

## JOURNAL OF THE CHEMICAL SOCIETY

**Perkin Transactions II**

## Physical Organic Chemistry

**CONTENTS**

- 1355 Hydrogen bonding. Part 9. Solute proton donor and proton acceptor scales for use in drug design **Michael H. Abraham, Philip P. Duce, David V. Prior, Derek G. Barratt, Jeffrey J. Morris, and Peter J. Taylor**
- 1377 Conformational analysis. Part 14. A lanthanide-induced shift n.m.r. analysis of indan-1-one and norcamphor **Raymond J. Abraham, Derek J. Chadwick, Paul E. Smith, and Fernando Sancassan**
- 1385 Trends in selectivity. Evidence from rates and products for simultaneous reaction channels in solvolyses of benzoyl chloride and substituted derivatives **T. William Bentley and In Sun Koo**
- 1393 Effects of  $\alpha$  and  $\gamma$  substituents on the relative reactivity of pyrylium and thiopyrylium cations **Giancarlo Doddi and Gianfranco Ercolani**
- 1397 N.m.r. spectroscopic and X-ray crystallographic studies on some *o*-NO<sub>2</sub> substituted aromatic sulphur amides **Pirkko Ruostesuo, Anna-Maija Häkkinen, Raikko Kivekäs, and Markku R. Sundberg**
- 1405 The formation of 2-oxopropyl-2-oxopropylidenediphenylphosphorane. Crystal and molecular structure of its lithium enolate **Olyana Angelova, Emil M. G. Kirilov, Marko Kirilov, Galin Petrov, José Kaneti, and Josef Macicek**
- 1409 Dynamic molecular motions of *p*-methylcinnamic acid included into  $\beta$ -cyclodextrin derivatives: a new type of free-energy relationship in complex formation **Yasuhisa Kuroda, Masahiko Yamada, and Iwao Tabushi**
- 1417 Reduction of dioxygen by an NADH model compound and 1,1'-dimethylferrocene catalysed by acids in homogeneous and heterogeneous systems **Shunichi Fukuzumi, Makoto Chiba, Masashi Ishikawa, Kunio Ishikawa, and Toshio Tanaka**
- 1425 Reactivity in S<sub>N</sub>Ar reactions of 2-(4-chloro-3-nitrophenyl)-1,3-diphenyl-1,3,4-triazol-1-ium-5-thiolate with some anionic and neutral nucleophiles **Aurea Echevarria and Joseph Miller**
- 1429 Photochromic formazans: X-ray crystal structure magnetic resonance and Raman spectra of 3-methyl-1,5-diphenylformazan and 3-*t*-butyl-1,5-diphenylformazan **Christopher W. Cunningham, Gary R. Burns, and Vickie McKee**
- 1437 Unusual co-ordination of water to iron(II) amino acid basket-handle porphyrins **P. Maillard, C. Schaeffer, C. Tétreau, D. Lavalette, J-M. Lhoste, and M. Momenteau**
- 1443 Characterization of two polymorphic forms of tolfenamic acid, *N*-(2-methyl-3-chlorophenyl)anthranilic acid: their crystal structures and relative stabilities **Kim Vilbour Andersen, Sine Larsen, Børge Alheda, Niels Gelting, and Ole Buchardt**
- 1449 Interchromophoric homoconjugation effect and intramolecular charge-transfer transition of the triptycene system containing a tetracyanoquinodimethane chromophore **Nobuyuki Harada, Hisashi Uda, Kazuhiro Nakasuji, and Ichiro Murata**
- 1455 Protonation of carboxylic acids by hydrogen bromide in dibromodifluoromethane: rates of proton exchange; relative basicities; and the acidity of HBr-CBr<sub>2</sub>F<sub>2</sub> **David R. Clark, John Emsley, and Frank Hibbert**
- 1459 Conformational study of bridgehead lactams. Preparation and X-ray structural analysis of 1-azabicyclo[3.3.1]nonane-2,6-dione **Peter H. McCabe, Neal J. Milne, and George A. Sim**
- 1463 An e.s.r. investigation of radical cations formed in Friedel-Crafts reactions **Hanqing Wang, Lowell D. Kispert, and Hong Sang**
- 1471 *N*-Nitroso compounds. Part 1. Structure and decomposition of *N*-nitroso-2-arylimidazolines in aqueous acidic media **Jim Iley, Fátima Norberto, and Eduarda Rosa**

- 1477 Photoresponsive peptide and polypeptide systems. Part 7. Reversible chiral photochromism and solubility change of azo aromatic L-lysine related compounds **Hiroyuki Yamamoto, Ayako Nishida, and Takashi Shimozawa**
- 1483 Unimolecular reactions of isolated  $C_4H_8O^{+}$  ions derived from unbranched butenols **Richard D. Bowen and Alex G. Harrison**
- 1491 Unusual host properties. X-Ray structures of three salt-like crystalline aggregates of 1,1'-binaphthyl-8,8'-dicarboxylic acid **Ingeborg Csöreg, Mátyás Czugler, Karl W. Törnroos, Edwin Weber, and Jochen Ahrendt**
- 1499 The tautomeric equilibria of thio analogues of nucleic acid bases. Part 1. 2-Thiouracil: background, preparation of model compounds, and gas-phase proton affinities **Alan R. Katritzky, Gokhan Baykut, Stanislaw Rachwal, Mirosław Szafran, Kenneth C. Caster, and John Eyler**
- 1507 The tautomeric equilibria of thio analogues of nucleic acid bases. Part 2.<sup>1</sup> AM1 and *ab initio* calculations of 2-thiouracil and its methyl derivatives **Alan R. Katritzky, Mirosław Szafran, and John Stevens**
- 1513 The reaction of triphenylmethyl halides with tributylphosphine and tributylamine in apolar solvents **Péter Huszthy, Gyöngyi Izsó, Károly Lempert, Mária Kajtár-Peredy, Miklós Győr, Antal Rockenbauer, and József Tamás**
- 1521 Chemical ionization mass spectra of urethanes **Andrew D. Wright, Richard D. Bowen, and Keith R. Jennings**
- 1529 Highly selective aromatic chlorination. Part 3. Kinetics and mechanism of chlorination of electron-rich aromatic compounds by *N*-chloroamines in acidic solution **John R. Lindsay Smith, Linda C. McKeer, and Jonathan M. Taylor**
- 1537 Highly selective aromatic chlorination. Part 4. The chlorination of aromatic hydrocarbons with *N*-chloroamines in acidic solution **John R. Lindsay Smith, Linda C. McKeer, and Jonathan M. Taylor**
- 1545 Cyclisation of 3-phenylpropan-1-ol *via* alkoxy radical and aryl radical-cation intermediates. A product and e.s.r. study **Bruce C. Gilbert and Cedric W. McClelland**
- 1553 Structure and conformation of polynitrodiphenylmethanes and related carbanions **Marie-Paule Simonnin, Hai-Qi Xie, François Terrier, Jacques Lelievre, and Patrick G. Farrell**
- 1559 Cyclisation of  $\omega$ -(isocyanatocarbonyl)alkyl radicals: acyclic precursors of imidyl radicals **Parveen Kaushal and Brian P. Roberts**
- 1569 Pulse radiolysis of monohalogenated biphenyls. Correlation of absorption spectra of the radical cations with photoelectron spectroscopic data **Elke Anklam, Klaus-Dieter Asmus, and Larry W. Robertson**
- 1573 Radical cations of polychlorinated and polybrominated biphenyls in 1,2-dichloroethane: a pulse radiolysis study **Elke Anklam, Klaus-Dieter Asmus, and Larry W. Robertson**
- 1577 The effect of the carboxy group on the chemical and  $\beta$ -lactamase reactivity of  $\beta$ -lactam antibiotics **Andrew P. Laws and Michael I. Page**
- 1583 Photoreduction of phenacyl halides by NADH analogues. Origins of different mechanistic pathways **Shunichi Fukuzumi, Seiji Mochizuki, and Toshio Tanaka**

## Corrigendum

- 
- 1591 Internal hydrogen bonding in benzo[*a*]pyrene diol and diol epoxide metabolites **Anthony C. Capomacchia, Vijay Kumar, and Robert N. Jennings**

## AUTHOR INDEX

- Abraham, Michael H., 1355  
Abraham, Raymond J., 1377  
Ahrendt, Jochen, 1491  
Alheda, Børge, 1443  
Andersen, Kim Vilbour, 1443  
Angelova, Olyana, 1405  
Anklam, Elke, 1569, 1573  
Asmus, Klaus-Dieter, 1569, 1573  
Barratt, Derek G., 1355  
Baykut, Gokhan, 1499  
Bentley, T. William, 1385  
Bowen, Richard D., 1483, 1521  
Buchardt, Ole, 1443  
Burns, Gary R., 1429  
Capomacchia, Anthony C., 1591  
Caster, Kenneth C., 1499  
Chadwick, Derek J., 1377  
Chiba, Makoto, 1417  
Clark, David R., 1455  
Csöreg, Ingeborg, 1491  
Cunningham, Christopher W., 1429  
Czugler, Mátyás, 1491  
Doddi, Giancarlo, 1393  
Duce, Philip P., 1355  
Echevarria, Aurea, 1425  
Emsley, John, 1455  
Ercolani, Gianfranco, 1393  
Eyler, John, 1499  
Farrell, Patrick G., 1553  
Fukuzumi, Shunichi, 1417, 1583  
Gelting, Niels, 1443  
Gilbert, Bruce C., 1545  
Győr, Miklós, 1513  
Häkkinen, Anna-Maija, 1397  
Harada, Nobuyuki, 1449  
Harrison, Alex G., 1483  
Hibbert, Frank, 1455  
Huszthy, Péter, 1513  
Iley, Jim, 1471  
Ishikawa, Kunio, 1417  
Ishikawa, Masashi, 1417  
Izsó, Gyöngyi, 1513  
Jennings, Keith R., 1521  
Jennings, Robert N., 1591  
Kajtar-Peredy, Mária, 1513  
Kaneti, José, 1405  
Katritzky, Alan R., 1499, 1507  
Kaushal, Parveen, 1559  
Kirilov, Emil M. G., 1405  
Kirilov, Marko, 1405  
Kispert, Lowell D., 1463  
Kivekäs, Raikko, 1397  
Koo, In Sun, 1385  
Kumar, Vijay, 1591  
Kuroda, Yasuhisa, 1409  
Larsen, Sine, 1443  
Lavalette, D., 1437  
Laws, Andrew P., 1577  
Lelievre, Jacques, 1553  
Lempert, Károly, 1513  
Lhoste, J.-M., 1437  
Macicek, Josef, 1405  
Maillard, P., 1437  
McCabe, Peter H., 1459  
McClelland, Cedric W., 1545  
McKee, Vickie, 1429  
McKeer, Linda C., 1529, 1537  
Miller, Joseph, 1425  
Milne, Neal J., 1459  
Mochizuki, Seiji, 1583  
Mometeau, M., 1437  
Morris, Jeffrey J., 1355  
Murata, Ichiro, 1449  
Nakasuji, Kazuhiro, 1449  
Nishida, Ayako, 1477  
Norberto, Fátima, 1471  
Page, Michael I., 1577  
Petrov, Galin, 1405  
Prior, David V., 1355  
Rachwal, Stanislaw, 1499  
Roberts, Brian P., 1559  
Robertson, Larry W., 1569, 1573  
Rockenbauer, Antal, 1513  
Rosa, Eduarda, 1471  
Ruostesuo, Pirkko, 1397  
Sancassan, Fernando, 1377  
Sang, Hong, 1463  
Schaeffer, C., 1437  
Shimozawa, Takashi, 1477  
Sim, George A., 1459  
Simonin, Marie-Paule, 1553  
Smith, John R. Lindsay, 1529, 1537  
Smith, Paul E., 1377  
Stevens, John, 1507  
Sundberg, Markku R., 1397  
Szafran, Miroslaw, 1499, 1507  
Tabushi, Iwao, 1409  
Tamás, József, 1513  
Tanaka, Toshio, 1417, 1583  
Taylor, Jonathan M., 1529, 1537  
Taylor, Peter J., 1355  
Tétreau, C., 1437  
Terrier, François, 1553  
Törnroos, Karl W., 1491  
Uda, Hisashi, 1449  
Wang, Hanqing, 1463  
Weber, Edwin, 1491  
Wright, Andrew D., 1521  
Xie, Hai-Qi, 1553  
Yamada, Masahiko, 1409  
Yamamoto, Hiroyuki, 1477

---

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

