

JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions 2

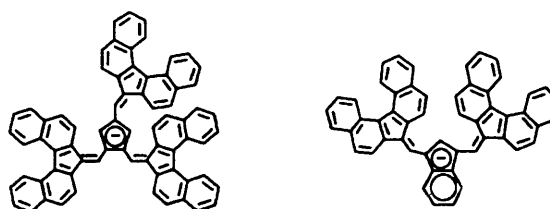
Physical Organic Chemistry

CONTENTS

Perkin Communications

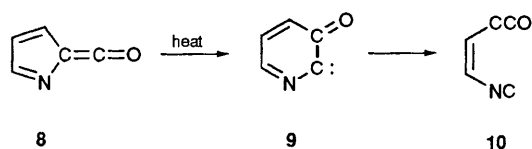
- 165 Hydrocarbon anions with high stability. Part I. Syntheses and properties of extremely stable cyclopentadienide ions with 7*H*-dibenzo[*c,g*]-fluorenylidene methyl substituents

Tomomi Kinoshita, Hiromi Kimura, Iwao Nakajima, Shigeo Tsuji and Ken'ichi Takeuchi



- 169 Theoretical evidence of a singlet α -oxocarbene intermediate in the retro-Wolff rearrangement of azafulvenone

Minh Tho Nguyen, Marie Rose Hajnal and L. G. Vanquickenborne

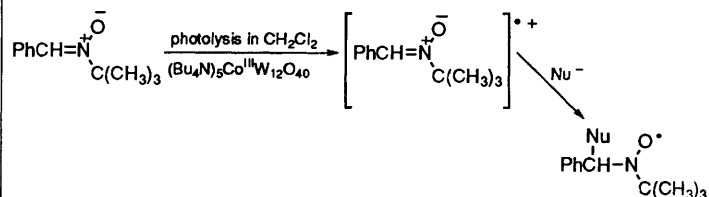


Ab initio calculations suggest the existence of **9** as a shallow potential energy minimum

Articles

- 171 Inverted spin trapping. Part III. Further studies on the chemical and photochemical oxidation of spin traps in the presence of nucleophiles

Lennart Ebersson



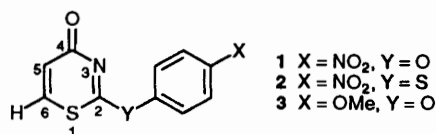
177 Mechanism of dediazonium of arenediazonium salts with triphenylphosphine and trialkyl phosphites. Generation of cation radicals from trivalent phosphorus compounds and their reactions

Shinro Yasui, Masayuki Fujii, Chihiro Kawano, Yukihiro Nishimura, Kosei Shioji and Atsuyoshi Ohno



185 Crystallographic and PM3-COSMO SCF-MO study of the structure and properties of aryloxy- or arylthio-thiazinones

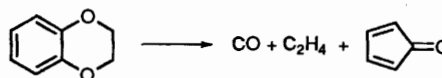
Mark Hilton, Peter Fisk, Barbara Odell, Henry S. Rzepa, David J. Williams and ManYin Yi



A strong C=O...H-C(6) hydrogen bond is observed in the crystal structure of **2** only, which also hydrolyses the fastest, and reveals the lowest calculated σ -type LUMO energy

189 Thermal decomposition of 2,3-dihydro-1,4-benzodioxin and 1,2-dimethoxybenzene

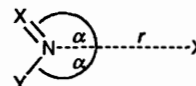
Gerrit-Jan Schraa, Isabel W. C. E. Arends and Peter Mulder



Rate parameters and mechanisms for the unimolecular decomposition between 750 and 900 K are described

199 Prediction of hydrogen bond basicity from computed molecular electrostatic properties: implications for comparative molecular field analysis

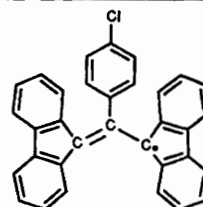
Peter W. Kenny



Electrostatic properties have been computed as functions of r and evaluated as predictors of hydrogen bond basicity for a series of 5- and 6-membered aromatic heterocycles

203 Molecular and crystal structure of 9-[\alpha-(9H-fluoren-9-ylidene)-4-chlorobenzyl]-9H-fluoren-9-yl; an organic antiferromagnet with $T_N = 3.25\text{ K}$

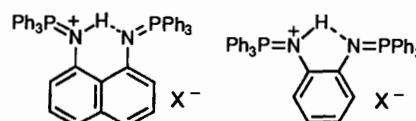
Nagao Azuma, Takehiro Ozawa and Jun Yamauchi



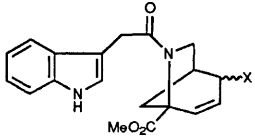
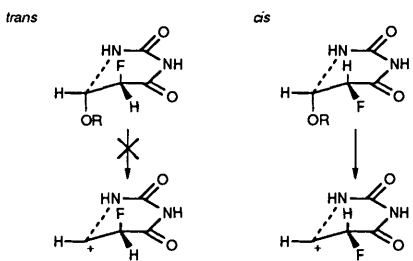
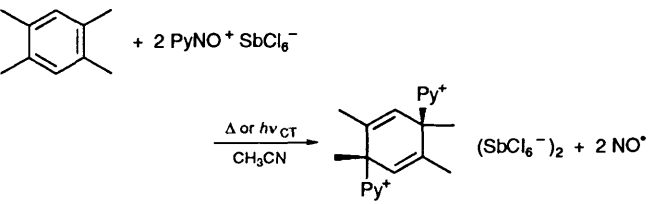
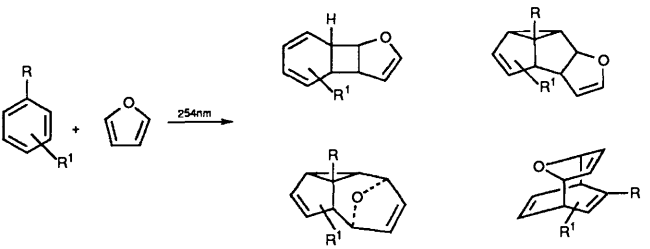
The exchange pathways are discussed based on the crystal structure and π -spin densities on the radical molecule

209 Iminophosphorane-substituted proton sponges. Part 5. Structures in the solid state. Correlation between solid state ³¹P MAS NMR spectra and crystal structures

Antonio L. Llamas-Saiz, Concepción Foces-Foces, José Elguero, Francisco Aguilar-Parrilla, Hans-Heinrich Limbach, Pedro Molina, Mateo Alajarín, Angel Vidal, Rosa Ma. Claramunt and Concepción López

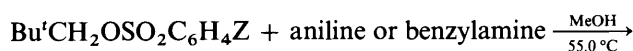


Good agreement between ³¹P MAS NMR results and X-ray structures have been found; the fluorene derivative shows a temperature-dependent exchange process

<p>213 NMR study of 6-azabicyclo[3.2.1]octene derivatives, by-products of catharanthine synthesis</p> <p>Eszter Gács-Baitz, Hedvig Bölcskei and Csaba Szántay</p>	 <p>Reports substituent and steric effects on long range ^{13}C-^1H couplings</p>
<p>219 A unified scale of solvent polarities for specific and non-specific interactions</p> <p>Russell S. Drago, Melissa S. Hirsch, Donald C. Ferris and Chris W. Chronister</p>	<p>The non-specific and specific donor-acceptor interactions of polar acceptor solvents with donor solute probes are included in a unified scale for predicting solvent polarity by using</p> $\Delta\chi = E_A'E_B^* + C_A'C_B^* + S'P + W$
<p>231 Fluorinated pyrimidines. Part 4. Synthesis, properties and stereochemical conversion of the <i>cis</i> and <i>trans</i> isomers of 6-alkoxy-5-fluoro-5,6-dihydrouracils</p> <p>Gerard W. M. Visser, Rinny Wedzinga, Robert P. Klok and Jacobus D. M. Herscheid</p>	 <p>Owing to the poor π-donor ability of the parallel C-F bond, upon substitution, the <i>trans</i> 5-fluoro-5,6-dihydrouracil adduct reacts <i>via</i> an intimate intermediate with inversion of configuration; the <i>cis</i> compound reacts <i>via</i> a solvent-separated intermediate followed by immediate front-side solvent collapse and consequently with retention of configuration</p>
<p>237 Charge-transfer activation of aromatic EDA complexes with <i>N</i>-nitrosopyridinium. Direct comparison with the <i>N</i>-nitrosopyridinium acceptor</p> <p>K. Y. Lee and J. K. Kochi</p>	
<p>247 Influence of arene substituents on the mode and regiochemistry of photocycloaddition of furan to the benzene ring</p> <p>Hermengildo Garcia, Andrew Gilbert and Owain Griffiths</p>	

- 253 **Bimolecular nucleophilic substitution (S_N2) reactions of neopentyl arenesulfonates with anilines and benzylamines in methanol**

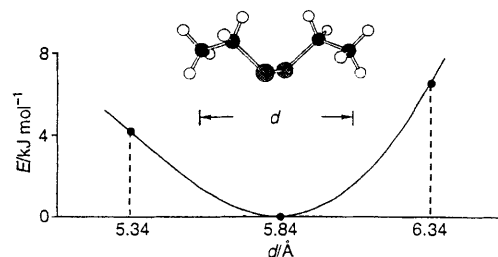
Han Joong Koh, Hai Whang Lee and Ikchoon Lee



Associative S_N2 process with $\rho_{XZ} = 0.30$

- 259 **Conformational properties of disulfide bridges. Part 3. An estimation of structural flexibility from a theoretical study of diethyl disulfide**

Carl Henrik Görbitz



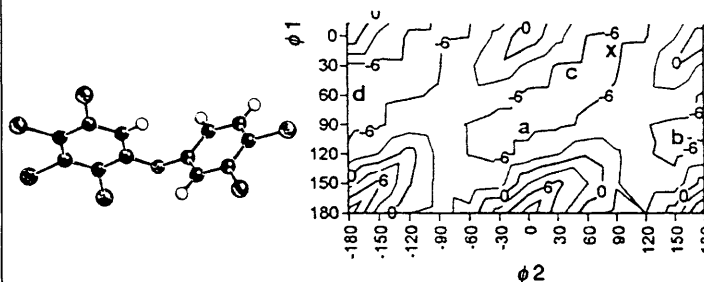
- 265 **Protonation sequence of linear aliphatic polyamines by ^{13}C NMR spectroscopy**

David N. Hague and Anthony D. Moreton

A simple method (based on ^{13}C δ -values) has been used to determine the protonation sites in 21 analytical intermediates formed during the pH titration of eight linear polyamines

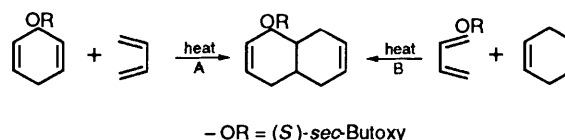
- 271 **AM1 and single-crystal X-ray diffraction study of the conformational properties of chlorinated diphenyl ethers**

Tapio Nevalainen and Kari Rissanen



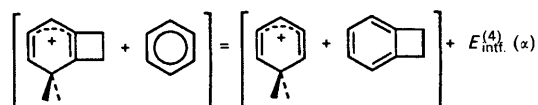
- 281 **A quantum chemical AM1 study of a Diels-Alder and retro-Diels-Alder tandem reaction**

Montserrat Ventura, Cristobal Segura and Miquel Solà

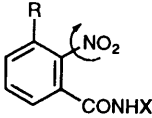
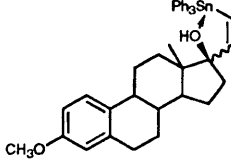
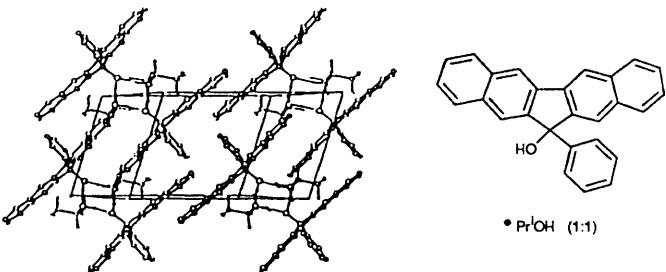
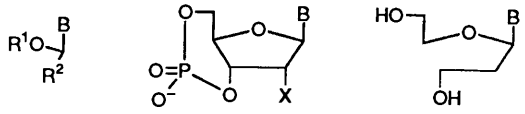
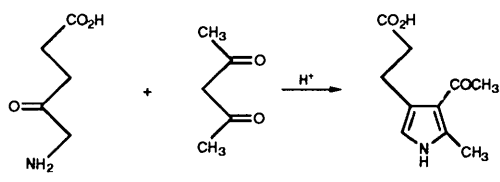
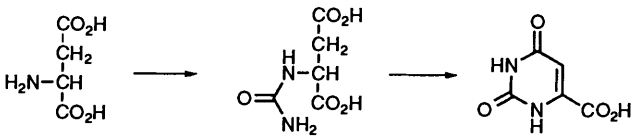


- 285 **Theoretical study of Wheland intermediates in benzocycloalkenes: vindication of the Mills-Nixon hypothesis**

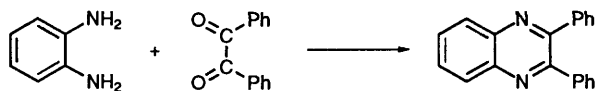
Mirjana Eckert-Maksić, Zvonimir B. Maksić and Martin Klessinger



Antagonistic action of σ and π electrons determines the reactivity difference of α - and β -positions in strained benzocycloalkanes

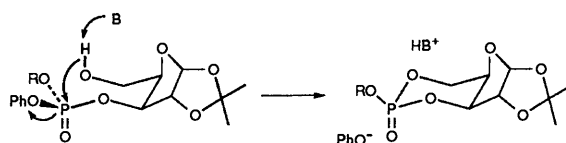
<p>291 Relationships between nitro group reduction potentials and torsion angles in di-ortho-substituted nitrobenzenes; a crystallographic and oxygen-17 NMR study</p> <p>Maruta Boyd, Ho H. Lee, Robert F. Anderson and William A. Denny</p>	 <p>X-ray data on nitroalkylbenzamides (R = H, Me, Et, Prⁱ, Bu^t) show nitro group torsion angles to be over-estimated by ¹⁷O NMR spectroscopy; the relationship between torsion angle and reduction potentials is discussed</p>
<p>297 Characterization by 2D-NMR and chemical properties of (20Z)-3-methoxy-17-[2-(triphenylstanny)vinyl]estra-1,3,5(10)-trien-17β-ol</p> <p>François Kayser, Monique Biesemans, Huade Pan, Marcel Gielen and Rudolph Willem</p>	 <p>The complete solution structure and conformation of (20Z)-3-methoxy-17-[2-(triphenylstanny)vinyl]estra-1,3,5(10)-trien-17β-ol were determined by 2D proton detected ¹H-¹³C HMQC-RELAY, 2D-NOESY build-up and proton detected ¹H-¹¹⁹Sn HMBC 1D and 2D NMR experiments</p>
<p>303 Crystalline alcoholic inclusions of singly-bridged triarylmethanol hosts. Synthesis, X-ray crystal structures and binding modes of five inclusion compounds</p> <p>Ingeborg Csöreg, Olga Gallardo, Edwin Weber and Norbert Dörpinghaus</p>	 <p>• PrⁱOH (1:1)</p>
<p>309 Additional evidence for the exceptional mechanism of the acid-catalysed hydrolysis of 4-oxypyrimidine nucleosides: hydrolysis of 1-(1-alkoxyalkyl)uracils, seconucleosides, 3'-C-alkyl nucleosides and nucleoside 3',5'-cyclic monophosphates</p> <p>Mikko Oivanen, Markku Rajamäki, Jaana Varila, Jari Hovinen, Sergey Mikhailov and Harri Lönnberg</p>	 <p>The effect of the structure on the glycone moiety on the acid-catalysed hydrolysis of 4-oxypyrimidine nucleosides has been studied</p>
<p>315 Mechanism of acid catalysis in the cyclisation of 5-aminovaleric acid and acetylacetone to 3-acetyl-4-(2-carboxyethyl)-2-methylpyrrole</p> <p>Anthony R. Butler and Sharon D. George</p>	
<p>319 Formation of N-carbamoylaspartic acid and its cyclisation to orotic acid</p> <p>Michael J. Bruce, Anthony R. Butler and Kate V. Russell</p>	

323 A mechanistic study of quinoxaline formation



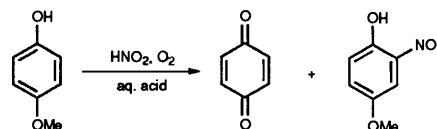
Lesley M. Anderson and Anthony R. Butler

327 Models for enzyme-catalysed phosphate transfer: comparisons of reactivity towards a neighbouring hydroxy group for phosphodiester anions and acids. General base catalysis of the cyclisation of a hydroxyalkyl phosphate triester

5 (R = H or Me) is some 10⁵ times more reactive than 5 (R = O⁻)

Anthony J. Chandler, Florian Hollfelder, Anthony J. Kirby, Fiona O'Carroll and Roger Strömberg

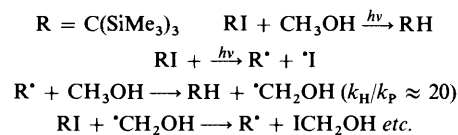
335 Nitration and oxidation of 4-methoxyphenol by nitrous acid in aqueous acid solution



Ben D. Beake, Jill Constantine and Roy B. Moodie

Numerical integrations simulate the observed product ratios and rates on the basis of a proposed radical mechanism

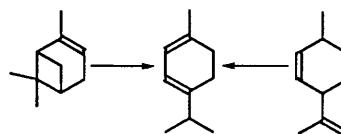
341 Light-catalysed reduction of tris(trimethylsilyl)methyl iodide by alcohols. A radical-chain process showing a large kinetic hydrogen isotope effect



Bruce M. Clark, Colin Eaborn and Duncan A. R. Happer

NaOMe and AgO₃SCF₃ promote reaction by removing radical trap I₂

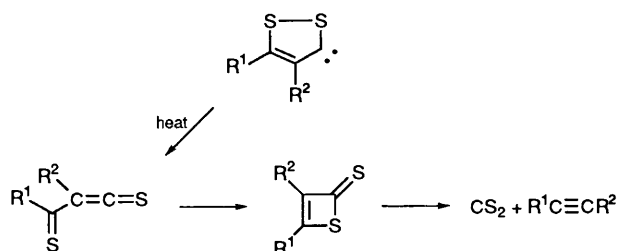
347 Oxidation of terpenes in H-mordenite



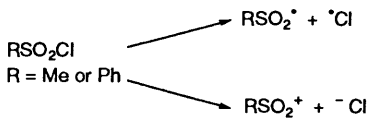
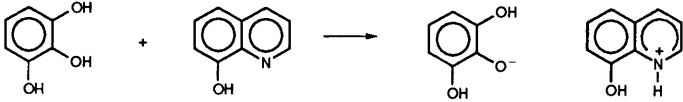
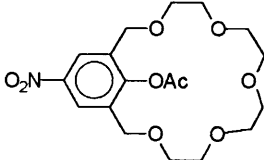
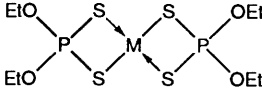
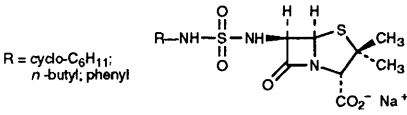
Rowena Crockett and Emil Roduner

The radical cation of α-terpinene was observed after the adsorption of α-pinene and isolimonene onto the zeolite H-mordenite

351 Thioacylthioketenes by pyrolysis of 1,3-dithiethanes and 1,2-dithiole derivatives



C. Oliver Kappe, Carl Th. Pedersen, Jean-Marie Catel and Yves Mollier

<p>357 Sulfur–Chlorine bond dissociation enthalpies in methane- and benzene-sulfonyl chlorides</p> <p>Chrysostomos Chatgililoglu, David Griller, Jolanta M. Kanabus-Kaminska and Fred P. Lossing</p>	 <p style="text-align: center;"> $\text{RSO}_2\text{Cl} \begin{cases} \longrightarrow \text{RSO}_2^+ + \cdot\text{Cl} \\ \longrightarrow \text{RSO}_2^+ + ^-\text{Cl} \end{cases}$ $\text{R} = \text{Me or Ph}$ </p>
<p>361 Study of the reaction between 1,2,3-trihydroxybenzene and 8-hydroxyquinoline in the solid state</p> <p>N. B. Singh, N. P. Singh, V. Amarendra Kumar and M. Nethaji</p>	
<p>367 Alkali-metal ion catalysis and inhibition of acetyl transfer from <i>p</i>-nitroaryl acetates to hexanoate ion</p> <p>Roberta Cacciapaglia, Luigi Mandolini and Alessandra Tomei</p>	 <p style="text-align: right;">2-AcO-5-NO₂-18C5</p> <p>Rates of reaction of 2-AcO-5-NO₂-18C5 with hexanoate ion in DMF are affected by the counterion in the order $\text{K}^+ > \text{Rb}^+ > \text{Cs}^+ > \text{Me}_4\text{N}^+ \approx \text{Na}^+ \gg \text{Li}^+$</p>
<p>373 Phosphorus-31 NMR investigation of the comparative hydrolytic breakdown of nickel(II) and cadmium(II) versus zinc(II) bis(<i>O,O</i>-diethyl dithiophosphates) in an aqueous medium</p> <p>Alan J. Burn, Sharwan K. Dewan, Ian Gosney, Kenneth G. McKendrick, Chris P. Warrens, John P. Wastle and Cameron W. Watson</p>	 <p>Hydrolysis of the complexes $\text{M}[\text{PS}_2(\text{OEt})_2]_2$ occurs by attack of water at the metal centre with cleavage of the M–S bond at different rates</p>
<p>381 Chemical and biological reactivity of sulfamidopenicillins</p> <p>Peter Davern, James Sheehy and Timothy Smyth</p>	 <p>R = cyclo-C₆H₁₁; n-butyl; phenyl</p> <p>Sulfamidopenicillins are similar to benzylpenicillin in terms of chemical (rate of hydrolysis) and conformational (thiazolidine ring flexibility) aspects but differ from benzylpenicillin in being biologically active against <i>S. aureus</i> but not against <i>E. coli</i></p>

Corrigenda

- 389 **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
- 389 **Formation of cyclopropylsulfones from 1-arylsulfonyl-2-chloromethylprop-2-enes** Stephen M. Jeffery and Charles J. M. Stirling

AUTHOR INDEX

- Aguilar-Parrilla, Francisco, 209
Alajarin, Mateo, 209
Anderson, Lesley M., 323
Anderson, Robert F., 291
Arends, Isabel W. C. E., 189
Azuma, Nagao, 203
Beake, Ben D., 335
Biesemans, Monique, 297
Bölskei, Hedvig, 213
Boyd, Maruta, 291
Bruce, Michael J., 319
Burn, Alan J., 373
Butler, Anthony R., 315, 319, 323
Cacciapaglia, Roberta, 367
Catel, Jean-Marie, 351
Chandler, Anthony J., 327
Chatgialoglu, Chrysostomos, 357
Chronister, Chris W., 219
Claramunt, Rosa Ma., 209
Clark, Bruce M., 341
Constantine, Jill, 335
Crockett, Rowena, 347
Csöreg, Ingeborg, 303
Davern, Peter, 381
Denny, William A., 291
Dewan, Sharwan K., 373
Dörpinghaus, Norbert, 303
Drago, Russell S., 219
Eaborn, Colin, 341
Eberon, Lennart, 171
Eckert-Maksić, Mirjana, 285
Elguero, José, 209
Ferris, Donald C., 219
Fisk, Peter, 185
Foces-Foces, Concepción, 209
Fujii, Masayuki, 177
Gács-Baitz, Eszter, 213
Gallardo, Olga, 303
Garcia, Hermengildo, 247
George, Sharon D., 315
Gielen, Marcel, 297
Gilbert, Andrew, 247
Görbitz, Carl Henrik, 259
Goosen, André, 389
Gosney, Ian, 373
Griffiths, Owain, 247
Griller, David, 357
Hague, David N., 265
Hajnal, Marie Rose, 169
Happer, Duncan A. R., 341
Herscheid, Jacobus D. M., 231
Hilton, Mark, 185
Hirsch, Melissa S., 219
Hollfelder, Florian, 327
Hovinen, Jari, 309
Jeffery, Stephen M., 389
Kanabus-Kaminska, Jolanta M., 357
Kappe, C. Oliver, 351
Kawano, Chihiro, 177
Kayser, François, 297
Kenny, Peter W., 199
Kimura, Hiromi, 165
Kinoshita, Tomomi, 165
Kirby, Anthony J., 327
Klessinger, Martin, 285
Klok, Robert P., 231
Kochi, J. K., 237
Koh, Han Joong, 253
Kumar, V. Amarendra, 361
Lee, Hai Whang, 253
Lee, Ho H., 291
Lee, Ikchoon, 253
Lee, K. Y., 237
Limbach, Hans-Heinrich, 209
Llamas-Saiz, Antonio L., 209
Lönnberg, Harri, 309
López, Concepción, 209
Lossing, Fred P., 357
Maksić, Zvonimir B., 285
Mandolini, Luigi, 367
McClelland, Cedric W., 389
McKendrick, Kenneth G., 373
Mikhailov, Sergey, 309
Molina, Pedro, 209
Mollier, Yves, 351
Moodie, Roy B., 335
Moreton, Anthony D., 265
Mulder, Peter, 189
Nakajima, Iwao, 165
Nethaji, M., 361
Nevalainen, Tapio, 271
Nguyen, Minh Tho, 169
Nishimura, Yukihiro, 177
O'Carroll, Fiona, 327
Odell, Barbara, 185
Ohno, Atsuyoshi, 177
Oivanen, Mikko, 309
Ozawa, Takehiro, 203
Pan, Huade, 297
Pedersen, Carl Th., 351
Rajamäki, Markku, 309
Rinaldi, Fabrizio C., 389
Rissanen, Kari, 271
Roduner, Emil, 347
Russell, Kate V., 319
Rzepa, Henry S., 185
Schraa, Gerrit-Jan, 189
Segura, Cristobal, 281
Sheehy, James, 381
Shioji, Kosei, 177
Singh, N. B., 361
Singh, N. P., 361
Smyth, Timothy, 381
Solà, Miquel, 281
Stirling, Charles J. M., 389
Strömberg, Roger, 327
Szántay, Csaba, 213
Takeuchi, Ken'ichi, 165
Tomei, Alessandra, 367
Tsuji, Shigeo, 165
Vanquickenborne, L. G., 169
Varila, Jaana, 309
Ventura, Montserrat, 281
Vidal, Angel, 209
Visser, Gerard W. M., 231
Warrens, Chris P., 373
Wastle, John P., 373
Watson, Cameron W., 373
Weber, Edwin, 303
Wedzinga, Rinny, 231
Willem, Rudolph, 297
Williams, David J., 185
Yamauchi, Jun, 203
Yasui, Shinro, 177
Yi, ManYin, 185

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 of the enolisation reactions of 2-acetylpyrrole and of 2-, 4- and 5-acetylthiazoles **P. de Maria, A. Fontana, M. Arlotta, S. Chimichi and D. Spinelli**

The Honig-Flory-Huggins combinatorial entropy correction - is it valid for aqueous solutions? **M. H. Abraham and P. Sakellariou**

Dioxirane Chemistry. Part 25. The effect of solvent on the dimethyldioxirane carbon-hydrogen bond insertion reaction **R. W. Murray and D. Gu**

Quantitative analysis of solvent effects on the keto-enol equilibrium of pentane-2,4-dione in aqueous solutions **W. Blokzijl, J. B. F. N. Engberts and M. J. Blandamer**

Rotational isomerism of disubstituted benzenes in the alkylphenyldi(1-adamantyl)-methanol series **J. S. Lomas and V. Bru Capdeville**

Solvents effects on chemical processes. 7. Quantitative description of the composition dependence of the solvent polarity measure $E_T(30)$ in binary aqueous-organic solvent mixtures **R. D. Skwierczynski and K. A. Connors**

Characterization of solute-solvent interaction at the transition state by thermodynamic and quantum-mechanical approaches. Reactions of imide ions with ethyl iodide in acetonitrile-methanol
Y. Kondo, O. Nonaka, K. Iwasaki, T. Kuwamoto and T. Takagi

Hydrogen bond basicity of esters, lactones and carbonates
F. Besseau, C. Laurence and M. Bethelot

Hydrogen-bond basicity of nitro-compounds
C. Laurence, M. Berthelot, M. Lucon and D. G. Morris

Volumes of activation for catalysed Diels-Alder reactions
N. S. Isaacs, L. Maksimović and A. Laila

Laser-desorption mass spectrometry of standard polynuclear aromatic hydrocarbons and fullerenes **A. A. Herod, B. J. Stokes, P. Hancock, R. Kandiyoti, J. E. Parker, C. A. F. Johnson, P. John and G. Smith**

Mono[6-(2-mercaptoethylamino)-6-deoxy]- β -cyclodextrin as an efficient glyoxalase mimic
S. Tamagaki, A. Katayama, M. Maeda, N. Yamamoto and W. Tagaki

Synthesis and spectral properties of new fluorescent probes for potassium
R. Crossley, Z. Goolamali, J. J. Gosper and P. G. Sammes

Position of side-chain branching and handedness of turns and helices of homopeptides from chiral C ^{α} -methylated amino acids. Crystal-state structural analysis of (OMe)Leu trimer and tetramer **A. Aubry, D. Bayeul, G. Précigoux, M. Pantano, F. Formaggio, M. Crisma, C. Toniolo, W. H. J. Boesten, H. E. Schoemaker and J. Kamphuis**

Conformational studies of substituted dibenzo-14-crown-4 ethers : a 1D and 2D ¹H and ¹³C NMR investigation **Z. Chen and R. A. Sachleben**

Collision induced dissociations of carbanions in the gas phase: the formation of vinylidene carbene intermediates from deprotonated prop-2-ynyl ethers
S. Dua, J. H. Bowie and J. C. Sheldon

Synthesis and EPR investigations of fluorocatecholamines
H. B. Stegmann, G. Deuschle and P. Schuler

Autoxidation of straight chain hydrocarbons: a product study
A. Goosen and D. H. Morgan

Ab initio SCF and force-field calculations on low-energy conformers of 2-acetylamino-2,N-dimethylpropanamide **C. Alemán and J. Casanovas**

Optical resolution of *trans*-bicyclo[2.2.1]heptane-2,3-diamine: chiral recognition in the crystal of its complex with (2*R*,3*R*)-*O,O'*-dibenzoyltartaric acid
K. Hatano, T. Takeda and R. Saito

Electron transfer photoisomerization of norbornadiene to quadricyclane cosensitized by dibenzoylmethanoboron difluoride and aromatic hydrocarbons
Z-L. Liu, M-X. Zhang, L. Yang, Y-C. Liu, Y. L. Chow and C. I. Johansson

Crystal structure and conformation of pakyonol, a macrocyclic bis(bibenzyl) constituent of *Mannia fragrans* **Z. Böcskei and G. M. Keserű**

Three fundamental mechanisms of base-catalysed reactions of isocyanates with hydrogen-acidic compounds **K. Schwetlick, R. Noack and F. Stebner**

ENDOR and EPR studies of highly isotopically ¹³C-enriched ubiquinone radicals
**R. I. Samoilova, W. van Liemt, W. F. Steggerda, J. Lugtenburg, A. J. Hoff,
A. P. Spoyalov, A. M. Tyryshkin, N. P. Gritzan and Y. D. Tsvetkov**

On the mechanism of the alkylation of quinoline and naphthyridine derivatives
G. Makara, G. M. Keserú and A. Kovács

Chemistry and kinetics of α - and β -naphthyl(phosphonyl)carbenes. Effects of positions on neighboring phosphonate participation **H. Tomioka, K. Hirai and Y. Tanimoto**

Synthetic strategies towards C₇₀. Molecular mechanics and MNDO calculations on pinakene, C₂₈H₁₄, and related molecules **E. D. Jemmis, G. N. Sastry and G. Mehta**

Highly efficient intramolecular general acid catalysis of enol ether hydrolysis, with rapid proton transfer to carbon **A. J. Kirby and F. O'Carroll**

Efficient intramolecular general acid catalysis of enol ether hydrolysis. Hydrogen-bonding stabilisation of the transition state for proton transfer to carbon
A. J. Kirby and N. H. Williams

Stoichiometric solvation effects. Part 2. A new product-rate correlation for solvolyses of *p*-nitrobenzenesulfonyl chloride in alcohol-water mixtures
T. W. Bentley, R. O. Jones and I. S. Koo

Evidence for the Möbius aromatic character of eight π electron conrotatory transition structure. Magnetic criteria **H. Jiao and P. von Ragué Schleyer**

The origins of the dichotomy of amine effects in aromatic nucleophilic substitution reactions **R. E. Akpojivi, T. A. Emokpae and J. Hirst**

An approach to functionalized cubanes. Regioselectivities and frontier molecular orbital analysis in the addition of 1,2-dicarbomethoxycyclobutadiene to quinones
G. Mehta, M. B. Viswanath, E. D. Jemmis and G. N. Sastry

Regioselective Rh₂(OAc)₄-promoted reactions of methyl diazoacetate with terminal triple bond enynes **E. A. Shapiro, A. V. Kalinin, B. I. Ugrak and O. M. Nefedov**

Inclusion compounds of cholic acid with aliphatic esters
M. R. Cairra, L. R. Nassimbeni and J. L. Scott

On the redox reactions of dopamine transients in aqueous solution: a pulse radiolysis study **D. K. Maity, H. Mohan and J. P. Mittal**

N-Aminoazoles. Part 3. Molecular structure and multinuclear NMR study of 1,3-diaminobenzimidazolium chloride hydrate and 1-amino-3-methylbenzimidazolium iodide
**A. F. Pozharshkii, V. V. Kuz'menko, C. Foces-Foces, A. L. Llamas-Saiz,
R. Ma. Claramunt, D. Sanz and J. Elguero**

Condensation products from the reactions of glyoxal with 2-substituted benzylamines. The formation and crystal structure of 2,2'-bi(1,2,3,4-tetrahydroquinazoline), and the crystal structure of 2,4,6,8,10,12-hexakis(2-methylbenzyl)-2,4,6,8,10,12-hexaazaisowurtzitane
A. Batsanov, J. C. Cole, M. R. Crampton, J. Hamid, J. A. K. Howard and R. Millar

Kinetic studies of the reactions of some phenyl aryl sulfides with aliphatic amines in dimethyl sulfoxide; the mechanism of base catalysis
R. A. Chamberlin and M. R. Crampton

Geometrical isomerization of carotenoids in dichloromethane
A. S. Jeevarajan, C. C. Wei and L. D. Kispert

Facile aerial oxidation of porphyrins. Part 16. Phenolic porphyrins without *t*-butyl substituents **L. R. Milgrom, J. P. Hill and W. D. Flitter**

A crystallographic and PM3 SCF-MO investigation of strong OH... π -alkene and alkyne hydrogen bonding interactions **H. S. Rzepa, M. H. Smith and M. L. Webb**

Photochemical reactions of 1H-pyrazolo[1,5-b][1,2,4]triazole azomethine dyes
K. Furuya, N. Furutachi, S. Oda and K. Maruyama

Ion associates and hydrogen bonded complexes of bromocresol green and quinine in dichloromethane **A. H. Gainza and M. T. Q. Rivera**