


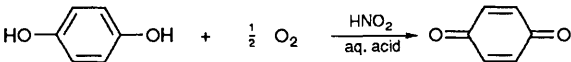
## JOURNAL OF THE CHEMICAL SOCIETY

## Perkin Transactions 2

## Physical Organic Chemistry

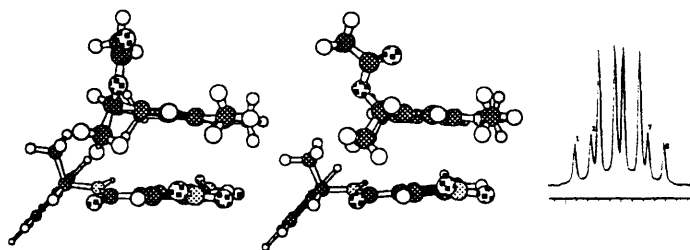
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<p>945 <b>Improved procedures for determining second-derivative cross-interaction coefficients and for establishing a relationship between the value and reaction type</b></p> <p>Dennis N. Kevill and Malcolm J. D'Souza</p>	<p>The intensity of cross-interaction between substituents can be determined without the need to incorporate external substituent constants into the multiple regression analysis</p>
<p>949 <b>Conformational analysis. Part 22. An NMR and theoretical investigation of the <i>gauche</i> effect in fluoroethanols</b></p> <p>Raymond J. Abraham, Eric J. Chambers and W. Anthony Thomas</p>	<p><i>p</i>-Br-C<sub>6</sub>H<sub>4</sub>·CH(OH)·CH<sub>2</sub>F</p> <p>CH<sub>2</sub>F·CH(OH)·CH<sub>2</sub>F</p>
<p>957 <b>The kinetics and mechanism of oxidation of hydroquinone and chlorohydroquinone in the presence of nitrous acid in aqueous acid solution</b></p> <p>Ben D. Beake, Roy B. Moodie and John P. B. Sandall</p>	 <p>Homolysis of a nitroso intermediate, forming nitric oxide, is rate-determining</p>

- 961 **Spectroscopic and molecular mechanics calculations of discrimination between enantiomers possessing an electron rich aromatic group directly attached to the chiral carbon atom with optically pure benzoyl derivatives**

Branko S. Jursic



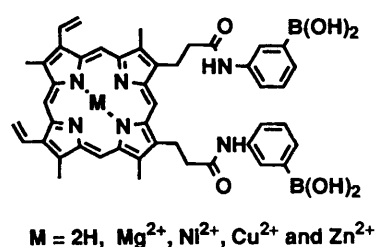
- 971 **Aromaticity and superaromaticity in cyclopolyacenes**

Jun-ichi Aihara

The topological resonance energy (TRE) method revealed that linear cyclopolyacenes are much less aromatic than are the zigzag isomers. Large linear and zigzag cyclopolyacenes are predicted to be as aromatic as their respective large polyacenes. The presence of a super-ring structure does not significantly affect the aromatic character of sizable cyclopolyacenes

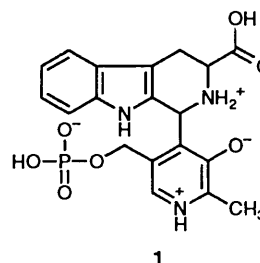
- 975 **Sugar sensing utilizing aggregation properties of boronic-acid-appended porphyrins and metalloporphyrins**

Hiroto Murakami, Takeshi Nagasaki, Itaru Hamachi and Seiji Shinkai



- 983 **Conformational analysis of the cyclised pyridoxal Schiff base of L-tryptophan. X-ray crystal structure, nuclear magnetic resonance and molecular orbital studies of 3-carboxy-1-{3-hydroxy-2-methyl-5-[(phosphonoxy)-methyl]-4-pyridyl}-1,2,3,4-tetrahydro-β-carboline**

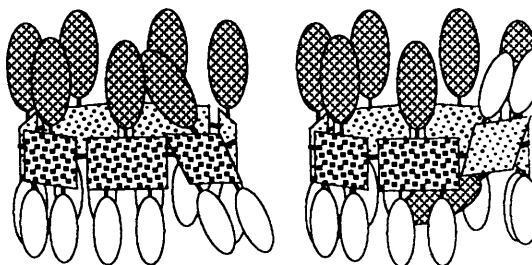
Hiroomi Nagata, Mitsunobu Doi, Masatoshi Inoue, Toshimasa Ishida, Miyoko Kamigauchi, Makiko Sugiura and Akio Wakahara



The stable and rigid conformation of **1** has been investigated by X-ray single crystal analysis, <sup>1</sup>H NMR measurements and molecular orbital calculations

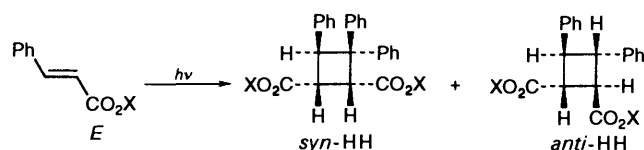
- 989 **Analysis of the conformational behaviour of perfunctionalized β-cyclodextrins. Part 1. Evidence for insertion of one of the rim substituents into the cyclodextrin cavity in organic solvents**

Ludovic Jullien, Josette Canceill, Liliane Lacombe and Jean-Marie Lehn

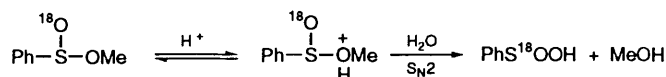


1003 **Organized photodimerization of unsaturated carboxylates. Selectivity control by normal and reversed micelles**

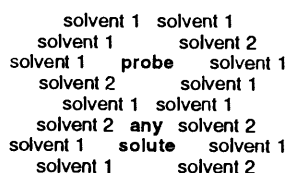
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1011 **On the mechanism of hydrolysis of sulfinate esters: oxygen isotope exchange and theoretical studies**

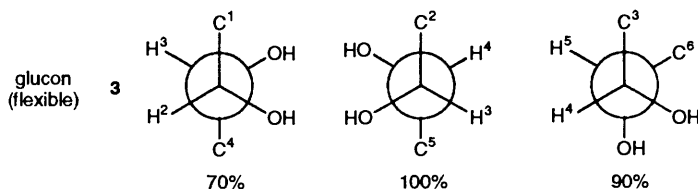
Tadashi Okuyama and Shigeru Nagase

1015 **Use of chemical probes for the characterization of solvent mixtures. Part 1. Completely non-aqueous mixtures**

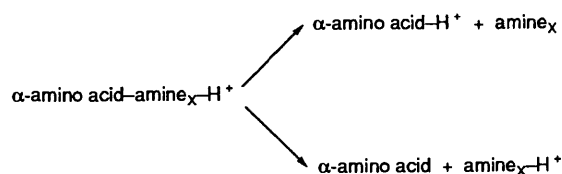
Yizhak Marcus

1023 **Conformational effects of 1,3-*syn*-diaxial repulsion and 1,2-*gauche* attraction between hydroxy groups in monomolecular *N*-octyl-D-hexonamide solutions. A  $^{13}\text{C}$  and  $^1\text{H}$  NMR spectroscopic study**

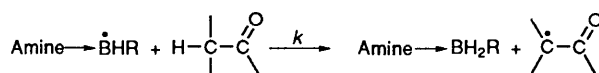
Sönke Svenson, Andreas Schäfer and Jürgen-Hinrich Fuhrhop

Attractive *gauche* interactions determine the conformations of open-chain hexonamides in DMSO solution1029 **On the proton affinity of some  $\alpha$ -amino acids and the theory of the kinetic method**

Gustav Bojesen and Torben Breindahl

A theoretical analysis of this reaction in the gas phase has been developed and the proton affinities of 17  $\alpha$ -amino acids have been determined1039 **Homolytic reactions of ligated boranes. Part 19. Relationships between structure, reactivity and enantioselectivity for hydrogen-atom abstraction by chiral amine-boryl radicals**

Hai-Shan Dang, Valérie Diart, Brian P. Roberts and Derek A. Tocher



1. X-ray crystal structures of amine $\rightarrow$ BH<sub>2</sub>R
2. Relative reactivities of amine $\rightarrow$ BHR determined by EPR spectroscopy
3. MO calculations of transition states

1047 **Conformational studies on peptides as enzyme inhibitors: chymotrypsin inhibitors using Bowman-Birk type as models**

Vincenzo Pavone, Carla Isernia, Michele Saviano, Lucia Falcigno, Angelina Lombardi, Livio Paolillo, Carlo Pedone, Solfrid Buøen, Hilde Merete Naess, Hege Revheim and Jon Amund Eriksen

H-Cys-Ala-Leu-Ser-Tyr-Pro-Ala-Gln-Cys-OH

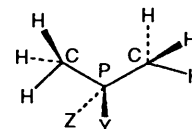
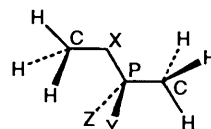
Peptide 197

Ac-Cys-Thr-Leu-Ser-Asn-Pro-Pro-Gln-Cys-NH<sub>2</sub>

Peptide 212

1055 **Ab initio studies on organophosphorus compounds. Part 2. Monoanionic methyl methylphosphonate and methyl methylphosphinate and their sulfur analogues**

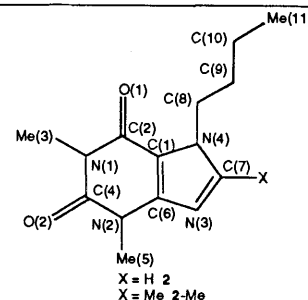
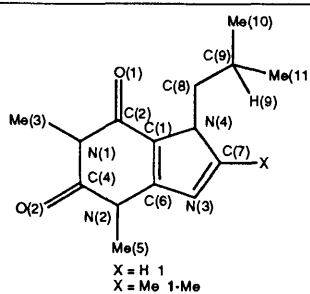
Jari P. Räsänen, Mikael Peräkylä, Esko Pohjala and Tapani A. Pakkanen



X, Y, Z = O or S

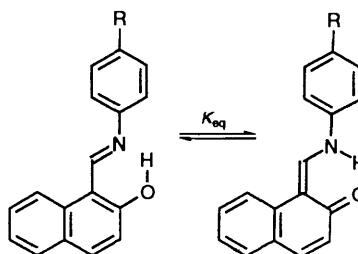
1061 **Structure and dynamics of theophylline derivatives by X-ray, NMR and molecular mechanics studies**

Orenzo Agostini, Graziano Bonacchi, Paolo Dapporto, Paola Paoli, Lionello Pogliani and Emilio Toja



1067 **<sup>13</sup>C NMR spectroscopic and AM1 study of the intramolecular proton transfer in anils of salicylaldehyde and 2-hydroxynaphthalene-1-carbaldehyde**

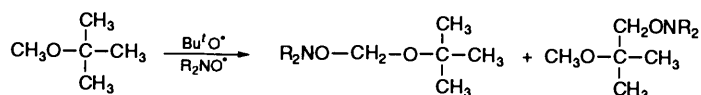
Sergio H. Alarcón, Alejandro C. Olivieri and Manuel González-Sierra



Variable-temperature <sup>13</sup>C NMR data show that, in contrast to salicylideneanilines, anils of 2-hydroxynaphthalene-1-carbaldehyde exist as equilibrium mixtures of two tautomers

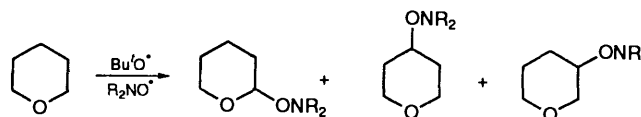
1071 **Reactions of *tert*-butoxyl radicals with acyclic ethers studied by the radical trapping technique**

W. Ken Busfield, I. Darren Grice, Ian D. Jenkins and Michael J. Monteiro



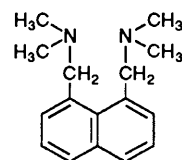
1079 **Reactions of *tert*-butoxyl radicals with cyclic ethers studied by the radical trapping technique**

W. Ken Busfield, I. Darren Grice and Ian D. Jenkins



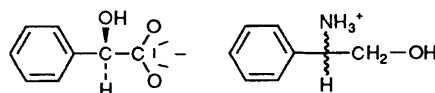
- 1087 **X-ray and Fourier-transform infrared studies of 1,8-bis(dimethylaminomethyl)naphthalene. Comparison with 1,8-bis(dimethylamino)naphthalene**

L. van Meervelt, K. Platteborze and Th. Zeegers-Huyskens



- 1091 **The role of solvates in optical resolution. A study of the diastereoisomeric salts formed from enantiomeric 2-amino-2-phenylethanol and (*R*)-mandelic acid, their crystal structures and physico-chemical properties**

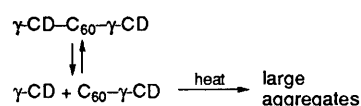
Sine Larsen, Dávid Kozma and Maria Ács



Diastereoisomeric salts formed in water-containing and water-free ethyl acetate

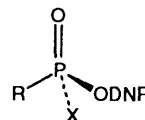
- 1097 **NMR and UV-VIS investigation of water-soluble fullerene-60- $\gamma$ -cyclodextrin complex**

Thomas Andersson, Gunnar Westman, Olof Wennerström and Mikael Sundahl



- 1103 **Kinetic study on the alkaline hydrolysis of some tetracoordinate P<sup>V</sup> esters of 2,4-dinitrophenol**

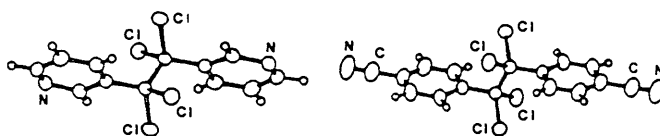
Giorgio Cevasco and Sergio Thea



DNP = 2,4-Dinitrophenyl. 1: R = PhCH<sub>2</sub>, X = Ph; 2: R = PhCH<sub>2</sub>, X = EtO; 3: R = PhCH<sub>2</sub>, X = Et<sub>2</sub>N; 4: R = X = Ph; 5: R = Ph, X = EtO; 6: R = Ph, X = Et<sub>2</sub>N

- 1107 **Internal rotation and conformational preferences in 1,2-diaryl derivatives of 1,1,2,2-tetrachloroethane: a <sup>1</sup>H DNMR and X-ray structural study**

Luciano Antolini, Ugo Folli, Adele Mucci, Silvia Sbardellati and Ferdinando Taddei



Multiple internal rotation is evidenced by DNMR in solution

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Environmentally friendly chemistry using supported reagent catalysts: structure–property relationships for clayzic **J. H. Clark, S. R. Cullen, S. J. Barlow and T. W. Bastock**

Solvent effects on chemical processes. Part 6. The phenomenological model applied to the solubility of naphthalene and 4-nitroaniline in binary aqueous–organic solvent mixtures **J. M. LePree, M. J. Mulski and K. A. Connors**

The rôle of powder diffraction in establishing structure–property relationships for crystalline solids: a new structural assignment of the photoreactive and photostable phases of *p*-formyl-*trans*-cinnamic acid **K. D. M. Harris and I. L. J. Patterson**

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Photochemistry of triethylamine–acid chloride charge-transfer complexes **S. Das, C. S. Rajesh, T. L. Thanulingam, D. Ramaiah and M. V. George**

1,8-Dimethyl-1,8-dihalo-1,8-digermacyclotetradecanes. The first germamacrocycles with anion transport capability **S. Aoyagi, K. Tanaka and Y. Takeuchi**

Oxidation reduction reactions involving nitro groups in trifluoromethanesulfonic acid. Part 2. The reactions of chloromethylbenzenes with aromatic nitro compounds **R. P. Austin and J. H. Ridd**

Nonlinear optical properties of organic molecules. Part 15. Calculation of the structure and hyperpolarisabilities of arylalkenes containing weak donors and acceptors **J. O. Morley**

A mechanistic study of the oxidation of phenols in aqueous solution by oxoiron(IV) tetra(*N*-methylpyridyl)porphyrins. A model for horseradish peroxidase compound II? **N. Colclough and J. R. Lindsay Smith**

Crystalline inclusion compounds of substituted 2,2'-bis(9-hydroxy-9-fluorenyl)biphenyls. Synthesis, X-ray crystal structures and thermal analysis study of inclusion compounds with butyronitrile, cyclohexanone, cyclopentanol and dimethylformamide **S. A. Bourne, L. R. Nassimbeni, M. L. Niven, E. Weber and A. Wierig**

Studies in crystal engineering: structure–reactivity correlations of substituted styrylcoumarins and related systems **J. N. Moorthy, S. D. Samant and K. Venkatesan**

Kinetic study of the reaction of naphthyllithium with carbon monoxide in hexane:THF solution **N. S. Nudelman and F. Doctorovich**

Conformational studies on analogues of the invertebrate peptide pyroGlu-Asp-Pro-Phe-Leu-Arg-Phe-NH<sub>2</sub> using <sup>1</sup>H NMR **D. J. S. Guthrie, R. F. Geraghty, G. B. Irvine and C. H. Williams**

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Structure and photophysics of deazabipyridyls. Excited internally hydrogen-bonded systems with one proton transfer reaction site **L. Kaczmarek, R. Balicki, J. Lipkowski, P. Borowicz and A. Grabowska**

Protonation tendencies of *p*-Azacyclophanes. A thermodynamic and NMR study **A. Bianchi, B. Escuder, E. García-España, S. V. Luis, V. Marcelino, J. F. Miravet and J. A. Ramírez**

Studies of substrate selectivity in the aromatic iodination and in other substitution reactions reinforce previous conclusions about the nature of the mechanism of electrophilic aromatic substitutions **C. Galli and S. Di Giammarino**

Dynamic aspects in host–guest interactions. Part 2. Directional inclusion reactions of some azo guest molecules with  $\alpha$ -cyclodextrin **N. Yoshida and K. Hayashi**

A multinuclear NMR study of some mesoionic 1,3-dimethyltetrazoles, 1- and 2-methyltetrazoles and related compounds **W. Bocian, J. Jaźwiński, W. Koźmiński, L. Stefaniak and G. A. Webb**

Peroxidatic activity of haem octapeptide complexes with anilines, naphthols and phenols **I. D. Cunningham, J. L. Bachelor and J. M. Pratt**

X-Ray structures and physical properties of tropone-annelated *p*-benzoquinones substituted with X–Ar groups  $\alpha$  to tropone carbonyls and first examples of the trione substituted with an electron-withdrawing group **K. Furuichi, H. Tada, A. Itoh, Y. Takeuchi, M. Mitoori, M. Kato, S. Matsumoto and M. Hashimoto**

# International Symposium

## RECOGNITION PROCESSES

University of Birmingham  
24-29 July 1994

### INVITED SPEAKERS

Y Aoyama  
E C Constable  
F D Cramer  
P B Dervan  
F N Diederich  
B Fraser Reid  
J M J Fréchet  
S E Halford

A D Hamilton  
W L Jorgensen  
G von Kiedrowski  
J-M Lehn  
R A Lerner  
D Lilley  
G R Newkome  
V Percec

H Ringsdorf  
R Roberts  
J K M Sanders  
J L Sessler  
P Sinay  
J A Stubbe  
D M Walba  
K Wüthrich

#### MAIN TOPICS INCLUDE:

- Biological Catalysts
- Biopolymer Interactions
- Catalytic Antibodies
- Coordination Chemistry
- Electrochemical Processes
- Enzyme Modelling
- Host-Guest Chemistry
- Liquid Crystals
- Molecular Devices
- Supramolecular Catalysts
- Synthetic Methodology
- Biomimetic Chemistry
- Carbohydrate Science
- Computational Methods
- Dendritic Macromolecules
- Enzyme Analogues
- Genetic Engineering
- Information Storage
- Membrane Science
- Molecular Receptors
- Noncovalent Interactions
- Polymer Science
- Molecular Recognition
- Nucleic Acids
- Protein Engineering
- Self-Organisation
- Separation Science
- Structural Studies
- Transport Processes
- Supramolecular Photochemistry
- Self-Assembly
- Self-Replication
- Spectroscopic Properties

#### Contact:

Dr John F Gibson, Secretary (Scientific), Royal Society of Chemistry, Burlington House, London UK W1V 0BN  
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Fax: +44 (0) 71 437 8883



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