

JOURNAL OF THE CHEMICAL SOCIETY

**Perkin Transactions 2**

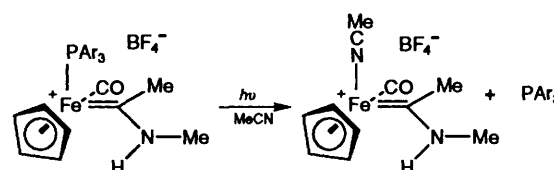
Physical Organic Chemistry

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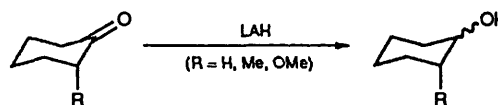
- 1005 **Photolabilisation of phosphine ligands bound to iron: Photofragmentation voltammetry analysis**

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



- 1009 **A probe of Cieplak's proposal: effect of 2-axial substitution on reactivity in the LiAlH<sub>4</sub> reduction of cyclohexanones**

Yasuhisa Senda, Sigeru Nakano, Hiromi  
Kunii and Hiroki Itoh

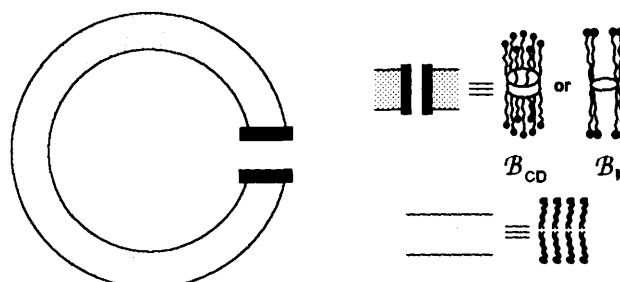


The relative reactivities of LAH reduction of the title compounds, and MO calculations, strongly suggest the importance of orbital overlap control on the stereochemistry

## Articles

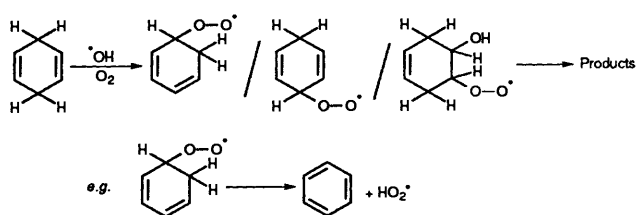
- 1011 **An approach to channel-type molecular structures. Part 3. Incorporation studies of the bouquet-shaped B<sub>M</sub> and B<sub>CD</sub> in phosphatidylcholine vesicles**

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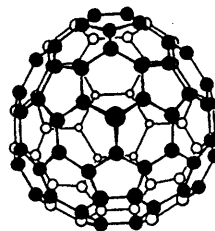
- 1021 **Hydroxyl-radical-induced oxidation of cyclohexa-1,4-diene by  $O_2$  in aqueous solution. A pulse radiolysis and product study**

Xian-Ming Pan, Man Nien Schuchmann and Clemens von Sonntag



- 1029  **$^{13}C$  NMR spectroscopy of  $C_{76}$ ,  $C_{78}$ ,  $C_{84}$  and mixtures of  $C_{86}$ – $C_{102}$ ; anomalous chromatographic behaviour of  $C_{82}$ , and evidence for  $C_{70}H_{12}$**

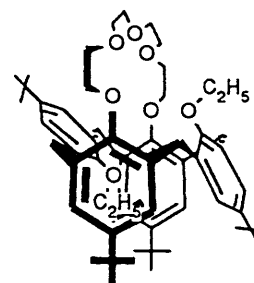
Roger Taylor, G. John Langley, Anthony G. Avent, T. John S. Dennis, Harold W. Kroto and David R. M. Walton



The HPLC retention time of  $C_{82}$  is abnormally long in this work, indicating that the polar  $C_3$  isomer is present

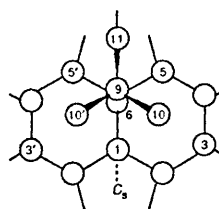
- 1037 **Transduction of selective recognition by preorganized ionophores;  $K^+$  selectivity of the different 1,3-diethoxycalix[4]arene crown ether conformers**

Zbigniew Brzozka, Ben Lammerink, David N. Reinhoudt, Eleonora Ghidini and Rocco Ungaro



- 1041 **Electron paramagnetic resonance spectra of R– $C_{60}$  radicals part 2: hindered rotation in alkyl- and silyl- $C_{60}$  radicals**

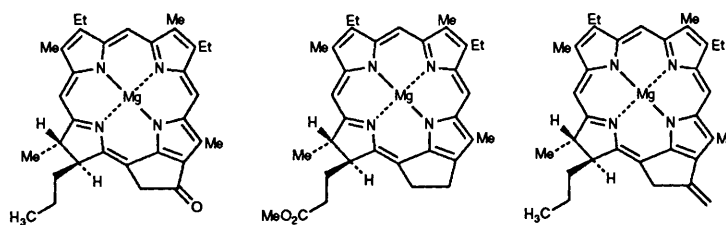
P. N. Keizer, J. R. Morton, K. F. Preston and P. J. Krusic



When alkyl and silyl radicals (R) react with  $C_{60}$  the EPR hyperfine interactions of the R– $C_{60}$  adducts vary with temperature, indicating hindered rotation about the R– $C_{60}$  bond

- 1047 **NMR spectra of the porphyrins. Part 42. The synthesis and aggregation behaviour of some chlorophyll analogues**

Raymond J. Abraham, Alan E. Rowan, Norman W. Smith and Kevin M. Smith



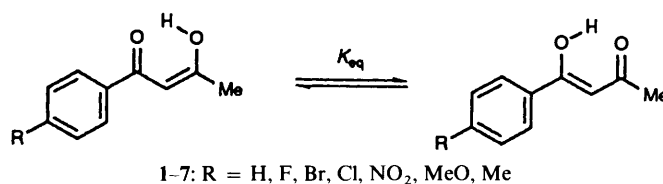
- 1061 **Conformational analysis. Part 21. Conformational isomerism in *cis*-cyclohexane-1,3-diol**

Raymond J. Abraham, Eric J. Chambers and W. Anthony Thomas



- 1067  $^{13}\text{C}$  NMR spectroscopic study of the tautomeric equilibrium in *p*-phenyl substituted benzoylacetones

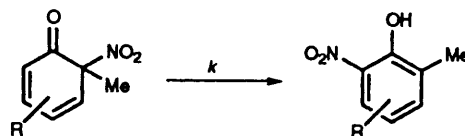
Raquel M. Cravero, Manuel González-Sierra and Alejandro C. Olivieri



$^{13}\text{C}$  NMR spectroscopic data for benzoylacetones 1–7 and related model compounds allow the calculation of the value of  $K_{\text{eq}}$

- 1073  $^{15}\text{N}$  Nuclear polarisation in nitration and related reactions. Part 8. The mechanisms of rearrangement of 2-methyl-2-nitrocyclohexa-3,5-dienones

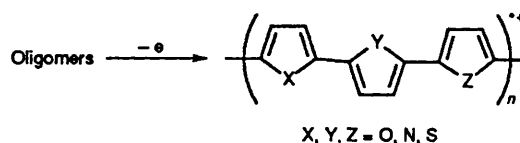
John H. Ridd, Susan Trelvelick and John P. B. Sandall



No  $^{15}\text{N}$  nuclear polarisation is found unless the 6-position is blocked

- 1081 Synthesis, electrical conductivity and electron paramagnetic resonance spectroscopy of polymers derived from NOPF<sub>6</sub>-doped XYZ-triheterocycles based on pyrrole, furan and thiophene

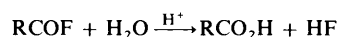
Makarand V. Joshi, Christine Hemler, Michael P. Cava, Jason L. Cain, Martin G. Bakker, Allan J. McKinley and Robert M. Metzger



Oxidation of the title oligomers with NOPF<sub>6</sub> gives polymers of varying conductivities

- 1087 The Brønsted acid-catalysed hydrolysis of acyl fluorides in aqueous media

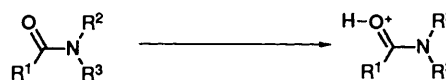
Richard E. Motie, Derek P. N. Satchell and Wasfy N. Wassef



Two mechanisms of acid catalysis are found for both aliphatic and aromatic acyl fluorides in dioxane–water mixtures

- 1091 Thermodynamics of protonation and hydration of aliphatic amides

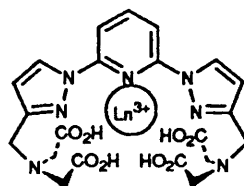
Alessandro Bagno, Giancarlo Lovato and Gianfranco Scorrano



R<sup>1</sup> = H, Me, Et, Pr<sup>i</sup>, Bu<sup>t</sup>  
R<sup>2</sup>, R<sup>3</sup> = H, Me

- 1099 Synthesis and luminescence properties of europium(III) and terbium(III) complexes with polyacid chelates derived from 2,6-bis(*N*-pyrazolyl)pyridine

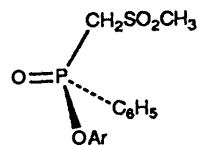
Modesto J. Remuñán, Herminia Román, Maria Teresa Alonso and Juan C. Rodríguez-Ubis



Eu<sup>III</sup> and Tb<sup>III</sup> ions of the title complexes show quite interesting luminescence properties as a consequence of highly efficient ligand-to-metal energy transfer and good protection of the metal ion from solvent

## 1103 The quest for carbanion-promoted dissociative pathways in the hydrolysis of aryl phosphinates

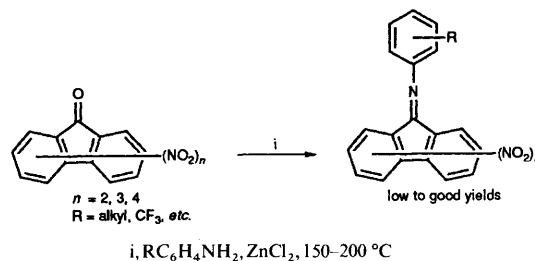
Giorgio Cevasco and Sergio Thea



Results of a kinetic study on the alkaline hydrolysis of aryl (methylsulfonyl)methylphenylphosphinates are reported, and mechanistic implications are discussed

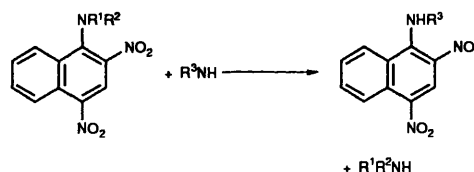
1107 Synthesis of *N*-(nitrofluorenylidene)anilines and their application as electron transport materials in positive charge electrophotography

Masaki Matsui, Katsuyuki Fukuyasu, Katsuyoshi Shibata and Hiroshige Muramatsu

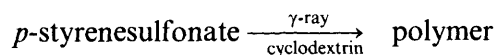


## 1111 Kinetic studies of the reaction of 1-dialkylamino-2,4-dinitronaphthalenes with butylamine in dimethyl sulfoxide

Shizen Sekiguchi, Masaru Hosokawa, Tohru Suzuki and Mitsuo Sato

1119 Hydrophobic acceleration of *p*-styrenesulfonate polymerization by  $\gamma$ -cyclodextrin

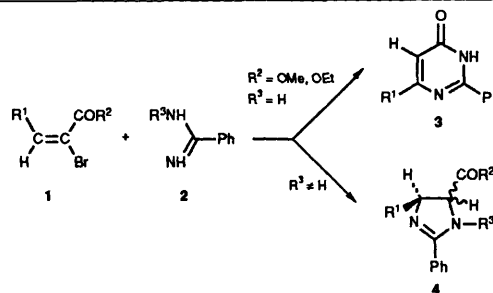
Yukio Yamamoto, Shinji Shiraki and Due Gao



Radical polymerization in aqueous solution is accelerated by complexation of the monomer with  $\gamma$ -cyclodextrin

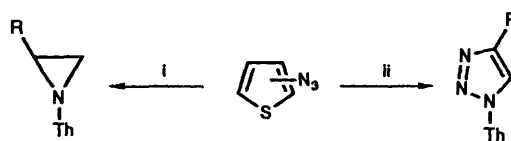
1123 Reaction of 2-bromo 2-alkenoic carbonyl compounds with amidines: experimental and theoretical (PM3) studies of the mechanism of heterocyclisation into dihydroimidazole and pyrimidin-4(3*H*)-one

Pascale Friant, Catherine Soula, Jean-Louis Rivail, Alain Cartier and Alain Marsura



## 1129 On the chemical, NMR and kinetic properties of 2-azido- and 3-azido-thiophene: recent developments

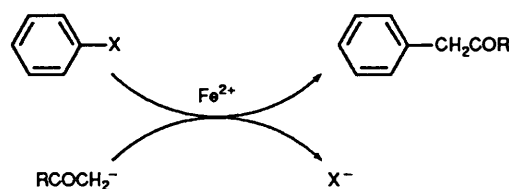
Domenico Spinelli and Paolo Zanirato



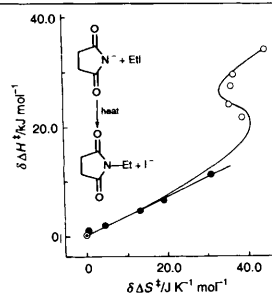
i = Trimethyl(vinyl)silane     $R = SiMe_3$   
 ii = (Trimethylsilyl)acetylene     $Th = 2\text{- or }3\text{-Thienyl}$

1135 **Catalysis by ferrous ion in nucleophilic aromatic substitution reactions**

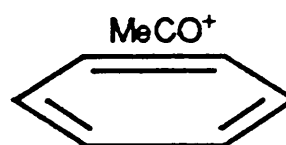
Carlo Galli and Patrizia Gentili

1141 **Nucleophilic reactivity and solvation of succinimide and phthalimide anions in acetonitrile-methanol mixtures**

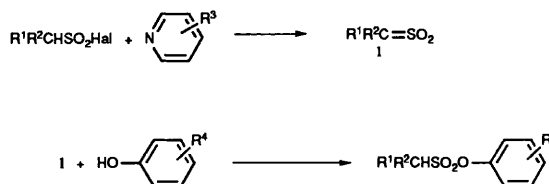
Yasuhiko Kondo, Kunio Kondo and Shigekazu Kusabayashi

1147 **Aromatic acylation in homogeneous solution and in the gas-phase: the mechanistic relevance of the mesitylene/durene reactivity ratio**

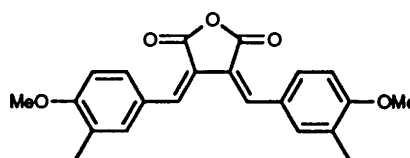
Carlo Galli and Simonetta Fornarini

1153 **Sulfene mechanism in the pyridine-catalysed reactions of alkanesulfonyl halides with phenols**

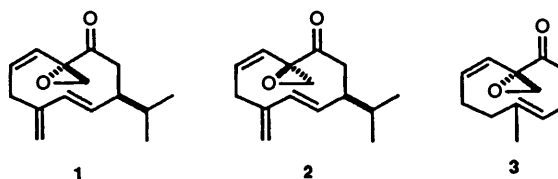
Serge N. Lyashchuk, Yuri G. Skrypnik and Vladimir P. Besrodnyi

The sulfene route has been quantitatively estimated by the use of kinetic methods and  $\rho\sigma$ -analysis1161 **Rotamers and isomers in the fulgide series. Part 3. Structures of the bis(4-methoxy-3-methylbenzylidene)succinic anhydrides**

Jan C. A. Boeyens, Christine C. Allen and Guido W. Perold

1167 **Combined molecular mechanics (MM2) and molecular orbital (AM1) study of periplanone-A and analogues. Evaluation of biological activity from electronic properties and geometries. Part 2**

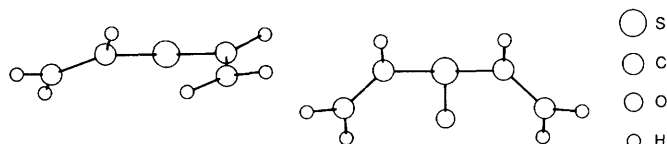
Kazuko Shimazaki, Masataka Mori, Kentaro Okada, Tatsuji Chuman, Shigefumi Kuwahara, Takeshi Kitahara, Kenji Mori, Hitoshi Gotō, Eiji Ōsawa, Kazuhisa Sakakibara and Minoru Hirota



To improve the structure-activity study on the periplanone analogues, conformational properties of periplanone-A (1), the epoxy epimer (2) and a structurally-related analogue (3) have been obtained by the use of MM2

1175 **The molecular structures of divinyl sulfide and divinyl sulfoxide in the gas phase from electron diffraction**

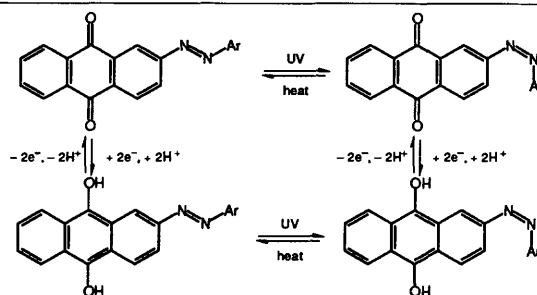
Béla Rozsondai and Zsolt E. Horváth



The C=C bonds tend to eclipse other bonds or a sulfur lone pair in the free molecules

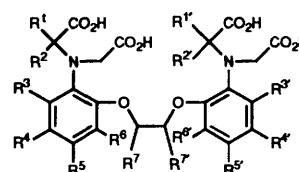
1181 **Multi-mode chemical transducers. Part 2. Electrochromic and photochromic properties of azoquinone compounds**

Tetsuyuki Saika, Tomokazu Iyoda, Kenichi Honda and Takeo Shimidzu



1187 **Design and properties of new  $^{19}\text{F}$  NMR  $\text{Ca}^{2+}$  indicators: modulation of the affinities of BAPTA derivatives *via* alkylation**

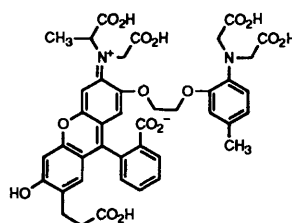
Sonia D. Clarke, James C. Metcalfe and Gerry A. Smith



Variation in  $K_{\text{Ca}}$  with different R and  $^{19}\text{F}$  NMR properties with  $\text{R}^4$  and  $\text{R}^5$  as F or  $\text{CF}_3$

1195 **The design and properties of a series of calcium indicators which shift from rhodamine-like to fluorescein-like fluorescence on binding calcium**

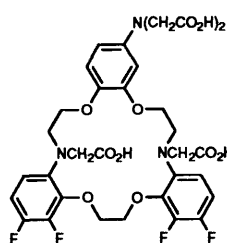
Garry A. Smith, James C. Metcalfe and Sonia D. Clarke



	$\lambda_{\text{exc}}/\text{nm}$	$\lambda_{\text{em}}/\text{nm}$
Free	537	566
+ $\text{Ca}^{2+}$	480	537
$K_{\text{d}}(\text{Ca})$	1.07 $\mu\text{mol dm}^{-3}$	

1205 **A new  $^{19}\text{F}$  NMR indicator for intracellular sodium**

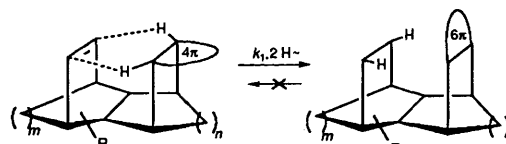
Gerry A. Smith, Heide L. Kirschenlohr, James C. Metcalfe and Sonia D. Clarke



$K_{\text{d}}(\text{Na})$	11 $\text{mol dm}^{-3}$
$\Delta_{\text{Na}}\delta_{\text{F}}$	4.6 and 0 ppm
$K_{\text{Na}}/K_{\text{K}}$	173

1211 **On intramolecular dyotropy: structural effects on reaction rates, crystal structure-molecular mechanics correlations and primary deuterium kinetic isotope effects**

Kenneth Mackenzie, Judith A. K. Howard, Sax Mason, Edward C. Gravett, K. Brian Astin, Liu Shi-Xiong, Andrei S. Batsanov, Djordje Vlaovic, John P. Maher, Martin Murray, Deborah Kendrew, Claire Wilson, Robert E. Johnson, Thomas Preiß and Robert J. Gregory

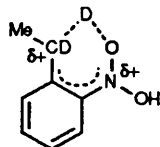
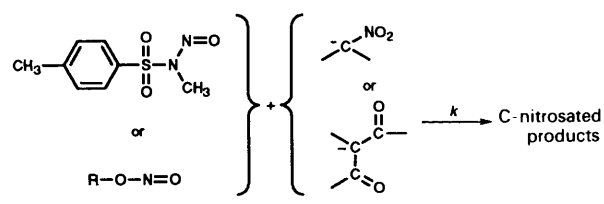
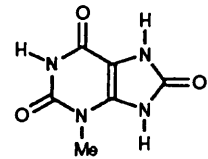


$$E_{\text{a}} = 20\text{--}34 \text{ kcal mol}^{-1} \text{ across 22 cases}$$

$$m = n = 1 \quad \text{R = variously H, Cl, OR}$$

$$m = 1 \quad n = 2 \quad 4\pi = [\text{C}=\text{C}]_2 \text{ or Ar}\ddot{\text{N}}\text{--N}=\text{CAr}$$

$$m = 2 \quad n = 1$$

<p>1229 <b>The mechanism of cyclisation of 1-ethyl-2-nitrobenzene to give 3-methylantranil in trifluoromethanesulfonic acid. Evidence for an intramolecular hydrogen transfer</b></p> <p>Rupert P. Austin and John H. Ridd</p>	 <p>Kinetic isotope effect on intramolecular hydrogen transfer in conjugate acid</p>
<p>1233 <b>Non-anomalous nucleophilic reactivity of carbanions towards the nitroso group</b></p> <p>J. Ramón Leis, M. Elena Peña and Ana Ríos</p>	 <p>C-nitrosated products</p>
<p>1241 <b>Comparison of electrochemical and enzymic oxidation of 3-methyluric acid</b></p> <p>Rajendra N. Goyal and (Miss) Madhu Shri Verma</p>	 <p>Peroxidase-catalysed oxidation was found to follow a chemical pathway quite similar to electrooxidation</p>

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