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Physical Organic Chemistry

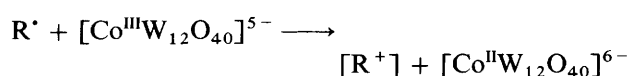


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- 1261 **Reactivity of $[\text{Co}^{\text{III}}\text{W}_{12}\text{O}_{40}]^{5-}$ with organic radicals in aqueous solution. Evidence for an electron transfer mechanism**

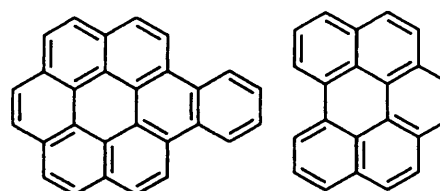
Enrico Baciocchi, Massimo Bietti and Steen Steenken



Articles

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

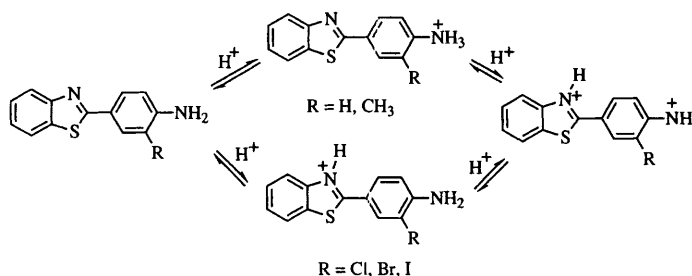
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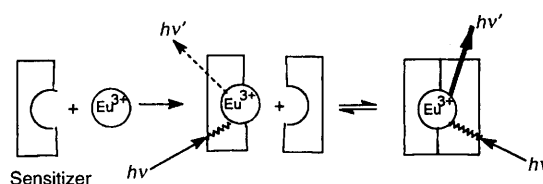
- 1271 **Antitumour benzothiazoles. Part 4. An NMR study of the sites of protonation of 2-(4-aminophenyl)benzothiazoles**

Richard T. Wheelhouse, Dong-Fang Shi, Derry E. V. Wilman and Malcolm F. G. Stevens



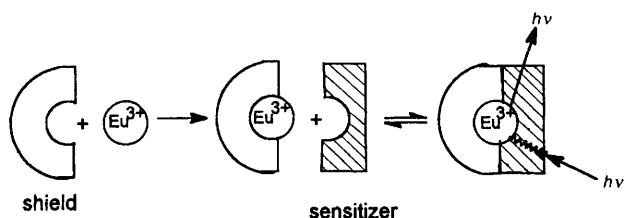
1275 **Enhancement of luminescence of europium(III) ions in water by use of synergistic chelation. Part 1. 1:1 and 2:1 complexes**

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



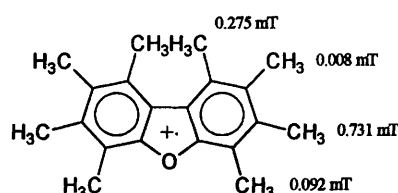
1283 **Enhancement of luminescence of europium(III) ions in water by use of synergistic chelation. Part 2. 1:1:1 complexes**

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



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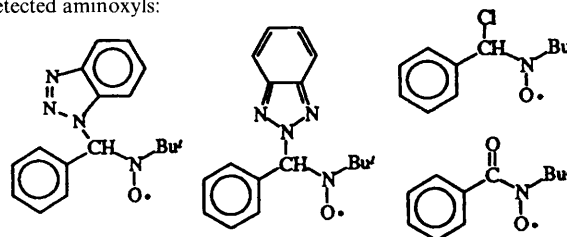
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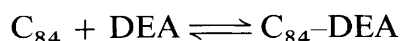
Patricia Carloni, Lennart Eberson, Lucedio Greci, Paolo Sgarabotto and Pierluigi Stipa

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



1311 **^{115}Sn NMR spectroscopy: a useful satellite pattern assignment method in gem-distannyl compounds**

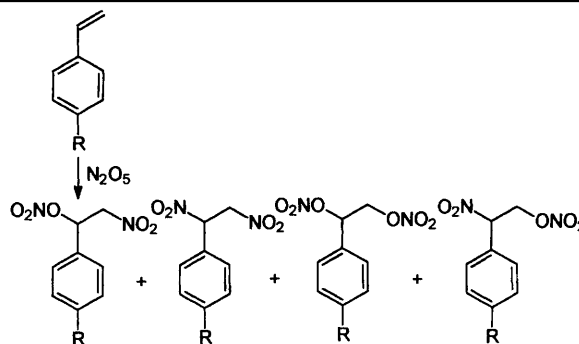
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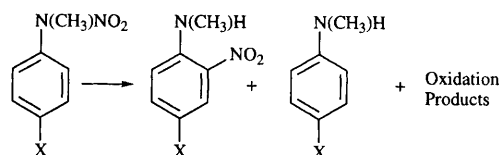
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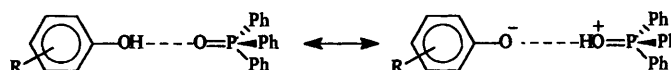


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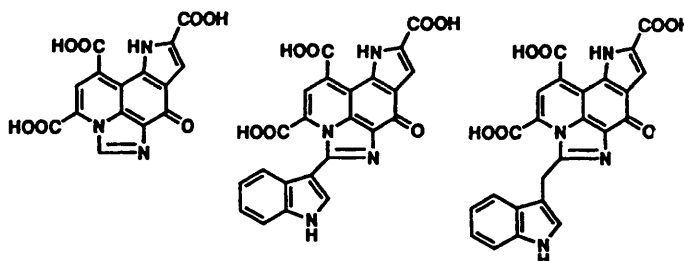
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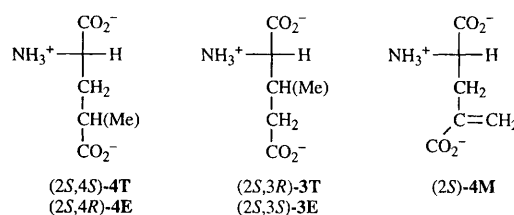
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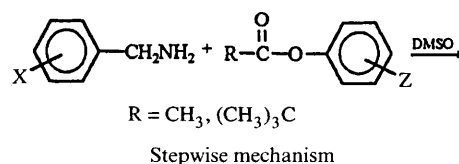
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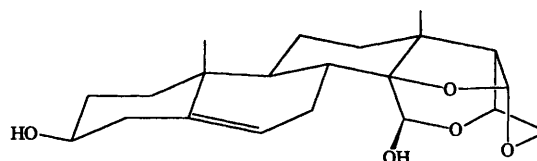
1353 Kinetics and mechanism of aminolysis of phenyl acetates and phenyl trimethylacetates in dimethyl sulfoxide

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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**

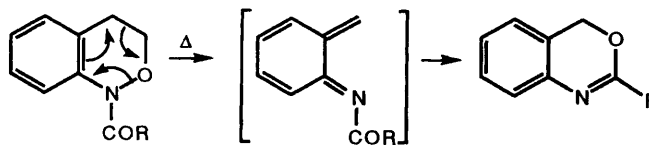
Edson S. Bento, João B. Calixto, Geoffrey E. Hawkes, Moacir G. Pizzolatti, Antonio E. G. Sant'Ana and Rosendo A. Yunes



The structure of velutinol A, a potent bradykinin antagonist, has been confirmed by the combined use of quantitative interproton NOEs and molecular mechanics and dynamics calculations

- 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**

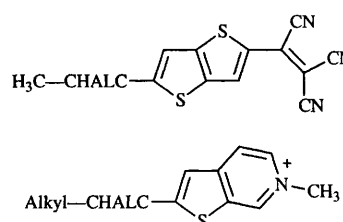
Stephen A. Glover, Katherine M. Jones, Ian R. McNee and Colleen A. Rowbottom



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

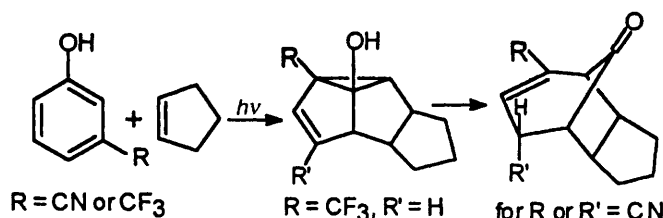
- 1377 **Chalcogens as electron donors for selected nonlinear optic phores**

Martin Blenkle, Peter Boldt, Christoph Bräuchle, Walter Grahn, Isabelle Ledoux, Heiko Nerenz, Stefan Stadler, Jürgen Wichern and Joseph Zyss



- 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



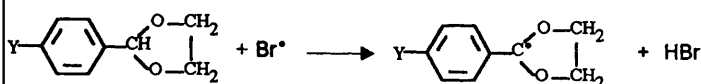
R = CN or CF₃

R = CF₃, R' = H

for R or R' = CN

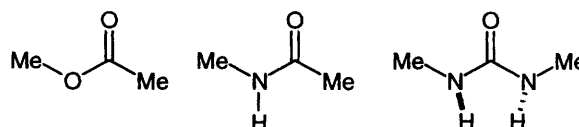
- 1391 **How does an alkoxy group at the benzylic carbon affect the transition state of the hydrogen-atom abstraction reaction? Correlation analysis of relative rates for 14 *p*-Y-substituted α,α -ethylene-dioxytoluenes**

Xi-Kui Jiang, Yu-Huang Zhang and William Fa-Xiang Ding



- 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

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

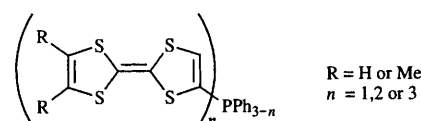
Bernd Kallies and Rolf Mitzner



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

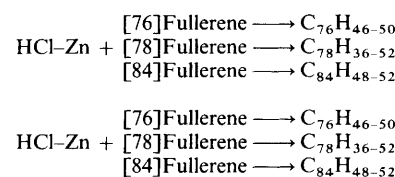
- 1409 Oxidation of phosphines containing two or three tetrathiafulvalene (TTF) or *o*-dimethyl-TTF moieties. Evidence for formation of radical polycations

Fabian Gerson, Axel Lamprecht and Marc Fourmigué



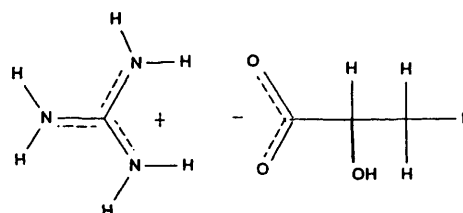
- 1415 Hydrogenation of [76]-, [78]- and [84]-fullerenes: cage degradation

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

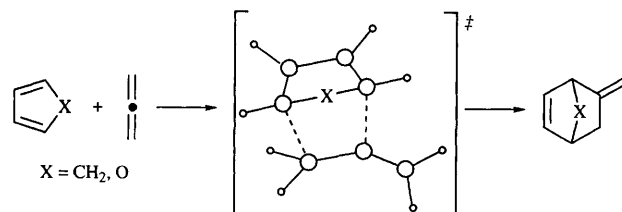
Péter Horváth, András Gergely and Béla Noszál



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

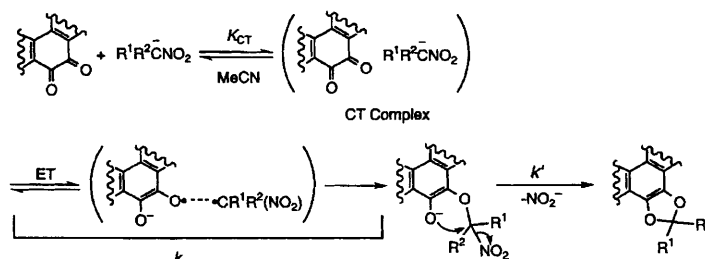
- 1423 Allene and fluoroallenes as dienophiles in Diels–Alder reactions: an AM1 and PM3 study

Mariappan Manoharan and Ponnambalam Venuvanalingam



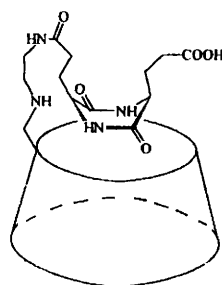
- 1429 Addition–cyclization reaction of nitroalkane anions with *o*-quinone derivatives via electron transfer in the charge-transfer complexes

Shinobu Itoh, Junichi Maruta and Shunichi Fukuzumi



1435 **Synthesis and high field NMR study of a new cyclodipeptide- β -cyclodextrin derivative**

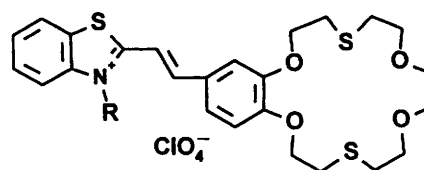
Giuseppe Impellizzeri, Giuseppe Pappalardo, Enrico Rizzarelli and Corrado Tringali



The synthesis and high field NMR study of a new cyclodipeptide functionalized- β -cyclodextrin β -CDen-c-(Glu-Glu) (3) in aqueous solution are reported

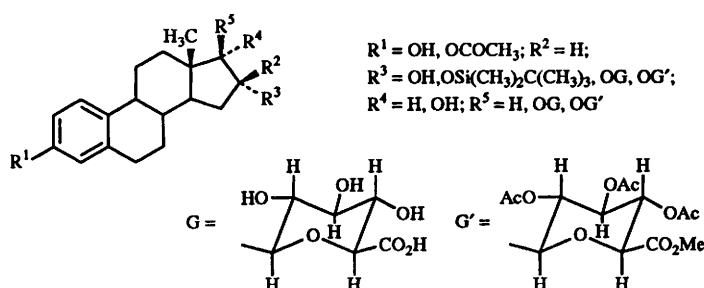
1441 **Synthesis and spectroscopic studies of novel photochromic benzodithiacrown ethers and their complexes**

Michael V. Alfimov, Yuri V. Fedorov, Olga A. Fedorova, Sergey S. Gromov, Ronald E. Hester, Igor K. Lednev, John N. Moore, Vladimir P. Oleshko and Artem I. Vedernikov



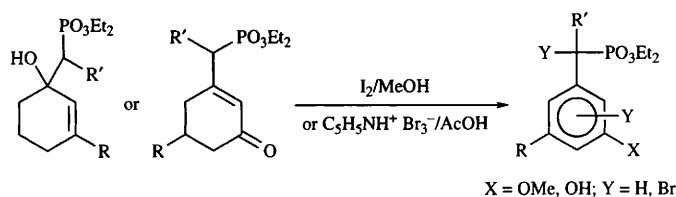
1449 **X-Ray crystal structure analysis and ^{13}C NMR investigation of estriol 16- and 17-monoglucuronide derivatives**

Wu Yinqiu, Joyce M. Waters and Leonard F. Blackwell



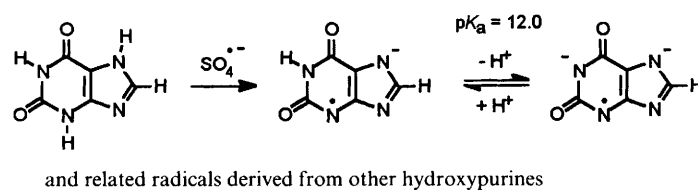
1455 **Reaction of phosphorus-stabilized carbanions with cyclic enones. Aromatization of the substitution and addition products**

Malose J. Mphahlele, André Pienaar and Tomasz A. Modro



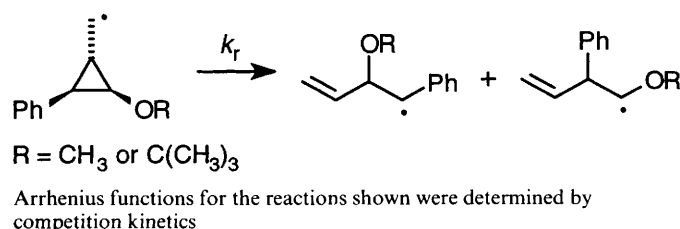
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Stephen R. Langman, M. Cândida B. L. Shohoji, João P. Telo, Abel J. S. C. Vieira and Horácio M. Novais



1467 **Picosecond radical kinetics. Rate constants for ring openings of (2-alkoxy-3-phenyl-cyclopropyl)methyl radicals**

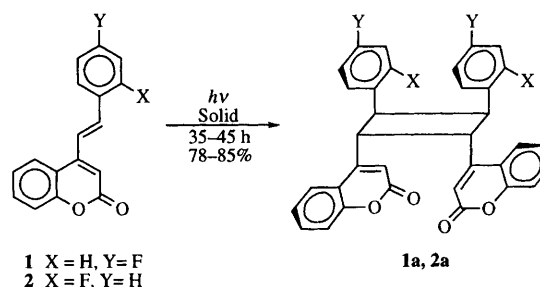
Marie-Hélène Le Tadic-Biadatti and Martin Newcomb



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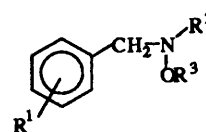
- 1475 **Studies in crystal engineering: effect of fluorine substitution in crystal packing and topological photodimerization of styryl coumarins in the solid state**

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**

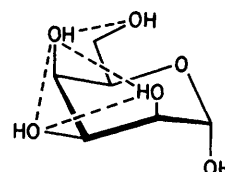
Sk. Asrof Ali, Azfar Hassan and Mohammed I. M. Wazeer



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

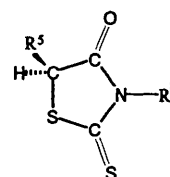
- 1485 **Intramolecular hydrogen bonds in monosaccharides in dimethyl sulfoxide solution**

Stephen J. Angyal and John C. Christofides



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

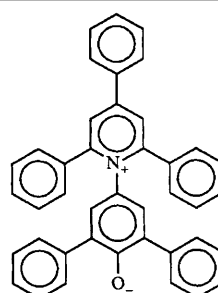
Knut Rang, Roland Isaksson and Jan Sandström



Chromatographic enantiomer separation, stereochemical stability and the UV and CD spectra of rhodanines, $R^5 = \text{Me}$ 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**

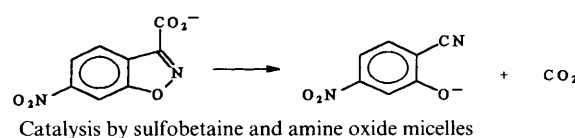
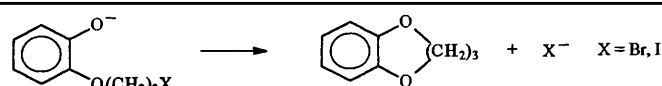
José Ortega, Clara Ràfols, Elisabeth Bosch and Martí Rosés



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



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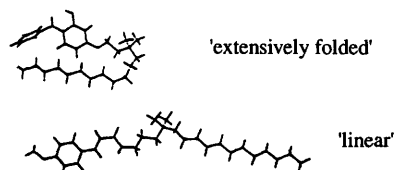
1511 Racemic compound formation–conglomerate formation. Part 3. Investigation of the acidic salts of α -phenylethylamine by achiral dicarboxylic acids. Optical resolution by preferential crystallization and a structural study of (*R*)- α -phenylethylammonium hydrogen itaconate

Zsolt Böcskei, Csaba Kassai, Kálmán Simon, Elemér Fogassy and Dávid Kozma

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 (*R*)- α -phenylethylammonium hydrogen itaconate and its optical resolution by preferential crystallization is described

1517 Comparative conformational and dynamical study of some *N*-quaternarized UV filters: structure–activity relationships

Cecilia Anselmi, Marisanna Centini, Marco Francioli and Alessandro Segà



The main conformers are dependent on structure and/or solvent

Corrigendum

- 1525 EPR studies of pyrazoline radicals that are potential precursors to non-Kekulé polyene radicals ions** Richard J. Bushby and Kai M. Ng

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9th International Symposium on Molecular Recognition and Inclusion

Lyon, France 7-12 September 1996

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