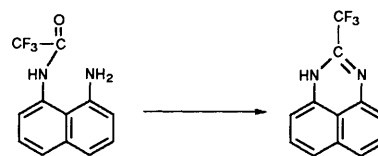




## Articles

- 1711 **General acid catalysis and kinetic isotope effects for intramolecular addition–elimination between amino and amide groups in 1-amino-8-trifluoroacetylaminonaphthalene; observation of a biphasic Brønsted plot**

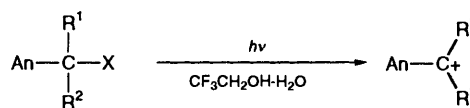
Andrew S. Baynham, Frank Hibbert and Muhammad A. Malana



The intramolecular addition–elimination shown above involves rate-limiting protonation of the zwitterionic intermediate formed by addition of the amino group to the amide carbonyl

- 1717 **Direct observation of  $\beta$ -fluoro-substituted 4-methoxyphenethyl cations by laser flash photolysis**

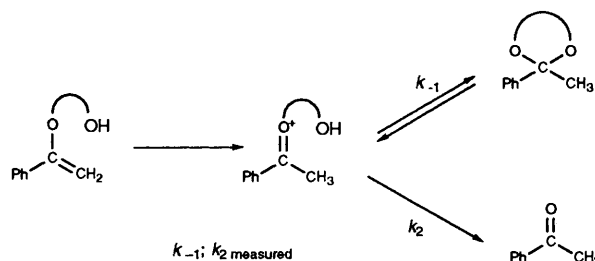
Robert A. McClelland, Frances L. Cozens, Steen Steenken, Tina L. Amyes and John P. Richard



$R^1 = \text{H}, R^2 = \text{CH}_2\text{F}, \text{CHF}_2, \text{CF}_3; R^1 = R^2 = \text{CF}_3$

- 1723 **Reversibility of the ring-opening step in the acid hydrolysis of cyclic acetophenone acetals**

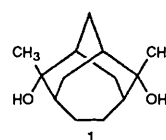
Robert A. McClelland, Brian Watada and Calvin S. Q. Lew



$k_{-1}; k_2$  measured

- 1729 **2,7-Dimethyltricyclo[4.3.1.1<sup>3,8</sup>]undecane-*syn*-2,*syn*-7-diol: structural analysis of the ellipsoidal clathrate and hemihydrate crystal forms**

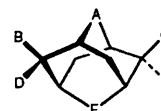
Stephen C. Hawkins, Roger Bishop, Ian G. Dance, Tony Lipari, Donald C. Craig and Marcia L. Scudder



Two cocrystalline forms of **1** are described in detail, and reasons for formation of its four alternative lattice types are discussed

- 1737 **Syntheses and crystal structures of four alicyclic diols which crystallise in different lattices involving helical extensions**

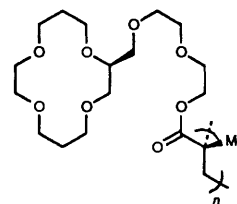
Stephen C. Hawkins, Roger Bishop, Donald C. Craig, Ian G. Dance, A. David Rae and Marcia L. Scudder



Crystal engineering aspects of the different helical lattices formed by diols of the above type are described and discussed

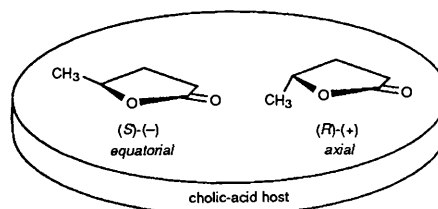
- 1747 **Synthesis of functionalised 12-, 13- and 14-membered crown ethers bearing exocyclic polymerisable groups and the binding properties and conductivities of their lithium doped polymers**

Luke Collie, James E. Denness, David Parker, Fiona O'Carroll and Christine Tachon



- 1759  **$^{13}\text{C}$  Solid-state NMR study on populations, conformations, and molecular motions of  $\gamma$ -valerolactone enantiomers enclathrated in the chiral cholic acid host**

Fumio Imashiro, Daisuke Kuwahara and Takehiko Terao



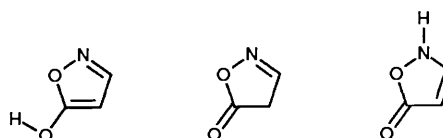
- 1765 **Thermochemical and crystallographic studies of some  $\beta$ -ketoimine derivatives**

Manuel A. V. Ribeiro Da Silva, Maria D. M. C. Ribeiro Da Silva, José P. A. Paiva, Isabel M. C. S. Nogueira, A. Margarida Damas, James V. Barkley, Marjorie M. Harding, Margaret J. Akello and Geoffrey Pilcher

Enthalpies of formation in the gaseous state and crystal structures of some  $\beta$ -ketoimines,  $\text{RCOCH}=\text{C}(\text{CH}_3)\text{NHR}^1$  are reported

- 1771 **Modelling of tautomeric equilibria of 5-hydroxyisoxazole in aqueous solution**

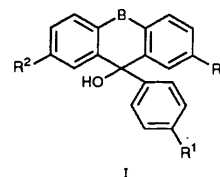
Ian R. Gould and Ian H. Hillier



Energies of three tautomers have been calculated in the gas phase and in water

- 1775 **Clathrate design for dioxane inclusion involving singly bridged triarylmethanol hosts. Synthesis, X-ray crystal structures and thermal stabilities of five inclusion compounds**

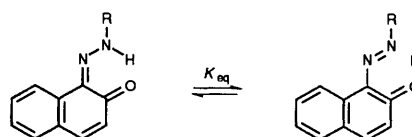
Ingeborg Csöreg, Edwin Weber, Luigi R. Nassimbeni, Olga Gallardo, Norbert Dörpinghaus, Anne Ertan and Susan A. Bourne



Different host molecules, represented by the general formula I, can be used for stabilization, storage and sensing of 1,4-dioxane

- 1783  **$^{13}\text{C}$  CPMAS NMR study of solid arylazonaphthols. Evidence of  $^{13}\text{C}$ ,  $^{14}\text{N}$  self-decoupling induced by a solid-state proton transfer reaction**

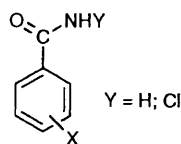
Sergio H. Alarcón, Alejandro C. Olivieri and Paul Jonsen



The proton transfer reaction shown ( $\text{R} = \text{H}; \text{MeO}; \text{N}=\text{N}-\text{Ph}$ ) causes  $^{13}\text{C}$ ,  $^{14}\text{N}$  self-decoupling in the  $^{13}\text{C}$  CPMAS spectra

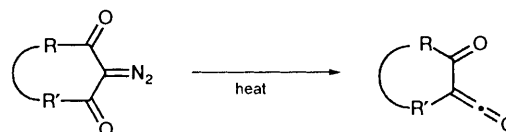
1787  $^{13}\text{C}$  Nuclear magnetic resonance study of  $\pi$ -polarization in 3- and 4-substituted benzamides and *N*-chlorobenzamides

Michael De Rosa, Keith Brown, Mary McCoy, Kevin Ong and Kimberley Sanford

Transmission of substituent effects by  $^{13}\text{C}$  NMR

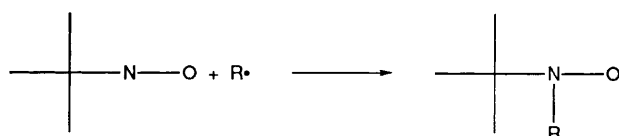
## 1791 Stereochemistry and thermal stability of diazodiketones

Vladimir V. Popik and Valerij A. Nikolaev

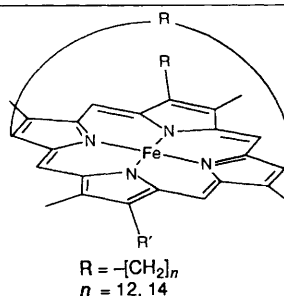
Thermal stability of diazodiketones mainly depends on distortion of the  $-\text{CO}-\text{CN}_2-\text{CO}-$  fragment of molecule

## 1795 Autoxidation of linoleic acid methyl ester studied by spin trapping

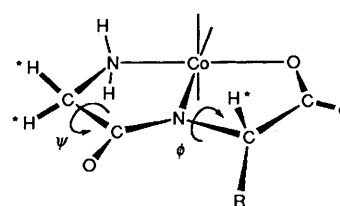
Thor Bernt Melø

1799 Kinetic parameters and linear free energy relationships of  $\text{O}_2$  and  $\text{CO}$  binding with closely related heme models of hemoglobins and cytochromes P-450

Driss El-Kasmi, Catherine Tetreau, Daniel Lavalette and Michel Momenteau

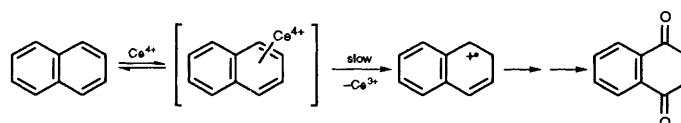
The binding of  $\text{O}_2$  and  $\text{CO}$  with various nitrogenous bases and thiolate derivatives of these  $\text{Fe}^{\text{II}}$  porphyrins has been investigated using laser flash photolysis1805 Interproton coupling across the *trans*-peptide bond ( $^5J_{\alpha\alpha'}$ ) in chelated dipeptides

Nenad Juranić, Vladimir Likić, Tanja Parac and Slobodan Macura



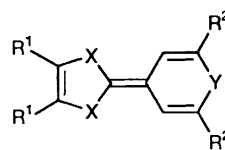
## 1811 Kinetics of ceric ion oxidation of naphthalene and its derivatives. Formation of the radical cation intermediate in the rate limiting step

M. Vivekananda Bhatt and Mariappan Periasamy

Oxidation of naphthalene to 1,4-naphthoquinone by  $\text{Ce}^{\text{IV}}$  takes place through the sequence outlined

1815 **Syntheses and properties of derivatives of 2-(thiopyran-4-ylidene)-1,3-dithiole and selenium analogues as novel unsymmetrical electron donors**

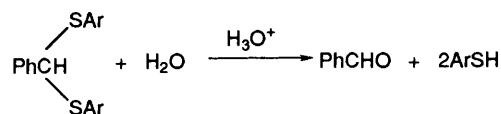
Tetsuo Otsubo, Yutaka Shiomi, Masayuki Imamura, Raita Kittaka, Akiko Ohnishi, Hiromi Tagawa, Yoshio Aso and Fumio Ogura



X, Y = S, Se  
R<sup>1</sup>, R<sup>2</sup> = H, Me, Ph, MeS, S CH<sub>2</sub>CH<sub>2</sub>S

1825 **Kinetics and mechanism of the acid-catalysed hydrolysis of benzaldehyde diaryl thioacetals and of benzaldehyde *S*-aryl, *S*-ethyl acetals in aqueous perchloric acid**

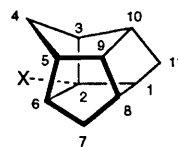
Muhammad Ali and Derek P. N. Satchell



Kinetic analysis for hydrolysis in concentrated aqueous perchloric acid

1829 **Synthesis of 2-substituted pentacyclo-[6.3.0.0<sup>2,6</sup>.0<sup>3,10</sup>.0<sup>5,9</sup>]undecanes (*D*<sub>3</sub>-trishomocubanes) and a study of their <sup>13</sup>C spin-lattice relaxation times in solution**

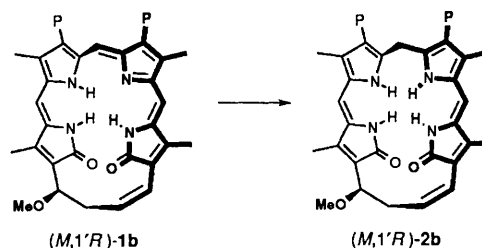
Martin Schwartz, Alan P. Marchand, Kuen-Shian Wang, S. Pulla Reddy, G. Madhusudhan Redda, V. R. Gadgil, William H. Watson, Ram P. Kashyap and Mariusz Krawiec



Five 2-substituted *D*<sub>3</sub>-trishomocubanes were synthesized. The results of <sup>13</sup>C NMR *T*<sub>1</sub> and NOE measurements are reported

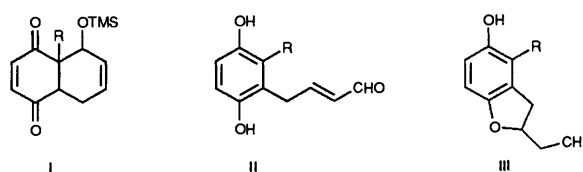
1837 **Helically shaped bilirubins: natural optical activity and chemical correlation of *M* and *P* backbone helicity with biliverdins**

Daniel Krois and Harald Lehner



1841 **Kinetic studies on the rearrangement of Diels-Alder adducts of activated benzoquinones with (*E*)-1-trimethylsiloxybuta-1,3-diene**

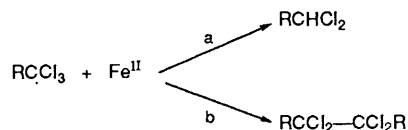
José G. Santos, Paz Robert and Jaime A. Valderrama



On the basis of kinetic evidence the probable mechanism of the acid-induced rearrangement of adducts **I** (R = COMe, CHO, CN) into compounds of type **II** and **III** is reported

1847 **Electron transfer in the reactions of organic trichloromethyl derivatives with iron(II) chloride**

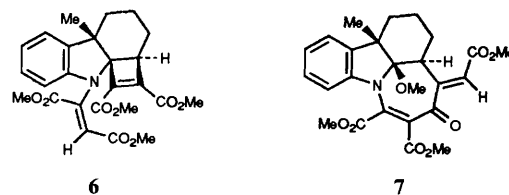
Andrea Cornia, Ugo Folli, Silvia Sbardellati and Ferdinando Taddei



R = Ph, PhC(O), EtOC(O): hydrogen abstraction (route a) and dimerization (route b) depend on the structure of the R group

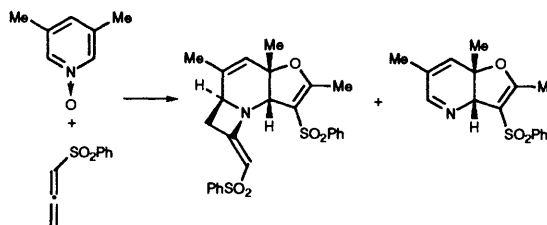
1855 **Interaction of 1,2,3,4-tetrahydro-4a-methyl-4aH-carbazole with dimethyl acetylenedicarboxylate: a re-examination. Crystal structures of 6 and 7**

Neil Barnwell, Claire B. Murphy, Stephen J. W. Holgate, Michael B. Mitchell, Gordon A. Leonard, William N. Hunter and John A. Joule



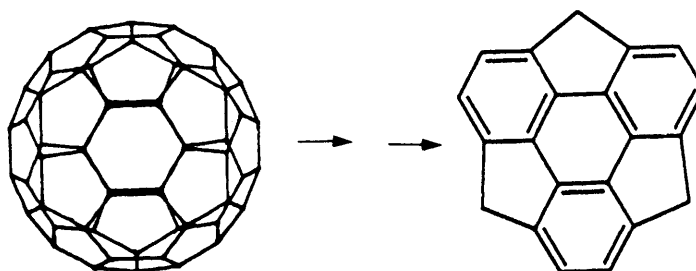
1859 **Reaction of aromatic N-oxides with dipolarophiles. Part 18. Formation mechanism and X-ray structure of the cycloadduct from sequential pericyclic reaction of pyridine N-oxides with phenylsulfonyllallene**

Toshikazu Matsuoka, Tomoaki Hasegawa, Masashi Eto, Kazunobu Harano and Takuzo Hisano



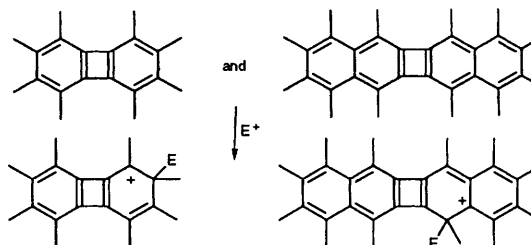
1867 **Synthetic strategies towards C<sub>60</sub>. Molecular mechanics and MNDO study on sumanene and related structures**

G. Narahari Sastry, Eluvathingal D. Jemmis, Goverdhan Mehta and Shailesh R. Shah



1873 **Oxidative and electrophilic chemistry (protonation, acetylation, trimethylsilylation) of octamethylbiphenylene and dodecamethylbinaphthylene; a mass spectral and superacid solution study**

Kenneth K. Laali

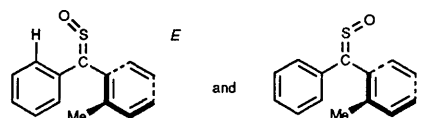


Decomposition pathways probed by MS/MS (E = H, MeCO, Me<sub>3</sub>Si)

1881 **NMR of terminal oxygen. Part 12. SO<sub>2</sub> and isoelectronic compounds with a true π-bond: <sup>17</sup>O NMR spectra of sulfinylamines R-N=S=O and sulfines RR'C=S=O. The conformation of *ortho*-substituted diaryl sulfines**

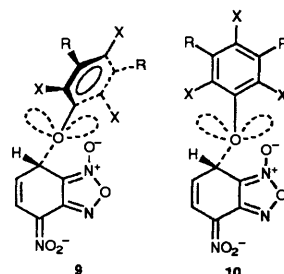
Hans Dahn, Péter Péchy, Vien Van Toan, Bianca F. Bonini, Lodovico Lunazzi, Germana Mazzanti, Giovanni Cerioni and Binne Zwanenburg

The <sup>17</sup>O NMR signals of the π<sub>p</sub>-bond compounds O=S=O, RN=S=O and RR'C=S=O appear several hundred ppm downfield from RR'S<sup>+</sup>-O<sup>-</sup>. Conformations deduced from <sup>17</sup>O and <sup>1</sup>H spectra are



1887 **Regioselectivity and stereoelectronic factors in the reactions of aryloxide nucleophiles with 4-nitrobenzofuroxan**

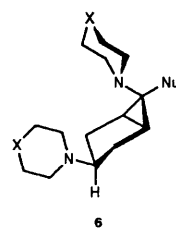
Richard A. Manderville and Erwin Runcel



Kinetic and thermodynamic preferences for C-5 vs. C-7 adduct formation by ambident aryloxides with 4-nitrobenzofuroxan are discussed on the basis of stereoelectronic factors

1895 **Functionalized chloroenamines in aminocyclopropane synthesis part 11. Bicyclo[3.1.0]hexane derivatives preferring a chair conformation**

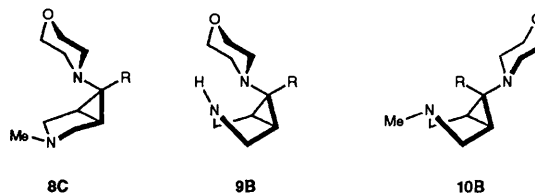
Elmar Vilsmaier, Joachim Fath, Claus Tetzlaff and Gerhard Maas



A chair conformation of a bicyclo[3.1.0]hexane skeleton was found to be present in diamines **6**

1901 **Conformation of 6-morpholino-3-azabicyclo[3.1.0]hexane derivatives**

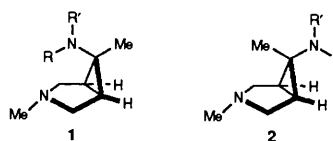
Claus Tetzlaff, Volker Butz, Elmar Vilsmaier, Rolf Wagemann, Gerhard Maas, Andreas Ritter von Onciul and Timothy Clark



Different conformations were deduced for 6-morpholino-3-azabicyclo[3.1.0]hexane compounds **8–10** (R = CN, CH<sub>3</sub>)

1907 **Functionalized chloroenamines in aminocyclopropane synthesis part 12. Basicity and protonation behaviour of 6-amino-3-azabicyclo[3.1.0]hexane derivatives**

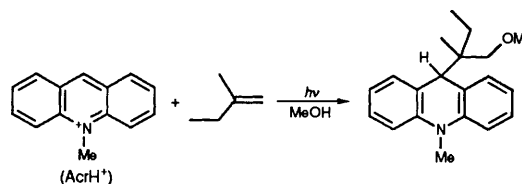
Volker Butz, Elmar Vilsmaier and Gerhard Maas



The basicity of diastereomeric diamines **1** and **2** has been determined; structures of monoammonium salts of **1** were studied

1915 **Reduction of 10-methylacridinium ion by alkenes via photoinduced electron transfer**

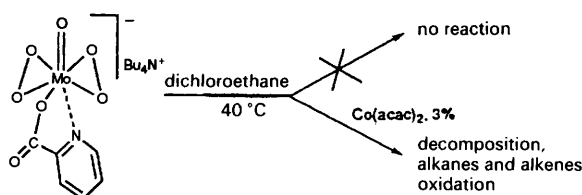
Morifumi Fujita and Shunichi Fukuzumi



Addition of various alkenes with AcrH<sup>+</sup> via photoinduced electron transfer has been investigated

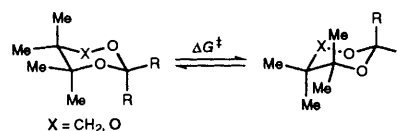
1923 **Co<sup>II</sup>-induced radical oxidations by peroxomolybdenum complexes**

Marcella Bonchio, Valeria Conte, Fulvio Di Furia, Tommaso Carofiglio, Franco Magno and Paolo Pastore



1927 **Chair–chair interconversion in some highly substituted 1,2,4-trioxanes and 1,3-dioxanes. A dynamic NMR study of a striking effect of skeletal substitution**

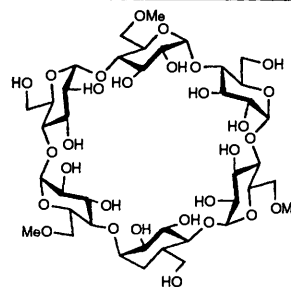
J. Edgar Anderson, A. J. Bloodworth and Aneela Shah



$\Delta G^\ddagger$  ranges from 6.5 to 12.3 kcal mol<sup>-1</sup>

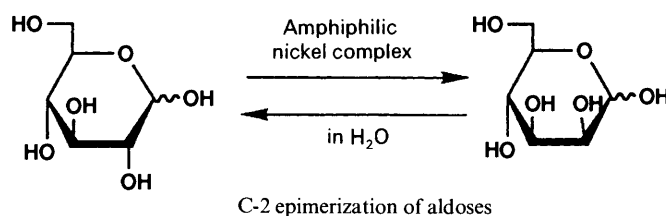
1931 **Crystal structure of hydrated 6<sup>A</sup>,6<sup>C</sup>,6<sup>E</sup>-Tri-*O*-methylcyclohexaamylose and its conformation in solution**

Viviane Durier, Georges Buisson, Emile Duée, Hugues Driguez and François-R. Taravel



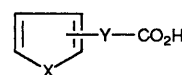
1937 **Epimerization of aldoses catalysed by self-organized metallomicelles in an aqueous solution**

Shuichi Osanai, Ryoji Yanagihara, Kimitake Uematsu, Atsuo Okumura and Sadao Yoshikawa



1941 **Thermodynamics of protonation of some five-membered heteroaryl-carboxylates, -alkanoates and -*trans*-propenoates**

Giuseppe Arena, Rosario Cali, Emanuele Maccarone and Amedeo Passerini

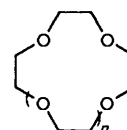


X = O, S, Se, NH, NCH<sub>3</sub>; Y = —  
X = O, S; Y = CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>, CH=CH.

$pK_a$ ,  $\Delta G^\circ$ ,  $\Delta H^\circ$ ,  $\Delta S^\circ$

1947 **Complexation thermodynamics of crown ethers. Part 3. 12-Crown-4 to 36-crown-12: from rigid to flexible ligand**

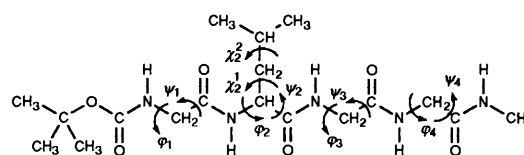
Yoshihisa Inoue, Yu Liu, Lin-Hui Tong, Mikio Ouchi and Tadao Hakushi



$n = 1-9$

1951 **Conformational analysis by molecular mechanics energy minimizations of the tetrapeptide Boc-Gly-Leu-Gly-Gly-NMe, a recurring sequence of elastin**

Vincenzo Villani and Antonio M. Tamburro



The set of the tetrapeptide Boc-Gly-Leu-Gly-Gly-NMe conformers has been determined by molecular mechanics energy minimizations using a strategy based on the build-up method

1963 **Chromogenic ligands for lithium based on calix[4]arene tetraesters bearing nitrophenol residues**

Mary McCarrick, Bei Wu, Stephen J. Harris, Dermot Diamond, Geraldine Barrett and M. Anthony McKervey

Three novel calix[4]arenes bearing nitrophenol residues which act as chromogenic indicators have been synthesised and found to display between a 10 and 40 fold selectivity for lithium against sodium, in the presence of a lipophilic base



- 1969 **Mechanism of the Beckmann rearrangement of formaldehyde oxime and formaldehyde hydrazone in the gas phase**

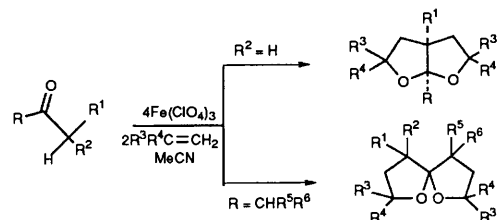
Minh Tho Nguyen and L. G. Vanquickenborne



High-level MO calculations suggest that the Beckmann rearrangement is a concerted process

- 1973 **Oxidation of ketones by ferric perchlorate in the presence of conjugated dienes to hexahydrofuro[2,3-*b*]furans and 1,6-dioxaspiro[4,4]nonanes**

Attilio Citterio, Magaly Caceres Carvajal, Andrea Mele, Marco Nicolini, Roberto Santi and Roberto Sebastiano



## Corrigendum

- 1981 **Reactions of the carbonyl group with nitroso compounds. The cases of pyruvic acid and acetaldehyde** Stanko Uršić, Viktor Pilepić, Valerije Vrček, Mario Gabričević and Branka Zorc

xi Conference Diary

## AUTHOR INDEX

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