

## **ORGANIC REACTIONS MECHANISMS GROUP**

Following the annual general meeting of the Organic Reactions Mechanisms Group (ORMG) of The Royal Society of Chemistry on 5th January 1988, membership of the ORMG will be open to non-members of the RSC from 1989. This initiative by the ORMG is intended to widen its membership to all chemists, especially those in continental Europe, who are interested in its subject area: experimental and theoretical investigations into mechanisms of reactions and reactivity of organic compounds including reactive intermediates and biologically important molecules. For further details and information during 1988, please contact the secretary/treasurer of the ORMG: **Dr. H. Maskill, Department of Chemistry, University of Stirling, Stirling FK9 4LA, Scotland.**



## JOURNAL OF THE CHEMICAL SOCIETY

## Perkin Transactions II

## Physical Organic Chemistry

---

CONTENTS

- 427 Stacking structure with trimolecular units of donor-acceptor-donor in a charge-transfer complex of dinaphtho[1,2-*b*:1',2'-*e*]-1,4-dithiin with tetracyanoquinodimethane **Keiji Kobayashi, Miyuki Takahashi, and Hayao Kobayashi**
- 431 Synthetic and stereochemical studies of the octahydro-1-benzopyran system **D. Vaughan Griffiths and Geoffrey Wilcox**
- 437 Theoretical investigations of methanesulphonamide as a hydroxy group equivalent in drugs. Examples from possible  $\beta$ -adrenergic agents and analysis of computational methods **Sid Topiol, Michael Sabio, and Paul W. Erhardt**
- 443 Substituent effects on electron spin distribution and conformation of radical ions obtained from 9-diphenylmethylene-fluorenes **M. Luisa T. M. B. Franco, Bernardo J. Herold, Jeffrey C. Evans, and Christopher C. Rowlands**
- 451 Kinetics and mechanism of the reaction of 2,3-dimethoxy-1,4-naphthoquinone with alkoxide ions in alcoholic solvents **Vivian M. Flaten, José G. Santos, and Jaime A. Valderrama**
- 457  $\pi$ -Electron transfer as calculated at various levels of basis set. A redefinition of the theoretical scale of  $\sigma_R^\circ$  values **Stephen Marriott, Anthony Silvestro, and Ronald D. Topsom**
- 461 Studies on the benzoxazine series. Part 1. Preparation and  $^1\text{H}$  and  $^{13}\text{C}$  nuclear magnetic resonance structural study of some substituted 3,4-dihydro-2*H*-1,3-benzoxazines **Kari Neuvonen and Kalevi Pihlaja**
- 469 Conformational analysis of *peri*-interactions in naphthalene derivatives. Ring inversion in  $\text{CH}_2\text{-X-CH}_2$ -bridged *peri*-naphthalenes **J. Edgar Anderson and Flemming S. Jørgensen**
- 473 Ionization constants of 5-arylmethylenehydantoins in 80% (w/w) dimethyl sulphoxide-water at 25 °C **Sau-Fun Tan, Kok-Peng Ang, Yoke-Fan Fong, and Harilakshmi Jayachandran**
- 477 An *ab initio* study of the hydrogen addition to methyl isocyanide ( $\text{CH}_3\text{N}\equiv\text{C}$ ) and methanediazonium ion ( $\text{CH}_3\text{N}\equiv\text{N}^+$ ): a case of a bifurcating point on the potential energy surface **Seamus Malone, Anthony F. Hegarty, and Min Tho Nguyen**
- 485 Kinetics of protideacylation of 1-benzoylnaphthalene and its homologous in 89.8% sulphuric acid **Peter H. Gore, Baljit Singh Moonga, and Eric L. Short**
- 489 One-electron redox chemistry of amsacrine, mAMSA [9-(2-methoxy-4-methylsulphonylaminoanilino)acridinium], its quinone di-imine, and an analogue. A radiolytic study **Robert F. Anderson, John E. Packer, and William A. Denny**
- 497 Gas-phase carbanion rearrangements. Deprotonated benzyl and allyl ethers **Peter C. H. Eichinger and John H. Bowie**
- 507 Application of Penning ionization electron spectroscopy to assignments of electron spectroscopic bands of anthracene **Takashi Kajiwara, Shigeru Masuda, Koichi Ohno, and Yoshiya Harada**
- 513 Kinetics and mechanism of *S*-nitrosation of some thiol-containing amino acids and other thiols **Pip A. Morris and D. Lyn H. Williams**
- 517 Nucleophilic catalysis in the nitrosation of sarcosine and proline **Thomas A. Meyer and D. Lyn H. Williams**
- 523 Correlation and prediction of gas-liquid partition coefficients in hexadecane and olive oil **Michael H. Abraham and Richard Fuchs**

- 529 Barriers to rotation in intramolecularly hydrogen-bonded 2-phenylazoresorcinols **Frank Hibbert** and **Rowena J. Sellens**
- 533 Oxidation of secondary alcohols with t-butyl hypochlorite in the presence of pyridine **Jovan N. Milovanović**, **Miorad Vasojević**, and **Svetislav Gojkovic**
- 537 A mainly  $^{13}\text{C}$  nuclear magnetic resonance investigation of some indolo[2,3-*a*]quinolizinylium salts **Csaba Szántay, jr.**, **Gábor Tóth**, **Ede Márványos**, **György Thaler**, and **Helmut Duddeck**
- 543 Complex formation of phenol, aniline, and their nitro derivatives with  $\beta$ -cyclodextrin **Agnes Buvári** and **Lajos Barcza**
- 547 Oxidation of aliphatic alcohols by pyridinium fluorochromate: a kinetic study **Kalyan K. Banerji**
- 551 Prediction of selective bioreductive anti-tumour, anti-folate activity using a modified *ab initio* method for calculating enzyme-inhibitor interaction energies **Christopher A. Reynolds**, **W. Graham Richards**, and **Peter J. Goodford**
- 557 The *E1cb* route for ester hydrolysis; volumes of activation as an additional criterion of mechanism **Neil S. Isaacs** and **Tariq S. Najem**
- 563 Collision-induced dissociations of aryl-substituted alkoxide ions. Losses of dihydrogen and rearrangement processes **Mark J. Raftery**, **John H. Bowie**, and **John C. Sheldon**
- 571 Kinetics of hydrolysis of 1-acetoxy-, 1-acetoxy-8-hydroxy-, and 1,8-diacetoxy-naphthalenes; intramolecular participation by a hydroxy group **Frank Hibbert** and **Karen J. Spiers**
- 575 An electron spin resonance study of the regioselectivity of the cyclization of protonated and unprotonated pent-4-en-1-oxyl and pent-4-en-1-peroxyl radicals **A. J. Bloodworth**, **Alwyn G. Davies**, and **Robyn S. Hay-Motherwell**
- 583 Radical-nucleophilic ( $S_{\text{RN}}1$ ) reactions: electron spin resonance studies of electron-capture processes. Part 5. *p*-Nitrobenzyl and *p*-nitrocumyl systems **Martyn C. R. Symons** and **W. Russell Bowman**
- 591 Combined use of kinetic and crystallographic data to probe the hydrolysis of a simple amide **Patrick Camilleri**, **Joseph V. Carey**, **Barbara Odell**, and **David J. Williams**

## AUTHOR INDEX

- Abraham, Michael H., 523  
Anderson, J. Edgar, 469  
Anderson, Robert F., 489  
Ang, Kok-Peng, 473  
Banerji, Kalyan K., 547  
Barcza, Lajos, 543  
Bloodworth, A. J., 575  
Bowie, John H., 497, 563  
Bowman, W. Russell, 583  
Buvári, Agnes, 543  
Camilleri, Patrick, 591  
Carey, Joseph V., 591  
Davies, Alwyn G., 575  
Denny, William A., 489  
Duddeck, Helmut, 537  
Eichinger, Peter C. H., 497  
Erhardt, Paul W., 437  
Evans, Jeffrey C., 443  
Flaten, Vivian M., 451  
Fong, Yoke-Fan, 473  
Franco, M. Luisa T. M. B., 443  
Fuchs, Richard, 523  
Gojkovic, Svetislav, 533  
Goodford, Peter J., 551  
Gore, Peter H., 485  
Griffiths, D. Vaughan, 431  
Harada, Yoshiya, 507  
Hay-Motherwell, Robyn S., 575  
Hegarty, Anthony F., 477  
Herold, Bernardo J., 443  
Hibbert, Frank, 529, 571  
Isaacs, Neil S., 557  
Jørgensen, Flemming S., 469  
Jayachandran, Harilakshmi, 473  
Kajiwara, Takashi, 507  
Kobayashi, Hayao, 427  
Kobayashi, Keiji, 427  
Malone, Seamus, 477  
Marriott, Stephen, 457  
Márványos, Ede, 537  
Masuda, Shigeru, 507  
Meyer, Thomas A., 517  
Milovanović, Jovan N., 533  
Moonga, Baljit Singh, 485  
Morris, Pip A., 513  
Najem, Tariq S., 557  
Neuvonen, Kari, 461  
Nguyen, Min Tho, 477  
Odell, Barbara, 591  
Ohno, Koichi, 507  
Packer, John E., 489  
Pihlaja, Kalevi, 461  
Raftery, Mark J., 563  
Reynolds, Christopher A., 551  
Richards, W. Graham, 551  
Rowlands, Christopher C., 443  
Sabio, Michael, 437  
Santos, José G., 451  
Sellens, Rowena J., 529  
Sheldon, John C., 563  
Short, Eric L., 485  
Silvestro, Anthony, 457  
Spiers, Karen J., 571  
Symons, Martyn C. R., 583  
Szántay, jr., Csaba, 537  
Takahashi, Miyuki, 427  
Tan, Sau-Fun, 473  
Thaler, György, 537  
Tóth, Gábor, 537  
Topiol, Sid, 437  
Topsom, Ronald D., 457  
Valderrama, Jaime A., 451  
Vasojević, Miorad, 533  
Wilcox, Geoffrey, 431  
Williams, D. Lyn H., 513, 517  
Williams, David J., 591

---

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

