

JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions 2

Physical Organic Chemistry

CONTENTS

- 1501 Prototropic tautomerism in *N,N*-dimethyl-*N'*-(1-nitro-9-acridyl)propane-1,3-diamine and its nitro isomers. Application of MNDO and PPP methods for the examination of structure and electronic absorption spectra **Anna Tempczyk, Janusz Rak, and Jerzy Błażejowski**
- 1509 An ESR study of thermal and photo-induced formation of radicals from anthralin and acylated derivatives **Pierre Lambelet, Elizabeth Prior, Jürg Löliger, and Braham Shroot**
- 1515 A structural study of 3- and 4-iodosylbenzoic acids, 3- and 4-iodylbenzoic acids, and their sodium salts **Alan R. Katritzky, G. Paul Savage, John K. Gallos, and H. Dupont Durst**
- 1519 A linear dichroism and cyclic voltammetric study of substituted naphthoquinones and an ESR investigation of the corresponding anion and cation radicals **Giovanni Gottarelli, Marco Lucarini, Gian Franco Pedulli, Gian Piero Spada, and Sergio Roffia**
- 1523 Synthesis of 1,10-dithia-4,7,13,16-tetra-azacyclo-octadecane, 1-aza-4,7-dithiacyclononane, and *N,N'*-1,2-bis(1-aza-4,7-dithiacyclononyl)ethane. Structural and solution studies of their silver complexes **Andrew S. Craig, Ritu Katakya, Robert C. Matthews, David Parker, George Ferguson, Alan Lough, Harry Adams, Neil Bailey, and Hermann Schneider**
- 1533 Base-catalysed aromatic nucleophilic substitution reactions of *O*-aryl oximes with pyrrolidine in non-polar aprotic, dipolar aprotic, and protic solvents **Ajay K. Jain, Vinod K. Gupta, and Anurag Kumar**
- 1539 Mechanistic interpretation of the simultaneous hydrolysis and methanolysis of chloromethyl chloroacetate in weakly acidic aqueous methanol solutions of varying solvent composition **Liisa T. Kanerva**
- 1545 Empirical correlations of partial molar volumes at infinite dilution of organic solutes and transition states for S_N1 and S_N2 ethanolsysis of alkyl halides **Hidenori Itsuki, Hisashi Yamamoto, Haruo Okazaki, and Seiji Terasawa**
- 1551 Amidines. Part 33. Full *ab initio* 3-21G optimization of the molecular structures of fluoro derivatives of formamidine and their protonation products. Quantitative structure-basicty relations of amidines **Janusz Oszczapowicz, Claus U. Regelmann, and Günter Häfelinger**
- 1559 Isolation, structure elucidation, and synthesis of novel penicillin degradation products: thietan-2-ones **Kirk A. Ashline, Robin P. Attrill, Edward K. Chess, J. Peter Clayton, Ernest A. Cutmore, Jeremy R. Everett, John H. C. Nayler, David E. Pereira, Walter J. Smith III, John W. Tyler, Michael L. Vieira, and Michal Sabat**
- 1567 A survey of the high-field 1H NMR spectra of the steroid hormones, their hydroxylated derivatives, and related compounds **David N. Kirk, Harold C. Toms, Christal Douglas, Karen A. White, Kelvin E. Smith, Shahid Latif, and Robert W. P. Hubbard**
- 1595 On the lack of reactivity of Buckminsterfullerene. A theoretical study **Dragan Amić and Nenad Trinajstić**
- 1599 Macro-rings designed for uncharged molecule complexation. Synthesis, complex formation, and structural studies of new pyridino crowns incorporating resorcinol and hydroquinone building blocks. X-Ray crystal and molecular structure of a 22-membered pyridino crown **Edwin Weber, Hans-Jürgen Köhler, Kaliyamoorthy Panneerselvam, and Kizakkekoikkal K. Chacko**
- 1607 A novel electro-organic synthesis of pyrrolopyrazole derivatives **Hussein M. Fahmy, Mohey E. Sharaf, Mohammed A. Aboutabl, Mahmoud M. M. Ramiz, Magdi Abdel El-Azzem, and Hassan Abd El-Rahman**

- 1615 ^{13}C NMR and AM1 study of the intramolecular proton transfer in solid 1,3-diphenylpropane-1,3-dione **Alejandro J. Vila, Claudia M. Lagier, and Alejandro C. Olivieri**
- 1619 2,5-Dihydro-1,2,3,5-thiazotriazole 1-oxides, 2*H*-1,2,3,5-thiazotriazol-1-ium salts, and 2,5-dihydro-1,2,3,5-thiazotriazol-5-yl radicals. X-Ray molecular structure of 2,5-dihydro-2,4-diphenyl-1,2,3,5-thiazotriazole 1-oxide and 2,4-diphenyl-2*H*-1,2,3,5-thiazotriazol-1-ium bromide **Franz A. Neugebauer, Hans Fischer, Rowena Crockett, and Claus Krieger**
- 1627 A theoretical approach to the vibrational analysis of the nitroenamine system **Jose Luis Chiara, Antonio Gómez-Sánchez, and Enrique Sánchez Marcos**
- 1637 Substituent effects on the hydrolysis of analogues of nitracrine {9-[3-(*N,N*-dimethylamino)propylamino]-1-nitroacridine} **Charmian J. O'Connor, Duncan J. McLennan, William A. Denny, and Bridget M. Sutton**

Corrigenda

- 1643 Application of coupled oscillator theory to conformational analysis of glycosides with aromatic groups **Masato Kodaka**

AUTHOR INDEX

- Aboutabl, Mohammed A., 1607
Adams, Harry, 1523
Amić, Dragan, 1595
Ashline, Kirk A., 1559
Attrill, Robin P., 1559
Bailey, Neil, 1523
Błażejowski, Jerzy, 1501
Chacko, Kizakkekoikkal K., 1599
Chess, Edward K., 1559
Chiara, Jose Luis, 1627
Clayton, J. Peter, 1559
Craig, Andrew S., 1523
Crockett, Rowena, 1619
Cutmore, Ernest A., 1559
Denny, William A., 1637
Douglas, Christal, 1567
Durst, H. Dupont, 1515
El-Azzem, Magdi Abdel, 1607
El-Rahman, Hassan Abd, 1607
Everett, Jeremy R., 1559
Fahmy, Hussein M., 1607
Ferguson, George, 1523
Fischer, Hans, 1619
Gallos, John K., 1515
Gómez-Sánchez, Antonio, 1627
Gottarelli, Giovanni, 1519
Gupta, Vinod K., 1533
Häfelinger, Günter, 1551
Hubbard, Robert W. P., 1567
Itsuki, Hidenori, 1545
Jain, Ajay K., 1533
Kanerva, Liisa T., 1539
Katak, Ritu, 1523
Katritzky, Alan R., 1515
Kirk, David N., 1567
Kodaka, Masato, 1643
Köhler, Hans-Jürgen, 1599
Krieger, Claus, 1619
Kumar, Anurag, 1533
Lagier, Claudia M., 1615
Lambelet, Pierre, 1509
Latif, Shahid, 1567
Lölinger, Jürg, 1509
Lough, Alan, 1523
Lucarini, Marco, 1519
Marcos, Enrique Sánchez, 1627
Matthews, Robert C., 1523
McLennan, Duncan J., 1637
Nayler, John H. C., 1559
Neugebauer, Franz A., 1619
O'Connor, Charmian J., 1637
Okazaki, Haruo, 1545
Olivieri, Alejandro C., 1615
Oszczapowicz, Janusz, 1551
Panneerselvam, Kaliyamoorthy, 1599
Parker, David, 1523
Pedulli, Gian Franco, 1519
Pereira, David E., 1559
Prior, Elizabeth, 1509
Rak, Janusz, 1501
Ramiz, Mahmoud M. M., 1607
Regelmann, Claus U., 1551
Roffia, Sergio, 1519
Sabat, Michal, 1559
Savage, G. Paul, 1515
Schneider, Hermann, 1523
Sharaf, Mohey E., 1607
Shroot, Braham, 1509
Smith, Kelvin E., 1567
Smith, Walter J., III, 1559
Spada, Gian Piero, 1519
Sutton, Bridget M., 1637
Tempczyk, Anna, 1501
Terasawa, Seiji, 1545
Toms, Harold C., 1567
Trinajstić, Nenad, 1595
Tyler, John W., 1559
Vieira, Michael L., 1559
Vila, Alejandro J., 1615
Weber, Edwin, 1599
White, Karen A., 1567
Yamamoto, Hisashi, 1545

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

