

JOURNAL
OF
THE CHEMICAL SOCIETY

PERKIN TRANSACTIONS II
Physical Organic Chemistry

CONTENTS

	PAGE
An INDO molecular orbital study of [1,3] π interactions in 2-substituted allyl cations By BARRY K. CARPENTER	1
Molecular polarisability. The anisotropy of the C_{ar} -F group By MANUEL J. ARONEY, GEORGINA CLEAVER, RAYMOND K. PIERENS, and RAYMOND J. W. LE FÈVRE	3
Rate enhancement of ester saponification in aqueous dimethyl sulphoxide: a case for the importance of transition state solvation By M. BALAKRISHNAN, G. VENKOBA RAO, and N. VENKATASUBRAMANIAN	6
Conformational analysis of cyclohexane derivatives. The A value of a benzyl group By J. EDGAR ANDERSON	10
Kinetics and mechanism of the Fischer-Hepp rearrangement. Part III. Rearrangement and denitrosation in the presence of urea and other nucleophiles By D. LYN H. WILLIAMS and JOHN A. WILSON	13
Stereochemistry of the Diels-Alder reaction: steric effects of the dienophile on <i>endo</i> -selectivity By JOHN M. MELLOR and COLIN F. WEBB	17
Stereochemistry of the Diels-Alder reaction: effect of diene structure on <i>endo</i> -selectivity By BARRIE C. C. CANTELLO, JOHN M. MELLOR, and COLIN F. WEBB	22
Stereochemistry of the Diels-Alder reaction: reaction of dienophiles with cyclopentadiene and methylcyclopentadiene By JOHN M. MELLOR and COLIN F. WEBB	26
Elimination reactions. Part I. Reaction of bis-(4-nitrophenyl)methyl chloride with sodium hydroxide in aqueous dioxan By RASMY TEWFIK, FOUAD M. FOUAD, and PATRICK G. FARRELL	31
Is squaric acid square? A combined X-ray and neutron diffraction study of 3,4-dihydroxycyclobut-3-ene-1,2-dione By YU WANG, GALEN D. STUCKY, and JACK M. WILLIAMS	35
The chemistry of terpenes. Part VI. Reactions involving the isomeric pinan-10-yl carbonium ions By EE CHONG-SEN, R. ALAN JONES, and TERENCE C. WEBB	38
Nucleophilic substitution at bivalent sulphur. Part III. Kinetics and mechanism of the base-catalysed hydrolysis of ethyl 2-nitro-4-trifluoromethylbenzenesulphenate, the corresponding sulphenyl chloride, and the disulphide By DONALD R. HOGG and JOSEPH STEWART	43
Application of reaction field theory to the calculation of solvent effects on the <i>t</i> -butyl chloride solvolysis, and on the $Me_4N^+Cl^-$ ion pair By MICHAEL H. ABRAHAM and RAYMOND J. ABRAHAM	47

Ambident neighbouring groups. Part V. Mechanism of cyclization of 2-halogenoethylsulphonamides to aziridines By JOHN H. COY, ANTHONY F. HEGARTY, EDWARD J. FLYNN, and FRANCIS L. SCOTT.	53
Extended conjugation in di- and tri-arylmethane dyes. Part IV. Electronic absorption spectra of some phenanthrene analogues of Malachite Green By GEOFFREY HALLAS and RODNEY M. POTTS	59
The role of the carboxy-group in intramolecular catalysis of acetal hydrolysis. The hydrolysis of substituted 2-methoxymethoxybenzoic acids By GABRIELLE-ANNE CRAZE and ANTHONY J. KIRBY	61
Ground state and transition state effects in the acylation of α -chymotrypsin in organic solvent-water mixtures By RONALD P. BELL, JOHN E. CRITCHLOW, and MICHAEL I. PAGE	66
Ultraviolet and nuclear magnetic resonance spectra of protonated benzamide and [^{15}N]benzamide in concentrated sulphuric acid and pure fluorosulphuric acid By MILICA LILER	71
The kinetics of the reactions of picryl chloride with some substituted anilines. Part II By SUNDAY I. ETTE and JACK HIRST	76
Kinetics and mechanism of the autoxidation of the 2-amino-4-hydroxy-5,6,7,8-tetrahydropteridines By JOHN A. BLAIR and ANTHONY J. PEARSON	80
Photoreactions of substituted 4-methylenebicyclo[3.2.0]hept-2-enes By NEIL K. HAMER and A. JIM WILLS	88
Boron trifluoride complexes. Part VII. Ground-state properties of complexes of aromatic aldehydes By AMIRAM GRINVALD and MORDECAI RABINOVITZ	94
Aromatic sulphonation. Part XLIV. Sulphonation of some <i>meta</i> -substituted benzenesulphonic acids with fuming sulphuric acid. Preparation of arene-1,2-disulphonic anhydrides By (MRS.) ANKIE KOEBERG-TELDER, CORNELIS RIS, and HANS CERFONTAIN	98
Stereochemistry of anticholinergic agents. Part III. Crystal and molecular structure of piperidolate (<i>N</i> -ethyl-3-piperidyl diphenylacetate) hydrochloride By JOHN J. GUY and THOMAS A. HAMOR	101
Crystal and molecular structure of 2,4-di- <i>O</i> -methyl α -D-galactopyranose monohydrate By IAIN C. M. DEA, PETER MURRAY-RUST, and WILLIAM E. SCOTT	105

INDEX OF AUTHORS' NAMES

- ABRAHAM, M. H., and Abraham, R. J., 47
Abraham, R. J. See Abraham, M. H., 47
Anderson, J. E., 10
Aroney, M. J., Cleaver, G., Pierens, R. K., and Le Fèvre,
R. J. W., 3
Balakrishnan, M., Rao, G. V., and Venkatasubramanian, N., 6
Bell, R. P., Critchlow, J. E., and Page, M. I., 66
Blair, J. A., and Pearson, A. J., 80
Cantello, B. C. C., Mellor, J. M., and Webb, C. F., 22
Carpenter, B. K., 1
Cerfontain, H. See Koeberg-Telder, A., 98
Chong-Sen, E., Jones, R. A., and Webb, T. C., 38
Cleaver, G. See Aroney, M. J., 3
Coy, J. H., Hegarty, A. F., Flynn, E. J., and Scott, F. L., 53
Craze, G-A., and Kirby, A. J., 61
Critchlow, J. E. See Bell, R. P., 66
Dea, I. C. M., Murray-Rust, P., and Scott, W. E., 105
Ette, S. I., and Hirst, J., 76
Farrell, P. G. See Tewfik, R., 31
Flynn, E. J. See Coy, J. H., 53
Fouad, F. M. See Tewfik, R., 31
Grinvald, A., and Rabinovitz, M., 94
Guy, J. J., and Hamor, T. A., 101
Hallas, G., and Potts, R. M., 59
Hamer, N. K., and Wills, A. J., 88
Hamor, T. A. See Guy, J. J., 101
Hegarty, A. F. See Coy, J. H., 53
Hirst, J. See Ette, S. I., 76
Hogg, D. R., and Stewart, J., 43
Jones, R. A. See Chong-Sen, E., 38
Kirby, A. J. See Craze, G-A., 61
Koeberg-Telder, A., Ris, C., and Cerfontain, H., 98
Le Fèvre, R. J. W. See Aroney, M. J., 3
Liler, M., 71
Mellor, J. M., and Webb, C. F., 17, 26
Mellor, J. M. See also Cantello, B. C. C., 22
Murray-Rust, P. See Dea, I. C. M., 105
Page, M. I. See Bell, R. P., 66
Pearson, A. J. See Blair, J. A., 80
Pierens, R. K. See Aroney, M. J., 3
Potts, R. M. See Hallas, G., 59
Ral inovitz, M. See Grinvald, A., 94
Rao, G. V. See Balakrishnan, M., 6
Ris, C. See Koeberg-Telder, A., 98
Scott, F. L. See Coy, J. H., 53
Scott, W. E. See Dea, I. C. M., 105
Stewart, J. See Hogg, D. R., 43
Stucky, G. D. See Wang, Y., 35
Tewfik, R., Fouad, F. M., and Farrell, P. G., 31
Venkatasubramanian, N. See Balakrishnan, M., 6
Wang, Y., Stucky, G. D., and Williams, J. M., 35
Webb, C. F. See Cantello, B. C. C., 22; and Mellor, J. M.,
17, 26
Webb, T. C. See Chong-Sen, E., 38
Williams, D. L. H., and Wilson, J. A., 13
Williams, J. M. See Wang, Y., 35
Wills, A. J. See Hamer, N. K., 88
Wilson, J. A. See Williams, D. L. H., 13

* The author to whom correspondence should be addressed is indicated by an asterisk after his name in the heading of the Paper.

