

JOURNAL
OF
THE CHEMICAL SOCIETY

PERKIN TRANSACTIONS II
Physical Organic Chemistry

CONTENTS

	PAGE
The photo-oxidation of aliphatic alcohols as monolayers on aqueous solutions of 1,1'-dimethyl-4,4'-bipyridylium (paraquat) dichloride	
By NORMAN M. D. BROWN, DAVID J. COWLEY, and WILLIAM J. MURPHY	1769
Kinetics of base-catalysed condensation of 5-methylfuran-2(3 <i>H</i>)-one with 2-hydroxybenzaldehyde	
By IGNAZIO R. BELLOBONO, ALMA DAL POZZO, and MARIO T. CATALDI	1773
Aromatic sulphonation. Part 52. Ionization, sulphation, sulphonation, and alkylation of ω -phenylalkan-1-ols in sulphuric acid	
By ANKIE KOEBERG-TELDER and HANS CERFONTAIN	1776
Aromatic sulphonation. Part 53. Kinetics and mechanism of sulphonation of ω -phenylalkane-1-sulphonic acids in sulphuric acid. Comparison of the side-chain SO ₃ H and OSO ₃ H substituent effects	
By HANS CERFONTAIN and (MRS.) ZWAANTJE R. H. SCHAASBERG-NIENHUIS	1780
Equilibria and reactions of acetylsulphuric acid in liquid sulphur dioxide	
By ENZO MONTONERI, MIRCO FORNAROLI, LUIGI GIUFFRÉ, EZIO TEMPESTI, and GIANCARLO SIOLI	1784
The role of intermediate complexes in benzofuran protonations	
By ESTANISLAO SILLA, JUAN BERTRÁN, ENRIC CANADELL, and J. I. FERNÁNDEZ-ALONSO	1789
Conformational studies by dynamic nuclear magnetic resonance. Part 4. Rotational isomers and torsional barriers of pyridinecarbaldehydes	
By LODOVICO LUNAZZI, DANTE MACCIANTELLI, and GIOVANNI CERIONI	1791
Nematic phase nuclear magnetic resonance investigations of rotational isomerism. Part IV. Conformational study on the rotamers of 3,3'-bithienyl	
By LODOVICO LUNAZZI, FRANCO SALVETTI, and C. ALBERTO VERACINI	1796
The carbonyl group frequency. Part VI. Alkyl carbonates	
By J. SYDNEY BYRNE, PAUL F. JACKSON, and KEITH J. MORGAN	1800
Kinetics of the oxidation of some <i>meta</i> - and <i>para</i> -substituted dimethylanilines with lead tetra-acetate	
By GUIDO GALLIANI, BRUNO RINDONE, and PIER LUIGI BELTRAME	1803
Linear free energy <i>ortho</i> -correlations in the thiophen series. Part IV. Kinetics of alkaline hydrolysis of some methyl 3-substituted thiophen-2-carboxylates in aqueous methanol	
By DOMENICO SPINELLI, RENATO NOTO, GIOVANNI CONSIGLIO, and ALBA STORACE	1805
Crystal and molecular structure of thiosemicarbazide hydrochloride	
By LEANDRO COGHI, ANNA MARIA MANOTTI LANFREDI, and ANTONIO TIRIPICCHIO	1808
Reduction of some ketones using sulphurated sodium borohydride (NaBH ₂ S ₃): kinetics and mechanism	
By V. M. SADAGOPA RAMANUJAM and NORMAN M. TRIEFF	1811
Vapour-phase chemistry of arenes. Part 3. Vapour-phase chlorination of benzene derivatives catalysed by ultraviolet light	
By WIM DORREPAAL and ROBERT LOUW	1815
Chiroptical properties of cyclo-L-cystine	
By ROBIN W. STRICKLAND and FREDERICK S. RICHARDSON	1818

	PAGE
Chlorinated pyridine compounds: quantum chemical calculations and chlorine-35 nuclear quadrupole resonance frequencies By MAVIS REDSHAW	1821
The electron spin resonance spectra of alkyl aryl ether radical cations By WILLIAM T. DIXON and DAVID MURPHY	1823
1,3-Dipolar character of six-membered aromatic rings. Part XXIX. Kinetic rates and equilibria for the addition of 2π -electron addends to 3-oxidopyridinium betaines By GEORGES GUIHENEUF, CHRISTIAN LAURENCE, and ALAN R. KATRITZKY	1829
Crystal structure of a very hindered olefin: 1,1-diphenyl-2,2-di- <i>t</i> -butylethylene at $-155\text{ }^{\circ}\text{C}$ By ANGELO MUGNOLI and MASSIMO SIMONETTA	1831
Nucleophilic character of acyl radicals. Absolute rate constant for the acylation of protonated benzothiazole by pivaloyl radical By MARTA BELLATTI, TULLIO CARONNA, ATTILIO CITTERIO, and FRANCESCO MINISCI	1835
Denitrosation of <i>N</i> -methyl- <i>N</i> -nitrosotoluene- <i>p</i> -sulphonamide in acid solution By D. LYN H. WILLIAMS	1838
Kinetics of oxidation of organic compounds by silver(II) in aqueous perchloric acid solution. Part 2. Aliphatic carboxylic acids By EDOARDO MENTASTI, EZIO PELIZZETTI, and CLAUDIO BAIOCCHI	1841
Dipole moment, spectroscopic, and theoretical study of di-2-pyridyl sulphones By ADRIANO BIGOTTO, VINICIO GALASSO, GIUSEPPE C. PAPPALARDO, and GIUSEPPE SCARLATA	1845
The photochemistry of benz[<i>de</i>]anthracen-7-ones. Part III. Fluorescence quantum yield and continuous photolysis studies By PETER BENTLEY and JOHN F. MCKELLAR	1850
Molecular polarisability. The conformations of some substituted pentafluorobenzenes By MANUEL J. ARONEY, (MRS.) GEORGINA CLEAVER, RAYMOND K. PIERENS, and RAYMOND J. W. LE FÉVRE	1854
Evidence for formation of carbanions in cleavage of carbon-silicon bonds by methanolic sodium methoxide. Some large kinetic isotope effects for reactions of carbanions with methanol By COLIN EABORN, DAVID R. M. WALTON, and GIANCARLO SECONI	1857
The conformational analysis of saturated heterocycles. Part 72. Tetrahydro-1,3,4-oxadiazines By IAN J. FERGUSON, ALAN R. KATRITZKY, and DAVID M. READ	1861
Thermal isomerization of 3,6-dimethyltricyclo[3.1.0.0 ^{2,4}]hexane By HENRY M. FREY, HENNING HOPF, and ROBERT A. SMITH	1865
Nuclear quadrupole resonance and stereochemistry. Part 6. Transmission of substituent effects through a double bond By Z. ARDALAN DE WECK, F. DELAY, M. GEOFFROY, E. A. C. LUCKEN, and S. MASSON	1867
Basicity and nucleophilic reactivity of carbonyl-stabilized sulphimides By HIDEO KISE, YUKIO SUGIYAMA, and MANABU SENŌ	1869
Correlation of the loss of solvent with the crystal structure of a 1 : 1 solvate. Indanetrione 2-(<i>N-p-t</i> -butylbenzoyl- <i>N</i> -phenylhydrazone) acetone solvate By SHERRILL A. PUCKETT, IAIN C. PAUL, and DAVID Y. CURTIN	1873
Structures and conformations of the fourteen-membered ring diterpene ovatodiolide and its acid cyclization product: nuclear Overhauser effect studies in solution and <i>X</i> -ray crystal structure analyses of ovatodiolide and ovatodiolic acid By RAOUL TOUBIANA, MARIE-JOSÉPHE TOUBIANA, ANDREW T. MCPHAIL, RICHARD W. MILLER, and KAZUO TORI	1881
Bridgehead β -deuterium secondary kinetic isotope effect in the solvolysis of <i>endo</i> -norbornan-2-yl <i>p</i> -bromobenzenesulphonate By H. MASKILL	1889
Kinetics of solvolysis of substituted ω -bromo-2-acetonaphthones in aqueous ethanol By P. ANANTHAKRISHNA NADAR and C. GNANASEKARAN	1893
Carbonylation of organomagnesium compounds: catalysis by hexamethylphosphoric triamide By WILHELMUS J. J. M. SPRANGERS and ROBERT LOUW	1895

	PAGE
Photochemical oxetan formation: the Paterno-Büchi reaction of aliphatic aldehydes and ketones with alkenes and dienes	
By CAREL W. FUNKE and HANS CERFONTAIN	1902
Electrophilic participation in phosphonodiester hydrolysis	
By RICHARD A. NAYLOR and ANDREW WILLIAMS	1908
Role of hydrogen bonding in the mechanism of hydrogen atom abstraction from alkyl-substituted phenols by polyvinyl acetate radicals	
By MIKLÓS SIMONYI, JULIANNA KARDOS, ILONA FITOS, ILONA KOVÁCS, and JAN POSPIŠIL	1913
Molecular mechanics calculations on lactones; an interpretation of the preferential C(8) relactonization of germacranolides containing C(6) and C(8) lactonizable α -oxygen functions	
By MICHAEL H. P. GUY, GEORGE A. SIM, and DAVID N. J. WHITE	1917
Additivity of substituent effects in the alkaline hydrolysis of alkyl benzoates	
By JAMEEL FAROOQI, PETER H. GORE, and ABDUR RAHIM	1921

INDEX OF AUTHORS' NAMES

- ARONEY, M. J., Cleaver, G., Pierens, R. K., and Le Fèvre, R. J. W., 1854
- Baiocchi, C. See Mentasti, E., 1841
- Bellatti, M., Caronna, T., Citterio, A., and Minisci, F., 1835
- Bellobono, I. R., Dal Pozzo, A., and Cataldi, M. T., 1773
- Beltrame, P. L. See Galliani, G., 1803
- Bentley, P., and McKellar, J. F., 1850
- Bertrán, J. See Silla, E., 1789
- Bigotto, A., Galasso, V., Pappalardo, G. C., and Scarlata, G., 1845
- Brown, N. M. D., Cowley, D. J., and Murphy, W. J., 1769
- Byrne, J. S., Jackson, P. F., and Morgan, K. J., 1800
- Canadell, E. See Silla, E., 1789
- Caronna, T. See Bellatti, M., 1835
- Cataldi, M. T. See Bellobono, I. R., 1773
- Cerfontain, H., and Schaasberg-Nienhuis, Z. R. H., 1780
- Cerfontain, H. See also Funke, C. W., 1902; and Koeberg-Telder, A., 1776
- Cerioni, G. See Lunazzi, L., 1791
- Citterio, A. See Bellatti, M., 1835
- Cleaver, G. See Aroney, M. J., 1854
- Coghi, L., Lanfredi, A. M. M., and Tiripicchio, A., 1808
- Consiglio, G. See Spinelli, D., 1805
- Cowley, D. J. See Brown, N. M. D., 1769
- Curtin, D. Y. See Puckett, S. A., 1873
- Dal Pozzo, A. See Bellobono, I. R., 1773
- de Weck, Z. A., Delay, F., Geoffroy, M., Lucken, E. A. C., and Masson, S., 1867
- Delay, F. See de Weck, Z. A., 1867
- Dixon, W. T., and Murphy, D., 1823
- Dorrepaal, W., and Louw, R., 1815
- Eaborn, C., Walton, D. R. M., and Seconi, G., 1857
- Farooqi, J., Gore, P. H., and Rahim, M. A., 1921
- Ferguson, I. J., Katritzky, A. R., and Read, D. M., 1861
- Fernández-Alonso, J. I. See Silla, E., 1789
- Fitos, I. See Simonyi, M., 1913
- Fornaroli, M. See Montoneri, E., 1784
- Frey, H. M., Hopf, H., and Smith, R. A., 1865
- Funke, C. W., and Cerfontain, H., 1902
- Galasso, V. See Bigotto, A., 1845
- Galliani, G., Rindone, B., and Beltrame, P. L., 1803
- Geoffroy, M. See de Weck, Z. A., 1867
- Giuffré, L. See Montoneri, E., 1784
- Gnanasekaran, C. See Nadar, P. A., 1893
- Gore, P. H. See Farooqi, J., 1921
- Guiheneuf, G., Laurence, C., and Katritzky, A. R., 1829
- Guy, M. H. P., Sim, G. A., and White, D. N. J., 1917
- Hopf, H. See Frey, H. M., 1865
- Jackson, P. F. See Byrne, J. S., 1800
- Kardos, J. See Simonyi, M., 1913
- Katritzky, A. R. See Ferguson, I. J., 1861; and Guiheneuf, G., 1829
- Kise, H., Sugiyama, Y., and Senō, M., 1869
- Koeberg-Telder, A., and Cerfontain, H., 1776
- Kovács, I. See Simonyi, M., 1913
- Lanfredi, A. M. M. See Coghi, L., 1808
- Laurence, C. See Guiheneuf, G., 1829
- Le Fèvre, R. J. W. See Aroney, M. J., 1854
- Louw, R. See Dorrepaal, W., 1815; and Sprangers, W. J. J. M., 1895
- Lucken, E. A. C. See de Weck, Z. A., 1867
- Lunazzi, L., Macciantelli, D., and Cerioni, G., 1791
- Lunazzi, L., Salvetti, F., and Veracini, C. A., 1796
- Macciantelli, D. See Lunazzi, L., 1791
- McKellar, J. F. See Bentley, P., 1850
- McPhail, A. T. See Toubiana, R., 1881
- Maskill, H., 1889
- Masson, S. See de Weck, Z. A., 1867
- Mentasti, E., Pelizzetti, E., and Baiocchi, C., 1841
- Miller, R. W. See Toubiana, R., 1881
- Minisci, F. See Bellatti, M., 1835
- Montoneri, E., Fornaroli, M., Giuffré, L., Tempesti, E., and Sioli, G., 1784
- Morgan, K. J. See Byrne, J. S., 1800
- Mugnoli, A., and Simonetta, M., 1831
- Murphy, D. See Dixon, W. T., 1823
- Murphy, W. J. See Brown, N. M. D., 1769
- Nadar, P. A., and Gnanasekaran, C., 1893
- Naylor, R. A., and Williams, A., 1908
- Noto, R. See Spinelli, D., 1805
- Pappalardo, G. C. See Bigotto, A., 1845
- Paul, I. C. See Puckett, S. A., 1873
- Pelizzetti, E. See Mentasti, E., 1841
- Pierens, R. K. See Aroney, M. J., 1854

- Pospišil, J. See Simonyi, M., 1913
 Puckett, S. A., Paul, I. C., and Curtin, D. Y., 1873
 Rahim, A. See Farooqi, J., 1921
 Ramanujam, V. M. S., and Trieff, N. M., 1811
 Read, D. M. See Ferguson, I. J., 1861
 Redshaw, M., 1821
 Richardson, F. S. See Strickland, R. W., 1818
 Rindone, B. See Galliani, G., 1803
 Salvetti, F. See Lunazzi, L., 1796
 Scarlata, G. See Bigotto, A., 1845
 Schaasberg-Nienhuis, Z. R. H. See Cerfontain, H., 1780
 Seconi, G. See Eaborn, C., 1857
 Senō, M. See Kise, H., 1869
 Silla, E. Bertrán, J., Canadell, E., and Fernández-Alonso, J. I., 1789
 Sim, G. A. See Guy, M. H. P., 1917
 Simonetta, M. See Mugnoli, A., 1831
 Simonyi, M., Kardos, J., Fitos, I., Kovács, I., and Pospíšil, J., 1913
 Sioli, G. See Montoneri, E., 1784
 Smith, R. A. See Frey, H. M., 1865
 Spinelli, D., Noto, R., Consiglio, G., and Storace, A., 1805
 Sprangers, W. J. J. M., and Louw, R., 1895
 Storace, A. See Spinelli, D., 1805
 Strickland, R. W., and Richardson, F. S., 1818
 Sugiyama, Y. See Kise, H., 1869
 Tempesti, E. See Montoneri, E., 1784
 Tiripicchio, A. See Coghi, L., 1808
 Tori, K. See Toubiana, R., 1881
 Toubiana, M-J. See Toubiana, R., 1881
 Toubiana, R., Toubiana, M-J., McPhail, A. T., Miller, R. W., and Tori, K., 1881
 Trieff, N. M. See Ramanujam, V. M. S., 1811
 Veracini, C. A. See Lunazzi, L., 1796
 Walton, D. R. M. See Eaborn, C., 1857
 White, D. N. J. See Guy, M. H. P., 1917
 Williams, A. See Naylor, R. A., 1908
 Williams, D. L. H., 1838

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