

## JOURNAL OF THE CHEMICAL SOCIETY

## Perkin Transactions 2

## Physical Organic Chemistry

## CONTENTS

- 1865 Ionization energies of triazines and tetrazines. Application of Green's function method coupled with semiempirical molecular orbital calculations **David Danovich** and **Yitzhak Apeloig**
- 1875 Alkynylhalocarbenes: generation from 1,1-dihaloalk-2-yne by base solvolysis and reaction with alkenes **Konstantin N. Shavrin**, **Irina V. Krylova**, **Inna B. Shvedova**, **Galina P. Okonnishnikova**, **Igor E. Dolgy** and **Oleg M. Nefedov**
- 1883  $pK_a$  Determination of water-soluble calix[4]arenes **Seiji Shinkai**, **Koji Araki**, **Peter D. J. Grootenhuis** and **David N. Reinhoudt**
- 1887 Isomerization and fragmentation of aliphatic thioether radical cations in the gas phase: ion-neutral complexes in the reactions of metastable ethyl propyl thioether ions **Herman W. Zappey**, **Steen Ingemann** and **Nico M. M. Nibbering**
- 1893 Cycloalkylmethyl radicals. Part 8. A conformational study of dioxo- and dithia-cyclohexylmethyl radicals by EPR spectroscopy **Finlay MacCorquodale**, **John C. Walton**, **Lise Hughes** and **Keith U. Ingold**
- 1901 An open transition state in carbonyl acyl group transfer in aqueous solution **Salem A. Ba-Saif**, **Matthew Colthurst**, **Mark A. Waring** and **Andrew Williams**
- 1909 Kinetic and equilibrium solvent isotope effects on the ionisation of a hydrogen-bonded proton and studies of the intramolecular hydrogen bond in phenylazoresorcinols **Frank Hibbert** and **Siân C. Phillips**
- 1913 Control of peptide conformational preferences by intramolecular ion-pairing: a NMR and molecular mechanics analysis of glycol-containing dipeptides in aqueous solutions **Craig Beeson** and **Thomas A. Dix**
- 1919 Kinetics and mechanism of the aminolysis of phenyl dithioacetate in aqueous solution **Enrique A. Castro**, **Fernando Ibáñez**, **José G. Santos** and **Carmen Ureta**
- 1925 Kinetics and mechanism of the addition of triphenylphosphoniocyclopentadienide to tetrachloro-*p*-benzoquinone **Francisco Pérez Plá**, **Juan Palou**, **Rosa Valero**, **C. Dennis Hall** and **Peter Speers**
- 1933 Hydrolysis and alkylating reactivity of aromatic nitrogen mustards **Charmian J. O'Connor**, **William A. Denny**, **Jun-Yao Fan**, **G. Lance Gravatt**, **Bruce A. Grigor** and **Duncan J. McLennan**
- 1941 Reactions of indolic radicals produced upon one-electron oxidation of 5,6-dihydroxyindole and its N(1)-methylated analogue **Akeel T. Al-Kazwini**, **Peter O'Neill**, **Gerald E. Adams**, **Robert B. Cundall**, **Gerard Lang** and **Alex Junino**
- 1947 Trico-ordinate phosphorus compounds as catalysts for the isomerization of (*Z*)- to (*E*)-azobenzene **C. Dennis Hall** and **Paul D. Beer**
- 1951 Rate and product analytical study of the solvolysis of 3-chlorobenzyl arenesulfonates in aqueous 2,2,2-trifluoroethanol **Isobel M. Gordon** and **H. Maskill**
- 1955 EPR study of radical intermediates from the oxidation of 6-ethoxy-2,2,4-trimethyl- and 6-ethoxy-2,2,4,8-tetramethyl-1,2-dihydroquinoline **Frank D. Gunstone**, **Raphael C. Mordi**, **Snorri Thorisson**, **John C. Walton** and **Richard A. Jackson**
- 1959 Redox behaviour and stable anion radicals of cyclic polycalixenes **Jun Yamauchi**, **Toyonari Sugimoto**, **Yoshihisa Arai**, **Masashi Sakaguchi** and **Zen-ichi Yoshida**
- 1963 Improved synthesis and crystal structure of tetrakis(benzoylthio)tetrathiafulvalene. A useful precursor to functionalised bis(ethylenedithio)tetrathiafulvalene derivatives **Thomas K. Hansen**, **Ian Hawkins**, **K. Sukumar Varma**, **Stephen Edge**, **Sine Larsen**, **Jan Becher** and **Allan E. Underhill**
- 1967 Arylation of heterocyclic ketene aminals with 2,4-dinitrohalobenzenes by a radical nucleophilic substitution mechanism **Wen-Yi Zhao** and **Zhi-Tang Huang**

- 1971 Optical resolution of amino acid and hydroxycarboxylic acid esters by complexation with optically active host compounds: a crystallographic result **Fumio Toda, Atsushi Sato, Luigi R. Nassimbeni and Margaret L. Niven**
- 1977 Mechanism of the photoreaction between 1,4-dicyanonaphthalene and benzylic donors **Nicola d'Alessandro, Elisa Fasani, Mariella Mella and Angelo Albini**
- 1981 Nucleophilic substitution reactions of allyl arenesulphonates with anilines and *N,N*-dimethylanilines **Hyuck Keun Oh, Han Joong Koh and Ikchoon Lee**
- 1985 Gas-phase reactions of  $F^-$  with phenyl acetates. Translational energy and substituent effects on product distribution **Jose M. Riveros, Steen Ingemann and Nico M. M. Nibbering**
- 1991 Interception of an iminium ion equivalent by intramolecular nucleophilic attack by a silyl ether during lithium aluminium hydride reduction of a tertiary lactam **Nigel G. Ramsden, George W. J. Fleet and Sung Keon Namgoong**
- 1995 Nitric acid equilibrium in concentrated trifluoromethanesulfonic acid studied by Raman spectroscopy **Nunziata C. Marziano, Alberto Tomasin and Marco Sampoli**
- 1999 3-Hydroxypyrroles and 1*H*-pyrrol-3(2*H*)-ones. Part 11.  $^1H$  and  $^{13}C$  NMR spectra of 1-substituted and 1,2-disubstituted 3-hydroxy- and 3-alkoxy-pyrroles **Hamish McNab and Lilian C. Monahan**
- 2003 Variable-temperature NMR and X-ray crystallographic studies of 5-dimethylaminomethylene-, 5-dimethylamino-propenylidene- and 5-(5-dimethylaminopenta-2,4-dienylidene)- derivatives of Meldrum's acid and related dimethyl malonate derivatives **Alexander J. Blake, Hamish McNab and Lilian C. Monahan**
- 2011 Ene reactions of allylic tin compounds with singlet oxygen and with 4-phenyl-1,2,4-triazoline-3,5-dione **Hai-Shan Dang and Alwyn G. Davies**
- 2021 An EPR study of 1-adamantylmethyl radicals **Alwyn G. Davies and Anthony G. Neville**
- 2025 Combined quantum mechanical–molecular mechanical study of catalysis by the enzyme phospholipase  $A_2$ : an investigation of the potential energy surface for amide hydrolysis **Bohdan Waszkowycz, Ian H. Hillier, Nigel Gensmantel and David W. Payling**
- 2033 Iminophosphorane-substituted proton sponges. Part 3. Preparation and crystal structure of three salts of protonated 1-dimethylamino-8-triphenylphosphoranylideneammonionaphthalene **Antonio L. Llamas-Saiz, Concepción Foces-Foces, José Elguero, Pedro Molina, Mateo Alajarin and Angel Vidal**
- 2041 Photocycloaddition of cyanonaphthalenes with acetylacetone: enhancement of quantum yields by sulphuric acid **Yuan L. Chow, Gonzalo E. Buono-Core, Yu-Hang Zhang and Xiao-Yun Liu**
- 2047  $^1H$  and  $^{13}C$  NMR studies on the conformation of *N*-methyl diastereomers of (+)-glauoine hydrotrifluoroacetate, an aporphine alkaloid salt **Robert Glaser and Michael A. Bernstein**
- 2055 Metal-catalysed ionization of a cyclic 1,3-diketone. The effects of nickel(II) and copper(II) on the ionization of 2-acetylcyclohexanone **Michael J. Hynes, Carlos A. Blanco and Marie T. Mooney**
- 2061 Photochemical reaction of 2,4,4,6-tetraaryl-4*H*-pyrans and -4*H*-thiopyrans with colour change by a 1,5-electrocyclic reaction. X-Ray molecular structure of 4-methyl-2,3,6-triphenyl-2*H*-thiopyran **Yukie Mori and Koko Maeda**
- 2067 Evidence for the formation of nitrenium ions in the acid-catalysed solvolysis of mutagenic *N*-acetoxy-*N*-alkoxy-benzamides **John J. Campbell, Stephen A. Glover, Gerard P. Hammond and Colleen A. Rowbottom**
- 2081 Solid state conformations of six 1,3,2-oxazaphospholidines derived from (–)-ephedrine: X-ray crystal structures of the 2-phenoxy-2-oxo, 2-phenyl-2-oxo and 2-phenyl-2-thio analogues **Carl H. Schwalbe, Geetanjee Chopra, Sally Freeman, John M. Brown and Joseph V. Carey**
- 2091 Solvent-induced mechanistic changes in nitrosation reactions. Part 2. Effect of acetonitrile–water mixtures in the nitrosation of ureas **Carlos Bravo, Pablo Hervés, J. Ramón Leis and M. Elena Peña**
- 2097 Photochemical reaction between acenaphthene and arenecarbonitriles **Enrico Boggeri, Elisa Fasani, Mariella Mella and Angelo Albini**
- 2103 Kinetics and mechanism of reserpine oxidation by nitrous acid. A reinterpretation of recent results **M. A. Muñoz, D. González-Arjona, M. Balón and D. Lyn H. Williams**

## AUTHOR INDEX

- Adams, Gerald E., 1941  
Alajarin, Mateo, 2033  
Albini, Angelo, 1977, 2097  
Al-Kazwini, Akeel T., 1941  
Apeloig, Yitzhak, 1865  
Arai, Yoshihisa, 1959  
Araki, Koji, 1883  
Balón, M., 2103  
Ba-Saif, Salem A., 1901  
Becher, Jan, 1963  
Beer, Paul D., 1947  
Beeson, Craig, 1913  
Bernstein, Michael A., 2047  
Blake, Alexander J., 2003  
Blanco, Carlos A., 2055  
Boggeri, Enrico, 2097  
Bravo, Carlos, 2091  
Brown, John M., 2081  
Buono-Core, Gonzalo E., 2041  
Campbell, John J., 2067  
Carey, Joseph V., 2081  
Castro, Enrique A., 1919  
Chopra, Geetanlee, 2081  
Chow, Yuan L., 2041  
Colthurst, Matthew, 1901  
Cundall, Robert B., 1941  
d'Alessandro, Nicola, 1977  
Dang, Hai-Shan, 2011  
Danovich, David, 1865  
Davies, Alwyn G., 2011, 2021  
Denny, William A., 1933  
Dix, Thomas A., 1913  
Dolgy, Igor E., 1875  
Edge, Stephen, 1963  
Elguero, José, 2033  
Fan, Jun-Yao, 1933  
Fasani, Elisa, 1977, 2097  
Fleet, George W. J., 1991  
Foces-Foces, Concepción, 2033  
Freeman, Sally, 2081  
Gensmantel, Nigel, 2025  
Glaser, Robert, 2047  
Glover, Stephen A., 2067  
González-Arjona, D., 2103  
Gordon, Isobel M., 1951  
Gravatt, G. Lance, 1933  
Grigor, Bruce A., 1933  
Grootenhuis, Peter D. J., 1883  
Gunstone, Frank D., 1955  
Hall, C. Dennis, 1925, 1947  
Hammond, Gerard P., 2067  
Hansen, Thomas K., 1963  
Hawkins, Ian, 1963  
Hervés, Pablo, 2091  
Hibbert, Frank, 1909  
Hillier, Ian H., 2025  
Huang, Zhi-Tang, 1967  
Hughes, Lise, 1893  
Hynes, Michael J., 2055  
Ibáñez, Fernando, 1919  
Ingemann, Steen, 1887, 1985  
Ingold, Keith U., 1893  
Jackson, Richard A., 1955  
Junino, Alex, 1941  
Koh, Han Joong, 1981  
Krylova, Irina V., 1875  
Lang, Gerard, 1941  
Larsen, Sine, 1963  
Lee, Ikchoon, 1981  
Leis, J. Ramón, 2091  
Liu, Xiao-Yun, 2041  
Llamas-Saiz, Antonio L., 2033  
MacCorquodale, Finlay, 1893  
Maeda, Koko, 2061  
Marziano, Nunziata C., 1995  
Maskill, H., 1951  
McLennan, Duncan J., 1933  
McNab, Hamish, 1999, 2003  
Mella, Mariella, 1977, 2097  
Molina, Pedro, 2033  
Monahan, Lilian C., 1999, 2003  
Mooney, Marie T., 2055  
Mordi, Raphael C., 1955  
Mori, Yukie, 2061  
Muñoz, M. A., 2103  
Namgoong, Sung Keon, 1991  
Nassimbeni, Luigi R., 1971  
Nefedov, Oleg M., 1875  
Neville, Anthony G., 2021  
Nibbering, Nico M. M., 1887, 1985  
Niven, Margaret L., 1971  
O'Connor, Charmian J., 1933  
Oh, Hyuck Keun, 1981  
Okonnishnikova, Galina P., 1875  
O'Neill, Peter, 1941  
Palou, Juan, 1925  
Payling, David W., 2025  
Peña, M. Elena, 2091  
Pérez Plá, Francisco, 1925  
Phillips, Siân C., 1909  
Ramsden, Nigel G., 1991  
Reinhoudt, David N., 1883  
Riveros, Jose M., 1985  
Rowbottom, Colleen A., 2067  
Sakaguchi, Masashi, 1959  
Sampoli, Marco, 1995  
Santos, José G., 1919  
Sato, Atsushi, 1971  
Schwalbe, Carl H., 2081  
Shavrin, Konstantin N., 1875  
Shinkai, Seiji, 1883  
Shvedova, Inna B., 1875  
Speers, Peter, 1925  
Sugimoto, Toyonari, 1959  
Thorisson, Snorri, 1955  
Toda, Fumio, 1971  
Tomasin, Alberto, 1995  
Underhill, Allan E., 1963  
Ureta, Carmen, 1919  
Valero, Rosa, 1925  
Varma, K. Sukumar, 1963  
Vidal, Angel, 2033  
Walton, John C., 1893, 1955  
Waring, Mark A., 1901  
Waszkowycz, Bohdan, 2025  
Williams, Andrew, 1901  
Williams, D. Lyn H., 2103  
Yamauchi, Jun, 1959  
Yoshida, Zen-ichi, 1959  
Zappey, Herman W., 1887  
Zhang, Yu-Hang, 2041  
Zhao, Wen-Yi, 1967

---

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

## Communications in Physical Organic Chemistry

Following the highly successful introduction of a communications section into the journal *Perkin Transactions 1*, we are pleased to announce that from January 1992 the same facility will be offered in the sister journal *Perkin Transactions 2*. Scientists having results in all areas of physical organic chemistry that warrant urgent publication should send three copies of the manuscript to the following address:

Dr. Sheila R. Buxton  
Royal Society of Chemistry  
Thomas Graham House  
Science Park  
Milton Road  
Cambridge CB4 4WF, UK

Authors should provide written justification for urgent publication and, where appropriate, key experimental data should be included in the paper.