

JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions 2

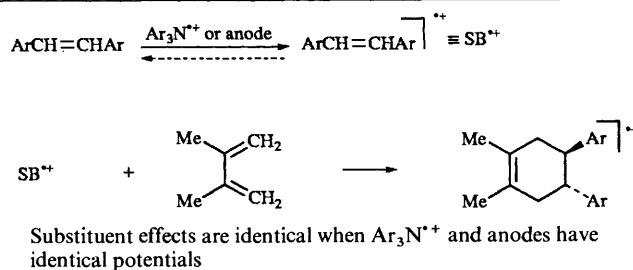
Physical Organic Chemistry

CONTENTS

Perkin Communications

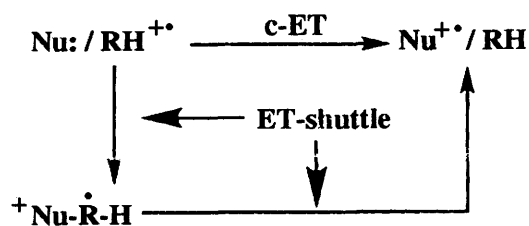
- 1715 **Electrochemical mechanistic criteria for the diagnosis and elucidation of cation radical mechanisms: the quantitative simulation of aminium salt catalysis by anodes of the same potential**

Wang Yueh, Haripada Sarker and Nathan L. Bauld



- 1717 **Electron transfer mechanisms: a mechanistic changeover induced by an intramolecular spacer in a model reaction of the $\text{NH}_3/\text{C}_2\text{H}_4^{\cdot+}$ pair**

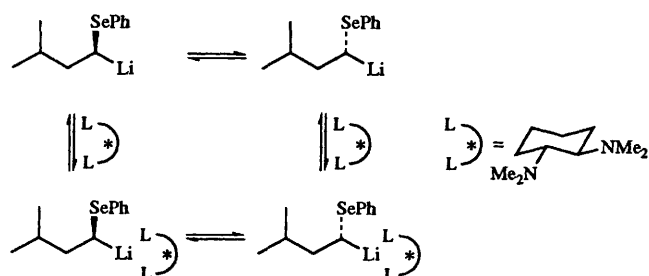
A. Chandrasekhar Reddy, G. Narahari Sastry and Sason Shaik



Articles

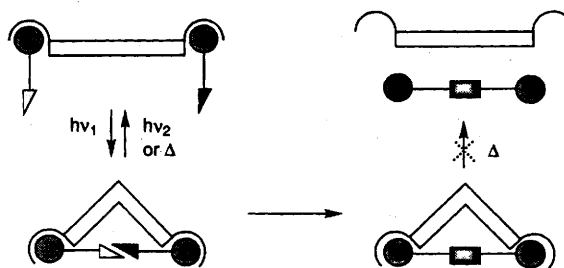
- 1721 **Chiral organometallic reagents. Part XVII. Formation of diastereoisomeric complexes between α -phenylselenanylalkyllithium compounds and chiral diamines**

Reinhard W. Hoffmann, Wolfgang Klute, Ruprecht K. Dress and Andreas Wenzel

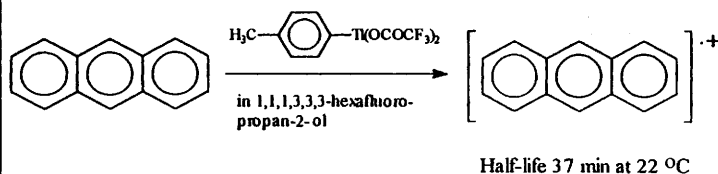


1727 **Photoresponsive synthetic receptors: binding properties and photocontrol of catalytic activity**

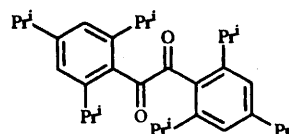
Frank Würthner and Julius Rebek, Jr.

1735 **1,1,1,3,3,3-Hexafluoropropan-2-ol as a solvent for the generation of highly persistent radical cations**

Lennart Ebersson, Michael P. Hartshorn and Ola Persson

1745 **Crystal structure of the solid state photoreactive 2,2',4,4',6,6'-hexaisopropylbenzil**

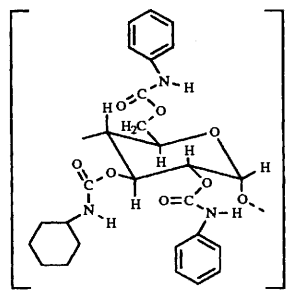
Joseph Frey, Erez Faraggi, Zvi Rappoport and Menahem Kaftory



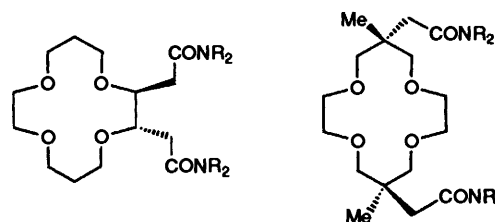
The crystal structure of 2,2',4,4',6,6'-hexaisopropylbenzil has been determined and hydrogen atoms which can participate in a known solid state photocyclization have been located

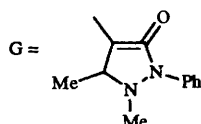
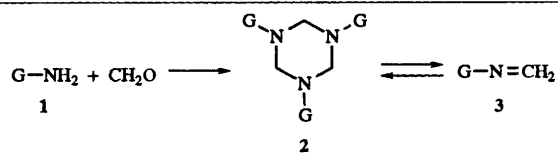
1749 **Enantiorecognition of a new chiral selector, β -cyclodextrin perphenylcarbamate, as studied by NMR spectroscopy and molecular energy calculation**

Yoshihiro Kuroda, Yoshiyuki Suzuki, Jingyi He, Takahiro Kawabata, Akimasa Shibukawa, Hiroo Wada, Hiroya Fujima, Yasuhiko Go-oh, Eiji Imai and Terumichi Nakagawa

1761 **Lithium-selective ionophores based on pendant arm substituted crown ethers**

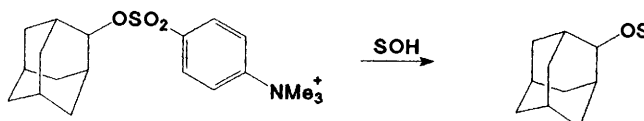
Stephen Faulkner, Ritu Katakya, David Parker and Andrew Teasdale



1771 An NMR observation of the *N*-methylideneamine–hexahydrotriazine equilibrium

Aminoantipyrine (1) reacted with paraformaldehyde to yield the trimer 2, which was found to equilibrate with its monomer in CD_2Cl_2 and $[\text{}^2\text{H}_6]\text{DMSO}$; X-ray structural data of 2 were obtained

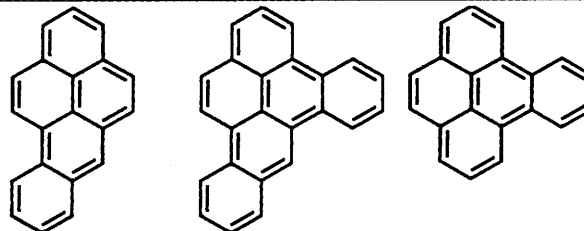
Angelo G. Giumanini, Giancarlo Verardo, Fausto Gorassini, Tiziano Scubla, Paolo Strazzolini, Franco Benetollo and Gabriella Bombieri

1777 Application of the Grunwald–Winstein equation to the solvolysis of the 2-adamantyl *p*-(trimethylammonio)benzenesulfonate (amsylate) cation. Absence of significant perturbation by a remote positive charge

$$\log(k/k_0) = 0.92Y_{\text{OTs}} + 0.07$$

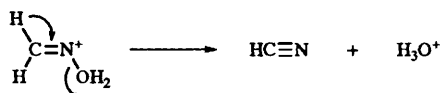
$$r = 0.990$$

Dennis N. Kevill and Richard W. Bahnke

1781 Protonation of benzo[*a*]pyrene, dibenzo[*a,e*]pyrene and benzo[*e*]pyrene in superacids: NMR studies of charge distribution in persistent arenium ions and AM1 calculations

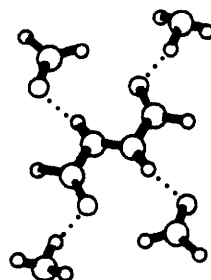
Persistent monoarenium ions were generated in $\text{FSO}_3\text{H}/\text{SO}_2\text{ClF}$ (NMR and AM1 theory)

Kenneth K. Laali, Poul Erik Hansen, John J. Houser and Maximilian Zander

1791 Important role of the Beckmann rearrangement in the gas phase chemistry of protonated formaldehyde oximes and their $[\text{CH}_4\text{NO}]^+$ isomers

Ab initio MO calculations show that the Beckmann rearrangement is the most facile unimolecular reaction of protonated formaldoximes and their isomers

Minh Tho Nguyen, Greet Raspoet and Luc G. Vanquickenborne

1797 Molecular conformation of isolated and hydrogen bonded *N,N'*-diformohydrazide: an *ab initio* study

The effect of hydrogen bonding on the structure and vibrational spectrum of *N,N'*-diformohydrazide was studied by *ab initio* methods

Fabio Ramondo and Luigi Bencivenni

AUTHOR INDEX

- Bahnke, Richard W., 1777
Bauld, Nathan L., 1715
Bencivenni, Luigi, 1797
Benetollo, Franco, 1771
Bombieri, Gabriella, 1771
Dress, Ruprecht K., 1721
Duca, José S., 1821
Eberson, Lennart, 1735
Ehara, Tsuguhisa, 1829
Faraggi, Erez, 1745
Faulkner, Stephen, 1761
Frey, Joseph, 1745
Fujima, Hiroya, 1749
Giumanini, Angelo G., 1771
Go-oh, Yasuhiko, 1749
Gorassini, Fausto, 1771
Grévy, Jean-Michel, 1809
Grosu, I., 1829
- Guerra, Maurizio, 1817
Hansen, Poul Erik, 1781
Hartshorn, Michael P., 1735
He, Jingyi, 1749
Hoffmann, Reinhard W., 1721
Houser, John J., 1781
Ikuta, Shigeru, 1805
Imai, Eiji, 1749
Jelokhani-Niaraki, Masood, 1829
Kaftory, Menahem, 1745
Kamigata, Nobumasa, 1805
Katakya, Ritu, 1761
Kawabata, Takahiro, 1749
Kevill, Dennis N., 1777
Klute, Wolfgang, 1721
Kodama, Hiroaki, 1829
Kondo, Michio, 1829
- Kuroda, Yoshihiro, 1749
Laali, Kenneth K., 1781
Mager, S., 1829
Matsuhisa, Ayumi, 1805
Mulliez, Michel, 1809
Nakagawa, Terumichi, 1749
Nguyen, Minh Tho, 1791
Parker, David, 1761
Persson, Ola, 1735
Pierini, Adriana B., 1821
Plé, G., 1829
Ramondo, Fabio, 1797
Rappoport, Zvi, 1745
Raspoet, Greet, 1791
Rebek, Julius, 1727
Reddy, A. Chandrasekhar, 1717
Sarker, Haripada, 1715
- Sastry, G. Narahari, 1717
Scubla, Tiziano, 1771
Shaik, Sason, 1717
Shibukawa, Akimasa, 1749
Shimizu, Toshio, 1805
Strazzolini, Paolo, 1771
Suzuki, Yoshiyuki, 1749
Teasdale, Andrew, 1761
Vanquickenborne, Luc G., 1791
Verardo, Giancarlo, 1771
Wada, Hiroo, 1749
Wenzel, Andreas, 1721
Würthner, Frank, 1727
Yueh, Wang, 1715
Zander, Maximilian, 1781

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

Forthcoming Articles in *Perkin Transactions 2*

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

R. A. Chamberlin and M. R. Crampton

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 **M. Bělohradský, P. Holý and J. Závada**

Kinetics of the iron porphyrin catalysed oxidation of cyclohexene with substituted iodosylbenzenes **G. J. Harden**

Sugar-induced conformational changes in boronic acid-appended poly(L- and D-lysine)s and sugar-controlled orientation of a cyanine dye on the polymers **T. Kimura, S. Arimori, M. Takeuchi, T. Nagasaki and S. Shinkai**

Photoinduced benzylation of 1,4-dimethoxynaphthalene by benzyl halides

A. Albini, E. Siviero, M. Mella, C. Long and A. C. Pratt

Photophysics of enediones **L. H. Catalani, V. G. Toscano and I. P. de Arruda Campos**

Intramolecular hydrogen bonding and tautomerism of acylpyran-2,4-diones, -2,4,6-triones and acylpyridinediones and benzannelated derivatives. Deuterium isotope effects on ¹³C NMR chemical shifts **P. E. Hansen, S. Bolvig and T. Kappe**

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

H. Mihara, Y. Tanaka, T. Fujimoto and N. Nishino

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

H. Komber

Interactions between metal cations and the ionophore lasalocid. Part 13. Structure of 1:1 and 2:1 lasalocid anion–divalent cation complexes in methanol **M. Mimouni, P. Malfreyt, R. Lyazghi, M. Palma, Y. Pascal, G. Dauphin and J. Juillard**

Selective sensing of guanidinium and tetraalkylammonium ions using lipophilic cyclodextrins

P. M. Kelly, R. Katakay, D. Parker and A. F. Patti

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

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

A study of the mechanism of solvolysis of allylcarbinyl 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]pagodanes, biseco-, seco- and dodecahedra (di) enes: stability of caged 4c/3e radical cations and 4c/2e dications **K. Weber, G. Lutz, L. Knothe, J. Mortensen, J. Heinze and H. Prinzbach**

Partition between phases of a solute that exists as two interconverting species **M. H. Abraham and A. J. Leo**

Factors that influence tadpole narcosis. An LFER analysis **M. H. Abraham and C. Rafols**

Interactions between amines and aromatic fluoro derivatives **L. Forlani and E. Mezzina**

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**

Molecular recognition of alkyl and arylalkylamines 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 T. Inoue**

Reviewing homolysis in benzylic systems: photolysis of a series of α -brominated *o*-xylenes in apolar solvents

D. de B. Rezende, I. P. de Arruda Campos, C. G. Toscano and L. H. Catalani

Conformational properties of 3,3'-, 3,4'- and 4,4'-dimethyl and bis(methylthio) 2,2'-bithiophenes

G. Barbarella, M. Zambianchi, L. Antolini, U. Folli, F. Goldoni, D. Iarossi, L. Schenetti and A. Bongini