

JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions 2

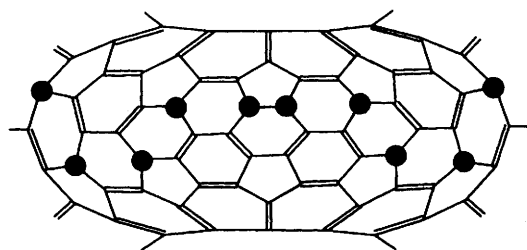
Physical Organic Chemistry

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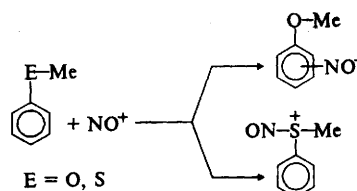
Perkin Communications

1027 **Theoretical characterisation of $C_{70}Cl_{10}$: the rôle of 1,4-addition across hexagonal rings**

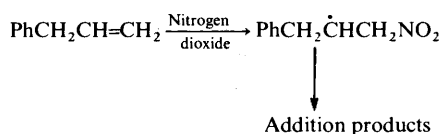
Sarah J. Austin, Patrick W. Fowler, John P. B. Sandall, Paul R. Birkett, Anthony G. Avent, Adam D. Darwish, Harold W. Kroto, Roger Taylor and David R. M. Walton

1029 **Interaction of anisole and thioanisole with the nitrosonium cation: π - vs. n -complex formation**

Gennady I. Borodkin, Vladimir A. Podryvanov, Makhmut M. Shakirov and Vyacheslav G. Shubin

1031 **Mechanism of reaction of nitrogen dioxide with alkenes in solution**

Julie Chatterjee, Robert G. Coombes, Julian R. Barnes and Melanie J. Fildes

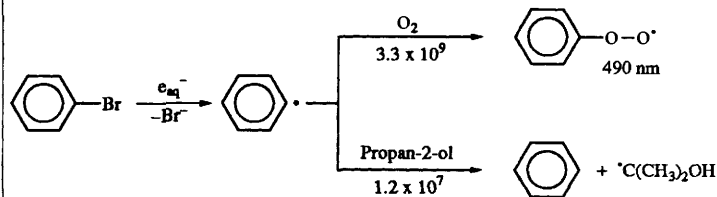


Both NO_2^{\cdot} and N_2O_4 are reactive species with allylbenzene and other alkenes

Articles

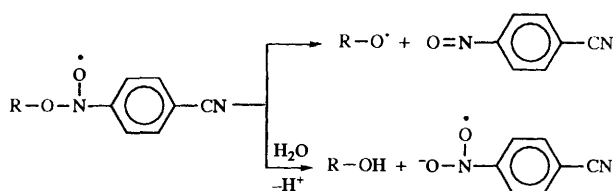
- 1033 **Pulse radiolysis of aryl bromides in aqueous solutions: some properties of aryl and arylperoxyl radicals**

Xingwang Fang, Ralf Mertens and Clemens von Sonntag



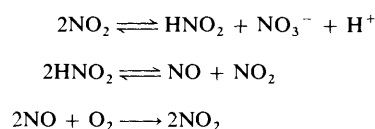
- 1037 **Oxidation vs. fragmentation in radiosensitization. Reactions of α -alkoxyalkyl radicals with 4-nitrobenzonitrile and oxygen. A pulse radiolysis and product analysis study**

Chandrasekhar Nese, Man Nien Schuchmann, Steen Steenken and Clemens von Sonntag



- 1045 **Role of the reaction of nitric oxide with oxygen in the decomposition of nitrous acid in aqueous acid solution**

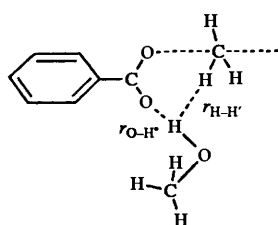
Ben D. Beake and Roy B. Moodie



This mechanism satisfactorily describes both the decomposition of nitrous acid and the oxidation of nitric oxide in air-saturated aqueous acid solution

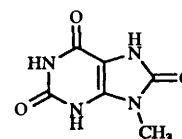
- 1049 **Solvation of carboxylate ions and of transition-state anions for the reaction of carboxylate ion with ethyl iodide in acetonitrile-methanol mixtures. Thermodynamic and quantum mechanical approaches**

Yasuhiko Kondo, Wataru Sugitani, Masaki Tokui and Tatsuya Takagi



- 1055 **Electrochemical and enzymic oxidation of 9-methyluric acid at solid electrodes**

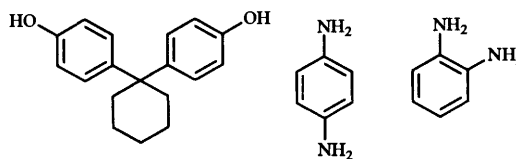
Rajendra N. Goyal, Ajay K. Jain and Neena Jain



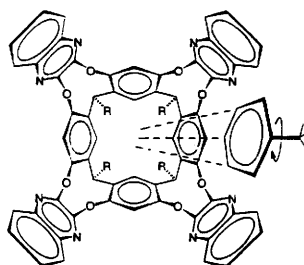
Electrochemical oxidation at solid electrode is similar to enzymic oxidation by horseradish peroxidase

1063 **Selective inclusion of phenylenediamine isomers by 1,1-bis(4-hydroxyphenyl)cyclohexane**

Mino R. Caira, Alicia Horne, Luigi R. Nassimbeni, Koichi Okuda and Fumio Toda

1069 **Host-guest complexation in the gas phase. Investigation of the mechanism of interaction between cavitands and neutral guest molecules**

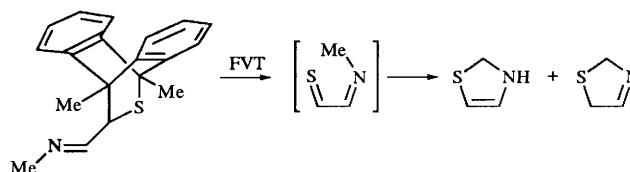
Marco Vincenti and Enrico Dalcanale



The gas-phase processes leading to the formation of host-guest complexes are investigated in the ion-source and in the octapole collision cell of a hybrid mass spectrometer

1077 **Theoretical study of the cyclization of α -iminothioaldehydes into dihydrothiazoles**

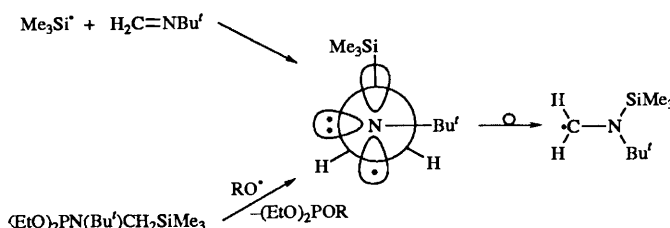
Roger Arnaud, Nadia Pelloux-Léon, Jean-Louis Ripoll and Yannick Vallée



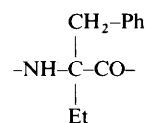
Flash vacuum thermolysis (FVT)

1087 **EPR spectroscopic studies of *N*-alkyl-*N*-trialkylsilylmethylaminyl radicals in solution**

Brian P. Roberts and Anthony R. Vazquez-Persaud

1097 **Linear oligopeptides. Part 329. Synthesis, characterization and solution conformational analysis of C $^{\alpha}$ -ethyl, C $^{\alpha}$ -benzylglycine [α (Et)Phe] containing peptides**

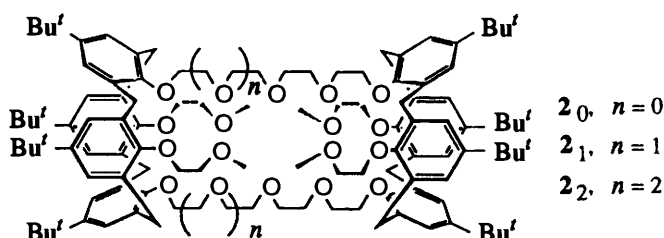
Fernando Formaggio, Monica Pantano, Marco Crisma, Gian Maria Bonora, Claudio Toniolo and Johan Kamphuis



(α Et)Phe is a strong β -turn and helical former

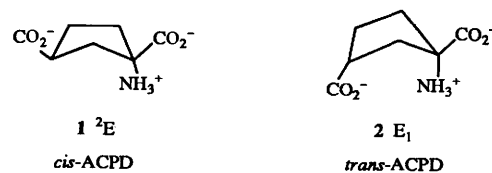
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Fumio Ohseto and Seiji Shinkai



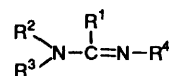
- 1111 **Conformational analysis by NMR spectroscopy, molecular dynamics simulation in water and X-ray crystallography of glutamic acid analogues: isomers of 1-aminocyclopentane-1,3-dicarboxylic acid**

Valéry Larue, Josyane Gharbi-Benarous, Francine Acher, Giovanni Valle, Marco Crisma, Claudio Toniolo, Robert Azerad and Jean-Pierre Girault



- 1127 **Amidines. Part 34. ¹⁵N NMR Spectra of trisubstituted amidines. Substituent effects**

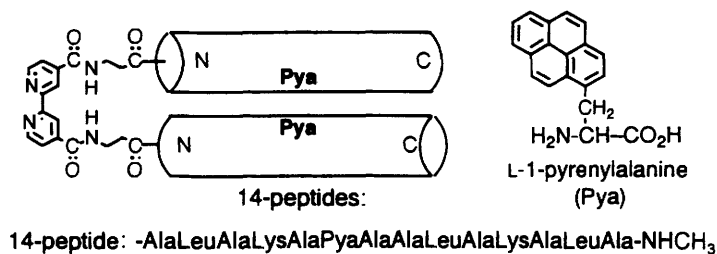
Janusz Oszczapowicz, Iwona Wawer, Manfred Dargatz and Erich Kleinpeter



The influence of substitution at any of the sites on the ¹⁵N NMR chemical shifts depends on substituents at the other two sites

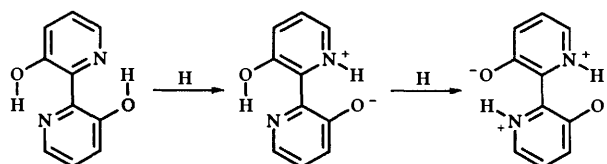
- 1133 **A pair of pyrene groups as a conformational probe for designed two α -helix polypeptides**

Hisakazu Mihara, Yuji Tanaka, Tsutomu Fujimoto and Norikazu Nishino



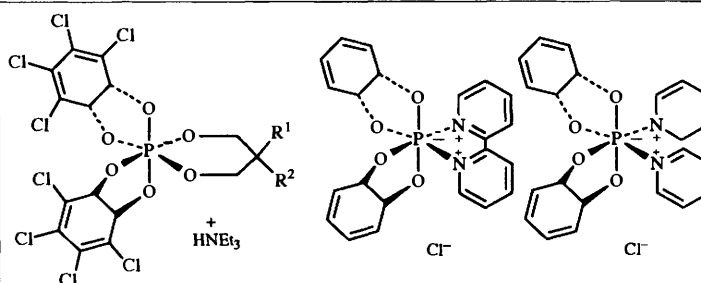
- 1141 **Proton transfer in the ground and excited electronic states of [2,2'-bipyridyl]-3,3'-diol. A semiempirical study**

Vincenzo Barone, Giuseppe Milano, Laura Orlandini and Carlo Adamo



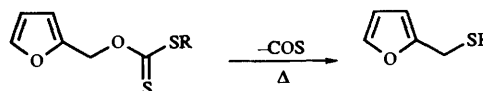
- 1149 **Correlation of ³¹P chemical shift parameters to molecular structures of hexacoordinate organophosphorus compounds in the solid state**

Marek J. Potrzebowski, Jacek Kowara, Włodzimierz Ciesielski and Aleksandra Skowrońska



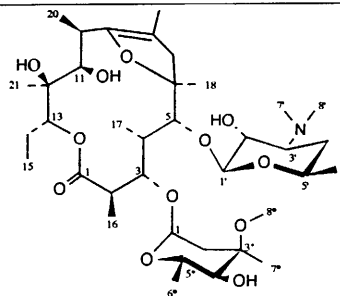
- 1155 **Simple synthesis of furfuryl sulfides *via* extrusion of COS from the xanthates and its mechanistic aspects**

Masashi Eto, Mituhiro Nishimoto, Toshihiro Uemura, Takuzo Hisano and Kazunobu Harano



- 1163 **Structural studies on erythromycin A enol ether: full assignments of the ^1H and ^{13}C NMR spectra**

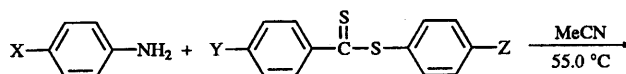
Perwaiz Alam, P. Christopher Buxton,
John A. Parkinson and Jill Barber



Erythromycin A enol ether

- 1169 **Kinetics and mechanism of the aminolysis of phenyl dithiobenzoates**

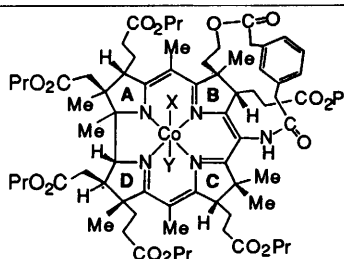
Hyuck Keun Oh, Chul Ho Shin and Ikchoon Lee



$\rho_{XY} > 0$, $\rho_{YZ} < 0$ and $\rho_{XZ} > 0 \longrightarrow$ rate-limiting breakdown of T^\ddagger

- 1175 **Hydrophobic vitamin B_{12} . Part 12. Preparation, characterization and enantioselective alkylation of strapped hydrophobic vitamin B_{12}**

Yukito Murakami, Yoshio Hisaeda, Teruhisa Ohno, Hiroshi Kohno and Takuya Nishioka

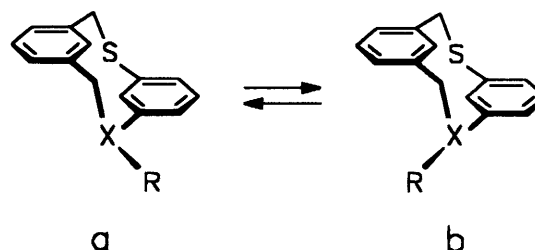


Strapped vitamin B_{12}

The enantioselective alkylation of hydrophobic vitamin B_{12} derivatives with racemic 3-bromo-2-methylpropionic esters was carried out, and the highest *S*-selectivity (75% ee) was observed with the strapped vitamin B_{12}

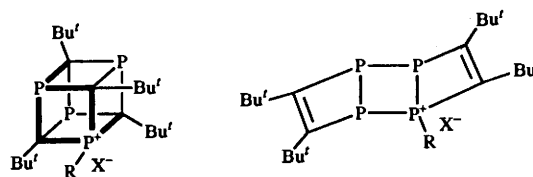
- 1185 **A study of the *N*-inversion barrier and the circular dichroism spectra of 1-thia-10-aza[2.2]metacyclophane**

Dorit Wortmann-Saleh, Stefan Grimme, Bernd Engels, Dirk Müller and Fritz Vögtle



- 1191 **Phosponium ions of 2,4,6,8-tetra-*tert*-butyl-1,3,5,7-tetraphosphacubane and 1,2,5,6-tetraphosphatricyclo[4.2.0.0^{2,5}]octa-3,7-diene in the gas phase: host-guest complexes, phosponium ion decomposition pathways and interaction with onium ions (and carbocations). A field desorption (FD), fast atom bombardment (FAB) and tandem mass spectrometry (CAD-MS/MS) study**

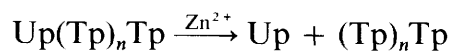
Kenneth K. Laali, Chrys Wesdemiotis, Michael Polce and Sárka Beranová



Desorption/ionization (FD, FAB) and CAD-MS/MS mass spectrometric studies of the mono- and di-phosponium salts; host-guest clusters

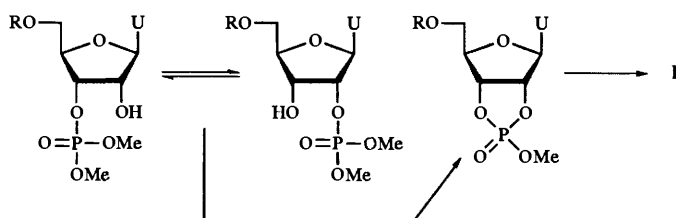
- 1197 **The effect of the 3'-terminal monophosphate group on the metal-ion-promoted hydrolysis of the phosphodiester bonds of short oligonucleotides**

Satu Kuusela, Alex Azhayev, Andrei Guzaev and Harri Lönnberg



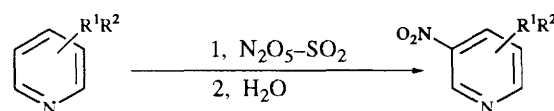
- 1203 **General and specific acid/base catalysis of the hydrolysis and interconversion of ribonucleoside 2'- and 3'-phosphotriesters: kinetics and mechanisms of the reactions of 5'-O-pivaloyluridine 2' and 3'-dimethylphosphates**

Markus Kosonen and Harri Lönnberg



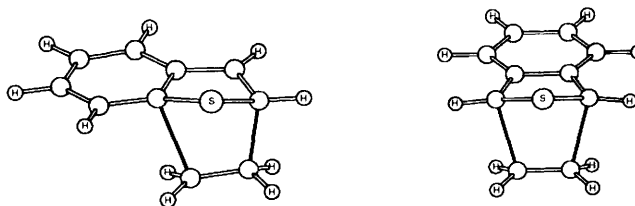
- 1211 **Nitration of pyridine by dinitrogen pentoxide in sulfur dioxide: investigation of the reaction mechanism**

Jan M. Bakke and Ingrid Hegbom



- 1217 **AM1 Semiempirical study of the reactivity of benzo[*b*]- and benzo[*c*]-thiophene as dienes in Diels–Alder reactions**

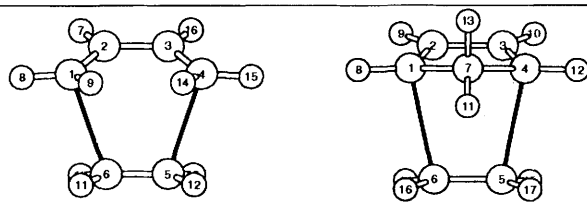
Branko S. Jursic



Theoretical study of the benzothiophene reactivity in the Diels–Alder reactions is prepared

- 1223 **DFT study of the Diels–Alder reactions between ethylene with buta-1,3-diene and cyclopentadiene**

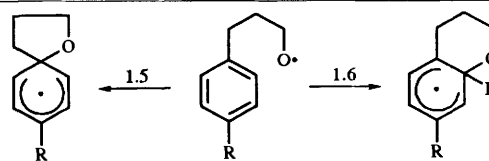
Branko Jursic and Zoran Zdravkovski



The activation energies for ethylene addition to butadiene and cyclopentadiene were calculated by DFT methods and compared with experimental values

- 1227 **Reactions of γ -arylalkanols *via* aryl radical cation and alkoxy radical intermediates. Part 3. Reactions of 3-arylprop-1-yl hydroperoxides with iron(II) in the presence of copper(II)**

André Goosen, Charles F. Marais, Cedric W. McClelland and Fabrizio C. Rinaldi



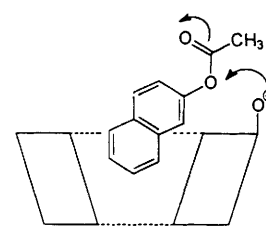
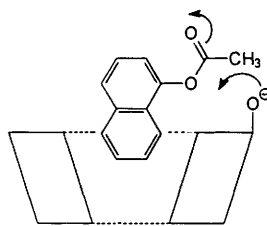
R = Me, Cl, OMe

The cyclisation reactions of 3-arylpropan-1-oxyl radicals are compared

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Oswald S. Tee and Michael J. Boyd



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1245 **Ab initio study of the homolytic additions of aminyl radicals and ammoniumyl cation radicals to alkenes** Brendan J. Maxwell, Carl H. Schiesser, Bruce A. Smart and John Tsanaktsidis

1245 **Preparation and properties of some crown ethers incorporating stable carbocations** Owen S. Mills, Nichola J. Mooney, Peter M. Robinson, C. Ian F. Watt and Brian G. Cox

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