

## JOURNAL OF THE CHEMICAL SOCIETY

## Perkin Transactions 2

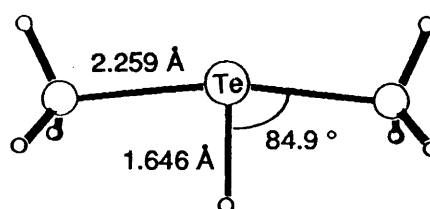
## Physical Organic Chemistry

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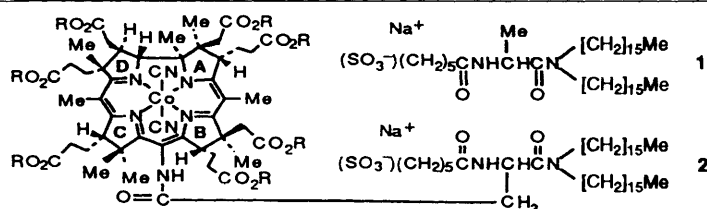
- 2269 On the stability of trivalent chalcogen radicals—a pseudopotential study of homolytic substitution by a methyl radical at methanethiol, methaneselenol and methanetellurol

Bruce A. Smart and Carl. H. Schiesser



- 2271 Isomerization catalysis by hydrophobic vitamin B<sub>12</sub> covalently bound to a lipid species in a bilayer membrane

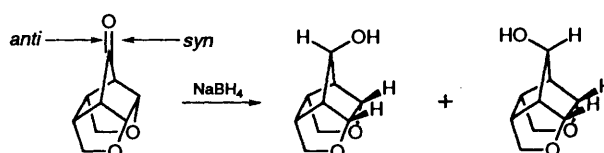
Teruhisa Ohno, Akihiro Ogawa, Yoshio Hisaeda and Yukito Murakami



A novel artificial vitamin B<sub>12</sub> holoenzyme composed of 1 and 2 remarkably enhanced a methylmalonyl-CoA mutase model reaction

- 2275  $\pi$ -Facial diastereoselection in reductions of sterically unbiased ketones containing the norbornyl framework: further tests for theoretical models

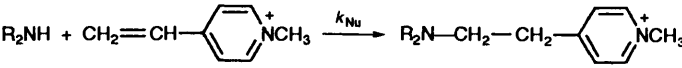
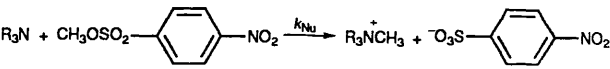
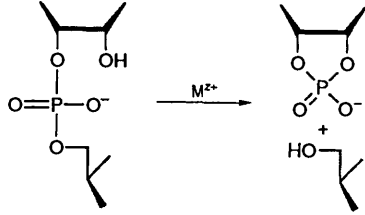
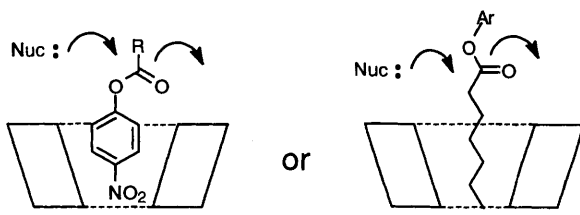
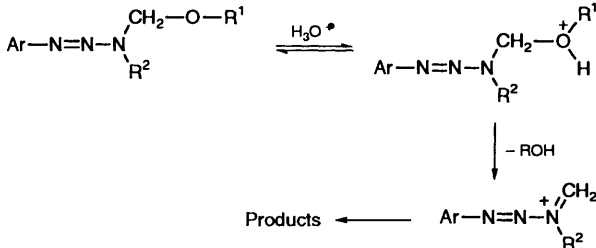
Goverdhan Mehta, Faiz Ahmed Khan, Biswajit Ganguly and Jayaraman Chandrasekhar



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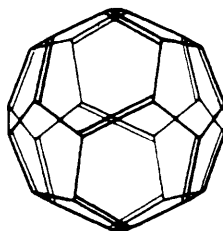
*endo*-Bridged norbornanones exhibit *syn*-selectivity which has been probed using MNDO and *ab initio* calculations

## Articles

<p>2279 <b>Nucleophilicity towards a vinylic carbon atom: rate constants for the addition of amines to the 1-methyl-4-vinylpyridinium cation in aqueous solution</b></p> <p>Christina K. M. Heo and John W. Bunting</p>	 <p>The addition of primary and secondary amines to the 1-methyl-4-vinylpyridinium cation is a suitable reference reaction for the definition of <math>N_+</math> parameters for amines in aqueous solution</p>
<p>2291 <b>Nucleophilicity towards a saturated carbon atom: rate constants for the aminolysis of methyl 4-nitrobenzenesulfonate in aqueous solution. A comparison of the <math>n</math> and <math>N_+</math> parameters for amine nucleophilicity</b></p> <p>John W. Bunting, Jacqueline M. Mason and Christina K. M. Heo</p>	 <p>Second-order rate constants for the aminolysis of methyl 4-nitrobenzenesulfonate correlate with second-order rate constants for the addition of amines to the 1-methyl-4-vinylpyridinium cation and demonstrate a linear relationship between <math>n</math> and <math>N_+</math> for amine nucleophiles in aqueous solution: <math>N_+ = 2.1n - 4.3</math></p>
<p>2301 <b>Metal-ion-promoted hydrolysis of polyuridylic acid</b></p> <p>Satu Kuusela and Harri Lönnberg</p>	
<p>2307 <b>Acyl transfer mediated by complexation. The effect of cyclodextrins on the reaction of nucleophiles with <math>p</math>-nitrophenyl acetate and hexanoate</b></p> <p>Oswald S. Tee and Timothy A. Gadosy</p>	
<p>2313 <b>Triazene drug metabolites. Part 14. Kinetics and mechanism of the acid-catalysed hydrolysis of 3-alkoxymethyl-3-alkyl-1-aryltriazenes</b></p> <p>Leonor Fernandes, Ana Paula Francisco, Jim Iley and Eduarda Rosa</p>	

2319 **Bond-stretch isomerism and the fullerenes**

Sarah J. Austin, Jon Baker, Patrick W. Fowler and David E. Manolopoulos



K2

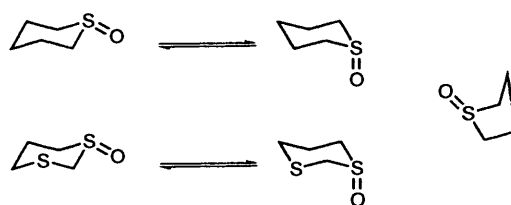
Fullerenes may have multiple totally symmetric Kekulé structures and hence may exhibit bond-stretch isomerism

2325 **Reaction of gaseous sulfur mustard with zeolite 13X**

Anthony J. Bellamy

Interaction of gaseous sulfur mustard with zeolite 13X, both dried and impregnated with H<sub>2</sub>O and various amines has been studied; the dried zeolite exhibited the highest absorption/reaction capacity2329 **Conformational analysis. Part 23. A lanthanide-induced shift investigation of some cyclic and acyclic sulfoxides**

Raymond J. Abraham, Leonard Pollock and Fernando Sancassan

2337 **The hydrogen bonding of alcohols, cholesterol and phenols with cyanate and azide ions**

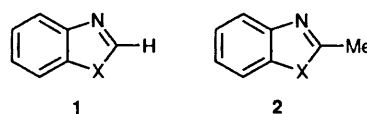
Pawel Goralski, Michel Berthelot, Jean Rannou, Didier Legoff and Martial Chabanel



Cyanate and azide anions as probes for measuring hydrogen bonding acidities

2341 **Gas phase basicities of 1,3-benzazoles: benzimidazole, benzoxazole, benzothiazole, benzoselenazole and benzotellurazole**

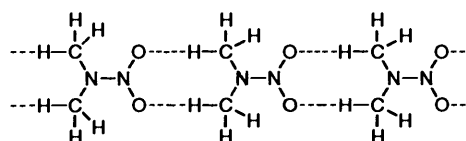
Rafael Notario, Marta Herreros, Emilio Ballesteros, M'hamed Essefar, José-Luis M. Abboud, Igor D. Sadekov, Vladimir I. Minkin and José Elguero



The gas-phase basicities of the above compounds have been determined and discussed using semiempirical PM3 calculations

2345 **C-H...O hydrogen bond patterns in crystalline nitro compounds: studies in solid-state molecular recognition**

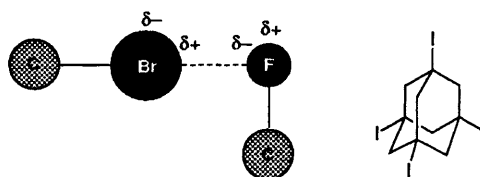
C. V. Krishnamohan Sharma and Gautam R. Desiraju



Nitro groups in organic crystals form several C-H...O hydrogen bond patterns which have been studied with data from the Cambridge Structural Database

- 2353 **The nature of halogen . . . halogen interactions and the crystal structure of 1,3,5,7-tetraiodoadamantane**

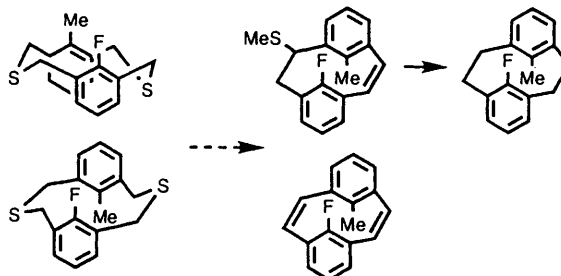
V. R. Pedireddi, D. Shekhar Reddy, B. Satish Goud, Donald C. Craig, A. David Rae and Gautam R. Desiraju



The presence of unsymmetrical halogen . . . halogen contacts demonstrate the importance of polarisability in these interactions and I . . . I interactions are present in an unusual twinned crystal structure of 1,3,5,7-tetraiodoadamantane

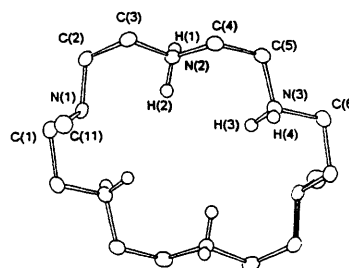
- 2361 **Synthesis, properties and conformational studies of *anti*-8-fluoro-16-methyl[2,2]metacyclophane and *anti*-8-fluoro-16-methyl[2,2]metacyclophane-1,9-diene**

Yee-Hing Lai and Zhao-Lin Zhou



- 2367 **1,10-Dimethyl-1,4,7,10,13,16-hexaazacyclooctadecane L and 1,4,7-trimethyl-1,4,7,10,13,16,19-heptaazacycloheicosane L1: two new macrocyclic receptors for ATP binding. Synthesis, solution equilibria and the crystal structure of (H<sub>4</sub>L)(ClO<sub>4</sub>)<sub>4</sub>**

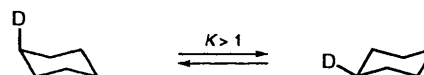
Antonio Andrés, Carla Bazzicalupi, Andrea Bencini, Antonio Bianchi, Vieri Fusi, Enrique Garcia-España, Claudia Giorgi, Nicoletta Nardi, Piero Paoletti, José Antonio Ramirez and Barbara Valtancoli



The title polyazamacrocycles are good receptors for binding ATP anions in solution. Comparison with some other analogous ligands shows selective ATP recognition by L. The crystal structure of (H<sub>4</sub>L)(ClO<sub>4</sub>)<sub>4</sub> shows that in spite of the electrostatic repulsion between positive charges, all the ammonium groups of H<sub>4</sub>L<sup>4+</sup> converge inside the macrocyclic cavity

- 2375 **<sup>13</sup>C, <sup>2</sup>H coupling constants and <sup>2</sup>H-induced <sup>13</sup>C NMR isotope chemical shifts in deuteriated cyclohexanes: application for measurements of conformational equilibrium isotope effects**

Vasiliy A. Uvarov, Vyacheslav A. Chertkov and Nickolai M. Sergeev



Shift of the equilibrium towards the conformer with equatorial deuterium leads to a small but significant increase of the averaged <sup>13</sup>C, <sup>2</sup>H vicinal coupling constant by ca. 3 mHz

## Corrigenda

- 2379 **Ring opening of a formal cyclopentylmethyl radical in the thermolysis of di(*tert*-alkyl)(1-norbornyl)methanols** John S. Lomas and Sylvette Briand
- 2379 **Rotational isomerism of disubstituted benzenes in the alkylphenyldi(1-adamantyl)methanol series** John S. Lomas and Veronique Bru-Capdeville

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

## Forthcoming Articles in *Perkin Transactions 2*

Kinetics and mechanism of the addition of triphenylphosphoniocyclopentadienide to tetrahalogeno-*p*-benzoquinones. Part 4. The substitution reactions of fluoranil **F. P. Pla, C. D. Hall, P. Speers and J. Palou**

Kinetics and equilibria of reactions between acetic anhydride and substituted phenolate ions in aqueous and chlorobenzene solutions **S. A. Ba-Saif, A. B. Maude and A. Williams**

Factors affecting rates of thermal decomposition of 5-azidopyrazoles: a comparison with other aromatic azides **G. L'abbé, L. Dyall, K. Meersman and W. Dehaen**

*N,N*-Coupled heterobicycles from cyclic hydrazine derivatives. Part 7. Investigations on the synthesis and structures of 1-(*N'*,*N'*-alkanediylcarbamimidoyl)pyrazolidine derivatives **O. Morgenstern, M. Ahlgrén J. Vepsäläinen, P. H. Richter and P. Vainiotalo**

Investigations on diastereoisomeric tetraorganotin compounds: the use of <sup>119</sup>Sn NMR spectroscopy for the direct determination of the diastereoisomeric composition **J. Klein, S. Neels and R. Borsdorf**

The effects of β-alkoxy substituents on radical reactions: halogen-atom abstraction from alkyl chlorides **B. P. Roberts and A. J. Steel**

The EPR spectrum of the dibenzo[*b,h*]biphenylene radical anion and cation: the pairing principle and the Mills-Nixon effect **A. G. Davies, G. Gescheidt, K. M. Ng and M. K. Shepherd**

Flavocyclodextrins as artificial redox enzymes. Part 4. Catalytic reactions of alcohols, aldehydes and thiols **H. Ye, W. Tong and V. T. D'Souza**

Solvato- and halo-chromic behaviour of some 4-[(*N*-methylpyridinium)methylideneamino]phenolate dyes **C. Machado, M. da Graça Nascimento and M. C. Rezende**

One- and two-electron reduction potentials of peroxy radicals and related species **G. Merényi, J. Lind and L. Engman**

The relevance of third-derivative cross interaction coefficients in Hammett-type treatments of nucleophilic substitution reactions **D. N. Kevill and M. J. D'Souza**

Solvent independent transition-state structures. Part III. Sulfonyl transfer reactions **R. M. Tarkka, W. K. C. Park, P. Liu, E. Bunce and S. Hoz**

Photoinduced electron transfer reactions of chloranil with benzodioxoles **B.-Z. Yan, Z.-G. Zhang, H.-C. Yuan, L.-C. Wang and J.-H. Xu**

Semiempirical study of the solvent effect on the Menshutkin reaction **U. Maran, T. A. Pakkanen and M. Karelson**

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**

Keto-enol tautomerism of phenacylpyrazine: acid catalysis with protonation at nitrogen **A. R. E. Carey, R. A. More O'Ferrall, M. G. Murphy and B. A. Murray**

<sup>1</sup>H and <sup>13</sup>C NMR spectra of α-heterocyclic ketones and assignment of keto, enol and enamino tautomeric structures **R. A. More O'Ferrall and B. A. Murray**

Equilibrium constants for ionisation and enolisation of 2-phenylacetyl furan **A. Fontana and R. A. More O'Ferrall**

Structural studies on some 1,3,4-thiadiazolium-2-aminides and their rearrangement isomers using <sup>15</sup>N and <sup>13</sup>C NMR **C. A. Montanari, J. P. B. Sandall, Y. Miyata and J. Miller**

Attractive interactions between an alkyne group and two carbonyl oxygen atoms: the crystal and molecular structure of 2,2'-ethynylenedibenzoic acid at 150 K **M. Pilkington, S. Tayyip and J. D. Wallis**

Reactivity of 1-iodoadamantane with carbonions by the S<sub>RN</sub>1 mechanism **R. A. Rossi, A. B. Pierini and G. L. Borosky**

*Ab Initio* studies on organophosphorus compounds. Part 3. Cationic calcium binding to phosphonate and phosphinate monoanions and their sulfur analogues **J. P. Räsänen, E. Pohjala and T. A. Pakkanen**

Naphthalene photocatalysed decomposition of chlorobenzenes in exciplex forming systems **C. A. Chesta, V. Avila, A. T. Soltermann, C. M. Previtali and J. J. Cosa**

Kinetic and thermodynamic investigation of the aluminium-anthocyanin complexation in aqueous solution **O. Dangles, M. Elhabiri and R. Brouillard**