

## JOURNAL OF THE CHEMICAL SOCIETY

## Perkin Transactions 2

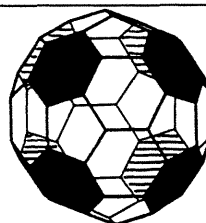
## Physical Organic Chemistry

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## Perkin Communications

- 275 **Is aromaticity a useful concept for  $C_{60}$  and its derivatives? Aromatisation of  $C_{60}$  by regioselective addition**

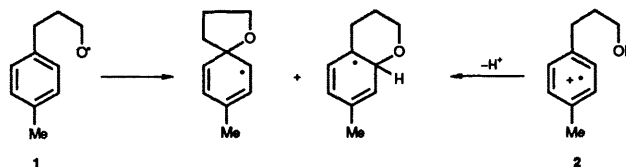
Patrick W. Fowler, David J. Collins and Sarah J. Austin



Aromatisation of  $C_{60}$  may be an important factor driving regioselective addition

- 279 **Cyclisation of 3-(*p*-methylphenyl)propan-1-ol via its alkoxy radical and aryl radical cation intermediates. A comparison of regioselectivities**

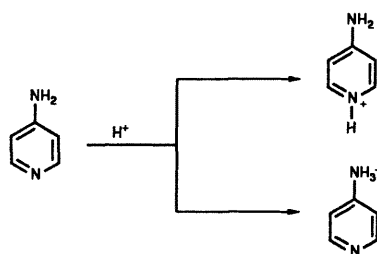
André Goosen, Cedric W. McClelland and Fabrizio C. Rinaldi



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- 283 **A novel method for the determination of ionization sites in polyfunctional acids and bases by NMR relaxation rate measurements**

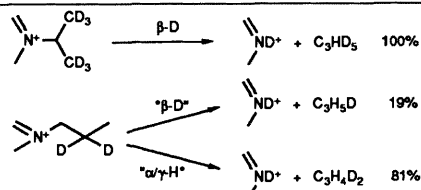
Alessandro Bagno, Clara Comuzzi and Gianfranco Scorrano



Alternative sites of ionization have been probed by NMR relaxation rates

- 285 **The mechanism of propene elimination from the immonium ions  $CH_2=N^+(CH_3)CH(CH_3)_2$  and  $CH_2=N^+(CH_3)CH_2CH_2CH_3$**

Richard D. Bowen, Alex W. Colburn and Peter J. Derrick

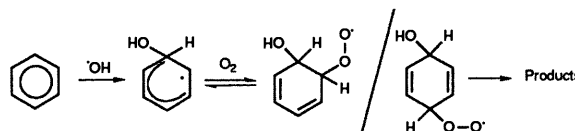


Propene loss from  $CH_2=N^+(CH_3)CH(CH_3)_2$  involves specific  $\beta$ -H transfer, but the corresponding fragmentation of  $CH_2=N^+(CH_3)CH_2CH_2CH_3$  involves mainly  $\alpha$ - and  $\gamma$ -H transfer

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- 289 **Oxidation of benzene by the OH radical. A product and pulse radiolysis study in oxygenated aqueous solution**

Xian-Ming Pan, Man Nien Schuchmann and Clemens von Sonntag



- 299 **Hydrogen bonding. Part 25. The solvation properties of methylene iodide**

Michael H. Abraham, Jenik Andonian-Haftvan, Juliet P. Osei-Owusu, Panos Sakellariou, José S. Urieta, María C. López and Richard Fuchs

Analysis of Ostwald solubility coefficients for 37 solvents on  $\text{CH}_2\text{I}_2$  at 298 K by the solvation equation of Abraham shows that solvation of solutes is aided only weakly by solvent polarisability, but more so by solvent hydrogen-bond acidity and basicity

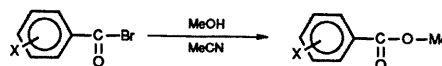
- 305 **Hydrogen bonding. Part 26. The calorimetric acidity scale of Laynez**

Michael H. Abraham and Robert W. Taft

The calorimetric acidity scale of Laynez can be used to obtain bulk solvent hydrogen bond acidities, as  $\alpha_1$  values

- 307 **Nucleophilic substitution at a trigonal carbon. Part 5. Substituent effects in the reactions of aromatic acyl bromides with methanol in acetonitrile**

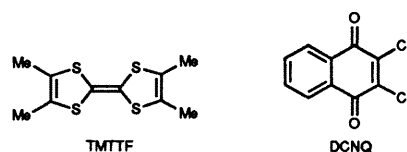
Dennis N. Kevill and (the late) Donald C. Knauss




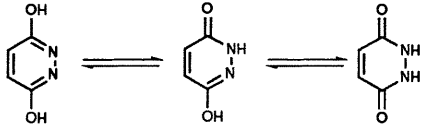
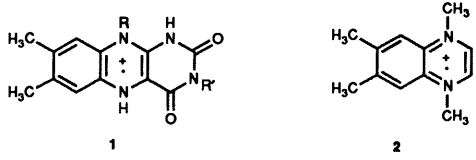
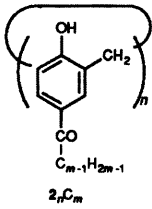
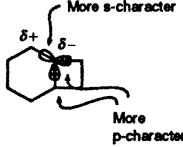
Simultaneously operating overall second- and third-order kinetic schemes are each analysed in terms of two competing reaction channels

- 313 **Studies on  $\pi$ -acceptor molecules containing the dicyanomethylene group. X-Ray crystal structure of the charge-transfer complex of tetramethyltetraathiafulvalene and 2,3-dicyano-1,4-naphthoquinone:  $(\text{TMTTF})_3^+-(\text{DCNQ})_2^-$**

Andrei S. Batsanov, Martin R. Bryce, Stephen R. Davies, Judith A. K. Howard, Roger Whitehead and Brian K. Tanner

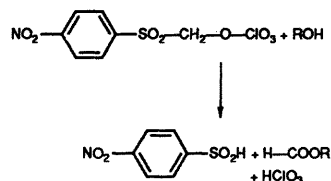


A range of new  $\pi$ -electron acceptor molecules based on 2-dicyanomethyleneindane-1,3-dione and 2,3-dicyano-1,4-naphthoquinone (DCNQ) have been studied

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<p>337 <b>Highly electrophilic heteroaromatics: the hydrolysis of 7-chloro-4,6-dinitrobenzofurazan and 7-chloro-4,6-dinitrobenzofuroxan in aqueous solution</b></p> <p>François Terrier, Lan Xiao, Miloudi Hlaibi and Jean-Claude Halle</p>	<p>Catalysis of the hydrolysis of highly electrophilic 7-chloro-4,6-dinitrobenzofurazan by carboxylate anions and water occurs <i>via</i> a concerted mechanism. However, the transition states for the water reactions are destabilized by important electrostatic effects</p>
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<p>347 <b>Molecular design and characterizations of new calixarene-based gelators of organic fluids</b></p> <p>Masayoshi Aoki, Kazuaki Nakashima, Hirosuke Kawabata, Satoru Tsutsui and Seiji Shinkai</p>	 <p>2, C<sub>m</sub></p> <p>(n, m) = (4, 18), (8, 12), (8, 18)</p> <p>Gel formation mechanism: C=O...HO hydrogen bonding interaction</p>
<p>355 <b>Electron paramagnetic resonance spectra of some benzocyclobutenes, benzocyclopentenes and benzocyclohexenes</b></p> <p>D. V. Avila, A. G. Davies, E. R. Li and K. M. Ng</p>	 <p>More s-character</p> <p>More p-character</p> <p>Rehybridisation of the bridgehead carbon atoms stabilises the <math>\psi_s</math> MO</p>

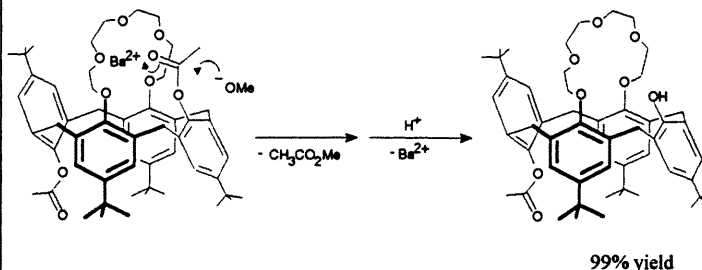
- 363 **Analysis of the kinetics of solvolysis of *p*-nitrophenylsulfonylmethyl perchlorate in binary alcoholic mixtures in terms of the thermodynamic properties of the solvent mixtures**

Jan W. Wijnen, Jan B. F. N. Engberts and Michael J. Blandamer



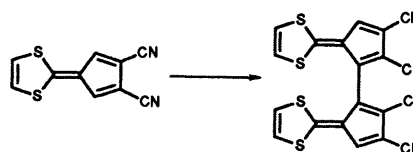
- 369 **Barium(II)-ion assisted monodeacetylation of partial-cone calix[4]arene-crown-5 diacetate. A convenient preparation of partial-cone calix[4]arene-crown-5 monoacetate**

R. Cacciapaglia, A. Casnati, L. Mandolini, S. Schiavone and R. Ungaro



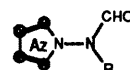
- 373 **Preparation, crystal and molecular structure and properties of 5,5'-bis-(1,3-dithiol-2-ylidene)[bicyclopenta-1,3-dien-1-yl]-2,2',3,3'-tetracarbonitrile**

David Nalewajek, Matthew H. Luly, Martin L. Kaplan, Melvyn R. Churchill, Joseph Ziller and Peter M. Schaber



- 377 **The structure of *N*-(azol-*N*-yl)formamides: a crystallographic and dynamic NMR spectroscopy study**

L. Salazar, M. Espada, D. Sanz, R. M. Claramunt, J. Elguero, S. García-Granda, M. Rosario Diaz and F. Gomez-Beltrán



1, R = H, Az = pyrazol-1-yl; 2, R = Me, Az = pyrazol-1-yl; 3, R = Bz, Az = pyrazol-1-yl; 4, R = H, Az = 1,2,4-triazol-4-yl; 5, R = H, Az = indazol-1-yl; 6, R = H, Az = indazol-2-yl

Some representative molecular structures (1, 5) and rotational barriers about the amide bond (1, 3, 4, 5) have been determined

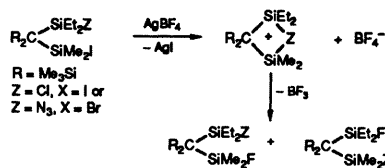
- 385 **Cyclotrimerization of aliphatic aldehydes catalysed by Keggin-type heteropoly acids and concomitant phase separation**

Satoshi Sato, Hiromi Furuta, Toshiaki Sodesawa and Fumio Nozaki

Keggin-type heteropoly acids catalyse the cyclotrimerization of aliphatic aldehyde to 2,4,6-trialkyl-1,3,5-trioxane accompanied by spontaneous phase separation into two phases, catalyst and product phase

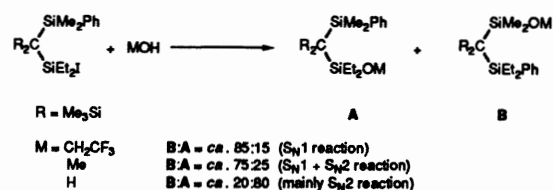
- 391 **1,3-Migration of chloride and azide ligands in reactions of highly sterically hindered organosilicon halides**

Colin Eaborn, Paul D. Lickiss and Sabah T. Najim



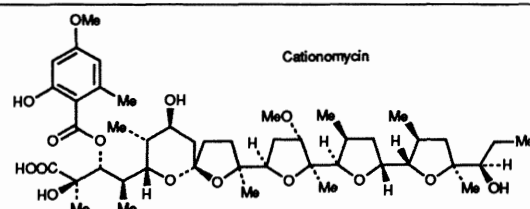
395 **Proportion of 1,3-phenyl migration in trifluoroethanolysis, methanolysis, and hydrolysis of  $(\text{Me}_3\text{Si})_2\text{C}(\text{SiMe}_2\text{Ph})(\text{SiEt}_2\text{I})$**

Colin Eaborn, Karen L. Jones, Paul D. Lickiss and Włodzimierz A. Stańczyk



399 **Conformation in solution of carboxylic ionophore cationomycin: acid form and  $\text{Li}^+$ ,  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Rb}^+$ ,  $\text{Cs}^+$ ,  $\text{NMe}_4^+$  complexes**

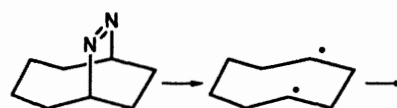
Gérard Dauphin, Georges Jeminet and Françoise Vaufrey



Very similar globular conformations are observed by NMR spectroscopy for the title compounds

405 **Deazetation of a bicyclic azo compound: product and mechanistic studies**

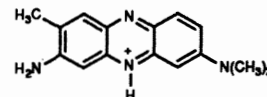
Christopher J. Samuel



It is argued that the product distribution from cyclo-octanediyl may be derived from two singlet and one triplet state of the biradical

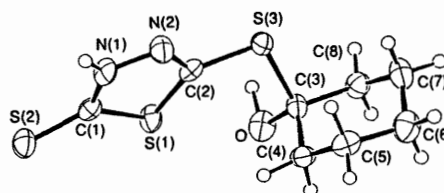
409 **Redox reactions of neutral red. A pulse radiolysis study**

Shambu N. Guha, Pervaje N. Moorthy and Jai P. Mittal



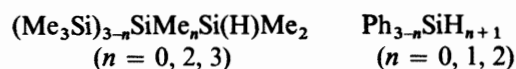
417 **Synthesis, crystal and molecular structure, and spectroscopic characterization of 5-(1-hydroxycyclohexylthio)-1,3,4-thiadiazole-2-thione**

Luciano Antolini, Andrea Cornia, Antonio C. Fabretti and Luisa Schenetti



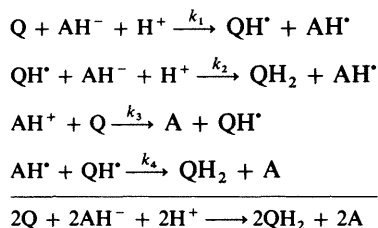
421 **Organosilanes as radical-based reducing agents with low hydrogen donating abilities**

Marco Ballestri, Chrystostomos Chatgialloglu, Maurizio Guerra, Andrea Guerrini, Marco Lucarini and Giancarlo Seconi



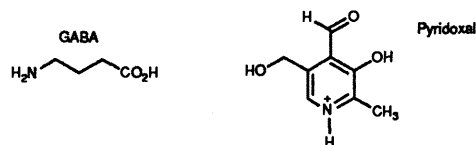
- 427 **Reduction kinetics of 2,3-dimethoxy-5-methyl-1,4-benzoquinone by ascorbic acid in acid solution**

Maria Constanza Soriano Cano and Juan Vera Sanchez



- 431 **Transamination of  $\gamma$ -aminobutyric acid; a semiempirical molecular orbital study of the transaminase mechanism**

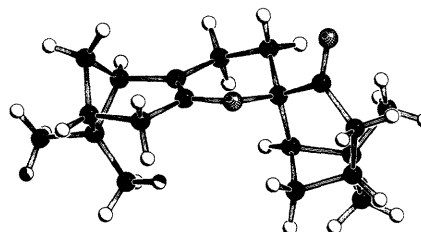
Tracy L. Nero, Magdy N. Iskander and Margaret G. Wong



A semiempirical molecular orbital study of the GABA-T mechanism and evaluation of the role of the PLP ring nitrogen

- 437  **$^{13}\text{C}$  NMR chemical shift assignment based on  $^{13}\text{C}$  INADEQUATE and heteronuclear  $^{13}\text{C}$ ,  $^1\text{H}$ -COSY experiments and absolute configuration of a new chiral pentacyclic pinocarovone dimer**

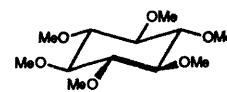
Erkki Kolehmainen, Kari Rissanen, Katri Laihia, Petteri Malkavaara, Jorma Korvola and Reijo Kauppinen



Pinocarovone dimer  $\text{C}_{20}\text{H}_{28}\text{O}_2$

- 441 **The six eclipsed sidechains in *scyllo*-inositol hexamethyl ether. A molecular mechanics study**

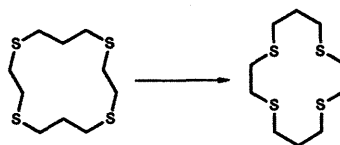
J. Edgar Anderson



Each exocyclic bond is calculated (MM3) to be eclipsed, and further eclipsed examples are found from calculations of stereoisomers

- 445 **Electronic properties of free and coordinating polythioether macrocycles. A spectroscopic and computational analysis**

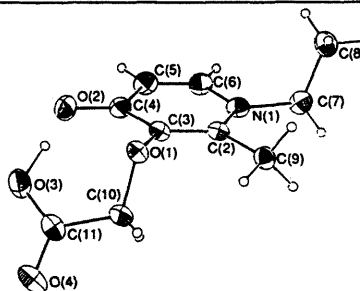
Marcus C. Durrant, Raymond L. Richards and Steven Firth



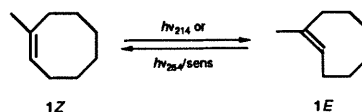
Variations in electronic properties with conformation are investigated

- 451 **Study of hydrogen bonding in 1-ethyl-2-methyl-4-oxo-1,4-dihydropyridin-3-yloxyethanoic acid and 3-(1,2-diethyl-4-oxo-1,4-dihydropyridin-3-yloxy)propanoic acid by  $^1\text{H}$  NMR spectroscopy and X-ray crystallography**

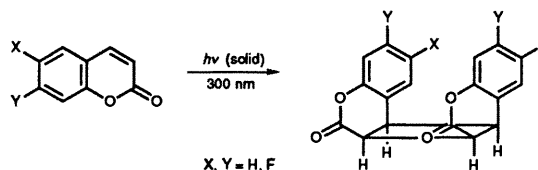
Paul S. Dobbin, Robert C. Hider, Safia K. Rizvi, Kim L. Maki and Dick van der Helm



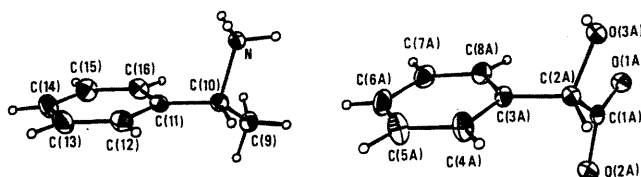
1-Ethyl-2-methyl-4-oxo-1,4-dihydropyridin-3-yloxyethanoic acid forms an unprecedented eight-membered chelate ring by very strong hydrogen bonding

457 **Direct and sensitized geometrical photoisomerization of 1-methylcyclooctene**

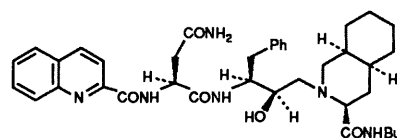
Hiroshi Tsuneishi, Yoshihisa Inoue, Tadao Hakushi and Akira Tai

463 **Crystal engineering: fluorine as a new steering group**

V. Amarendra Kumar, Noor Shahina Begum and K. Venkatesan

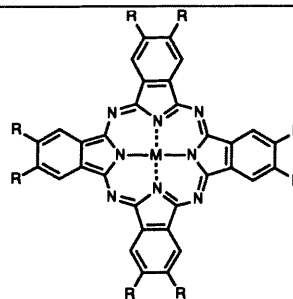
469 **Isolation of different enantiomers caused by variation in the stoichiometric ratio of racemate and resolving agent. The crystal structure of (*R*)-1-phenylethylammonium (*S*)-mandelate-dimandelic acid**

Sine Larsen and Heidi Lopez de Diego

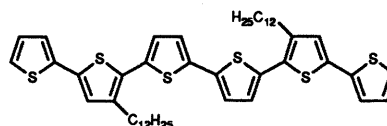
475 **NMR studies of four isomers of decahydroisoquinoline-3(*S*)-carboxylic acid and a potent HIV proteinase inhibitor incorporating the (*S,S,S*) isomer**

HIV proteinase inhibitor Ro 31-8959; solution conformation investigated by NMR spectroscopy

Jenny C. Gilbert, Sally Redshaw, Heather S. Simmonite, W. Anthony Thomas and Ian W. A. Whitcombe

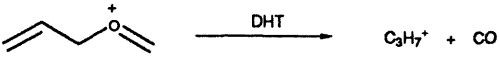
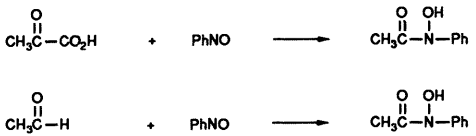
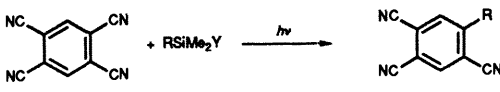
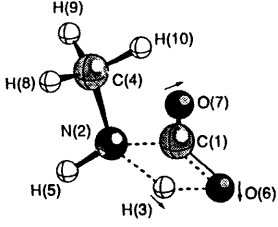
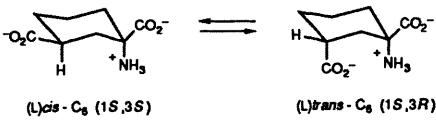
481 **Photochemical stability of various porphyrins in solution and as thin film electrodes**

Abdol Khezer Sobbi, Dieter Wöhrle and Derck Schlettwein

489 **Synthesis and structural characterization of alkyl oligothiophenes—the first isomerically pure dialkylsexithiophene**

Regioselective synthesis and definitive structural assignment of a didodecyl sexithiophene and representative precursors are described

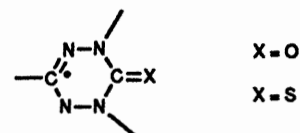
Peter Bäuerle, Frederike Pfau, Helge Schlupp, Frank Würthner, Kai-Uwe Gaudl, Miguel Balparda Caro and Peter Fischer

<p>495 <b>Selective cathodic cleavage of unsymmetrical imidodicarbonates, acylcarbamates and diacylamides</b></p> <p>Hernani L. S. Maia, Luís S. Monteiro, Fredrik Degerbeck, Leif Grehn and Ulf Ragnarsson</p>	$P^1P^2NR + e \longrightarrow P^2NHR$ $P^1, P^2 = R'OCO, R'CO, R'SO_2$ $P^1 \neq P^2$
<p>501 <b>Unimolecular reactions of isolated organic ions: loss of carbon monoxide from the oxonium ion <math>CH_2=CHCH_2^+O=CH_2</math> via double hydrogen transfer</b></p> <p>Richard D. Bowen, Andrew D. Wright and Peter J. Derrick</p>	 <p>Metastable <math>CH_2=CHCH_2^+O=CH_2</math> loses CO via double hydrogen transfer, rather than <math>CH_2O</math> by <math>\sigma</math>-cleavage</p>
<p>509 <b>Reaction of the carbonyl group with nitroso compounds. The cases of pyruvic acid and acetaldehyde</b></p> <p>Stanko Uršić, Viktor Pilepić, Valerije Vrček, Mario Gabričević and Branka Zorc</p>	
<p>515 <b>Photochemical reaction of arenecarbonitriles in the presence of alkylsilanes, silyl ethers and silyl amines</b></p> <p>Mariella Mella, Nicola d'Alessandro, Mauro Freccero and Angelo Albini</p>	 <p><math>Y = Me, OR', OSiMe_3, NMeSiMe_3</math></p> <p>With benzene-1,2,4- and -1,3,5-tricarbonitrile, alkylation occurs at unsubstituted positions</p>
<p>521 <b>A theoretical study of the addition mechanism of carbon dioxide to methylamine. Modelling <math>CO_2</math>-biotin fixation</b></p> <p>Juan Andrés, Vicente Moliner, Jiri Krechl and Estanislao Silla</p>	 <p>The addition reaction of <math>CO_2</math> to <math>MeNH_2</math> which can be considered as a first step for modelling the <math>CO_2</math> biotin fixation, is investigated using an <i>ab initio</i> MO method</p>
<p>525 <b>Conformational analysis of cyclohexane-derived analogues of glutamic acid by X-ray crystallography, NMR spectroscopy in solution, and molecular dynamics</b></p> <p>Nathalie Morelle, Josyane Gharbi-Benarous, Francine Acher, Giovanni Valle, Marco Crisma, Claudio Toniolo, Robert Azerad and Jean-Pierre Girault</p>	 <p>(L)cis-<math>C_6</math> (1S,3S)      (L)trans-<math>C_6</math> (1S,3R)</p>



- 535 **Verdazyls. Part 33. EPR and ENDOR studies of 6-oxo- and 6-thioxoverdazyls. X-Ray molecular structure of 1,3,5-triphenyl-6-oxoverdazyl and 3-tert-butyl-1,5-diphenyl-6-thioxoverdazyl**

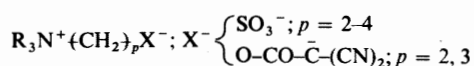
Franz A. Neugebauer, Hans Fischer and Claus Krieger



- 545 **Dielectric increments, interchange distances and conformation of quaternary ammonioalkylsulfonates and alkoxydicyanoethenolates in aqueous and trifluoroethanol solutions**

Monique Galin, Alain Chapoton and Jean-Claude Galin

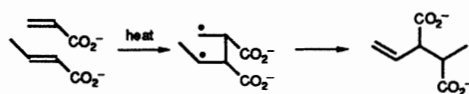
Basicity, dipole moment and conformation of zwitterions of the type



are described

- 555 **Thermal cross-coupled dimerization of sodium acrylate/crotonate and methacrylate/crotonate binary systems in the solid state**

Masaaki Kudoh, Kiyoshi Naruchi, Fumihiko Akutsu and Masatoshi Miura



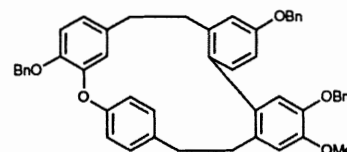
- 559  **$\alpha,\beta$ -Unsaturated enamino-ketones with trifluoromethyl groups. Infrared spectra and structure**

Sergei I. Vdovenko, Igor I. Gerus and Marina G. Gorbunova

Spatial and electronic structure of enamino-ketones  $O=C(R^1)CH=CHNR^2R^3$  (1,  $R^1 = CF_3$ ,  $R^2 = Me$ ,  $R^3 = H$ ; 2,  $R^1 = CF_3$ ,  $R^2 = R^3 = Me$ ) have been discussed on the basis of spectral analysis

- 563 **Determination of the preferred conformation of a macrocyclic bis(bibenzyl) by NMR spectroscopy and molecular mechanics calculations**

Mária Katjár-Peredy, György M. Keser and Mihály Nógrádi



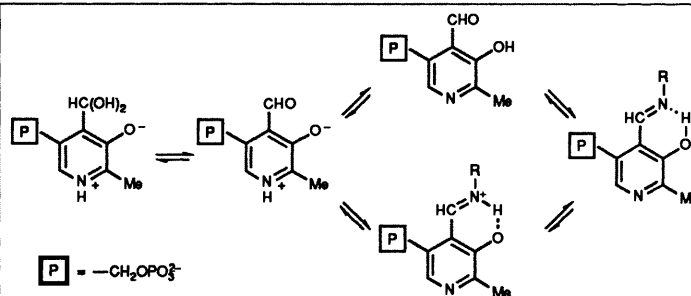
- 567 **Geometry changes of aryl amino groups resulting from changes in electron withdrawal: an *ab initio* molecular orbital study**

David B. Adams



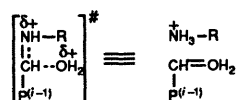
- 573 **A potentiometric study into the stability of the Schiff's base formed between pyridoxal 5'-phosphate and hexylamine in water-dioxane mixtures**

Isabel M. Plaza del Pino and Jose M. Sanchez-Ruiz



- 581 **Kinetics of the formation and hydrolysis of the Schiff's base of pyridoxal 5'-phosphate with hexylamine in water-dioxane**

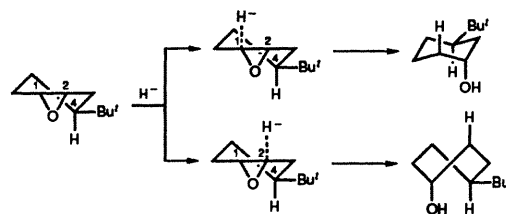
Isabel M. Plaza del Pino, Juan Llor and Jose M. Sanchez-Ruiz



Transition state

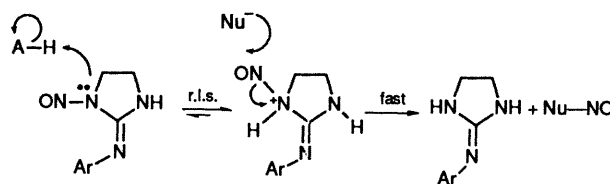
- 585 **Reactive cleavage of epoxides. Molecular mechanics model for regiochemical control of the ring-opening reactions**

Ljiljana I. Došen-Mićović and Bogdan Šolaja



- 591 **N-Nitroso compounds. Part 2. The synthesis of N-nitrosoclonidine and its decomposition in aqueous acidic media**

Jim Iley, Fátima Norberto, Eduarda Rosa and in part, Victor Cardoso and Carlos Rocha



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

