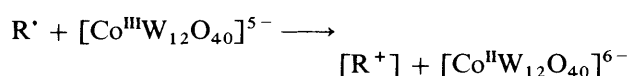


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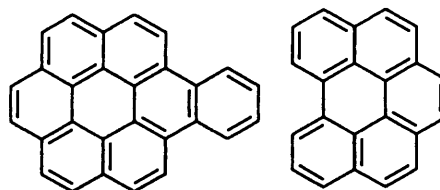
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- 1265 **Protonation-oxidation manifold in large PAHs. Benzo[*a*]coronene and benzo[*ghi*]perylene; stable ion studies in superacid media and AM1 calculations**

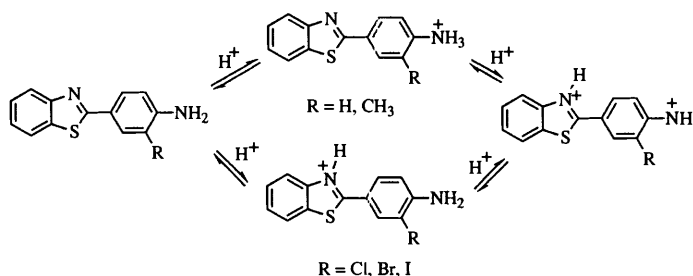
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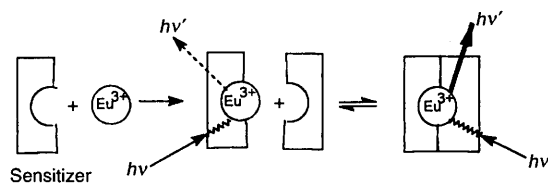
- 1271 **Antitumour benzothiazoles. Part 4. An NMR study of the sites of protonation of 2-(4-aminophenyl)benzothiazoles**

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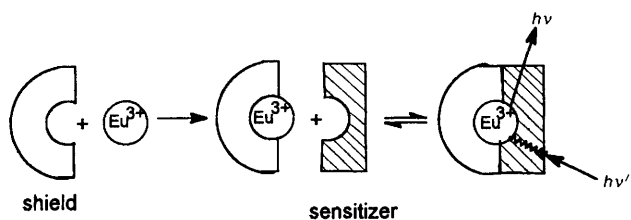
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John Coates, Peter G. Sammes and Richard M. West



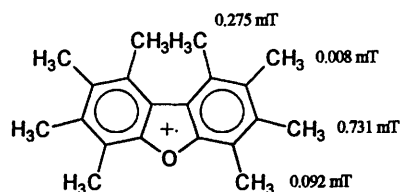
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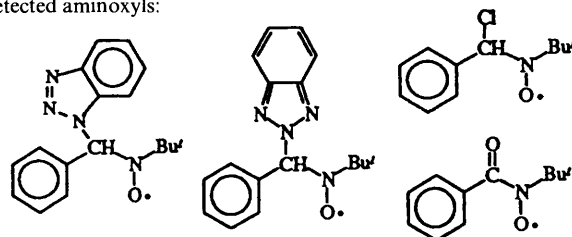
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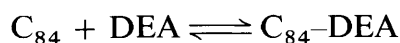
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Detected aminoxyls:



1307 **Ground state charge transfer complex of [84]fullerene and *N,N*-diethylaniline**

Christopher E. Bunker, Harry W. Rollins and Ya-Ping Sun



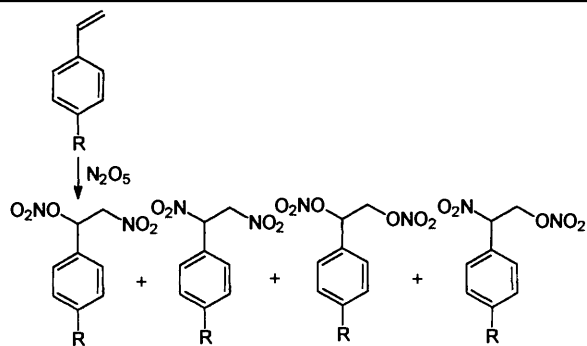
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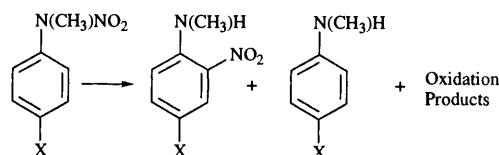
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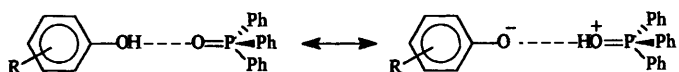


1321 Thermal decomposition of arylnitramines

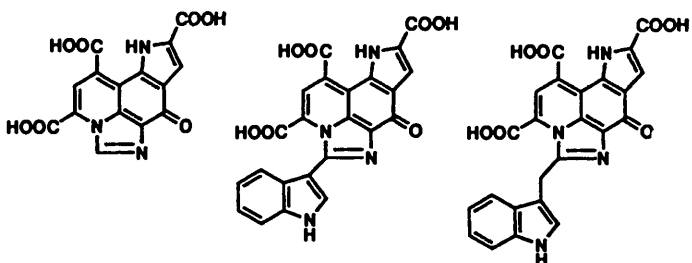
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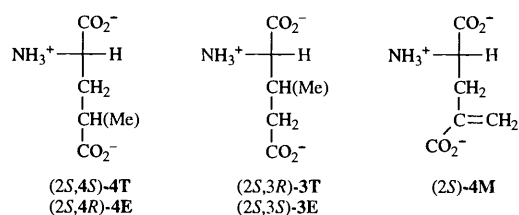
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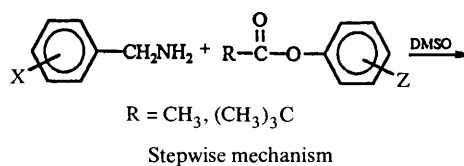
1337 Conformational analysis by NMR spectroscopy and molecular simulation in water of methylated glutamic acids, agonists at glutamate receptors

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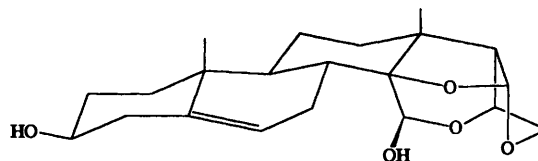
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- 1359 The structure of velutinol A is (15*R*,16*R*,20*S*)-14,16:15,20:16,21-triepoxy-15,16-seco-14 β ,17 α -pregn-5-ene-3 β ,15-diol. A combined quantitative Overhauser effect and molecular modelling study

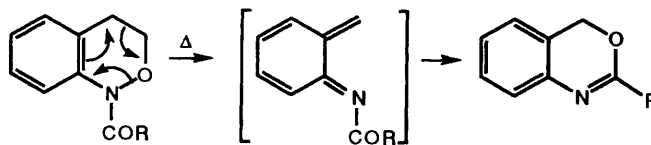
Edson S. Bento, João B. Calixto, Geoffrey E. Hawkes, Moacir G. Pizzolatti, Antonio E. G. Sant'Ana and Rosendo A. Yunes



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- 1367 Rearrangement of *N*-acyl-3,4-dihydro-1*H*-2,1-benzoxazines to 2-substituted-4*H*-3,1-benzoxazines through a retro-Diels–Alder extrusion of formaldehyde

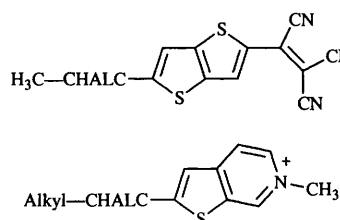
Stephen A. Glover, Katherine M. Jones, Ian R. McNee and Colleen A. Rowbottom



R = Ph, Me, Bu^t, Prⁱ, Bu, 3-pentyl, Et, 2-butyl

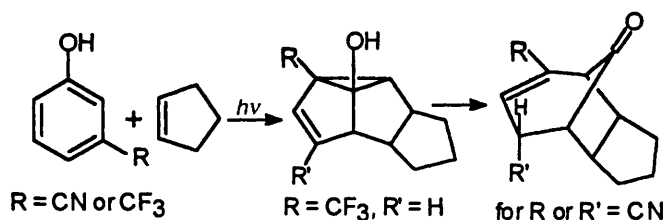
- 1377 Chalcogens as electron donors for selected nonlinear optic phores

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- 1385 Formation of bicyclo[3.2.1]oct-2-en-8-ones and 1-hydroxydihydrosemibullvalenes from the *meta*-photocycloaddition of cyclopentene to phenols

Andrew Gilbert and Damian T. Jones



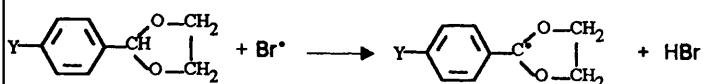
R = CN or CF₃

R = CF₃, R' = H

for R or R' = CN

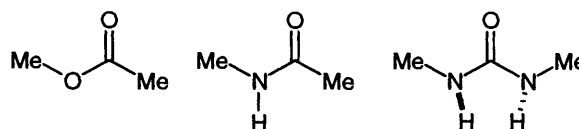
- 1391 How does an alkoxy group at the benzylic carbon affect the transition state of the hydrogen-atom abstraction reaction? Correlation analysis of relative rates for 14 *p*-*Y*-substituted α,α -ethylene-dioxytoluenes

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- 1397 Study of electron densities of methyl acetate, *N*-methylacetamide and *N,N*-dimethylurea by quantum mechanical investigations. Part 1. Gas phase

Bernd Kallies and Rolf Mitzner



The details of electron delocalization are studied

- 1403 Study of electron densities of methyl acetate, *N*-methylacetamide and *N,N*-dimethylurea by quantum mechanical investigations. Part 2. Solvent models

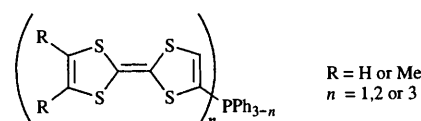
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N,N'-Dimethylurea hydrogen bonded to six water molecules

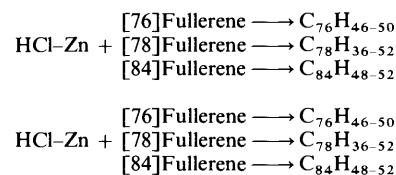
- 1409 Oxidation of phosphines containing two or three tetrathiafulvalene (TTF) or *o*-dimethyl-TTF moieties. Evidence for formation of radical polycations

Fabian Gerson, Axel Lamprecht and Marc Fourmigué



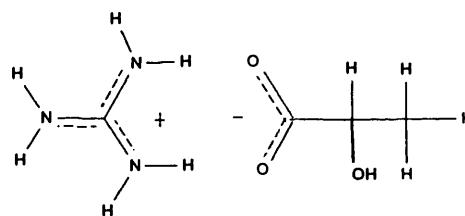
- 1415 Hydrogenation of [76]-, [78]- and [84]-fullerenes: cage degradation

Adam D. Darwish, Harold W. Kroto, Roger Taylor and David R. M. Walton



- 1419 Characterization of lactate-guanidinium and lactate-lactate interactions in aqueous solution by spectropolarimetry

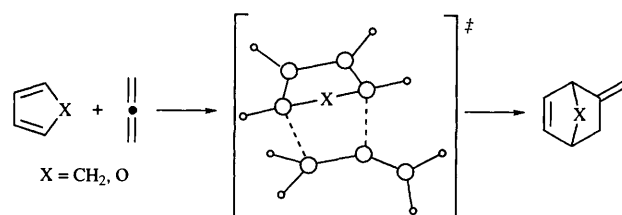
Péter Horváth, András Gergely and Béla Noszál



The association constant for the above guanidinium-lactate interaction is 6.11; the analogous value for the lactate dimerization is 1.12

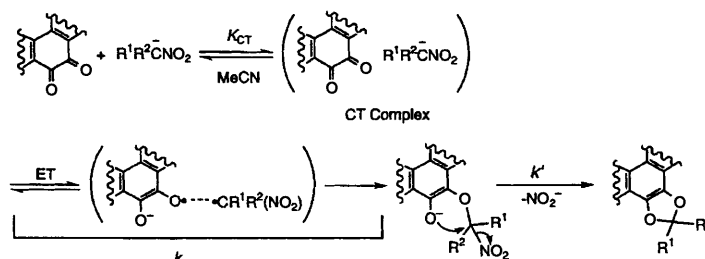
- 1423 Allene and fluoroallenes as dienophiles in Diels-Alder reactions: an AM1 and PM3 study

Mariappan Manoharan and Ponnambalam Venuvanalingam



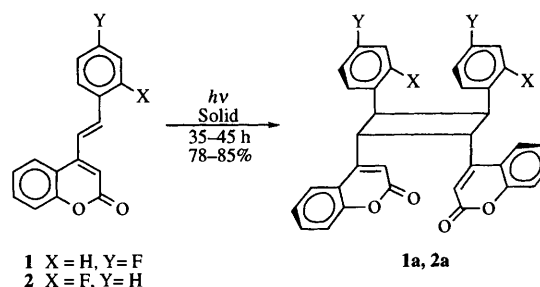
- 1429 Addition-cyclization reaction of nitroalkane anions with *o*-quinone derivatives via electron transfer in the charge-transfer complexes

Shinobu Itoh, Junichi Maruta and Shunichi Fukuzumi



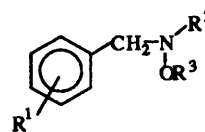
- 1475 **Studies in crystal engineering: effect of fluorine substitution in crystal packing and topological photodimerization of styryl coumarins in the solid state**

Kodumuru Vishnumurthy, Tayur N. Guru Row and Kailasam Venkatesan



- 1479 **Nitrogen inversion and N–O bond rotation processes in di- and tri-substituted hydroxylamines. A dynamic NMR study**

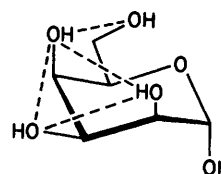
Sk. Asrof Ali, Azfar Hassan and Mohammed I. M. Wazeer



Substitution effects on the nitrogen inversion/N–O rotation barriers are discussed

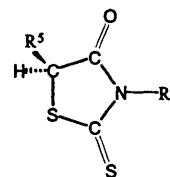
- 1485 **Intramolecular hydrogen bonds in monosaccharides in dimethyl sulfoxide solution**

Stephen J. Angyal and John C. Christofides



- 1493 **Chromatographic enantiomer separation and circular dichroism spectra of chiral rhodanines**

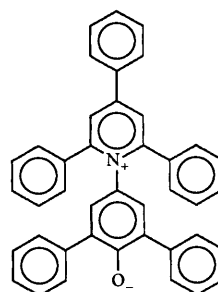
Knut Rang, Roland Isaksson and Jan Sandström



Chromatographic enantiomer separation, stereochemical stability and the UV and CD spectra of rhodanines, R⁵ = Me and Ph, have been studied

- 1497 **Solute–solvent and solvent–solvent interactions in binary solvent mixtures. Part 3. The $E_T(30)$ polarity of binary mixtures of hydroxylic solvents**

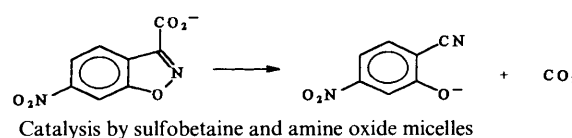
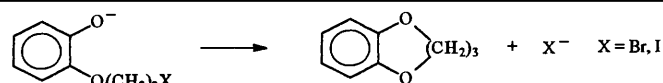
José Ortega, Clara Ràfols, Elisabeth Bosch and Martí Rosés

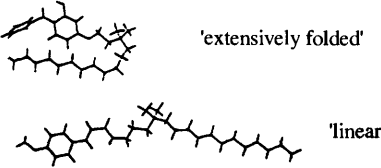


Solvent exchange models can be successfully applied to describe the transition energy of the Dimroth–Reichardt $E_T(30)$ solvatochromic indicator in binary solvent mixtures

- 1505 **Cyclisation and decarboxylation in zwitterionic micelles: effects of head group structure**

Pietro Di Profio, Raimondo Germani, Gianfranco Savelli, Giorgio Cerichelli, Nicoletta Spreti and Clifford A. Bunton



<p>1511 Racemic compound formation–conglomerate formation. Part 3. Investigation of the acidic salts of α-phenylethylamine by achiral dicarboxylic acids. Optical resolution by preferential crystallization and a structural study of (<i>R</i>)-α-phenylethylammonium hydrogen itaconate</p> <p>Zsolt Böcskei, Csaba Kassai, Kálmán Simon, Elemér Fogassy and Dávid Kozma</p>	<p>Acidic salts of eight achiral dicarboxylic acids with α-phenylethylamine are investigated and it is found that conglomerate formation takes place when the protonated and deprotonated carboxylic groups form hydrogen bonded chains, rather than forming a cyclic intramolecular hydrogen bond; the crystal structure of (<i>R</i>)-α-phenylethylammonium hydrogen itaconate and its optical resolution by preferential crystallization is described</p>
<p>1517 Comparative conformational and dynamical study of some <i>N</i>-quaternarized UV filters: structure–activity relationships</p> <p>Cecilia Anselmi, Marisanna Centini, Marco Francioli and Alessandro Segà</p>	<div style="text-align: center;">  <p>'extensively folded'</p> <p>'linear'</p> </div> <p>The main conformers are dependent on structure and/or solvent</p>

Corrigendum

<p>1525 EPR studies of pyrazoline radicals that are potential precursors to non-Kekulé polyene radicals ions</p>	<p>Richard J. Bushby and Kai M. Ng</p>
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9th International Symposium on Molecular Recognition and Inclusion

Lyon, France 7-12 September 1996

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Mr M Munoz (Committee Secretary), IBCP, CNRS UPR 412,
7 passage du Vercors, Lyon cedex 07, F69367 FRANCE
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