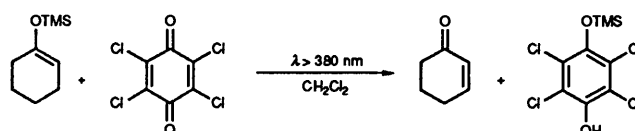


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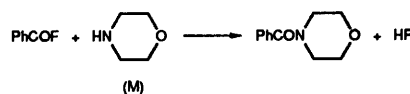
Perkin Communications

- 595 Dehydrosilylation *versus* α -coupling in the electron-transfer of enol silyl ethers to quinones. Strong solvent effect on photogenerated ion pairs



T. Michael Bockman, Serge Perrier and Jay K. Kochi

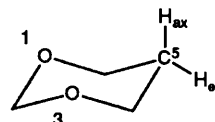
- 599 The kinetics of aminolysis of acyl halides



$$-d[\text{PhCOF}]/dt = \{k_1[\text{M}] + k_2[\text{M}]^2\}[\text{PhCOF}]$$

Maria Jedrzejczak, Richard E. Motie and Derek P. N. Satchell

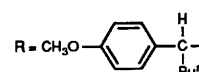
- 601 An NMR and *ab initio* MO study of the effect of β -oxygen in 1,3-dioxanes



The effect at the 5-position of the two β -oxygen atoms is to reduce $^1J_{\text{C-H}_{\text{eq}}}$ (ca. 125 Hz) below $^1J_{\text{C-H}_{\text{ax}}}$ (ca. 132 Hz)

J. Edgar Anderson, A. J. Bloodworth, Jiaqiang Cai, Alwyn G. Davies and Carl H. Schiesser

- 603 The acetolysis of 2,2-dimethyl-1-(*p*-methoxyphenyl)propyl chloride.—The first example of $\text{S}_{\text{N}}2\text{C}^+$ -type solvolysis under typical solvolysis conditions in the absence of additives

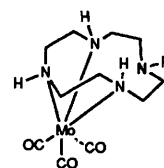


Tomomi Kinoshita, Hiroshi Ueda and Ken'ichi Takeuchi

Articles

- 605 **Synthesis of charged and uncharged complexes of gadolinium and yttrium with cyclic polyazaphosphinic acid ligands for *in vivo* applications**

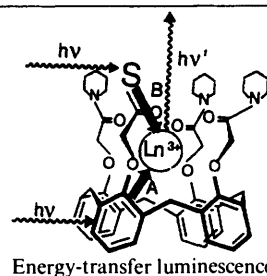
Kanthi P. Pulukkody, Timothy J. Norman, David Parker, Louise Royle and (in part) Christopher J. Broan



Charged and uncharged complexes of gadolinium and yttrium (stable *in vivo*) have been prepared and characterised. Uncharged and cationic ligands were prepared using the monoalkylated 12-N-4 cycle

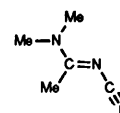
- 621 **Energy-transfer luminescence of lanthanide ions encapsulated in sensitizer-modified calix[4]arenes**

Nariaki Sato and Seiji Shinkai



- 625 **Super-basic nitriles**

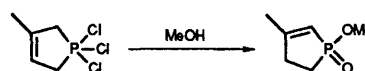
Michel Berthelot, Maryvonne Helbert, Christian Laurence, Jean-Yves Le Questel, Frederick Anvia and Robert W. Taft



This nitrile is more basic than amines on the hydrogen-bonding basicity scale

- 629 **Improved synthesis of 1-methoxy-3-methyl-2-phospholene oxide utilising multivariate optimization analysis**

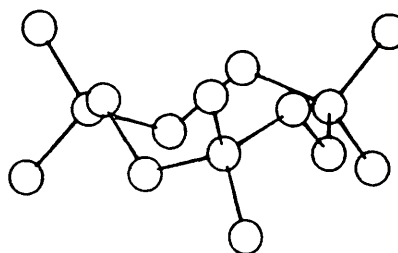
Gregory V. Coleman, Dennis Price, A. Richard Horrocks and James E. Stephenson



Multivariate optimization increased yield from 25% to >90%

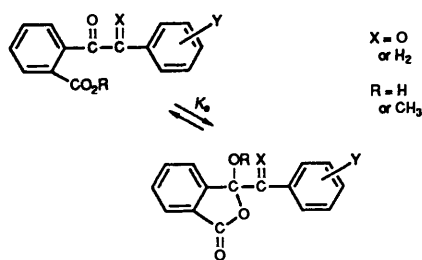
- 633 **1,1,4,4,7,7-Hexamethylcyclononane: synthesis and crystal structure**

Paul Binger, Hannelore Schäfer and Richard Goddard



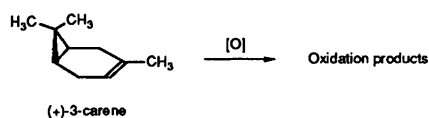
- 635 **Ring-chain tautomerism. Part 7.¹ Substituted benzil-2-carboxylic and 2-phenylacetylbenzoic acids and their methyl esters**

Keith Bowden and Faisal P. Malik



- 641 **Oxygen-containing bicyclic monoterpenes. ¹H, ¹³C and ¹⁷O NMR spectroscopic and X-ray diffraction studies of seven oxidation products of (+)-3-carene**

Erkki Kolehmainen, Katri Laihia, Mika Heinänen, Kari Rissanen, Roland Fröhlich, Jorma Korvola, Pia Mänttari and Reijo Kauppinen



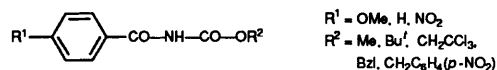
- 649 **Basicity (pK_{BH}) and acidity constants (pK_a^*) of some 3-X-, 4-X-, and 2,6-dimethyl-4-X-benzoic acids**

Paolo De Maria, Antonella Fontana, Domenico Spinelli, Carlo Dell'Erba, Marino Novi, Giovanni Petrillo and Fernando Sancassan

Substituent effects on pK_{BH} and pK_a^* in some benzoic acids have been compared with those in 2,6-dimethyl analogues where steric inhibition to coplanarity between the carboxyl group and the aromatic ring is sizeable

- 655 **Acidity of benzoylcarbamates in dimethyl sulfoxide. Confirmation of mixed *N/O* alkylation in the Mitsunobu reaction**

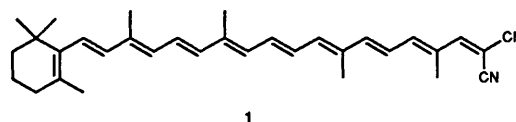
Ilmar Koppel, Juta Koppel, Ivar Koppel, Ivo Leito, Viljar Pihl, Annelie Wallin, Leif Grehn and Ulf Ragnarsson



The above compounds have been made, their pK_a s in dimethyl sulfoxide determined and selected derivatives reacted under Mitsunobu conditions

- 659 **AM1 Electron density and NMR spectral studies of carotenoids with a strong terminal electron acceptor**

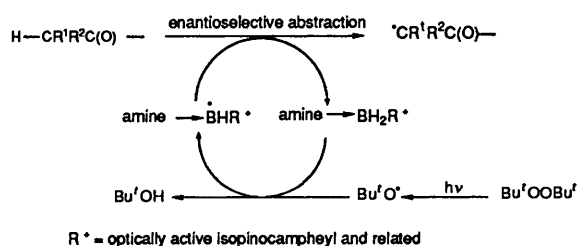
Elli S. Hand, Kenneth A. Belmore and Lowell D. Kispert



NMR spectral analyses and AM1 calculated electron densities of 1 are used to assess the effect of a terminal strong electron acceptor on the structure of carotenoids

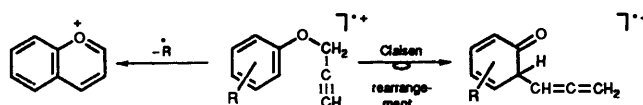
- 665 **Homolytic reactions of ligated boranes. Part 16. Enantioselective hydrogen-atom abstraction by chiral amine-boryl radicals: catalytic kinetic resolution of esters and of camphor**

Pearl L. H. Mok, Brian P. Roberts and (in part) Paula T. McKetty



- 675 Claisen rearrangements and cyclisations in phenyl propargyl ethers under electron impact conditions

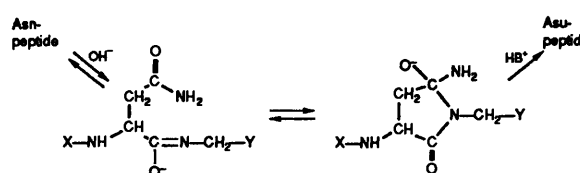
Devalla V. Ramana and Marimanikuppam S. Sudha



Phenyl propargyl ethers undergo both Claisen rearrangement and cyclisation reactions on electron impact

- 679 Kinetics and mechanism of succinimide ring formation in the deamidation process of asparagine residues

Sante Capasso, Lelio Mazzarella, Filomena Sica, Adriana Zagari and Severo Salvadori



Proposed mechanism for Aminosuccinyl (Asu) formation

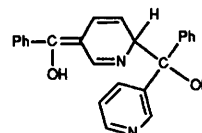
- 683 Reactivity of planar and twisted amides in vacuum and aqueous environments: an *ab initio* MEP study

Francisco J. Luque and Modesto Orozco



- 691 The photoreduction of 3-benzoylpyridine: an experimental and theoretical study of the formation of the intermediate LAT

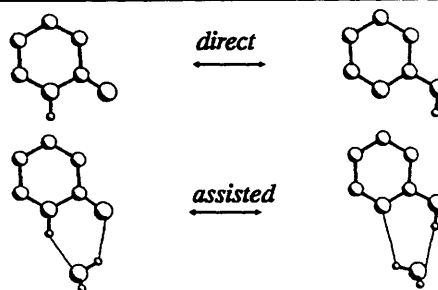
Angelo Albini, Pietro Bortolus, Elisa Fasani, Sandra Monti, Fabrizia Negri and Giorgio Orlandi



Evidence is given for the structure of the LAT of 3-benzoylpyridine as an aromatic ketyl radical dimer

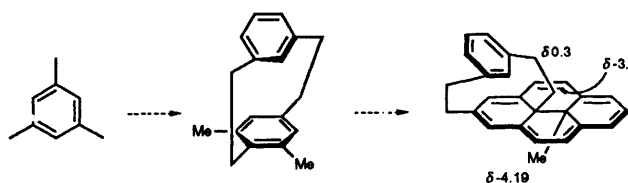
- 697 Protomeric equilibria in the ground and excited states of 2-pyridone. A semiempirical study including solvent effects

Carlo Adamo, Vincenzo Barone, Sandrine Loison and Camilla Minichino



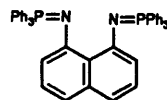
- 703 Synthesis and diatropicity of a *trans*-10c-methyl-10b,10c-dihydropyrene-containing cyclophane: a novel aromatic molecule with a (1,3)cyclophane within the π -cloud of a [14]annulene

Yee-Hing Lai and Angeline Hui-Tin Yap



- 709 **Iminophosphorane-substituted proton sponges. Part 4. Comparison of X-ray molecular structures with solution properties (pK_a , 1H and ^{13}C NMR spectroscopy)**

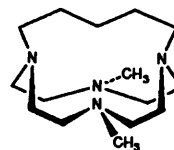
José Laynez, Margarita Menéndez, José Luis Saiz Velasco, Antonio L. Llamas-Saiz, Concepción Foces-Foces, José Elguero, Pedro Molina, Mateo Alajarin and Angel Vidal



The basicity of the above compound has been estimated to be $pK_a = 15.64$ in water at 25 °C, much higher than that of 1,8-bis(dimethylamino)naphthalene (DMAN, $pK_a = 12.1$)

- 715 **Synthesis and characterization of an aza-cage, basicity behaviour and crystal structure of its diprotonated species**

Andrea Bencini, Antonio Bianchi, Carla Bazzicalupi, Mario Ciampolini, Paolo Dapporto, Vieri Fusi, Mauro Micheloni, Nicoletta Nardi, Paola Paoli and Barbara Valtancoli



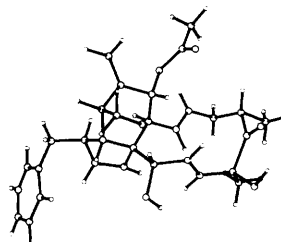
- 721 **Aromatic sulfonation. Part 120. Reaction of dihydroxy- and dimesyloxy-naphthalenes with sulfur trioxide in nitromethane. Directing effects and the influence of initial sulfation on the product distributions**

Harold R. W. Ansink, Erwin Zelveler, Erik J. de Graaf and Hans Cerfontain

The mono- and di-sulfonation of a series of dihydroxy- and dimesyloxy-naphthalenes with SO_3 has been studied: the influence of initial hydrogen sulfate information with the former type of substrates is discussed

- 729 **The conformation of cytochalasin D in DMSO solution from 1H and ^{13}C NMR relaxation rates**

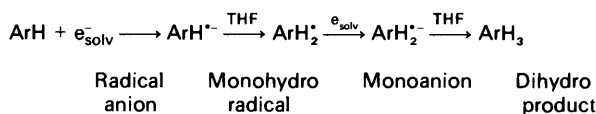
Antonella Maccotta, Gianni Valensin, Nicola Gaggelli and Elena Gaggelli



Molecular model of cytochalasin D in DMSO solution was obtained with the aid of NMR parameters. The conformation is similar to that of cytochalasin B in the same solvent

- 733 **Transients formed during reduction of polynuclear aromatics: a pulse radiolysis study**

Tomi Nath Das and K. Indira Priyadarsini



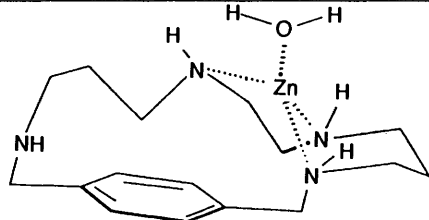
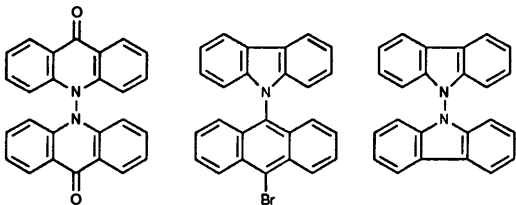

Reduction scheme for polynuclear aromatics in the presence of solvated electron

- 741 **Latent inhibitors. Part 9. Substrate activated time-dependent inhibition of carboxypeptidase A by aminocyclopropanecarboxylic acid derivatives and analogues**

Alison Kemp, Surjit K. Ner, Liliias Rees, Colin J. Suckling, M. Catriona Tedford, Andrew R. Bell and Roger Wrigglesworth



R = Ph, Pro
 = COR', CH(OH)R'
 = COCH₂SO₂R'

<p>749 Polyazacyclophanes. 2,6,9,13-Tetraaza[14]paracyclophane as a cationic and anionic receptor</p> <p>Antonio Andrés, M. Isabel Burguete, Enrique García-España, Santiago V. Luis, Juan E. Miravet and Conxa Soriano</p>	 <p>2,6,9,13-Tetraaza[14]paracyclophane shows some interesting properties in its interaction with anions and cations</p>
<p>757 Synthesis and structure of new hosts related to 9,9'-bianthryl</p> <p>Gérard Boyer, Rosa M. Claramunt, José Elguero, Mohamed Fathallah, Concepción Foces-Foces, Carlos Jaime and Antonio L. Llamas-Saiz</p>	 <p>The molecular structures of the above compounds are reported</p>
<p>767 Oxidative behaviours and relative reactivities of some alkanols and aryl alcohols towards bis(dihydrogentellurato)-cuprate(III) and -argentate(III) in alkaline medium</p> <p>Kalyan Kali Sen Gupta, Bijay Kumar Nandy and Shipra Sen Gupta</p>	$R^1R^2CHOH + M^{III} \xrightarrow{OH^-} R^1R^2\dot{C}OH + M^{II}$ $R^1R^2\dot{C}OH + M^{III} \longrightarrow R^1R^2CO + M^{II}$ $M^{III} = [Ag^{III} \text{ or } Cu^{III}(H_2TeO_6)_2]^{5-}$ $R^1, R^2 = H, \text{ alkyl, aryl}$
<p>773 Using theoretical descriptors in quantitative structure–activity relationships: gas phase acidity</p> <p>George R. Famini, Benjamin C. Marquez and Leland Y. Wilson</p>	<p>Gas phase acidity parameters for some carboxylic acids, alcohols, anilines, silanols, hydrocarbons and oximes are correlated with computationally derived molecular parameters involving size, polarizability, acidity and basicity.</p>
<p>783 Proton transfer from carbon. A study of the acid–base-catalysed relaxation and the bromination of aryl-substituted methane-disulfones</p> <p>Fiona Aiken, Brian G. Cox and Poul E. Sørensen</p>	 <p>Proton transfer from an aryl- and sulfonyl-activated carbon acid</p>

Corrigendum

- 791 **Reactivity of nucleophilic nitrogen compounds towards the nitroso group** Luis Garcia-Rio, Emilia Iglesias, J. Ramon Leis, M. Elena Pena and Ana Rios

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

