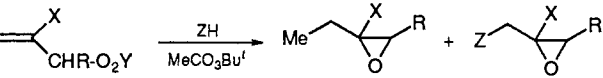


C...HO distances in π -alkene hydrogen bonding can be as short as 2.1 Å in compounds showing wide structural diversity; PM3 calculations overestimate the lengths by ≈ 0.3 Å

- 709 Regioselective Rh₂(OAc)₄-promoted reactions of methyl diazoacetate with terminal triple bond enynes

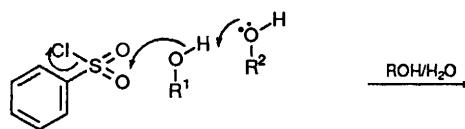
Evgeny A. Shapiro, Alexey V. Kalinin, Bogdan I. Ugrak and Oleg M. Nefedov



<p>715 The kinetics of basic cleavage of nitrophenyl alkanooate esters by 'hydroxypropyl-β-cyclodextrin' in aqueous solution</p> <p>Timothy A. Gadosy and Oswald S. Tee</p>	 <p>Sensitive to position of X; insensitive to length of RCO</p> <p>Insensitive to position of X; sensitive to length of RCO</p>
<p>723 Hammett equation and micellar effects upon deacylation</p> <p>Antonella Bartoletti, Simona Bartolini, Raimondo Germani, Gianfranco Savelli and Clifford A. Bunton</p>	 <p>X = H, OMe, Me, Cl, CN</p> <p>Substituent effects for reactions mediated by micelles of cationic surfactants</p>
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<p>735 The radical anion of tetraphenylene revisited</p> <p>Markus Scholz and Georg Gescheidt</p>	 <p>Formerly it was reported that the radical anion of tetraphenylene exists in two geometries of different symmetry. This EPR study indicates that the reason for these different symmetries is ion-pair formation</p>
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<p>745 Intramolecular homolytic displacements. Part 22. Polar effects in the homolytic induced decompositions of allyl peroxides</p> <p>Daniel Colombani and Bernard Maillard</p>	 <p>ZH = <i>c</i>-C₆H₁₂, CH₂(CO₂Me), PhH X = CO₂Et, R = Me, Y = Bu^t or SiMe₃ or C(Me)₂Ph or C(Me)₂OMe X = R = H, Y = Bu^t Influence of the various factors X, Y and Z on the yields of epoxides</p>

- 753 **Stoichiometric solvation effects. Part 2. A new product–rate correlation for solvolyses of *p*-nitrobenzenesulfonyl chloride in alcohol–water mixtures**

T. William Bentley, Robert O. Jones and In Sun Koo



ester: $R^1 = R^2 = R$ and $R^1 = R, R^2 = H$
acid: $R^1 = R^2 = H$ and $R^1 = H, R^2 = R$

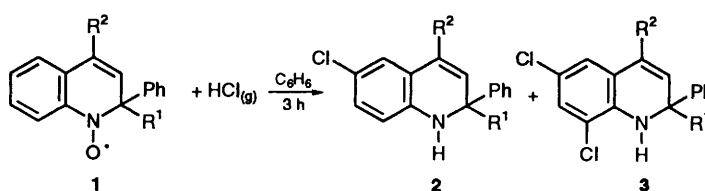
- 761 **A relationship between selectivity and solvent composition for nucleophilic attack on carbocations in alcohol–water mixtures**

T. William Bentley and Zoon Ha Ryu



- 769 **Hydrogen chloride treatment of quinolinic aminoxy radicals. Part 2. Crystal structures of 6-chloro-1,2-dihydro-2,2-diphenyl- and 6,8-dichloro-1,2-dihydro-2,2-diphenylquinoline**

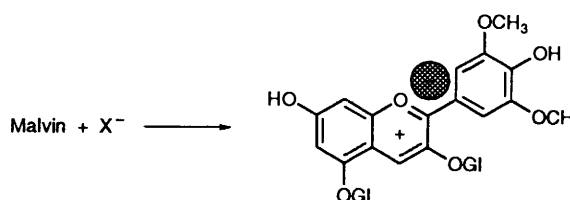
Liberato Cardellini, Patricia Carloni, Elisabetta Damiani, Lucedio Greci, Pierluigi Stipa, Corrado Rizzoli and Paolo Sgarabotto



Quinolinic aminoxy radicals (1) react with hydrogen chloride to give the corresponding mono- (2) and di- (3) chlorinated amines

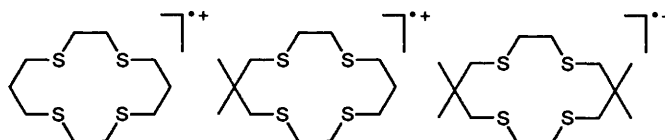
- 775 **Formation of anthocyanin ion-pairs. A co-pigmentation effect**

Paulo Figueiredo and Fernando Pina



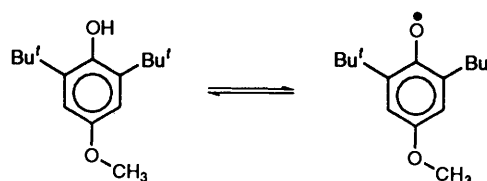
- 779 **Intramolecular interactions between sulfur atoms in cyclotetrathioether radical cations**

Jacek Rogowski, Jan Adamus, Jerzy Gebicki and Stephen F. Nelsen



- 785 **Entropic and enthalpic effects of 4-methoxy substitution in phenoxy radicals**

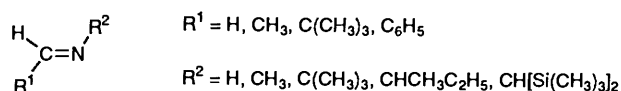
Marta E. J. Coronel and Agustin J. Colussi



$\Delta H = 322.2 \pm 1.6 \text{ kJ mol}^{-1}$; $\Delta S = -18.5 \pm 5.6 \text{ J K}^{-1} \text{ mol}^{-1}$

789 **Ultraviolet photoelectron, electron transmission and *ab initio* study of the factors determining the stability of imines**

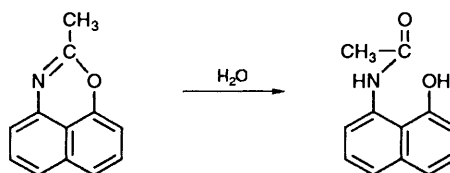
Maurizio Dal Colle, Giuseppe Distefano, Derek Jones, Andrea Guerrino, Giancarlo Seconi and Alberto Modelli



The stability of imines is discussed in terms of frontier orbitals energy and total electron charge distribution

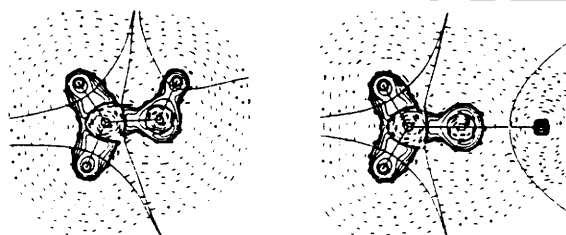
795 **Rate-pH profile for the formation of 1-hydroxy-8-acetylamino-naphthalene from 2-methylnaphth[1,8-*de*]-1,3-oxazine in aqueous solution; acid catalysis and inhibition and comparison with the reaction of 1-amino-8-trifluoroacetylamino-naphthalene**

Wendy J. Dixon and Frank Hibbert



799 **Theoretical studies of protonation and lithiation of first- and second-row aldehydes**

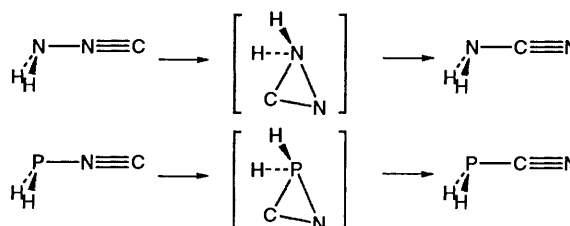
Peter Speers and Keith E. Laidig



Laplacian maps show that protonation of aldehydes, left, is a strongly shared interaction and lithiation, right, is a closed-shell interaction

807 **A theoretical comparison of phosphino and amino groups in the isocyanide-cyanide rearrangement**

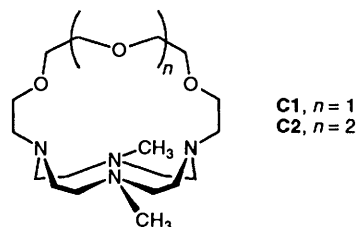
Minh Tho Nguyen, Peter J. Groarke, Seamus Malone and Anthony F. Hegarty



The energy barrier (27 kcal mol⁻¹) for the rearrangement of the phosphinoisocyanide to the more stable phosphinocyanide suggests that it might be a synthetic target

815 **Synthesis, characterization and basicity properties of two new oxa-aza macrobicyclic receptors. Crystal structure of a 'water cryptate'**

Carla Bazzicalupi, Andrea Bencini, Antonio Bianchi, Vieri Fusi, Piero Paoletti and Barbara Valtancoli



A water molecule is deeply embedded into the macrobicyclic cavity, held by an arrangement of hydrogen bonds

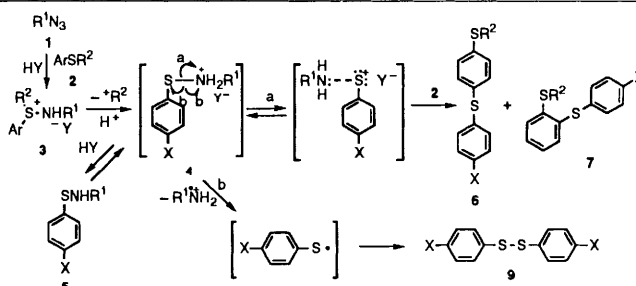
821 **NMR study on a SRYD-containing fibronectin-like sequence (250–257) of *Leishmania* gp63: contribution of residual water in the dimethyl sulfoxide solution structure**

Vassilios Tsikaris, Mahn Thong Cung, Constantinos Sakarellos, Athina K. Tzinia, Ketty P. Soterladou and Maria Sakarellos-Daitsiotis

An NMR analysis of I²⁵⁰ASRYDQL²⁵⁷ has shown that, after treatment with molecular sieves of the DMSO solution at pH 2, residual water is redistributed between the peptide functional groups and a new conformational state, similar to that at pH 5, is adopted

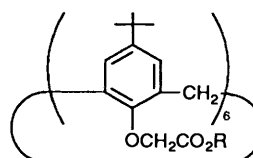
827 **Novel generation of arylsulfenium ion intermediates and efficient aromatic arylthiolation by the intermediates**

Hiroshi Takeuchi, Hiromi Ōya, Takehiro Yanase, Katsutaka Itou, Taki Adachi, Hiroshi Sugiura and Noriyuki Hayashi



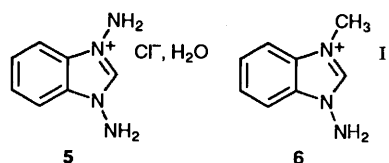
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Sang-Yoon Han, Myong-Hee Kang, YeonEui Jung and Suk-Kyu Chang



841 ***N*-Aminoazoles. Part 3. Molecular structure and multinuclear NMR study of 1,3-diaminobenzimidazolium chloride hydrate and 1-amino-3-methylbenzimidazolium iodide**

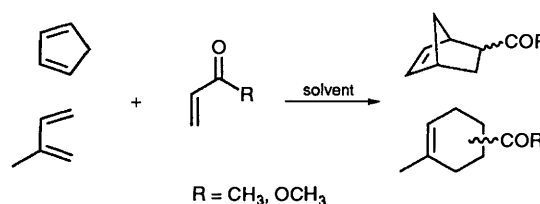
Alexander F. Pozharskii, Valery V. Kuz'menko, Concepción Foces-Foces, Antonio L. Llamas-Saiz, Rosa M^a. Claramunt, Dionisia Sanz and José Elguero



The X-ray structure, NMR spectroscopy (¹H, ¹³C, ¹⁵N) and AM1 calculations of compounds 5 and 6 are reported

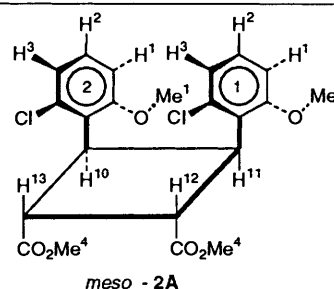
847 **Solvent effects on *endo/exo*- and regioselectivities of Diels–Alder reactions of carbonyl-containing dienophiles**

Carlos Cativiela, José I. García, José A. Mayoral and Luis Salvatella



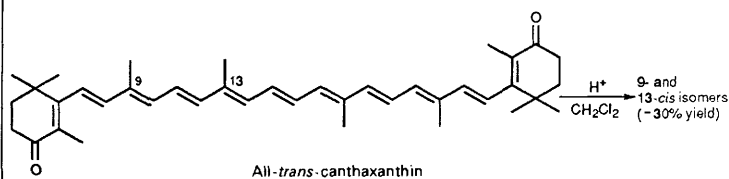
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David A. Ben-Efraim and Rina Arad-Yellin

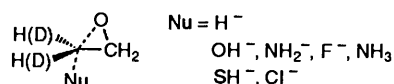


861 Geometrical isomerization of carotenoids in dichloromethane

Antony S. Jeevarajan, Chih-Chang Wei and Lowell D. Kispert

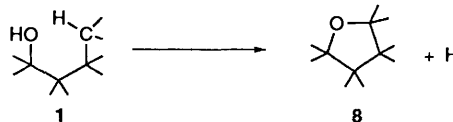
871 *Ab initio* Study of the nucleophilic ring opening of ethylene oxide. Connection between secondary kinetic isotope effects and transition structures

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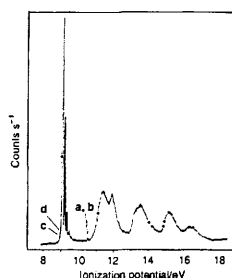
Ivan O. Juranić, Mihailo Lj. Mihailović and Milan M. Dabović



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883 Thermal decomposition of thiirane and 2-methylthiirane: an experimental and theoretical study

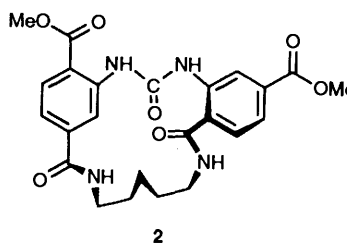
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Spectrum of thiirane and pyrolysis products at 900 °C

891 Metal-ion complexation by a new urea macrocyclophane

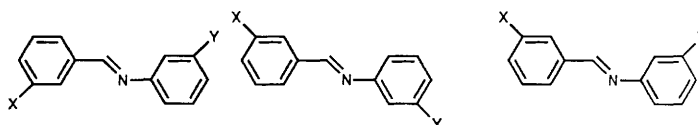
Didier Cordier and Pierre R. Coulet



Design, synthesis, characterization and complexation behaviour in water of the fluorescent urea macrocyclophane **2** with Cd^{II} and Zn^{II} ions

895 Conformational studies of the *N*-(3-halobenzylidene)-3-haloaniline system. Part 2. Molecular energetics

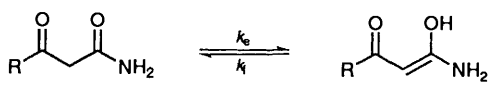
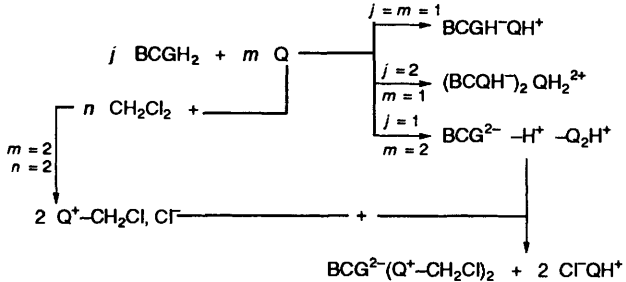
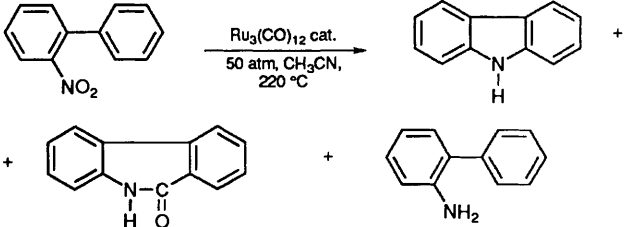
Sharona Zamir, Joel Bernstein, Alexander Ioffe, Jon Brunvoll, Mária Kolonits and Istvan Hargittai



Observed solid-state molecular conformations

Gas-phase molecular conformations

X, Y = Br, Cl

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<p>913 Role of alkali halides in the synthesis of nitrogen containing heterocycles by reductive carbonylation of aromatic nitro-derivatives catalysed by $Ru_3(CO)_{12}$</p>	 <p>Maddalena Pizzotti, Sergio Cenini, Silvio Quici and Stefano Tollari</p> <p>Alkali halides behave as co-catalysts, strongly affecting reaction rates and selectivities towards formation of heterocyclic compounds</p>
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