

Communications

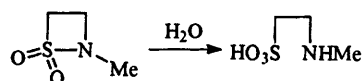
- 2241 A remarkable mechanistic dichotomy in the acid-catalysed decomposition of the N- and C-adducts of indolide anions with 1,3,5-trinitrobenzene

Patricia Sepulcri, Régis Goumont,
François Terrier and Erwin Buncel

N- and C-adducts of indolide anions with 1,3,5-trinitrobenzene are found to decompose through different acid-catalysed processes in aqueous solution; in the case of the C-adducts, the overall process is simply a S_EAr substitution of the trinitrocyclohexadienyliide moiety by hydronium ion

- 2245 The hydrolytic reactivity of β -sultams

Nicholas J. Baxter, Andrew P. Laws,
Laurent Rigoreau and Michael I. Page



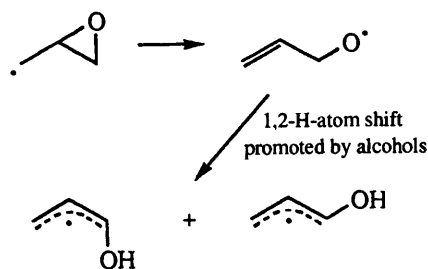
> 10^7 rate enhancement in base

> 10^9 rate enhancement in acid

Articles

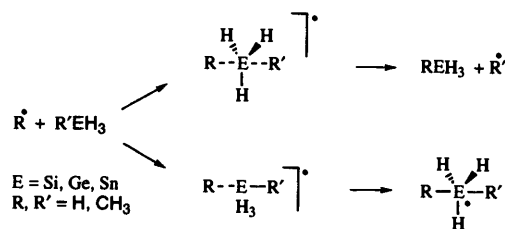
- 2247 EPR studies of the formation and transformation of isomeric radicals $[C_3H_5O]^\cdot$. Rearrangement of the allyloxyl radical in non-aqueous solution involving a formal 1,2-hydrogen-atom shift promoted by alcohols

Patrick E. Elford and Brian P. Roberts



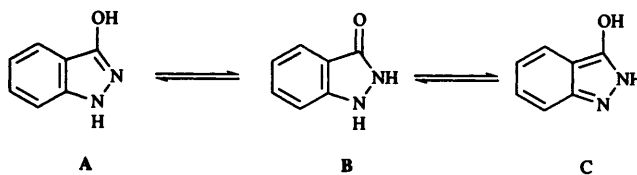
- 2257 *Ab initio* study of some free-radical homolytic substitution reactions at silicon, germanium and tin

Carl H. Schiesser, Michelle L. Styles and
Lisa M. Wild



2263 The tautomerism of indazolinone in aqueous solution. A note on the 'principle of vinylogy'

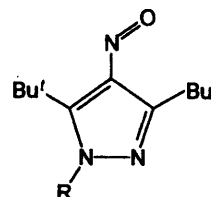
Pierre Bruneau, Peter J. Taylor and Anthony J. Wilkinson



About 95% of **B** is present, with *ca.* $10^{-4.7}$ of **C**

2271 Studies in nitrosopyrazoles. Part 1. Preparative and spectroscopic studies of some 3,5-dialkyl-4-nitrosopyrazoles

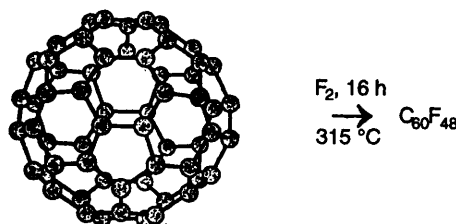
Mailer Cameron, Brian G. Gowenlock and Alan S. F. Boyd



^{13}C NMR studies demonstrate that the steric effects of the flanking *tert*-butyl groups upon the NO are smaller than in 2,4,6-tri-*tert*-butylnitrosobenzene

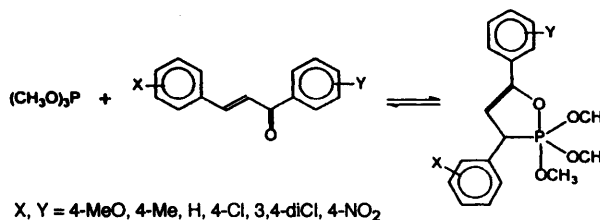
2275 Formation of $\text{C}_{60}\text{F}_{48}$ and fluorides of higher fullerenes

Olga V. Boltalina, Lev N. Sidorov, Vladimir F. Bagryantsev, Viktor A. Seredenko, Adolf S. Zapol'skii, Joan M. Street and Roger Taylor



2279 The kinetics and mechanism of the reaction of trimethyl phosphite with benzylideneacetophenones

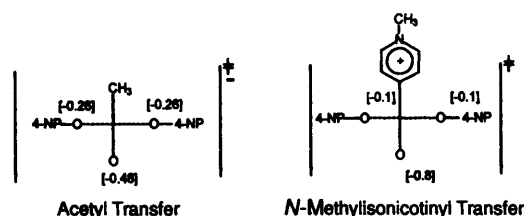
Imre Petneházy, György Clementis, Zsuzsa M. Jászay, László Töke and C. Dennis Hall



X, Y = 4-MeO, 4-Me, H, 4-Cl, 3,4-diCl, 4-NO₂

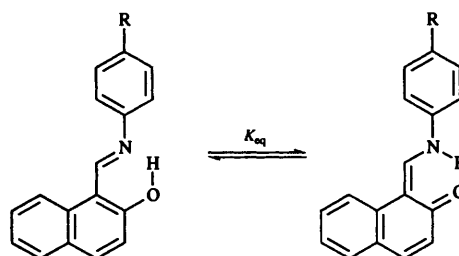
2285 Transfer of a positively charged acyl group between substituted phenolate ion nucleophiles: the Brønsted β for the calibrating equilibrium for *N*-methylisonicotinyl (4-carbonyl-*N*-methylpyridinium) transfer

Matthew J. Colthurst, Matilde Nanni and Andrew Williams



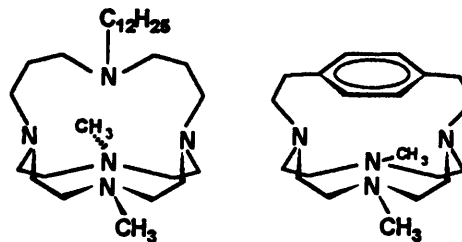
2293 Solid-state electronic absorption, fluorescence and ^{13}C CPMAS NMR spectroscopic study of thermo- and photo-chromic aromatic Schiff bases

Sergio H. Alarcón, Alejandro C. Olivieri, Alison Nordon and Robin K. Harris



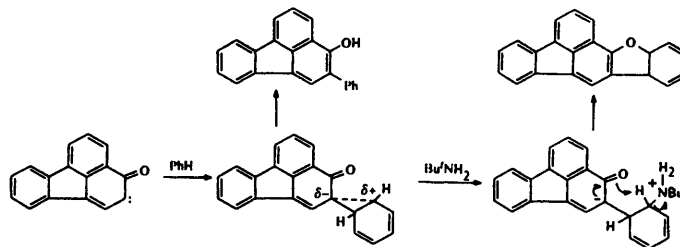
2297 **Aza-macrocycles bearing lipophilic functions. Their synthesis and selective lithium complexation**

Andrea Bencini, Vieri Fusi, Claudia Giorgi, Mauro Micheloni, Nicoletta Nardi and Barbara Valtancoli



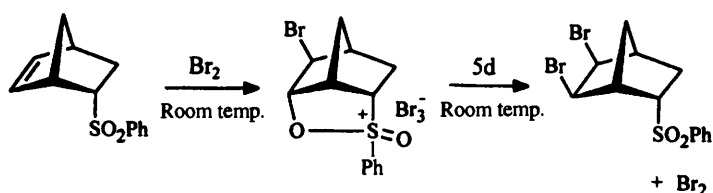
2303 **Photolytic decomposition of some polycyclic α -diazoketones: generation and reactivity of 1,2-oxocarbenes in benzene with and without *tert*-butylamine**

Peter J. N. Brown, J. I. G. Cadogan, Ian Gosney, Alexander Johnstone, R. Michael Paton and Norman H. Wilson



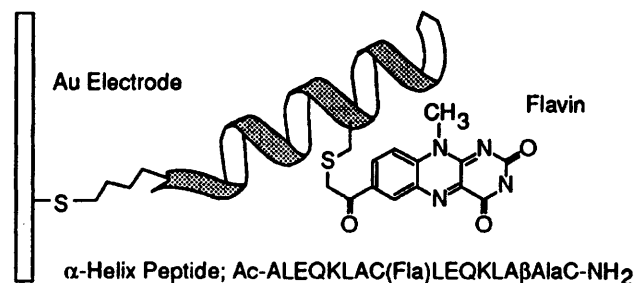
2309 **Intramolecular nucleophilic interception by the sulfonyl group of reaction intermediates arising from electrophilic addition to unsaturated non-conjugated bicyclic sulfones**

J. I. G. Cadogan, Donald K. Cameron, Ian Gosney, John R. A. Millar, Stephen F. Newlands and David Reed



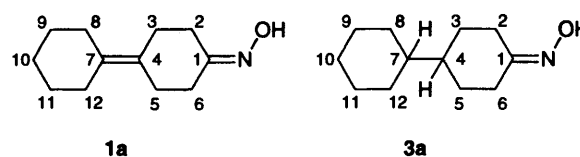
2319 **Design and synthesis of flavin-conjugated peptides and assembly on a gold electrode**

Seiji Sakamoto, Haruhiko Aoyagi, Naotoshi Nakashima and Hisakazu Mihara



2327 **Oligo(cyclohexylidene) oximes and derivatives as probe molecules for long-range substituent effects on ^{13}C NMR chemical shifts**

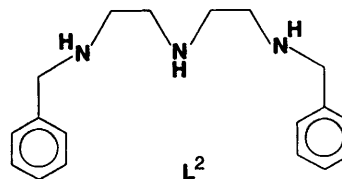
Frans J. Hoogesteger, David M. Grove, Leonardus W. Jenneskens, Theodorus J. M. de Bruin and Bart A. J. Jansen



Long-range substituent effects on ^{13}C NMR chemical shifts

2335 **Thermodynamic, NMR and photochemical study on the acid-base behaviour of N,N' -dibenzylated polyamines and on their interaction with hexacyanocobaltate(III)**

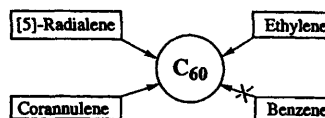
M. Alexandra Bernardo, José A. Guerrero, Enrique García-España, Santiago V. Luis, José M. Linares, Fernando Pina, José A. Ramírez and Conxa Soriano



Acid-base behaviour of dibenzylated polyamines has been studied by potentiometry, NMR, UV-VIS and steady-state fluorescence emission and adduct formation with hexacyanocobaltate(III) by steady-state fluorescence emission

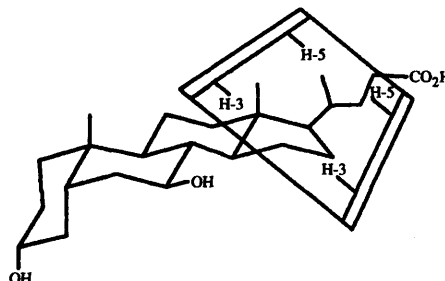
2343 **Molecular electrostatic potential topographical studies on the structural motifs of C_{60}**

Eluvathingal D. Jemmis, G. Subramanian, G. Narahari Sastry, G. Mehta, Rajendra N. Shirsat and Shridhar R. Gadre



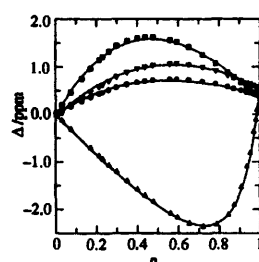
2347 **One- and two-dimensional NMR study of complexation of ursodeoxycholic acid with β -cyclodextrin**

Adele Mucci, Luisa Schenetti, Maria A. Vandelli, Flavio Forni, Paolo Ventura and Gianfranco Salvioli



2351 **General approach to measurements of pK_a differences by ^{13}C NMR spectroscopy**

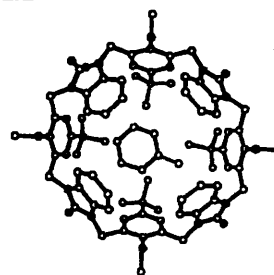
Tonis Pehk, Ene Kiirend, Endel Lippmaa and Ulf Ragnarsson



Relative pK_a values of multi-component mixtures are obtained by using, instead of pH , the degree of protonation of reference compound and plotting it against the chemical shift differences between the reference and investigated compounds

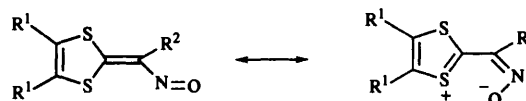
2359 **Heterocalixarenes featuring the benzimidazol-2-one subunit. Synthesis and X-ray structural studies of solvent inclusions**

Edwin Weber, Jörg Trepte, Karsten Gloe, Manfred Piel, Mátyás Czugler, Victor Ch. Kravtsov, Yurri A. Simonov, Janusz Lipkowski and Edward V. Ganin



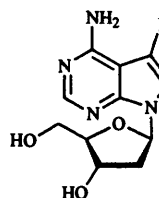
2367 **Nitroso derivatives of 1,3-dithiol-2-ylidene stabilised by intramolecular oxygen... sulfur interactions: synthesis and X-ray crystal structures**

Martin R. Bryce, Michael A. Chalton, Andrei S. Batsanov, Christian W. Lehmann and Judith A. K. Howard



2373 **The DNA-stabilising nucleoside 7-iodo-2'-deoxytubercidin: its structure in the solid state and in solution**

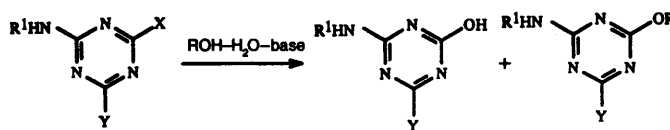
Frank Seela, Matthias Zulauf, Helmut Rosemeyer and Hans Reuter



The structure of 7-iodo-2'-deoxytubercidin is compared with those of 2'-deoxytubercidin and 2'-deoxyadenosine

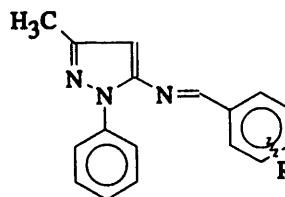
2377 **Rate-product correlations for concurrent nucleophilic displacements of halotriazines by hydroxide and alkoxides in water**

T. William Bentley, Joanne Ratcliff,
A. Hunter M. Renfrew and John A. Taylor



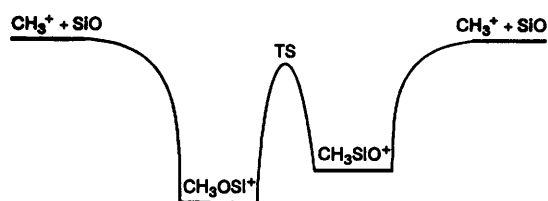
2383 **1-Phenyl-3-methyl-5-*N*-benzylideneamino-pyrazoles. Substituent effects and protonation sites studied by NMR and *ab initio* (6-31G*) MO calculations**

Erkki Kolehmainen, Agnieszka Puchała,
Reijo Suontamo, Danuta Rasała and
Robert Lysek



2389 **Combined quantum chemical and mass spectrometric study of $[\text{Si}, \text{C}, \text{H}_3, \text{O}]^+$ isomers**

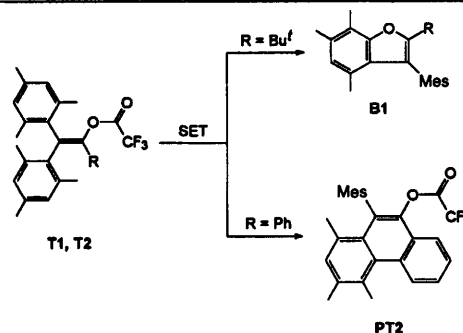
Max C. Holthausen, Detlef Schröder,
Waltraud Zummack, Wolfram Koch and
Helmut Schwarz



Silicon methoxide cation H_3COSi^+ ($\Delta_f H = 151 \text{ kcal mol}^{-1}$) represents the global minimum on the potential energy surface of $[\text{Si}, \text{C}, \text{H}_3, \text{O}]^+$, followed by the two silaacetyl cations H_3SiCO^+ ($\Delta_f H = 172 \text{ kcal mol}^{-1}$) and H_3CSiO^+ ($\Delta_f H = 180 \text{ kcal mol}^{-1}$)

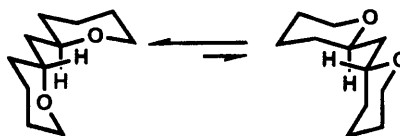
2401 **Electroactive protecting groups and reaction units. Part 4. Mesolytic O-CO bond cleavage versus intramolecular cyclization reaction in enol trifluoroacetate cation radicals. A kinetic and mechanistic investigation**

Michael Schmittl and Holger Trenkle



2407 **Flexible molecules with defined shape. Part 3. Conformational analysis of bis(tetrahydropyran-2-yl)methanes**

Reinhard W. Hoffmann, B. Colin Kahrs,
Jan Schiffer and Jörg Fleischhauer



The bis(tetrahydropyran-2-yl)methane system is biconformational with a strong preference for the O,O-proximal conformer. This preference can be further enhanced by suitably placed methyl substituents

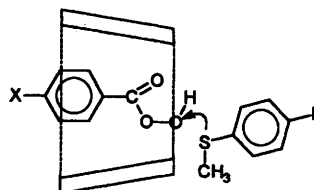
- 2415 The interaction of α -cyclodextrin with aliphatic, aromatic and inorganic peracids, the corresponding parent acids and their respective anions

D. Martin Davies and Michael E. Deary



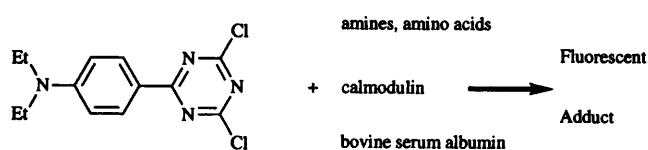
- 2423 Effect of α -cyclodextrin on the oxidation of aryl alkyl sulfides by peracids

D. Martin Davies and Michael E. Deary



- 2431 Triazinylaniline derivatives as fluorescence probes. Part 4. Kinetics and selectivity in the reactions of *N,N*-diethyl-4-(dichloro-1,3,5-triazinyl)aniline with amines, amino acids and proteins relevant to fluorescence labelling

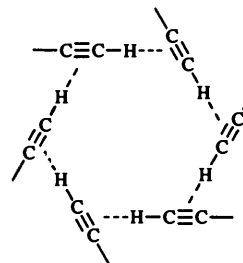
David J. Cowley



Hydrophobic interactions strongly influence the reaction kinetics and the positional selectivity of coupling to the amino group(s) in the substrate

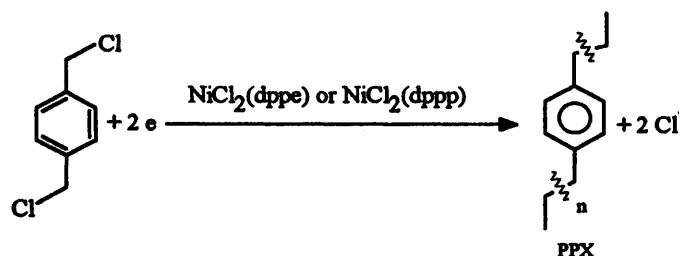
- 2441 Weak hydrogen bonding. Part 5. Experimental evidence for the long-range nature of $C\equiv C-H \cdots \pi$ interactions: crystallographic and spectroscopic studies of three terminal alkynes

Thomas Steiner, Matthias Tamm, Alexander Grzegorzewski, Niels Schulte, Nora Veldman, Antoine M. M. Schreurs, Jan A. Kanters, Jan Kroon, John van der Maas and Bert Lutz



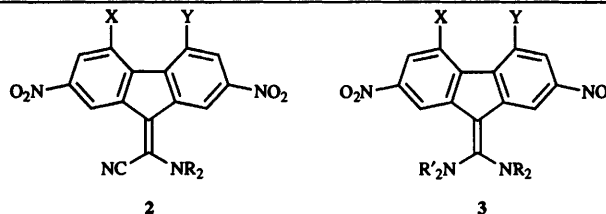
- 2447 Mechanistic and synthetic aspects of a novel route to poly-*p*-xylylene (PPX) via nickel complex catalysed electropolymerisation of 1,4-bis(chloromethyl)benzene

Christian Amatore, Florence Gaubert, Anny Jutand and James H. P. Utley



- 2453 Electron acceptors of the fluorene series. Part 5. Intramolecular charge transfer in nitro-substituted 9-(aminomethylene)fluorenes

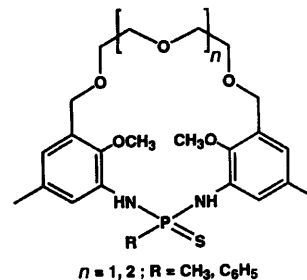
Igor F. Perepichka, Anatolii F. Popov, Tatyana V. Orekhova, Martin R. Bryce, Alexander N. Vdovichenko, Andrei S. Batsanov, Leonid M. Goldenberg, Judith A. K. Howard, Nikolai I. Sokolov and (in part) Joanne L. Megson



Intramolecular charge-transfer in compounds **2** and **3** has been studied in solution (NMR and UV-VIS spectroscopy, and cyclic voltammetry) and in the solid state, by an X-ray crystal structure analysis of a derivative of **2**

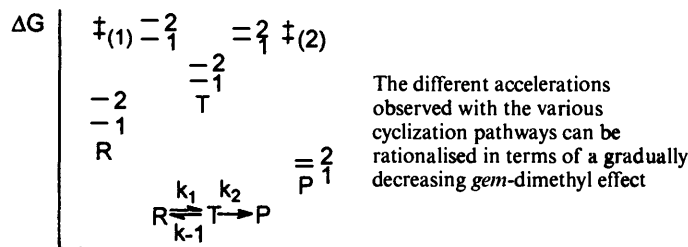
2471 **Synthesis and molecular structure of new phosphorous-crown compounds containing the thiophosphoryl group**

Jean-Paul Declercq, Pascale Delangle, Jean-Pierre Dutasta, Luc Van Oostenryck, Pascal Simon and Bernard Tinant



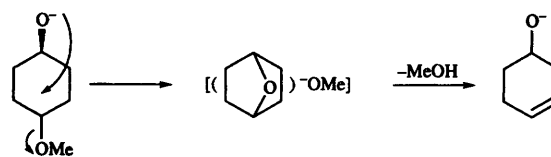
2479 **The *gem*-dimethyl effect on reactivities in cyclizations through tetrahedral intermediates. Cyclization of methyl-substituted methyl amides of 5-(*p*-nitrophenyl)hydantoic acids**

Asen H. Koedjikov, Iva B. Blagoeva, Ivan G. Pojarlieff and Anthony J. Kirby



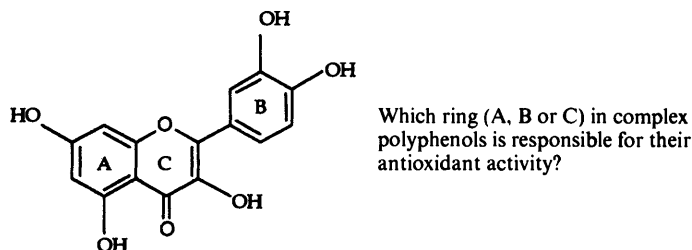
2489 **The mechanism of methanol loss from the (*M* - H)⁻ ions of *cis*- and *trans*-4-methoxycyclohexanol. The application of experiment and theory in concert**

Suresh Dua, Mark A. Buntine, Mark J. Raftery, Peter C. H. Eichinger and John H. Bowie



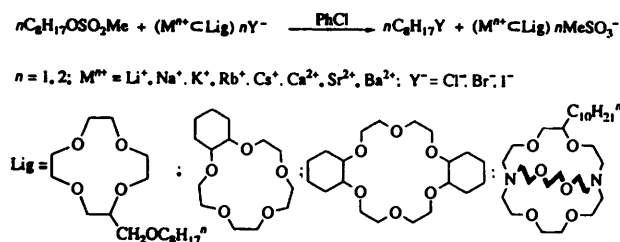
2497 **Reduction potentials of flavonoid and model phenoxy radicals. Which ring in flavonoids is responsible for antioxidant activity?**

Slobodan V. Jovanovic, Steen Steenken, Yukihiko Hara and Michael G. Simic



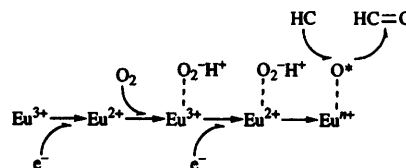
2505 **Cation participation in nucleophilic substitution reactions promoted by complexes of polyether ligands with alkali and alkaline-earth metal salts**

Alessandro Gobbi, Dario Landini, Angelamaria Maia and Michele Penso



2511 **Reactivity of active oxygen species generated in the EuCl₃ catalytic system for monoxygenation of hydrocarbons**

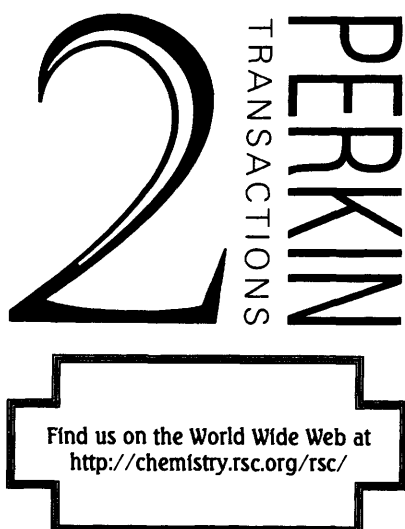
Ichiro Yamanaka, Katsumi Nakagaki, Takashi Akimoto and Kiyoshi Otsuka



Monoxygenation of hydrocarbons (HC) with O₂ by EuCl₃-Zn-MeCO₂H catalytic system was investigated for nature of the active oxygen species (O*)

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