

JOURNAL  
OF  
THE CHEMICAL SOCIETY

---

PERKIN TRANSACTIONS II  
Physical Organic Chemistry

CONTENTS

	PAGE
Substituent effects on the kinetics of pyridine-catalysed hydrolysis of aromatic sulphonyl chlorides; Brønsted and Hammett correlations By O. ROGNE . . . . .	489
Kinetics of the reaction of trimethyl phosphite with cyclic $\alpha$ -diketones By Y. OGATA and M. YAMASHITA . . . . .	493
Kinetics and salt effects on the alkaline hydrolysis of perbenzoate ion By F. SECCO, M. VENTURINI, and S. CELSI . . . . .	497
A probe for homolytic reactions in solution. Part VI. Reactions of polyhalogenomethyl radicals with nitrosobutane By C. M. CAMAGGI, R. J. HOLMAN, and M. J. PERKINS . . . . .	501
A probe for homolytic reactions in solution. Part VII. Hindered phenols as spin traps By C. M. CAMAGGI and M. J. PERKINS . . . . .	507
Electrolytic reduction and cleavage of cyclohexane-1,4-dione By E. KARIV and B. J. COHEN . . . . .	509
Nitrogen-15 chemical shifts in ring-substituted benzamides and benzonitriles By P. S. PREGOSIN, E. W. RANDALL, and A. I. WHITE . . . . .	513
Intramolecular nucleophilic assistance in reactions of acetals By E. ANDERSON and B. CAPON . . . . .	515
The kinetics and mechanism of the hydrolysis of 2,3-(phenylmethylenedioxy)benzene ( <i>OO'</i> -benzylidene-catechol) and benzaldehyde diphenyl acetal By B. CAPON and M. I. PAGE . . . . .	522
The kinetics and mechanism of the hydrolysis of 2,3-(phenylmethylenedioxy)benzoic acid ( <i>OO'</i> -benzylidene-2,3-dihydroxybenzoic acid) By B. CAPON, M. I. PAGE, and G. H. SANKEY . . . . .	529
Nuclear magnetic resonance studies of rate processes and conformations. Part XX. Nitrogen inversion in the gas phase By T. DRAKENBERG and J. M. LEHN . . . . .	532
The structural dependence of the inductive effect. Part VI. The calculation of vicinal proton-proton spin-spin coupling constants in substituted ethanes By L. PHILLIPS and V. WRAY . . . . .	536
Benzoquinone imines. Part IX. Mechanism and kinetics of the reaction of <i>p</i> -benzoquinone di-imines with <i>m</i> -aminophenols By JOHN F. CORBETT . . . . .	539
Application of the RRKM theory of unimolecular reactions to the thermal reactions of spiropentane By M. C. FLOWERS and A. R. GIBBONS . . . . .	548

The kinetics of the thermal gas phase reactions of methylspiro[2,2]pentane at low pressure By M. C. FLOWERS and A. R. GIBBONS . . . . .	555
Crystal and molecular structure of 5-chloro-2,1-benzisothiazole By M. DAVIS, M. F. MACKAY, and W. A. DENNE . . . . .	565
The kinetics and mechanism of the oxidation of benzyl alcohol to benzaldehyde by bromine By PETER AUKETT and I. R. L. BARKER . . . . .	568
Conjugation in sulphones. Electronic spectra and polarographic behaviour of thiophen dioxides By FEIKE de JONG and MATTHIJS JANSSEN . . . . .	572
The photoreaction of aromatic carbonyl compounds with amines: evidence for electron transfer from tertiary aromatic amines to triplet benzophenone By R. F. BARTHOLOMEW, R. S. DAVIDSON, P. F. LAMBETH, J. F. MCKELLAR, and P. H. TURNER. . . . .	577
Crystal structure of 3,6-anhydro- $\alpha$ -D-glucosyl-1,4:3,6-dianhydro- $\beta$ -D-fructoside By N. W. ISAACS and C. H. L. KENNARD . . . . .	582
Application of the MINDO method to the tautomers of purine By ZOHAR NEIMAN . . . . .	585
Oxidation of 4a,4b-dihydrophenanthrene. Part V. Tunnelling effect on the kinetics of the initiation step By A. BROMBERG, K. A. MUSZKAT, E. FISCHER, and F. S. KLEIN . . . . .	588
Crystal and molecular structure of 6-chloro-5,6,7,12-tetrahydro-2,5,7,10-tetramethyldibenzo[ <i>d,g</i> ][1,3,2]diazaphosphocine 6-oxide By T. S. CAMERON . . . . .	591
Acetolysis of 2-(2,3-dihydro-1 <i>H</i> -cyclopenta[ <i>l</i> ]phenanthren-2-yl)ethyl derivatives: participation by the 9,10-bond of phenanthrene to give an analogue of a classical norbornyl cation By R. M. COOPER, M. C. GROSSEL, and M. J. PERKINS . . . . .	594
Liquid crystal proton magnetic resonance spectrum of thieno[2,3- <i>b</i> ]thiophen By C. A. BOICELLI, A. MANGINI, L. LUNAZZI, and M. TIECCO . . . . .	599
Conformational study of some component peptides of pentagastrin By J. FEENEY, G. C. K. ROBERTS, J. P. BROWN, A. S. V. BURGEM, and H. GREGORY . . . . .	601
Further refinement of the crystal structure of neovitamin B <sub>12</sub> By HELEN STOECKLI-EVANS, E. EDMOND, and DOROTHY CROWFOOT HODGKIN . . . . .	605
Proton magnetic resonance studies of cyclic compounds. Part VIII. The conformations of <i>cis</i> - and <i>trans</i> -decahydroquinolines and their acyl derivatives By H. BOOTH and A. H. BOSTOCK. . . . .	615
Proteolytic enzymes. Papain-catalysed hydrolysis of specific aryl esters By A. WILLIAMS, E. C. LUCAS, and A. R. RIMMER . . . . .	621
Proteolytic enzymes. Nature of binding forces between papain and its substrates and inhibitors By A. WILLIAMS, E. C. LUCAS, A. R. RIMMER, and (MRS.) H. C. HAWKINS. . . . .	627
Studies on the nuclear magnetic resonance contact shifts induced by interaction with free radicals. Part IV. Utility of <sup>13</sup> C contact shifts for the study of weak hydrocarbon-radical interaction By ISAO MORISHIMA, TAKESHI MATSUI, TEIJIRO YONEZAWA, and KOJITSU GOTO. . . . .	633
A spectroscopic study of carbanions and corresponding nitranions: ion pair formation in the ground state and the first excited state By H. W. VOS, H. H. BLOM, N. H. VELTHORST, and C. MACLEAN . . . . .	635
The chemistry of reactive lignin intermediates. Part I. Transients in coniferyl alcohol photolysis By GORDON LEARY . . . . .	640
Crystal and molecular structure of hexamethylmelamine [2,4,6-tris(dimethylamino)-1,3,5-triazine] By G. J. BULLEN, D. J. CORNEY, and F. S. STEPHENS . . . . .	642
Proton magnetic resonance spectra of amino-acids and peptides relevant to wool structure. Part II. Relative residence times of sulphur-containing $\alpha$ -amino-acids By K. D. BARTLE, D. W. JONES, and R. L'AMIE . . . . .	646

Proton magnetic resonance spectra of amino-acids and peptides relevant to wool structure. Part III. Relative residence times of dipeptides of asparagine, aspartic acid, phenylalanine, and tyrosine By K. D. BARTLE, D. W. JONES, and R. L'AMIE . . . . .	650
Rearrangements accompanying the formation of alkynyl- and allyl-cobaloximes and their reactions with sulphur dioxide By C. J. COOKSEY, D. DODD, C. GATFORD, M. D. JOHNSON, G. J. LEWIS, and D. M. TITCHMARSH. . . . .	655
<i>N</i> -Oxides and related compounds. Part XL. Chemical and <i>X</i> -ray crystallographic investigation of the oxidation products of $\alpha$ -diketone bisacylhydrazones By H. BAUER, A. J. BOULTON, W. FEDELI, A. R. KATRITZKY, A. MAJID-HAMID, F. MAZZA, and A. VACIAGO . . . . .	662
<i>N</i> -Oxides and related compounds. Part XLI. Substituent-ring interactions in methyl- and chloro-pyrazines and -pyrazine 1-oxides By R. P. DUKE, RICHARD A. Y. JONES, A. R. KATRITZKY, J. M. LAGOWSKI, and YU. SHEINKER . . . . .	668
Acidity functions and the protonation of weak bases. Part VII. The protonation behaviour of dimethyl-aminopyridines and their <i>N</i> -oxides By P. FORSYTHE, R. FRAMPTON, C. D. JOHNSON, and A. R. KATRITZKY . . . . .	671
The conformational analysis of saturated heterocycles. Part XLV. <i>N</i> -Alkyldihydro-1,3,5-dithiazines and <i>N</i> -alkyltetrahydro-1,3,5-thiadiazines By L. ANGIOLINI, R. P. DUKE, RICHARD A. Y. JONES, and A. R. KATRITZKY . . . . .	674
The validity of the spectrophotometric method for determination of the kinetics of the reduction of ketones with sodium borohydride By DONALD C. WIGFIELD and DAVID J. PHELPS . . . . .	680
Temperature effects in the photochemistry of cycloalkanones in solution By J. D. COYLE . . . . .	683
Crystal structure of di- <i>p</i> -tolylcarbodi-imide, MeC <sub>6</sub> H <sub>4</sub> ·N:C:N·C <sub>6</sub> H <sub>4</sub> Me By A. T. VINCENT and P. J. WHEATLEY. . . . .	687

---

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

## INDEX OF AUTHORS' NAMES

- ANDERSON, E., and Capon, B., 515  
 Angiolini, L., Duke, R. P., Jones, R. A. Y., and Katritzky, A. R., 674  
 Aukett, P., and Barker, I. R. L., 568  
 Barker, I. R. L. See Aukett, P., 568  
 Bartholomew, R. F., Davidson, R. S., Lambeth, P. F., McKellar, J. F., and Turner, P. H., 577  
 Bartle, K. D., Jones, D. W., and L'Amie, R., 646, 650  
 Bauer, H., Boulton, A. J., Fedeli, W., Katritzky, A. R., Majid-Hamid, A., Mazza, F., and Vaciago, A., 662  
 Blom, H. H. See Vos, H. W., 635  
 Boicelli, C. A., Mangini, A., Lunazzi, L., and Tiecco, M., 599  
 Booth, H., and Bostock, A. H., 615  
 Bostock, A. H. See Booth, H., 615  
 Boulton, A. J. See Bauer, H., 662  
 Bromberg, A., Muszkat, K. A., Fischer, E., and Klein, F. S., 588  
 Brown, J. P., See Feeney, J., 601  
 Bullen, G. J., Corney, D. J., and Stephens, F. S., 642  
 Burgen, A. S. V. See Feeney, J., 601  
 Camaggi, C. M., and Perkins, M. J., 507  
 Camaggi, C. M., Holman, R. J., and Perkins, M. J., 501  
 Cameron, T. S., 591  
 Capon, B., and Page, M. I., 522  
 Capon, B., Page, M. I., and Sankey, G. H., 529  
 Capon, B. See also Anderson, E., 515  
 Celsi, S. See Secco, F., 497  
 Cohen, B. J. See Kariv, E., 509  
 Cooksey, C. J., Dodd, D., Gatford, C., Johnson, M. D., Lewis, G. J., and Titchmarsh, D. M., 655  
 Cooper, R. M., Grossel, M. C., and Perkins, M. J., 594  
 Corbett, J. F., 539  
 Corney, D. J. See Bullen, G. J., 642  
 Coyle, J. D., 683  
 Davidson, R. S. See Bartholomew, R. F., 577  
 Davis, M., Mackay, M. F., and Denne, W. A., 565  
 de Jong, F., and Janssen, M., 572  
 Denne, W. A. See Davis, M., 565  
 Dodd, D. See Cooksey, C. J., 655  
 Drakenberg, T., and Lehn, J. M., 532  
 Duke, R. P., Jones, R. A. Y., Katritzky, A. R., Lagowski, J. M., and Sheinker, Yu., 668  
 Duke, R. P. See also Angiolini, L., 674  
 Edmond, E. See Stoekli-Evans, H., 605  
 Fedeli, W. See Bauer, H., 662  
 Feeney, J., Roberts, G. C. K., Brown, J. P., Burgen, A. S. V., and Gregory, H., 601  
 Fischer, E. See Bromberg, A., 588  
 Flowers, M. C., and Gibbons, A. R., 548, 555  
 Forsythe, P., Frampton, R., Johnson, C. D., and Katritzky, A. R., 671  
 Frampton, R. See Forsythe, P., 671  
 Gatford, C. See Cooksey, C. J., 655  
 Gibbons, A. R. See Flowers, M. C., 548, 555  
 Goto, K. See Morishima, I., 633  
 Gregory, H. See Feeney, J., 601  
 Grossel, M. C. See Cooper, R. M., 594  
 Hawkins, H. C. See Williams, A., 627  
 Hodgkin, D. C. See Stoekli-Evans, H., 605  
 Holman, R. J. See Camaggi, C. M., 501  
 Isaacs, N. W., and Kennard, C. H. L., 582  
 Janssen, M. See de Jong, F., 572  
 Johnson, C. D. See Forsythe, P., 671  
 Johnson, M. D. See Cooksey, C. J., 655  
 Jones, D. W. See Bartle, K. D., 646, 650  
 Jones, R. A. Y. See Angiolini, L., 674; and Duke, R. P., 668  
 Katritzky, A. R. See Angiolini, L., 674; Bauer, H., 662; Duke, R. P., 668; and Forsythe, P., 671  
 Kariv, E., and Cohen, B. J., 509  
 Kennard, C. H. L. See Isaacs, N. W., 582  
 Klein, F. S. See Bromberg, A., 588  
 Lagowski, J. M. See Duke, R. P., 668  
 Lambeth, P. F. See Bartholomew, R. F., 577  
 L'Amie, R. See Bartle, K. D., 646, 650  
 Leary, G., 640  
 Lehn, J. M. See Drakenberg, T., 532  
 Lewis, G. J. See Cooksey, C. J., 655  
 Lucas, E. C. See Williams, A., 621, 627  
 Lunazzi, L. See Boicelli, C. A., 599  
 Mackay, M. F. See Davis, M., 565  
 McKellar, J. F. See Bartholomew, R. F., 577  
 MacLean, C. See Vos, H. W., 635  
 Majid-Hamid, A. See Bauer, H., 662  
 Matsui, T. See Morishima, I., 633  
 Mangini, A. See Boicelli, C. A., 599  
 Mazza, F. See Bauer, H., 662  
 Morishima, I., Matsui, T., Yonezawa, T., and Goto, K., 633  
 Muszkat, K. A. See Bromberg, A., 588  
 Neiman, Z., 585  
 Ogata, Y., and Yamashita, M., 493  
 Page, M. I. See Capon, B., 522, 529  
 Perkins, M. J. See Camaggi, C. M., 501, 507; and Cooper, R. M., 594  
 Phelps, D. J. See Wigfield, D. C., 680  
 Phillips, L., and Wray, V., 536  
 Pregosin, P. S., Randall, E. W., and White, A. I., 513  
 Randall, E. W. See Pregosin, P. S., 513  
 Rimmer, A. R. See Williams, A., 621, 627  
 Roberts, G. C. K. See Feeney, J., 601  
 Rogne, O., 489  
 Sankey, G. H. See Capon, B., 529  
 Secco, F., Venturini, M., and Celsi, S., 497  
 Sheinker, Yu. See Duke, R. P., 668  
 Stephens, F. S. See Bullen, G. J., 642  
 Stoekli-Evans, H., Edmond, E., and Hodgkin, D. C., 605  
 Tiecco, M. See Boicelli, C. A., 599  
 Titchmarsh, D. M. See Cooksey, C. J., 655  
 Turner, P. H. See Bartholomew, R. F., 577  
 Vaciago, A. See Bauer, H., 662  
 Velthorst, N. H. See Vos, H. W., 635  
 Venturini, M. See Secco, F., 497  
 Vincent, A. T., and Wheatley, P. J., 687  
 Vos, H. W., Blom, H. H., Velthorst, N. H., and MacLean, C., 635  
 Wheatley, P. J. See Vincent, A. T., 687  
 White, A. I. See Pregosin, P. S., 513  
 Wigfield, D. C., and Phelps, D. J., 680  
 Williams, A., Lucas, E. C., and Rimmer, A. R., 621  
 Williams, A., Lucas, E. C., Rimmer, A. R., and Hawkins, H. C., 627  
 Wray, V. See Phillips, L., 536  
 Yamashita, M. See Ogata, Y., 493  
 Yonezawa, T. See Morishima, I., 633