

JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions II

Physical Organic Chemistry

CONTENTS

- 1289 ^{13}C Nuclear magnetic resonance spectroscopy of nitrogen heterocycles. Part 4. *intra-extra* Configuration of the *N*-acetyl group in phenothiazine and related systems with a ‘butterfly’ shape **Enzio Ragg, Giovanni Fronza, Rosanna Mondelli, and Giancarlo Scapini**
- 1293 Improvement of the applicability of Taft–Kamlet solvent polarity parameters to chemical reactivity **Vojtěch Bekárek**
- 1297 *Ab initio* calculation of the molecular structure and electronic properties of carbodi-imide, $\text{HN}=\text{C}=\text{NH}$ **Minh-Tho Nguyen and Tae-Kyu Ha**
- 1301 One-electron oxidation of closed-shell molecules. Part 3. Oxidative cleavage of 1,2,2,2-tetrakis-(*p*-methoxyphenyl)-ethanone with dibenzoyl and bis-(3,5-dinitrobenzoyl) peroxides: mechanistic changeover of the peroxide function from radical to molecular oxidation **Ken'ichi Takeuchi, Osamu Murai, Shin Matsui, Takeshi Inoue, Toshikazu Kitagawa, and Kunio Okamoto**
- 1311 Studies in decarboxylation. Part 16. Steric inhibition of resonance in a 1,5-sigmatropic reaction **Amal al-Borno and David B. Bigley**
- 1313 Photochemistry in micelles as a model for the *in vivo* phototoxicity of chlorpromazine **Gary A. Epling, Carole Black, and Viresh Rawal**
- 1317 1,3-Dipolar cycloaddition of azonium dicyanomethylides **Enrique Díez-Barra, Carmen Pardo, José Elguero, and Jean Arriau**
- 1321 β -Thioxoketones. Part 9. A dynamic ^1H nuclear magnetic resonance spectroscopic study of thioacetylacetone and related β -thioxoketones. Direct observation of the enol and enethiol tautomeric constituents and their interconversion **Ulf Berg, Jan Sandström, Lars Carlsen, and Fritz Duus**
- 1327 Effect of poly(diallyldimethylammonium chloride) and of poly(ethyleneimine) on the esterolysis of 8-acetoxy-quinoline **Antonio Arcelli and Carlo Concilio**
- 1333 Reactivity of certain piperidin-4-ols towards oxidation with cerium(IV) **Chenniappan Vasantha Devi, Kuppusamy Selvaraj, Kondareddiar Ramalingam, and Krishnasamy Ramarajan**
- 1337 Nucleophilic attack at $\alpha\beta$ -unsaturated carbonyl systems. The reactions of acrolein and methyl acrylate with CF_3O^- , $[\text{F}^- \cdots \text{HOME}]$, RO^- , and $\text{RO}^- \cdots \text{HOR}$. An *ab initio* and ion cyclotron resonance study **Gunter Klass, John C. Sheldon, and John H. Bowie**
- 1343 Photochemistry of 1,2-diketones. Part 5. Formation of dihydrodioxines, oxetanes, allylic ethers, and 1,2-adducts from alicyclic 1,2-diketones and alkenes **Paul L. Verheijdt and Hans Cerfontain**
- 1351 Conformations and barriers to inversion of some cyclic seven-membered α -diketones. A study by dynamic nuclear magnetic resonance spectroscopy and molecular mechanics calculations **Roland Isaksson and Tommy Liljefors**
- 1357 High-resolution ^{13}C nuclear magnetic resonance spectra of some solid anthraquinone dyestuffs and related species **A. Margaret Chippendale, Alan Mathias, Rajinder S. Aujla, Robin K. Harris, Kenneth J. Packer, and Barry J. Say**
- 1363 Quasiphosphonium intermediates. Part 3. Preparation, structure, and reactivity of alkoxyphosphonium halides in the reactions of neopentyl diphenylphosphinite, dineopentyl phenylphosphonite, and trineopentyl phosphite with halogeno-

- methanes and the effect of phenoxy-substituents on the mechanism of alkyl–oxygen fission in Michaelis–Arbusov reactions **Harry R. Hudson, Aloysius Kow, and John C. Roberts**
- 1369 Degradation of *O*-arylisoureas in alkali: a low temperature Chapman-type rearrangement **Nicola A. Suttle and Andrew Williams**
- 1373 An electron spin resonance study of aminoallyl, aminopropynyl, and aminocyanomethyl radicals **David Griller, Derek C. Nonhebel, and John C. Walton**
- 1381 A comparison of the mechanisms of hydrolysis of diphenylketene and dimethylketene in diethyl ether solution **Nai L. Poon and Derek P. N. Satchell**
- 1385 Stabilities of electron donor–acceptor complexes of aromatic hydrocarbons with 1-(2,4,6-Trinitrophenyl)propan-2-one in solution from nuclear magnetic resonance shift measurements **John A. Chudek, Roy Foster, and David R. Twiselton**
- 1391 ^{14}N and ^2H quadrupole double resonance in substituted imidazoles **Maria L. S. Garcia, John A. S. Smith, P. M. G. Bayin, and C. R. Ganellin**
- 1401 ^{14}N and ^2H quadrupole double resonance in salts of cytosine and adenine **Maria L. S. Garcia and John A. S. Smith**
- 1409 Nitrogen bridgehead compounds. Part 29. Tautomerism and *Z*–*E* isomerism of ethyl 9-aminomethylene-4-oxo-6,7,8,9-tetrahydro-4*H*-pyrido[1,2-*a*]pyrimidine-3-carboxylates and their homologues **Gábor Tóth, Áron Szöllősy, Benjamin Podányi, István Hermecz, Ágnes Horváth, Zoltán Mészáros, and István Bitter**
- 1413 Nitrogen bridgehead compounds. Part 32. Absolute configuration and circular dichroism of 6-methyl-tetrahydro-4*H*-pyrido[1,2-*a*]pyrimidin-4-ones **István Hermecz, Péter R. Surján, Tibor Breining, Kálman Simon, Gábor Horváth, Zoltán Mészáros, Márton Kajtár, and Gábor Tóth**
- 1421 Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 8. Conductimetric and spectrophotometric rate constants for the reactions of pyridinium and related cations with piperidine in chlorobenzene **Alan R. Katritzky, Yu Xiang Ou, Joan Ellison, and Giuseppe Musumarra**
- 1427 Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 9. *N*-Substituted 2,4,6-triphenylpyridiniums, 5,6-dihydro-2,4-diphenylbenzo[*h*]quinoliniums, and 5,6,8,9-tetrahydro-7-phenyldibenzo[*c,h*]acridiniums: kinetic rate variation with structure of the *N*-substituent **Alan R. Katritzky, Kumars Sakizadeh, Yu Xiang Ou, Bratislav Jovanovic, Giuseppe Musumarra, Francesco P. Ballistreri, and Roberto Crupi**
- 1435 Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 10. Reactions of *s*-alkyl primary amines with pyryliums **Alan R. Katritzky, Jorge Marquet, Jeremy M. Lloyd, and James G. Keay**
- 1443 Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 11. ρ^* Plots for the solvolysis of 1-*s*-alkyl-5,6-dihydro-2,4-diphenylbenzo[*h*]quinolinium cations **Alan R. Katritzky, Jorge Marquet, and Maria L. Lopez-Rodríguez**
- 1449 Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 12. Regio- and stereochemistry of nucleophilic displacement and solvolysis reactions of *N*-(α -Methylallyl)- and *N*-(α -Phenylethyl)-pyridiniums **Alan R. Katritzky, Yu Xiang Ou, and Giuseppe Musumarra**
- 1455 Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 13. Penta- and nonacyclic derivatives **Alan R. Katritzky and Charles M. Marson**
- 1463 Kinetics and mechanisms of nucleophilic displacements with heterocycles as leaving groups. Part 14. The preparation and reactions of some further α -heteroarylpyridinium salts **Alan R. Katritzky, Jacek Z. Brzezinski, Yu Xiang Ou, and Giuseppe Musumarra**
- 1471 Oxygen-17 and selenium-77 nuclear magnetic resonance of carbonyl and selenocarbonyl compounds. Correlation of oxygen-17 and selenium-77 chemical shifts **Tuck W. Wong, Frank S. Guziec, Jr., and Christine A. Moustakis**

AUTHOR INDEX

- al-Borno, A., 1311
Arcelli, A., 1327
Arriau, J., 1317
Aujla, R. S., 1357
Ballistreri, F. B., 1427
Bavin, P. M. G., 1391
Bekárek, V., 1293
Berg, U., 1321
Bigley, D. B., 1311
Bitter, I., 1409
Black, C., 1313
Bowie, J. H., 1337
Breining, T., 1413
Brzezinski, J. K., 1463
Carlsen, L., 1321
Cerfontain, H., 1343
Chippendale, A. M., 1357
Chudek, J. A., 1385
Concilio, C., 1327
Crupi, R., 1427
Devi, C. V., 1333
Diez-Barra, E., 1317
Duus, F., 1321
Elguero, J., 1317
- Ellison, J., 1421
Epling, G. A., 1313
Foster, R., 1385
Fronza, G., 1289
Ganellin, C. R., 1391
Garcia, M. L. S., 1391, 1401
Griller, D., 1373
Guziec, F. S. (Jr.), 1471
Ha, T.-K., 1297
Harris, R. K., 1357
Hermecz, I., 1409, 1413
Horváth, A., 1409
Horváth, G., 1413
Hudson, H. R., 1363
Inoue, T., 1301
Isaksson, R., 1351
Jovanovic, B., 1427
Kajtár, M., 1413
Katritzky, A. R., 1421, 1427,
 1435, 1443, 1449, 1455,
 1463
Keay, J. G., 1435
Kitagawa, T., 1301
Klass, G., 1337
- Kow, A., 1363
Liljefors, T., 1351
Lloyd, J. M., 1435
Lopez-Rodriquez, M. L.,
 1443
Marquet, J., 1435, 1443
Marson, C. M., 1455
Mathias, A., 1357
Matsui, S., 1301
Mészáros, Z., 1409, 1413
Mondelli, R., 1289
Moustaki, C. A., 1471
Murai, O., 1301
Musumarra, G., 1421, 1427,
 1449, 1463
Nguyen, M-T., 1297
Nonhebel, D. C., 1373
Okamoto, K., 1301
Ou, Y. X., 1421, 1427, 1449,
 1463
Packer, K. J., 1357
Pardo, C., 1317
Podányi, B., 1409
Poon, N. L., 1381
- Ragg, E., 1289
Ramalingam, K., 1333
Ramarajan, K., 1333
Rawal, V., 1313
Roberts, J. C., 1363
Sakizadeh, K., 1427
Sandström, J., 1321
Satchell, D. P. N., 1381
Say, B. J., 1357
Scapini, G., 1289
Selvaraj, K., 1333
Sheldon, J. C., 1337
Simon, K., 1413
Smith, J. A. S., 1391, 1401
Surján, P. R., 1413
Suttle, N. A., 1369
Szöllösy, Á., 1409
Takeuchi, K., 1301
Tóth, G., 1409, 1413
Twiselton, D. R., 1385
Verheijdt, P. L., 1343
Walton, J. C., 1373
Williams, A., 1369
Wong, T. C., 1471

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

