

JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions 2

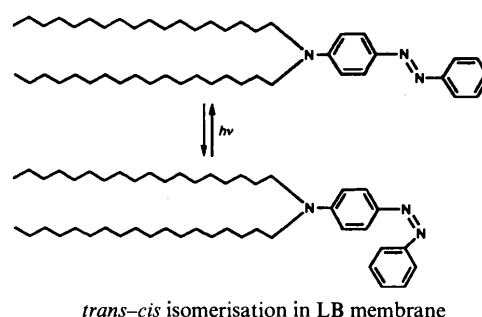
Physical Organic Chemistry

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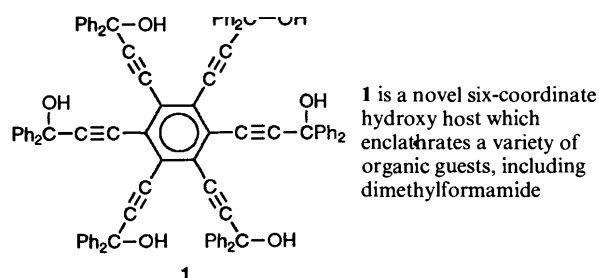
1897 Photoinduced reversible *trans-cis* isomerisation of an azobenzene amphiphile bearing dialkyl side chains in Langmuir-Blodgett membranes

Jun-ichi Anzai, Naoko Sugaya and Tetsuo Osa



1899 Inclusion by a novel sexipedal host. Crystal structure and thermal analysis

Susan A. Bourne, Mino R. Caira, Luigi R. Nassimbeni, Muneyoshi Sakamoto, Koichi Tanaka and Fumio Toda

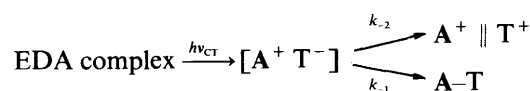


Articles

Keynote Article

1901 From solvolysis to electron transfer: direct observation of ion-pair dynamics by time-resolved spectroscopy

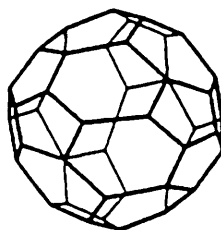
T. Michael Bockman and Jay K. Kochi



Charge-transfer photolysis ($h\nu_{\text{CT}}$) generates the contact ion pair, which reacts *via* the competitive processes of internal return (k_{-1}) and solvent separation (k_{-2})

1917 Predictions of spectral signatures of fullerenes. Second-order Jahn–Teller effects on the structures of C_{44} , C_{56} , C_{68} and C_{92}

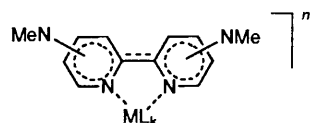
Patrick W. Fowler and John P. B. Sandall



Fullerenes with pseudo-closed π shells are susceptible to loss of symmetry

1923 Diquaternized heterocycles with strong electronic coupling between a metal-chelating site and a methylviologen-type redox function: EPR/ENDOR detected coordination of metal ions and complexes by radical cation intermediates

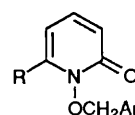
Walter Matheis, Jürgen Poppe, Wolfgang Kaim and Stanislav Zális



The most typical bipyridine features, *i.e.* redox reactivity and metal chelate binding, can be integrated in a single biaryl system in different ways

1929 Characterization of the β -cyclodextrin inclusion complexes with bichromophoric 1-benzyloxy-2-pyridone and related compounds

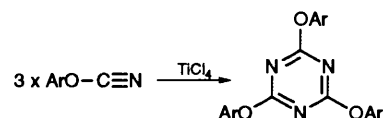
Tadamitsu Sakurai, Eiko Saitou, Narumi Hayashi, Yukiko Hirasawa and Hiroyasu Inoue



Methyl- and aryl-substituent effects on the structure and stability of the β -cyclodextrin inclusion complexes with bichromophoric guest molecules are presented

1937 Kinetics and mechanism of the titanium tetrachloride-catalysed cyclotrimerisation of aryl cyanates

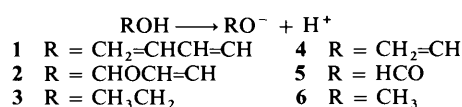
Ian D. Cunningham, Andrew Brownhill, Ian Hamerton and Brendan J. Howlin



Aryl cyanates undergo $TiCl_4$ -catalysed cyclotrimerisation *via* rate-limiting nucleophilic attack by cyanate on a cyanate-catalyst complex

1945 Acidity of carboxylic acids: resonance delocalization or induction?

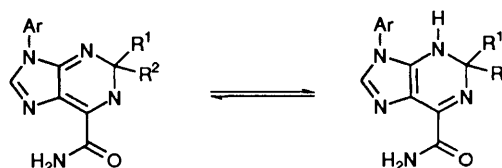
T. Darrah Thomas



Delocalization of charge in the anion plays a role in the acidity of 1 relative to 4 and of 2 relative to 5, but the relative acidities of 3, 4 and 5 and of 1 and 2 are due to the charge distribution in the initial molecule

1949 Synthesis of 9-aryl-6-carbamoyl-1,2-dihydropurines and a study of their tautomerism

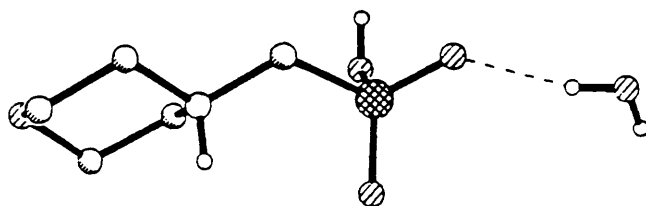
M. Jose Alves, Brian L. Booth, Alice Carvalho, Paul R. Eastwood, Lida Nezhat, Robin G. Pritchard and M. Fernanda J. R. P. Proença



X-Ray structures of both tautomers (Ar = Ph) have been obtained and the effects of changing Ar, R^1 and R^2 have been studied

1957 NMR, crystal structure and FAB mass spectral studies of morphinomethylphosphonic acid

Mark P. Lowe, Joyce C. Lockhart, Craig J. Matthews, William Clegg, Mark R. J. Elsegood and Lynne Horsburgh



1965 Eclipsed ground-state conformations for methoxycyclohexanes with adjacent methyl-group substitution. An NMR criterion and molecular mechanics calculations

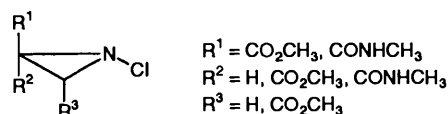
J. Edgar Anderson and Anthony I. Ijeh



In axial or equatorial methoxycyclohexanes with equatorial methyl groups in the 2- and 6-positions, the exocyclic carbon-oxygen bond is eclipsed as shown by a large $^3J_{\text{H-C-O-C}}$ coupling of about 7.4 Hz

1969 Structural studies of *N*-chloroaziridine-carboxylates by multinuclear NMR spectroscopy

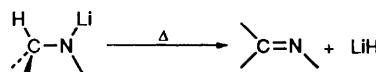
Arrigo Forni, Irene Moretti, Alberto Pirondi, Fabio Prati and Luisa Schenetti



A multinuclear ^1H , ^{13}C , ^{15}N , ^{17}O NMR study affords relative configurations

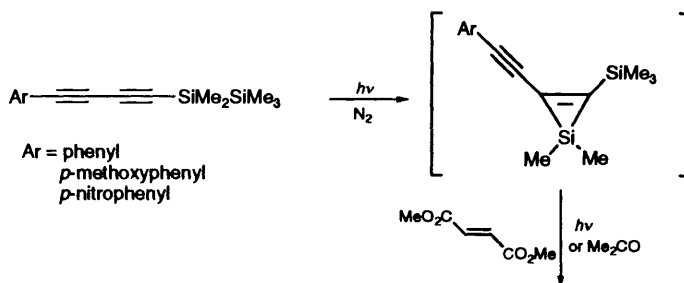
1973 Thermal decomposition of lithium amides: a matrix isolation investigation

Robert Withnall, Ian R. Dunkin and Ronald Snaith

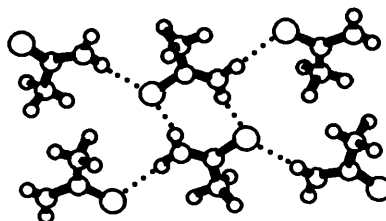


1979 Photochemistry of 1-aryl-4-(pentamethyldisilanyl)buta-1,3-diyne: photoreaction with acetone and dimethyl fumarate

Sang Chul Shim and Seong Taek Lee

1985 Effect of hydrogen bonding on the methyl conformation of thioacetamide: an *ab initio* study

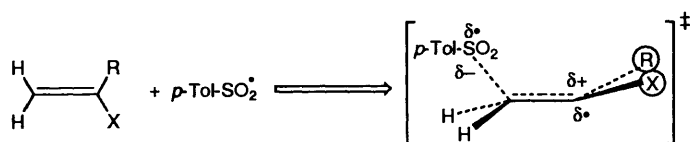
Fabio Ramondo and Luigi Bencivenni



The geometries and methyl rotation barriers of thioacetamide monomer, dimer and hexamer were investigated by *ab initio* methods

1993 **The importance of polar, resonance, steric and solvent effects in the addition of sulfonyl radicals to alkenes**

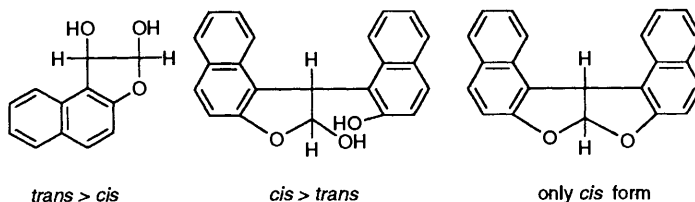
Carlos M. M. da Silva Corrêa, M. Daniela C. M. Fleming, M. Augusta B. C. S. Oliveira and Ermelinda M. J. Garrido



Polar, resonance, steric and solvent effects

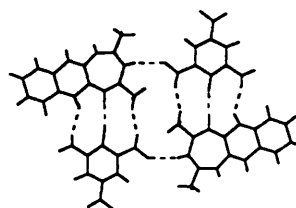
2001 **Stereochemistry of the products from the alkylation of 2-naphthol with glyoxal**

Xiaobo Fan, Makoto Yamaye, Yoshio Kosugi, Hiroshi Okazaki, Hoyou Mizobe, Tomoko Yanai and Taketoshi Kito



2007 **Structure of 2,4-dimethyl-1*H*-naphtho[2,3-*b*]-[1,4]diazepine hydropicrate. Solid-state assembly via C–H...O hydrogen bonding**

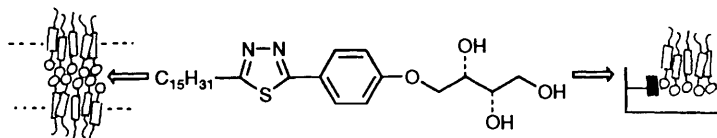
V. Agafonov, P. Dubois, F. Moussa, J. M. Cense and S. Toscani



Hydrogen bond motifs in the crystal of naphthodiazepine hydropicrate

2011 **Investigation of bulk properties and monolayer behaviour of amphiphilic mesogens: structural variations of the head group**

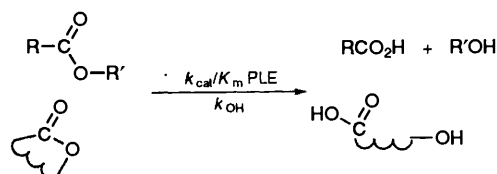
Detlev Joachimi, André Öhlmann, Willi Rettig and Carsten Tschierske



Amphiphilic rod-like molecules self-organize to thermotropic and lyotropic liquid crystalline phases as well as to monomolecular films at the air–water interface, with properties strongly depending on the nature of the hydrophilic head group

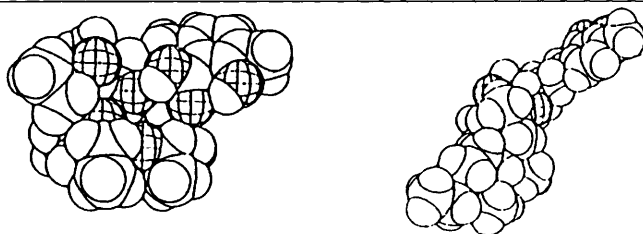
2021 **Structure–activity relationships in the esterase-catalysed hydrolysis and transesterification of esters and lactones**

Patrick Barton, Andrew P. Laws and Michael I. Page



2031 **Open and closed forms of the ionophore lasalocid free acid and free anion. Obtaining the most probable conformations using AM1 semi-empirical quantum mechanical calculations**

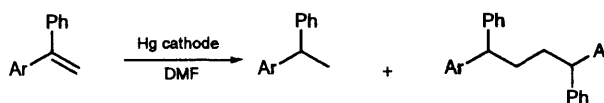
Patrice Malfreyt, Yves Pascal and Jean Juillard



Closed and unfolded conformations

2039 **Electrochemical reduction of 1,1-diaryl-substituted ethenes in dimethylformamide**

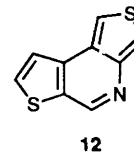
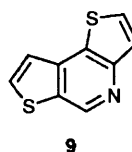
Michelina Fruianu, Mauro Marchetti,
Giovanni Melloni, Gavino Sanna and
Renato Seeber



Ar = phenyl, 2-naphthyl, 2-pyridyl, 2-thienyl, 2-furyl

2045 **Structural chemistry of polycyclic heteroaromatic compounds. Part 4. Electronic structures of angular dithienopyridines**

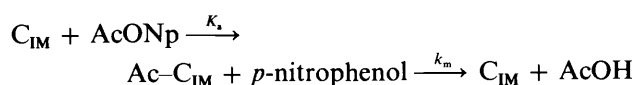
Waldemar A. Brett, Paul Rademacher,
Roland Boese, Salo Gronowitz and
Youhua Yang



The HeI photoelectron spectra of nine isomeric [b,d]-annellated dithienopyridines are reported, the structures of isomers **9** and **12** have been determined by X-ray diffraction

2053 **Theoretical study on the mechanism of ester hydrolysis in micellar catalysis using model systems**

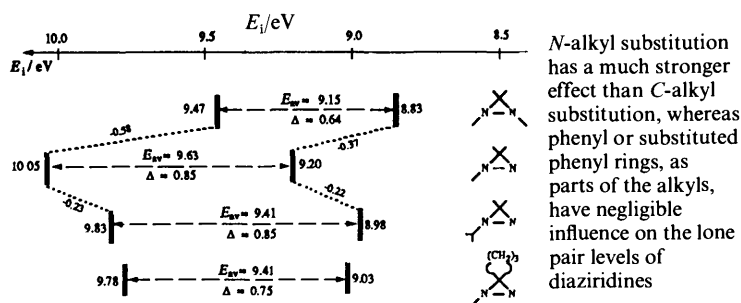
Kenzi Hori, Akio Kamimura, Junko Kimoto,
Sachiko Gotoh and Yasuji Ihara



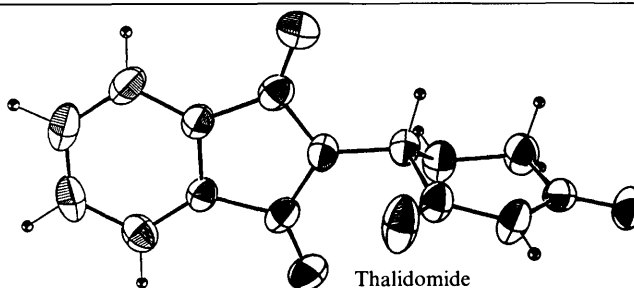
AcONp, *p*-nitrophenyl ester; C_{IM}, imidazole catalyst;
Ac-C_{IM}, acylated intermediate

2059 **Photoelectron spectra of alkyldiaziridines**

Leo Klasinc, Albrecht Mannschreck, Mladen
Mintas and Sean P. McGlynn

2063 **Characterization and crystal structure of two polymorphic forms of racemic thalidomide**

John C. Reepmeyer, Myron O. Rhodes, Don
C. Cox and James V. Silverton



Corrigendum

2069 **The kinetics of basic cleavage of nitrophenyl alkanooate esters by 'hydroxypropyl-β-cyclodextrin' in aqueous solution**
Timothy A. Gadosy and Oswald S. Tee

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

Forthcoming Articles in *Perkin Transactions 2*

- Substituent effects in the reaction of triphenylphosphine with diazodiphenylmethane: the interpretation of a U-shaped Hammett correlation in an elementary biphilic reaction **D. Bethell, R. Bourne and M. Kasran**
- NMR spectroscopic and X-ray crystallographic studies of calix[4]arene-Ag⁺ complexes. Influence of bound Ag⁺ on C_{2v}-C_{2v} interconversion in *cone*-calix[4]arenes **A. Ikeda, H. Tsuzuki and S. Shinkai**
- Is the collision induced loss of methanol from deprotonated 4-methoxybut-1-yne in the gas phase a charge remote reaction? **S. Dua and J. H. Bowie**
- Factors affecting the rates of thermal decomposition of azidothiophenes **L. K. Dyal, P. M. Suffolk, W. Dehaen and G. L'abbé**
- Bicyclopentene addend on [60]fullerene: epoxidation and *cis*-bromine addition **M. F. Meidine, A. G. Avent, A. D. Darwish, G. J. Langley, W. Locke, O. Ohashi, H. W. Kroto, R. Taylor and D. R. M. Walton**
- Alkene epoxidations catalysed by molybdenum(VI) supported on imidazole-containing polymers. Part 3. Epoxidation of oct-1-ene and propene **M. M. Miller, D. C. Sherrington and S. Simpson**
- The relationship between structure and second hyperpolarisability in conjugated hydrocarbons **R. Thomas**
- Conformationally restricted Criegee intermediates: evidence for formation and stereoelectronically controlled fragmentation **S. Chandrasekhar and C. D. Roy**
- A detailed study defining the extent of preorganization of an aza macrocycle containing the phenyldinaphthomethane subunit (a three bladed propeller) using dynamic NMR and molecular dynamics **P. J. Cooper, M. N. S. Hill and J. C. Lockhart**
- Remote substituent effects on polar and non-polar covalent bonds **M. Jonsson, J. Lind, G. Merényi and T. E. Eriksen**
- An extended form of the Evans–Polanyi equation: a simple empirical relationship for the prediction of activation energies for hydrogen-atom transfer reactions **B. P. Roberts and A. J. Steel**
- Electrophilic chemistry (protonation, nitration, bromination) of crowded (*Z*)-2,2,5,5-tetramethyl-3,4-diphenylhex-3-ene; formation of phenanthrenium ions by facial ring protonation/transannular cyclization in superacid media; *p,p*-dinitration and *p,p*-dibromination with NO₂⁺ BF₄⁻ and Br₂-SO₂ **K. K. Laali, J. E. Gano, C. W. Gundlach IV and D. Lanoir**
- ¹³C, ¹H and two-dimensional NMR studies of charge distribution in sterically congested persistent cycloalkyl- and alkyl-pyrenium ions generated by protonation in superacid media **K. K. Laali and P. E. Hansen**
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- Nucleophilic substitution in benzylic thiophosphinyl and thiophosphonyl chlorides: the contribution of elimination–addition pathways with methylenethioxophosphorane (thiophosphene) intermediates **M. P. Coogan and M. J. P. Harger**
- The kinetics of cleavage of nitrophenyl alkanooates by γ-cyclodextrin and by 'dimethyl-β-cyclodextrin' in basic aqueous solution **O. S. Tee and T. A. Gadosy**
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- Hemiacetals of acetophenone. Aromatic substituent effects in the H⁺- and general-base-catalysed decomposition in aqueous solution **R. A. McClelland, K. M. Engell, T. S. Larsen and P. E. Sørensen**
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- Triazene drug metabolites. Part 14. Kinetics and mechanism of the acid catalysed hydrolysis of 3-alkoxymethyl-3-alkyl-1-aryltriazenes **L. Fernandes, A. P. Francisco, J. Iley and E. Rosa**

The accurate prediction of the solvation of nucleotide base pairs using an *ab initio* continuum model
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