

JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions 2

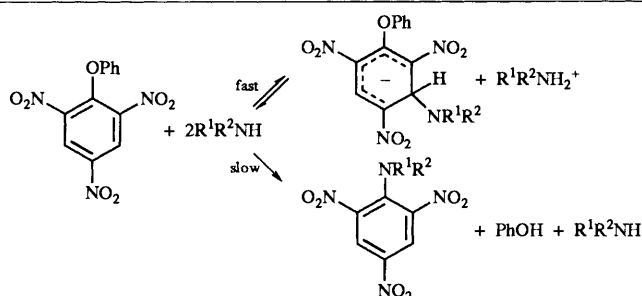
Physical Organic Chemistry

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Articles

- 1831 **Mechanism of base catalysis in the reactions of phenyl aryl ethers with aliphatic amines in dimethyl sulfoxide**

Rachel A. Chamberlin and Michael R. Crampton



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

- 1839 **Partition between phases of a solute that exists as two interconverting species**

Michael H. Abraham and Albert J. Leo

Assignment of descriptors can be made for interconverting species such as conformers or keto-enol tautomers, and can be used to estimate partition coefficients for the individual species as well as the equilibrium mixture of isomers

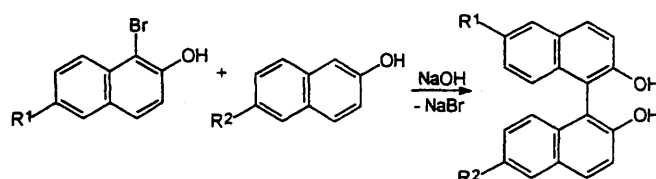
- 1843 **Factors that influence tadpole narcosis. An LFER analysis**

Michael H. Abraham and Clara Rafols

For 84 solutes studied by Overton, and for 114 solutes in total, an LFER analysis is used to elucidate the solute factors that influence narcosis and to probe the properties of the anaesthetic binding site

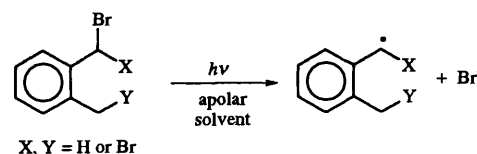
1853 **Nucleophilic coupling of alkali 2-naphthoxides with 1-bromo-2-naphthols. Ion-pairing and halogen dance in the formation of 1,1'-binaphthalene-2,2'-diols**

Martin Bělohradský, Petr Holý and Jiří Závada



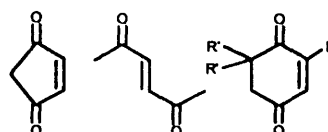
1857 **Photolysis of a series of α -brominated *ortho*-xylenes in apolar solvents**

Daisy de B. Rezende, Ivan P. de Arruda Campos, Vicente G. Toscano and Luiz H. Catalani



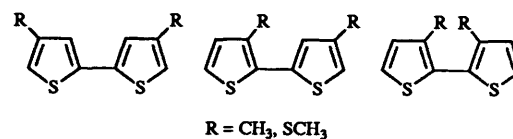
1863 **Photophysics of enediones**

Luiz H. Catalani, Vicente G. Toscano and Ivan P. de Arruda Campos



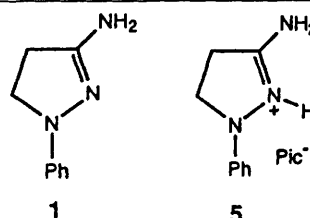
1869 **Conformational properties of 3,3'-, 3,4'- and 4,4'-dimethyl- and -bis(methylsulfanyl)-2,2'-bithiophenes**

Giovanna Barbarella, Massimo Zambianchi, Luciano Antolini, Ugo Folli, Francesca Goldoni, Dario Iarossi, Luisa Schenetti and Alessandro Bongini



1875 **Structure of 3-amino-4,5-dihydropyrazoles in acid media: X-ray structure of 3-amino-1-phenyl-4,5-dihydropyrazol-2-ium picrate and the origin of broad signals in ¹H NMR spectroscopy**

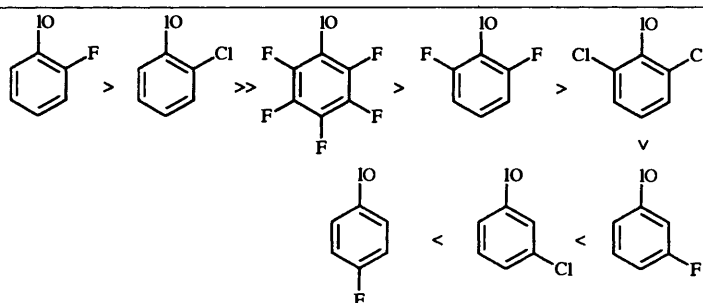
Rosa María Claramunt, Pietro Cozzini, Paolo Domiano, José Elguero, Isabelle Forfar and Alain Fruchier



The broadening of NMR signals in 3-amino-4,5-dihydropyrazoles is due to the presence of acid in some solvents, like deuteriochloroform; to determine the protonation site of 3-amino-1-phenyl-4,5-dihydropyrazole **1**, the crystal structure of its picrate **5** was determined: contrary to other dihydropyrazoles, **1** protonates on N² like an amidine

1883 Kinetics of the iron porphyrin catalysed oxidation of cyclohexene with substituted iodosylbenzenes

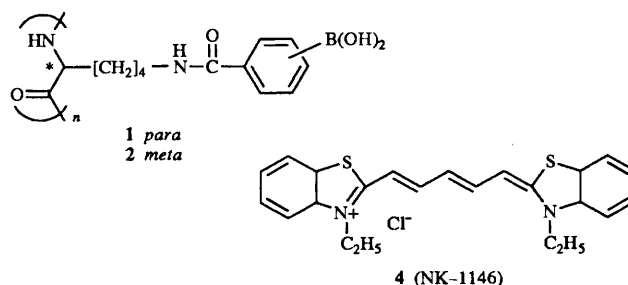
Grahame J. Harden



Incorporating electronegative aryl substituents on iodosylbenzene leads to a rate enhancement for iron porphyrin catalysed alkene epoxidation

1889 Sugar-induced conformational changes in boronic acid-appended poly(L- and D-lysine) and sugar-controlled orientation of a cyanine dye on the polymers

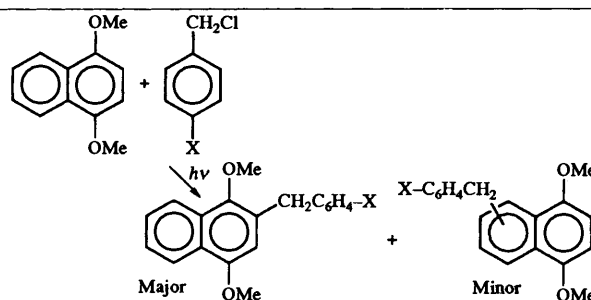
Taro Kimura, Susumu Arimori, Masayuki Takeuchi, Takeshi Nagasaki and Seiji Shinkai



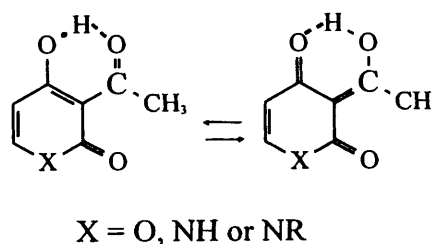
The conformation of 1 and 2 was changed by adding saccharides; the chiral orientation of cyanine dye (4) was induced on 1 or 2 in the presence of saccharides

1895 Photoinduced benzylation of 1,4-dimethoxynaphthalene by benzyl halides

Angelo Albini, Enrico Siviero, Mariella Mella, Conor Long and Albert Pratt

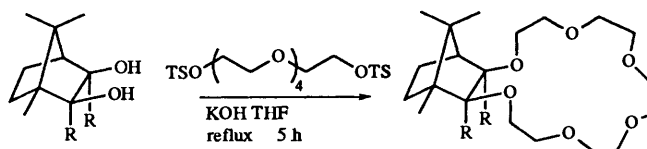
1901 Intramolecular hydrogen bonding and tautomerism of acylpyran-2,4-diones, -2,4,6-triones and acylpyridinediones and benzannulated derivatives. Deuterium isotope effects on ^{13}C NMR chemical shifts

Poul Erik Hansen, Simon Bolvig and Thomas Kappe



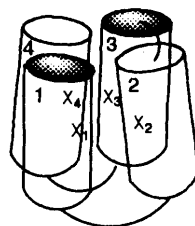
1909 Synthesis of camphor based chiral crown ethers and their interactions with amino acid derivatives

Brian J. Brisdon, Richard England, Mary F. Mahon, Khalid Reza and Malcolm Sainsbury



1915 A pair of pyrene groups as a conformational probe for designed four- α -helix bundle polypeptides

Hisakazu Mihara, Yuji Tanaka, Tsutomu Fujimoto and Norikazu Nishino

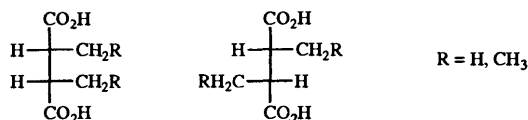


$\text{DAPeLLKAX}_1\text{AeLLK-}$
 $\text{DAPeLLKAX}_2\text{AeLLK-}$
 $\text{DAPeLLKAX}_3\text{AeLLK-}$
 $\text{DAPeLLKAX}_4\text{AeLLK-}$

$X_1=X_3=\text{L-1-pyrenylalanine (Pya)}$
 $X_2=X_4=\text{Phe}$

1923 NMR conformational study of the neutralisation of *meso*- and *rac*-2,3-dimethyl- and 2,3-diethylsuccinic acids in aqueous solution

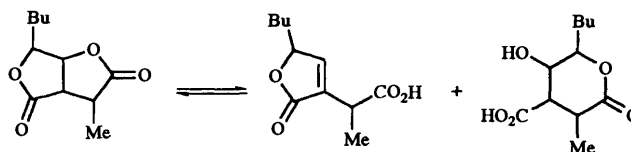
Hartmut Komber



The changes of both the vicinal methine protons coupling constants and the ^{13}C chemical shifts of the isomers of 2,3-dimethyl- and 2,3-diethylsuccinic acid have been determined in the course of titration and were attributed to changes of the conformational equilibrium

1929 Rates and mechanisms for the ring opening, ring closure and ring transformation reactions of the di- γ -lactone dihydrocanadensolide (DHC)

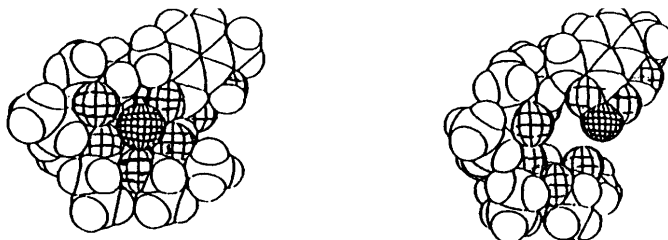
David C. Aldridge, Stuart Nicholson and Peter J. Taylor



+ various hydrolysis products; some unusual ΔS^\ddagger values are found

1939 Interactions between metal cations and the ionophore lasalocid. Part 13. Structure of 1:1 and 2:1 lasalocid anion-divalent cation complexes in methanol

Mostafa Mimouni, Patrice Malfreyt, Rachid Lyazghi, Marc Palma, Yves Pascal, Gérard Dauphin and Jean Juillard



Barium and magnesium 1:1 complexes

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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*

A study of the mechanism of solvolysis of but-3-enyl bromide (4-bromobut-1-ene) using the extended (two-term) Grunwald-Winstein equation **D. N. Kevill and M. H. Abduljaber**

Electrochemical oxidation of [1.1.1]paracyclophanes, biseco-, seco- and dodecahedra(dienes): stability of caged 4c/3e radical cations and 4c/2e dications **K. Weber, G. Lutz, L. Knothe, J. Mortensen, J. Heinz and H. Prinzbach**

Conformational analysis. Part 24. A lanthanide-induced-shift (LIS) NMR investigation of aromatic ketones. Lutetium versus lanthanum reagents in probing diamagnetic complexation shifts **F. Sancassan, G. Petrillo and R. J. Abraham**

Interactions between amines and aromatic fluoro derivatives. ¹⁹F NMR investigation in [2H₆] toluene **L. Forlani and E. Mezzina**

Molecular recognition of alkyl and arylalkylamines in dichloromethane and chloroform by calix[4]-crown ethers **Y. E. Jung, B. M. Song and S.-K. Chang**

Design, synthesis and solution structure of a helix-loop-helix dimer—a template for the rational design of catalytically active polypeptides **S. Olofsson, G. Johansson and L. Baltzer**

Enantiodifferentiating photoisomerization of 1-methylcyclooctene sensitized by chiral alkyl benzenecarboxylates: steric effects upon stereodifferentiation **H. Tsuneishi, T. Hakushi, A. Tai and Y. Inoue**

Hydrogen-bond basicity of thioamides and thioureas **C. Laurence, M. Berthelot, J.-Y. Le Questel and M. J. El Ghomari**

New 'multi-site' phase transfer catalyst for the addition of dichlorocarbene to styrene **T. Balakrishnan and J. P. Jayachandran**

ENDOR and EPR studies of highly isotopically ¹³C-enriched ubiquinone radicals. Part 2 **R. I. Samoilova, N. P. Gritsan, A. J. Hoff, W. van Liemt, J. Lugtenburg, A. P. Spoyalov and Y. D. Tsvetkov**

Infrared spectroscopic studies of vancomycin and its interactions with *N*-acetyl-D-ala-D-ala and *N,N'*-diacetyl-L-lys-D-ala-D-ala **C. J. Salter, R. C. Mitchell and A. F. Drake**

Selective sensing of guanidinium and tetraalkylammonium ions using lipophilic cyclodextrins **P. M. Kelly, R. Katakly, D. Parker and A. F. Patti**

Conformational Analysis. Part 25. The evaluation of molecular geometries by the lanthanide induced shift (LIS) technique **R. J. Abraham, S. Angiolini, M. Edgar and F. Sancassan**

Triplet state properties of flavone in homogeneous and micellar solutions. A laser flash photolysis study **C. Avila and C. M. Previtali**

Complementary hydrogen bonding in diamides: a study on the influence of remote substituents using density functional theory **J. E. McGrady and D. M. P. Mingos**

Organic sonoelectrochemistry. The reduction of fluorescein in the presence of 20 kHz power ultrasound. An EC' reaction **J. C. Eklund, D. N. Waller, T. O. Rebbitt, F. Marken and R. G. Compton**

Detropylations of *N*-tropyldimethylamine and *N*-troylacetylamide **J. Palou, P. M. Robinson and C. I. F. Watt**

Rate constants for the reaction of peroxy free radical with flavonoids and related compounds as determined by the kinetic chemiluminescence method **V. A. Belyakov, V. A. Roginsky and W. Bors**

Influence of magnesium(II) ions on cathodic reactions in aprotic solvents: the reduction of benzoate esters **D. Pletcher and L. Slevin**

Cation-exchanged fluorotetrasilicic mica (Mⁿ⁺-TSM; Mⁿ⁺ = Mn²⁺, Cr³⁺, Co²⁺ and Cu²⁺) -catalysed oxidation of alkanes with *tert*-butyl hydroperoxide **J.-I. Tateiwa, H. Horiuchi and S. Uemura**

Quantitative structure-sublimation enthalpy relationship studied by neural networks, theoretical crystal packing calculations and multilinear regression analysis **M. H. Charlton, R. Docherty and M. G. Hutchings**

Solvent-induced changes in nitrosation mechanisms. Part 3. The effects of tetrahydrofuran–water and dimethylsulfoxide–water mixtures on the nitrosation of ureas **P. Hervés and J. R. Leis**

Characterization of the 1-indanone keto–enol system **E. A. Jefferson, J. R. Keeffe and A. J. Kresge**

S_N2 reactions of a sulfonate ester in mixed cationic/phosphine oxide micelles **A. Blaskó, C. A. Bunton, E. A. Toledo, P. M. Holland and F. Nome**