

JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions 2

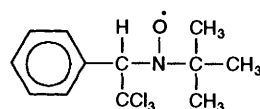
Physical Organic Chemistry

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Papers Presented at the 26th International ESR Conference

1983 Study of the isolation and stability of α -trichloromethylbenzyl(*tert*-butyl)aminoxyl, the trichloromethyl radical adduct of α -phenyl-*tert*-butylnitron (PBN)

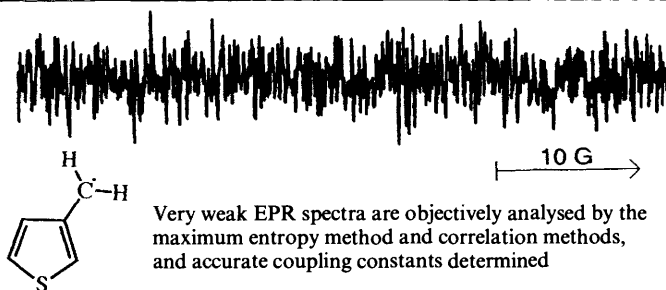
Edward G. Janzen, Guoman Chen, Tammy M. Bray, Lester A. Reinke, J. Lee Poyer and Paul B. McCay



The stability of the trichloromethyl radical adduct of PBN is explored in a variety of solvents

1991 Objective analysis of EPR spectra by computer methods

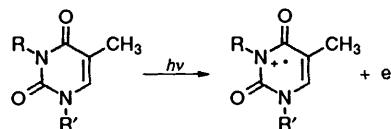
Richard A. Jackson



Very weak EPR spectra are objectively analysed by the maximum entropy method and correlation methods, and accurate coupling constants determined

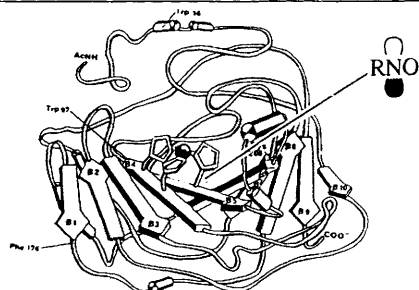
1995 Electronic structure, methyl group reorientation and reactions of radical cations of 1,2,4-trimethylcyclohexanes: An EPR study

Masaru Shiotani, Michinobu Matsumoto and Mikael Lindgren



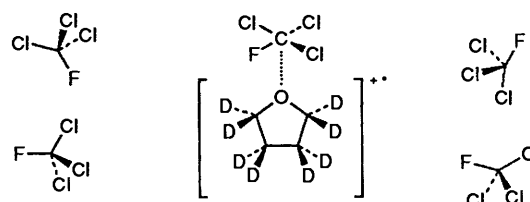
2003 Probing local mobility in carbonic anhydrase: EPR of spin-labelled SH groups introduced by site-directed mutagenesis

Mikael Lindgren, Magdalena Svensson, Per-Ola Freskgård, Uno Carlsson, Bengt-Harald Jonsson, Lars-Göran Mårtensson and Per Jonasson

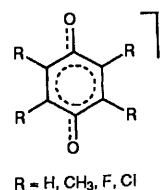


2009 The $[^2\text{H}_8]\text{THF}$ radical cation in CF_3CCl_3 and CFCl_3 . An EPR and ENDOR study

Mikael Lindgren, Roland Erickson, Nikolas P. Benetis and Oleg N. Antzutkin

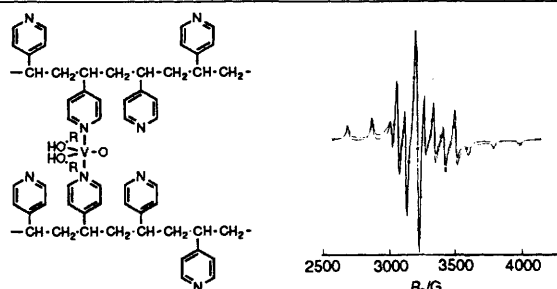
2015 EPR and flash photolysis investigations of some *p*-quinone radical cations

Günter Grampp and Kurt Neubauer



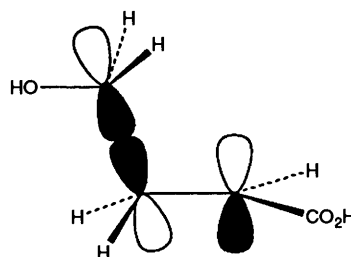
2021 Simulation of EPR spectra with automatic fitting of the spectroscopic parameters and of the reorientational correlation time

Edgar J. Soulié and Claude Chachaty



2025 Kinetic-EPR studies of the addition of aliphatic radicals to acrylic acid and related alkenes: the interplay of steric and electronic factors

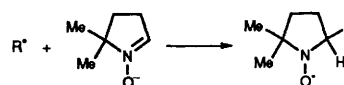
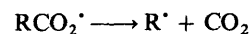
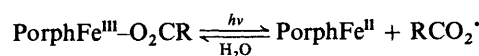
Bruce C. Gilbert, John R. Lindsay Smith, Elizabeth C. Milne, Adrian C. Whitwood and Philip Taylor



Typical transition-state for the addition of pyramidal oxygen-conjugated radicals to acrylic acid

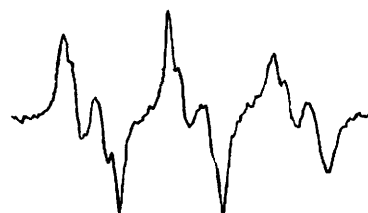
2033 Photolytic cleavage of the iron-carboxyalkyl ligand bond in some iron(III) tetra(*N*-methylpyridyl)porphyrins: Evidence for reversible photodecomposition and fragmentation from EPR and UV spectroscopy

Bruce C. Gilbert, John R. Lindsay Smith, Philip MacFaul and Philip Taylor



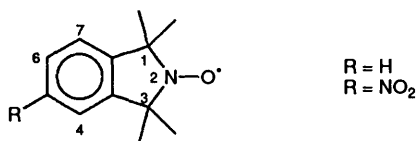
2039 EPR spin-trapping studies of the reaction of the hydroxyl radical with pyrimidine nucleobases, nucleosides and nucleotides, polynucleotides and RNA. Direct evidence for sites of initial attack and for strand breakage

Helen Catterall, Michael J. Davies, Bruce C. Gilbert and Natalie P. Polack

EPR spectrum of uridine-OH spin-adducts generated by HO^\bullet attack and subsequent enzymatic cleavage of RNA

2049 **An EPR and NMR study of some tetramethylisoindolin-2-yloxyl free radicals**

Roger Bolton, Duncan G. Gillies, Leslie H. Sutcliffe and Xiaoping Wu

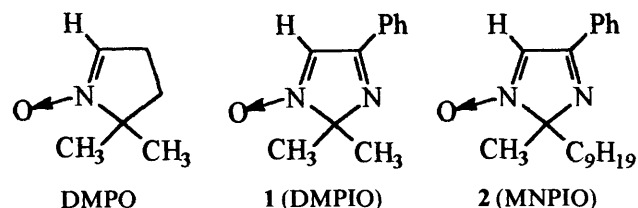
¹H and ¹³C hyperfine coupling constants have been derived from EPR and NMR spectra2053 **Comparative study of the reduction rates of various types of imidazoline radicals in tissues**

V. Yelinova, A. Krainev, A. Savelov and I. Grigor'ev

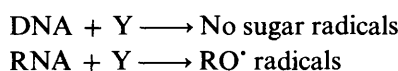
Various types of imidazoline radical have been studied for potential utility as contrast-enhancing agents in nuclear magnetic resonance (NMR) imaging

2057 **Spin-trapping study of free radical penetration into liposomal membranes**

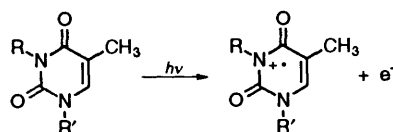
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2061 **The effects of ionizing radiation on frozen aqueous RNA: an electron paramagnetic resonance study**

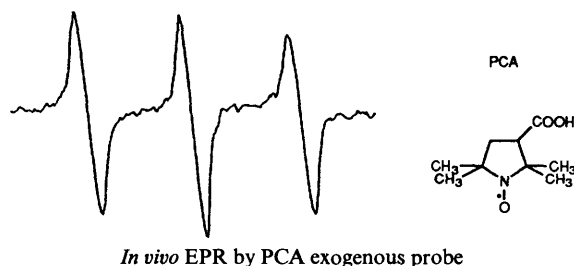
Philip J. Boon, Aidan O'Connell, Ian D. Podmore and Martyn C. R. Symons

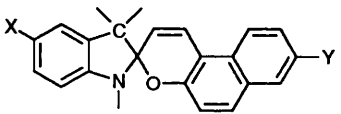
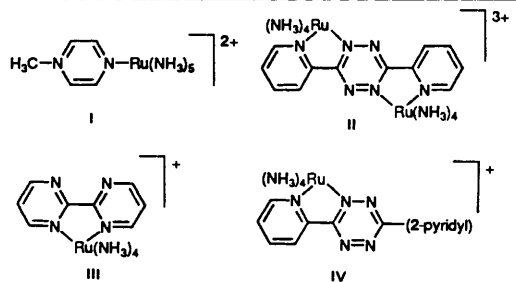
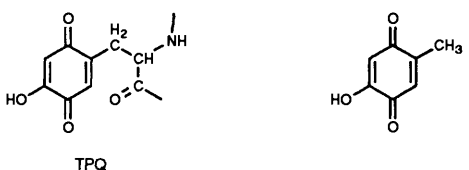
2067 **An EPR study of photoionised thymine and its derivatives at 77 K**

Mark E. Malone, Martyn C. R. Symons* and Anthony W. Parker

2077 **New experimental procedures for *in vivo* L-band and radio frequency EPR spectroscopy/imaging**

Silvia Colacicchi, Marcello Alecci, Giancaterino Gualtieri, Valentina Quaresima, Cinzia Lucia Ursini, Marco Ferrari and Antonello Sotgiu

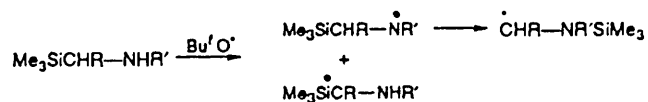


<p>2083 Spontaneous and photoinduced formation of radical anions in the reaction of borohydrides with unsaturated compounds</p> <p>Marco Lucarini, Gian Franco Pedulli, Angelo Alberti, Carmen Paradisi and Sergio Roffia</p>	$A + BH_4^- \longrightarrow A^{\cdot-} + BH_3 + \frac{1}{2} H_2$ $A \xrightarrow{h\nu} A^*$ $A^* + BH_4^- \longrightarrow AH + BH_3^{\cdot-}$ $A + BH_3^{\cdot-} \longrightarrow ABH_3^{\cdot-}$
<p>2089 Radical ions and gertyloxyaminoxyls from nitrospiro[indoline-naphthopyrans]. A combined electrochemical and EPR study</p> <p>Mylène Campredon, Gérard Giusti, Robert Guglielmetti, André Samat, Gérard Gronchi, Angelo Alberti and Massimo Benaglia</p>	 <p style="text-align: center;">X, Y = H, NO₂</p> <p>EPR spectroscopy reveals unexpected behaviour in the dinitro spiro compound towards chemical reduction</p>
<p>2095 An <i>in-situ</i> radiolysis EPR study of spin trapping by 2-methyl-2-nitrosopropane: steric and electronic effects influencing the trapping of hydroxyalkyl radicals derived from pentanols and substituted pentanols</p> <p>Keith P. Madden and Hitoshi Taniguchi</p>	$(CH_3)_3C-N=O + \dot{C}(OH)RR' \longrightarrow$ $(CH_3)_3C-N(\dot{O})-C(OH)RR' \text{ or}$ $(CH_3)_3C-N(\dot{O})H + C(O)RR'$
<p>2105 EPR characteristics of radical complexes with coordinated ammineruthenium(II) fragments. Evidence for the metal-to-ligand charge transfer (MLCT) nature of the low-lying excited states in precursor complexes</p> <p>Jürgen Poppe, Wolfgang Kaim, Aída Ben Altabef and Néstor E. Katz</p>	
<p>2109 Ruthenium(II) coordination to a model for the topasemiquinone cofactor of amine oxidases. Resolution of ¹H and ^{99,101}Ru EPR hyperfine structure</p> <p>Eberhard Waldhör, Brigitte Schwederski and Wolfgang Kaim</p>	 <p style="text-align: center;">TPQ</p> <p>The effect of metal chelate coordination on the electronic structure of <i>o,p</i>-(semi)quinonoid systems has been studied</p>
<p>2113 Spin-lattice relaxation times of phospholipid aminoxy spin labels in cardiolipin-cytochrome <i>c</i> bilayers: a pulse saturation-recovery EPR study</p> <p>Teresa J. T. Pinheiro, Peter J. Bratt, Ian H. Davis, David C. Doetschman and Anthony Watts</p>	<p>Spin-lattice (T_1) relaxation times of aminoxy spin-labels have been measured in lipid bilayers by pulse saturation methods to monitor the perturbation of the dynamics of the bilayer lipid chains by the peripheral protein, cytochrome <i>c</i></p>

2119 **Hydrogen abstraction from silylamines; an investigation of the 1,2-migration of the trimethylsilyl group in aminyl radicals**

Joanna M. Harris, John C. Walton, Bernard Maillard, Stéphane Grelier and Jean-Paul Picard

Hydrogen abstraction from silylamines gave mixtures of aminyl and aminoalkyl radicals; rearrangement of the former was monitored by EPR spectroscopy



2125 **Measurement of the ^{13}C hyperfine tensors for cubyl and related bridgehead radicals**

Christopher J. Rhodes, John C. Walton and Ernest W. Della

Solid-state features from carbon-13 nuclei have been observed by EPR spectroscopy in a series of bridgehead radicals, leading to a determination of the geometries of their radical centres

2129 **Substituent effects in diphenylmercury radical cations: a very clear distinction between σ - and π -states**

Christopher J. Rhodes, Hikmet Agirbas, Henry J. Shine, A. K. M. Mansural Hoque and T. Krishnan Venkatachalam

Diphenylmercury radical cations are formed in the σ -state in a solid freon matrix at 77 K, and show a pronounced interaction with a single chlorine atom from the matrix; allyloxy derivatives, in contrast, are formed in their π -states

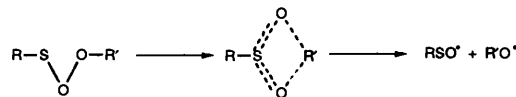
2135 **An EPR and theoretical investigation of azoalkane and azobenzene radical cations**

Christopher J. Rhodes, Hikmet Agirbas, Mikael Lindgren and Oleg N. Antzutkin

g - and A -tensors have been evaluated for a range of azoalkane and azobenzene radical cations by simulation of their EPR spectra as observed in solid freon matrices; the results are compared with those predicted from semiempirical calculations

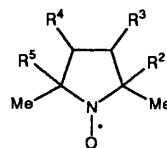
2141 **Post-irradiation decomposition of sulfanylperoxides and peroxy-cyclohexadienethiones formed from thiyl and peroxy radicals**

Brynmor Mile, Christopher C. Rowlands, Philip D. Sillman and Andrew J. Holmes



2149 **Ring pseudorotation in pyrrolidine N -oxyl radicals: an analysis of ^{13}C -hyperfine structure of EPR spectra**

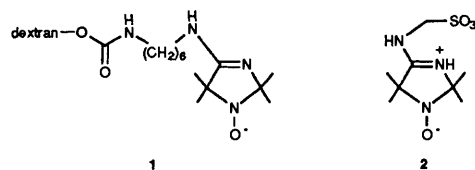
Antal Rockenbauer, László Korecz and Kálmán Hideg



- (i) EPR ^{13}C -satellites
- (ii) ring pseudorotation
- (iii) *cis-trans* configuration
- (iv) axial-equatorial position

2157 **New pH-sensitive aminoxyls: application to the study of biomembrane transport processes**

Maxim Balakirev and Valery Khramtsov

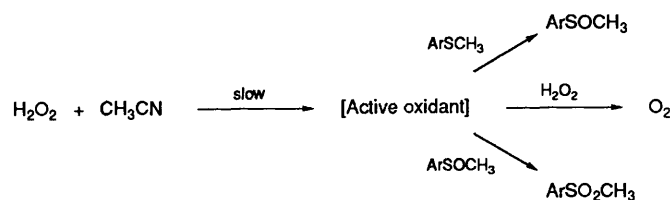


New pH-sensitive hydrophilic spin probes, **1** and **2**, have been used to determine the kinetics of pH variations inside large unilamellar phospholipid vesicles, and the membrane permeability coefficients for H^+ ($5 \times 10^{-4} \text{ cm s}^{-1}$), Cl^- ($10^{-10} \text{ cm s}^{-1}$) and Tl^+ ($10^{-8} \text{ cm s}^{-1}$)

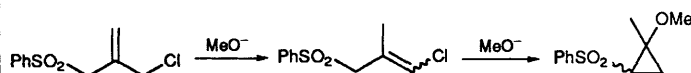
Perkin Communications

2161 **Reactivity and selectivity in the oxidation of aryl methyl sulfides and sulfoxides by hydrogen peroxide mediated by acetonitrile**

Donald Bethell, Andrew E. Graham, Jag P. Heer, Olga Markopoulou, Philip C. Bulman Page and B. Kevin Park

2163 **Formation of cyclopropylsulfones from 1-arylsulfonyl-2-chloromethylprop-2-enes**

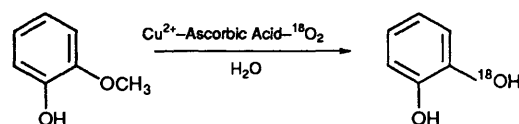
Stephen M. Jeffery and Charles J. M. Stirling

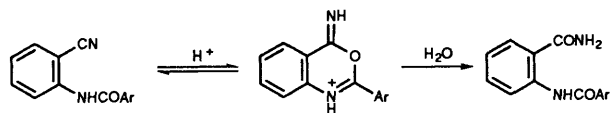


Regular Articles

2165 **Mechanistic studies of selective catechol formation from *o*-methoxyphenols using a copper(II)-ascorbic acid-dioxygen system**

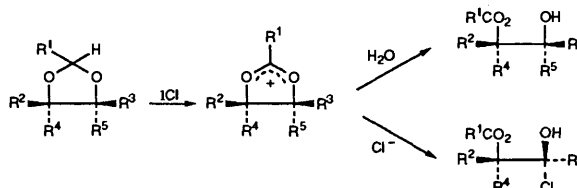
Kazuhiro Aihara, Yasuteru Urano, Tsunehiko Higuchi and Masaaki Hirobe



2171 **Anchimeric assistance in the specific acid-catalysed hydration of benzonitriles**

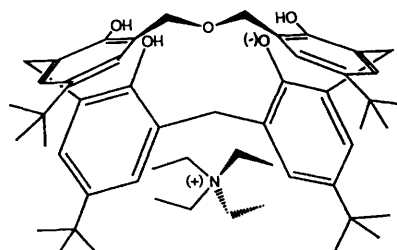
Richard M. Smyth and Andrew Williams

Anchimeric assistance by a neighbouring amido carbonyl increases the acid-catalysed hydration rate of a nitrile by a factor of 25 000

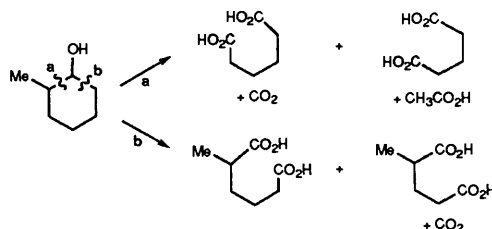
2175 **Reactions of 1,3-dioxolanes with iodine monochloride: formation of chlorohydrin esters and diol monoesters**

Beverley D. Glass, André Goosen and Cedric W. McClelland

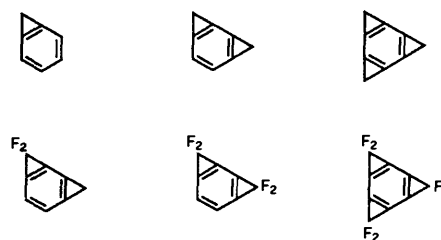
Dioxolanes react with ICl to form either diol monoesters (stereoselectively) or chlorohydrin esters (stereo- and regioselectively), depending on the reaction conditions

2183 **Cation-calixarene interactions: tetraalkylammonium cation binding by calixarene anions**

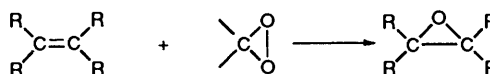
Jack M. Harrowfield, Mark I. Ogden, William R. Richmond, Brian W. Skelton and Allan H. White

2191 **Oxidation of α -substituted cyclohexanols by nitric acid**

John R. Lindsay Smith, C. Barry Thomas and Mark Whittaker

2195 **Fluorination effect on the structural properties of selected benzocyclopropenes**

Wolfram Koch, Mirjana Eckert-Maksić and Zvonimir B. Maksić

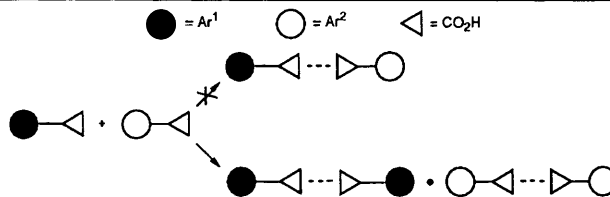
2203 **Dioxirane chemistry. Part 23. The effect of solvent on the dimethyldioxirane epoxidation reaction**

The rate of epoxidation of alkenes by dimethyldioxirane is increased by hydrogen bond donor solvents

Robert W. Murray and Daquan Gu

- 2209 **Molecular recognition involving an interplay of O-H...O, C-H...O and π ... π interactions. The anomalous crystal structure of the 1:1 complex 3,5-dinitrobenzoic acid-4-(*N,N*-dimethylamino)benzoic acid**

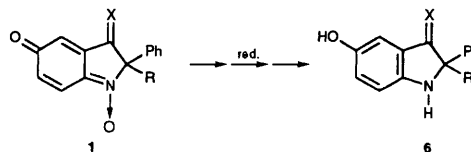
C. V. Krishnamohan Sharma, Kaliyamoorthy Panneerselvam, Tullio Pilati and Gautam R. Desiraju



The interplay of O-H...O, C-H...O and π - π interactions causes the formation of the unusual homodimer structure for the pair of title benzoic acids instead of the expected heterodimer

- 2217 **Chemical and electrochemical reduction of 2*H*-indole-3,5-dione and -dione 3-imine *N*-oxides**

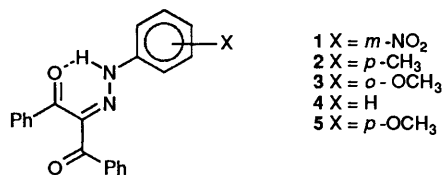
Patricia Carloni, Elisabetta Damiani, Lucedio Greci, Pierluigi Stipa, Angelo Alberti, Massimo Benaglia, Giancarlo Marrosu, Rita Petrucci and Antonio Trazza



A series of *N*-oxides (**1**) was reduced either chemically or electrochemically affording the corresponding 5-hydroxyindoles (**6**)

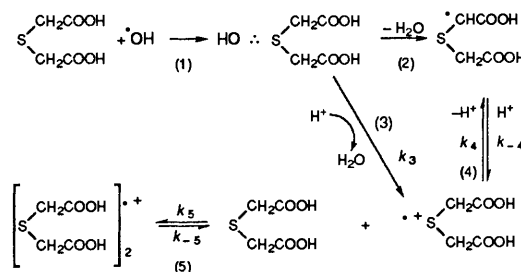
- 2223 **Intramolecular N-H...O hydrogen bonding assisted by resonance. Part 2. Intercorrelation between structural and spectroscopic parameters for five 1,3-diketone arylhydrazones derived from dibenzoylmethane**

Valerio Bertolasi, Valeria Ferretti, Paola Gilli, Gastone Gilli, Y. M. Issa and O. E. Sherif



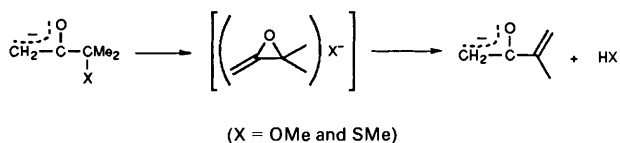
- 2229 **Electron transfer reactions of 2,2'-thiodiethanoic acid in aqueous solutions: a pulse radiolysis study**

Dilip K. Maity and Hari Mohan



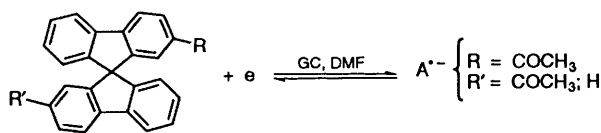
- 2235 **Rearrangement reactions of deprotonated α -substituted ketones in the gas phase**

Suresh Dua, Alan P. Pollnitz and John H. Bowie

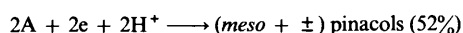


- 2243 **Electrochemistry of 9,9'-spirobifluorene derivatives: 2-acetyl- and 2,2'-diacetyl-9,9'-spirobifluorene. Preparation of stereoisomeric 2,3-bis(9,9'-spirobifluoren-2-yl)butane-2,3-diols**

Leonardo Mattiello and Liliana Rampazzo

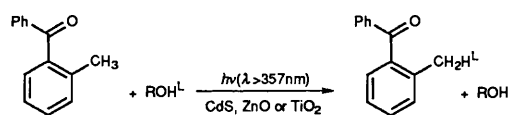


R' = H:



2249 Hydrogen isotope exchange in *ortho*-alkyl-phenyl ketones mediated by illuminated semiconductor powders

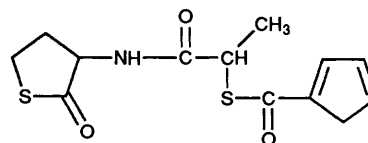
Jacek Michalak and Jerzy Gębicki



R = Me, Prⁱ
H^L = deuterium or tritium

2253 Crystal structure and NMR investigation of the serine proteinase inhibitor MR889, a cyclic thiolic compound

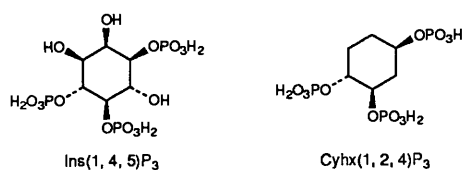
Menico Rizzi, Elena Casale, Paolo Ascenzi, Mauro Fasano, Silvio Aime, Concetta La Rosa, Maurizio Luisetti and Martino Bolognesi



Serine proteinase inhibitor MR889

2257 *myo*-Inositol 1,4,5-triphosphate and related compounds' protonation sequence: potentiometric and ³¹P NMR studies

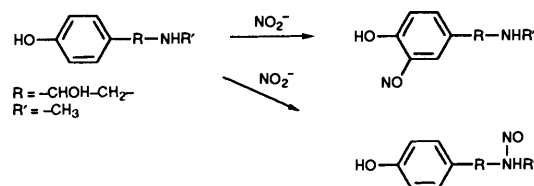
Laurent Schmitt, Patrick Bortmann, Gilbert Schlewer and B. Spiess



³¹P NMR shows the importance of phosphate interactions and the presence of the hydroxy groups on the ionization state of *myo*-inositol 1,4,5-triphosphate and analogues

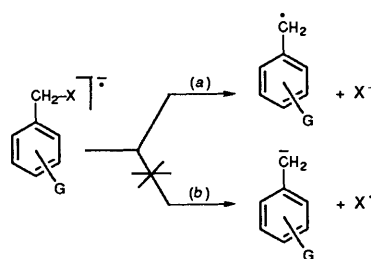
2265 Simultaneous *C*- and *N*-nitrosation of synephrine. A kinetic study

M. P. Fernández-Liencre, F. Carazo, M. C. Cabeza, B. Quintero, J. Thomas and J. M. Alvarez



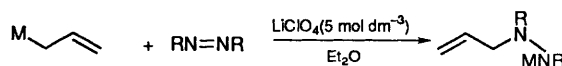
2275 Homolytic bond dissociation energies of the carbon-halogen bonds in the benzyl halide radical anion intermediates formed in radical nucleophilic substitution reactions

Xian-Man Zhang



2281 Catalysis of ene reactions by lithium perchlorate

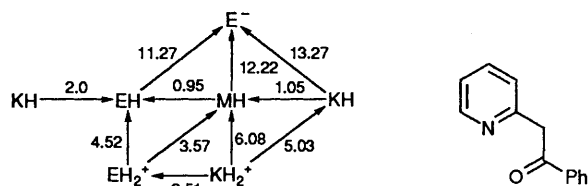
Alwyn G. Davies and Wojciech J. Kinart



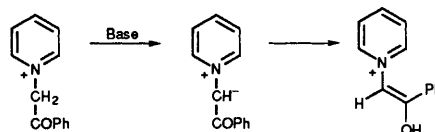
Lithium perchlorate catalyses the hydrogen-ene reaction of allyl-hydrogen compounds (M = H), and the metallo-ene reaction of allyl-tin compounds (M = SnR₃) with azo-compounds

2285 **Keto-enol and imine-enamine tautomerism of 2-, 3- and 4-phenacylpyridines**

A. R. Edwin Carey, Stephen Eustace, Rory A. More O'Ferrall and Brian A. Murray

2297 **Keto-enol tautomerism and ionisation of 1-phenacylpyridinium ions: a model for carbanion-stabilisation of azomethine ylides**

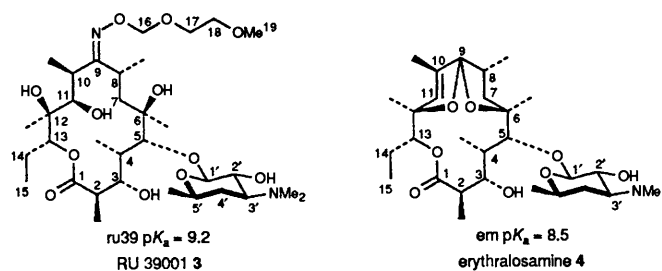
A. R. Edwin Carey, Rory A. More O'Ferrall and Brian A. Murray



An azomethine ylide intermediate relates keto-enol tautomerism of 1-phenacylpyridinium ion to catalysis by pyridoxal

2303 **Conformational analysis of major metabolites of macrolide antibiotics roxithromycin and erythromycin A with different biological properties by NMR spectroscopy and molecular dynamics**

Josyane Gharbi-Benarous, Patrick Ladam, Marcel Delaforge and Jean-Pierre Girault



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

