


JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions 2

Physical Organic Chemistry

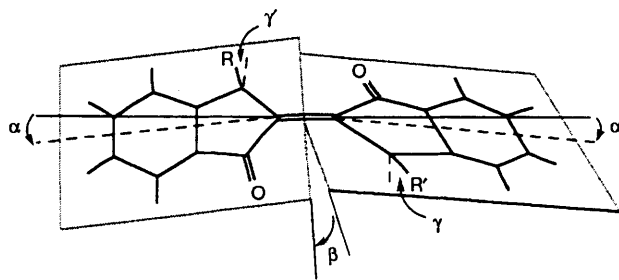
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Articles

<p>141 Nucleophilic substitution reaction of 1-phenylethyl chlorides in methanol</p> <p>Ikchoon Lee, Won Heui Lee, Hai Whang Lee and T. W. Bentley</p>	$\text{RX} \xrightleftharpoons[k_{-1}]{k_1} \text{R}^+ \cdot \text{X}^- \xrightarrow{k_{\text{N}}[\text{nuc}]} \text{Products}$ $k_2 = k_{\text{N}} \cdot K \quad K = \frac{k_1}{k_{-1}}$ <p>The title reaction proceeds by an ion-pair mechanism ($\text{S}_{\text{N}}2\text{C}^+$)</p>
<p>147 Electron-transfer <i>versus</i> nucleophilic substitution in the reactions of α-halogenated 4-nitrotoluenes with base</p> <p>Toh-Seok Kam and Tuck-Meng Lim</p>	$\text{ArCHXY} + \text{OH}^- \begin{cases} \xrightarrow{\text{ET/radical}} \text{Dimeric products} \\ \xrightarrow{\text{S}_{\text{N}}} \text{Solvolysis products} \end{cases}$ <p>(Ar = 4-NO₂C₆H₄-, X, Y = halogen)</p>
<p>151 Electron paramagnetic resonance studies of electron-capture processes. <i>p</i>-Nitrobenzyl and <i>p</i>-nitrobenzylidene systems</p> <p>Martyn C. R. Symons, Jane Wyatt, Toh-Seok Kam and Tuck-Meng Lim</p>	<p>$\text{S}_{\text{RN}}1$ reactions for</p> $\text{O}_2\text{N}-\text{C}_6\text{H}_4-\text{CX}_3 \quad \text{X} = \text{H, F, Cl, Br, I}$ <p>are probed using e⁻-addition at 77 K and EPR spectroscopy to study parent anions +</p> $\text{O}_2\text{N}-\text{C}_6\text{H}_4-\dot{\text{C}}\text{X}_2$
<p>157 Anti-aromaticity and colour in dyes containing unsaturated five-membered ring systems</p> <p>Fritz Dietz, Nikolai Tyutyulkov and Mordecai Rabinovitz</p>	 <p>It is shown that substituted or annellated anti-aromatic cyclopentadienyl cations are the basic chromophore of many dyes containing unsaturated five-membered ring systems</p>

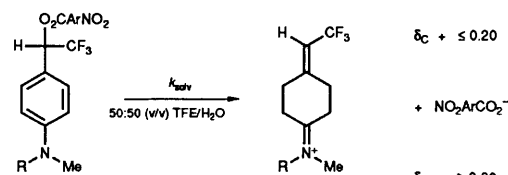
- 165 **A comparison of the structures of *N*-chloroacetylindigo (*N*-chloroacetyl-2,2'-bi-indolinylidene-3,3'-dione) and *N,N'*-bis(chloroacetyl)indigo [*N,N'*-bis(chloroacetyl)-2,2'-bi-indolinylidene-3,3'-dione] in the solid and solution state**

Bradley D. Smith, Marie-France Paugam and Kenneth J. Haller



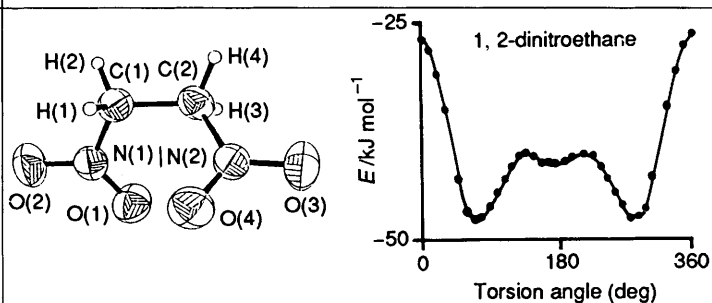
- 171 **How delocalised are resonance-stabilised 1-[4-(*N*-methyl-*N*-alkylamino)phenyl]-2,2,2-trifluoroethyl carbocations?**

Vandanapu Jagannadham, Tina L. Amyes and John P. Richard



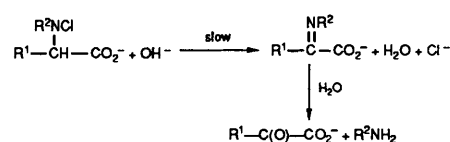
- 175 **IR spectra, crystal structure, dipole moment, *ab initio* and AM1 study of 1,2-dinitroethane**

Yu-Lin Lam, Lip Lin Koh and Hsing Hua Huang



- 181 **Decomposition of *N*-chloro- α -amino acids in alkaline medium**

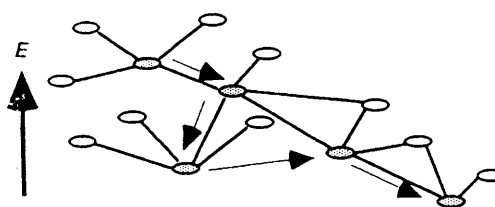
X. L. Armesto, M. Canle, M. Losada and J. A. Santaballa



($A_{xh}D_HD_N$) carbanion and reactant-like

- 187 **An efficient algorithm for searching low-energy conformers of cyclic and acyclic molecules**

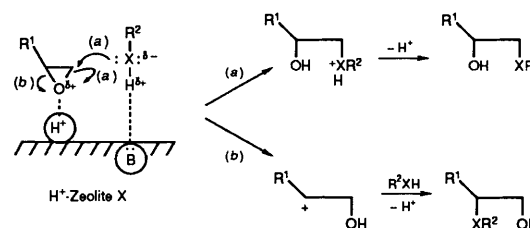
Hitoshi Gotō and Eiji Ōsawa



A new conformational space search algorithm has been developed

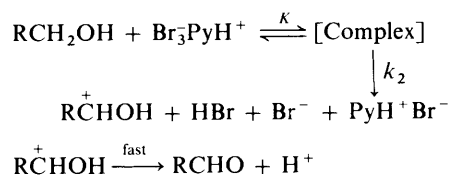
- 199 **The use of proton-exchanged X-type zeolite in catalysing ring-opening reactions of 2-substituted epoxides with nucleophiles and its effect on regioselectivity**

Hiroshi Takeuchi, Kunio Kitajima, Yasuhiro Yamamoto and Kiyokazu Mizuno



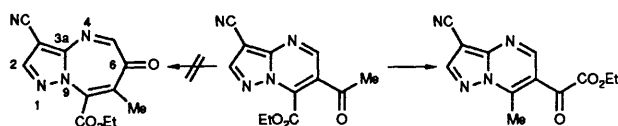
- 205 **Kinetics and mechanism of oxidation of primary alcohols by pyridinium hydrobromide perbromide**

Dipti Mathur, Pradeep K. Sharma and Kalyan K. Banerji



- 209 **Chemistry of substituted pyrazolo[1,5-*a*]-pyrimidines. Part 3. A structural correction of a pyrazolo[1,5-*a*][1,3]diazepine derivative on the basis of ^{13}C NMR spectroscopy**

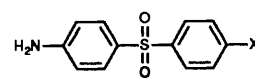
Stefano Chimichi, Barbara Cosimelli, Fabrizio Bruni and Annarella Costanzo



Ethyl 3-cyano-7-methylpyrazolo[1,5-*a*]pyrimidine-6-oxoacetate and not ethyl 3-cyano-7-methyl-6-oxopyrazolo[1,5-*a*][1,3]diazepine-8-carboxylate is shown to be the final product in the reaction of ethyl 6-acetyl-3-cyanopyrazolo[1,5-*a*]pyrimidine-7-carboxylate with aqueous acetic acid

- 213 **Molecular structure and crystal packing of five 4-aminophenyl(4-substituted phenyl) sulfones. Correlations between structural distortions, spectroscopic parameters and electronic substituent effects**

Valerio Bertolasi, Valeria Ferretti, Paola Gilli and Pier G. De Benedetti

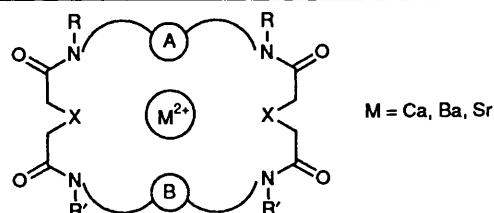


I

1; X = NO₂ 4; X = OCH₃
2; X = CN 5; X = NH₂
3; X = F

- 221 **Macrocyclic polyether tetralactams. Part 3. Spectroscopic study and molecular modelling of their complexes with alkaline-earth cations**

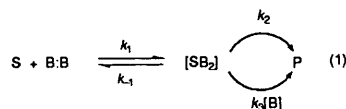
Thierry Pigot, Marie-Christine Duriez, Louis Cazaux, Claude Picard and Pierre Tisnès



Only one symmetric rotamer was evidenced for each complex in solution

- 229 **Reaction of 2,6-dinitroanisole with cyclohexylamine in toluene-octanol binary solvents. Further support for the 'dimer nucleophile mechanism' in aromatic nucleophilic substitution**

N. Sbarbati Nudelman, Mariel Marder and Alejandra Gurevich



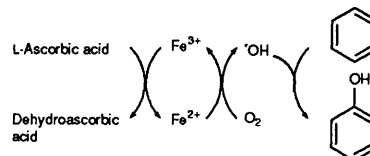
- 235 **Circular dichroism as a probe of chiral solvent structure around chiral molecules**

Julie Fidler, P. Mark Rodger and Alison Rodger

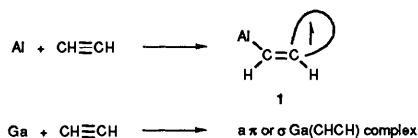
The solvation shell around a chiral molecule is found to be chiral even when the solvent itself is achiral. This solvent structure is found to modify chiral properties of the solute molecule

243 **Electron-transfer photochemistry of endoperoxides**Yasutake Takahashi, Kan Wakamatsu,
Shin-ichi Morishima and Tsutomu Miyashi

Photoinduced electron-transfer reactions of endoperoxides have been investigated

255 **Evidence for hydroxyl radicals as an active species generated from Udenfriend's reagent**Sotaro Ito, Kazuhiko Ueno, Akira Mitarai
and Kazuo SasakiUdenfriend's reagent (Fe^{2+} /EDTA/ascorbic acid/ O_2) generates $\cdot\text{OH}$ 261 **(Z/E)-Photoisomerization of C_{40} -carotenoids by iodine**

Péter Molnár and József Szabolcs

The phenomenon of iodine-catalysed *cis-trans* photoisomerization of the most prominent C_{40} -carotenoids has been studied267 **EPR spectroscopic study of the reaction of aluminium and gallium atoms with acetylenes in a rotating cryostat**Michael Histed, James A. Howard, Ruth
Jones and Mauro Tomietto**1** is unstable above 100 K and in adamantane a second $\text{Al}(\text{CHCH})$ complex is formed

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273 **Solution- and solid-state stereochemistry of (–)- α -lobeline hydrochloride and hydrobromide, a respiratory-stimulant drug** Robert Glaser, Paul Hug, Marc Drouin and André Michel

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

The SmithKline Beecham Research Symposium

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IN ORGANIC SYNTHESIS**

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PROFESSOR G E PATTENDEN, FRS

University of Nottingham

POSTER SESSION:

Posters are invited from participants and abstracts will be published in the Conference Proceedings. Closing date for the receipt of abstracts is 29th January 1993.

REGISTRATION:

The registration fee of £250.00 (£100.00 for registered under-graduate and graduate students) includes welcome buffet, conference dinner and all other meals, accommodation for two nights in Robinson College and a copy of the Symposium Proceedings.

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