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Journal of the Chemical Society, Faraday Transactions

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1 Manuscripts must be typed in double-line spacing, single sided on A4 paper, with margins at top, bottom and left-hand side of at least 4 cm.

2 The first page should be set out as follows:

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(ii) Title of the paper, with capitals for the first letter of each noun and adjective only.

(iii) Authors' names, including one forename for each author.

(iv) The address where the work was carried out; if this is different from the current address a footnote indicating the present address of this author should be included. Present addresses of other authors are not normally given.

(v) Abstract, preceded and followed by a horizontal line, and typed in double-line spacing.

3 Suitable headings and sub-headings should be used in the main text as appropriate (except for communications in which no headings are used).

References should be numbered serially in the text by means of superscript arabic numerals.

4 Bibliographic references (not footnotes) should follow the main text and should have the following format:

1 C. Jarque and A. D. Buckingham, *J. Chem. Soc., Faraday Trans.*, 1992, **88**, 1353.

2 R. M. Barrer and R. J. B. Craven, in *New Developments in Zeolite Science and Technology*, ed. Y. Murakame, A. Iijima and J.W. Ward, Kodansha, Tokyo, 1986, p. 521.

Journal titles should be abbreviated according to the Chemical Abstracts Service Source Index (CASSI).

5 Tables should be typed on separate sheets at the end of the manuscript.

6 Diagrams should be accompanied by a separately typed set of captions. Extensive identifying lettering should be placed in the caption rather than on lines on graphs, *etc.* Original artwork should be supplied wherever possible. Colour photographs will be accepted only when a black-and-white photograph fails to show some vital feature.

7 Bulk information (such as primary kinetic data, computer programs and output *etc.*) which accompanies papers published in *Faraday Transactions* may be deposited, free of charge, with the Society's Supplementary Publications Scheme, either at the request of the author and with the approval of the referees or on the recommendation of the referees with the approval of the author. Details are available from the Editorial Office.

8 Molecular modelling studies should be subject to the same rigorous scientific standard required of other types of experiment, such that objective evaluation by independent investigators is possible. Authors are therefore strongly encouraged to provide sufficient details of any computationally assisted modelling results they report that might assist in any such an evaluation. This information should include:

- (a) A precise description of any computer software used, including any version or revision numbers, the type of computer used and a reference to a source for the program or a published definition of the algorithm used.
- (b) A concise indication in a 'Computational Details Section' or a footnote of standard options involved such as basis sets, SCF methods, electronic states, parameter sets, charge distribution schemes, symmetry, geometry optimisation methods, convergence criteria, cut-offs, time constants, *etc.* More explicit details of any non-standard use of *e.g.* basis sets, force-field parameters, algorithmic options, *etc.* should be particularly provided.
- (c) Key stationary points in a potential surface which are essential to conclusions discussed in the text should be accurately characterised by reporting *e.g.* the calculated energy and im-

portant geometrical parameters. Authors are encouraged to provide more complete information such as atom types, molecular coordinates and connectivity data if available for these points in the form of supplementary tables, or preferably in computer-readable form as *e.g.* program input data sets or archive files.

Further details of proposed guidelines in molecular modelling are to be found in P. Gund, D. C. Barry, J. M. Blaney and N. C. Cohen, *J. Med. Chem.*, 1988, **31**, 2230.

Nomenclature

Current IUPAC nomenclature and symbolism should be used.

Attention is drawn to the following publications in which the rules themselves and guidance on their use are given:

Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H, Pergamon Press, Oxford, 1979 edn.

Nomenclature of Inorganic Chemistry, Blackwell Scientific Publications, Oxford, 1990.

Biochemical Nomenclature and Related Documents, The Biochemical Society, London, 1978.

Compendium of Chemical Terminology: IUPAC Recommendations, Blackwell Scientific Publications, Oxford, 1987.

Units and Symbols

The recommendations of IUPAC should be followed. Their basis is the 'Système Internationale d'Unités' (SI). A detailed treatment is given in the so-called Green Book: *Quantities, Units and Symbols in Physical Chemistry*, Blackwell Scientific Publications, Oxford, 1988 edn.

FARADAY DIVISION INFORMAL AND GROUP MEETINGS

*Surface Reactivity and Catalysis Group***Annual Conference Catalysis and Surface Science**

To be held at the University of Wales College of Cardiff on 7–9 July 1993

Further information from Dr G. Attard, School of Chemistry and Applied Chemistry, University of Wales College of Cardiff, PO Box 78, Cardiff CF1 3TB

*Division with the Institute of Physics***11th National Quantum Electronics Conference**

To be held at Queen's University, Belfast on 30 August to 1 September

Further information from Dr S. Swain, David Bates Building, Queen's University, Belfast BT7 1NN

*Division with the Institute of Physics***Sensors and their Applications VI**

To be held in Manchester on 12–15 September 1993

Further information from Ms J. Butler, The Institute of Physics, 47 Belgrave Square, London SW1X 8QX

*Surface Reactivity and Catalysis Group***1st European Congress on Catalysis**

To be held in Montpellier, France on 12–17 September 1993

Further information from Dr G. McDougall, Department of Chemistry, University of Edinburgh, West Mains Road, Edinburgh EH9 3JJ

*Polymer Physics Group***Physical Aspects of Polymer Science**

To be held at the University of Reading on 15–17 September 1993

Further information from Dr M. J. Richardson, Division of Materials Metrology, The National Physical Laboratory, Queens Road, Teddington TW11 0LW

*Colloid and Interface Science Group***Kinetics of Phase Growth**

To be held at the University of Hull on 20–21 September 1993

Further information from Dr I. D. Robb, Unilever Research, Port Sunlight Laboratory, Quarry Road East, Bebington, Wirral, L63 3JW

*Division***Autumn Meeting: Structural Investigations using Solid State NMR**

To be held at the University of Warwick on 21–23 September 1993

Further information from Dr J. F. Gibson, The Royal Society of Chemistry, Burlington House, Piccadilly, London W1V 0BN

*Colloid and Interface Science Group***Dynamics of Surfactant Monolayers**

To be held at the Scientific Societies Lecture Theatre, London on 17 December 1993

Further information from Dr I. D. Robb, Unilever Research, Port Sunlight Laboratory, Quarry Road East, Bebington, Wirral, L63 3JW

*High Resolution Spectroscopy Group***Title to be announced**

To be held at the University of Wales College of Cardiff on 19–21 December 1993

Further information from Dr T. P. Softley, Physical Chemistry Laboratory, South Parks Road, Oxford OX1 3QZ

*Division***Annual Congress: The Reactive Interface**

To be held at the University of Liverpool on 12–15 April 1994

Further information from Dr J. F. Gibson, The Royal Society of Chemistry, Burlington House, Piccadilly, London W1V 0BN

*Gas Kinetics Group***13th International Symposium on Gas Kinetics**

To be held at University College, Dublin in July 1994

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THE ROYAL SOCIETY OF CHEMISTRY, FARADAY DIVISION, jointly with ASSOCIAZIONE ITALIANA DI CHIMICA FISICA, DEUTSCHE BUNSEN GESELLSCHAFT FÜR PHYSIKALISCHE CHEMIE, SOCIÉTÉ FRANÇAISE DE CHIMIE, DIVISION DE CHIMIE PHYSIQUE, GENERAL DISCUSSION 96

Dynamics at the Gas/Solid Interface

University of Cambridge 13–15 September 1993

Organising Committee

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A powerful approach has recently emerged to study the ways in which molecules interact with and react at solid surfaces. State-of-the-art laser and supersonic molecular beam technologies are being deployed together with novel surface science techniques in studies of gas–solid interactions.

There is now a rather detailed understanding of a number of aspects of surfaces relating to crystallography and electronic structure. Problems such as adsorption, energy exchange, diffusion and reaction are, by comparison, less well understood. Recent developments have focused attention away from static problems to

The preliminary programme may be obtained from **Mrs Angela Fish**, The Royal Society of Chemistry, Burlington House, Piccadilly, London W1V 0BN.

dynamic studies.

Stimulated by recent advances, this discussion is intended to bring together experimentalists and theoreticians who are currently contributing to these new developments in the understanding of dynamic processes at the gas/solid interface. The object is to identify key areas of current knowledge and to provide a forum for presenting and discussing future developments in this exciting new field which will have a bearing in a range of applied surface problems, including heterogeneous catalysis, microelectronics fabrication and corrosion.

THE ROYAL SOCIETY OF CHEMISTRY, FARADAY DIVISION, SYMPOSIUM 29

Potential-energy Surfaces and Organic Reaction Paths

University of Oxford 15–17 December 1993

Organising Committee

Dr J. Gerratt (Chairman)
Dr H. Rzepa

Dr M. Robb
Dr I. H. Williams

Dr T. Clark
Dr I. Fleming

The determination of reaction paths, and the structure and nature of transition states is a fundamental problem in the study of organic reactivity. This is a rapidly developing field which poses great challenges for both experimentalists and theoreticians. An equally important objective is to gain insight into the mechanisms of reactions in order to formulate useful models which are able to rationalize known results and predict new phenomena. The purpose of this Faraday Symposium is to bring together experimentalists and theoreticians to survey the latest results, examine new ideas and concepts and to indicate important future directions of research.

The meeting will consist of three broad sections: (i) methodology, (ii) applications to organic reactivity and (iii) understanding organic reactivity.

The following invited speakers have agreed to attend:

- P. von Ragué Schleyer - OPENING SPEAKER, *Friedrich-Alexander Universität, Erlangen-Nürnberg, Germany*
- F. Bernardi, *Università di Bologna, Italy*
- W. T. Borden, *University of Washington, USA*
- K. N. Houk, *University of California, USA*
- W. L. Jorgensen, *Yale University, USA*
- J. Michl, *University of Texas at Austin, USA*
- G. D. Purvis III, *CAChe Scientific, USA*
- S. Shaik, *Ben Gurion University, Israel*
- H. B. Schlegel, *Wayne State University, USA*
- J. Tomasi, *Università di Pisa, Italy*
- D. G. Truhlar, *University of Minnesota, USA*

The preliminary programme may be obtained from **Mrs Angela Fish**, The Royal Society of Chemistry, Burlington House, Piccadilly, London W1V 0BN.

THE ROYAL SOCIETY OF CHEMISTRY, FARADAY DIVISION, GENERAL DISCUSSION 97

Structure and Dynamics of Van der Waals Complexes

University of Durham, 6–8 April 1994

Organising Committee:

Dr B. J. Howard (Chairman)
 Dr J. M. Hutson
 Professor A. C. Legon
 Dr P. R. R. Langridge-Smith

Dr P. Hamilton
 Dr D. C. Clary
 Dr B. Soep

Since Faraday Discussion No. 73 on Van der Waals molecules, in 1982, the study of weakly bound molecular complexes has developed rapidly. Spectroscopic studies can now yield detailed information on intermolecular potential-energy surfaces in molecular systems. Studies of trimers, tetramers and higher clusters are giving insight into solvation effects and providing information on many-body forces, which are important in understanding the properties of condensed phases.

Investigations of photodissociation and predissociation processes are helping us to understand the dynamics of fundamental chemical

processes such as molecular rearrangement and energy transfer. In addition, Van der Waals complexes provide an opportunity to control the orientation of colliding molecules and the energies and impact parameters of reactive collisions, and have added significantly to our understanding of the pathways of simple chemical reactions.

This discussion will bring together experimentalists and theoreticians who are involved in the study of Van der Waals molecules.

Contributions are invited for consideration by the Organising Committee: Abstracts of about 300 words should be submitted by **30 June 1993** to: **Dr B. J. Howard, Physical Chemical Laboratory, Oxford University, South Parks Road, Oxford OX1 3QZ.**

Full papers for publication in the Discussion volume will be required by December 1993.

THE ROYAL SOCIETY OF CHEMISTRY, FARADAY DIVISION, GENERAL DISCUSSION 98

Polymers at Surfaces and Interfaces

University of Bristol, 12–14 September 1994

Organising Committee:

Professor Sir Sam Edwards (Chairman)
 Professor R. H. Ottewill
 Professor J. S. Higgins
 Dr R. A. L. Jones

Dr R. Buscall
 Dr T. Cosgrove
 Dr R. W. Richards

New experimental methods and new theoretical and computational techniques have recently led to great progress in understanding the difficult but technologically important problems associated with the conformation of polymer molecules at surfaces and interfaces. The purpose of this Discussion is to bring together experimentalists and theoreticians working towards a molecular understanding of polymers at surfaces and interfaces to survey the progress in the

area to date and to indicate future directions of research.

The meeting will attempt to bring a unified approach to the problem, encompassing problems of the structure of surfaces and interfaces in polymer melts, the conformation of polymers at solid/liquid and liquid/liquid interfaces, and extensions towards more complicated biological systems.

Contributions are invited for consideration by the Organising Committee. Abstracts of about 300 words should be submitted by **30 September 1993** to: **Dr R. A. L. Jones, Cavendish Laboratory, University of Cambridge, Madingley Road, Cambridge CB3 0HE**

Full papers for publication in the discussion volume will be required by May 1994.

THE ROYAL SOCIETY OF CHEMISTRY, FARADAY DIVISION, GENERAL DISCUSSION 99

Vibrational Optical Activity: from Fundamentals to Biological Applications

University of Glasgow, 19–21 December 1994

Organising Committee

Professor L. D. Barron (Chairman)
 Dr D. L. Andrews
 Professor A. D. Buckingham

Dr A. F. Drake
 Professor R. E. Hester

Traditional optical activity measurements such as CD are confined to the visible and near-ultraviolet spectral regions where they provide stereochemical information on chiral molecules via polarized electronic transitions. Thanks to prompting from theory and new developments in instrumentation, optical activity measurements are now being made in the vibrational spectrum using both infrared and Raman methods. Studies over the past decade on a large range of chiral molecules, from small organics to biological macromolecules, have demonstrated that vibrational optical activity opens up a whole new world of fundamental studies and practical applications undreamt of in the realm of conventional electronic optical activity.

The meeting seeks to bring together experimentalists and theoreticians to discuss the current and future experimental possibilities and the development of theories, including *ab initio* computational methods, which can relate the observations to stereochemical details. The increasing importance now being attached to molecular chirality and solution conformation in the life sciences should also encourage the participation of biomolecular scientists.

Contributions are invited for consideration by the Organising Committee. Abstracts of about 300 words should be submitted by **31 January 1994** to **Professor L. D. Barron, Department of Chemistry, The University, Glasgow G12 8QQ.**

Full papers for publication in the Discussion volume will be required by August 1994.