

JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions 2

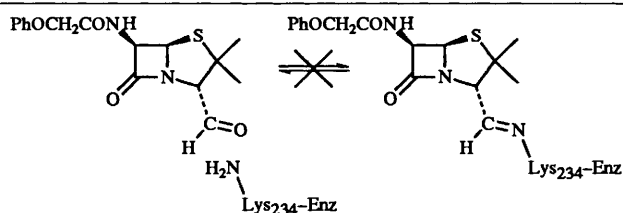
Physical Organic Chemistry

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- 869 Penicillin 3-aldehyde is a good substrate and not an inhibitor of β -lactamases A and C

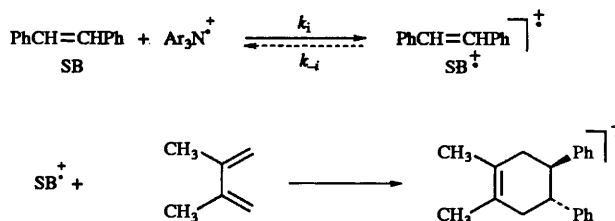
Nicola J. Layland, Andrew P. Laws, Bartolomé Vilanova and Michael I. Page



Normal pH-rate profile for hydrolysis catalysed by β -lactamase; no inhibition by imine formation

- 871 Criteria for the cation radical vs. electrophilic mechanistic distinction: the aminium salt-catalysed Diels-Alder reaction

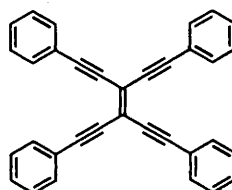
Wang Yueh and Nathan L. Bauld



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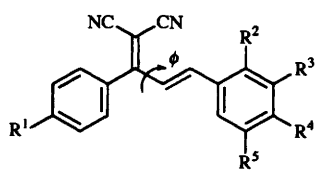
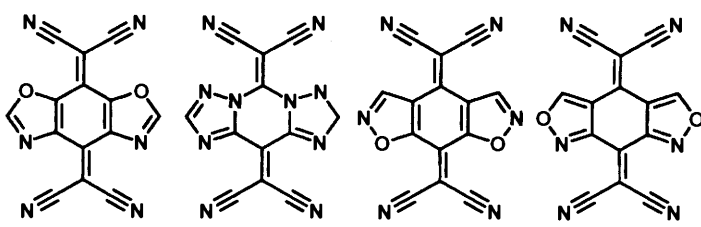
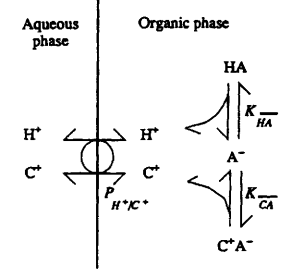
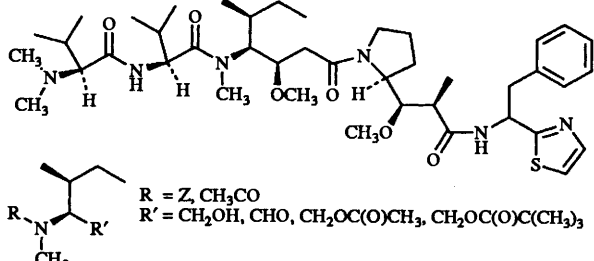
- 875 π -Complexes incorporating tetrakis(phenylethynyl)ethene

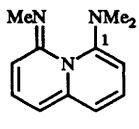
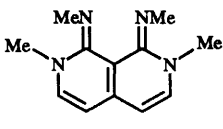
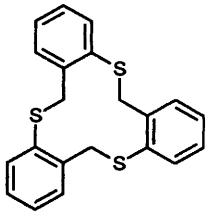
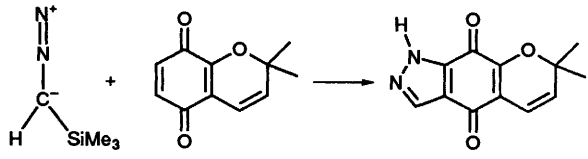
Douglas Philp, Volker Gramlich, Paul Seiler and François Diederich



Tetrakis(phenylethynyl)ethene

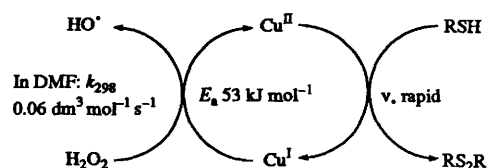
The formation of π -complexes between tetrakis(phenylethynyl)ethene and π -acceptors is controlled by electrostatic interactions rather than by orbital interactions

<p>887 Hydrogen bonding. Part 40. Factors that influence the distribution of solutes between water and sodium dodecylsulfate micelles</p> <p>Michael H. Abraham, Harpreet S. Chadha, Julian P. Dixon, Clara Rafols and Claude Treiner</p>	<p>An equation set up for the distribution of 132 varied solutes between water and SDS micelles shows that the two main factors that influence distribution are solute hydrogen-bond basicity that favours water and solute volume that favours the SDS micellar pseudo phase</p>
<p>895 EPR Spin-trapping studies of the reaction of radicals derived from hydroperoxide tumour-promoters with nucleic acids and their components</p> <p>Clare Hazlewood and Michael J. Davies</p>	<p>EPR spin trapping studies using MNP are reported which are consistent with the following behaviour:</p> $\text{Ti}^{\text{III}} + \text{Bu}'\text{O}_2\text{H} \longrightarrow \text{Ti}^{\text{IV}} + \text{HO}^- + \text{Bu}'\text{O}^{\bullet}$ <p>Bu'O[•] + Pyrimidine bases → Base adducts at C₅-C₆ double bond Bu'O[•] + Pyrimidine nucleosides → Base adducts at C₅-C₆ double bond plus sugar radicals Bu'O[•] + Purine nucleosides → Base adducts? Bu'O[•] + DNA or RNA → Signals similar to pyrimidine base adducts</p>
<p>903 Effects of conformation, substituents and solvent on molecular hyperpolarizabilities of push-pull diaryl-alkenes and -dienes: a computational study</p> <p>Walter M. F. Fabian, Renate Dworczak, Hans Junek and Barburao N. Pawar</p>	
<p>907 Prediction of planarity and reduction potential of derivatives of tetracyanoquinodimethane using <i>ab initio</i> molecular orbital theory</p> <p>Peter W. Kenny</p>	 <p>MO calculations identify novel planar TCNQ derivatives and predict reduction potentials</p>
<p>911 Behaviour of hydrophobic pH indicators in aqueous-organic two-phase systems</p> <p>Peter J. Halling, Yuchao Han, Grant A. Johnston, Colin. J. Suckling and Rao H. Valivety</p>	 <p>Spectroscopically measurable dissociation of HA reports aqueous pH</p>
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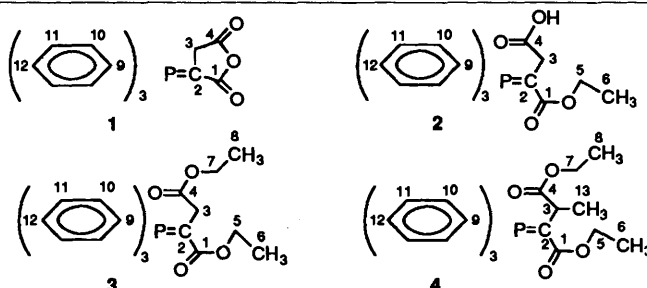
<p>923 Semiempirical (AM1, PM3 and SAM1) calculations of the protonation enthalpies of proton sponges related to 1,8-diaminonaphthalene. Estimation of the aqueous basicity of new designed superbases</p> <p>Antonio L. Llamas-Saiz, Concepción Foces-Foces, Ana Martínez and José Elguero</p>	<div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;">  <p>6</p> </div> <div style="text-align: center;">  <p>8</p> </div> </div> <p>SAM1 and AM1 calculations have been used to predict that compounds 6 and 8 should be superbases (aqueous pK_a between 19 and 22)</p>
<p>929 Critical re-evaluation of FABMS analysis of ligand-cation interactions</p> <p>G. John Langley, Darren G. Hamilton and Martin C. Grossel</p>	<p>The use of FABMS for quantitative studies of ligand-metal binding requires the use of an internal standard and relevant calibration of each system to produce meaningful results</p>
<p>935 Conformation of 6<i>H</i>,12<i>H</i>,18<i>H</i>-tribenzo[<i>b</i>,<i>f</i>,<i>j</i>]-[1,5,9]trithiacyclododecin revisited</p> <p>György M. Keserű, Mihály Nógrádi, Attila Kovács and Uwe Himmelreich</p>	
<p>939 Regioselectivity in Diels-Alder reactions of pyranobenzoquinones</p> <p>Fernando Zuloaga, Ricardo Tapia and Carmina Quintanar</p>	
<p>945 Neutral hydrolysis and imidazole-catalysed decomposition of bis(4-nitrophenyl) oxalate. 1,1'-Oxalyldiimidazole as an intermediate</p> <p>Helmi Neuvonen</p>	$\text{ArOCOCO}_2\text{Ar} \xrightarrow{\text{ImH or 2ImH}} \text{ImCOCO}_2\text{Ar} + \text{ArOH}$ <p style="text-align: center;">1</p> $\text{ImCOCO}_2\text{Ar} \xrightarrow{\text{ImH}} \text{ImCOCOIm} + \text{ArOH} + \text{ImH}$ <p style="text-align: center;">2</p> <p style="text-align: center;">↓ ImH, H₂O</p> <p style="text-align: center;">Hydrolysis products</p> <p>ImH = Imidazole Ar = -C₆H₄-NO₂</p> <p>Formation of 1 is fast compared with its reaction to 2</p>
<p>951 Effect of the acyl group in the reaction of imidazole with acyl-substituted 4-nitrophenyl acetates in acetonitrile and in aqueous acetonitrile with a low water content</p> <p>Helmi Neuvonen</p>	<p>In MeCN and in aqueous MeCN</p> $\text{RC(=O)-O-C}_6\text{H}_4\text{-NO}_2 + \text{Imidazole (ImH)} \longrightarrow \text{Products}$ $k_{\text{obs}} = k_1[\text{ImH}] + k_2[\text{ImH}]^2$ <p>R = CF₃, CHCl₂, CH₂Cl, CH₃</p> <p>Comparison of the effect of the acyl group on the mechanisms of the overall second- and third-order reactions</p>

955 EPR studies of the copper-catalysed oxidation of thiols with peroxides

Garry Scrivens, Bruce C. Gilbert and Timothy C. P. Lee

965 Structural and conformational analysis of 2-triphenylphosphoranylidene succinic acid derivatives by ^1H , ^{13}C and ^{31}P one and two dimensional NMR spectroscopy and molecular modelling

Radu Bacaloglu, Andrei Blaskó, Clifford A. Bunton, Giorgio Cerichelli, Fernando Castaneda and Enrique Rivera

973 Considerably improved Grunwald–Winstein correlations for solvolyses of several secondary and tertiary benzylic derivatives upon inclusion of a term governed by the aromatic ring parameter (I)

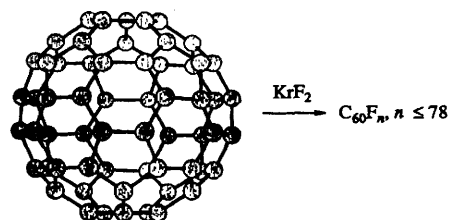
Dennis N. Kevill and Malcolm J. D'Souza

$$\log(k/k_0) = lN + mY + hI + c$$

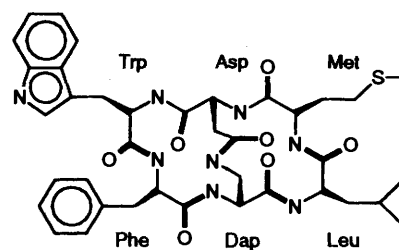
Consideration of the utility of the aromatic ring parameter (I)

981 Hyperfluorination of [60]fullerene by krypton difluoride

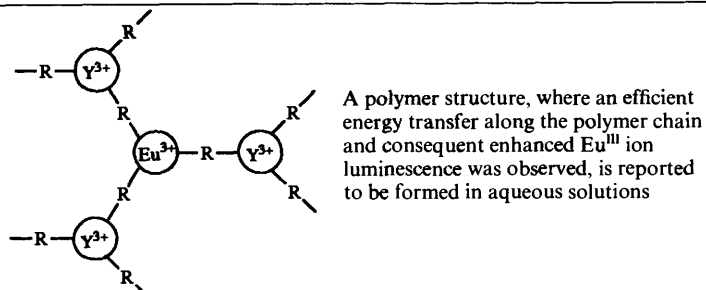
Olga V. Boltalina, Ala'a K. Abdul-Sada and Roger Taylor

987 Design and structure of a novel Neurokinin A receptor antagonist cyclo(-Met¹-Asp²-Trp³-Phe⁴-Dap⁵-Leu⁶-)-cyclo(2 β -5 β)

Vincenzo Pavone, Angelina Lombardi, Flavia Natri, Michele Saviano, Ornella Maglio, Gabriella D'Auria, Laura Quartara, Carlo Alberto Maggi and Carlo Pedone

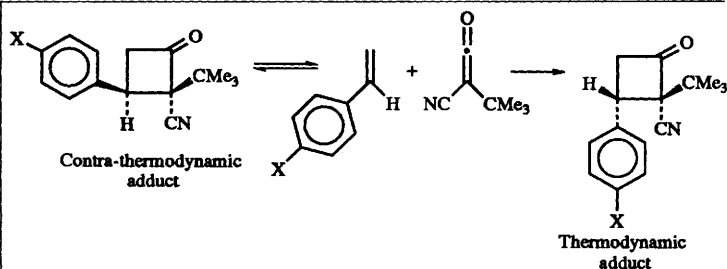
995 Enhanced Eu^{III} ion luminescence and efficient energy transfer between lanthanide chelates within the polymeric structure in aqueous solutions

Martti Latva, Harri Takalo, Katariina Simberg and Jouko Kankare



1001 *tert*-Butylecyanoketene-substituted styrene cycloadditions. A kinetic study

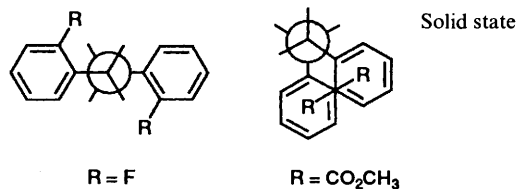
Sk. Asrof Ali, Mohammed Muqtar and Abdulrahman H. Al-Husaini



Kinetics of ketene-styrene additions are discussed

1007 Effect of *ortho* substituents on the internal rotation processes and conformational preferences of 1,2-diaryl-1,1,2,2-tetrachloroethanes: a ¹H and ¹³C NMR variable temperature and X-ray structural study

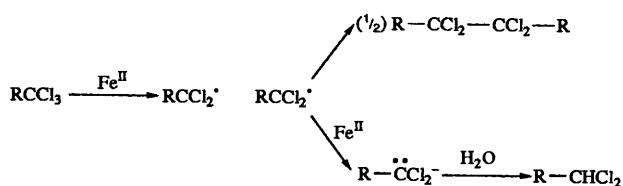
Luciano Antolini, Ugo Folli, Dario Iarossi, Adele Mucci, Silvia Sbardellati and Ferdinando Taddei



The *gauche* forms are preferred in solution

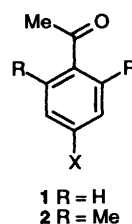
1017 Selectivity towards hydrodehalogenation and dehalo-coupling in the reduction of trichloromethyl derivatives with iron(II) chloride

Ugo Folli, Francesca Goldoni, Dario Iarossi, Silvia Sbardellati and Ferdinando Taddei



1021 Differential substituent effects in 4-X-acetophenones and 4-X-2,6-dimethylacetophenones: basicity constants (pK_{BH^+}) and ¹⁷O chemical shifts

Stefano Chimichi, Carlo Dell'Erba, Michelangelo Gruttadauria, Renato Noto, Marino Novi, Giovanni Petrillo, Fernando Sancassan and Domenico Spinelli



The pK_{BH^+} (in sulfuric acid) and the ¹⁷O NMR chemical shifts (in CDCl₃) of acetophenones have been determined; in going from 1 to 2, the 2,6-dimethyl substitution brings about remarkable variations in the electronic array of the probe group, as measured by either protonation equilibria or carbonyl oxygen chemical shifts

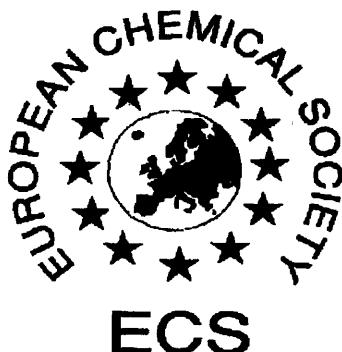
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- Reversible intramolecular 1,3-chlorine migration in the triad carbon—carbon—sulphur
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- Electrochemical and enzymic oxidation of 9-methyluric acid at solid electrodes **R. N. Goyal, A. K. Jain and N. Jain**



European Chemical Society

The Organic Division of the ECS organises its

First European Symposium

**August 12-17th, 1995
Louvain-la-Neuve, Belgium**

First Circular

The following distinguished speakers have already agreed to deliver a plenary lecture

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D. Craig (U.K.)	I. Marek (France)
P. Declercq (Belgium)	R. Neier (Switzerland)
B. Feringa (The Netherlands)	I. Paterson (U.K.)
C. Gennari (Italy)	A. Perczel (Hungary)
D. Gilheany (Ireland)	K. Rissanen (Finland)
K.-A. Jorgensen (Denmark)	I. Stary (Czech Republic)
W. Kerr (U.K.)	M. Taddei (Italy)
J. Koca (Czech Republic)	D. Tanner (Sweden)
M. Maier (Germany)	N. Turner (U.K.)

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