ISSN 0300-9580 JCPKBH(12) 2561–2778(1996)

JOURNAL OF THE CHEMICAL SOCIETY

Physical Organic Chemistry

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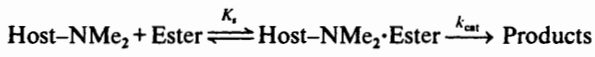
Communication

2561 **A calixresorcinarene provides the framework for an artificial esterase**

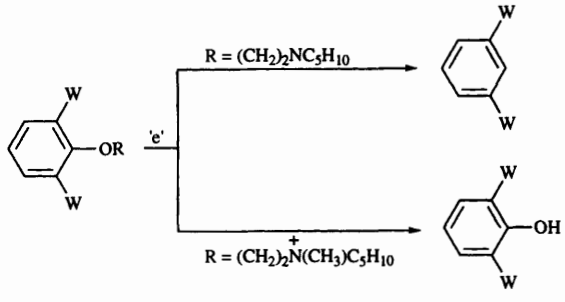
Necmettin Pirrincioglu, Flora Zaman and Andrew Williams



Articles

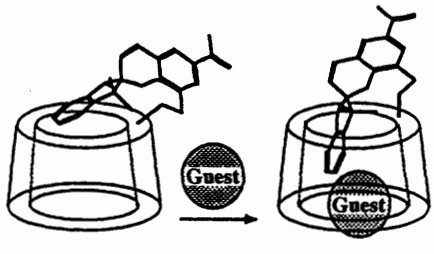
2563 **The effect of topologically controlled coulombic interactions on the regioselectivity of the reductive cleavage of alkyl phenyl ethers**

Ugo Azzena, Francisco Casado, Pierfrancesco Fois, Iluminada Gallardo, Luisa Pisano, Jordi Marquet and Giovanni Melloni



2567 **Photochromic molecular recognition of β-cyclodextrin bearing spiropyran moiety for organic guests**

Fumio Hamada, Koutarou Hoshi, Yutaka Higuchi, Kouichi Murai, Youichi Akagami and Akihiko Ueno



2571 **The kinetics and mechanism of the reaction of *p*-nitrocumyl bromide with azide ions in dimethyl sulfoxide. Evidence for a heterolytic reaction**

Stuart W. Paine and John H. Ridd

$$ArCMe_2Br + N_3^- \xrightarrow[(CD_3)_2SO]{} ArCMe_2N_3$$

Heterolytic, not $S_{RN}1$

2577 **The kinetics and mechanism of the reaction of *p*-nitrocumyl bromide with nitrite ions in dimethyl sulfoxide. Evidence for a non-chain reaction giving a high nitro/nitrite ratio in the product**

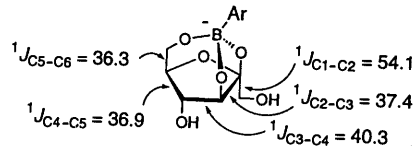
Stuart W. Paine and John H. Ridd

$$ArCMe_2Br + NO_2^- \xrightarrow[(CD_3)_2SO]{} \begin{matrix} ArCMe_2NO_2 \\ + \\ ArCMe_2ONO \end{matrix}$$

Not $S_{RN}1$, but with a high $[RNO_2]/[RONO]$ ratio

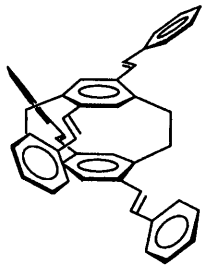
2583 **Boronic acids as fructose sensors. Structure determination of the complexes involved using $^1J_{CC}$ coupling constants**

Jens Chr. Norrild and Hanne Eggert



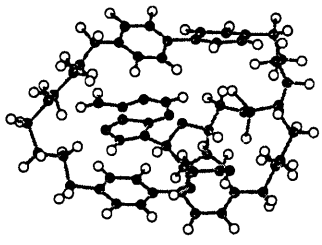
2589 **Charged cyclophanes with extended conjugation: the effect of the cyclophane hub on the charge distribution**

E. Shabtai, M. Rabinovitz, B. König, B. Knieriem and A. de Meijere



2597 **Nucleotide complexes with azoniacyclophanes containing phenyl-, biphenyl- or bipyridyl-units**

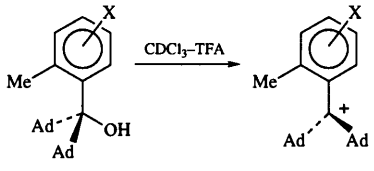
Kaliappa G. Ragunathan and Hans-Jörg Schneider



One cyclophane shows selectivity between AMP5′ and AMP3′ and the lowest affinity for GMP5′; and unusually a similar affinity for the pyrimidine nucleotide TMP5′. Another cyclophane shows the highest affinity for GMP5′

2601 **^{13}C NMR spectroscopic comparison of sterically stabilized *meta*- and *para*-substituted *o*-tolyldi(adamant-1-yl)methyl cations with conjugatively stabilized benzyl cations**

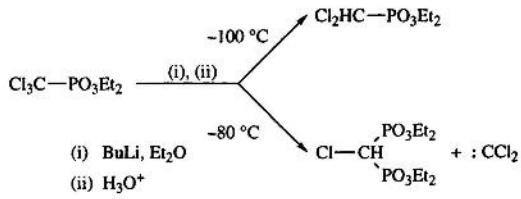
John S. Lomas



^{13}C NMR indicates some resonance stabilization

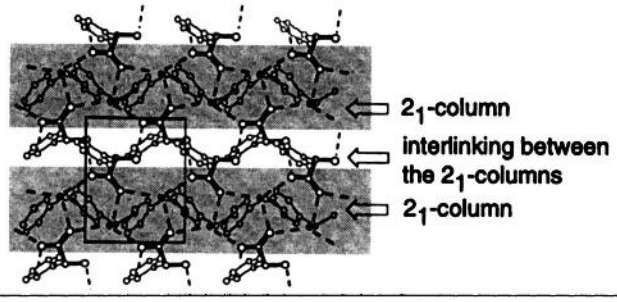
2611 **Lithiation of diethyl trichloromethylphosphonate and the transformations of the α-lithiated derivative**

Wieslawa Perlikowska, Agnes M. Modro, Tomasz A. Modro and Malose J. Mphahlele



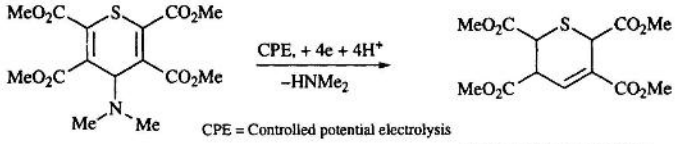
2615 **Chiral discrimination upon crystallisation of the diastereomeric salts of 1-arylethylamines with mandelic acid or *p*-methoxymandelic acid: interpretation of the resolution efficiencies on the basis of the crystal structures**

Kazushi Kinbara, Kenichi Sakai, Yukihiko Hashimoto, Hiroyuki Nohira and Kazuhiko Saigo



2623 **Electrochemical access to functionalized dihydrothiopyran derivatives. Part 1. Electroreduction of tetraactivated 4*H*-thiopyrans**

D. Rondeau, E. Raoult, A. Tallec, S. Sinbandhit, L. Toupet, A. Imberty and J. P. Pradère

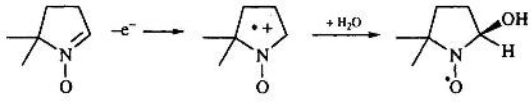


CPE = Controlled potential electrolysis

Ratio of diastereoisomers depends on the experimental conditions

2631 **Radical cations from nitrone spin-traps: reaction with water to give OH adducts**

Shakti Bhattacharjee, Md N. Khan, Harish Chandra and Martyn C. R. Symons



2635 **The first examples of persistent dimethyldihydropyrenium cations: reversal of ring current effects**

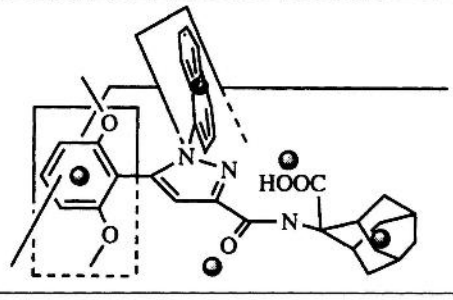
Kenneth K. Laali, Simon Bolvig, Todd J. Raeker and Reginald H. Mitchell

δ_{Me} = –4.23
diatropic Hückel [14] annulene

δ_{Me} = 1.70; 1.32
paratropic 4nπ [12] annulenium ions

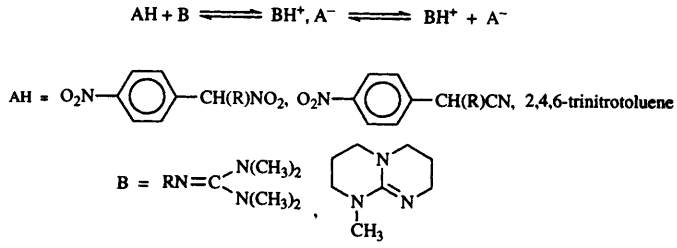
2639 **Structural requirements of non-peptide neurotensin receptor antagonists**

Luc Quéré, Robert Boigegrain, Francis Jeanjean, Danielle Gully, Guy Evrard and François Durant



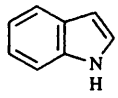
2647 **The influence of common cation BH^+ on the products of reactions between C-acids and strong guanidine bases in acetonitrile solvent**

Włodzimierz Gałęzowski, Małgorzata Stańczyk, Iwona Grześkowiak and Arnold Jarczewski



2653 **Structural and vibrational analysis of indole by density functional and hybrid Hartree–Fock/ density functional methods**

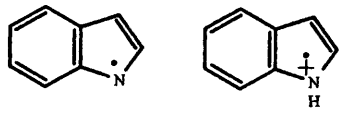
Susan E. Walden and Ralph A. Wheeler



Through utilization of density functional methods, we provide complete assignments for the fundamental vibrations of indole, without scaling or fitting to experiment

2663 **Structural and vibrational analysis of indolyl radical and indolyl radical cation from density functional methods**

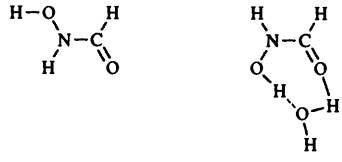
Susan E. Walden and Ralph A. Wheeler



Through utilization of density functional methods, we provide the first set of complete assignments for the fundamental vibrations of the indolyl radical and cation radical

2673 **Conformational behaviour of hydroxamic acids: *ab initio* and structural studies**

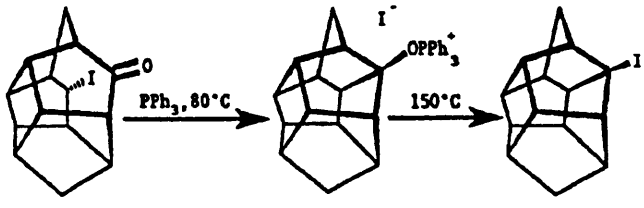
David A. Brown, Raymond A. Coogan, Noel J. Fitzpatrick, William K. Glass, Dau E. Abukshima, Loreto Shiels, Markku Ahlgrén, Kimmo Smolander, Tuula T. Pakkanen, Tapani A. Pakkanen and Mikael Peräkylä



The more stable *E* conformer of hydroxamic acids is shown to be preferentially stabilized in the *Z* form by hydrogen bonding with water

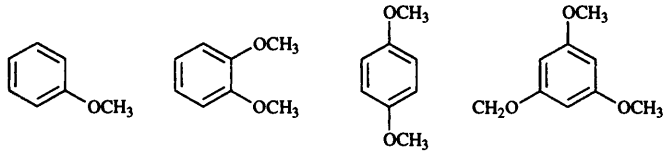
2681 **Reactions of phosphine with hexacyclo[6.6.0.0^{2,6}.0^{3,13}.0^{4,11}.0^{5,9}]-tetradecan-10-one derivatives**

Tahsin J. Chow, Lih-Pyng Li, Vincent Y. R. Lee, Kuan-Jiuh Lin and Chong-Yow Chen



2687 **Solid-state structure of 1,2-dimethoxybenzene (veratrole) and related methoxybenzenes. X-Ray crystallography and ^{13}C nuclear magnetic resonance tensor analysis**

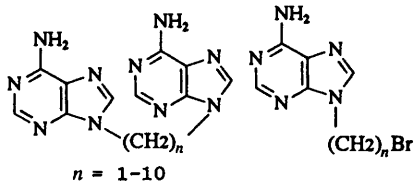
Marielle Gerzain, Gerald W. Buchanan, Alex B. Driega, Glenn A. Facey, Gary Enright and Robert A. Kirby



From variable spinning rate ^{13}C CPMAS NMR, principal shielding tensors have been measured for the above compounds. The low temperature X-ray crystallographic structure for 1,2-dimethoxybenzene shows that the methoxy groups are slightly out of the aromatic plane

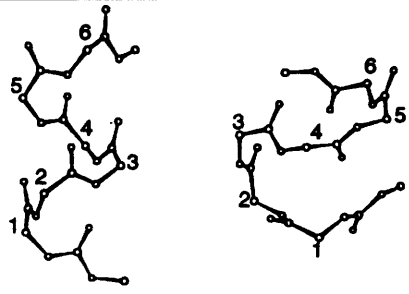
2695 **NMR study of 9,9′-(alkane-α,ω-diyl)-diadenine**

Toshio Itahara



2701 **Conformational variability in short acyclic peptides. Stabilization of multiple β-turn structures in organic solvents**

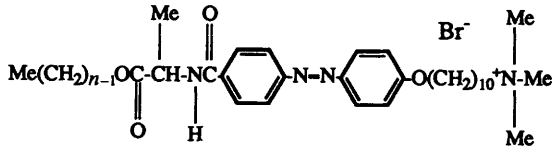
Satish Kumar Awasthi, Srinivasa Rao Raghothama and Padmanabhan Balaram



Configurational inversion at position 2 of a hexapeptide causes a major conformational change

2707 **Periodic change in absorption maxima due to different chain packing between the bilayers of amphiphiles possessing even and odd numbers of carbons in the hydrophobic chain**

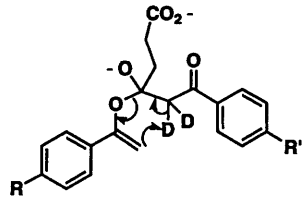
Norihiro Yamada, Kenji Okuyama, Takeshi Serizawa, Masashi Kawasaki and Shinichiro Oshima



$\lambda_{max.}$ 350 nm, n = 6, 8, 10, 12
320 nm, n = 7, 9, 11, 13

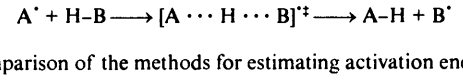
2715 **On the mechanism of succinyl transfer from aryl enolsuccinates to enolates of arylketones: addition–elimination *vs.* alkoxide-assisted retro-ene reaction**

William V. Murray, Ignatius J. Turchi and Jacqueline C. Bussolari



2719 **Understanding the rates of hydrogen-atom abstraction reactions: empirical, semi-empirical and *ab initio* approaches**

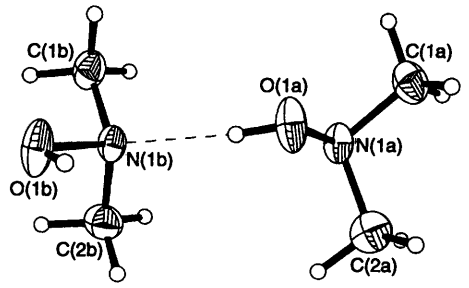
Brian P. Roberts



Comparison of the methods for estimating activation energies

2727 ***N,N*-Dimethylhydroxylamine: structural studies of the free molecule and of hydrogen-bonding in the solid state**

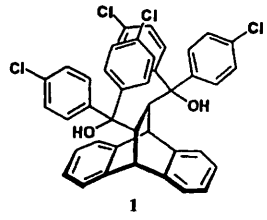
Norbert W. Mitzel, Bruce A. Smart, Simon Parsons, Heather E. Robertson and David W. H. Rankin



N,N-Dimethylhydroxylamine is monomeric in the gas phase and aggregated by hydrogen bonds in chains in the crystal, but the geometry of the C_2NO core is not significantly affected by the phase change

2733 **Simultaneous electrophile–nucleophile Cl···π interactions stabilizing solid state inclusions: a new tool for supramolecular crystal engineering**

Ingeborg Csöregh, Edwin Weber, Thomas Hens and Mátyás Czugler

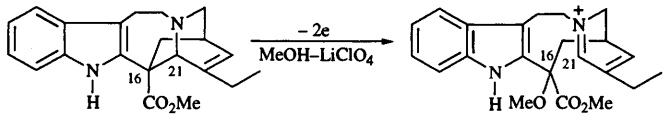


1

1a 1•pentan-2-ol (1:1)
1b 1•1,4-dioxane (2:5)
1c 1•*o*-xylene (1:2)

2741 **Anodic C16–C21 fragmentation of catharanthine in methanol. Synthesis of 16-methoxycleavamine**

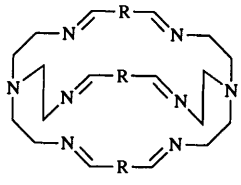
Ibro Tabakovic, Esmir Gunic and Miroslav J. Gasic



Cath 2

2747 **Hexa Schiff-base cryptands: solution thermodynamic and X-ray crystallographic studies of main group, transition and heavy metal ion complexes**

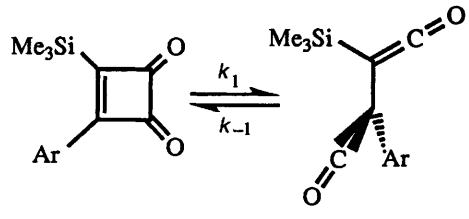
Rym Abidi, Françoise Arnaud-Neu, Michael G. B. Drew, Sarah Lahély, Debbie Marrs, Jane Nelson and Marie-José Schwing-Weill



The formation of mono- and bi-nuclear species is ligand and cation dependent and the stoichiometries detected in solution are always in agreement with those of the solid complexes. The weak selectivities result from a remarkable enthalpy-entropy compensation

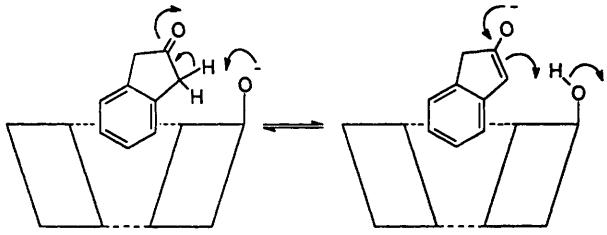
2757 **Aryl substituent effects on the thermal interconversion of cyclobutenediones and 1,2-bisketenes**

Ronghua Liu and Thomas T. Tidwell



2763 **Catalysis of the enolization of indan-2-one by cyclodextrins in aqueous solution**

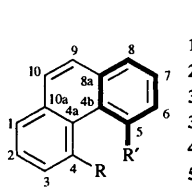
Oswald S. Tee and Robert A. Donga



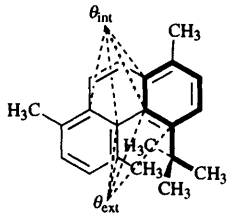
Cyclodextrins catalyse the enolization of indan-2-one

2771 **X-Ray and quantum chemical studies of strained phenanthrenes**

Stefan Grimme, Ivo Pischel, Martin Nieger and Fritz Vögtle



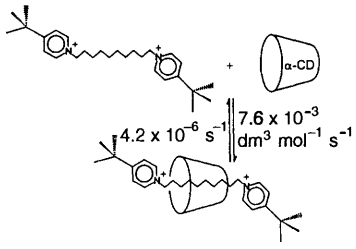
1 R = R′ = H
2 R = R′ = F
3 R = R′ = Cl
3a Decachloro
4 R = R′ = Me
5 R = R′ = Bu^t



6

2775 **The self-assembly of a [2]pseudorotaxane of α-cyclodextrin by the slippage mechanism**

Donal H. Macartney



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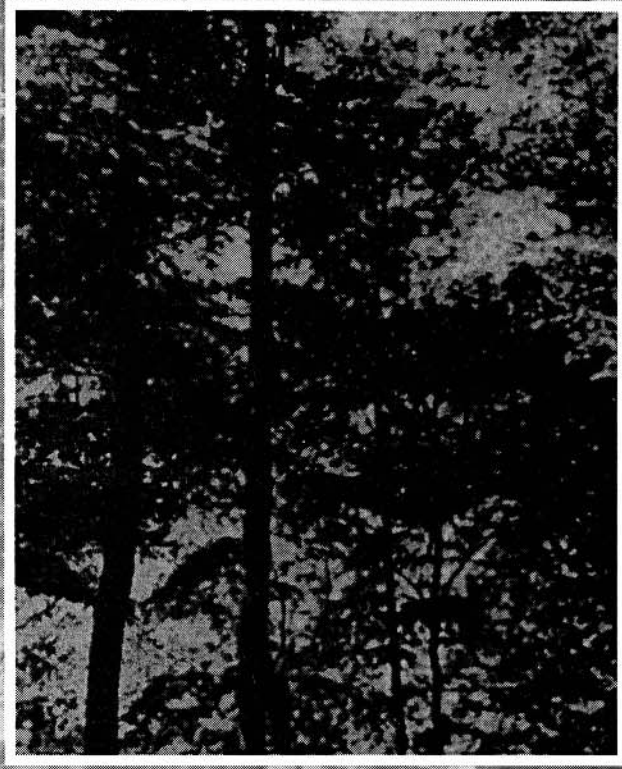

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