

SCIENTIFIC PROGRAMME

INTRODUCTION

The 5th World Congress of Theoretically Oriented Chemists will take place at Imperial College London, from Sunday 1 August to Friday 6 August 1999, with participants arriving during the afternoon of Sunday 1 August.

The Congress is being organised by the Royal Society of Chemistry and it follows previous meetings held in

1996 Jerusalem
1993 Toyohashi, Japan
1990 Toronto, Canada
1987 Budapest, Hungary

LOCATION

Imperial College of Science, Technology and Medicine is an independent constituent part of the University of London, founded in 1907. Its location in South Kensington provides an excellent opportunity to explore some of London's most famous Museums, including the Victoria & Albert, the Natural History and Science Museums, all of which are within easy walking distance. The traditional and famous tourist attractions, including Buckingham Palace, Tower of London, St Paul's Cathedral and many more are within easy reach by public transport.

More information on Imperial College is available on their Web site:

<http://www.ic.ac.uk/>

TRAVEL

London's five airports (Heathrow, Gatwick, Stansted, Luton and City Airport) provide links to over 200 cities worldwide. There are direct links from each by either rail and/or underground to central London. More information on travel can be obtained from the following web sites:

| | |
|---------------------------------|---|
| WATOC '99 Information | http://www.chemsoc.org/watoc99/directn.htm |
| Rail Travel | http://www.railtrack.co.uk/ |
| National Express Coaches | http://www.nationalexpress.co.uk/ |
| British Midland | http://www.iflybritishmidland.com/ |
| British Airways | http://www.british-airways.com/ |
| KLM UK | http://www.airuk.co.uk/ |

SCIENTIFIC PROGRAMME

The Scientific Programme will comprise 30 invited lectures and 48 contributed papers, which will cover the following topics

- ★ New Directions
- ★ Modelling Organic Structure and Reactivity
- ★ Inorganic: Organometallic & Reactivity
- ★ Solution Phase and other Hybrid Methods
- ★ DFT (applications oriented)
- ★ Materials
- ★ Excited States
- ★ Bio Applications

| SUNDAY 1 AUGUST | |
|------------------------|--|
| 12:30 | LUNCH |
| 14:00 | Opening |
| 14:15 | I1 Theoretically Oriented Chemistry: 1996 - 1999 <i>H. F. Schaefer III University of Georgia, USA</i> |
| 15:15 | I2 Tools for Exploring Potential Energy Surfaces <i>H. B. Schlegel Wayne State University, USA</i> |
| 16:00 | TEA |
| 16:30 | I3 Density Functional Theory As a Practical Tool in Transition Metal Chemistry. Modelling the Real Thing <i>T. Ziegler University of Calgary, Canada</i> |
| 17:15 | I4 Direct Dynamics Calculations in the Gas Phase and in Liquid Solution Based on Reaction Paths and Reaction Swaths <i>D. Truhlar University of Minnesota, USA</i> |
| 18:00 | CLOSE OF SESSION |

+ denotes presenter *denotes principal author

SCIENTIFIC PROGRAMME

Monday 2 August

| MONDAY 2 AUGUST | | | | | |
|-----------------|--|----------------------|----------------------|---|---|
| 09:30 | I5 Pericyclic Reactions: From Femtosecond Dynamics to Catalytic Antibodies K. N. Houk <i>University of California, Los Angeles, USA</i> | | | | |
| 10:15 | COFFEE | | | | |
| 10:45 | I6 Ab Initio QM/MM Simulation of Chemical Processes J. Gao <i>State University of New York at Buffalo, USA</i> | C3 10:45 to 11:05 | C5 10:45 to 11:05 | Extrapolating the Correlation Energy G. E. Scuseria <i>Rice University, Houston, USA</i> | Parallelization of Incore SCF Algorithm on cc-NUMA Machines Using OpenMP C.P.Sosa*, G. Scalmani, R. Gomperts, and M. J. Frisch <i>Silicon Graphics Computer Systems, USA</i> |
| 11:30 to 11:50 | C1 Some Difficulties in Computing BSSE-Corrected Potential Surfaces of Chemical Reactions G. Lendvai, I. Mayer* <i>Hungarian Academy of Sciences, Budapest, Hungary</i> | C4 11:10 to 11:30 | C6 11:10 to 11:30 | Geometry Optimization of Biomolecules in Internal Coordinates B. Paizs†, G. Fogarasi, S. Suhai and P. Pulay* <i>German Cancer Research, Heidelberg, Germany</i> | A New IMOMM and IMOMMM Implementation In Gaussian '98 I. Komáromi†, S. Dapprich, T. Vreven, K.S. Byun, and K. Morokuma*, M. J. Frisch <i>Gaussian Inc, USA</i> |
| 11:55 to 12:15 | C2 Computationally Inexpensive Theoretical Thermochemistry J. Cioslowski*, M. Schimeczek, G. Liu, and V. Stoyanov <i>Florida State University, USA</i> | I7 11:30 | C7 11:30 to 11:50 | Cytochrome P-450: Electronic Structure and Reactivity Patterns S. Shaik <i>Hebrew University, Israel</i> | A Massively Parallel Implementation of the State-Selecting Multi Reference Configuration Interaction Method P. Stampfuss and W. Wenzel** <i>Dortmund University, Germany</i> |
| 12:15 | LUNCH | | C7 11:55 to 12:15 | | Parallel MOPAC H.A. Früchtl**†, R.H. Nobes, A.A. Bliznyuk <i>Fujitsu European Centre for Information Technology, UK</i> |

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SCIENTIFIC PROGRAMME

Monday 2 August

| | | | | | | | | | |
|----------------|-----|---|----------------|-----|--|----------------|----------------|-----|---|
| 13:45 to 14:05 | C9 | New Approaches to Order-Disorder in Oxides N. L. Allan <i>University of Bristol, UK</i> | 13:45 to 14:05 | C11 | Modelling of Lanthanide Macrocyclic Complexes in Vacuo and in Solution A. Villa ^{†*} , U. Cosentino, G. Moro, D. Pitea, V. Barone, A. Maiocchi <i>Università degli Studi di Milano, Italy</i> | 13:45 to 14:05 | 13:45 to 14:05 | 18 | Conversion of Light into "Molecular Motion" in Biology: Retinal and other Chromophores M. Olivucci <i>University of Siena, Italy</i> |
| 14:10 to 14:30 | C10 | First Principles Modelling of Electrode Materials for Lithium Intercalation Batteries J.L. Barras ^{†*} , C.A. Daul, E. Deiss, L. Benco, M. Atanasov <i>University of Fribourg, Switzerland</i> | 14:10 to 14:30 | C12 | Understanding and Predicting Magnetic Resonance Parameters for Heavy-Element Compounds M. Kaupp ^{†*} , J. Vaara, B. Schimmelpfennig, M. Munzarová, O. L. Malkina, V. G. Malkin <i>Max-Planck-Institute, Germany</i> | 14:30 to 14:50 | 14:30 to 14:50 | C15 | The Effect Of Corrosion Inhibitor Films On Deposition Of Wax To Metal Oxide Surfaces M. A. San-Miguel ^{†*} and P. M. Rodger <i>University of Reading, UK</i> |
| 14:30 to 14:50 | C13 | Density Functional Theory Applied to Very Large Systems J-L. Rivail <i>Université Henri Poincaré, France</i> | 14:30 to 14:50 | C13 | Ferromagnetism in Transition Metals: A Chemical Bonding View G. A. Landrum ^{†*} and R. Dronskowski [*] <i>RWTH-Aachen, Germany</i> | 14:55 to 15:15 | 14:55 to 15:15 | C16 | Ab Initio Many-Body Model Potentials and the Study of Binding in Small Metal Clusters I. Kaplan <i>UNAM, Mexico</i> |
| 15:15 | | | | | | | | | |
| 15:45 | 110 | Conformational Study on Informational Biomolecules. A Prelude to Ab Initio Drug Design I. Csizmadia <i>University of Toronto, Canada</i> | | | | | | | |
| 16:30 | 111 | Evaluation of Cyclic Electron Delocalization P. von Ragué Schleyer <i>University of Georgia, USA</i> | | | | | | | |
| 17:15 | | POSTER VIEWING - SESSION A | | | | | | | |

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SCIENTIFIC PROGRAMME

Tuesday 3 August

| TUESDAY 3 AUGUST | | Computer Simulation of Enzymatic Reactions A. Warshel <i>University of Southern California, USA</i> | |
|------------------|-----|--|---|
| 09:30 | I12 | COFFEE | |
| 10:15 | | COFFEE | |
| 10:45 to 11:05 | C17 | Local Regularity and Non-recrossing Path in Transition State -A New Strategy in Chemical Reaction Theories T. Komatsuzaki ^{*,†} , R. S. Berry <i>University of Chicago, USA</i> | 10:45 to 11:05 Recent Developments and Applications of Hybrid Quantum Mechanical/Molecular Mechanical Methods I. H. Hillier <i>University of Manchester, UK</i> |
| 11:10 to 11:30 | C18 | Semiclassical Simulations of Azomethane Photochemistry M. Persico ^{*,†} and P. Cattaneo <i>University of Pisa, Italy</i> | 11:10 to 11:30 Conceptual and Computational Aspects of DFT : Recent Developments and Applications in Organic and Inorganic Chemistry F De Proft ^{*,†} and P. Geerlings <i>Vrije Universiteit Brussel, Belgium</i> |
| 11:30 to 11:50 | C19 | Application of Ab Initio Molecular Dynamics methods in Solution Chemistry M Sprik <i>University of Cambridge, UK</i> | 11:30 to 11:50 Selectivity in Asymmetric Synthesis from QM-Guided Molecular Mechanics Per-Ola Norrby <i>Royal Danish School of Pharmacy, Denmark</i> |
| 11:55 to 12:15 | C20 | Modern Valence-Bond Description of Organic Reaction Mechanisms D.L. Cooper [†] , P.B. Karadakov <i>University of Liverpool, UK</i> | 11:30 to 11:50 Group Functions, Loewdin Partition, and Hybrid QC/MM Methods for Large Molecular Systems A.L. Tchougreff <i>Karpov Institute of Physical Chemistry, Russia</i> |
| 11:30 to 11:05 | C23 | | 11:30 to 11:05 Electron Propagators with Highly Correlated Reference States J. V. Ortiz [*] + <i>Kansas State University, USA</i> |
| 11:30 to 11:50 | C21 | | 11:30 to 11:50 Quantum Mechanical Description of the Picosecond Photoprocess Initiating Proton Pumping in the Protein Bacteriorhodopsin K. Schulten <i>University of Illinois, Urbana-Champaign, USA</i> |
| 12:15 | | LUNCH | |

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SCIENTIFIC PROGRAMME

Tuesday 3 August

| | | | | | | | |
|----------------|--|----------------|--|---|----------------|---|--|
| 13:45 to 14:05 | C27 | 13:45 to 14:05 | Theoretical Modeling of Silicon Oxynitride Chemical Vapor Deposition: Initial Reactions of NO with Si(100) Surface A. A. Korkin,*†, A. Demkov, N. Tanpipat, K. Wilson and R.J. Bartlett <i>Motorola Inc, USA</i> | 13:45 to 14:05 | C29 | Theoretical Models of Polymerization of Ethylene over a Phillips Catalyst Ø. Espelid and K.J.Børve <i>University of Bergen, Norway</i> | |
| 13:45 I15 | Recent Developments in Semiempirical Hybrid Approaches W. Thiel <i>University of Zürich, Switzerland</i> | 14:10 to 14:30 | C28 | A Non-Empirical Intermolecular Potential for Oxalic Acid and its Application to Crystal Structure Prediction I. Nobeli*, T. Beyer, S.L. Price† <i>University College London, UK</i> | 14:10 to 14:30 | C30 | Carbon-Hydrogen Bond Activation by Iridium(III): Oxidative-Addition vs. Sigma-Bond Metathesis Pathways, Inter- vs. Intra-Molecular Activation, and Catalytic vs. Non-Catalytic Alkane Dehydrogenation M. B. Hall**†, S. Niu <i>Texas A&M University, USA</i> |
| 14:30 to 14:50 | C25 | | Empirical Potential for Borosilazane Ceramics C. M. Marian **†, M. Gastreich <i>GMD Center for Information Technology, St. Augustin, Germany</i> | 14:30 to 14:50 | C31 | Density Functional Modelling of the Reactions of 3d Transition Metals with N₂O and NO₂ A. Stirling <i>Institute of Isotope and Surface Chemistry, Hungarian Academy of Science, Budapest, Hungary</i> | |
| 14:55 to 15:15 | C26 | 14:30 | I16 | Computational Studies of Organic Reactions from the Gas Phase to Enzymes W. Jorgensen <i>Yale University, USA</i> | 14:55 to 15:15 | C32 | Towards a Catalyst for Alkene Hydroamination - Static and Dynamic Ab Initio DFT Studies H.M. Senn**†, P.E. Blöchl, A. Togni <i>ETH Zürich, Switzerland</i> |
| 15:15 | | | | TEA | | | |
| 15:45 | I17 | | | Simulation of Reactions in Solution and Enzymes P. D. Lyne <i>University of Oxford, UK</i> | | | |
| 16:30 | I18 | | | Applications of Ab Initio Quantum Chemistry to Atmospheric Chemistry and Spectroscopy T. J. Lee <i>NASA Ames Research Center, USA</i> <i>Dirac Medallist</i> | | | |
| 17:15 | | | | POSTER VIEWING - SESSION B | | | |

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SCIENTIFIC PROGRAMME

Wednesday 4 August

| WEDNESDAY 4 AUGUST | |
|--------------------|--|
| 09:15 | I19 Theoretical Chemical Models J. A. Pople <i>Northwestern University, USA</i> |
| 10:15 | COFFEE |
| 10:45 | I20 Density Functional Theory for Molecular Properties N. J. Handy <i>University of Cambridge, UK</i> <i>Schrödinger Medallist</i> |
| 11:45 | I21 Molecular Excited States and Electronic Spectroscopy B. Roos <i>University of Lund, Sweden</i> <i>Schrödinger Medallist</i> |
| 12:45 | CLOSE OF SESSION LUNCH and Excursions |

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There are no scientific sessions on
Wednesday afternoon.

A programme of half-day excursions,
all of which include dinner, has been planned.

Details of the programme can be found
on pages 18 and 19.

SCIENTIFIC PROGRAMME

Thursday 5 August

| THURSDAY 5 AUGUST | |
|-------------------|---|
| 09:30 | I22 Ab Initio Simulation of Water and Water Solutions M. Parrinello <i>Max-Planck Institute, Germany</i> |
| 10:15 | COFFEE |
| 10:45 to 11:05 | C33 Alkylcesiums: Computed and Experimental Basicities A. Streitwieser**+, S. S.-W. Leung, F. Abu-Hasanayn <i>University of California, Berkeley, USA</i> |
| 11:10 to 11:30 | C34 Design Of Potent Organic Superbases By Ab Initio Quantum Chemistry Z. B. Maksic <i>Rudjer Boskovic Institute, Zagreb, Croatia</i> |
| 10:45 to 11:05 | C35 Ab Initio Studies Toward Accurate Protein Circular Dichroism Calculations J. D. Hirst**+, N. A. Besley <i>The Scripps Research Institute, La Jolla, USA</i> |
| 11:10 to 11:30 | C36 Electronic Spectroscopy of Polypeptides L. Serrano-Andrés**+, M. P. Fülischer <i>University of València, Spain</i> |
| 11:30 to 11:50 | C37 Tunneling Mechanism Prevails in the Formation of Zwitterionic Forms of Aminoacids in Aqueous Solution Z. Smedarchina**+, A. Fernandez-Ramos, M. Z. Zgierski and W. Siebrand <i>Steacie Institute For Molecular Sciences, NRC, Canada</i> |
| 11:30 to 11:50 | C39 Cobalt Complexes as Redox Active Therapeutic Agents: A Combined Theoretical - Experimental Approach C. A. Reynolds*, J. H. Wu, P. J. Winn, G. G. Ferenczy, Y. Zheng and J. R. Dilworth <i>University of Essex, UK</i> |
| 11:30 to 11:50 | C38 Principles of Chiral Recognition. An Investigation of Suitable Computational Approaches S. Topiol*, P. U Biedermann, S. Garten, T.P. Radhakrishnan, and I Agranat <i>Core Technologies Area, Novartis Institute</i> |
| 11:55 to 12:15 | C40 Digitally Filtered Molecular Dynamics: The Frequency Specific Control of Molecular Dynamics Simulations S. C. Phillips*, C. M. Edge and J. W. Essex+ <i>University of Southampton, UK</i> |
| 12:15 | LUNCH |

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SCIENTIFIC PROGRAMME

Thursday 5 August

| | | | | | | | | |
|----------------|----------------------------------|--|----------------|-----|--|----------------|-----|--|
| 13:15 to 13:35 | C41 | Molecular Orbital Study of [2+2]Cycloaddition Reaction of Substituted Benzene Y. Osamura ^{*,†} , K. Suzuki, K. Morokuma <i>Rikkyo University, Tokyo, Japan</i> | 13:15 | I25 | Insight into the Chemical Bonds of Transition Metal Complexes G. Frenking <i>Philipps University Marburg, Germany</i> | 13:15 to 13:35 | C47 | Quantum Chemical Insights Into Green Fluorescent Protein V. Helms ^{*,†} , W. Weber [*] , J.A. McCammon, P. Langhoff <i>Max-Planck-Institute of Biophysics, Frankfurt, Germany</i> |
| 13:40 to 14:00 | C42 | The Aromaticity of Bent Benzene Rings: A Valence Bond Study F. Dijkstra ^{*,†} , J.H. van Lenthe <i>Debye Institute, Utre, The Netherlands</i> | 13:40 to 14:00 | C48 | Design of New 'Warheads' for Eneidyne Anti-Cancer Drugs E. Krafka and D. Cremer <i>Göteborg University, Sweden</i> | 13:40 to 14:00 | C48 | Design of New 'Warheads' for Eneidyne Anti-Cancer Drugs E. Krafka and D. Cremer <i>Göteborg University, Sweden</i> |
| 14:00 to 14:20 | C43 | How do benzylic Amide Catenane Rings Rotate M.S. Deleuze ^{*,†} , D.A. Leigh, F. Zerbetto <i>Limburgs Universitair Centrum, Belgium</i> | 14:00 to 14:20 | C45 | Biological Nitrogen Fixation. Density Functional Modeling the Fe-Mo-Cofactor Bound Homocitrate Ligand: Bi- vs. Monodentate Coordination R. K. Szilagy ^{†*} , D. G. Musaev, and K. Morokuma, <i>Emery University, USA</i> | 14:00 to 14:00 | I26 | Predictions For New, Simple Chemical Species P. Pyykko <i>University of Helsinki, Finland</i> |
| 14:25 to 14:45 | C44 | Nature of the Metal-Alkene Bond in Platinum Complexes of Strained Olefins B. F. Yates ^{*,†} <i>University of Tasmania, Australia</i> | 14.25 to 14.45 | C46 | The Role of DNA Flexibility in Sequence Specific Recognition S. A. Harris ^{*,†} , C. E. Bostock-Smith, M. S. Searle and C. A. Laughton <i>University of Nottingham, UK</i> | 14:25 to 14:45 | C46 | The Role of DNA Flexibility in Sequence Specific Recognition S. A. Harris ^{*,†} , C. E. Bostock-Smith, M. S. Searle and C. A. Laughton <i>University of Nottingham, UK</i> |
| 14:45 | I27 | New Tools for Calculation and Interpretation P. Gill <i>University of Cambridge, UK</i> <i>Dirac Medallist</i> | | | | | | |
| 15:30 | TEA + POSTER VIEWING - SESSION C | | | | | | | |

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SCIENTIFIC PROGRAMME

Friday 6 August

| FRIDAY 6 AUGUST | |
|-----------------|---|
| 09:30 I28 | Saturated Backbones: Conformation and Electronic Excitation J. Michl <i>University of Colorado, USA</i> |
| 10:15 | COFFEE |
| 10:45 I29 | Solvent Effects on Molecular Spectra M. Frisch <i>Lorentzian Inc, USA</i> |
| 11:30 I30 | Applications of Molecular Dynamics and Quantum Chemistry to Proteins and Nucleic Acids P. Kollman <i>University of California, San Francisco, USA</i> |
| 12:15 | CLOSE OF MEETING + Lunch |

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POSTERS

Poster presentations will form a significant part of the meeting and two formal poster viewing sessions are included within the scientific programme. Contributions were called for in Circular 1 and over 400 offers have been accepted for presentation at the meeting.

Late contributions can still be considered for poster presentation and abstracts should be submitted, in the format shown below.

Authors are asked to observe the following criteria:

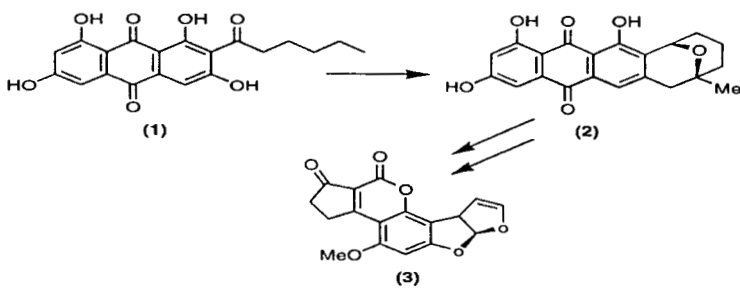
- The title of the abstract should be concise.
- The name of the speaker or poster presenter should be clearly indicated. The name of the Main Author should be underlined, and the name of the presenter (i.e. the individual who will attend the meeting to present the work) should be marked with an asterisk (*).
- Abstracts should **not** be folded and should be **typed** in English using **double line** spacing on white paper.
- The preferred font should be Arial, Avant Garde, Courier, Helvetica or Times New Roman.
- The preferred font size should be 12 point and not less than 10 point.
- Where possible, the printed abstract should be submitted together with a PC-formatted disk containing the abstract as a word-processed document (Microsoft Word for Windows v6.0 or Office Word 98).
- Chemical structures may be drawn using ChemDraw, ChemWindow or ISIS/Draw.
- A full one-page abstract will be reproduced by a photo-offset method directly from authors' originals.
- The whole of the abstract **must** be contained within a rectangle of size 242 mm HIGH x 165 mm WIDE (9.5 x 6.5 inches) in portrait layout.
- The heading should be presented in the format as shown on the example abstract including the full line separating text and heading.
- References, denoted by superscript numbers in the text, should be listed at the end of the text using standard Chemical Abstracts Source Service Index (CASSI) terminology followed by YEAR, VOLUME, PAGE.

SUBSTRATE SPECIFICITY OF NORSOLORINIC ACID SYNTHASE

Nicola J. Willett, * * Carole McNicholas^b and Thomas J. Simpson^a

^a School of Chemistry, University of Bristol, Cantock's Close, Bristol, BSS ITS
^b Natural Products Chemistry Department, Xenova Limited, 240 Bath Road, Slough, Berkshire, SL 1 4EF

Norsolorinic acid (1) is the first enzyme-free intermediate on the biosynthetic pathway to aflatoxin B₁ (3). It is the product of the polyketide synthase, norsolorinic acid synthase, and a greater understanding of this enzyme, its substrate specificity and mode of action provides the first intrinsic target for the inhibition of aflatoxin B₁ biosynthesis.



Previous feeding experiments have shown intact incorporation of [1-¹³C] hexanoic acid into averufin (2), implying that norsolorinic acid is formed via a condensation of a hexanoate starter unit with seven malonates.¹

Norsolorinic acid synthase substrate specificity has been investigated further by carrying out incorporation studies with a variety of analogues of the essential hexanoate starter unit, using ¹H, ¹³C and ¹⁹F isotopic labels.² This results in the efficient production of a number of structural analogues of (1).

1. C. A. Townsend, S. B. Christensen and K. Trautwein, *J. Am. Chem. Soc.*, 1984, **106**, 3868; S. W. Brobst and C. A. Townsend, *Can. J. Chem.*, 1994, **72**, 200
2. D. S. J. McKeown, C. McNicholas, T. J. Simpson and N. J. Willett, *J. Chem. Soc., Chem. Commun.*, 1996., 301

Sample Abstract

Electronic Submission of Abstracts

Alternatively, abstracts can be submitted electronically via the WATOC '99 web site:

<http://www.chemsoc.org/watoc99/home.htm>

or sent by Email (as a file attachment in Word format) to Paula Whelan (whelanp@rsc.org)

Abstracts submitted in the prescribed format will be published in the Book of Abstracts to be distributed to all participants at the meeting. The closing date for receipt of abstracts is **Friday 28 May**. It will not be possible to publish any abstracts received after the closing date.

EXHIBITION AND SPONSORS

In addition to poster presentations, there will be an exhibition featuring companies associated with theoretical chemistry. A number of companies have already committed to attend and any others interested in exhibiting should contact Mrs Paula Whelan at the Royal Society of Chemistry. (Email: whelanp@rsc.org)

There will also be a display of scientific books and enquiries concerning this should be directed to Penny Head, Wisepress Limited, The Old Church Hall, Wimbledon, London SW19 1EX. Tel: 0181 715 1812.

The organisers are pleased to acknowledge the following organisations which have, so far, agreed to support WATOC '99

| | |
|------------------------------|--|
| Compaq | http://www.compaq.com |
| Elsevier Science | http://www.elsevier.nl |
| Gaussian | http://www.gaussain.com |
| IBM UK | http://www.ibm.com |
| Molecular Simulations | http://www.msi.com |
| Oxford Molecular | http://www.oxmol.com |
| Q-Chem | http://www.q-chem.com |
| Silicon Graphics | http://www.sgi.com |
| John Wiley & Sons | http://www.wiley.co.uk |
| Wisepress | genaral@wisepress.co.uk |

WORKSHOPS/USERS MEETINGS

Gaussian will be holding a Users Meeting
For further information please contact: info@gaussian.com

Molecular Simulations will be running a Workshop
For further information please contact: byronk@msicam.co.uk

ATTENDANCE

Attendance at any part of the meeting, including the Accompanying Person's programme, is restricted to those who have registered in advance using the enclosed Application Form. The closing date for application is **MONDAY 21 JUNE 1999**. To qualify for the **Early Bird Registration fee**, applications must be received, together with the appropriate payment, by **MONDAY 17 MAY 1999**.

Multiple applications may be made on one form provided all individual requirements are clearly indicated. Photocopies of Application Forms are acceptable, as are faxed applications.

Completed applications, together with the appropriate payment, should be sent to:

Paula Whelan
WATOC99
The Royal Society of Chemistry
Burlington House
London W1V 0BN UK
Tel: +44 (0)171 437 8656
Fax: +44 (0)171 734 1227
Email: conferences@rsc.org (please use subject header: 'WATOC99')

COSTS

The registration fees shown below include Value Added Tax (VAT) at the prevailing rate (17.5%).

EARLY BIRD REGISTRATION FEES will apply if both the payment and application form are received **BEFORE MONDAY 17 MAY 1999**.

| | |
|---|----------------|
| Active Participant - member of RSC or WATOC | £250.00 |
| Active Participant | £350.00 |
| Student | £100.00 |
| *Accompanying Person | £30.00 |

STANDARD REGISTRATION: BEFORE MONDAY 21 JUNE 1999

| | |
|---|----------------|
| Active Participant - member of RSC or WATOC | £300.00 |
| Active Participant | £400.00 |
| Student | £150.00 |
| *Accompanying Person | £30.00 |

* An Accompanying Person is the guest of a fully registered participant and as such is expected **NOT** to attend the scientific sessions.

ACCOMMODATION

Campus Accommodation

Standard Rooms (with shared bathroom facilities) are available in the Imperial College Linstead Halls of Residence which are within short walking distance of the Sherfield Building where the scientific sessions will take place. There are single or twin-bedded rooms, with wash hand basin, and shared bathroom facilities. There are no en-suite rooms (ie rooms with private bathroom) available at Linstead Hall.

The cost of the accommodation package, which includes five nights' accommodation, on a bed and full breakfast basis (Sunday to Thursday inclusive), is

| | |
|--|---------------------------|
| Single room (shared bathroom facilities) | £190.00 per person |
| *Twin-bedded room (shared bathroom facilities) | £290.00 per room |

A limited number of rooms are available for the nights of Saturday 31 July and Friday 6 August (bed and full breakfast basis), the costs are as follows

| | |
|-------------------|-------------------------------------|
| Single room | £38.00 per person, per night |
| *Twin-bedded room | £58.00 per room, per night |

*There are a very limited number of twin-bedded rooms available and these will be allocated strictly on a first-come-first-served basis.

Rooms with Private Bathroom Facilities are available in the Pembridge Gardens Hall of Residence. Pembridge Gardens is approximately 25 minutes' walk from the Lecture Theatres where the scientific

sessions will take place. The numbers of rooms available are limited and will be allocated strictly on a first-come-first served basis.

The cost of the accommodation package, which includes five nights' accommodation, on a bed and continental breakfast basis (Sunday to Thursday inclusive), is

| | |
|---|---------------------------|
| Single room with private facilities | £235.00 per person |
| *Twin-bedded room with private facilities | £330.00 per room |

Evening meals have not been included as part of the accommodation package and participants will be free to make their own arrangements for dinner.

Hotel Accommodation

The Organisers are pleased to announce that special rates have been negotiated through the British Hotel Reservation Centre (BHRC). Details including costs, are given on Form B (enclosed). Anyone wishing to book accommodation through this organisation should complete and return Form B directly to BHRC.

The Organisers cannot accept responsibility for bookings made through other hotels or organisations.

LUNCHES

Lunches are not included as part of the registration or accommodation fees. Lunch will be available on Sunday and on the five days of the scientific programme and should be pre-booked via the Application Form. Tickets will be issued for all lunches and it will not be possible to give refunds on any pre-booked lunches at the time of the meeting. The cost for lunch (including VAT @ 17.5%) is £12.50 per day.

SPECIAL DIET/DISABILITY

Special diets can be provided only if advance notice is given to the Organisers. Participants who require special diets should give details of diet required on Application Form A. Similarly, the Organisers are anxious to assist wherever possible with special needs in respect of any disability and requirements should be indicated on the Application Form.

METHOD OF PAYMENT

Payment can only be accepted in UK Sterling

Cheques/Money Orders Cheques or money orders should be made payable to
"The Royal Society of Chemistry"

Credit Cards Credit card payment of fees is permitted for participants. **Payments must be made in full** and the following credit/charge cards are accepted: Visa, Eurocard, Mastercard and American Express. The Society regrets that payment cannot be made by Diners or Visa Electron. The particular card to be debited, together with the **Account Number, Expiry Date,** and the **Registered Name and Address** of the Card Holder, must be specified on the Application Form.

Bank Transfer Participants transferring money from overseas are reminded that bank charges are made. These charges are usually deducted by the bank before passing on the cheque/money order to the Society. These fees have to be recouped by the Society and it is therefore essential that such transfer of money should include any surcharge. Deductions suffered by the Society should be paid at the Registration Desk on arrival.

BACS Payment can now be made by BACS to the following account:

NatWest Bank plc

King's Parade Branch, 10 Benet Street, Cambridge CB2 3PU, UK

A/C Name: RSC Conferences - WATOC99

A/C Number: 24052558 Sort Code: 60-04-23

Payments from overseas by bank transfer/BACS are subject to a charge of approximately £30.00. These charges are usually deducted by the bank before payment is passed into the Society bank account. Any such deductions incurred by the Society should be paid at the Registration Desk on arrival. **A copy of the payment advice must be attached to the application form.**

If it is necessary to send payment separately from the Application Form, every care should be taken to ensure that the cheque/money order includes both the **title of the meeting** and the **individual** concerned. All application forms received at The Royal Society of Chemistry will be acknowledged.

GENERAL INFORMATION

CANCELLATIONS

Applications may be cancelled by Monday 5 July 1999 in which case a partial refund of 75% of fees already paid will be made. It will not be possible to offer any refunds if details of cancellations are received after this date.

BURSARIES

A limited number of bursaries are available to students whose attendance cannot be covered by any other source. Anyone wishing to apply should contact Paula Whelan (Email: whelanp@rsc.org or tel: +44 (0)171 440 3316) for an Application Form as soon as possible. The closing date for returning applications for bursaries is **Monday 21 June**.

REGISTRATION MATERIAL

In advance of the meeting, all registered participants will receive confirmation of registration and any accommodation reservations, together with maps and arrival instructions.

Conference material, including tickets, Final Programme and Book of Abstracts, etc., will **NOT** be sent out in advance. This material should be collected at the Registration Desk on arrival at the meeting.

On Sunday 1 August the Registration/Information Desk will be situated in the Sherfield Building where the scientific sessions will take place, and will open from 10.30 to 17.30. From Monday 2 August to Friday 6 August the Desk will remain open each day whilst the scientific sessions are in progress.

CORRESPONDENCE

Correspondence concerning the meeting may be referred as follows:

Scientific Matters

Professor M A Robb
School of Chemistry
King's College
The Strand
London WC2R 2LS
Tel No: +44 (0)171 873 2098
Fax No: +44 (0)171 873 2810
Email: mike.robb@kcl.ac.uk
(Please use subject header WATOC 99)

Local Matters

Dr H S Rzepa
Department of Chemistry
Imperial College
South Kensington
London SW7 2AY
Tel No: + 44 (0)171 594 5774
Fax No: + 44 (0)171 594 5804
Email: rzepa@ic.ac.uk;
(Please use subject header WATOC 99)

For Administrative Matters

Mrs Paula Whelan
WATOC '99
The Royal Society of Chemistry
Burlington House
London W1V 0BN
Tel No: +44 (0)171 437 8656
Fax No: +44 (0)171 734 1227
E-mail: whelanp@rsc.org
(please use subject header WATOC 99)

WEB SITES

The URL for the WATOC '99 home page is
<http://www.chemsoc.org/watoc99/>

The URL for the WATOC Association home page is
<http://www.ch.ic.ac.uk/watoc/>

QUANTUM BIOINORGANIC CHEMISTRY (QBIC) - Satellite Meeting

This satellite meeting is being held at the University of Warwick from 29 July to 30 July 1999. Further information may be obtained from Dr R Deeth, Department of Chemistry, University of Warwick, Coventry CV4 7AL. E-mail: r.j.deeth@warwick.ac.uk

COMMITTEES

International Advisory Committee:

H F Schaefer III (*The President, WATOC Association*), F Bernardi, J Bertran, R J Boyd, T Clark, K N Houk, S Iwata, P A Kollmann, K Morokuma, L Radom, B Roos, C Still, W Thiel, and S Shaik.

National Scientific Organising Committee:

M A Robb and H S Rzepa (*co-chairman, WATOC '99*), C R A Catlow, D C Clary, N C Handy, I H Hillier, R Hubbard and W G Richards

WATOC '99 Steering Group:

M A Robb, H S Rzepa, J Gale, I Gould, J F Gibson, S Riaz and P Whelan

SOCIAL PROGRAMME

Tickets for all social events must be booked via Application Form A. Even those events which are free of charge, must be booked in advance. **Tickets for social events are available only to registered participants and accompanying persons.**

EVENING SOCIAL EVENTS

| | | |
|--------------------------|------------------------|---|
| Sunday 1 August | 18.30 - 21.00 | Welcome Buffet Reception at the Science Museum <i>Ticket Cost: Free of charge</i> |
| Thursday 5 August | 19.00 for 19.30 | Conference Dinner at the Victoria & Albert Museum The V&A is one of the world's great museums, a treasure-house of art and design reflecting every civilisation, style and subject. It is a magnificent Victorian building with remarkable rooms of the period. The dinner will be held in The Dome, an impressive arcaded and pillared room with sculptures, marble floors and glittering decor. The pre-dinner reception will be held in the delightful Italiante Pirelli Garden (weather permitting). The ticket price includes the reception, dinner, wines, gratuities and VAT. Ticket Cost: £58.50 per person |

DAYTIME EXCURSIONS - Wednesday 3 August

There are no formal scientific sessions on Wednesday afternoon and evening and the following excursions have been planned.

The cost of excursions includes transport, entrance fees and guides (if applicable), VAT, gratuities and Dinner (where indicated).

EXCURSION 1

Cost: £85.00 per person

Tour of London/St Paul's Cathedral/Globe Theatre including supper and Shakespearean Play

Participants will be taken by luxury coach and Blue Badge guide from Imperial College on a panoramic tour of the heart of London. There will be a guided tour of St Paul's Cathedral, after which participants will be taken to the famous Globe Theatre on the south side of the River Thames. Guests will be welcomed with an introductory talk on the history of the Globe Theatre and the development of this amazing new theatre built in the same style as the original Globe of Shakespeare's day. After a private buffet supper, guests will be shown into the Galleries to their pre-booked seats for a performance of Antony and Cleopatra

EXCURSION 2

Cost: £76.00 per person

Black Horse Pub and Canal Cruise including dinner

Participants will travel by luxury coach to the Black Horse Pub, often thought of as one of the birthplaces of the modern fine chemicals industry, being the home of William Perkin's factory. Guests can enjoy a leisurely drink at this attractive pub which overlooks the Grand Union Canal. This offers a pretty start to a fascinating Canal cruise which will show guests a side to London they will probably never have seen before. The areas through which the Canal passes encompass many worlds, from industry to great luxury, showing off some hidden gems en route. During the cruise there will be a three course dinner served, and a singer/guitarist will provide entertainment afterwards. The cruise will end at Camden Lock, where a coach will be waiting to take participants back to Imperial College.

EXCURSION 3

Cost: £45.00 per person

Hampton Court Palace and Barbecue Supper

Hampton Court Palace, the Tudor home of Henry VIII is a visit not to be missed. The Palace features a blend of Tudor and Wren baroque architecture, set in 60 acres of formal gardens and parkland. Its many attractions include the vast Tudor kitchens, the Great Hall, William III's maze and Great Vine and the King's Apartments. Following a guided tour of the Palace, participants will be taken by coach to the Imperial Arms Inn for a barbecue supper.

Maximum and minimum numbers are fixed for all the excursions, and participants are asked to indicate a second choice in the event of an excursion being over or under subscribed. The Organisers reserve the right to cancel any excursions due to lack of demand, etc.

ACCOMPANYING PERSONS

Monday 2 August

Free of Charge

Welcome and Introductory Talk on London

There is no formal programme of events for Accompanying Persons, but an introductory talk on London will be given on Monday morning. Tourist information and guidance on how to make the most of a visit to London will be available. Tickets to the talk are free to registered accompanying persons and should be requested via Application Form A.

5th World Congress of Theoretically Oriented Chemists



Proposed Hotels for Congress Participants

| HOTELS | Nearest Underground |
|---|------------------------|
| 4 Star - Holiday Inn Kensington - The Holiday Inn is in one of the best locations in London and is surrounded by many of London's attractions. The Holiday Inn Kensington is situated in its own landscaped gardens and offers Health/Fitness/Sauna facilities on site. | Gloucester Road |
| 4 Star - Jurys Kensington - Situated in the exclusive "Little Paris" area in the heart of South Kensington, the Jurys has earned an RAC recommendation for customer service. The Jury also has an affiliation with the Imperial College where residents can use the sports/gym facilities at a discount. | Gloucester Road |
| 4 Star - Swallow International - The Swallow International is one of London's long standing 4 Star hotels, offering all the amenities a modern day guest could wish for, catering for business travellers, and discerning tourists alike. Comprehensive Leisure facilities can be found on site. | Gloucester Road |
| 4 Star - Forum - The Forum Hotel has on of the most convenient locations in London for both tourists and business people. The hotel is unique among London hotels in its variety of bars and restaurants. Health/Fitness facilities can be found on site. | Gloucester Road |
| 4 Star - Strathmore - Once the London Residence of the 14th Earl of Strathmore, the Queen Mother's father. The Strathmore Hotel provides a spectacular blend of Victorian grandeur and contemporary luxury, providing sumptuous comfort in one of the world's most exclusive and fashionable neighbourhoods. | Gloucester Road |
| 4 Star - Kensington Moat House - The Kensington Moat House is an elegant Victorian hotel located in the centre of Kensington and within easy reach of the worlds most famous renowned museums. The Kensington Moat is a glamorous, yet informal hotel. All the rooms are larger than average and are individually decorated. | South Kensington |
| 3 Star - Novotel Hammersmith - Located between Heathrow and the West End, the hotel is an ideal base for both business and pleasure. There are 333 designated non-smoking rooms as well as a number of disabled rooms. | Hammersmith |
| 3 Star - Jarvis Embassy House - This is an elegant Grade II listed Victorian building, with magnificent features which have been preserved. The Embassy House has wonderful charm and character, with an informal and relaxing atmosphere as well as some of the best service to be found anywhere in London. | Gloucester Road |
| 3 Star - The Paragon - Situated opposite Earls Court Exhibition Centre, this modern hotel has 500 en-suite bedrooms. Convenient for London's West End and tourist attractions. | West Brompton |
| 3 Star - Park International - The Park International was originally 5 Victorian town houses, which have been converted to an hotel, although most features still remain. Excellent standard of facilities throughout. | Gloucester Road |
| 3 Star - The Burns - The Burns is in the residential area of Earl's Court close to Chelsea, Belgravia and Knightsbridge. Previously a Victorian town house, sympathetically restored. | Earls Court |
| 3 Star - Kensington Plaza - The Kensington Plaza has been converted from 6 Victorian town houses. It still retains its original features, with high ceilings and its original staircase, although there are lifts. | Gloucester Road |
| 3 Star - Posthouse Kensington - A thoroughly modern hotel in one of the capital's most historic boroughs. Graded as a three star hotel even though a recent extensive refurbishment programme has raised it to a four star standard. It also offers comprehensive leisure facilities. | High Street Kensington |
| 3 Star - De Vere Park - The hotel is a fine example of Victorian architecture with many rooms offering views over Kensington Gardens and Hyde Park. Its proximity to Hyde Park makes it a perfect venue for those who enjoy strolling. Lovely large rooms offset by an excellent standard of service throughout. | High Street Kensington |
| 3 Star - Adelphi - Centrally situated in the Royal Borough of Kensington and Chelsea and just a minute away from London's main attractions. The Adelphi Hotel is a perfect base for visitors to one of the worlds most exclusive and fashionable neighbourhoods. | Gloucester Road |
| 3 Star - Comfort Inn Kensington - Situated on one of central London longest roads and surrounded by numerous museums and in one of the most sought after areas in London makes this a wonderful place to stay. | Earls Court |
| B&B Star - Eden Plaza - The Eden Plaza is ideally located for some of London's exclusive and more glamorous sights. At the Plaza you will be met by friendly and efficient staff and the rooms are extremely comfortable and offering great value for money. | Gloucester Road |
| B&B - Stuart - A small friendly hotel, situated amidst the historic surrounds of the Royal Borough of Kensington. | Gloucester Road |

The Royal Society of Chemistry
5th World Congress of Theoretically Oriented Chemists



Imperial College, London

The Corporate Team in association with The Royal Society of Chemistry has arranged special discounted rates for delegates attending the 5th Congress.

| HOTEL | | SINGLE | DOUBLE | Distance from Venue |
|----------------------------|--------|-----------|-----------|---------------------|
| Holiday Inn Kensington | 4 Star | £118.00 | £138.00 | 15 min. walk |
| Jurys Kensington | 4 Star | £110.00 | £110.00 | 5 min. walk |
| The Swallow International | 4 Star | £103.00 ♦ | £123.00 ♦ | 20 min. walk |
| Forum | 4 Star | £103.00 + | £123.00 + | 10 min. walk |
| Strathmore | 4 star | £87.00 ♦ | £99.00 ♦ | 5 min. walk |
| Kensington Moat House | 3 Star | £90.00 ♦ | £100.00 ♦ | 10 min. walk |
| Novotel Hammersmith | 3 Star | £89.00 ♦ | £99.00 ♦ | 4 Tube Stops |
| Jarvis Embassy House | 3 Star | £87.00 ♦ | £102.00 ♦ | 5 min. walk |
| Paragon | 3 Star | £75.00 | £85.00 | 2 Tube Stops |
| The Park International | 3 Star | £85.00 | £109.00 | 10 min. walk |
| Burns Hotel | 3 Star | £82.00 ♦ | £101.00 ♦ | 20 min. walk |
| Kensington Plaza | 3 Star | £75.00 | £95.00 | 5 min. walk |
| Forte Posthouse Kensington | 3 Star | £75.00 ♦ | £85.00 ♦ | 10 min. walk |
| De Vere Park | 3 Star | £69.00 | £79.00 | 10 min. walk |
| Adelphi Hotel | 3 Star | £65.00 ♦ | £79.00 ♦ | 10 min. walk |
| Comfort Inn Kensington | 3 Star | £60.00 ♦ | £80.00 ♦ | 20 min. walk |
| Eden Plaza | B & B | £59.00 ♦ | £72.00 ♦ | 10 min. walk |
| The Stuart Hotel | B & B | £48.00 ♦ | £64.00 ♦ | 10 min. walk |

All rates include VAT & Service + Continental breakfast included. ♦ English breakfast included. Rates are subject to change without prior notice.

For a wider range of hotels in different locations and price ranges, please contact BHRC with your requirements

To make your reservation, please complete the form opposite and return it to:

British Hotel Reservation Centre
13 Grosvenor Gardens
London SW1W 0BD
Tel: +44 (0)171 828 1075
Fax: +44 (0)171 828 6439
Email: events@corporateteam.co.uk

Or visit their website at

http://www.corporateteam.co.uk/events/123_QE for an online booking form.

APPLICATION FORM B



5th World Congress of
Theoretically Oriented Chemists
WATOC '99
Imperial College, London SW7
1 - 6 August 1999

Please quote ID Number 123 QE when you contact us

PLEASE DO NOT RETURN THIS FORM TO THE ROYAL SOCIETY OF CHEMISTRY

Kindly complete the form below and return by either:

Post to: British Hotel Reservation Centre
13 Grosvenor Gardens
London SW1W 0BD
Tel: +44 (0)171 828 1075
Fax: +44 (0)171 828 6439
Email: events@corporateteam.co.uk

Or Visit our website at <http://www.corporateteam.co.uk/events/123 QE> for an online booking form.

Priority Reservation Form - 123 QE

| | | |
|-------------------|-----------------------------|--------------------------|
| Name: | | |
| Company: | First Hotel Choice: | |
| Address: | Second Hotel Choice: | |
| | Arrival Date: | Approx. Time: |
| | No. Of Nights: | Smoking Room: Y/N |
| Postcode: | Room Type: | No of rooms: |
| Telephone: | Credit Card Type: | Expiry Date: |
| Facsimile: | Number: | |
| E-Mail: | Card Holder: | |

Please Note: Reservations will only be held until 1200 hours on the day of arrival unless guaranteed by a credit card. If you expect to arrive after 1200 hours, credit card details must be given above. No charge is made by TCT. Guests should settle their account at the hotel upon departure, unless otherwise arranged. There is no charge if the room is cancelled up to 24 hours before the arrival date. Non arrival or cancellation after this time may result in a charge being incurred.

The Corporate Team is a division of The Polyglobe Group • Tel: 0171-828 1075 • Fax: 0171-828 6439

| OFFICE USE | | | | |
|------------|------|-----|----------|--------|
| OWES | PAID | REF | ID NO | REG NO |
| | | | 99WATOC/ | |

5th World Congress of Theoretically Oriented Chemists



Imperial College, London, 1-6 August 1999

APPLICATION FORM A

Please type or write clearly

This form should be completed and returned, together with the appropriate remittance, to Mrs Paula Whelan, WATOC99, The Royal Society of Chemistry, Burlington House, London W1V 0BN, not later than **Monday 21 June 1999 (Early Bird Registration: Monday 17 May 1999)**.

GENERAL INFORMATION

- Title: Mr Miss Ms
 Mrs Dr Professor
Sex: M F
RSC Members Associate Student LRSC
 GRSC CChem MRSC CChem FRSC
WATOC Member

First Name:
(for badge)

Middle Initials:

Surname:

Mailing Address:

Post Code:* Country:

Fax No:
(inc. dialling code)

e-mail Address:

Affiliation:
(e.g. name of University, College, Company)

Employer's
Postcode*:

Special Diet/Disability:

Name of
Accompanying Person(s):
(Not participating in the Scientific Programme)

*by supplying this information, we will be able to process your application more efficiently

Please complete the form by indicating your choices in the boxes and entering your remittance in this column →

| | | Remittance | Office Use 11015 11093 |
|--|--|--------------------|---------------------------|
| Registration | Early Bird: Before 17 May 1999 | | |
| | <input type="checkbox"/> Member of the Royal Society of Chemistry/WATOC | £250.00 | |
| | <input type="checkbox"/> Non Member | £350.00 | |
| | <input type="checkbox"/> Student | £100.00 | |
| | <input type="checkbox"/> Accompanying Person | £30.00 | 530003 |
| | Standard: Before 21 June 1999 | | |
| | <input type="checkbox"/> Member of the Royal Society of Chemistry/WATOC | £300.00 | |
| | <input type="checkbox"/> Non Member | £400.00 | |
| <input type="checkbox"/> Student | £150.00 | | |
| <input type="checkbox"/> Accompanying Person | £30.00 | 530003 | |
| Accommodation | FULL CONFERENCE PERIOD <i>For 5 nights (bed & breakfast) arriving Sunday 1 August and departing on Friday 6 August</i> | | |
| | On Campus <u>Standard Accommodation</u> with Shared Bathroom Facilities (bed and breakfast) | | |
| | <input type="checkbox"/> Single Standard Room | per person £190.00 | 530002 |
| | <input type="checkbox"/> Twin-bedded Standard Room | per room £290.00 | |
| | EXTRA NIGHTS - Saturday 31 July 1999 | | |
| | <input type="checkbox"/> Single Standard Room | per person £38.00 | 530002 |
| | <input type="checkbox"/> Twin-bedded Standard Room | per room £58.00 | |
| | Friday 6 August 1999 | | |
| | <input type="checkbox"/> Single Standard Room | per person £38.00 | 530002 |
| | <input type="checkbox"/> Twin-bedded Standard Room | per room £58.00 | |
| | On Campus <u>Ensuite Accommodation</u> (private bathroom facilities and continental breakfast for 5 nights) | | |
| | <input type="checkbox"/> Single Ensuite Room | per person £235.00 | 530002 |
| <input type="checkbox"/> Twin-bedded Ensuite Room | per room £330.00 | | |
| HOTEL ACCOMMODATION should be booked via Application Form B and sent directly to BHRC | | | |
| Total carried forward | | £ | |

ALL PAYMENTS SHOULD BE MADE IN UK POUNDS STERLING

PERSONAL CHEQUE - Made payable to 'The Royal Society of Chemistry'

COMPANY CHEQUE - Made payable to 'The Royal Society of Chemistry'

CREDIT CARD

PLEASE CHARGE MY *EUROCARD / MASTERCARD/ VISA / AMERICAN EXPRESS*
(Delete appropriate)

ACCOUNT NUMBER:

Diners/Visa Electron CANNOT be accepted

EXPIRY DATE / Amount to be debited **UK£**

Authorised Address of Cardholder

.....

.....

.....

Authorised Signature of Cardholder

.....

BANK TRANSFER (A COPY OF PAYMENT ADVICE MUST BE ATTACHED)

Payment can be made by BACS to the following account:

National Westminster Bank

Kings Parade

10 Benet Street

Cambridge CB2 3PU

A/C Name:

RSC Conferences - WATOC 99

A/C No:

24052558

Sort Code:

60-04-23

Payments from overseas by bank transfer are subject to a charge of approximately £30.00. These charges are usually deducted by the bank before passing into the Society bank account. Any such charges should be met by the applicant.

The data you supply on this Registration Form will be held on computer by The Royal Society of Chemistry for the purposes of administering this Conference. A list of participants, which will include e-mail addresses, will be published for distribution at the conference. If you **DO NOT** wish to be included in this list, please tick the box

The Royal Society of Chemistry may include your address on its records in order that information on any future meetings related to this subject and RSC products and services may be sent to you. If you **DO NOT** wish to receive details, please tick the box.

Your name, address and affiliation may be passed onto exhibitors at the meeting. If you **DO NOT** wish your details to be forwarded, please tick the box.

All cheques, postal orders or money orders should be made payable to 'THE ROYAL SOCIETY OF CHEMISTRY' and crossed. If for any reason it should be necessary for the remittance to be sent separately from this application, every effort should be taken to ensure that the cheque/money order is identifiable with the **APPLICANT** and **WATOC99**. The Royal Society of Chemistry VAT Registration no. is: GB 342 1764 71. *THIS IS NOT A TAX INVOICE.*



The Royal Society of Chemistry is the professional body for chemists and the learned society for chemistry in the UK. Income generated by the Society's activities is used to provide services for members and benefit the chemical community.

Conferences and Awards
Royal Society of Chemistry
Burlington House, Piccadilly
London, UK W1V 0BN

Tel +44 (0) 171 437 8656
Fax +44 (0) 171 734 1227
E-mail conferences@rsc.org
WWW <http://www.rsc.org/conferences>

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