ISSN 0300-9580 JCPKBH(12) 2087–2378(1995)

JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions 2

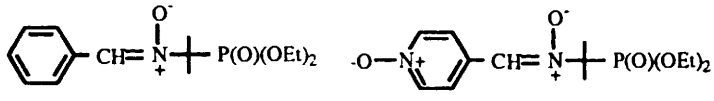
Physical Organic Chemistry

CONTENTS

Perkin Communications

2087 **β-Phosphorylated α-phenyl-*N*-*tert*-butylnitrone (PBN) analogues: a new series of spin traps for oxyl radicals**

Abdelhamid Zeghdaoui, Béatrice Tuccio, Jean-Pierre Finet, Viviane Cerri and Paul Tordo



PPN 4-PyOPN

PPN and 4-PyOPN trap efficiently HO˙ and HOO˙

Papers presented at the 28th International ESR Conference

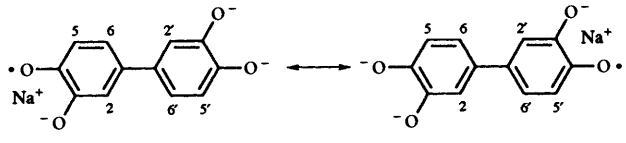
2091 **Free radicals from biogenic volatile organic compounds (VOCs): an electron spin resonance investigation**

Andrew Hudson, Daniel Waterman and Angelo Alberti

ESR spectrum formed by hydrogen abstraction from β-pinene

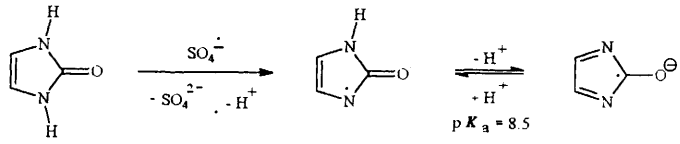
2095 **Electron-spin resonance investigation of the cation exchange of the semiquinone of 3,3′,4,4′-tetrahydroxybiphenyl**

Jens A. Pedersen



2101 **Electron spin resonance study of the reaction of $SO_4^{\bullet -}$ with azolinones**

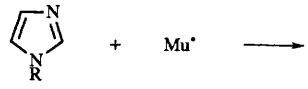
M. Câmdida B. L. Shohoji, Horácio M. Novais and Abel J. S. C. Vieira



and radicals derived from related azolinones

2107 **Patterns of muonium addition to imidazoles: a model of radiation-produced hydrogen-atom reactivity with key biological subunits**

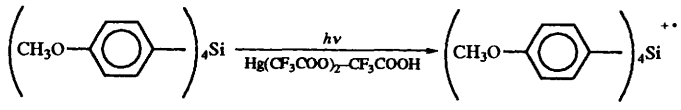
Christopher J. Rhodes, Harry Morris and Ivan D. Reid



The regioselectivity of reactions of muonium atoms with the imidazole ring has been determined

2115 **Radical cations from aryl-silanes, -germanes and -digermanes**

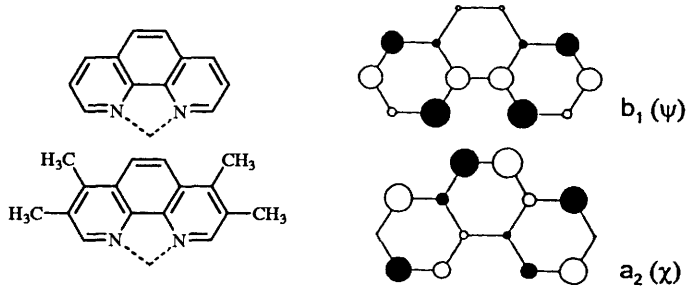
Heino Klaukien, Manfred Lehnig, Thomas Reiche, Susanne Reiß and Peter Such



EPR and ENDOR spectra are given

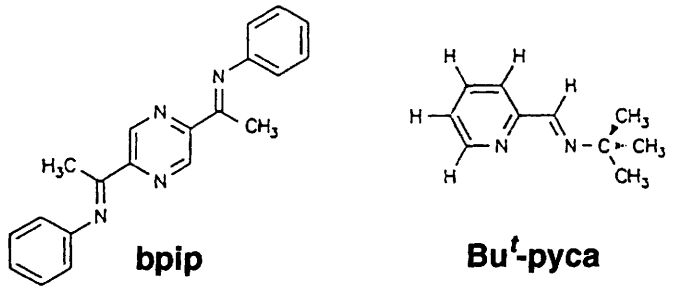
2121 **Different orbital occupation by an added single electron in 1,10-phenanthroline and its 3,4,7,8-tetramethyl derivative. Evidence from electron paramagnetic resonance spectroscopy of the anion radicals and of their dimesitylplatinum(II) complexes. X-Ray molecular structure of dimesityl(1,10-phenanthroline)platinum(II)**

Axel Klein, Wolfgang Kaim, Eberhard Waldhör and Hans-Dieter Hausen



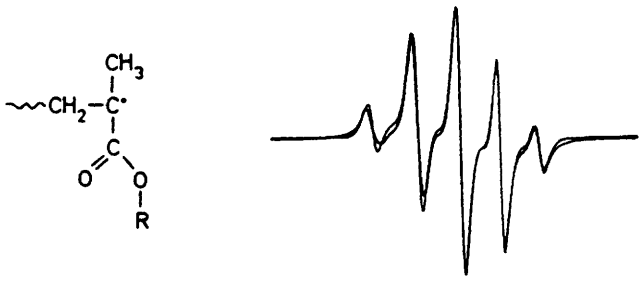
2127 **Conformational equilibria of 2,5-bis(1-phenyliminoethyl)pyrazine anion radical, bpip$^{\bullet -}$. An electron paramagnetic resonance/electron–nuclear double resonance study of bpip$^{\bullet -}$, (bpip$^{\bullet -}$)(RMg$^+$)$_2$, and of the related anion radical of *N-tert*-butylpyridine-2-carbaldimine (Bu^t-pyca)**

Thomas Stahl, Volker Kasack and Wolfgang Kaim



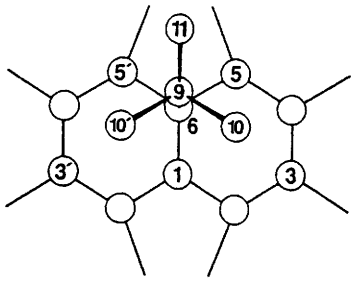
2133 **Electron paramagnetic resonance and electron–nuclear double resonance characterization of radicals in photopolymerized multifunctional methacrylates**

Cesare Oliva, Elena Selli, Silvia Di Blas and Giorgio Termignone



2141 **Electrostatic effects on the C_{60} surface of alkyl-C_{60} radicals**

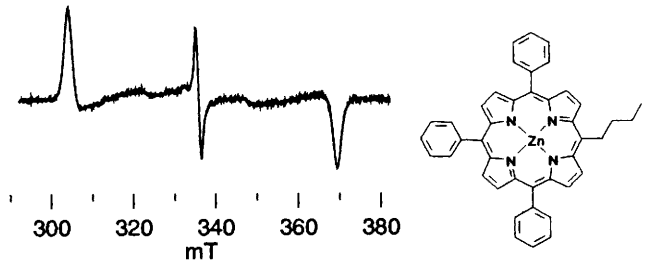
John R. Morton, Fabrizia Negri, Keith F. Preston and Géraldine Ruel



In XYZC-C_{60} radicals the most electronegative of X, Y or Z gains the pentagon position 11

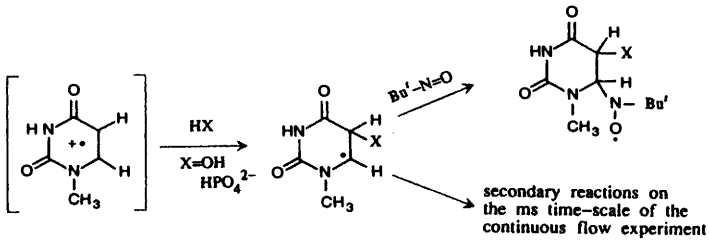
2147 **Continuous-wave electron spin resonance studies of porphyrin and porphyrin-quinone triplet states**

Burkhard Kirste, Peizhu Tian, Werner Kalisch and Harry Kurreck



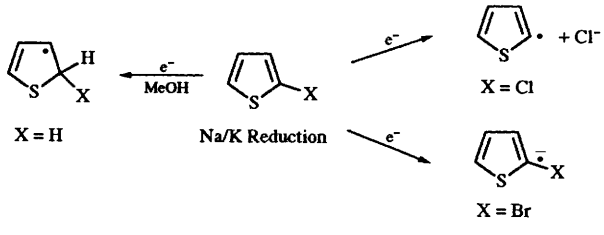
2153 **Spin-trapping studies of the reaction of the sulfate radical anion with N^1-substituted pyrimidine bases. Comparison with continuous-flow electron paramagnetic resonance experiments**

Knut Hildenbrand



2163 **Electron paramagnetic resonance studies of electron attachment to thiophene, bi(thienyl) and some halogen-substituted thiophenes**

Robert D. Farley, Bruce C. Gilbert, Peter Hanson, Allan W. Timms and Martyn C. R. Symons



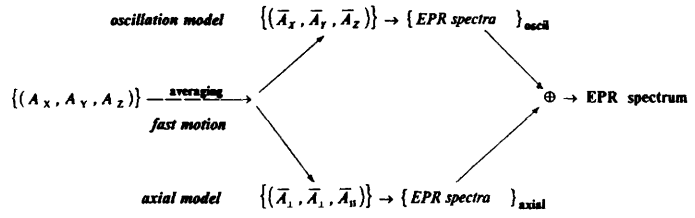
2167 **Electron paramagnetic resonance spin-trapping studies of the reaction of aryl radicals with nucleic acids and their components**

Clare Hazlewood, Michael J. Davies, Bruce C. Gilbert and John E. Packer

EPR spin trapping studies using MNP are reported which are consistent with the following behaviour:
$PhN_2^+ + e^- \longrightarrow N_2 + Ph^\bullet$
$Ph^\bullet$ + Pyrimidine bases ⟶ Base adducts at C^5–C^6 double bond
$Ph^\bullet$ + Pyrimidine nucleosides ⟶ Base adducts at C^5–C^6 double bond plus sugar radicals
$Ph^\bullet$ + Adenosine triphosphate ⟶ Base adducts?
$Ph^\bullet$ + DNA or tRNA ⟶ DNA and RNA radicals, together with low-molecular-weight fragments from strand-breaks

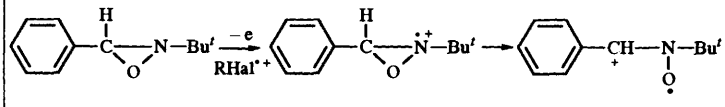
2175 **Dynamics of macromolecule spin-labelled side-chain groups by electron paramagnetic resonance spectra simulation**

Vladimir Timofeev and Boris Samarianov



2183 **Generation of α-aminoxylcarbenium ions by electron-transfer oxidation of *N-tert*-butyl-3-phenyloxazirane and their role in nitrone spin trapping chemistry**

Valentin E. Zubarev and Ortwin Brede



Articles

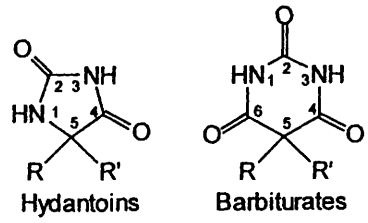
2189 **Electrostatic *vs.* orbital effects as stereoinductive factors in nucleophilic additions to the *endo*-substituted norbornan-7-one ring system**

Goverdhan Mehta, Faiz Ahmed Khan and William Adcock

Polar-field susceptibility parameters as well as a ^{13}C NMR probe based on the transmission of polar substituent effects in *endo*-norbornan-7-ones points to the involvement of electrostatic effects in determining π-face selectivities during nucleophilic additions to this ring system

2191 **Molecular dynamics of hydantoins and barbiturates assessed by ^{1}H, ^{13}C and ^{15}N relaxation data**

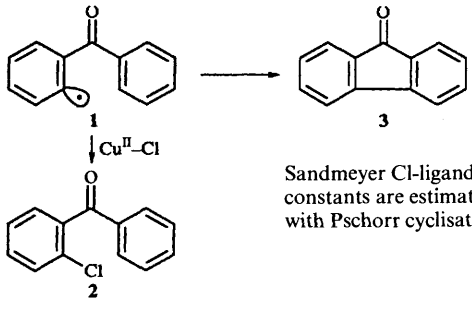
Petra Gruhlke, Christa G. Seipelt, Andreas Dölle, Manfred D. Zeidler, Paula Zaderenko, Paloma Ballesteros and Sebastián Cerdán



Molecular dynamics and pharmacological activity of hydantoins and barbiturates

2195 **Sandmeyer reactions. Part 3. Estimation of absolute rate constants for the transfer of chloride ligands from Cu^{II} to 2-benzoylphenyl radical (Pschorr radical clock) and further investigation of the relative rates of transfer of chloride and water ligands to other substituted phenyl radicals**

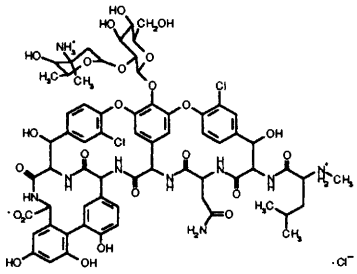
Peter Hanson, Roger C. Hammond, Bruce C. Gilbert and Allan W. Timms



Sandmeyer Cl-ligand transfer rate constants are estimated by comparison with Pschorr cyclisation

2203 **Infrared spectroscopic studies of vancomycin and its interactions with *N*-acetyl-D-Ala-D-Ala and *N,N'*-diacetyl-L-Lys-D-Ala-D-Ala**

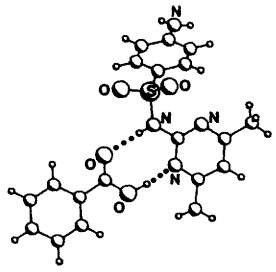
Colin J. Salter, Robert C. Mitchell and Alex F. Drake



The IR spectra of vancomycin and two peptide models, in D_2O solutions, have been assigned and the interactions of the peptides with vancomycin have been studied

2213 **Selective formation of hydrogen bonded cocrystals between a sulfonamide and aromatic carboxylic acids in the solid state**

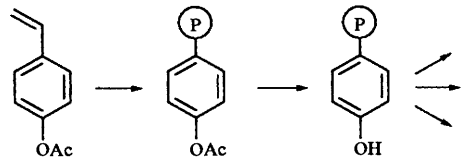
Mino R. Caira, Luigi R. Nassimbeni and Alexander F. Wildervanck



1 : 1 Cocrystal between sulfadimidine and benzoic acid

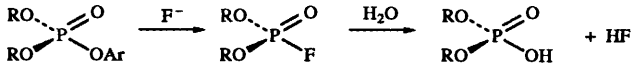
2217 **Poly(*p*-acetoxystyrene) resin: a prospective new support for combinatorial synthesis**

Hervé Deleuze and David C. Sherrington



2223 **Fluoride ion in phosphoryl transfer. A catalyst or an inhibitor?**

Marian Mentz and Tomasz A. Modro



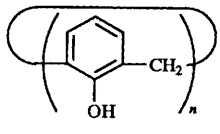
2227 **Effect of cations in the hydrolysis of phosphate esters**

Marian Mentz and Tomasz A. Modro

The hydrolysis of the P–OAr bond in diethyl 2-pyridyl phosphate is acid-catalysed and for *N*-methyl-8-(dimethylphosphoryloxo)-quinolinium ion occurs in alkaline medium, but for both substrates the reaction is subject to electrophilic catalysis by the cationic species present

2231 **Combined NMR spectroscopy and molecular mechanics studies on the stable structures of calix[*n*]arenes**

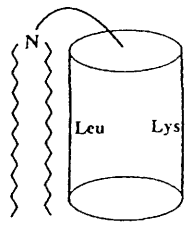
Takaaki Harada and Seiji Shinkai



1$_n$ (n = 4 ~ 7)

2243 **Amphiphilic α-helical structure in water stabilized by dioctadecyl chain**

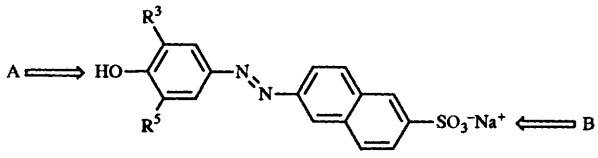
Jinbao Zhao, Shunsaku Kimura and Yukio Imanishi



Stabilized amphiphilic helical structure

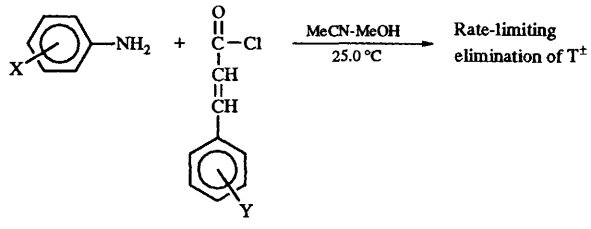
2249 **Dynamic aspects in host–guest interactions. Part 4. Kinetic and ^{1}H NMR evidence for multi-step directional binding in the molecular recognition of some 2-naphthylazophenol guests with α-cyclodextrin**

Noboru Yoshida



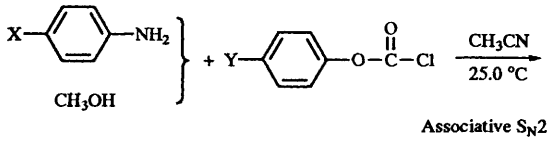
2257 **Nucleophilic substitution reactions of cinnamoyl chlorides with anilines in acetonitrile and acetonitrile–methanol mixtures**

Tae-Hyoung Kim, Chul Huh, Bon-Su Lee and Ikchoon Lee



2263 **Nucleophilic substitution reactions of phenyl chloroformates**

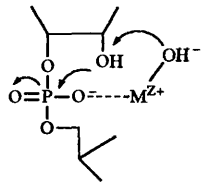
Kyoung Han Yew, Han Joong Koh, Hai Whang Lee and Ikchoon Lee



Associative S_N2

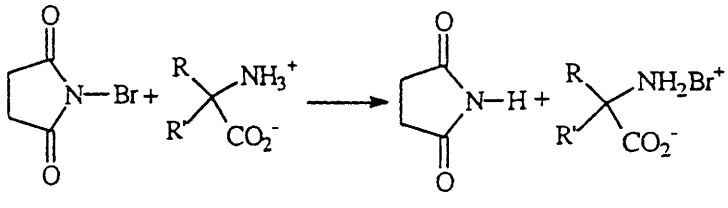
2269 **Metal-ion-promoted hydrolysis of uridylyl(3′,5′)uridine: internal *vs.* external general base catalysis**

Satu Kuusela, Mika Rantanen and Harri Lönnberg



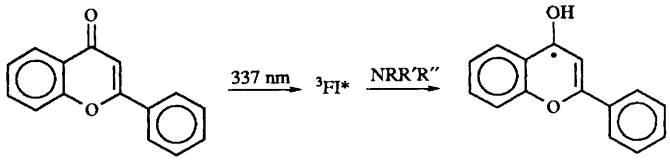
2275 **Kinetics of electrophilic bromine transfer from *N*-bromosuccinimide to amines and amino acids**

Juan M. Antelo, Florencio Arce and Juan Crugeiras



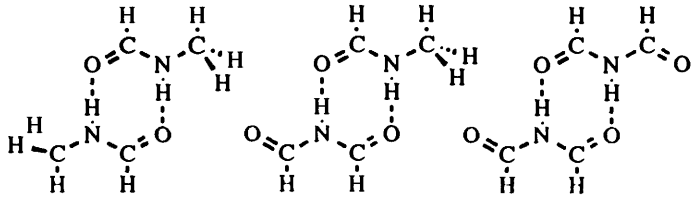
2281 **Triplet state properties of flavone in homogeneous and micellar solutions. A laser flash photolysis study**

Vicente Avila and Carlos M. Previtali



2287 **Complementary hydrogen bonding in diamides: a study on the influence of remote substituents using density functional theory**

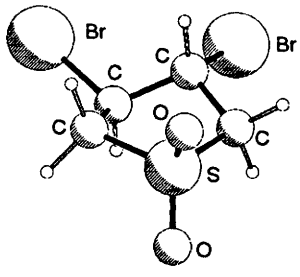
John E. McGrady and D. Michael P. Mingos



ΔE_{int} = 54.5 kJ mol^{-1} ΔE_{int} = 45.9 kJ mol^{-1} ΔE_{int} = 34.5 kJ mol^{-1}

2293 **Structure of (*E*)-3,4-dibromotetrahydrothiophene 1,1-dioxide, $C_4H_6Br_2SO_2$, as determined in the gas phase by electron diffraction, in the crystalline phase at 150 K by X-ray diffraction and by *ab initio* computations**

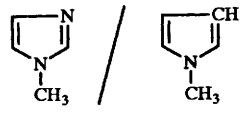
Alexander J. Blake, Paul T. Brain, Ian Gosney, Robert O. Gould, David W. H. Rankin, Heather E. Robertson, Peter Trickey and Michael Bühl



In both phases, the ring adopts the half-twist conformation with C_2 symmetry; in the solid phase the bromine atoms occupy *equatorial* positions, whereas in the gas phase the optimum fit is for a mixture of *axial* and *equatorial* conformers [proportion of *axial* conformer = 47.2(23)%]

2301 **Calorimetric quantification of the hydrogen-bond acidity of solvents and its relationship with solvent polarity**

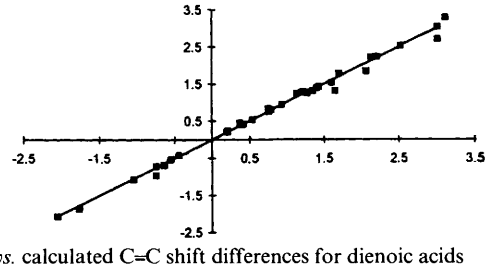
Javier Catalán, Javier Gómez, José L. Saiz, Angeles Couto, Marisa Ferraris and José Laynez



The hydrogen-bond acidity of organic solvents has been evaluated by measuring differences between the solvation enthalpies of *N*-methylimidazole and *N*-methylpyrrole in organic solvents and considering the solvent polarity

2307 **The σ-inductive effects of C=C and C≡C bonds: predictability of NMR shifts at sp^2 carbon in non-conjugated polyenoic acids, esters and glycerides**

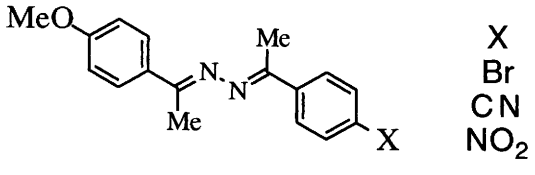
Oliver W. Howarth, Christopher J. Samuel and Giovanna Vlahov



Observed *vs.* calculated C=C shift differences for dienoic acids

2311 **Push–pull substitution *versus* intrinsic or packing related N–N *gauche* preferences in azines. Synthesis, crystal structures and packing of asymmetrical acetophenone azines**

Grace Shiahuy Chen, Jason K. Wilbur, Charles L. Barnes and Rainer Glaser



Stereoelectronics of asymmetrical acetophenone azines

2319 **Rate constants for the reaction of peroxyl free radical with flavonoids and related compounds as determined by the kinetic chemiluminescence method**

The late Vladimir A. Belyakov, Vitalij A. Roginsky and Wolf Bors

The following reactions are basic to ROO• scavenging by diphenols,

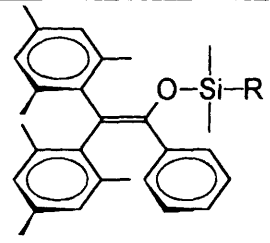
$$Ph(OH)_2 + ROO^{\bullet} \longrightarrow Ph(OH)O^{\bullet} + ROOH$$
$$Ph(OH)O^{\bullet} + ROO^{\bullet} \longrightarrow Ph(=O)_2 + ROOH$$
$$2\,Ph(OH)O^{\bullet} \longrightarrow Ph(=O)_2 + Ph(OH)_2$$

while for the kinetic deviations caused by flavonoids, an intramolecular rearrangement and subsequent chain propagation reactions are proposed:

$$PhO^{\bullet} \longrightarrow r^{\bullet} + O_2 \longrightarrow rOO^{\bullet}$$
$$r^{\bullet}(rOO^{\bullet}) + RH + O_2 \longrightarrow ROO^{\bullet} + rH(rOOH)$$
$$r^{\bullet}(rOO^{\bullet}) + PhOH \longrightarrow PhO^{\bullet} + rH(rOOH)$$
$$r^{\bullet}(rOO^{\bullet}) + PhO^{\bullet} \longrightarrow \text{products}$$

2327 **Silyl enol ether cation radicals in solution: nucleophile assisted Si–O bond cleavage**

Michael Schmittel, Manfred Keller and Armin Burghart

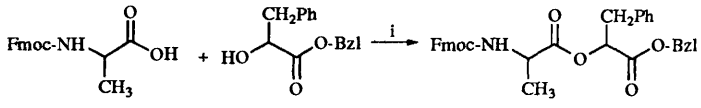


1–3 R = CH_3, Bu^t, 4-MeO-Ph

The chemistry of the cation radicals of silyl enol ethers **1–3** has been investigated, providing evidence for a nucleophile assisted Si–O bond cleavage

2335 **A model reaction for assessing the coupling and chiral efficiency of reagents in depside bond formation**

John S. Davies, Joanne Howe and Murielle Le Breton

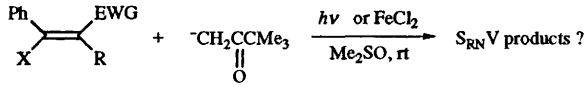


(Fmoc-L-Ala-OH) (L-H-Phlac-OBzl) (Fmoc L-Ala-L-Phlac-OBzl)

(i) Various coupling conditions

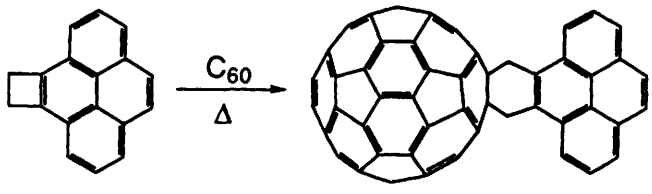
2341 **Effect of substituents on the competition between several mechanisms of nucleophilic vinylic substitution**

Christian Amatore, Carlo Galli, Patrizia Gentili, Alessandra Guarnieri, Ettie Schottland and Zvi Rappoport



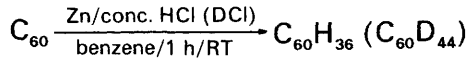
2351 **Synthesis and electronic properties of C_{60}–*o*-quinodimethane adducts**

Yosuke Nakamura, Toshiyuki Minowa, Seiji Tobita, Haruo Shizuka and Jun Nishimura



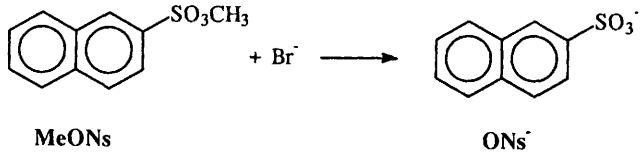
2359 **Polyhydrogenation of [60]- and [70]-fullerenes**

Adam D. Darwish, Ala'a K. Abdul-Sada, G. John Langley, Harold W. Kroto, Roger Taylor and David R. M. Walton



2367 **S_N2 Reactions of a sulfonate ester in mixed cationic/phosphine oxide micelles**

Andrei Blaskó, Clifford A. Bunton, Eduardo A. Toledo, Paul M. Holland and Faruk Nome



MeONs **ONs⁻**

in micelles of $C_{16}H_{33}NMe_3Br$ + $C_{12}H_{25}PMe{=}O$

Corrigenda

2375 **Structural studies on some 1,3,4-thiadiazolium-2-aminides and their rearrangement isomers using ^{15}N and ^{13}C NMR spectroscopy** C.A. Montanari, J. P. B. Sandall, Y. Miyata and J. Miller

2376 **1,2-Diphenylethane-1,2-diamine: an effective NMR chiral solvating agent for chiral carboxylic acids** R. Fulwood and D. Parker

2377 **The effective 'size' of the tris(trimethylsilyl)silyl group in several molecular environments** J. Frey, E. Schottland, Z. Rappoport, D. Bravo-Zhivotovskii, M. Nakash, M. Botoshansky, M. Kaftory and Y. Apeloig

2378 **^{13}C CP/MAS NMR studies of tetraazaannulenes: fast proton transfer in the solid state** A. C. McGregor, P. J. Lukes, J. R. Osman and J. A. Crayston

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Hydroxyl-radical-induced reactions of poly(acrylic acid); a pulse radiolysis, EPR and product study. Part II. Oxygenated aqueous solutions **P. Ulanski, E. Bothe, K. Hildenbrand, M. Rosiak and C. von Sonntag**

Hydroxyl-radical-induced reactions of poly(acrylic acid); a pulse radiolysis, EPR and product study. Part I. Deoxygenated aqueous solutions **P. Ulanski, E. Bothe, K. Hildenbrand, J.M. Rosiak and C. von Sonntag**

Synthesis, NMR spectroscopy and conformational studies of two vicinally disubstituted trisaccharides
P.E. Jansson, A. Kjellberg, T. Rundlöf and G. Widmalm

Ab initio studies on organophosphorus compounds. Part 4. Intramolecular hydrogen bonding and water interactions of bisphosphonates **J.P. Räsänen, E. Pohjala and T.A. Pakkanen**

The low intrinsic reactivity of picrylacetone: an index for the π-acceptor capability of a 2,4,6-trinitrophenyl structure
G. Moutiers, B.E. Fahid, A.G. Collot and F. Terrier

Importance of aromaticity on the relative stabilities of indazole annular tautomers: an *ab initio* study
J. Catalán, J.L.G. de Paz and J. Elguero

Mechanism of asymmetric photocyclization of α-oxoamides
D. Hashizume, H. Kogo, A. Sekine, Y. Ohashi, H. Miyamoto and F. Toda

Conformational behaviour of methyl *p-tert*-butylcalix[6]arene ester: interconversions among 1,2,3-alternate conformations
S. Ahn, J.W. Lee and S-K. Chang

Inverted spin trapping. Part V. 1,1,1,3,3,3-Hexafluoropropan-2-ol as a solvent for the discrimination between proper and inverted spin trapping **L. Eberson, M.P. Hartshorn and O. Persson**

On the existence of quinone radical cations. A study in 1,1,1,3,3,3-hexafluoropropan-2-ol
L. Eberson and M.P. Hartshorn

Stability and IR spectra of isomers of $C_{60}F_{48}$ **S.J. Austin, P.W. Fowler and J.P.B. Sandall**

Kinetic study of the stability of $(NH_2)_2CSSC(NH_2)_2^{2+}$ **L.G. Rio, C.G. Munkley and G. Stedman**

EPR spectra of tris(trimethylsilyl)methyl(hydroxy)silyl radicals, $(Me_3Si)_3CSi(R)OH$ and of tris(trimethylsilyl)methylsilanone radical anions, $(Me_3Si)_3CSi(R)=O^-$(R=H,Me,Et,Bu,PhF) **A.G. Davies, C. Eaborn, P.D. Lickiss and A.G. Neville**

Kinetic constraints on possible reaction pathways for the osmium-catalysed asymmetric dihydroxylation (AD)
P.O. Norrby and K.P. Gable

Spectroscopic detection of diols and sugars by a colour change in boronic-acid-appended spirobenzoypyrans
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Synthesis and studies on surface and self-assembly properties of polyphenylsulfonates in aqueous solution. Part 2. Sodium 2'-methyl-5'-phenyl-1,1':3',1"-terphenyl-4-sulfonate **J. Czapkiewicz and P. Milart**

3-Acetyoxyaminoquinazolin-4(3H)ones as aziridinating agents: relative rate of inversion at the exocyclic nitrogen
R.S. Atkinson and P.J. Williams

Tertiary: secondary: primary C–H bond relative reactivity in the one electron side-chain oxidation of alkylbenzenes. A tool to distinguish electron transfer from hydrogen atom transfer mechanisms
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IUPAC draft for public comment

Glossary of Terms in Computational Drug Design

Computational drug design is a rapidly growing field which is now an important component in the discipline of medicinal chemistry. At the same time many medicinal chemists lack significant formal training in this field and may not have a clear understanding of some of the terminology used; however they need to grasp concepts, follow research results, define problems, and utilize the findings. In this context IUPAC felt it would be useful to develop a glossary of terms used in computational drug design for easy reference purposes. Accordingly a working party of seven experts in the field have constructed a glossary of some 108 terms. Concise but explanatory definitions have been formulated based on a variety of literature sources and selected key references provided.

Copies of the text may be obtained from Dr Alan McNaught, The Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge CB4 4WF. IUPAC would welcome comments (by **31 May 1996**) before preparation of a final draft for publication in *Pure Appl. Chem.*