

JOURNAL OF THE CHEMICAL SOCIETY

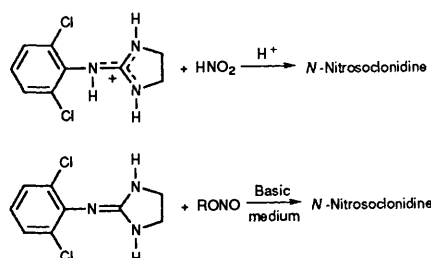
Perkin Transactions 2

Physical Organic Chemistry

CONTENTS**Articles**

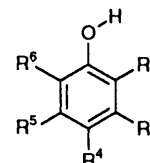
- 1561 **Kinetics and mechanism of nitrosation of clonidine: a bridge between nitrosation of amines and ureas**

Fátima Norberto, José A. Moreira, Eduarda Rosa, Jim Iley, J. Ramón Leis and M. Elena Peña



- 1567 **O-H Bond strengths and one-electron reduction potentials of multisubstituted phenols and phenoxy radicals. Predictions using free energy relationships**

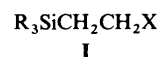
Mats Jonsson, Johan Lind, Trygve E. Eriksen and Gabor Merényi



A general equation for determination of O-H bond strengths of multisubstituted phenols based on linear free energy relationships is presented

- 1569 **Conformational effects in β -functional acyclic organosilicon compounds**

Martin S. Beevers, Susan Bratt, Ann W. P. Jarvie and Michael C. Perry



Theoretical and experimental evaluation of R and X on the conformation of **I**

- 1575 **Reactivity-selectivity relationship and kinetic solvent isotope effects in nucleophilic substitution reactions**

Ikchoon Lee, Han Joong Koh, Young Sook Park and Hai Whang Lee

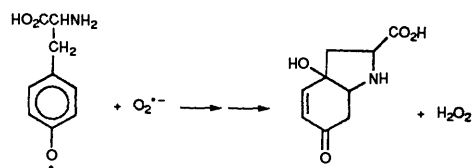
$$\log k_N/k_S = \Delta\rho_Y \times \sigma_Y$$

$$\log \text{KSIE} = \Delta\rho_Y \times \sigma_Y$$

Signs of $\Delta\rho_Y$ are indicative of reaction mechanism

1583 **The superoxide radical reacts with tyrosine-derived phenoxyl radicals by addition rather than by electron transfer**

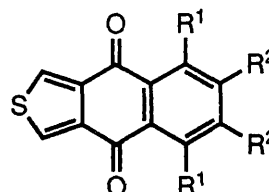
Faming Jin, Johannes Leitich and Clemens von Sonntag



The superoxide radical reacts with tyrosine-derived phenoxyl radicals by addition rather than by electron transfer

1589 **Preparation and characterisation of thienonaphthoquinones and their radical ions**

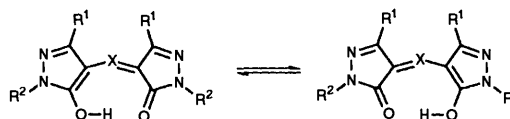
Joe A. Crayston, Ahmed Iraqi, Philip Mallon and John C. Walton



Redox reactions of three naphtho[2,3-*c*]thiophene-4,9-diones were studied electrochemically and by EPR spectroscopy

1597 **Proton transfer in rubazoic acid derivatives in solution and in the solid state. An NMR study**

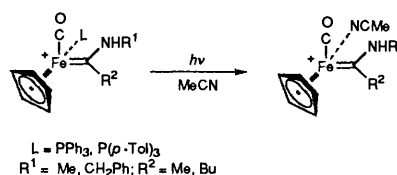
Alejandro C. Olivieri, Dionisia Sanz, Rosa M^a. Claramunt and José Elguero



¹H, ¹³C, ¹⁵N and ²H NMR in solution, and ¹³C solid-state NMR data are reported for rubazoic acid derivatives

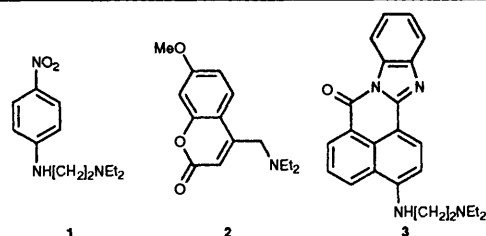
1603 **Photofragmentation voltammetry studies of the aminocarbene complexes**
 $[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})(\text{L})\{\text{C}(\text{NHR}^1)(\text{R}^2)\}]\text{BF}_4$
 [L = PPh₃, P(*p*-Tol)₃; R¹ = Me, CH₂Ph; R² = Me, Bu]

Stephen G. Davies, Michael R. Metzler, W. Carl Watkins, Richard G. Compton, Jonathan Booth and John C. Eklund



1611 **Luminescence and charge transfer. Part 3. The use of chromophores with ICT (internal charge transfer) excited states in the construction of fluorescent PET (photoinduced electron transfer) pH sensors and related absorption pH sensors with aminoalkyl side chains**

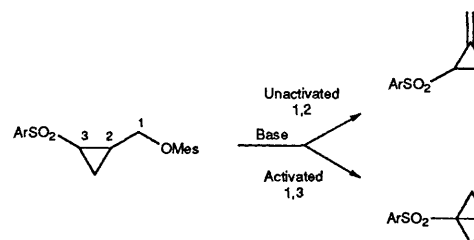
A. Prasanna de Silva, H. Q. Nimal Gunaratne, P. L. Mark Lynch, Alan J. Patty and Graham L. Spence



1-3 are absorption pH sensors while 2 and 3 also show fluorescent pH sensor action

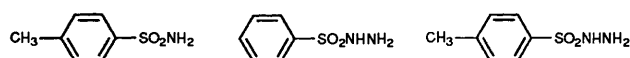
1617 **The strain limit in intramolecular nucleophilic substitution**

Stephen M. Jeffery and Charles J. M. Stirling



1625 **Investigation and rationalisation of hydrogen bonding patterns in sulfonylamino compounds and related materials: crystal structure determination of microcrystalline solids from powder X-ray diffraction data**

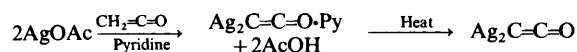
Philip Lightfoot, Maryjane Tremayne, Christopher Glidewell, Kenneth D. M. Harris and Peter G. Bruce



The crystal structures of these compounds, solved from powder X-ray diffraction data, are reported and their hydrogen bonding patterns, and those of related materials, are discussed in terms of graph set analysis

1631 **Preparation, properties and structure of crystalline silver ketenide (μ -oxoethenylidene disilver) and its pyridine complex**

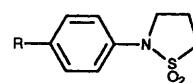
Ernest T. Blues, Derek Bryce-Smith, Ronald Shaoul, Hans Hirsch and Michael J. Simons



Silver ketenide and its pyridine complex have unusual structures involving monolayers of silver atoms separated by rod-like ketenide groups normal to the sheets of silver atoms

1643 **Acid-catalysed hydrolysis and protonation behaviour of *N*-arylpropane-1,3-sultams**

Yunus Bekdemir, John G. Tillett and Romuald I. Zalewski

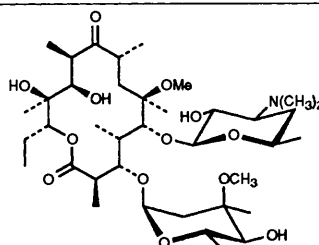


1 R = a, MeO; b, Me; c, H; d, Cl; e, NO₂

The rate maxima observed in the acid-catalysed hydrolyses of sultams are shown to be associated with extensive protonation of these substrates in strong acid

1647 **Origin of regioselectivity in the *O*-methylation of erythromycin as elucidated with the aid of computational conformational space search**

Hitoshi Gotō, Yutaka Kawashima, Masato Kashimura, Shigeo Morimoto and Eiji Ōsawa

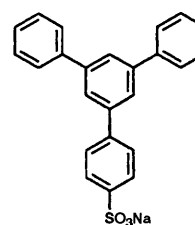


6-*O*-methylethromycin A (1, Clarithromycin)

Populations of reactive conformers for the title reaction have been predicted by the use of program CONFLEX which effectively generates low-energy conformers

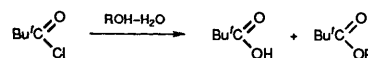
1655 **Synthesis and studies on surface and self-assembly properties of polyphenylsulfonates in aqueous solution. Part 1: sodium 5'-phenyl-1,1':3',1''-terphenyl-4-sulfonate**

Jan Czapkiewicz, Piotr Milart and Bożena Tutaj



1659 **Dual reaction channels for solvolyses of acyl chlorides in alcohol-water mixtures**

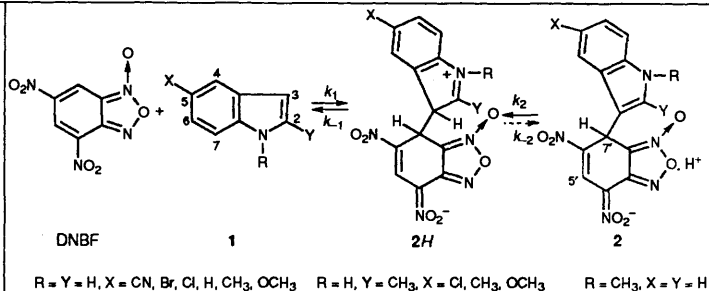
T. William Bentley and Chang Sub Shim



Rates and products of the above reaction are interpreted in terms of both competing nucleophiles, and competing reaction channels in contrast to the transition state variation model

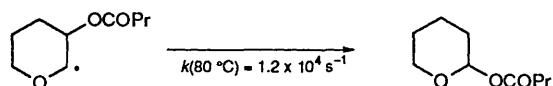
1665 **Electrophilic heteroaromatic substitutions: reactions of 5-X-substituted indoles with 4,6-dinitrobenzofuroxan**

François Terrier, Marie-José Pouet, Jean-Claude Halle, Stephen Hunt, John R. Jones and Erwin Buncel



1673 **The mechanism of the β -acyloxyalkyl radical rearrangement. Part 2: β -acyloxytetrahydropyranyl radicals**

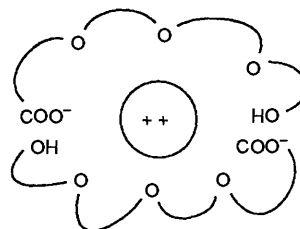
Athelstan L. J. Beckwith and Peter J. Duggan



This rearrangement proceeds, at least in part, by a dissociative process involving the intermediacy of an intimate radical-cation anion pair

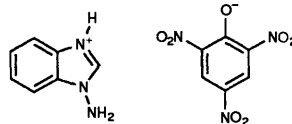
1681 **Interactions between metal cations and the ionophore lasalocid. Part 12. Alkaline-earth-lasalocid 1-2 complex salts in chloroform. Formation and structure**

Rachid Lyazghi, Yvon Pointud, Gérard Dauphin and Jean Juillard



1687 ***N*-Aminoazoles. Part 2. Basicity and protonation site of *N*-aminoazoles: an experimental (pK_a , ^{13}C and ^{15}N NMR spectroscopy and crystallography) and theoretical study**

Rosa M^a. Claramunt, Dionísia Sanz, Javier Catalán, Fernando Fabero, Norman A. García, Concepción Foces-Foces, Antonio L. Llamas-Saiz and José Elguero



The X-ray structures of two polymorphic forms of *N*-aminobenzimidazolium picrate have been determined

Corrigendum

1701 **The reaction of imidazole with some 1-halogeno-2,4-dinitrobenzenes** Elizabeth T. Akinyele, Delanson F. Crist and Jack Hirst

vii Conference Diary

AUTHOR INDEX

- Akinyele, Elizabeth T., 1701
Beckwith, Athelstan L. J., 1673
Beevers, Martin S., 1569
Bekdemir, Yunus, 1643
Bentley, T. William, 1659
Blues, Ernest T., 1631
Booth, Jonathan, 1603
Bratt, Susan, 1569
Bruce, Peter G., 1625
Bryce-Smith, Derek, 1631
Buncel, Erwin, 1665
Catalán, Javier, 1687
Claramunt, Rosa M^a., 1597, 1687
Compton, Richard G., 1603
Crayston, Joe A., 1589
Crist, Delanson F., 1701
Czapkiewicz, Jan, 1655
Dauphin, Gérard, 1681
Davies, Stephen G., 1603
de Silva, A. Prasanna, 1611
Duggan, Peter J., 1673
Eklund, John C., 1603
Elguero, José, 1597, 1687
Eriksen, Trygve E., 1567
Fabero, Fernando, 1687
Foces-Foces, Concepción, 1687
García, Norman A., 1687
Glidewell, Christopher, 1625
Gotō, Hitoshi, 1647
Gunaratne, H. Q. Nimal, 1611
Halle, Jean-Claude, 1665
Harris, Kenneth D. M., 1625
Hirsch, Hans, 1631
Hirst, Jack, 1701
Hunt, Stephen, 1665
Iley, Jim, 1561
Iraqi, Ahmed, 1589
Jarvie, Ann W. P., 1569
Jeffery, Stephen M., 1617
Jin, Faming, 1583
Jones, John R., 1665
Jonsson, Mats, 1567
Juillard, Jean, 1681
Kashimura, Masato, 1647
Kawashima, Yutaka, 1647
Koh, Han Joong, 1575
Lee, Hai Whang, 1575
Lee, Ikchoon, 1575
Leis, J. Ramón, 1561
Leitich, Johannes, 1583
Lightfoot, Philip, 1625
Lind, Johan, 1567
Llamas-Saiz, Antonio L., 1687
Lyazghi, Rachid, 1681
Lynch, P. L. Mark, 1611
Mallon, Philip, 1589
Merényi, Gabor, 1567
Metzler, Michael R., 1603
Milart, Piotr, 1655
Moreira, José A., 1561
Morimoto, Shigeo, 1647
Norberto, Fátima, 1561
Olivieri, Alejandro C., 1597
Osawa, Eiji, 1647
Park, Young Sook, 1575
Patty, Alan J., 1611
Peña, M. Elena, 1561
Perry, Michael C., 1569
Pointud, Yvon, 1681
Pouet, Marie-José, 1665
Rosa, Eduarda, 1561
Sanz, Dionisia, 1597, 1687
Shaoul, Ronald, 1631
Shim, Chang Sub, 1659
Simons, Michael J., 1631
Spence, Graham L., 1611
Stirling, Charles J. M., 1617
Terrier, François, 1665
Tillett, John G., 1643
Tremayne, Maryjane, 1625
Tutaj, Bożena, 1655
von Sonntag, Clemens, 1583
Walton, John C., 1589
Watkins, W. Carl, 1603
Zalewski, Romuald I., 1643

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

