



**International
Union of
Crystallography**

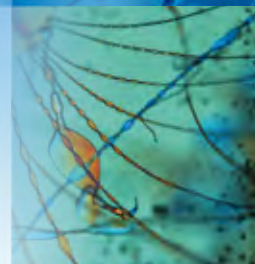
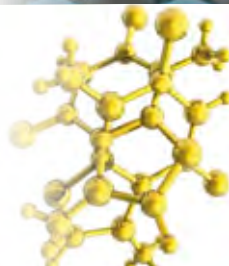
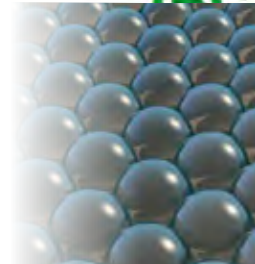
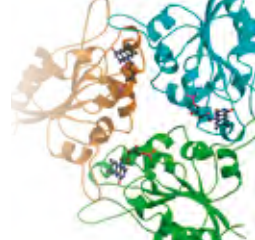
**Madrid
22-30
August
2011**

XXII Congress and General Assembly

**Second
Announcement**

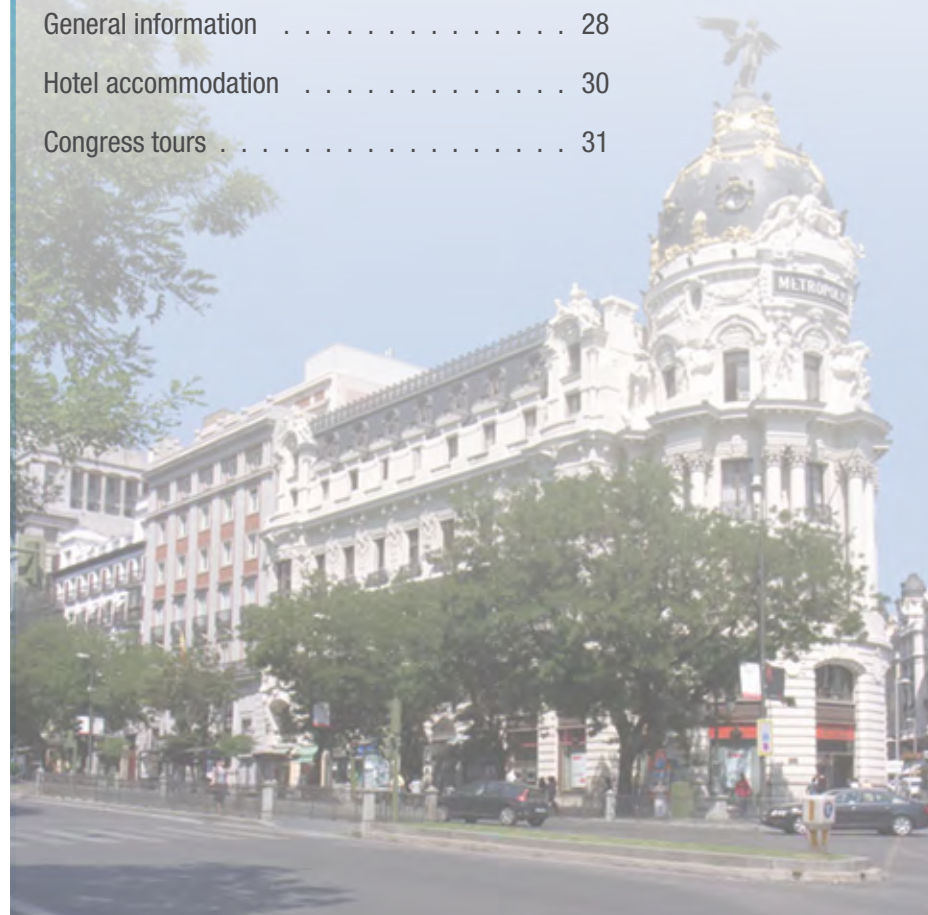


<http://www.iucr2011madrid.es>



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Welcome

The triennial meetings of the International Union of Crystallography represent a highlight for crystallographers worldwide. In August 2011 we have the opportunity to meet again in Madrid for the XXII International Congress and General Assembly of the IUCr that is being organized by our Spanish colleagues.

As you can see from this circular, the International Program Committee has put together a rich scientific program of Microsymposia and Keynote Lectures that in an excellent way illustrates all the new achievements of crystallography in its many facets.

Another important component of the meeting is the General Assembly where the delegates from 50 IUCr member countries get together to review the work of the IUCr, elect the members of the Executive Committee and Commissions and decide on the venue for the 2017 Congress.

I have had the opportunity to meet with the Spanish organizers and visit the beautiful conference venue in Madrid. From these experiences I can tell you that our Spanish hosts are doing everything to make the Congress a success and make you feel at home in Madrid, so you can enjoy both the science at the Congress and the charm and beauty of the city.

So everything is in place for a successful IUCr Congress, and I hope that you will accept this invitation from our Spanish colleagues, so I can look forward to seeing many crystallographers from all parts of the world in Madrid next August.

Sine Larsen
President
International Union of Crystallography

The Spanish Crystallographic Community warmly invites you to participate in the XXII Congress and General Assembly of the International Union of Crystallography (IUCr) to be held in Madrid, Spain, in August 2011. The Local Organizing Committee together with the International Program Committee, are working hard to offer a scientific program of the highest quality, aimed at showing the latest developments and topics in the field of one of the most interdisciplinary sciences that links together frontier areas of research.

With an attractive and weighty Scientific Program and taking into account all the different research interests, the timetable has been organized trying to avoid any overlap in topics, making sure that every attendant can make the most of their participation.

Crystallography plays a key role for the development of many important scientific fields, from Mineralogy up to Chemistry, Physics, Material Sciences, Nanotechnology, Biochemistry, Biology and Biomedicine. No scientist is a stranger to the crystallographic forum.

Learning about new trends in all these scientific areas surrounded by Madrid's friendly and cosmopolitan atmosphere, a European city privileged with its cultural and historical heritage, will be an unforgettable experience.

We look forward to welcoming you in Madrid!

Enrique Gutiérrez-Puebla
Chairperson
XXII IUCr Madrid 2011 Congress

Honorary Committee

Presidency:

The King and Queen of Spain

Members:

The Minister of Science and Innovation

The President of the Community of Madrid

The Mayor of the City of Madrid

The President of the Spanish National Research Council (CSIC)

The Rector of the University of Alcalá

The Rector of the University Complutense of Madrid

The Rector of the Autonomous University of Madrid

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Sakura Pascarelli (France)

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Jill Trehwella (Australia)

Pamela Whitfield (Canada)

Jian-Min Zuo (USA)

James F. Britten (Canada) *Ex-officio*

Yasuhiko Fujii (Japan) *Ex-officio*

Chris Gilmore (UK) *EC Representative*

Technical Secretariat

Grupo Pacífico, S.A.

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Important dates

- **January 15, 2011:** Opening of abstracts submission
- **March 15, 2011:** Deadline for bursary applications
- **April 15, 2011:** Deadline for abstracts submission
- **May 15, 2011:** Deadline for "Early Bird" registration
- **June 15, 2011:** Deadline for payment registration fees for validation and publication of submitted abstracts.

The organization strongly recommends communicating your interest in exhibition, hotel & tours reservations as follows:

- **By May 15, 2011:** For exhibitors stand reservations.
- **By June 1, 2011:** For hotel & tours registration.

Timetable

Monday, August 22	Registration Opens (11:00) Pre-Congress Workshops Opening Ceremony (18:30-19:30) Ewald Prize Lecture (19:30-20:30) Welcome Reception (20:30-22:00)
Tuesday, August 23	Scientific Session Exhibition Evening: IUCr General Assembly
Wednesday, August 24	Scientific Session Exhibition Evening: IUCr General Assembly
Thursday, August 25	Scientific Session Exhibition Evening: Cultural Activity
Friday, August 26	Scientific Session Exhibition Evening: Congress Dinner
Saturday, August 27	Scientific Session Exhibition Evening: IUCr General Assembly
Sunday, August 28	Scientific Session Exhibition Evening: IUCr General Assembly
Monday, August 29	Scientific Session Closing Ceremony
Tuesday, August 30	Congress Tours

Scientific program

Please note that the scientific program, elaborated by the International Program Committee and approved by the IUCr Executive Committee, is still subject to the acceptance of some of the invited speakers and Chairs. Please refer to the website for the revised information.

Tuesday, August 23, 2011

- 09:00 - 09:50 **PL 1** Thomas A. Steitz
Understanding the Structural Basis of Ribosome Function
Chair: Sine Larsen
- 09:50 - 10:15 **Coffee Break**
- 10:15 - 12:50 **MS 1 Hot Structures in Biology I**
Chairs: Poul Nissen, Guillermo Montoya
MS 2 Hybrid Methods: the EM-Crystallography Interface
Chairs: Eva Nogales, Jorge Navaza
MS 3 Polymer and Gel Structure: Arriving at a Structural Model
Chairs: Parthasarathi Dastidar, Beatriu Escuder Gil
MS 4 Industrial Applications of SAXS and SANS
Chairs: Robert Knott, Aldo F. Craievich
MS 5 Non-Ambient Powder Diffraction
Chairs: Dave Billing, Tiziana Boffa-Ballaran
MS 6 Crystal Structure Prediction: Practice and Applications
Chairs: Sally L. Price, John Kendrick
MS 7 Coherent Diffraction and Imaging
Chairs: Vincent Favre-Nicolin, John Rodenburg
- 12:50 - 15:00 **Lunch and Poster Session**
- 15:00 - 17:35 **MS 8 Large Biological Assemblies**
Chairs: Andrew Leslie, Keiichi Namba
MS 9 Topological Correlations and Crystal Structure Interconnections
Chairs: Jean-Guillaume Eon, Hans-Joachim Klein
MS 10 Determination of Ab-Initio Crystal Structures from Powder Diffraction and their Applications in Pharmaceutical Industry
Chairs: Fabia Gozzo, Maryjane Tremayne
MS 11 Standardization, Validation, and Automation in Modern Biological Small-Angle Scattering
Chairs: Javier Pérez, Mario de Oliveira Neto
MS 12 Non-Covalent Interactions in Molecular Crystals and Biomolecular Systems under Pressure
Chairs: Simon Parsons, Kamil Dziubek
MS 13 Automation of Data Collection and Remote Control of Experiments
Chairs: Olof Svensson, Masaki Yamamoto
MS 14 Biomineralization and Biomimetic Materials
Chairs: Dino Aquilano, Jaime Gómez-Morales
- 17:40 - 18:30 **KN 1** Tomitake Tsukihara
Large Macromolecular Assemblies
Chair: Yasushi Kai
KN 2 Ian Robinson
Coherent X-Ray Diffraction
Chair: Janos Kirz
KN 3 Michael O'Keefe
Topological Characterization of Coordination Networks & Metal-Organic Frameworks
Chair: Davide Proserpio
- 18:30 - 19:30 **Poster Session**

Scientific program

Wednesday, August 24, 2011

- 09:00 - 09:50 **KN 4** Peter Kwong
Crystallography and the Design of An Effective HIV-1 Vaccine
Chair: David Stuart
KN 5 Iris Torriani
X-Ray Diffraction and Small-Angle Scattering to the Study of Polycrystalline Materials, Polymers and Soft Matter
Chair: To be confirmed
KN 6 Makoto Fujita
Crystal Engineering
Chair: Mike Zarawotko
- 09:50 - 10:15 **Coffee Break**
- 10:15 - 12:50 **MS 15 Nucleosome Processing and Epigenetics**
Chairs: Daniela Rhodes, K. Morikawa
MS 16 Crystallography in Disease and Therapy
Chairs: Hugo L. Monaco, Colin Groom
MS 17 Synthons: from Small to Macromolecules
Chairs: Pinak Chakrabarti, Catalina Ruiz-Pérez
MS 18 Powder Diffraction at the Nanoscale
Chairs: Antonella Guagliardi, Yuri Andreev
MS 19 Synthesis, Structure and Properties of Novel Materials at High Pressure
Chairs: Olga Degtyareva, Valentín García Baonza
MS 20 Beyond Space-Group Symmetry in Periodic Structures
Chairs: Marco Pasero, Bernd Souvignier
MS 21 Surfaces & Interfaces
Chairs: Ullrich Pietsch, María Varela del Arco
- 12:50 - 15:00 **Lunch and Poster Session**
- 15:00 - 17:35 **MS 22 Cell Signalling and Protein-Protein Interactions**
Chairs: Michael Parker, M.V. Hosur
MS 23 Difficult Phasing and Difficult Structures
Chairs: Phil Evans, Manfred Weiss
MS 24 New Challenges in Crystal Engineering: Correlating Structure and Properties
Chairs: Piero Sozzani, Alicia Beatty
MS 25 Crystallography of Materials with Exchange, Sequestration and Storage Properties
Chairs: Thomas Albrecht-Schmitt, Elena Bonaccorsi
MS 26 SAXS/SANS, Total Scattering and the Nanostructure Problem
Chairs: Simon Billinge, Michael V. Avdeev
MS 27 Developments and Directions for Crystallographic Databases
Chairs: Saulius Gražulis, John Westbrook
MS 28 Wide Band Semiconductor and Other Crystals Used in Optoelectronics
Chairs: Ewa Talik, Enrique Calleja
- 17:40 - 18:30 **KN 7** Eva Nogales
EM, Hybrid Methods
Chair: Michael Rossmann
KN 8 Roberto Fornari
New Trends in the Growth from the Melt of Semiconductors: the Use of External Fields
Chair: Jiyang Wang
KN 9 Kei Hirose
High-Pressure Geoscience/Mineralogy (with Particular Reference to Post-Perovskite)
Chair: Przemek Dera
- 18:35 - 19:25 **PL 2** Venkatraman Ramakrishnan
Title to be confirmed
Chair: Ted Baker

Scientific
program

Thursday, August 25, 2011

- 09:00 - 09:50 **KN 10** Ian Wilson
Exploration of Protein Structure Universe with Structural Genomics
Chair: Helen Berman
- KN 11** Yaroslav Filinchuk
Energy Related Materials: Borohydrides
Chair: Bjorn Hauback
- KN 12** Alessia Bacchi
Supramolecular Chemistry
Chair: Guy Orpen
- 09:50 - 10:15 **Coffee Break**
- 10:15 - 12:50 **MS 29** Viruses and Viral Proteins
Chairs: Fasseli Coulibaly, Ying-Fang Liu
- MS 30** Diffuse Scattering in Partially Ordered/Disordered Systems
Chairs: Thomas Weber, Ernesto Estevez Rams
- MS 31** Structural Implications in Catalytic Processes
Chairs: Arnold Rheingold, Jorge Rodríguez-Navarro
- MS 32** Crystallography in Industrial Process Control
Chairs: Jim Kaduk, Nikki Scarlett
- MS 33** New Sources (Neutrons, X-Rays, XFEL)
Chairs: Edgar F. Weckert, Christian Vettier
- MS 34** Descriptors of Electronic Structure and Chemical Bonding
Chairs: Louis J. Farrugia, Angel Martín Pendás
- MS 35** The Growth and Morphology of Crystals
Chairs: Arkady Glikin, Sol López-Andrés
- 12:50 - 15:00 **Lunch and Poster Session**
- 15:00 - 17:35 **MS 36** Understanding Bacterial Pathogenesis
Chairs: Jijie Chai, Dirk Heinz
- MS 37** X-Ray Lasers and Other New Frontiers in Synchrotron Applications to Structural Science
Chairs: Soichi Wakatsuki, Janet L. Smith
- MS 38** Fabrication and Macroscopic Properties of Flexible Frameworks
Chairs: Michaela Hardie, to be confirmed
- MS 39** Energy-Related Materials
Chairs: William I.F. David, Rosa Palacín
- MS 40** Pressure-Induced Phase Transitions
Chairs: Vadin Brazhkim, Karen Friese
- MS 41** Advanced Approaches in Charge Density Analysis and Derived Properties
Chairs: Nouzha Bouhmaida, Christian Jelsch
- MS 42** XAFS Studies in Biology Coupled to Crystallography
Chairs: Farideh Jalilehvand, Sofia Díaz-Moreno
- 17:40 - 18:30 **KN 13** Juan Hermoso
Bacterial Pathogenicity and Peptidoglycan Degradation Machines
Chair: Rita Berisio
- KN 14** John Spence
Ultrafast Crystallography with X-Ray Free Electron Lasers
Chair: Keith Hodgson
- KN 15** Len J. Barbour
Porous Materials. Structure of Solid Gas Materials
Chair: S. Natarajan
- 18:30 - 19:30 **Poster Session**

Scientific
program

Friday, August 26, 2011

- 09:00 - 09:50 **KN 16** Gerard Kleywegt
Validation and Error in Protein Structures
Chair: Gert Vriend
- KN 17** Helmut Coelfen
Prenucleation Clusters and Crystallization Control by Additives
Chair: Manuel Prieto
- KN 18** Steve Pennycook
Atomic Resolution Real-Space Imaging and Aberration Corrected Electron Microscopy
Chair: Carlos Otero
- 09:50 - 10:15 **Coffee Break**
- 10:15 - 12:50 **MS 43** Validation, Error Detection and Fraud Prevention
Chairs: Eleanor Dodson, Ian Bruno
- MS 44** Quantitative Real Space Electron Imaging
Chairs: Sandra Van Aert, Ángel Landa
- MS 45** Dynamical Structural Science
Chairs: Pance Naumov, Eric Collet
- MS 46** Powder Diffraction Methods in Archaeometry
Chairs: Gilberto Artioli, Petr Bezduka
- MS 47** Advances in High Pressure Techniques and Instrumentation
Chairs: Chris Tulk, Giuliana Aquilanti
- MS 48** Electron Momentum and Spin Densities in Correlated Electron Systems
Chairs: Bernardo Barbiellini, Masahisa Ito
- MS 49** Crystal Growth and Interface Phenomena at Nanoscale
Chairs: Katsuo Tsukamoto, Jim De Yoreo
- 12:50 - 15:00 **Lunch and Poster Session**
- 15:00 - 17:35 **MS 50** Structural Biology of the Immune System
Chairs: Dinakar M. Salunke, Yvonne Jones
- MS 51** Complementary Biophysical Methods: Adding Value to Protein Structures
Chairs: Nathan Cowieson, Dorothy Beckett
- MS 52** Graphitic Materials
Chairs: Kazutomo Suenaga, Pascale Launois
- MS 53** High-Throughput Crystallization and Polymorphic Search in Pharmaceuticals
Chairs: Ulrich Griesser, Susan M. Reutzel-Edens
- MS 54** Minerals as Advanced Materials
Chairs: Volker Kahlenberg, Claudia Weidenthaler
- MS 55** Structure and Dynamics by Inelastic Scattering
Chairs: Alfred Baron, Helmut Schober
- MS 56** Spectroscopic Approaches (XAFS, NMR, ...) in Crystallography
Chairs: M. Carmen Asensio, Carlo Castellano
- 17:40 - 18:30 **KN 19** Sunney Xie
Single-Molecule Methods
Chair: Ignacio Tinoco
- KN 20** Emil Makovicky
From Plane Groups to Quasilattices: Hispano-Islamic Ornamental Art of the Alhambra, Cordoba and Sevilla
Chair: Stephen Hyde
- KN 21** Bo Iversen
Materials Crystallography
Chair: Carlo Gatti

Scientific
program

Saturday, August 27, 2011

- 09:00 - 09:50 **KN 22** George Sheldrick
The SHELX Approach to Experimental Phasing of Macromolecules
Chair: David Brown
- KN 23** Ute Kolb
Ab-Initio Structure Solution of Complex Inorganic, Organic and Mineral Structures By Automated Electron Diffraction Tomography
Chair: Christian Baerlocher
- KN 24** José Elguero
Structural Motifs in Organic Chemistry
Chair: Andre Roodt
- 09:50 - 10:15 **Coffee Break**
- 10:15 - 12:50 **MS 57 New Perspectives in Structural Genomics**
Chairs: Celia Goulding, Shigeyuki Yokoyama
- MS 58 New Computational Approaches to Structure Solution and Refinement**
Chairs: Anastassis Perrakis, Paul Adams
- MS 59 Anion Recognition and Templatation in Halogen Bonding**
Chairs: Venkateswara R. Pedireddi, Melanie Rademeyer
- MS 60 Solid State Reactivity**
Chairs: Simona Galli, John B. Parise
- MS 61 Hot Structures in Chemical Crystallography**
Chairs: Shie-Ming Peng, Dietmar Stalke,
- MS 62 Crystallographic Software: the Library Approach**
Chairs: Ralf Grosse-Kunstleve, Luc Bourhis
- MS 63 Quasicrystals and Their Approximants: Structure and Physical Properties**
Chairs: Hiroyuki Takakura, N.K. Mukhopadhyay
- 12:50 - 15:00 **Lunch and Poster Session**
- 15:00 - 17:35 **MS 64 Hot Structures in Biology II**
Chairs: Tsuyoshi Inoue, Se Won Suh
- MS 65 Atomistic and Electronic Structures of Nanomaterials**
Chairs: Marek Malac, Quan Li
- MS 66 Electric, Magnetic and other Physical Properties of Molecular Crystals**
Chairs: Song Gao, Akiko Kobayashi
- MS 67 Layered Inorganic Materials and Layered Precursors of 3D Structures**
Chairs: Bernd Marler, Heloise Pastore
- MS 68 Data Reduction of Area Detector Measurements**
Chairs: Garry J. McIntyre, to be confirmed
- MS 69 Crystallographic Methods and Software for Periodic and Aperiodic Crystals**
Chairs: Michal Dusek, Lian-Mao Peng
- MS 70 Radiation Damage: Consequences and Uses**
Chairs: Vittal K. Yachandra, Gerd Rosenbaum
- 17:40 - 18:30 **KN 25** Christiane Schaffitzel
Ribosome Complexes
Chair: to be confirmed
- KN 26** S.V. Krivovichev
Topological Variations and Crystal Structure Interconnections
Chair: Elena Sokolova
- KN 27** Samar Hasnain
XAFS Contribution to Protein Structure-Function Investigations
Chair: Britt Hedman
- 18:35 - 19:25 **PL 3** Avelino Corma
Micro and Mesoporous Crystalline Materials: Structural and Composition Implications in Adsorption and Catalysis
Chair: Angeles Monge

Scientific
program

Sunday, August 28, 2011

- 09:00 - 09:50 **KN 28** Leemor Joshua Tor
Structural Basis of Cell Regulatory Processes
Chair: María Armenia Carrondo
- KN 29** Elena Boldyreva
Molecular Crystals at High Pressure
Chair: Andrzej Katrusiak
- KN 30** Reinhard Neder
Powder Diffraction at the Nanoscale: Structure and Defects
Chair: David Keen
- 09:50 - 10:15 **Coffee Break**
- 10:15 - 12:50 **MS 71 Machinery of RNA Processing**
Chairs: Ben Luisi, Mark Glover
- MS 72 Automated Data Processing and Structural Solution for High Throughput Crystallography**
Chairs: Frank Von Delft, Rocco Caliandro
- MS 73 Theory and Practice of Hydrogen Bond: An Evergreen Interaction for Molecular Recognition**
Chairs: Paola Gilli, Andrew Bond
- MS 74 Powder Diffraction and Complementary Techniques**
Chairs: Peter Chupas, Marco Milanese
- MS 75 Liquids, Amorphous and Nanocrystalline Solids at High Pressure**
Chairs: Chrystele Sanloup, Stanimir Bonev
- MS 76 Density Functional Methods for Electronic Structure Calculations**
Chairs: Angel Rubio, Risto Nieminen
- MS 77 XAFS Instrumentation: Automation, Standardization and Validation of XAFS Experiments**
Chairs: Christopher Chantler, Kiyotaka Asakura
- 12:50 - 15:00 **Lunch and Poster Session**
- 15:00 - 17:35 **MS 78 Transcription and Translation**
Chairs: Anders Liljas, Dmitry Vassilyev
- MS 79 Electron Diffraction and Crystallography**
Chairs: Philip Nakashima, Christop Koch
- MS 80 Solid State Photochemistry**
Chairs: Menahem Kaftory, Pilar Gómez Sal
- MS 81 The Crystallography of Functional Inorganic Materials and Their Applications**
Chairs: Dhananjai Pandey, Yoshihiro Kuroiwa
- MS 82 Biological Neutron Scattering and Deuteration**
Chairs: Trevor Forsyth, Joanna Krueger
- MS 83 Application of Crystal Structure Information in Chemical Education**
Chairs: Gary M. Battle, Lourdes Infantes
- MS 84 What is order, and how can one describe it? (Which kinds of matter diffract?)**
Chairs: Marjorie Senechal, Uwe Grimm
- 17:40 - 18:30 **KN 31** Yigong Shi
Membrane Proteins
Chair: Mitchell Guss
- KN 32** Ron McGrath
Structure of Quasicrystalline Surfaces
Chair: Ron Lifshitz
- KN 33** A.M. Balagurov
Magnetic Neutron Crystallography - Commensurate and Incommensurate Structures
Chair: E. Suard
- 18:30 - 19:30 **Poster Session**

Scientific
program

Monday, August 29, 2011

- 09:00 - 09:50 **KN 34** Janet Newman
Protein Crystallization
Chair: Alex McPherson
- KN 35** Gautam R. Desiraju
Molecular Recognition in Crystals
Chair: Carlo Mealli
- KN 36** Isabelle Mirebeau
Frustration and Spin-Lattice Coupling in Oxides
Chair: J.L. García Muñoz
- 09:50 - 10:15 **Coffee Break**
- 10:15 - 12:50 **MS 85 Membrane Protein Structures**
Chairs: So Iwata, María J. Sánchez-Barrena
- MS 86 Challenges of Low-Resolution Crystallography**
Chairs: Joel Sussman, Irene Margiolaki
- MS 87 Chirality in the Solid State, from Organic Molecules to Chiral MOF and Helical Materials**
Chairs: Jennifer Swift, Berta Gómez Lor
- MS 88 Crystal Chemistry and Physics of Modulated and Composite Crystals**
Chairs: Joke Haderman, Andreas Schönleber
- MS 89 Archiving, Exchange and Retrieval of Scientific Data in the 21st Century**
Chairs: James Hester, David Brown
- MS 90 Hydrogen Bonding: from the Solid State to Solution**
Chairs: Alan Soper, Mark E. Tuckerman
- MS 91 X-Ray Absorption, Diffraction and Imaging in Forensic Science and Ancient Materials**
Chairs: Simona Quartieri, Joaquín García-Ruiz
- MS 92 Crystallising Challenging Biological Targets**
Chairs: Kunio Miki, Abel Moreno
- 12:50 - 14:20 **Lunch**
- 14:25 - 17:00 **MS 93 Dissecting Enzyme Mechanisms**
Chairs: Xavier Gomis-Rüth, Andrea Mattevi
- MS 94 Molecular Recognition in the Crystal Bulk and in the Surface: Theory and Applications**
Chairs: Jürg Hulliger, Bart Kahr
- MS 95 Automated Data Processing and Structural Solution for Powder Crystallography**
Chairs: Rosanna Rizzi, Anton Meden
- MS 96 Complementary Use of Neutrons and Photons in Magnetism**
Chairs: Robert Cywinski, Valeria Lauter
- MS 97 Web Based Crystallography Teaching: the Use of Modern Communication Methods to Teach Crystallography**
Chairs: Katherine Kantardjieff, Gervais Chapuis
- MS 98 Complex Structure and Frustrated Systems: Simulation and Experiments**
Chairs: Olivier Perez, Guido Kreiner
- 17:10 - 18:00 **PL 4** Ada Yonath
The Spectacular Architecture of the Ribosome and Clues about its Origin
Chair: Peter Colman

Satellite
meetings

'Aperiodic Crystals for Beginners.'

August 31 - September 1, 2011,
Alcalá de Henares, Madrid, Spain.

Organizers:

M. de Boissieu (*Chair*), M. Perez Mato (*Co-chair*), A. Abakumov, G. Chapuis, S. van Smaalen

Scientific advisory board:

The IUCr commission on Aperiodic Crystals

Aperiodic crystals (incommensurately modulated phases, incommensurate composite crystals and quasicrystals) are found in many different systems such as minerals, the elements at high pressures, various inorganic compounds, molecular crystals and intermetallics. Their identification is nowadays easier thanks to the steady improvement of instrumentation, modern X-ray and neutron detectors and advanced transmission electron microscopes. The knowledge of the atomic structure of aperiodic crystals is a key point for the understanding of their chemical and physical properties. However, this still remains difficult for the non-specialist. This two-day satellite meeting offers a basic and tutorial introduction to structural analysis of aperiodic crystals. The general concepts of the high-dimensional crystallography will be introduced step by step and they will be applied to a few organic and inorganic materials. A hands-on exercise will be organized for simple examples.

The satellite meeting will take place in Alcalá de Henares, a beautiful historical Spanish city, conveniently located about 30 minutes from the Madrid international airport. Further details can be found on the web site: <http://sig3.ecanews.org/aperbeg2011/aperbeg2011.html>

Contact person: Marc de Boissieu - Marc.de-boissieu@simap.inpg.fr

2011 Crystallographic Computing School - Mieres

August 15-20, 2011

Universidad de Oviedo, Mieres, Asturias, Spain

Organizers:

Harry Powell (MRC, UK), Ralf Grosse-Kunstleve (LBNL, USA), Min Yao (Hokkaido University, Japan), Santiago García-Granda (Univ. de Oviedo, Spain), Laura Torre-Fernández, (Univ. de Oviedo, Spain), Laura Roces Fernández, (Univ. de Oviedo, Spain), Ángel Gutiérrez (Univ. de Oviedo, Spain).

The Mieres Crystallographic Computing School will build on the foundations laid by previous schools in Siena (Italy) and Kyoto (Japan). Senior developers of current major initiatives will be available throughout the school for discussions with those who are interested in contributing new software for crystallographic calculations. The school is structured to foster the exchange of ideas via formal lectures, afternoon tutorials, coding challenges and code comparison sessions. Special historical talks will be used to emphasize the ways in which the science of crystallography has been encapsulated in the software, from the early days of computing to the present day.

A major theme of the school will be to harvest the knowledge and experience of senior developers across the whole field, from small angle scattering, powder diffraction, to single crystal methods as implemented in both chemical and macromolecular crystallography. We are aiming for the "cross-pollination of minds" to which Ray Pepinsky referred in his opening address to the inaugural conference on Crystallographic Computing in April 1950.

With help from our sponsors, we hope to keep the registration cost (including accommodation

Satellite meetings

and meals) below 600 € (ca \$US 780). We expect to have student bursaries available to reduce the cost further for a limited number of attendees. The number of attendees is limited to 80 students. The registration deadline is July 22, 2011.

<http://www.iucr.org/resources/commissions/crystallographic-computing/schools>

Contact person: Harry Powell - harry@mrc-lmb.cam.ac.uk

Categorizing Halogen Bonding and Other Noncovalent Interactions Involving Halogen Atoms

August 20-21, 2011

Sigüenza, Guadalajara, Spain

Organizers:

Scientific Program Committee: Pierangelo Metrangolo, *Chairman* (Italy), Giuseppe Resnati, *Chairman* (Italy), Roberto Marquardt (France), Jane S. Murray (USA), Tullio Pilati (Italy), Giancarlo Terraneo (Italy).

Local Organizing Committee: Guillermo Mínguez Espallargas (Spain), Marcos Daniel Garcia Romero (Spain).

Halogen atoms in organic compounds typically can be found at the periphery of molecules. For this reason, they are ideally positioned to be involved in intermolecular interactions. For instance, halogen atoms are common place substituents in drugs and also occur naturally in biological systems.

The term halogen bonding has been introduced for describing any noncovalent interaction involving halogens as acceptors of electron density. The objective of this workshop is to gather several international leaders in the field around the task of giving a modern definition of halogen bonding that takes into account all current experimental and theoretical pieces of information on both gaseous and condensed halogen-bonded systems in chemical and biological systems (IUPAC Project no. 2009-032-1-100)

www.iupac.org/web/ins/2009-032-1-100; www.halogenbonding.eu.

The Workshop attendance is free and the number of participants is limited to 50.

The following leaders in the field have already accepted to deliver a lecture:

Christer Aakeröy (USA), Ibon Alkorta (Spain), Lee Brammer (UK), Duncan W. Bruce (UK), David Bryce (Canada), Gautam R. Desiraju (India), Francesco Devillanova (Italy), Wolf-W. du Mont (Germany), Marc Formigué (France), P. Shing Ho (USA), Pavel Hobza (Czech Republic), Lars Kloo (Sweden), Anthony C. Legon (UK), Peter A. Politzer (USA), Kari Rissanen (Finland), Antonio Togni (Switzerland), Hiroshi Yamamoto (Japan)

Further information: Scientific Secretariat

Serena Biella, Italy: serena.biella@polimi.it

Gabriella Cavallo, Italy: gabriella.cavallo@polimi.it

Online Edition of International Tables for Crystallography: Databases and Applications of Space Groups and their Symmetry Relations

September 1-3, 2011

Bilbao, Basque Country, Spain

Organizers:

Local Organizing Committee:

Gotzon Madariaga (Chair), Mois I. Aroyo, Josu Igartua, Emre Tasci, Gemma de la Flor

Satellite meetings

The workshop is organized by the Department of Condensed Matter Physics (Universidad del País Vasco, Spain) and the Commission on Mathematical and Theoretical Crystallography of IUCr. It is supported by the Commission of International Tables of IUCr.

The aim of the workshop is the introduction to the current state and the future developments of the new Online Edition of International Tables for Crystallography, Vol. A: Space-group symmetry, and Vol. A1: Symmetry relations between space groups. The new web server provides an excellent on-line tool for the study of crystallographic symmetry and its applications. It gives access to databases with symmetry information on crystallographic groups (plane, space and subperiodic). The available software includes computer tools for the study of group-subgroup relations between space groups (e.g. subgroups and supergroups, coset decompositions, splitting of Wyckoff positions). Possible applications of the available databases and computer tools related to specific problems of solid-state physics and chemistry as magnetic symmetry, phase transitions, structural pseudosymmetry, relations between crystal structures, etc., form an important part of the workshop program. The workshop aims at giving the necessary background and practical skills for an efficient use of the online databases and programs on the new web server of International Tables for Crystallography.

Lecturers

Nicola Ashcroft (IUCr-Chester, UK), Daniel Litvin (Reading, USA), Massimo Nespolo (Nancy, France), J Manuel Perez-Mato, Gotzon Madariaga, Mois I. Aroyo (Bilbao, Spain).

Contact person: Gotzon Madariaga - gotzon.madariaga@ehu.es

2011 International School on Charge Density – Theory and Practice

30 August – 4 September 2011

Zaragoza University Residence, Jaca, Huesca (Spain)

Organizers:

Prof. Claude Lecomte (CRM2 UMR 7036 Nancy-Université – CNRS, France)

Prof. Fernando J. Lahoz (CSIC – University of Zaragoza, Spain)

Secretary:

Dr. Pilar García Orduña (CSIC – University of Zaragoza, Spain)

The school is supported by the IUCr Commission on Charge, Spin and Momentum Densities.

Charge and spin density determination through high order X-ray and polarized neutrons diffraction experiments is a powerful method to get a detailed description of the chemical and physical properties of molecules and materials. This approach has become quite accessible for organic and first row transition metals complexes using user-friendly software. This school will cover all the aspects of the methods, from data collection procedures to the analysis of derived properties. Extension to proteins and heavy atoms will be discussed. Tutors of the school will be well known specialists in the area and main software authors will attend the school to demonstrate their programs. Software training will be extensively provided to the participants.

The school will be held in Jaca (Spanish Pyrenees), with a minimum of 32 teaching hours, equally distributed between theory and practice. The organization will arrange transport from/to Madrid, and cheap accommodation for participants. A tentative registration cost will be around 360 € including registration, half-board accommodation in a shared room and a half-day hiking activity. The number of attendees is strictly limited to 50 persons.

For more information and formalize registration see www.iucr2011madrid.es or contact directly with F.J. Lahoz at lahoz@unizar.es or C. Lecomte at claudel@crm2.uhp-nancy.fr.

Satellite meetings

Crystallography of Hispano-Islamic Ornamental Art: Visit to the Alhambra in Granada

August 30 - September 1

Granada, Spain

This event is proposed by the CrysAC "Crystallography in Art and Cultural heritage" IUCr commission; the lead person for its contents is Prof. Emil Makovicky, University of Copenhagen.

The palace complex of the Alhambra in Granada (Andalusia) is the most comprehensive collection of Hispano-Islamic ornamental art at its peak development and offers examples spanning a wide range from plane groups of symmetry to quasilattices. The two-day excursion from Madrid will present and analyze ornamental patterns based on simple plane groups, dichroic plane groups, analysis of Islamic approach to polychromatic patterns, the use of layer groups and 1-D groups, the conscious combinations of different symmetry principles in one pattern and, finally, two-dimensional decagonal and octagonal quasicrystalline patterns. An afternoon session with presentations and discussion will precede the in situ study of the ornaments the following day.

For more information and formalize registration see www.iucr2011madrid.es or contact directly with Emil Makovicky, Emilm@geo.ku.dk

All workshops will take place on Monday, August 22, 2011 from 9:00 to 18:00 at the Congress Palace. Registration for the workshop is additional to the Congress registration. Please refer to the website for the updated information.

Workshop n° 1:

XAFS Tutorials for crystallographers and beginners: General introduction and analytical methods for crystallographers and beginners in the field of XAFS

The purpose of the Tutorial is to give a general introduction and analytical methods for crystallographers and beginners in the field of XAFS. The number of participants is limited to 60.

Lectures will cover the fundamentals of XAFS: data analysis and its principles, theory and simulation of XAFS spectra, with applications to biology, chemistry, physics and materials science. Some tutorials will provide hands-on practice of EXAFS.

For more information please contact:

Isabella Ascone, isabella-ascone@chimie-paristech.fr

Joaquin García Ruiz, jgr@unizar.es

Workshop n° 2:

Current Research on Molecular Structures and Chemical Properties – A Young Perspective

This workshop, proposed by the ECA Special Interest Group 13 and supported by the IUCr Commission of Structural Chemistry, aims to the exchange of current experiences between different groups working in this area.

We invite young researchers to give short talks (< 30 min) to explain to the other participants the main objectives of the research carried out in their groups and on the specific research they are per-

Workshops

Software fayre

sonally involved. The main goal is to learn through these short talks the current work that is carried out on the binomial 'Molecular Structures/Chemical Properties' in different groups. We would like to stimulate the establishment of future collaboration, perhaps within the framework of international funding systems.

For more information please contact:

Teresa Duarte, teresa.duarte@ist.utl.pt

Fernando J. Lahoz, lahoz@unizar.es

With resources provided by the IUCr 2011 congress organizers, developers of academic and/or open-source crystallographic software are invited to present their new developments at the Crystallographic Software Fayre. This Fayre will be held throughout most of the IUCr 2011 congress in Madrid, from Tuesday, August 23 until Sunday, August 28, 2011.

A booking page showing booked time slots, and time slots remaining, is viewable via:

http://www.cryst.chem.uu.nl/lutz/software_fayre.html

The Software Fayre is being organized by:

Martin Lutz (Utrecht University)

Lourdes Infantes (Instituto Rocasolano, CSIC, Madrid)

Any queries should be sent to Martin Lutz (m.lutz@uu.nl) or Lourdes Infantes (xlourdes@iqfr.csic.es)

Open commission meetings

Open Commission Meetings will take place, as scheduled below, between 13.00-14.50

Tuesday, August 23, 2011

Commission on Crystal Growth and Characterization of Materials

Coordinator: Hanna A. Dabkowska

For further information: dabkoh@mcmaster.ca

Commission on Journals

Coordinator: Gernot Kosterz, Peter Strickland

For further information: ps@iucr.org

Wednesday, August 24, 2011

Commission on Mathematical and Theoretical Crystallography

Coordinator: Maximo Nespolo

For further information: massimo.nespolo@crm2.uhp-nancy.fr

Thursday, August 25, 2011

Commission on International Tables

Coordinator: Carolyn P. Brock, Peter Strickland

For further information: ps@iucr.org

Friday, August 26, 2011

Commission on Crystallographic Computing

Coordinator: Harry Powell

For further information: harry@mrc-lmb.cam.ac.uk

Commission on Synchrotron Radiation

Coordinator: Soichi Wakatsuki

For further information: soichi.wakatsuki@kek.jp

Saturday, August 27, 2011

Commission on Crystallography in Art and Cultural heritage

Coordinator: Eric Dooryhee

For further information: eric.dooryhee@grenoble.cnrs.fr

Commission on Charge, Spin and Momentum Densities

Coordinator: Carlo Gatti,

For further information: c.gatti@istm.cnr.it

Congress scope

The contributions, either poster or oral, should be assigned to one MS when submitted. In the following list the MS are ordered by different IUCr commissions, one MS could be under more than one commission.

Hot Topics 2010

- MS31** Structural Implications in Catalytic Processes
MS52 Graphitic Materials

1. Aperiodic Crystals

- MS30** Diffuse Scattering in Partially Ordered/Disordered Systems
MS55 Structure and Dynamics by Inelastic Scattering
MS63 Quasicrystals and their Approximants: Structure and Physical Properties
MS69 Crystallographic Methods and Software for Periodic and Aperiodic Crystals
MS84 What is order, and how can one describe it? (Which kinds of matter diffract?)
MS88 Crystal Chemistry and Physics of Modulated and Composite Crystals
MS98 Complex Structure and Frustrated Systems: Simulation and Experiments

2. Biological Macromolecules

- MS1** Hot Structures in Biology I
MS2 Hybrid Methods: the EM-Crystallography Interface
MS8 Large Biological Assemblies
MS11 Standardization, Validation, and Automation in Modern Biological Small-Angle Scattering
MS15 Nucleosome Processing and Epigenetics
MS16 Crystallography in Disease and Therapy
MS22 Cell Signalling and Protein-Protein Interactions
MS23 Difficult Phasing and Difficult Structures
MS29 Viruses and Viral Proteins
MS35 The Growth and Morphology of Crystals
MS36 Understanding Bacterial Pathogenesis
MS37 X-Ray Lasers and other New Frontiers in Synchrotron Applications to Structural Science
MS50 Structural Biology of the Immune System
MS51 Complementary Biophysical Methods: Adding Value to Protein Structures
MS57 New Perspectives in Structural Genomics
MS58 New Computational Approaches to Structure Solution and Refinement
MS64 Hot Structures in Biology II
MS70 Radiation Damage: Consequences and Uses
MS71 Machinery of RNA Processing
MS72 Automated Data Processing and Structural Solution for High Throughput Crystallography
MS78 Transcription and Translation
MS85 Membrane Protein Structures
MS86 Challenges of Low-Resolution Crystallography
MS92 Crystallizing Challenging Biological Targets
MS93 Dissecting Enzyme Mechanisms

3. Charge, Spin and Momentum Densities

- MS34** Descriptors of Electronic Structure and Chemical Bonding
MS41 Advanced Approaches in Charge Density Analysis and Derived Properties
MS48 Electron Momentum and Spin Densities in Correlated Electron Systems
MS55 Structure and Dynamics by Inelastic Scattering

Congress Scope

- MS76** Density Functional Methods for Electronic Structure Calculations
MS90 Hydrogen Bonding: From the Solid State to Solution
MS96 Complementary Use of Neutrons and Photons in Magnetism

4. Crystal Growth and Characterization of Materials

- MS14** Biomineralization and Biomimetic Materials
MS28 Wide Band Semiconductor and Other Crystals Used in Optoelectronics
MS35 The Growth and Morphology of Crystals
MS49 Crystal Growth and Interface Phenomena at the Nanoscale
MS53 High-Throughput Crystallization and Polymorphic Search in Pharmaceuticals

5. Crystallographic Computing

- MS6** Crystal Structure Prediction: Practice and Applications
MS13 Automation of Data Collection and Remote Control of Experiments
MS27 Developments and Directions for Crystallographic Databases
MS43 Validation, Error Detection and Fraud Prevention
MS58 New Computational Approaches to Structure Solution and Refinement
MS62 Crystallographic Software: the Library Approach
MS69 Crystallographic Methods and Software for Periodic and Aperiodic Crystals
MS72 Automated Data Processing and Structural Solution for High Throughput Crystallography
MS95 Automated Data Processing and Structural Solution for Powder Crystallography

6. Crystallographic Teaching

- MS83** Application of Crystal Structure Information in Chemical Education
MS97 Web Based Crystallography Teaching: the Use of Modern Communication Methods to Teach Crystallography

7. Electron Crystallography

- MS7** Coherent Diffraction and Imaging
MS21 Surfaces & Interfaces
MS44 Quantitative Real Space Electron Imaging
MS65 Atomistic and Electronic Structures of Nanomaterials
MS79 Electron Diffraction and Crystallography

8. High Pressure

- MS5** Non-Ambient Powder Diffraction
MS12 Non-Covalent Interactions in Molecular Crystals and Biomolecular Systems Under Pressure
MS19 Synthesis, Structure and Properties of Novel Materials at High Pressure
MS40 Pressure-Induced Phase Transitions
MS47 Advances in High Pressure Techniques and Instrumentation
MS60 Solid State Reactivity
MS75 Liquids, Amorphous and Nanocrystalline Solids at High Pressure

9. Inorganic and Mineral Structures

- MS14** Biomineralization and Biomimetic Materials
MS25 Crystallography of Materials with Exchange, Sequestration and Storage Properties
MS30 Diffuse Scattering in Partially Ordered/Disordered Systems
MS39 Energy-Related Materials
MS54 Minerals as Advanced Materials

Congress Scope

- MS67** Layered Inorganic Materials and Layered Precursors of 3D Structures
MS81 The Crystallography of Functional Inorganic Materials and Their Applications
MS88 Crystal Chemistry and Physics of Modulated and Composite Crystals
MS98 Complex Structure and Frustrated Systems: Simulation and Experiments
- 10. Mathematical and Theoretical Crystallography**
MS9 Topological Correlations and Crystal Structure Interconnections
MS20 Beyond Space-Group Symmetry in Periodic Structures
MS30 Diffuse Scattering in Partially Ordered/Disordered Systems
- 11. Neutron Scattering**
MS5 Non-Ambient Powder Diffraction
MS26 SAXS/SANS, Total Scattering and the Nanostructure Problem
MS33 New Sources (Neutrons, X-Rays, XFEL)
MS39 Energy-Related Materials
MS47 Advances in High Pressure Techniques and Instrumentation
MS55 Structure and Dynamics by Inelastic Scattering
MS68 Data Reduction of Area Detector Measurements
MS82 Biological Neutron Scattering and Deuteration
MS96 Complementary Use of Neutrons and Photons in Magnetism
- 12. Powder Diffraction**
MS5 Non-Ambient Powder Diffraction
MS9 Topological Correlations and Crystal Structure Interconnections
MS10 Determination of Ab-Initio Crystal Structures from Powder Diffraction and their Applications in Pharmaceutical Industry
MS18 Powder Diffraction at the Nanoscale
MS25 Crystallography of Materials with Exchange, Sequestration and Storage Properties
MS32 Crystallography in Industrial Process Control
MS39 Energy-Related Materials
MS46 Powder Diffraction Methods in Archaeometry
MS53 High-Throughput Crystallization and Polymorphic Search in Pharmaceuticals
MS60 Solid State Reactivity
MS74 Powder Diffraction and Complementary Techniques
MS81 The Crystallography of Functional Inorganic Materials and Their Applications
MS91 X-Ray Absorption, Diffraction and Imaging in Forensic Science and Ancient Materials
MS95 Automated Data Processing and Structural Solution for Powder Crystallography
- 13. Crystallography in Art and Cultural Heritage**
MS46 Powder Diffraction Methods in Archaeometry
MS91 X-Ray Absorption, Diffraction and Imaging in Forensic Science and Ancient Materials
- 14. Small Angle Scattering**
MS4 Industrial Applications of SAXS and SANS
MS11 Standardization, Validation, and Automation in Modern Biological Small-Angle Scattering
MS26 SAXS/SANS, Total Scattering and the Nanostructure Problem
MS51 Complementary Biophysical Methods: Adding Value to Protein Structures
MS74 Powder Diffraction and Complementary Techniques
MS82 Biological Neutron Scattering and Deuteration

Congress Scope

- 15. Structural Chemistry**
MS3 Polymer and Gel Structure: Arriving at a Structural Model
MS10 Determination of Ab-Initio Crystal Structures from Powder Diffraction and their Applications in Pharmaceutical Industry
MS17 Synthons: From Small to Macromolecules
MS24 New Challenges in Crystal Engineering: Correlating Structure and Properties
MS38 Fabrication and Macroscopic Properties of Flexible Frameworks
MS45 Dynamical Structural Science
MS53 High-Throughput Crystallization and Polymorphic Search in Pharmaceuticals
MS56 Spectroscopic Approaches (XAFS, NMR, ...) in Crystallography
MS59 Anion Recognition and Templatation in Halogen Bonding
MS61 Hot Structures in Chemical Crystallography
MS66 Electric, Magnetic and Other Physical Properties of Molecular Crystals
MS73 Theory and Practice of Hydrogen Bond: An Evergreen Interaction for Molecular Recognition
MS80 Solid State Photochemistry
MS83 Application of Crystal Structure Information in Chemical Education
MS87 Chirality in the Solid State, From Organic Molecules to Chiral MOF and Helical Materials
MS94 Molecular Recognition in the Crystal Bulk and in the Surface: Theory and Applications
- 16. Synchrotron Radiation**
MS7 Coherent Diffraction and Imaging
MS21 Surfaces & Interfaces
MS23 Difficult Phasing and Difficult Structures
MS33 New Sources (Neutrons, X-Rays, XFEL)
MS37 X-Ray Lasers and Other New Frontiers in Synchrotron Applications to Structural Science
MS47 Advances in High Pressure Techniques and Instrumentation
MS55 Structure and Dynamics by Inelastic Scattering
MS70 Radiation Damage: Consequences and Uses
MS77 XAFS Instrumentation: Automation, Standardization and Validation of XAFS Experiments
MS96 Complementary Use of Neutrons and Photons in Magnetism
- 17. XAFS**
MS42 XAFS Studies in Biology Coupled to Crystallography
MS56 Spectroscopic Approaches (XAFS, NMR, ...) in Crystallography
MS70 Radiation Damage: Consequences and Uses
MS77 XAFS Instrumentation: Automation, Standardization and Validation of XAFS Experiments
MS91 X-Ray Absorption, Diffraction and Imaging in Forensic Science and Ancient Materials
- 18. COMCIF**
MS89 Archiving, Exchange and Retrieval of Scientific Data in the 21st Century
- 19. Other Topics in Crystallography**

Abstract submission

Deadline for the submission of Bursary Applications:

March 15, 2011

Deadline for Submission of Abstracts:

April 15, 2011

Abstracts must be submitted on-line by connecting to the Web site **www.iucr2011madrid.es**. Please note that the abstract submission form on the Web site will be not available after the deadline so that there will be no chance of a late submission. Participants, who would like to make an oral or poster presentation at the congress, must submit an abstract for consideration and approval of the Scientific Committee. The topics of the Microsymposia (MS) are all defined and up to three speakers will be invited by the corresponding MS Chairpersons. The two additional speakers will be selected by the Chairpersons, after the evaluation of the abstracts proposed by the authors as oral contribution. This request together with the identification of the MS needs to be specified at the time of abstract submission. It will be responsibility of the two Chairpersons to complete the MS program by selecting the additional speakers among the applying participants. The contribution will be automatically redirected to the poster session if the request for an oral presentation cannot be fulfilled. The instructions for the preparation of the abstracts (specified below) will be available on the Web site. The presenting author is required to ensure that all co-authors are aware of the contents of the abstract before submission. To have an abstract accepted and included in the program and in the Book of Abstracts, the presenting author must have registered and paid the registration fee prior to **June 15, 2011**.

Abstract preparation

Abstract must be written in English and contain a brief, clear statement of conclusion; statements like "the findings will be discussed" must be avoided. All abbreviations must be defined before being used in the text.

Please note that in the preparation of the abstract it is compulsory to use the template available online (<http://www.iucr2011madrid.es/downloads/template.rtf>).

Title: Should be not more than 80 characters in length. Exceeding characters will be truncated.

Presenting author: The name of the presenting author must appear first in the list of authors. No one may be first author on more than ONE contribution. Invited speakers are, however, permitted to submit a poster presentation in addition to their talk.

Affiliation: Please report the information in a concise manner. The e-mail address of the presenting author is recommended.

Abstract: There is enough space for approximately 550 words (3500 characters) of text in Times New Roman, font size 9 in a maximum area of 8.5 x 24 cm. Do NOT use a smaller font size. Use single spacing. Include graphics (minimum resolution 300 dpi) only if necessary, and if they reproduce well in black and white. Note that although diagrams in color can be submitted for the electronic Book of Abstracts, the Program and Book of Abstracts will not be printed in color. Please remember that the area of the printed abstract is small and that the graphic will be correspondingly smaller. Please save your diagrams at the correct size before including them in your abstract, note that the maximum size allowed for the uploaded document will be 2 MB.

Keywords: Three keywords must be supplied as they will be used in indexing the Book of Abstracts. A list of suggested keywords is available online in the download section.

(<http://www.iucr2011madrid.es/downloads/keywords.pdf>)

Note that a printed version of the book of Abstracts will be given only on request and at an extra cost.

Abstract submission

Abstract submission

The prepared abstract file must be uploaded in the server to the congress by following the indicated steps, which are slightly different for invited speakers and other participants:

1. Access the Web site **www.iucr2011madrid.es** within the period 2011 January 15-April 15. Click on the Abstract link and once there, on the Abstract Submission.
2. a) Keynote speakers will receive the personalized instructions by e-mail from the Technical Secretariat.
- b) Poster presentation and oral contribution: if you do not have Username and Password, click on the "New Abstract" button. Please fill all the fields in the form.
 - I) "Title": write the abstract title (< 80 characters).
 - II) "Keywords": enter the three keywords already present in the abstract and separated by commas (use small letters).
 - III) Request for Oral Presentation or Poster Contribution: authors must check the preferred option.
 - IV) Contribution Category: please indicate the microsymposium chosen from the supplied list of Comissions and Microsymposia (also reported at pages 18-21 of this circular).
 - V) "Abstract File": use the "Browse" button to locate the prepared abstract file in your computer.
 - VI) After uploading your file click on the "next" button and fill the fields corresponding to first author personal data, and later those of the co-authors, if appropriate. Click "Next".
 - VII) If you consider all the data is correct click on "Submit Abstract".

Immediately after confirmation, you will automatically receive a Username and a Password by e-mail.

After submission, the presenting author will have only a 10 day period to modify the abstract by introducing your e-mail and password. After this time (or at the abstract deadline, if this comes first), any modifications will be rejected.

Abstracts should not be sent by email or fax as they will not be processed by the Secretariat nor forwarded to the Scientific Committee for review. Only in case of genuine difficulties, please contact the Technical Secretariat at **iucr2011@pacifico-meetings.com**.

Processing

The submitting author will receive an automatic confirmation that the abstract and other relevant information have been uploaded and the procedure finalized. In all correspondence with the organizers, please quote the assigned number.

Acceptance as speaker in a given MS will be communicated to the author after the decision has been made by the respective chairpersons, not later than **April 30, 2011**.

Acceptance of the poster contribution will be notified to the presenting authors by **April 30, 2011**. Final scheduling of the poster presentation will be communicated to the submitting author after payment of the registration fee (deadline: **June 15, 2011**).

The accepted contributions will be printed in the Book of Abstracts and will also be made available online in a special issue of Acta Crystallographica Section A, published at the end of the year 2011.

Poster prize awards

Poster awards will be given to the excellent young scientists posters by the IUCr and other organizations such as GE3C, CCDC, PDB, EMU, Crys. Eng. Commun, ...

Details on these awards will be given in the Congress web site: **www.iucr2011madrid.es**

Bursaries

Student bursaries

The organizers are currently involved in raising funds to be redistributed as attendance bursaries to young scientists, especially those coming from the less favoured regions. It is a policy of IUCr to convey significant amounts of money to this purpose, by utilizing funds from various international institutions and by using part of the congress income. In this respect, no reimbursements and honoraries of any sort are paid to the invited speakers and chairs of the Microsymposia.

The first requirement for obtaining a bursary is the submission of a regular abstract. Also an age limit of 35 applies. Application form must be submitted online not later than **March 15, 2011** and should be accompanied by the following documents (to be uploaded):

- Curriculum Vitae
- A headed paper letter from the Research Supervisor who certifies the student status of the applicant and whether the student has access to any source of funds to attend the congress.

The support of organizers, if granted, will include one or more of the following benefits (in a priority order):

- 1) reduced registration fee
- 2) accommodation in student dormitory
- 3) lump sum to cover part of the travel expenses (only in exceptional cases)

In no case, funds will be anticipated to the applicant by the organizers.

Travel support for senior scientists from President's Fund

Deadline: **March 30, 2011**

The president's Fund support senior scientists to attend IUCr Congresses. Details and an Application Form can be found on the following web site:

<http://www.iucr.org/iucr-top/cong/index.html>

Support program for retired scientists

The local organizing committee will offer a limited number of reduced fees for retired scientists over 70 years old.

A high quality commercial exhibition fair will be held as a central feature of XXII IUCr Madrid 2011. We are convinced that this meeting will be an excellent opportunity for companies to make direct contact with a large number of scientists leading research projects at international level.

The exhibition will run from August 23 to 28, 2011 in the Multipurpose Hall of the Madrid Municipal Conference Centre. More than 1500 m² for 100 booths are prepared to receive industrial and supplier companies.

Please, visit our web page www.iucr2011madrid.es to obtain further details on the sponsorship and exhibition fair.

The following program will be organized for participants and accompanying persons.

- **Welcome Reception: Monday, August 22, 20:30 – 22:00**
(Included in the registration fee) The welcome cocktail will take place immediately after the Opening Ceremony at the main Lobby of the venue, Palacio Municipal de Congresos.
- **Cultural Activity: Thursday August 25, 19:30 – 21:30**

Social Program

Registration

- **Congress Dinner: Friday August 26, 21:00 – 01:00**

It will take place at the Botanical Garden of the Universidad Complutense de Madrid (UCM). Please see registration.

- **Congress Tours:** Different tours will take place from **August 23 to 30**. Please see Tours.

Registration Fees in EUROS	Until May 15, 2011**	After May 15, 2011
Participant	560	640
Student*	270	320
Accompanying Person	180	200
Congress Dinner Fee for registered participants	40	40
Congress Dinner Fee for not registered person	90	90

* Students under 35 years old must attach a copy of their student ID or enclose a letter from the Head of the Department certifying their student status.

** In order to benefit from the early bird registration fee, payment must be made before May 16, 2011. Otherwise the full late registration will be applied.

How to register:

Registration should be made through the congress website www.iucr2011madrid.es, by filling the Registration & Accommodation on line form. Exceptionally, if you face any problem in sending your registration on-line, please contact the technical secretariat to send you a pdf format for manual registration.

Fee Includes:

- **Participant or Student:**

Attendance to all congress scientific sessions. Congress material (documentation & congress program). Certificate of attendance and/or participation. Lunches and Coffee-breaks. Welcome reception. Cultural Activity. Reduced fee for the congress dinner (40€). One ticket for free public transport in the period of August 22 to August 30, 2011.

- **Accompanying person:**

Welcome reception. Half day city tour to Madrid, on Thursday, August 25, 2011. Cultural Activity. Reduced fee for the congress dinner (40 €). One ticket for free public transport in the period of August 22 to August 30, 2011.

Method of payment:

- **All payments must be made in Euros (€) by credit card (Visa, Mastercard).** The organization strongly recommends using the credit card payment, otherwise, bank transfer will be accepted in Euros in favour of: **Grupo Pacífico, S.A.**

Bank Name: Banco Sabadell Atlántico

Account Number: 0081 5084 04 0001264536

IBAN Code: ES45 0081 5084 04 0001264536

SWIFT Code: BSAB ESBB

Commercial exhibition fair

Social Program

Registration

- Please do not forget to include the following reference in the bank transfer “IUCR 2011 REGISTRATION FEE”, as well as the name of the participant.
- All bank charges incurred will be borne by the payee.
- Participants must send by fax or e-mail, a copy of the receipt of the bank transfer to the technical secretariat within 5 working days. Otherwise registration and all other services required will not be confirmed.
- No confirmation will be sent until the technical secretariat has received the full payment.
- Any difference arising in the payments will be collected on site by the technical secretariat.
- In the case that registration funds are wired late or for unexpected reasons, are not credited to the congress account at the time of registration, the original bank receipt will be required. If no proof of payment can be presented, full payment will be required on site.
- Additional requests made after August 10, 2011 will be processed on site.

Registration cancellation policy:

- Cancellations must be notified in writing to iucr2011@pacifico-meetings.com.
- Any name change will be treated as a cancellation and a new registration will be made.
- 100 % refund cancellation by May 15, 2011 (an administrative charge of 50 € applies).
- 50 % refund cancellation by June 30, 2011.
- No refund cancellation after July 1, 2011 or registered participants who fail to attend.
- Corresponding refunds will be made from September 1, 2011 onwards.

• By Air: Barajas Airport

Madrid-Barajas Airport it is just 13 km away from the city, and its connections by public transportation are excellent. Besides bus or taxi, travelers may take the Metro, every five minutes a train to/from Madrid-Barajas Airport leaves from Nuevos Ministerios Station in the City Centre at a cost of 2 € while you will pay only 1 € for a ticket within the City!



The underground (Metro) is the most efficient and affordable way to move around Madrid. The city has a vast metropolitan network and covers almost all the points in the capital and many of the neighboring areas.

To take a taxi you must go to the appropriate taxi rank. Signs of taxi stops are well indicated at the arrival area of each terminal. The official taxis are white with red line. Ignore any drivers who offer their services unsolicited inside the terminals. Make sure that the taxi driver has started up the taximeter at the start of the journey (minimum fare). You may request a free receipt with the tax ID, amount, date, license number and vehicle registration number, or a printed receipt. The estimated cost of a taxi from the airport to the city centre is 30–40 €, and from the airport to the venue is 15–20 €.

Supplements:

- Journeys beginning or ending at the airport, including those within the airport grounds: 5.50 €.
- Journeys originating or ending at bus stations, train stations or the Parque Ferial Juan Carlos I (IFEMA near Venue) fairs complex: 2.95 €.

• By Train:

International trains arrive at Atocha or Chamartín train stations. Atocha is located in the south center of the city and Chamartín is in the north. Both stations have access to metro stations.

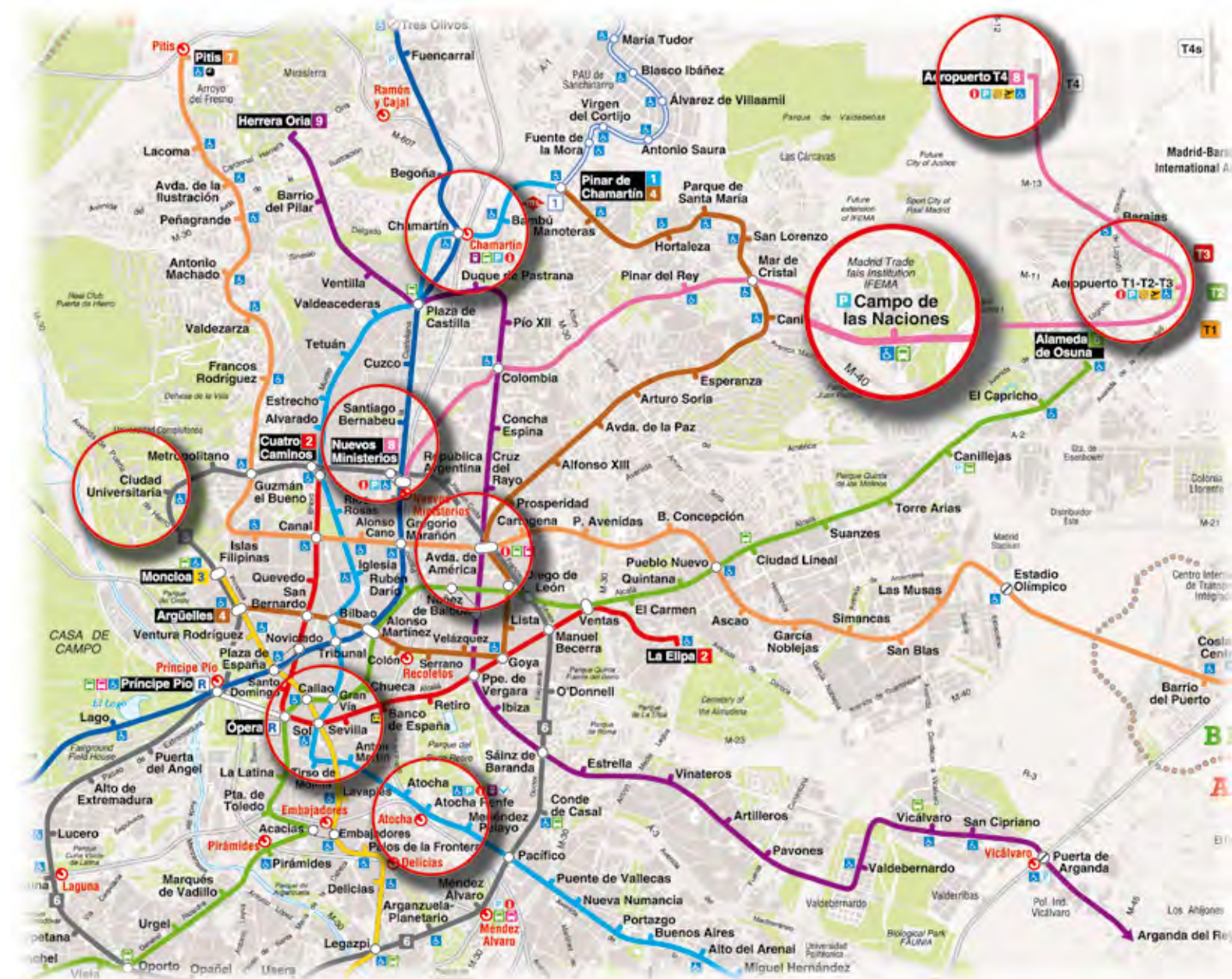
How to get to Madrid

• By Bus:

Avenida de América and Méndez Álvaro bus stations are the main bus stations in the city and have routes to other Spanish cities. Méndez Alvaro is located in the south of the city and Avenida de América is located in the north-east.

Bus Lines 204 and 200 connect Barajas airport with Avenida de América bus station.

Underground network map showing position and connections between the airport, venue (Campo de las Naciones), main stations, historical city center (Sol-Opera) and Halls of Residence (Ciudad Universitaria).



General information

The Venue: Palacio Municipal de Congresos de Madrid

Its avant-garde design has given it great versatility, with the technology and services that are necessary to absorb all market demands. Address: Av. de la Capital de España 7, 28042 - Madrid (Spain) www.madridespaciosycongresos.com

How to reach the Venue

- **By Metro:** Line 8 (Nuevos Ministerios-Aeropuerto), **Campo de las Naciones** station .
- **By Bus:** Line 122, Avda. de América to Feria de Madrid, **Campo de las Naciones** bus stop.
- **By Taxi:**
From the city centre, 15 minutes approximately. Estimated cost: 20 – 25 €.
From the airport, 10 minutes approximately. Estimated cost: 15 - 20 €.

Opening hours of the registration desk on site

- Registration desk will be open on Monday August 22, from 11:00 to 20:00h.
- From Tuesday August 23 to Monday August 29, it will be open from 08:00 to 19:00h.

Official web site

The official web site of the congress is www.iucr2011madrid.es

Participants will be able to submit abstracts, to register to the congress, to make reservations for hotels and tours and to find the updated version of the Scientific Program. Any news on the congress will be announced in the official web site.

Clothing

Informal for all the occasions.

Exhibition

A commercial exhibition is scheduled to take place in conjunction with the congress, from Tuesday August 23 to Sunday August 28, 2011. For further information please visit the web site www.iucr2011madrid.es

Internet and fax

Internet connection will be provided during the congress hours. However, no Fax machines will be available.

Language

The official language of the congress will be English. Therefore, sessions and posters will be presented in English.

Business hours & shops

Most shops open between 09.30 and 13.30h in the morning and 17.00 to 20.00h or even later in the afternoon. Department stores remain open all day from 10:00 to 22:00h. On Sundays shops are closed except those in the central area (around Puerta del Sol and Gran Vía) that are open every day.

General information

City transportation

The city of Madrid counts with excellent means of transport. Its underground network (metro) has modern trains and stations and links to most destinations reaching even some of the main towns in the surrounding areas of the city. Using the underground will be the best way to get from one part of the city to another. www.ctm-madrid.es is a useful website for planning your transportation in Madrid: you will find schedules for buses, trains and for the subway lines. All the vehicles, either buses or trains of the whole network are air-conditioned.

Climate

The average maximum temperature in Madrid in August is 90°F/32°C (probably lower at the end of the month) and the average minimum temperature is 61°F/16°C. Madrid will surprise you with its intense and enveloping blue sky. It has a dry climate with little rainfall.

Currency and banks

The national currency of Spain is the Euro (€). Exchange facilities are available at Barajas airport, most banks and also along main streets (ATMs). Debit cards and credit cards are widely accepted. However, it would be wise to check this with your bank before travelling.

Electricity

Spain's standard electricity supply is 220 Volts (V), 50 Hertz (Hz) AC. The plugs are round two pins, European standard.

Post office

The closest post office to the venue is: Avda. del Partenón s/n (Recinto Ferial Ifema) 28042 - Madrid
Hotels often provide simple postage services.

Smoking

Smoking restrictions apply in most public areas.

Time

The time in Madrid is the Central European Time (Summer Time GMT+2)

Tipping and consumer tax

Service is normally included. However, a small tip shows your appreciation of the service (~5%). There are two different tax rates in Spain: 8% and 18%. You will pay 8% tax on your hotel and restaurant bills, as well as other items considered "essential". Most physical items purchased in shops will be taxed at the 18% rate.

Visas

The Spanish Ministry of Foreign Affairs and Cooperation (<http://bit.ly/8XLyCa>) establishes some requirements for entry into Spain for a stay not exceeding ninety days in any six month period. Further information regarding these requirements and as well as the Visa issues can be found through the website <http://bit.ly/bNyvp0> and/or directly through the Spanish Embassies or Consulates whose addresses can be found through this web address <http://bit.ly/9ebe05>.

Hotel accommodation

In order to guarantee accommodation the organization recommends to send the reservation before **June 1, 2011**

A number of Hotels rooms have been blocked to guarantee accommodation for IUCr participants. Special care has been taken in selecting hotels with an easy reach of the venue by metro. Please check details on the hotels in the congress web page www.iucr2011madrid.es

Grupo Pacifico is the official IUCr2011 hotel handling agent. Therefore, please do all inquiries regarding accommodations to:

GRUPO PACÍFICO

Paseo del General Martínez Campos, 44 – 1º

E-28010 Madrid (Spain)

Telf: +34 913 836 000

Fax: +34 913 023 926

E-mail: iucr2011@pacifico-meetings.com

Reservation and payment

- Hotel reservations must be made by filling the Registration & Accommodation on line form (please visit the web site www.iucr2011madrid.es)
- Hotel reservations & rates are limited to the Congress dates (arrival August 22 and departure August 30, 2011). For extra nights, please contact Grupo Pacifico.

Hotel category	SINGLE	DOUBLE
	min / max	min / max
5-star	104 € - 147 €	109 € - 147 €
4-star	69 € - 115 €	78 € - 131 €
3-star	50 € - 90 €	50 € - 104 €

* All rates quoted are per room and per night, breakfast and taxes are included.

Accommodation cancellation policy

- Cancellations must be notified in writing to iucr2011@pacifico-meetings.com
For further information please visit the web site www.iucr2011madrid.es

Halls of Residence on Universidad Complutense de Madrid

Reservations must be made for the entire duration of the congress. Double rooms must be reserved under the name of two people.

Colegios Mayores UCM*	Ciudad Universitaria (L 6) or Moncloa (L 3, L 6)
Single Room with bathroom	42,00 €
Single Room with shared bathroom	37,00 €
Double Room with bathroom	58,00 € (29,00 € per person)
Room for handicapped people	42,00 €

*All rates quoted are per room and per night, breakfast and taxes are included.

Residencia Galdós*	Metropolitano (L 6)
Single Room	49,00 €
Double Room	65,00 € (32,50 € per person)
Room for handicapped people	49,00 €

*All rates quoted are per room and per night, taxes are included. Breakfast is not included.

Congress tours

Several tours are offered to congress delegates and accompanying persons to give a chance to experience the history, culture and environments of Madrid and the surrounding areas. Tours can be reserved on the congress website. For further details check the congress web page www.iucr2011madrid.es.

Tours	Rates	Tuesday, August 23	Wednesday, August 24	Thursday, August 25	Friday, August 26	Saturday, August 27	Sunday, August 28	Monday, August 29	Tuesday, August 30
Madrid Sightseeing Tour + Madrid de los Austrias (Half day tour)	35,00 €	• (AM)		• (AM)					• (AM)
Reina Sofia Museum + Royal Palace (Half day tour)	36,00 €		• (AM)		• (AM)			• (AM)	
Madrid Panoramic Sightseeing Tour + Prado Museum (Half day tour)	29,00 €		• (PM)			• (AM)	• (PM)		• (AM)
Aranjuez-Chinchón (Full day tour, Lunch included)	93,00 €	•		•			•		
El Escorial (Half day tour)	53,00 €		• (AM)			• (AM)			• (AM)
Alcala de Henares (Half day tour)	28,00 €				• (AM)			• (AM)	
Toledo (Full day tour, Lunch included)	101,00 €	•		•				•	
Segovia-La Granja (Full day tour, Lunch included)	102,00 €		•			•			•
Avila (Full day tour, Lunch included)	92,00 €				•		•		
Barcelona * (Full day tour, Lunch included)	122,00 €	•							
Sevilla * (Full day tour, Lunch included)	115,00 €		•						
Valencia * (Full day tour, Lunch included)	104,00 €			•					

*High Speed Train tickets are not included in the price, since rates may vary according to the booking date rates of train tickets on request.