

JOURNAL OF THE CHEMICAL SOCIETY

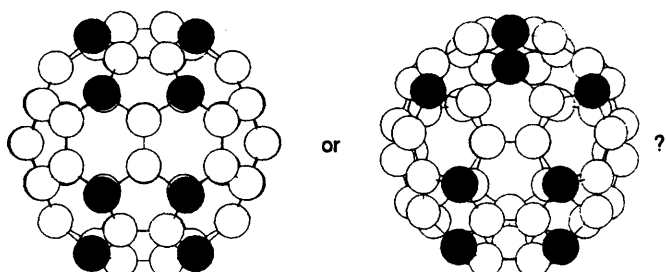
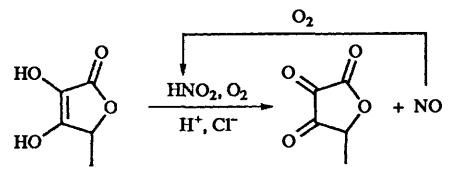
Perkin Transactions 2

Physical Organic Chemistry

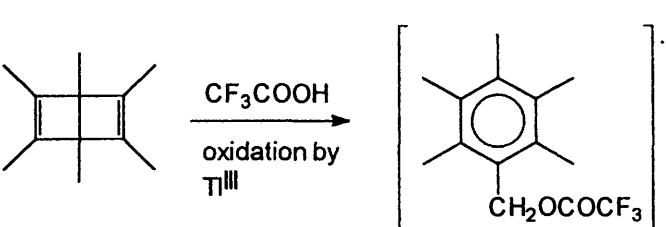
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Perkin Communications

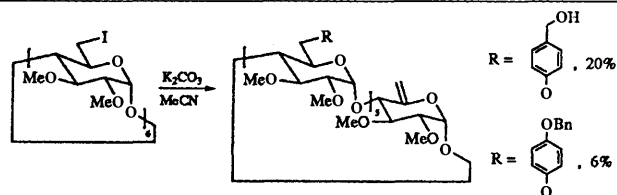
<p>1247 Relative stabilities of octabromo[60]fullerene isomers: limitations of semi-empirical methods</p> <p>Patrick W. Fowler and John P. B. Sandall</p>	
<p>1251 Oxidation of ascorbic acid by nitrous acid: conditions where autoxidation of nitric oxide is rate determining</p> <p>Ben D. Beake, Roy B. Moodie and Davina Smith</p>	

Articles

<p>1253 Formation and characterization of the radical cation of pentamethylbenzyl trifluoroacetate from the oxidation of hexamethyl (Dewar benzene) by thallium(III) trifluoroacetate in trifluoroacetic acid—a slow and complex reaction</p> <p>Lennart Eberson, Michael P. Hartshorn, Ola Persson and Jan O. Svensson</p>	
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1263 **The synthesis and structural mapping of unsymmetrical chemically modified α -cyclodextrins by high-field nuclear magnetic resonance spectroscopy**

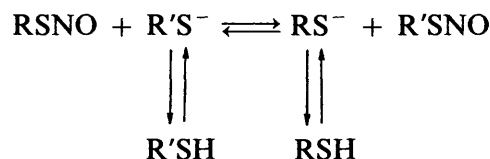
Peter R. Ashton, Edward Y. Hartwell, Douglas Philp, Neil Spencer and J. Fraser Stoddart



The elimination reaction, which has taken place to form the olefinic bond on one of the glucopyranose residues, is the first observation of its type in the cyclodextrin field

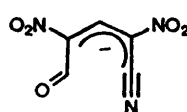
1279 **NO-Group transfer (transnitrosation) between S-nitrosothiols and thiols. Part 2**

D. Jonathan Barnett, Ana Rios and D. Lyn H. Williams



1283 **Solvent effects on aromatic nucleophilic substitution by the ANRORC mechanism. Hydrolysis of 2-chloro-3,5-dinitropyridine**

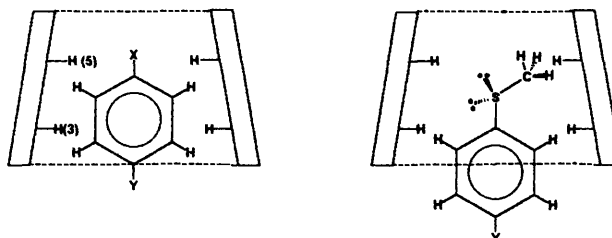
Hamad A. Al-Lohedan and Anthony J. Kirby



The title reaction goes through the remarkable intermediate shown; its formation and disappearance are followed separately in six mixed solvents and the rate ratio k_1/k_2 varies from 8 to over 1000

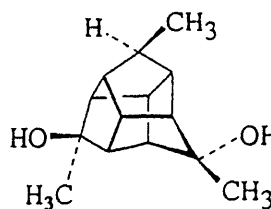
1287 **Cooperativity and steric hindrance: important factors in the binding of α -cyclodextrin with *para*-substituted aryl alkyl sulfides, sulfoxides and sulfones**

D. Martin Davies and Michael E. Deary



1295 **Disorder *versus* symmetry in the helical tubuland inclusion host lattice—a successful trishomocubyl diol probe**

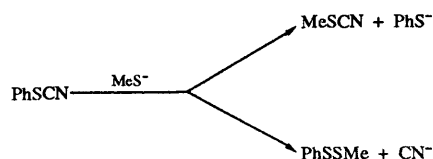
Roger Bishop, Donald C. Craig, Marcia L. Scudder, Alan P. Marchand and Zenghui Liu



The requisite helical tubuland C_2 symmetry is achieved through crystallographic disorder

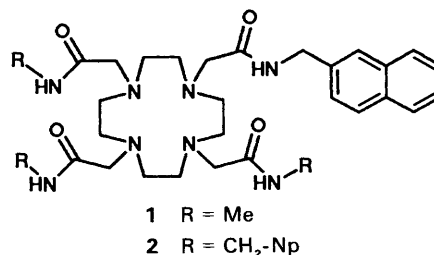
1301 **Theoretical studies on the biocidal activity of phenylthiocyanates**

John O. Morley and Memdoh Naji



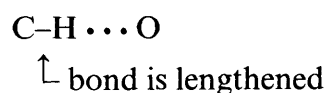
- 1305 Luminescence behaviour of cadmium, lead, zinc, copper, nickel and lanthanide complexes of octadentate macrocyclic ligands bearing naphthyl chromophores

David Parker and J. A. Gareth Williams



- 1315 Weak hydrogen bonding. Part 1. Neutron diffraction data of amino acid C_α-H suggest lengthening of the covalent C-H bond in C-H...O interactions

Thomas Steiner



- 1321 Weak hydrogen bonding. Part 2. The hydrogen bonding nature of short C-H...π contacts: crystallographic, spectroscopic and quantum mechanical studies of some terminal alkynes

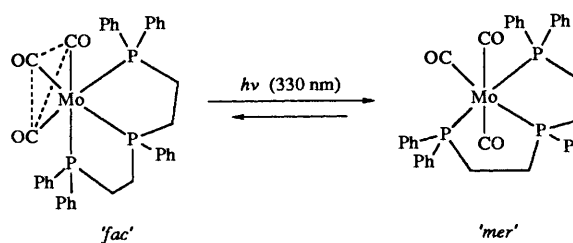
Thomas Steiner, Evgeni B. Starikov, Ana M. Amado and José J. C. Teixeira-Dias



Weak hydrogen bonding interactions

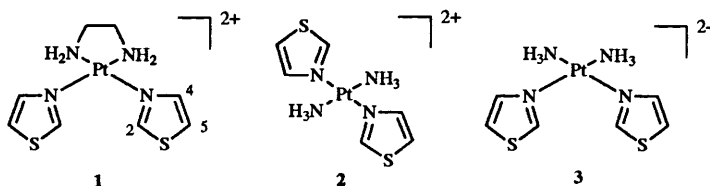
- 1327 Voltammetric study of the photolysis of *fac*-tricarbonyl-η³-(bis[2-(diphenylphosphino)ethyl]phenylphosphine)molybdenum

Richard G. Compton, John C. Eklund, Allan Hallik, Sunita Kumbhat, Alan M. Bond and Ray Colton



- 1333 Hydrogen isotope exchange in Pt^{II}-thiazole complexes

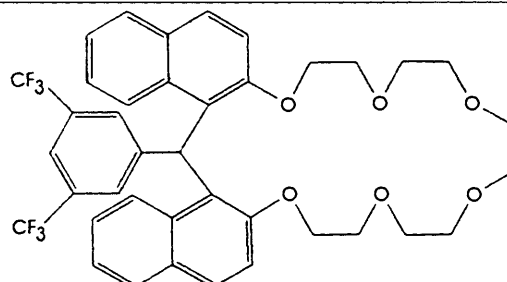
Erwin Buncel and Omoshile Clement



Study of H/D isotopic exchange has allowed exchange to be observed at all thiazole positions in 1, with C(2)-H ≧ C(5)-H > C(4)-H, while in 2 and 3 the reactivity order is C(2)-H ≧ C(5)-H; this is the first reported exchange at thiazole C(4)

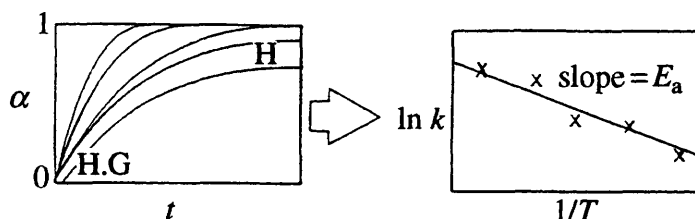
- 1339 Search for diastereoisomers of the 3,5-bis(trifluoromethyl)phenyldinaphtho propeller crowns: crystal structure and molecular dynamics simulations

William Clegg, Paul J. Cooper, George A. Forsyth and Joyce C. Lockhart



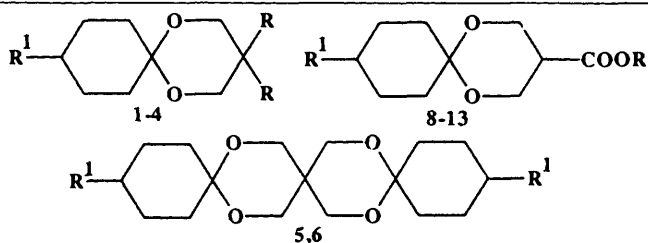
1345 Kinetics of desolvation of inclusion compounds of 9,10-derivatives of *trans*-9,10-dihydroxy-9,10-dihydroanthracene with benzene

Leonard J. Barbour, Mino R. Cairra, Anita Coetzee and Luigi R. Nassimbeni



1351 Conformational analysis of some spiro and polyspiro 1,3-dioxane compounds with axial and helical chirality

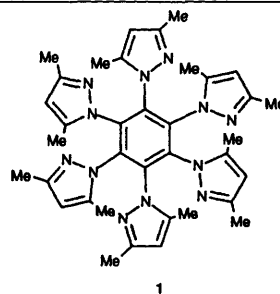
Ion Grosu, Sorin Mager and Gerard Plé



The axial and the helical chirality of 1,3-dioxanes 1-6 and 8-13 is discussed

1359 Aromatic propellenes. Part 1. NMR spectroscopy, X-ray crystal and molecular structure of hexa(3,5-dimethylpyrazol-1-yl)-benzene

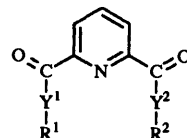
Concepción Foces-Foces, Antonio L. Llamas-Saiz, Rosa M^a Claramunt, Nadine Jagerovic, Maria Luisa Jimeno and José Elguero



The structure of the title compound 1 corresponds to an (*ududud*) conformation, where the pyrazole rings are almost perpendicular and successively up (*u*) and down (*d*); in solution, CDCl₃ + TFA, another isomer appears 2 (*uduud*); AM1 calculations of all possible conformers show that these two are the most stable

1365 Electrochemical reduction of some 2,6-disubstituted pyridine-based esters and thioic *S*-esters in acetonitrile

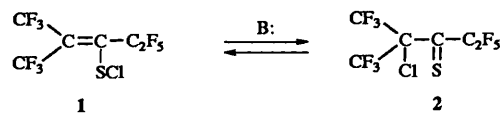
Richard D. Webster, Alan M. Bond and Thomas Schmidt



The mechanism for the electrochemical reduction of some 2,6-disubstituted esters of pyridine is described in depth
Y¹ = Y² = O or S
R¹ = R²

1375 Reversible intramolecular 1,3-chlorine migration in the triad 'carbon-carbon-sulfur'

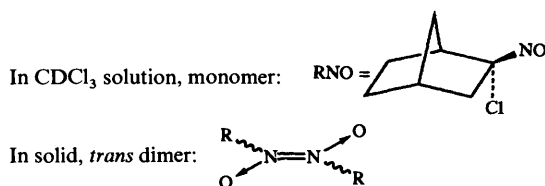
Vera Ya. Popkova, Victor M. Anisimov, Georgii N. Dolenko, Mikhail N. Semenenko and Vladimir M. Fedoseev



In the absence of nucleophilic solvents or catalyst's assistance (B:) both forms are completely stable and show no tautomerism on storage

1381 Magnetic resonance studies of the structure and the red photolysis reactions of 2-chloro-2-nitrosornbornane

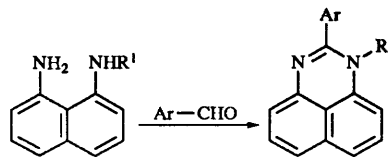
Mohamed-Chérif Boucenna, John S. Davidson, Anthony McKee, Andrew L. Porte and David C. Apperley



Photochemical reactions triggered by red light

1389 **2-Arylperimidine derivatives. Part 1. Synthesis, NMR spectroscopy, X-ray crystal and molecular structures**

Antonio L. Llamas-Saiz, Concepción Foces-Foces, Dionisia Sanz, Rosa M^a Claramunt, Julio Dotor, José Elguero, Javier Caltalán and Juan Carlos del Valle



The synthesis and molecular structures of seven derivatives of the perimidine system, namely 2-phenylperimidine (1), 2-(2-hydroxyphenyl)perimidine (2), 2-(2-methoxyphenyl)perimidine (3), 2-(9-anthryl)perimidine (4), 1-methyl-2-phenylperimidine (5), 1-methyl-2-(2-hydroxyphenyl)perimidine (6) and 1-methyl-2-(2-methoxyphenyl)perimidine (7)

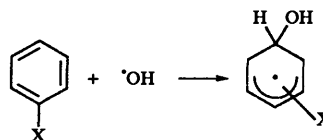
1399 **Molecular symmetry, melting temperatures and melting enthalpies of substituted benzenes and naphthalenes**

Angelo Gavezzotti

An old rule of thumb says that *para*-disubstituted benzenes melt at higher temperatures than *meta*- or *ortho*-disubstituted isomers; but why?

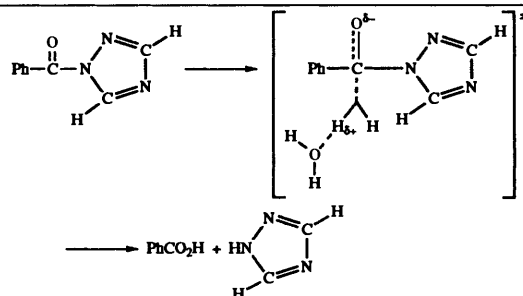
1405 **Ab initio molecular study on reactivity of phenol, biphenyl, benzoate and *p*-hydroxybenzoate in the $\cdot\text{OH}$ addition reaction and stability of the corresponding $\cdot\text{H}$ and $\cdot\text{OH}$ cyclohexadienyl adducts**

Mikael Peräkylä and Tapani A. Pakkanen



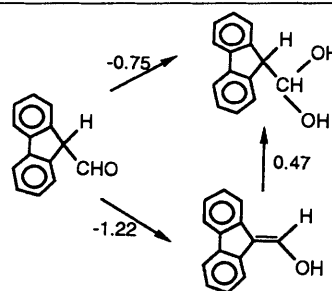
1411 **Kinetics of hydrolysis in aqueous solution of 1-benzoyl-1,2,4-triazole; the role of pairwise and triplet Gibbs energy interaction parameters in describing the effects of added salts and added alcohols**

Wouter H. Noordman, Wilfried Blokzijl, Jan B. F. N. Engberts and Michael J. Blandamer



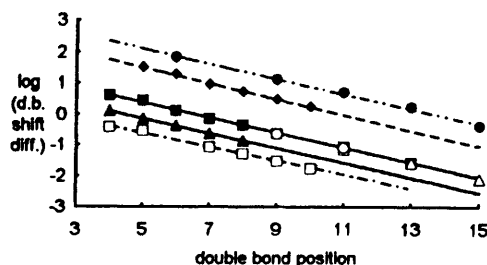
1415 **Keto-enol tautomerism and hydration of 9-acylfluorenes**

Myles P. Harcourt and Rory A. More O'Ferrall



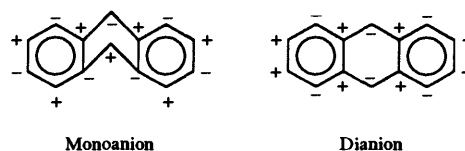
1427 **Long-range σ -inductive interactions through saturated C-C bonds in polymethylene chains**

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



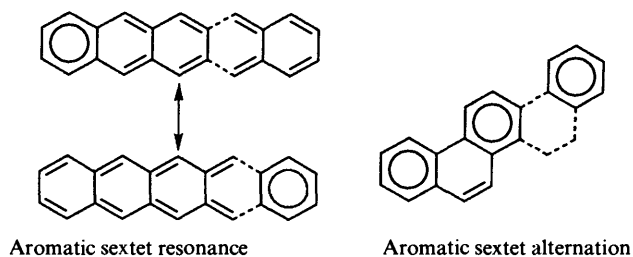
- 1433 **Acidity of dibasic carbon acids. Part 2. Geometry and electronic structure of mono- and di-anions of 9,10-dihydroanthracene and its derivatives in tetrahydrofuran**

Malka Nir, Roy E. Hoffman, Israel O. Shapiro and Mordecai Rabinovitz



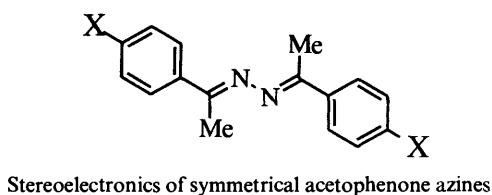
- 1443 **Precise PPP molecular orbital calculations of excitation energies of polycyclic aromatic hydrocarbons. Part 1. On the correlation between the chemical softness and the absolute hardness**

Kimihiro Hiruta, Sumio Tokita and Kichisuke Nishimoto



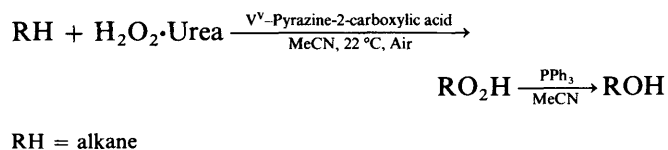
- 1449 **Comparative analysis of crystal structures of *E,E*-configured *para*-substituted acetophenone azines with halogen, oxygen, nitrogen and carbon functional groups**

Rainer Glaser, Grace Shiahuy Chen, Mitchell Anthamatten and Charles L. Barnes



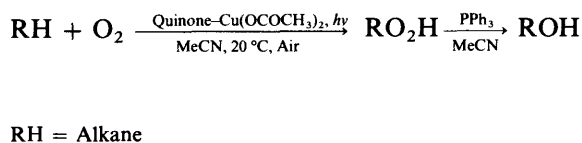
- 1459 **Oxidations by the reagent ' H_2O_2 -vanadium complex-pyrazine-2-carboxylic acid'. Part 4. Oxidation of alkanes, benzene and alcohols by an adduct of H_2O_2 with urea**

Georgiy B. Shul'pin and Georg Süß-Fink



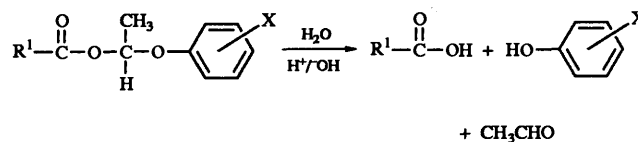
- 1465 **Aerobic oxidation of saturated hydrocarbons into alkyl hydroperoxides induced by visible light and catalysed by a 'quinone-copper acetate' system**

Georgiy B. Shul'pin, Marina M. Bochkova and Galina V. Nizova



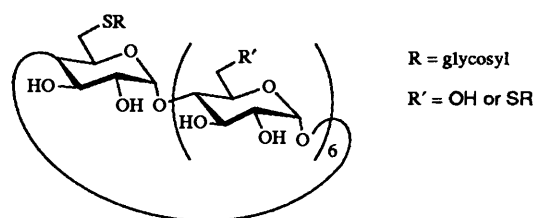
- 1471 **Kinetics and mechanism of the hydrolysis of 1-aryloxyethyl alkanoates**

C. Dennis Hall and Celia W. Goulding

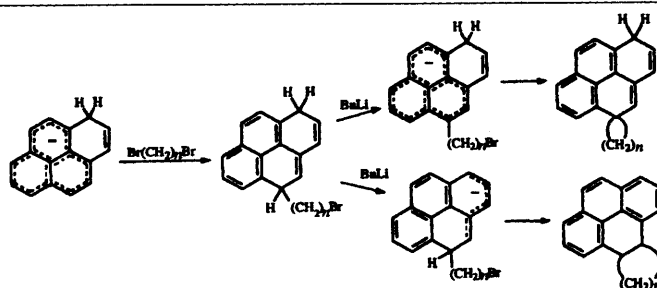


1479 Inclusion and solubilization properties of 6-*S*-glycosyl-6-thio derivatives of β -cyclodextrin

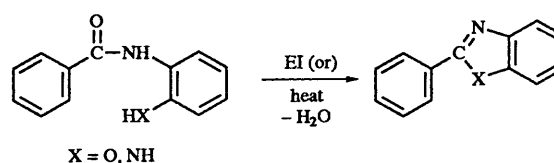
Valérie Lainé, Annie Coste-Sarguet, Andrée Gadelle, Jacques Defaye, Bruno Perly and Florence Djedaini-Pilard

1489 Reactivity of the 1-hydropyrenyl anion towards α,ω -dibromoalkanes

Joost T. M. van Dijk, Johan Lugtenburg and Jan Cornelisse

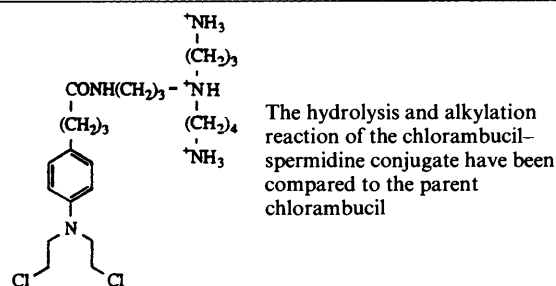
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Devalla V. Ramana and Ethirajulu Kantharaj



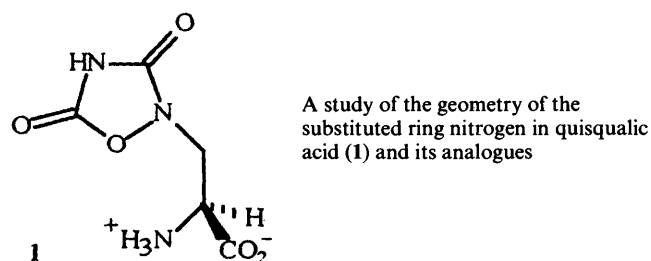
1503 Mechanism and reactivity of chlorambucil and chlorambucil-spermidine conjugate

Paul M. Cullis, Ruth E. Green and Mark E. Malone



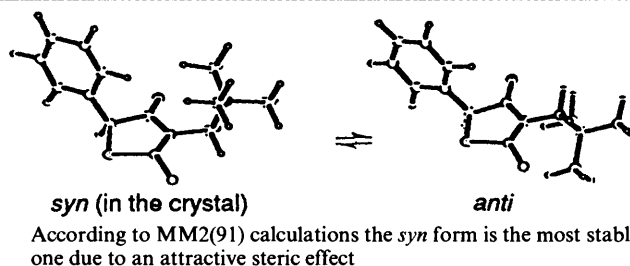
1513 A study of the nitrogen inversion barrier in quisqualic acid and its analogues

Cristina I. De Matteis and David E. Jackson



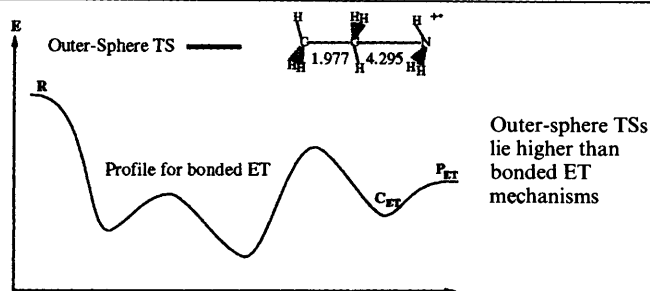
1521 Conformations and conformational changes of 3-isobutyl- and 3-neopentyl-rhodanines. A case of steric attraction studied by X-ray crystallography, NOE effects and force-field calculations

Knut Rang, Fen-Ling Liao, Jan Sandström and Sue-Lein Wang



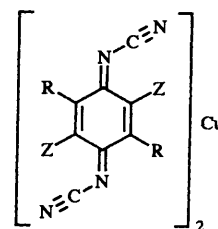
- 1525 **Electron transfer mechanistic manifold and variable transition state character. A theoretical investigation of model electron transfer processes between nucleophiles and ethane cation radical**

A. Chandrasekhar Reddy, David Danovich, Alexander Ioffe and Sason Shaik



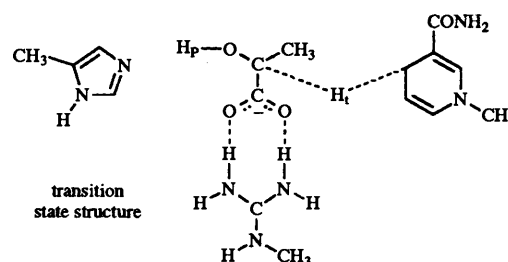
- 1541 **Chemical pressure effect by selective deuteration in the molecular-based conductor, 2,5-dimethyl-*N,N*-dicyano-*p*-benzoquinone diimine-copper salt, (DMe-DCNQI)₂Cu**

Shuji Aonuma, Hiroshi Sawa and Reizo Kato



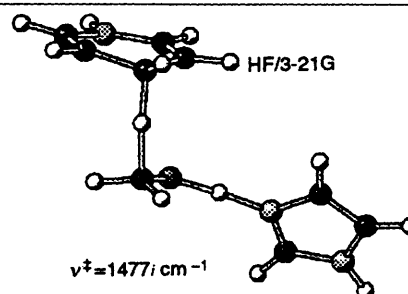
- 1551 **Transition state structures for the molecular mechanism of lactate dehydrogenase enzyme**

J. Andrés, V. Moliner, J. Krechl and E. Silla



- 1559 **Geometrical preferences for general acid-catalysed hydride transfer: comparative theoretical study of transition structures for reduction of formaldehyde**

John Wilkie and Ian H. Williams



Corrigendum

- 1569 **Reaction of diethylaminosulfur trifluoride with diols** Dale F. Shellhamer, D. Timothy Anstine, Kelly M. Gallego, Brian R. Ganesh, Aaron A. Hanson, Kelli A. Hanson, Rodney D. Henderson, Jeanie M. Prince and Victor L. Heasley

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