

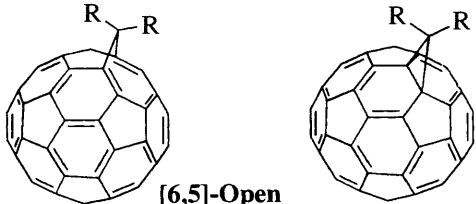
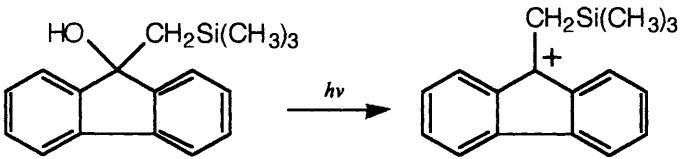
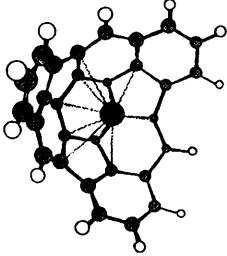
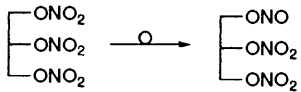
JOURNAL OF THE CHEMICAL SOCIETY

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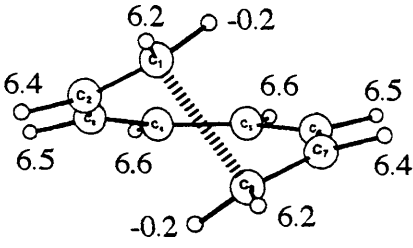
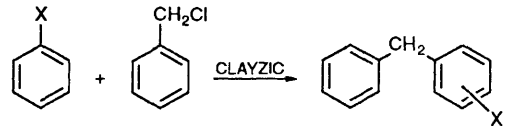

Physical Organic Chemistry

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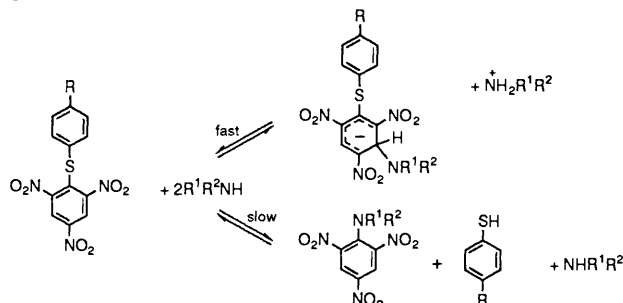
<p>391 Valence isomerism and rearrangements in methanofullerenes</p> <p>François Diederich, Lyle Isaacs and Douglas Philp</p>	 <p>PM3 computational and experimental study of the relative stabilities and interconversions of isomeric methanofullerenes</p>
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Articles

<p>405 The Honig–Flory–Huggins combinatorial entropy correction—is it valid for aqueous solutions?</p> <p>Michael H. Abraham and Panos Sakellariou</p>	<p>The Honig–Flory–Huggins combinatorial entropy correction, given as $-\Delta S = R(1-r)$, is not appropriate for dilute solutions in water</p>
<p>407 Evidence for the Möbius aromatic character of eight π electron conrotatory transition structure. Magnetic criteria</p> <p>Haijun Jiao and Paul von Ragué Schleyer</p>	
<p>411 Activation of clayzic and its effect on the relative rates of benzylation of aromatic substrates</p> <p>Simon J. Barlow, Tony W. Bastock, James H. Clark and Stephen R. Cullen</p>	 <p>X = H \approx F < Cl < Br, I (Unactivated catalyst), X = F < Cl < Br < H (<I) (Activated catalyst)</p> <p>Unexpected and activation dependent rate trends are observed in the Clayzic catalysed benzylations of benzene and the halobenzenes</p>
<p>415 Kinetics of the enolisation reactions of 2-acetylpyrrole and of 2-, 4- and 5-acetylthiazoles</p> <p>Paolo De Maria, Antonella Fontana, Marialuisa Arlotta, Stefano Chimichi and Domenico Spinelli</p>	<p>Kinetic results are reported on the rates of enolisation of title compounds in water, acetate buffers, hydrochloric acid, sodium hydroxide solutions and in the presence of metal-ion salts (Li^+, Cu^{2+}, Ni^{2+}, Cd^{2+} and Zn^{2+}). Metal catalysis is particularly effective with 'soft' acetyl groups (2-acetylpyrrole) or with ketones that can coordinate the metal cation through both the carbonyl oxygen and the heteroatom (2- and 4-acetylthiazoles)</p>
<p>421 Condensation products from the reactions of glyoxal with 2-substituted benzylamines. The formation and crystal structures of 2,2'-bi(1,2,3,4-tetrahydroquinazoline), and 2,4,6,8,10,12-hexakis(2-methylbenzyl)-2,4,6,8,10,12-hexaazaisowurtzitane</p> <p>Andrei Batsanov, Jason C. Cole, Michael R. Crampton, Javid Hamid, Judith A. K. Howard and Ross Millar</p>	

425 **Kinetic studies of the reactions of some phenyl aryl sulfides with aliphatic amines in dimethyl sulfoxide; the mechanism of base catalysis**

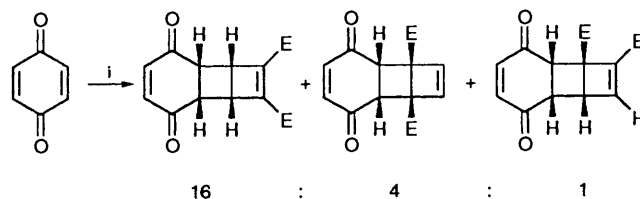
Rachel A. Chamberlin and Michael R. Crampton



Base catalysis in the substitution reaction is attributed to rate limiting proton transfer from a zwitterionic intermediate to amine

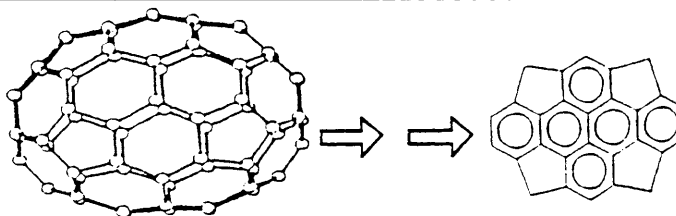
433 **An approach to functionalized cubanes. Regioselectivities and frontier molecular orbital analysis in the addition of dimethyl cyclobutadiene-1,2-dicarboxylate to quinones**

Goverdhan Mehta, M. Balaji Viswanath, Eluvathingal D. Jemmis and G. Narahari Sastry



437 **Synthetic strategies towards C₇₀: molecular mechanics and MNDO calculations on pinakene, C₂₈H₁₄ and related molecules**

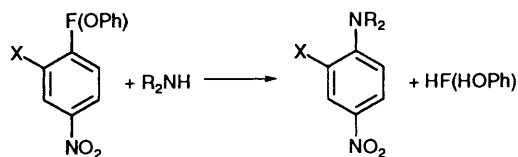
Eluvathingal D. Jemmis, G. Narahari Sastry and Goverdhan Mehta



Various synthetic approaches to pinakene, and from it to C₇₀, are discussed

443 **The origins of the dichotomy of amine effects in aromatic nucleophilic substitution reactions**

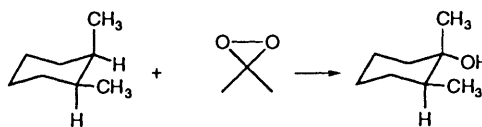
Raymond E. Akpojivi, Thomas A. Emokpae and Jack Hirst



Effect of X (NO₂, CF₃, CN) on mechanism of reaction of primary and secondary amines

451 **Dioxirane chemistry. Part 25. The effect of solvent on the dimethyldioxirane carbon-hydrogen bond insertion reaction**

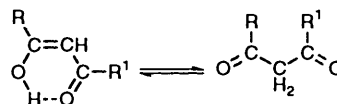
Robert W. Murray and Daquan Gu



Hydrogen bond donor solvents increase the rate of the insertion reaction

455 **Quantitative analysis of solvent effects on the keto-enol equilibrium of pentane-2,4-dione in aqueous solutions**

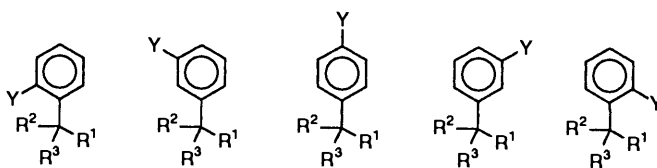
Wilfried Blokzijl, Jan B. F. N. Engberts and Michael J. Blandamer



A method is described for a quantitative analysis of solvent effects of monohydric alcohols on the keto-enol equilibrium of pentane-2,4-dione in dilute aqueous media

459 Rotational isomerism of disubstituted benzenes in the alkylphenyldi(1-adamanty)methanol series

John S. Lomas and Veronique Bru-Capdeville



$R^1 = \text{H or OH}; R^2 = R^3 = 1\text{-Ad}; Y = \text{Bu}^t \text{ (not } ortho \text{) or Me}$

467 Solvent effects on chemical processes. Part 7. Quantitative description of the composition dependence of the solvent polarity measure $E_T(30)$ in binary aqueous-organic solvent mixtures

Raymond D. Skwierzynski and Kenneth A. Connors

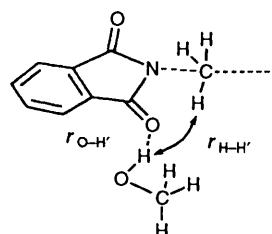
$$\Gamma = \frac{E_T(x_2) - E_1}{E_2 - E_1} = \frac{K_1 x_2}{x_1 + K_1 x_2}, \text{ if } E_2 > 47 \text{ or } \log P < -1$$

otherwise

$$\Gamma = \frac{K_1 x_1 x_2 / 2 + K_1 K_2 x_2^2}{x_1^2 + K_1 x_1 x_2 + K_1 K_2 x_2^2}$$

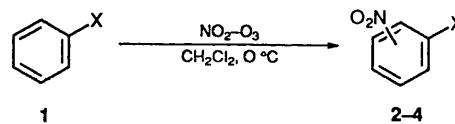
473 Characterization of solute-solvent interaction at the transition state by thermodynamic and quantum-mechanical approaches. Reactions of imide ions with ethyl iodide in acetonitrile-methanol

Yasuhiko Kondo, Osamu Nonaka, Kazuhiko Iwasaki, Tomoyuki Kuwamoto and Tatsuya Takagi



479 Ozone-mediated nitration of chloro- and bromo-benzenes and some methyl derivatives with nitrogen dioxide. High *ortho*-directing trends of the chlorine and bromine substituents

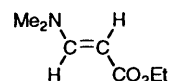
Hitomi Suzuki and Tadashi Mori



$o:p$ 1.14-0.45 ($X = \text{Cl}$), 1.11-0.68 ($X = \text{Br}$)

485 Hydrogen-bond basicity of esters, lactones and carbonates

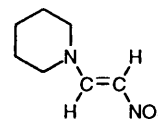
François Besseau, Christian Laurence and Michel Berthelot



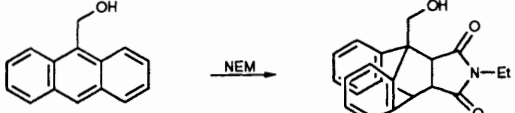
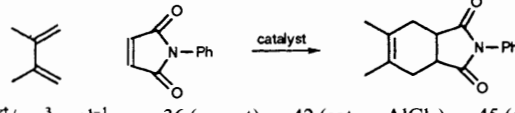
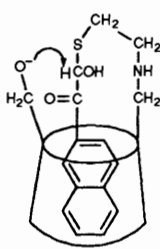
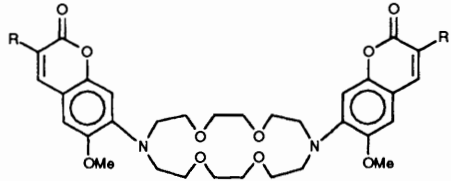
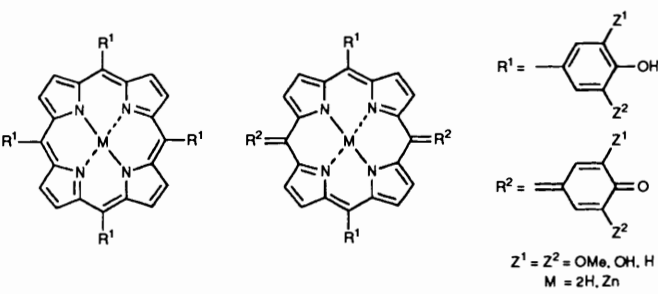
The compound shown is more basic on the pK_{HB} or β_2^{H} scales than Et_3N

491 Hydrogen-bond basicity of nitro-compounds

Christian Laurence, Michel Berthelot, Maryvonne Lucon and David G. Morris

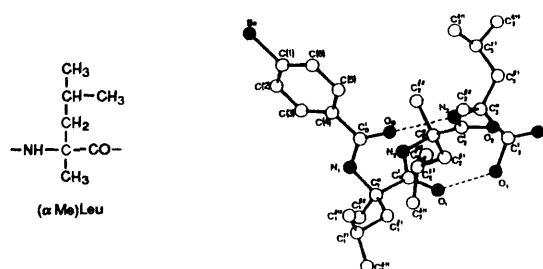


The nitro compound shown reaches the basicity of Bu_3N on the pK_{HB} or β_2^{H} scales

495 Volumes of activation for catalysed Diels–Alder reactions	 <p>$\Delta V^\ddagger/\text{cm}^3 \text{ mol}^{-1} = 36$ (water); -31 (butan-1-ol); -22 (heptane)</p>  <p>$\Delta V^\ddagger/\text{cm}^3 \text{ mol}^{-1} = -36$ (no cat); -42 (cat = AlCl_3); -45 (cat = LiClO_4)</p>
Neil S. Isaacs, Ljiliana Maksimovič and Abdulhameed Laila	
499 Laser-desorption mass spectrometry of standard polynuclear aromatic hydrocarbons and fullerenes	<p>Benzopyrene $\text{C}_{20}\text{H}_{12}$ (solid)</p> <p>LD-MS Nd: YAG 266 nm</p> <p>$\left\{ \begin{array}{l} \text{C}_{20}\text{H}_{(11-15)}^+ \\ \text{pseudo-molecular ions} \\ + \\ \text{C}_{(1-19)}\text{H}_{(0-3)}^{(+ \text{ or } -)} \\ \text{carbon clusters} \end{array} \right.$</p>
Alan A. Herod, Brian J. Stokes, Paul Hancock, Rafael Kandiyoti, John E. Parker, Chris A. F. Johnson, Philip John and Gerry Smith	
507 Mono[6-(2-mercaptoethylamino)-6-deoxy]-β-cyclodextrin as an efficient glyoxalase mimic	
Seizo Tamagaki, Atsushi Katayama, Masahiko Maeda, Noritaka Yamamoto and Waichiro Tagaki	
513 Synthesis and spectral properties of new fluorescent probes for potassium	 <p>1 R = CO_2H 2 R = H</p>
Roger Crossley, Zia Goolamali, Jeffrey J. Gosper and Peter G. Sammes	Compounds 1 and 2 behave as selective, fluorescent potassium probes
521 Facile aerial oxidation of porphyrins. Part 16. Phenolic porphyrins without <i>tert</i>-butyl substituents	 <p>$\text{R}^1 = \text{---} \text{C}_6\text{H}_3(\text{OH}) \text{---}$ $\text{R}^2 = \text{---} \text{C}_6\text{H}_3(\text{O}) \text{---}$ $\text{Z}^1 = \text{Z}^2 = \text{OMe, OH, H}$ $\text{M} = 2\text{H, Zn}$</p>
Lionel R. Milgrom, Jonathan P. Hill and William D. Flitter	Non- <i>tert</i> -butyl-substituted phenolic porphyrins undergo aerial oxidation in acidic and basic solutions to yield radicals with apparent extensive delocalisation of the unpaired electron

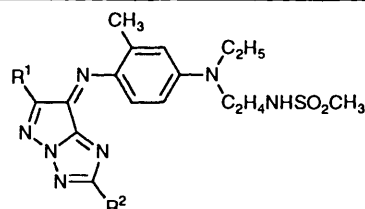
525 **Position of side-chain branching and handedness of turns and helices of homopeptides from chiral C^α-methylated amino acids. Crystal-state structural analysis of (αMe)Leu trimer and tetramer**

André Aubry, Daniel Bayeul, Gilles Précigoux, Monica Pantano, Fernando Formaggio, Marco Crisma, Claudio Toniolo, Wilhelmus H. J. Boesten, Hans E. Schoemaker and Johan Kamphuis



531 **Photochemical reactions of 1*H*-Pyrazolo[1,5-*b*][1,2,4]triazole azomethine dyes**

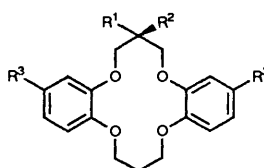
Kazuhiko Furuya, Nobuo Furutachi, Shohei Oda and Kazuhiro Maruyama



The fluorescence of dimers of pyrazolotriazole dyes is quenched by spiroindane derivatives

537 **Conformational studies of substituted dibenzo-14-crown-4 ethers: a 1-D and 2-D ¹H and ¹³C NMR investigation**

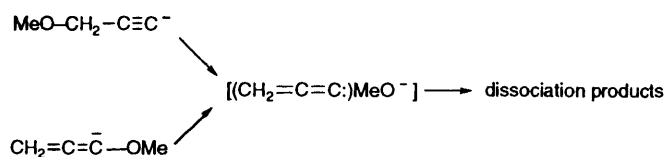
Zhihong Chen and Richard A. Sachleben



- 1 R¹ = R² = R³ = H
- 2 R¹ = CH₃, R² = R³ = H
- 3 R¹ = CH₂CH₂OH, R² = R³ = H
- 4 R¹ = CH₂CO₂H, R² = R³ = H
- 5 R¹ = CH₂CO₂H, R² = H, R³ = C(CH₃)₂CH₂C(CH₃)₃
- 6 R¹ = OH, R² = R³ = H
- 7 R¹ = OCH₃, R² = R³ = H
- 8 R¹ = OCH₂CH₂OH, R² = R³ = H
- 9 R¹ = OCH₂CO₂H, R² = H, R³ = C(CH₃)₂CH₂C(CH₃)₃

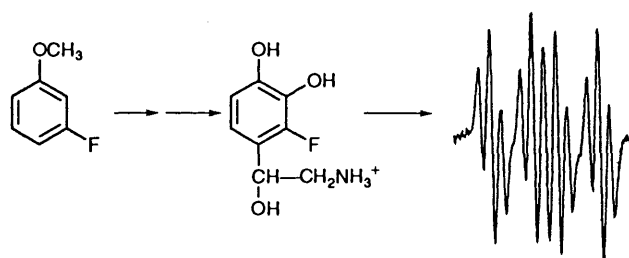
543 **Collision induced dissociations of carbanions in the gas phase: the formation of vinylidene carbene intermediates from deprotonated prop-2-ynyl ethers**

Suresh Dua, John H. Bowie and John C. Sheldon



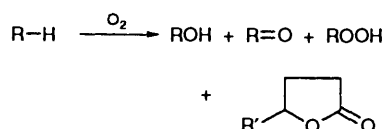
547 **Synthesis and EPR investigations of fluorocatecholamines**

Hartmut B. Stegmann, Gabriele Deuschle and Paul Schuler



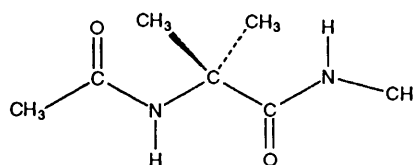
557 **Autoxidation of nonane and decane: a product study**

André Goosen and David H. Morgan



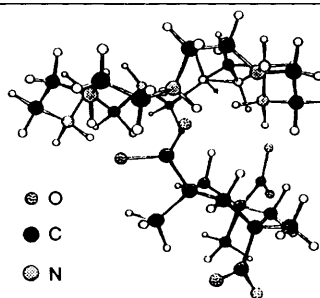
- 563 *Ab initio* SCF and force-field calculations on low-energy conformers of 2-acetylamino-2,N-dimethylpropanamide

Carlos Alemán and Jordi Casanovas



- 569 Selective recognition of carboxylate anions by polyammonium receptors in aqueous solution. Criteria for selectivity in molecular recognition

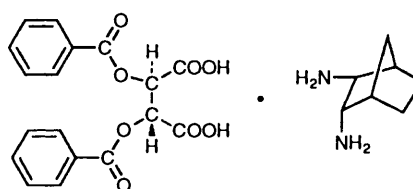
Andrea Bencini, Antonio Bianchi, M. Isabel Burguete, Paolo Dapporto, Antonio Doménech, Enrique García-España, Santiago V. Luis, Paola Paoli and José A. Ramírez



Interactions, in its protonated forms, of the macrocyclic receptor 1,4,7,10,13,16,19-heptaazacycloheptacosane with a series of di- and tri-carboxylic acids is described; potentiometric and electrochemical methods unambiguously define selectivity patterns independent of the degree of protonation of receptor and substrate

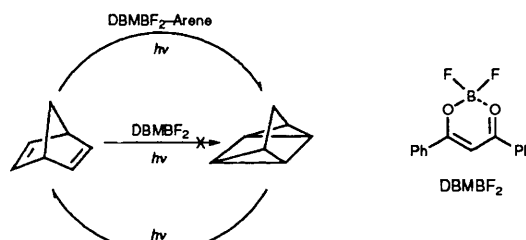
- 579 Optical resolution of *trans*-Bicyclo[2.2.1]heptane-2,3-diamine: chiral recognition in the crystal of its complex with (2*R*,3*R*)-*O*,*O'*-dibenzoyltartaric acid

Keiichiro Hatano, Tadahiro Takeda and Reiko Saito



- 585 Electron transfer photoisomerization of norbornadiene to quadricyclane cosensitized by dibenzoylmethanoboron difluoride and aromatic hydrocarbons

Zhong-Li Liu, Mao-Xi Zhang, Li Yang, You-Cheng Liu, Yuan L. Chow and Carl I. Johansson



The DBMBF₂-arene-NBD triplex is proposed to be responsible for the energetically unfavourable isomerization

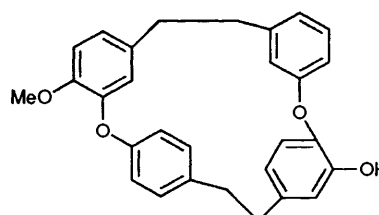
- 591 On the mechanism of the alkylation of quinoline and naphthyridine derivatives

Gergely Makara, György M. Keserű and Attila Kovács



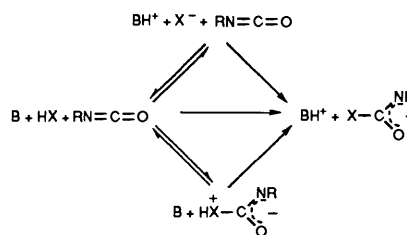
- 595 Crystal structure and conformation of pakyonol, a macrocyclic bis(bibenzyl) constituent of *Mannia fragrans*

Zsolt Böcskei and György M. Keserű



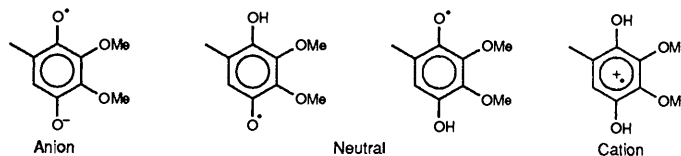
599 **Three fundamental mechanisms of base-catalysed reactions of isocyanates with hydrogen-acidic compounds**

Klaus Schwetlick, Rainer Noack and Fanziska Stebner



609 **ENDOR and EPR studies of highly isotopically ^{13}C -enriched ubiquinone radicals**

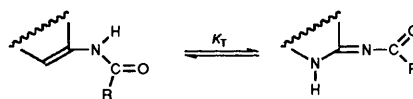
Rimma I. Samoilova, Willem van Liemt, Winand F. Steggerda, Johan Lugtenburg, Arnold J. Hoff, Andrei P. Spoyalov, Alexei M. Tyryshkin, Nina P. Gritzan and Yuri D. Tsvetkov



Ubiquinone 0 radicals

615 **Tautomerism in some acetamido derivatives of nitrogen-containing heterocycles: X-ray structural analysis of 2-amino and 2-imino forms of benzothiazole derivatives**

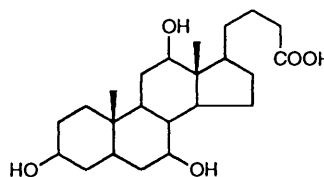
Marco Annese, Anna Bonamartini Corradi, Luciano Forlani, Corrado Rizzoli and Paolo Sgarabotto



A method for quantitative evaluation of tautomeric equilibrium is reported

623 **Inclusion compounds of cholic acid with aliphatic esters**

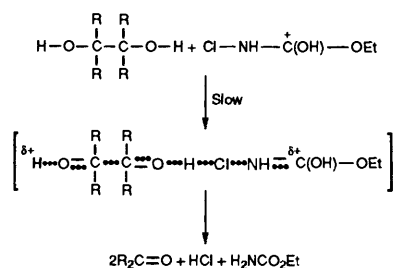
Mino R. Caira, Luigi R. Nassimbeni and Janet L. Scott



Cholic acid forms inclusion compounds with aliphatic esters crystallising in two packing motifs exhibiting different phases during decay

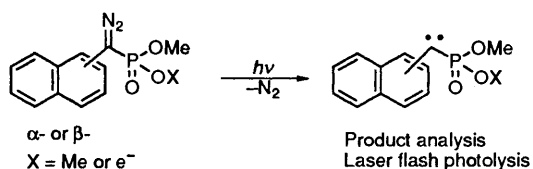
629 **Kinetics and mechanism of the oxidation of diols by ethyl *N*-chlorocarbamate**

Anjali Grover, Seema Varshney and Kalyan K. Banerji



633 **Chemistry and kinetics of α - and β -naphthyl(phosphonyl)carbenes. Effects of positions on neighbouring phosphonate participation**

Hideo Tomioka, Katsuyuki Hirai and Yoshifumi Tanimoto



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