

JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions 2

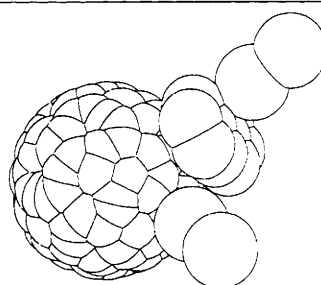
Physical Organic Chemistry

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Perkin Communications

1407 **Preparation and single crystal structure determination of the solvated intercalate $C_{60} \cdot I_2 \cdot \text{toluene}$**

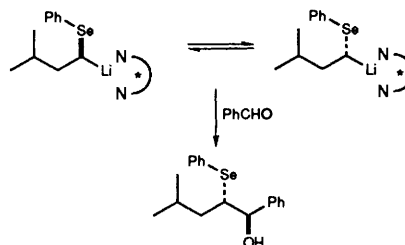
Paul R. Birkett, Christos Christides, Peter B. Hitchcock, Harold W. Kroto, Kosmas Prassides, Roger Taylor and David R. M. Walton



Iodine is shown to have molecular contacts with both C_{60} and toluene molecules in the solvated intercalate $C_{60} \cdot I_2 \cdot \text{toluene}$

1409 **Enantioselective transformations of configurationally labile α -phenylseleno-alkyllithium compounds**

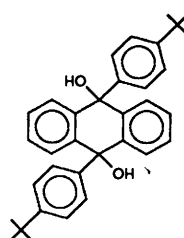
Wolfgang Klute, Ruprecht Dress and Reinhard W. Hoffmann



Factors that determine the e.e. of the product

1413 **Enclathration of diethyl ether**

Leonard J. Barbour, Mino R. Caira and Luigi R. Nassimbeni

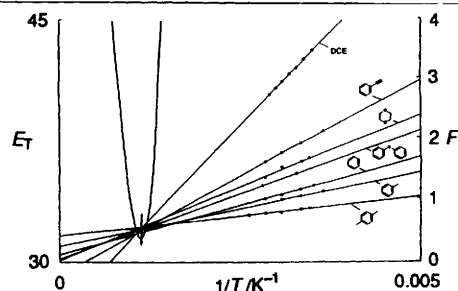


9,9'-Dihydroxy-9,9'-di(4-*tert*-butylphenyl)-9,9'-dihydroanthracene enclathrates diethyl ether from the vapour and forms a stable inclusion compound

Articles

- 1415 **Acceptor properties of solvents: the use of isokinetic relationships to elucidate the relationship between the acceptor number and the solvatochromism of *N*-phenolate betaine dyes**

Wolfgang Linert and Reginald F. Jameson



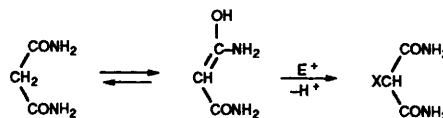
- 1423 **On the calculation of tetrahedral intermediate pK_a values**

Peter J. Taylor

In the context of $\Delta pK_a(Y) = \rho_1 \Sigma \sigma_1(X)$ for X_3CY , we derive a new value of $\rho_1 = -9.1$, and σ_1 values for charged substituents

- 1429 **Electrophilic substitution in malonamide. Evidence for reaction *via* the enol tautomer**

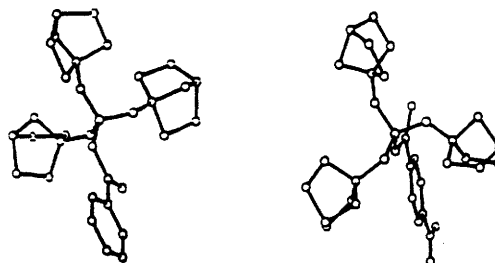
D. Lyn H. Williams and Ling Xia



Malonamide reacts with electrophiles (E^+) *via* the enol tautomer; enolisation or reaction of the enol can be rate limiting

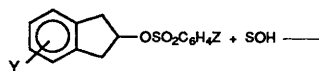
- 1433 **Quasiphosphonium intermediates. Part 7. The preparation of trinorborn-1-yl phosphite and its reactions with halogeno compounds: stable intermediates of the Arbuzov and Perkow reactions and their structural characterization by X-ray diffraction, NMR spectroscopy, and fast atom bombardment mass spectrometry**

Harry R. Hudson, Ray W. Matthews, Mary McPartlin, Michael A. Pryce and Oluyemisi O. Shode



- 1441 **Solvolysis mechanism of indan-2-yl arenesulfonates**

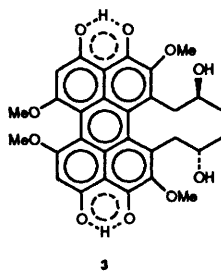
Ikchoon Lee, Young Sook Lee, Bon-Su Lee and Hai Whang Lee



The small value of cross-interaction constant ρ_{Y2} and its solvent and temperature dependence are consistent with the S_N2 mechanism

1447 NMR study of tautomerism in natural perylenequinones

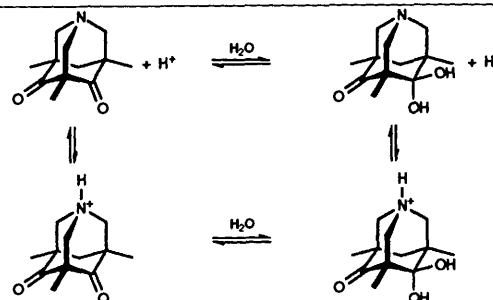
Alberto Arnone, Lucio Merlini, Rosanna Mondelli, Gianluca Nasini, Enzo Ragg, Leonardo Scaglioni and (the late) Ulrich Weiss



The influence of structural factors, solvent and concentration on the keto-enol tautomerism of 11 naturally occurring perylenequinones (e.g. 3) has been studied by ^1H , ^2H and ^{13}C NMR spectroscopy

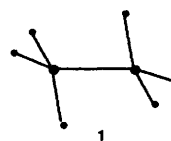
1455 Protonation and gem-diol formation of 1-azaadamantanones

Danilo Kardel, Wilhelm Knoche and Nikolaus Risch



1461 Ethane cation-radical isomers and their interconversion pathways. Electron shift isomerism in cation radicals

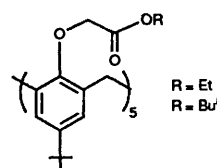
Alexander Ioffe and Sason Shaik



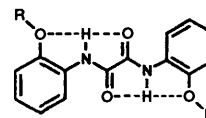
The $\text{C}_2\text{H}_6^{+\cdot}$ surface is computed. Seven isomers (e.g., 1) and five transition states are located. Non-traditional Jahn-Teller behaviour is observed and rationalized

1475 Cation complexation by chemically modified calixarenes. Part 6. Alkali and silver(I) cation complexation by *p*-*tert*-butylcalix[5]arene derivatives and X-ray structure determination of a pentaester

Geraldine Barrett, M. Anthony McKerverey, John F. Malone, Andrew Walker, Françoise Arnaud-Neu, Lourdes Guerra, Marie-Jose Schwing-Weill, C. David Gutsche and Don R. Stewart

1481 ^1H , ^{13}C , ^{15}N , 2D and variable temperature NMR study of the role of hydrogen bonding in the structure and conformation of oxamide derivatives

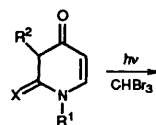
Francisco Javier Martínez-Martínez, Armando Ariza-Castolo, Hugo Tlahuext, Margarita Tlahuextl and Rosalinda Contreras



NMR determination of hydrogen bonding and conformation in oxamides

1487 Photochemistry of uracils in halogenated solvents

Claus Moltke-Leth and Karl Anker Jørgensen



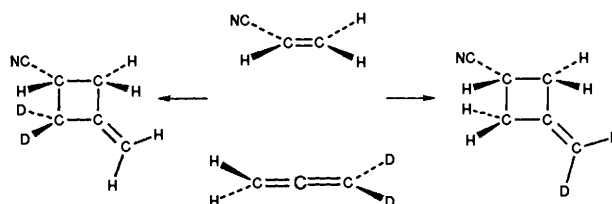
1491 Bent benzene—boat or chair?

George G. Hall

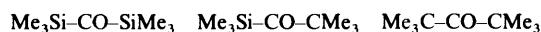
It is argued that a benzene ring should bend into boat form when compressed inside a molecule

1493 Cycloaddition of acrylonitrile to allene: computed reaction path (AM1) and intramolecular secondary isotope effect

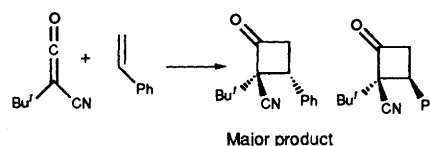
E. Amitai Halevi and Max Wolfsberg

1497 NMR of terminal oxygen. Part 11. ^{17}O NMR spectra of disilyl ketone and related compounds: a case of strong deshielding by electronic excitation energy

Hans Dahn, Péter Péchy and Hans Jürgen Bestmann

1499 An MCSCF study of the effect of substituents and solvent on the [2 + 2] cycloaddition of *tert*-butylcyanoketene to phenylethene

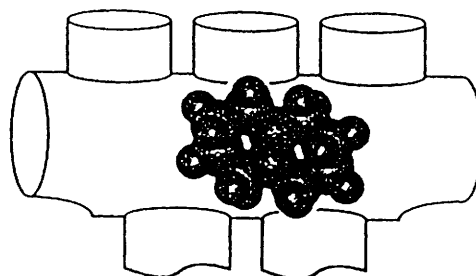
Mar Reguero, Rafael R. Pappalardo, Michael A. Robb and Henry S. Rzepa



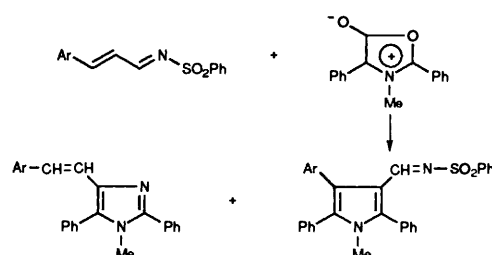
Ab initio MCSCF calculations with SCRF solvation correction for the [2 + 2] cycloaddition reaction predict that formation of the most hindered product proceeds *via* the least hindered biradical transition state

1503 Dimerisation and transannular reactions of cycloalkenes on H-mordenite

Rowena Crockett and Emil Roduner

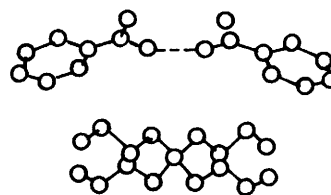
1511 Cycloaddition reactions of *N*-phenylsulfonyl-1-azabuta-1,3-dienes with mesoionic 2,4-diphenyl-1-methyl-1,3-oxazolium 5-oxide

Piero Dalla Croce, Raffaella Ferraccioli, Concetta La Rosa and Tullio Pilati



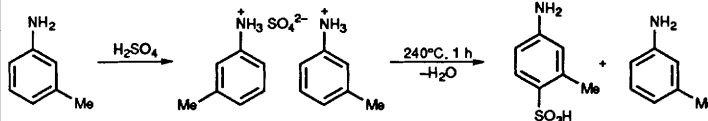
- 1517 **Tetrabutylammonium hydrogen bisbenzoate: crystal structure and study of short hydrogen bonds in hydrogen bisbenzoate anion system**

Vedavati G. Puranik, Sudam S. Tavale, Venkat S. Iyer, Jagdish C. Sehra and Swaminathan Sivaram



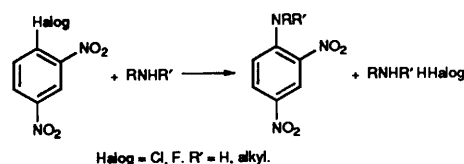
- 1521 **Kinetics of thermal decomposition of arylammonium sulfates. Part 2. *m*-Ditoluidinium sulfate**

Gurdip Singh, Inder Pal Singh Kapoor and Monica Jain



- 1525 **Catalysis in nucleophilic aromatic substitution reactions. The presence of molecular complexes on the pathway of reactions between 1-fluoro- and 1-chloro-2,4-dinitrobenzene and aliphatic amines**

Luciano Forlani



The self-catalysis of the reported reactions is explained by the presence of interactions substrate-amine

- 1531 **A ¹H NMR study on the interaction of aminoxyl paramagnetic probes with unfolded peptides**

Gennaro Esposito, Henriette Molinari, Monica Pegna, Neri Niccolai and Lucia Zetta

The use of soluble spin labels to filter out the cross peaks of outer nuclei in 2D NMR spectra has been proposed as a general method to obtain structural information about complex molecules

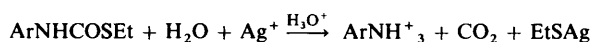
- 1535 **Origin of the additive relationship for ¹³C NMR chemical shifts of alkanes as studied by *ab initio* GIAO calculations**

Fumio Imashiro, Yuji Masuda, Masaru Honda and Shigeru Obara

A new additive relationship for ¹³C NMR chemical shifts of alkane conformers is constructed by employing substituent and conformation additive shift parameters

- 1543 **The kinetics and mechanism of the silver ion-promoted hydrolysis of thiolurethanes in aqueous solution**

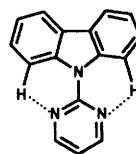
Derek P. N. Satchell, Rosemary S. Satchell and (in part) S. Bhavnani



Reaction occurs only *via* 2Ag⁺ : 1ArNHCOSet complexes

1547 **The problem of the existence of C(Ar)-H...N intramolecular hydrogen bonds in a family of 9-azaphenyl-9H-carbazoles**

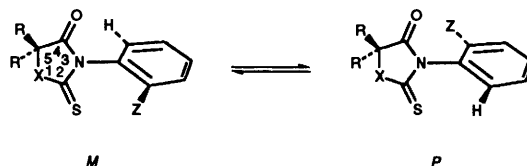
Carmen Avendaño, Modesta Espada, Blanca Ocaña, Santiago García-Granda, María del Rosario Díaz, Baudilio Tejerina, Fermín Gómez-Beltrán, Ana Martínez and José Elguero



X-ray diffraction and ^1H NMR studies clearly show a planar structure with C-H...N intramolecular hydrogen bonds in 9-(2-pyrimidinyl)carbazole

1557 **The enantiomers of *N*-aryl-2-thioxo-4-oxazolidinones and *N*-arylrhodanines. Investigation by liquid chromatography, circular dichroism and thermal racemization**

Ilknur Dogan, Nikola Pustet and Albrecht Mannschreck



These enantiomers ($X = \text{O}, \text{S}$) were enriched semi-preparatively: their relative configurations and barriers to C-N rotation are reported

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

