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WELCOME

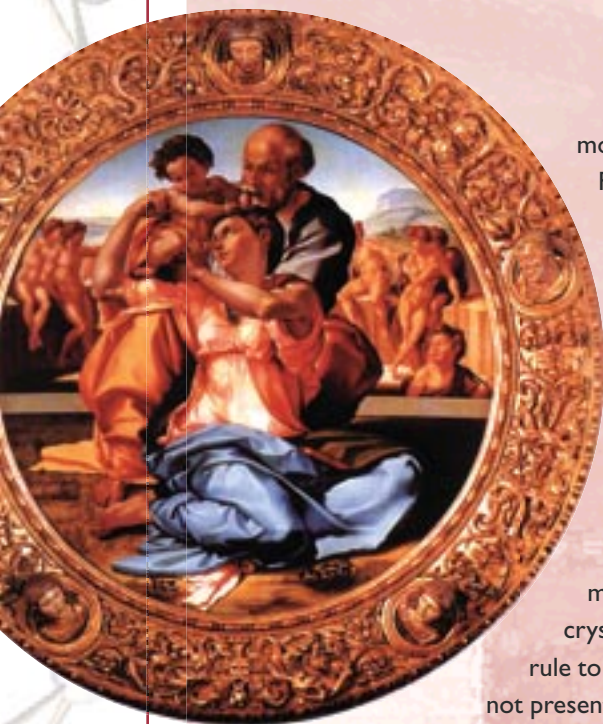
Dear Crystallographer,

I would like to extend a personal invitation to crystallographers everywhere to attend the XX congress and general assembly of the International Union of Crystallography in Florence, Italy August 23-31, 2005. It would give me great pleasure to welcome you to one of the most beautiful cities in the world to participate in what promises to be the most enlightening, exciting, and exhilarating IUCr Congress ever held. I feel certain that most attendees will have to make difficult choices when deciding which of the many excellent parallel sessions to attend. Come join your friends and colleagues from over fifty countries around the world as we work together to advance international science and cooperation.

William L. Duax

President

International Union of Crystallography



The crystallographic world community has the opportunity to attend its most important meeting immersed in the exciting and unique atmosphere of Florence. The city is famous for being the cradle of the Renaissance, the cultural phenomenon which spread through Europe in the XV century leaving for posterity famous masterpieces of architecture, sculpture and painting. Visiting the magnificent attractions is still a striking experience for both the first time and repeat visitors. Moreover, the congress organizers plan various initiatives that will give the delegates and accompanying persons the feeling of being not merely “just another tourist”.

The scientific program of the congress, which has been prepared by an international committee formed by 23 experts in the various branches of crystallography is very rich and of the highest level, with three Nobel Laureates and 33 other authorities presenting keynote lectures. As many as 98 micro-symposia with about 500 selected speakers will highlight the character of crystallography as the most multidisciplinary of sciences. As a generally accepted rule to favor the diffusion of new ideas, care has been taken to invite speakers who have not presented in the most recent IUCr congresses. The frontiers of crystallography will be discussed, but particular attention will be devoted to the structural aspects of matter and its relations with properties and functions. Since the understanding of the biological world represents the greatest challenge to modern science, the attention will be obviously centered on biological macromolecules. On the other hand, given our own scientific background, we have tried as organizers to give new impulse to the wider role of structural chemistry. In particular, organic, inorganic, pharmaceutical, solid-state and materials chemists, as well as mineralogists and all of those with an interest in structural properties will find the scientific program of the greatest interest. The invitation is extended to both the expert crystallographer and to the early stage researcher, since this congress is intended to consolidate and diffuse the crystallographic state of the art.

Carlo Mealli

Chairperson

Scientific Program Committee

Paola Paoli

Chairperson

Local Organizing Committee

SCIENTIFIC PROGRAM COMMITTEE

Carlo Mealli, ICCOM-CNR Florence, Italy (Chairperson)
 mealli@iucr2005.it

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LOCAL ORGANIZING COMMITTEE

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IMPORTANT DATES

Deadline for bursary applications (abstract should be included with application): **February 10, 2005**

Deadline for submission of abstract: **February 28, 2005**

Deadline for payment of registration fee at 'Early Bird' rate: **April 15, 2005**

Deadline for hotel reservation: **April 15, 2005**

Deadline for payment of registration fee for validation and publication of submitted abstract: **June 1, 2005**

Deadline for tours reservation: **June 30, 2005**

Deadline for payment of registration fee of workshops: **July 31, 2005**

TIMETABLE

Tuesday, August 23, 2005

Registration Opens
Pre-Congress Workshops
Exhibition Opens
Opening Ceremony
Ewald Prize Lecture
Welcome Cocktail

Wednesday, August 24, 2005

Scientific Session
Exhibition
Evening: **IUCr General Assembly**

Thursday, August 25, 2005

Scientific Session
Exhibition
Evening: **IUCr General Assembly**

Friday, August 26, 2005

Scientific Session
Exhibition

Saturday, August 27, 2005

Scientific Session
Exhibition
Evening: **Concert**

Sunday, August 28, 2005

Scientific Session
Evening: **IUCr General Assembly**

Monday, August 29, 2005

Scientific Session
Late Afternoon: **IUCr General Assembly**
Evening: **Social Banquet**

Tuesday, August 30, 2005

Scientific Session
Closing Ceremony

Wednesday, August 31, 2005

Congress Tours

SCIENTIFIC PROGRAM

Please note that the scientific program, elaborated by the Scientific Program Committee and approved by the IUCr Executive Committee, is still subject to the acceptance of the invited speakers and chairs.

Wednesday, August 24, 2005

- 8.30-9.30** **KN 1 - Roald Hoffmann**
"Luigi Sacconi" medal awarded by Luigi Sacconi Foundation and Italian Chemical Society (SCI)
Theoretician's View of Crystallography
 Chair: **Joel Bernstein**
- 9.30-10.00** **Break**
- 10.00-12.35** **MS 1 - Chairs: Naomi Chayen, Janet Newman**
When Bad Crystals Turn Good: Transforming Poorly Diffracting Crystals
MS 2 - Chairs: Lynne Reagan, Paul Curmi
Chameleon Proteins
MS 3 - Chairs: Shiv P. Halasyamani, Reiko Kuroda
Chiral and Non-centrosymmetric Structures
MS 4 - Chairs: Elias Vlieg, Robin D. Rogers
Polymorphism
MS 5 - Chairs: Juan Manuel Perez-Mato, Ulrich Bismayer
Structural Phase Transitions
MS 6 - Chairs: David Rendle, Izumi Nakai
Crystallography and Forensic Science
MS 7 - Chairs: Wulf Depmeier, Herta Effenberger
Crystal Chemistry of Inorganic and Mineral Compounds
- 12.35-13.45** **Lunch Break**
- 13.45-14.45** **Poster Session**
- 14.45-17.20** **MS 8 - Chairs: Jacqueline M. Gulbis, R. Michael Garavito**
Membrane Protein Structure and Function
MS 9 - Chairs: Settimio Mobilio, Joaquin Garcia-Ruiz
Combined XAS and XRD Techniques in Physics, Chemistry and Materials Science
MS 10 - Chairs: Andreas Roodt, Santiago Alvarez
Integrated Crystallographic, Spectroscopic and Computational Approaches
MS 11 - Chairs: Thomas Tschentscher, John Arthur
Instrumentation at Next Generation X-ray Sources
MS 12 - Chairs: Reinhard Neder, Thomas Proffen
Disorder Diffuse Scattering
MS 13 - Chairs: Brian H. Toby, Lachlan M. D. Cranswick
Advances in Computational Methods for Powder Diffraction
MS 14 - Chairs: Emil Mackoviky, Stefano Merlino
Modularity and Modulation in Inorganic and Mineral Structures
- 17.20-17.30** **Break**
- 17.30-18.30** **KN 2 - Martino Bolognesi**
Structure and Recognition in the CtBP-dependent Transcription Regulation
 Chair: **Dino Moras**
KN 3 - Chikashi Toyoshima
Calcium Pumps
 Chair: **Giuseppe Inesi**
KN 4 - Walter Reimers
Neutrons and X-rays for Microstructure: Strain/Stress Characterization in Materials
 Chair: **Anatoly Balagurov**

Thursday, August 25, 2005

SCIENTIFIC PROGRAM

- 8.30-9.30** **KN 5 - David Sayre**
Single-particle Diffraction
Chair: John Spence
KN 6 - Lynne McCusker
Zeolites
Chair: Reinhard Fischer
KN 7 - Vaclav Petricek
Structure Analysis of Modulated Crystals: Trends and Tendencies
Chair: Ray L. Withers
- 9.30-10.00** **Break**
- 10.00-12.35** **MS 15 - Chairs: Sung-Hou Kim, Edward N. Baker**
The Big Question in Structural Genomics: Getting Function from Structure
MS 16 - Chairs: Gian Carlo Ruocco, Alfred Baron
High Resolution X-ray Inelastic Scattering
MS 17 - Chairs: Gautam R. Desiraju, Mariusz Jaskolski
Non-covalent Interactions in Crystals of Small Molecules and Macromolecules
MS 18 - Chairs: Christian Baerlocher, Sergey Krivovichev
Powder Diffraction on Nano- and Mesoporous Materials
MS 19 - Chairs: Sander Van Smaalen, Sven Lidin
News from Incommensurate Crystals
MS 20 - Chairs: Simon Parsons, Giovanni Luca Cascarano
Advances in Computational Methods for Small Molecule Crystallography
Dedicated to the late Prof. Mario Nardelli
MS 21 - Chairs: Alain Lodini, Lyndon Edwards
Basic to Industrial Applications of Stress and Strain Analyses
with Synchrotron and Neutron Radiations
- 12.35-13.45** **Lunch Break**
- 13.45-14.45** **Poster Session**
- 14.45-17.20** **MS 22 - Chairs: Janos Hajdu, Henry Chapman**
Single Particle X-ray Diffraction Imaging
MS 23 - Chairs: E. Yvonne Jones, Peter R. Mittl
Putting the Pedal to the Metal: Speeding Up Biological Structure Determination
MS 24 - Chairs: Judith A. K. Howard, Jacqui Cole
Molecular Crystals Under Non-ambient Conditions
MS 25 - Chairs: Andrew Fitch, John Faber
Structure Determination from Powder Diffraction Data (Organics)
MS 26 - Chairs: Koh Saitoh, Ron Lifshitz
Recent Advances in Quasicrystal Research
MS 27 - Chairs: Naoto Yagi, Christian Broennimann
Detectors: Developments and Requirements for X-ray, Synchrotron and
Neutron Sources
MS 28 - Chairs: João Rocha, Alessandro Gualtieri
Structure/Properties Relationships of Technologically Relevant
Inorganic and Mineral Compounds
- 17.20-17.30** **Break**
- 17.30-18.30** **KN 8 - Raymond Stevens**
Structural Genomics
Chair: Mamannamana Vijayan
KN 9 - Peter Stephens
Structure Solution of Pharmaceutical Compounds from Powder Diffraction Data
Chair: Kenneth Shankland
KN 10 - Akiji Yamamoto
Quasicrystal Structure Analysis. The State of the Art
Chair: Marc De Boissieu

Friday, August 26, 2005

- 8.30-9.30** **KN 11 - Andrej Šali**
High Throughput Modelling
Chair: Janet Thornton
KN 12 - Roberto Dovesi
Quantum Mechanical Simulation of Crystalline Materials with the CRYSTAL Code
Chair: Davide Viterbo
KN 13 - Abraham Clearfield
In-situ Characterization during Crystal Growth
Chair: Roberto Fornari
- 9.30-10.00** **Break**
- 10.00-12.35** **MS 29** - *Chairs: Philip E. Bourne, R. Sowdhamini*
Improving Structures Using Bio-informatics
MS 30 - *Chairs: Edgar Meyer, Magdolna Hargittai*
Art and Crystallography
MS 31 - *Chairs: Franco Ugozzoli, Claire Gervais*
Supramolecular Chemistry
MS 32 - *Chairs: Angela Altomare, Holger Putz*
Structure Determination from Powder Diffraction Data (Inorganics)
MS 33 - *Chairs: Roger Fourme, Wilson Poon*
Soft Condensed Organical-Biological Material under Pressure
MS 34 - *Chairs: Louis Farrugia, Tibor Koritsanzky*
Advances in Computational Methods for Electron Density Studies
MS 35 - *Chairs: Giovanni Ferraris, Elena Belokoneva*
Polytypism and Twinning
- 12.35-13.45** **Lunch Break**
- 13.45-14.45** **Poster Session**
- 14.45-17.20** **MS 36** - *Chairs: Elspeth Garman, Ming Luo*
Combating Viruses
MS 37 - *Chairs: Yoshiro Yoneda, David Owen*
Intracellular Trafficking of Biomolecules
MS 38 - *Chairs: Christer Aakeröy, Alessia Bacchi*
Controlled Building of Crystals from Non-covalent Interactions
MS 39 - *Chairs: Robert Blessing, Jeremy Cockcroft*
Powder Diffraction of Proteins
MS 40 - *Chairs: Giulia Galli, Alessandro Pavese*
Computational Crystallography Applied to Extreme Conditions
MS 41 - *Chairs: Duncan E. McRee, James Holton*
Computational Solutions for High-Throughput Crystallography
MS 42 - *Chairs: Andreas Schreyer, Mark R. Daymond*
Complementarity of Neutron and X-rays
Methods in Material Science
- 17.20-17.30** **Break**
- 17.30-18.30** **KN 14 - Deborah Fass**
The Ins and Outs of *de Novo* Disulfide Bond Formation in the Cell
Chair: to be defined
KN 15 - Guy Orpen
Synthetic Crystallography
Chair: Frank Allen
KN 16 - John S. Tse
The Combination of Theory and Experiments in High Pressure Crystallography
Chair: Werner F. Kuhs

Saturday, August 27, 2005

SCIENTIFIC PROGRAM

- 8.30-9.30** **KN 17 - Harold Kroto**
Fullerenes
Chair: **Ivano Bertini**
- 9.30-10.00** **Break**
- 10.00-12.35** **MS 43 - Chairs: Adrian Goldman, Sthanam Narayana**
Extracellular Proteins and Cellular Adhesion
MS 44 - Chairs: Stephen Neidle, Eric Westhof
Nucleic Acids: Transcription, Translation and Repair
MS 45 - Chairs: Jonathan W. Steed, Carol Brock
Packing of Organic Molecular Compounds
MS 46 - Chairs: Tadashi Ohachi, Vladimir Kaganer
In-situ Observation of Crystal Growth Processes
MS 47 - Chairs: Colin Pulham, Nancy Ross
Novel Materials Under High Pressure
MS 48 - Chairs: Christian Riek, Atsuo Iida
Microbeam X-ray Scattering
MS 49 - Chairs: John Spence, Bo B. Iversen
Charge Spin and Momentum Densities in Material Science
- 12.35-13.45** **Lunch Break**
- 12.35-14.35** **Round Table on Data Mining from PDB**
- 13.45-14.45** **Poster Session**
- 14.45-17.20** **MS 50 - Chairs: Alexander Wlodawer, Silvia Onesti**
Enzymes and Allostery
MS 51 - Chairs: Wah Chiu, Lucia Banci
Complementary Approaches to Biological Structure Determination
MS 52 - Chairs: Christoph Janiak, Stuart R. Batten
Inorganic-Organic Framework Materials
MS 53 - Chairs: John Irvine, Torbjörn Gustafsson
Materials for Energy Conversion and Storage
MS 54 - Chairs: Guillaume Fiquet, Artem Oganov
Crystallography at Conditions of Earth and Planetary Interiors
MS 55 - Chairs: Jianming Cao, Hervé Cailleau
Time Resolved Diffraction
MS 56 - Chairs: José Teixeira, Roberto Triolo
Analyses Combining SANS and SAXS Experiments
- 17.20-17.30** **Break**
- 17.30-18.30** **KN 18 - Louise Johnson**
Mechanisms of Protein Kinase Inhibition
Chair: **John Helliwell**
KN 19 - Jim A. Ibers
Crystallography in Inorganic Solid-State Chemistry:
Importance, Pitfalls, Abuses
Chair: **Jan Boeyens**
KN 20 - Michael M. Thackeray
New Materials for Energy Storage
Chair: **Peter G. Bruce**

Sunday, August 28, 2005

- 8.30-9.30** **KN 21 - Michael W. Parker**
Pore-forming Toxins
Chair: **William L. Duax**
KN 22 - Malcolm I. McMahon
Complex Materials at High Pressure
Chair: **Osamo Shimomura**
KN 23 - Mark Spackman
Electrostatic and Related Properties from Accurate Charge Density Analyses
Chair: **Vladimir Tsirelson**
- 9.30-10.00** **Break**
- 10.00-12.35** **MS 57 - Chairs: Kunio Miki, David Stuart**
Large Protein Assemblies: Forming and Analysing Complexes
MS 58 - Chairs: Salvatore Siano, Henk Schenk
Crystallography and Understanding of Cultural Heritage
MS 59 - Chairs: Paul R. Raithby, Trevor Forsyth
Applications of Synchrotron and Neutron Facilities in Structural Chemistry
MS 60 - Chairs: Davor Balzar, Paolo Scardi
Microstructural Properties from Powder Diffraction Data
MS 61 - Chairs: Mohammed Mezouar, Nozomu Hamaya
Structures, Phase Transitions and Properties at High Pressure
MS 62 - Chairs: Piet Gros, Kevin D. Cowtan
Advances in Computational Methods for Protein Crystallography
MS 63 - Chairs: Nour Eddine Ghermani, Peter Blaha
Chemical Insights from Electron Density Studies and Wavefunctions
- 12.35-13.45** **Lunch Break**
- 13.45-14.45** **Poster Session**
- 14.45-17.20** **MS 64 - Chairs: Bi-Cheng Wang, Alexandre Urzhumtsev**
Difficult Phasing and Difficult Structures in Structural Biology
MS 65 - Chairs: Zihé Rao, Brian W. Matthews
Protein Interactions with Other Biological Macromolecules
MS 66 - Chairs: Davide M. Proserpio, Jean-Guillaume Eon
Topology of Crystal Structures: Nets, Knots and Surfaces
MS 67 - Chairs: Ivana Evans Radosavljevic, Roland Boese
Non-ambient Powder Diffraction and Kinetic Studies
MS 68 - Chairs: Christopher Tulk, Dennis Klug
Liquids and Amorphous Systems at High Pressure
MS 69 - Chairs: Eva Nogales, Ute Kolb
Electron Crystallography on Organic Crystals and Biomolecules
MS 70 - Chairs: Gernot Kostorz, Theyencheri Narayanan
New SAS Frontiers
- 17.20-17.30** **Break**
- 17.30-18.30** **KN 24 - Nenad Ban**
Carbohydrate Recognition
Chair: **Sherry Mowbray**
KN 25 - Lawrence Margulies
Micro Beam Diffraction
Chair: **Stefano Lagomarsino**
KN 26 - Dmitri Svergun
New Possibilities for Structure Determination of Biomolecular Complexes
Chair: **Giuseppe Zanotti**

Monday, August 29, 2005

SCIENTIFIC PROGRAM

- 8.30-9.30** **KN 27 - Michael Murphy**
Cu-Ligand Intermediate
Chair: Carrie Wilmot
KN 28 - Tim J. White
The Crystallo-Chemical Basis of Synthetic Mineral in Immobilization Technology
Chair: Ekkehart Tillmanns
KN 29 - Salvador Ferrer
The Surface Structure of Model Catalyst in Action Investigated by X-ray Diffraction
Chair: Mikhail Koval'chuk
- 9.30-10.00** **Break**
- 10.00-12.35** **MS 71 - Chairs: David Rose, Massimo Degano**
Structural Biology and the Immune System
MS 72 - Chairs: Glaucius Oliva, Andrew H.-J. Wang
Hot Structures in Protein Crystallography
MS 73 - Chairs: Catalina Ruiz-Perez, Alicia Beatty
Molecular Crystals with Novel Physical Properties
MS 74 - Chairs: Despina Louca, David Keen
Total Scattering and Local Order
MS 75 - Chairs: Laurence D. Marks, Maddalena Pedio
Surfaces
MS 76 - Chairs: Peter Erk, Samuel W.D. Motherwell
New Algorithms for Structure Prediction
MS 77 - Chairs: Masatoshi Arai, Ian Anderson
Perspective of Neutron Crystallography at High Power Sources
- 12.35-13.45** **Lunch Break**
- 13.45-14.45** **Poster Session**
- 14.45-17.20** **MS 78 - Chairs: Anders Liljas, Wayne Hendrickson**
Structuromes: Structures of Ribosomes, Nucleosomes and other -omes
MS 79 - Chairs: Jordi Rius, Evgeny Antipov
Inorganic and Mineral Structures Solved and Refined by Powder Diffraction Data
MS 80 - Chairs: Jean-Claude Daran, Pilar Gómez-Sal
Structural Knowledge and Catalysis
MS 81 - Chairs: Eric Kisi, Paul Barnes
Time-resolved Powder Diffraction for Materials Production and Processing
MS 82 - Chairs: Ugo Valbusa, Tilo Baumbach
X-ray Characterization of Nanostructures
MS 83 - Chairs: Christer Svensson, Vincent Favre-Nicolin
Computational Problems and Solutions for Aperiodic Crystals
MS 84 - Chairs: Szabolcs Vass, Salvino Ciccariello
Theoretical Methods for Analyses of Data from Solutions
- 17.20-17.30** **Break**
- 17.30-18.30** **KN 30 - Janet L. Smith**
Structural Biology of Imidazole Glycerol-phosphate Metabolism
Chair: Mitchell Guss
KN 31 - Myunghyun Paik Suh
Metal Organic Frameworks Self-assembly of Inorganic Materials
Chair: to be defined
KN 32 - Michiyoshi Tanaka
Nano Structures Studied by Convergent Beam Electron Diffraction
Chair: Yuji Ohashi

Tuesday, August 30, 2005

- 8.30-9.30** **KN 33 - Ahmed Zewail**
Ultrafast Electron Crystallography
Chair: **Xiadong Zou**
- 9.30-10.00** **Break**
- 10.00-12.35** **MS 85 - Chairs: Stefania Di Marco, William C. Stallings**
Biological Molecules as Targets for Drug Design
MS 86 - Chairs: Adriana Bigi, to be defined
Bio-inorganics in Biological Macromolecules
MS 87 - Chairs: Leonard MacGillivray, Fumio Toda
Reactions in Molecular Solids
MS 88 - Chairs: John J. Rehr, Keijo Hamalainen
Electronic Excitations
MS 89 - Chairs: José Martin-Gago, Giovanna Fragneto
Structural Characterization of Controlled Solid-Liquid Interfaces
MS 90 - Chairs: Ralf W. Grosse-Kunstleve, Maryjane Tremayne
Applying Non-crystallographic Algorithms to Crystallography
MS 91 - Chairs: Jacob Jansen, Vera Kletschkovskaia
Electron Crystallography on Inorganic Crystals
- 12.35-13.45** **Lunch Break**
- 13.45-14.45** **Poster Session**
- 14.45-17.20** **MS 92 - Chairs: Sine Larsen, Michael Becker**
Emerging Technologies for Structural Biology
MS 93 - Chairs: Marcello Mellini, Mihaly Posfai
Crystallography and Environmental Science
MS 94 - Chairs: Frank Leveillier, Michele Saviano
Crystallographic Knowledge in Drug Design Strategies
MS 95 - Chairs: Michele Catti, to be defined
Advanced Functional Materials (Including Molecular Biological Fuel Cell Battery)
MS 96 - Chairs: Åke Oskarsson, Randy J. Read
Crystallographic Teaching
MS 97 - Chairs: Herbert J. Bernstein, Brian McMahon
Programming Robust CIF and XML into Crystallographic Software
MS 98 - Chairs: Yoshiyuki Amemiya, Iris Torriani
Analysis of Anisotropic Materials
- 17.05-17.30** **Break**
- 17.30-18.30** **KN 34 - David Eisenberg**
Protein Interactions
Chair: **Maria Armenia Carrondo**
KN 35 - Gerhard Klebe
Structure-based Drug Design
Chair: **to be defined**
KN 36 - Lia Addadi
Strategies and Design Principles in Biological Mineralization
Chair: **Leslie Leiserowitz**

SATELLITE MEETINGS

Crystallographic Computing School

August 18-23, 2005

Siena, Italy

School organizers:

A. Spek, M. Mellini, A. Gualtieri, H. Powell and L. Cranswick

School consultants:

D. Watkin and S. Parsons

A school of Crystallographic Computing will be organized in the Certosa di Pontignano, in the environs of Siena, a magnificent historical town in Tuscany which is located at one hour driving south of Florence. A most generous support to the school is provided by the University of Siena, which owns the facilities. Even with a high ratio of speakers to students, the registration and accommodation costs are kept at a reasonable low level. The organisation will provide transportation to the XX IUCr Congress in Florence which starts just when the school is over.

For more information, please visit the web site:

<http://www.iucr.org/iucr-top/comm/ccom/siena2005/index.html>

ElCryst2005 - New Frontiers in Electron Crystallography

September 2-8, 2005

Brussels, Belgium

School organizer:

Stavros Nicolopoulos

Other members of the organizing team:

Anton-Jan Bons (ExxonMobil Chemical Europe, Belgium)

Jean Luc DelPlancke (Université Libre de Bruxelles, Belgium)

Jean-Paul Morniroli (University of Lille, France)

Thomas E. Weirich (Aachen University, Germany)

Topics

- Basics of Crystallography and TEM
- Dynamical Electron Diffraction
- Symmetry Determination by CBED
- Conventional and Dynamical Direct Methods
- Kinematical and Dynamical Structure Refinement
- Maximum Entropy and Likelihood in Electron Crystallography
- Crystallographic Image Processing
- FEG TEMs and Exit Wave Reconstruction
- Precession and Electron Diffractometry
- Imaging Plates Compared with other Electron Detectors
- Texture Patterns
- Electron Powder Diffraction
- Strategies for Determining Crystal Structures from Electron Microscopy Data
- Electron Crystallography Linked with X-ray Powder Diffraction and Quantum Mechanical Calculations
- Application of TEM to Solid State Chemistry Problems
- Electron Crystallography of Zeolites and Organic Compounds
- Local Structure and Bonding Determined by EELS

For more information, please visit the web site:

<http://www.elcryst2005.de>

WORKSHOPS

All workshops will take place on Tuesday, August 23, 2005 at the Fortezza da Basso, Main Pavilion. Registration for the workshop is additional to the Congress registration. Please register using the enclosed form or through the congress Web site. Workshop fee is € 100,00 (€ 60,00 for students). Deadline for registration: **July 31, 2005**.

WORKSHOP N. 1

Membrane Proteins: From Gene to Crystal

Half day workshop

For more information please contact **Adriana Zagari** at: zagari@unina.it

WORKSHOP N. 2

Putting the Pedal to the Metal: High Throughput Protocols for Crystallization

Half day workshop

For more information please contact **Adriana Zagari** at: zagari@unina.it

WORKSHOP N. 3

Introduction to Small-Angle Scattering

Full day workshop organized by Jan Skov Pedersen

The workshop will cover the following topics:

- introduction, basic theory (simple form factors, Porod, Guinier, Invariant) and contrast variation
- instrumentation and smearing effects
- modelling
- free-form approaches (Indirect Fourier transformation), ab-initio methods
- applications in: material science, molecular biology, polymer solutions and soft matter and bulk polymers

For more information please contact **Jan Skov Pedersen** at: jsp@chem.au.dk

WORKSHOP N. 4

Structural Analysis of Aperiodic Crystals

Full day workshop chaired by Sander van Smaalen and Ray L. Withers

This workshop is intended to give an overview of the state of the art of crystallographic analysis of incommensurately modulated crystals, incommensurate composite crystals, polytypes and quasicrystals. Introductory lectures will present the basic phenomena related to aperiodic order, including diffraction and morphology, and the fundamental principles of the superspace descriptions of their crystal structures. The afternoon session will be devoted to recent developments and applications of superspace crystallography.

<http://www.uni-bayreuth.de/departments/crystal/inc-workshop2005/>

For further information, please contact **Sander van Smaalen** at: smash@uni-bayreuth.de

WORKSHOP N. 5

Small Molecule Crystallization

Full day workshop chaired by Roland Boese (University of Essen, Germany) and **Chick Wilson** (University of Glasgow, UK); co-organized by European Crystallographic Association SIGs on Molecular Interaction and Recognition and Molecular Structure and Chemical Properties with the support of the IUCr Commissions on Structural Chemistry and Crystal Growth and Characterization of Materials.

Organizing Committee: **Paola Gilli** (University of Ferrara, Italy) and **Martin U. Schmidt** (University of Frankfurt, Germany).

This full-day workshop will cover theory and experimental techniques for the crystallization of molecular inorganic, organic and organometallic compounds (except biological compounds).

Topics include:

- Thermodynamic and kinetic factors in nucleation and crystal growth
- Crystallization techniques, including non-ambient methods
- *In-situ* crystallization of liquids and gases
- Co-crystallization (mixed crystals, solid solution, host-guest systems)
- Growth of large single crystals
- Polymorph screening

Grants are available. Requests should be sent to Martin U. Schmidt

For further information, please contact:

Paola Gilli at: paola.gilli@unife.it

Martin U. Schmidt at: m.schmidt@chemie.uni-frankfurt.de

COMPUTER FAYRE

With resources provided by the IUCr 2005 congress organizers, both non-commercial crystallographic software developers and software users are invited to participate in an informal Crystallographic Software Fayre that will be held throughout most of the IUCr 2005 congress in Florence.

This fayre will occur from Wednesday, August 24 until Tuesday, August 30, 2005.

User computers will consist of 8 PCs and a laser printer. They will be connected in a local network. The room will be also equipped with an audio system and video projector.

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

<http://www.ccp14.ac.uk/projects/iucr2005-softwarefayre>

The Software Fayre is being organized by:

Richard Stephenson (CCPI 4, University College London)

Lachlan Cranswick (NRC Canada, Chalk River Laboratories)

Any queries should be sent to **Richard Stephenson** at: r.stephenson@mail.cryst.bbk.ac.uk.

OPEN COMMISSION MEETINGS

Open Commission Meetings will take place, as scheduled below, between **12.35-14.35**

Wednesday, August 24, 2005 Commission on Journals (I)

Coordinator: **J. Helliwell**

For further information: hell@spec.ch.man.ac.uk

Thursday, August 25, 2005 Commission on Journals (II)

Coordinator: **J. Helliwell**

For further information: hell@spec.ch.man.ac.uk

Friday, August 26, 2005 COMCIFS

The Current Status and Future Prospects of CIF

Coordinator: **D. Brown**

For further information: idbrown@mcmaster.ca

Commission on Biological Macromolecules

Coordinator: **M. Guss**

For further information: M.Guss@mmb.usyd.edu.au

Saturday, August 27, 2005 Commission on Inorganic and Mineral Structures

Coordinator: **G. Ferraris**

For further information: giovanni.ferraris@unito.it

Commission on Charge, Spin and Momentum Densities

Coordinator: **C. Lecomte**

For further information: claude.lecomte@lcm3b.uhp-nancy.fr

Commission on International Tables of Crystallography

Coordinator: **H. Fuess**

For further information: hfuess@tu-darmstadt.de

Monday, August 29, 2005 Commission on High Pressure

Coordinator: **M. Kunz**

For further information: m.kunz@lbl.gov

Schedule to be defined

CONGRESS MAIN TOPICS

01 Instrumentation and Experimental Techniques

1. Conventional Sources of X-rays
2. Synchrotron Radiation I: Instrumentation and Techniques
3. Synchrotron Radiation II: Applications
4. New X-ray Sources
5. Electron Diffraction (LEED, RHEED, PED, AED)
6. Cryo-Electron Microscopy
7. X-ray Imaging
8. Neutron Scattering I: Techniques and Instrumentation
9. Neutron Scattering II: Applications
10. Area Detectors (Multi-wire, Image Plate, CCD)
11. Data Accuracy and Detectors
12. Cryo-Crystallography: Techniques and Instrumentation
13. Fast (pico-second) Crystallography
14. Free Electron Lasers for X-rays

02 Methods for Structure Determination

1. Difficult Structures
2. Direct Methods of Phase Determination
3. Maximum Entropy Methods
4. Anomalous Dispersion/MAD/MIR Phasing
5. Laue Time Resolved Methods
6. Incommensurate Structure Solution
7. EXAFS and XANES
8. High Resolution NMR and Macromolecules
9. Liquid Structure Determination
10. Structure Prediction: Computational Methods
11. Ab Initio Powder Diffraction Solutions: Molecular Compounds
12. Ab Initio Powder Diffraction Solutions: Inorganic Compounds
13. Ab Initio Powder Diffraction Solutions: Electron Diffraction
14. Ab Initio Low Resolution Macromolecular Phasing
15. X-ray and Neutron Complementarity
16. Rietveld Refinement Methods

03 Computers in Analysis, Molecular Modelling and Molecular Design

1. Programs for Refinement and Analysis
2. Atomic Displacement Analyses and Variable Temperature Analyses
3. Graphics and Virtual Reality
4. Rational Drug Design
5. Materials Design
6. Structure Simulations: Inorganic Crystals
7. Structure Simulations: Protein Folding Studies
8. Map Fitting and Modification
9. Image Reconstruction
10. Homology Modelling, Structural Families and Docking
11. Use Of Genetic Algorithms and Other Optimisation Methods

04 Crystallography of Biological Macromolecules

1. Peptide and Protein Crystallisation
2. Enzymes and Enzyme Catalysis
3. Metallo-Enzymes
4. Muscle and Motor Proteins
5. Nucleic Acids
6. Protein - DNA Interactions
7. Protein - RNA Interactions
8. Protein Design and Engineering
9. Protein Biosynthesis
10. Cryo-Crystallography: Applications to Macromolecules
11. Proteins of the Immune System
12. Receptor and Signal Transduction Proteins
13. Viruses and Viral Proteins
14. Macromolecular Assemblies
15. Macromolecular Based Drug Design
16. Multi-domain Proteins
17. Structural Motifs
18. Organelles
19. Diseases and Toxicity
20. NMR Applications to Macromolecules
21. Time Resolved Studies
22. Structural Genomics
23. High Resolution Protein Structures
24. Water and Other Solvent Structures In Macromolecules
25. Hot Macromolecular Structures

05 Crystallography of Biological Small Molecules

1. Peptides
2. CNS Agents
3. Antibiotics
4. Steroids
5. Other Natural Products
6. Other Biosynthetic and Exotic Molecules
7. Hydrogen Bonding and Included Water Structure

06 Crystallography of Organic Compounds

1. Sugars
2. Lipids
3. Alkaloids
4. Fused Ring Systems
5. Fullerenes and Carbon Cages
6. Supramolecular Assemblies
7. Inclusion Compounds and Complexes
8. Intercalates
9. Clathrates

07 Crystallography of Organometallic, Co-ordination and Main Group Compounds

1. Metal Atom Complexes ($N = 1-3$) and Metal Clusters ($N > 3$)
2. Molecular Recognition Complexes
3. Fullerene Metal Complexes
4. Supramolecular Co-ordination Complexes
5. Main Group Chemistry
6. Cage and Metallo-Cage Structures
7. Bio-Inorganic Structures

8. Bio-Mineralization and Modifications
9. Inclusion Compounds and Clathrates
10. Molecular Magnets

08 Structure/Property Relationships

1. Molecular Recognition
2. Chemical Crystallography of The Future
3. Dynamic Properties in Molecular Crystals
4. Solid State Reactions
5. Structural Thermodynamics and Kinetic Aspects
6. Phase Transitions
7. Analysis of Atomic Displacement Parameters
8. Intermolecular Interactions
9. Structure and Chemical Reactivity
10. Polymorphism and Isomorphism: Identification and Characterisation
11. Polymorphism: Applications
12. Time Resolved in situ Reactions
13. Hydrogen Bonding Studies
14. Structure Property Relationships

09 Crystal Engineering

1. General Applications and Strategy
2. Organic Compounds
3. Inorganic Compounds
4. Organometallic Complexes
5. Intermolecular Interactions: Exploitation
6. Non Centrosymmetric Systems: Creation and Applications

10 Inorganic Crystallography and Geosciences

1. General Geosciences
2. Systematics of Inorganic Compounds
3. Systematics in Geosciences
4. High Pressure and High Temperature Studies
5. Minerals: Characterisation Methods and Structures
6. Zeolites (Natural and Synthetic)
7. Exotic Molecules

11 Crystallography in Material Science

1. Superconducting and Semi-Conducting Materials
2. Catalysis: In situ Studies
3. Giant Magneto Resistance Materials
4. Fullerene Complexes: Applications
5. Non-crystalline Materials
6. Ceramics, Glasses and Amorphous Materials
7. Aperiodic and Incommensurate Structures
8. Polymers
9. Liquid Crystals
10. Nonlinear Optical and Electronic Materials
11. Perovskite Materials
12. Ferroic and Ferro-Electric Structures
13. Battery and Fuel Cell Materials
14. Residual Stress Measurements
15. Pore Framework Materials

12 Surfaces, Interfaces, Liquids and Thin Films

1. Surface and Interface Crystallography by X-ray and Neutron Diffraction

2. Surfaces and Catalysis
3. Dynamic Diffraction Methods
4. X-ray Reflectivity: Instrumentation and Applications
5. Neutron Reflectometry: Techniques and Applications
6. Recent Liquid Structure Determination
7. Small Angle Scattering
8. Diffuse Scattering
9. Interfacial Structures
10. Micelles
11. Thin Films and Multilayers
12. Magnetic and Conducting Properties of Thin Films

13 Fibre Diffraction

1. Polymers: Synthetic Fibres
2. Structure Determination of Fibres
3. Biological Fibre Diffraction
4. Non-Periodic and Disordered Fibres

14 Charge, Spin and Momentum Density

1. Multipole and Other Modelling Methods
2. Software Developments
3. Applications of Synchrotron Data
4. Maximum Entropy Applications
5. Experimental Methods and Techniques
6. Topological Analyses
7. Molecular and Crystal Properties From Charge Densities
8. Magnetisation and Spin Densities
9. New Frontiers

15 Diffraction Physics and Optics

1. Interferometry
2. Inelastic Scattering
3. Neutron Optics
4. X-ray Optics: Lenses, Guides and Focusing
5. Resonant Magnetic X-ray Diffraction
6. Anisotropic Resonant Scattering
7. Polarisation: Generation and Exploitation
8. Dynamical Diffraction
9. Extinction and Absorption
10. N-beam Diffraction
11. Grazing Angle Incidence

16 Crystal Growth: Techniques, Instrumentation and Applications

1. Systems that are Difficult to Crystallise
2. Industrial Mass Crystallisation
3. Crystal Growth from Solution and Gels
4. Crystal Growth and Characterisation from the Melt
5. Microgravity Crystallisation
6. Epitaxial Growth
7. Crystal Doping and Imperfections
8. Self-Assembled Crystals
9. Exploitation of Chirality
10. Crystal Growth: Modelling, and Predicting Morphology
11. Morphology Modification: Theory and Experiment

12. Twinning: Acceptance and Avoidance
13. Polymorphism: Recognition and Applications
14. Low Temperature in situ Crystallisation

17 Characterisation of Defects, Microstructures and Textures

1. Techniques, Theory and Instrumentation
2. Electron Microscopy
3. X-ray Topography
4. Diffraction
5. STM and AFM Microscopy
6. Other Techniques Including Polarised Light and Infrared Studies
7. Cathodo and Photo Luminescence

18 Electron Microscopy

1. Applications to Macromolecules
2. Cryo-Microscopy
3. New Techniques and New Instrumentation
4. Applications

19 Electron Diffraction

1. New Techniques and New Instrumentation
2. High Resolution Results
3. Other Applications and Advances

20 Non-Ambient Conditions

1. High Pressure Crystallography I: Extremes of Temperature and Pressure
2. High Pressure Crystallography II: Physical Properties Under Pressure
3. High Pressure Crystallography III: Phase Transitions and High Pressure
4. High Pressure Crystallography IV: Data Acquisition and Analysis
5. High Pressure Crystallography V: Biological and Soft Matter under Pressure
6. High Pressure Crystallography VI: New Frontiers
7. High Temperature Crystallography: Instrumentation, Techniques and Applications
8. Low Temperature Crystallography: Instrumentation, Techniques and Applications
9. Phase Transitions I: Characterisation and Applications
10. Phase Transitions II: Magnetic and Structural Identification
11. Applications of Light and Laser Irradiation
12. Crystallography of Excited States

21 Symmetry and its Generalisations

1. General Symmetry: Theory
2. Designer Symmetry: Theory and Practice
3. Pseudo-Symmetry: Recognition and Applications

22 Aperiodic and Incommensurate structures

1. Data Collection and Structure Solution
2. Identification and Refinement
3. Results and Applications

23 Crystallographic Topology

1. Group Theory and Topology
2. Tiling
3. Quasicrystals
4. Networks
5. Critical Points

24 Databases

1. Creation and Exploitation
2. Coping with Rapid Expansions of Data. The Next Generation Of Databases
3. Research Applications of the CSD
4. Research Applications of the PBD/ NADB
5. Research Applications of the ICSD
6. Research Applications of the PDF
7. Data Mining and Knowledge Generation
8. Bio-informatics: The Future

25 Industrial Crystallography

1. Instrumentation and Techniques
2. Stress-Strain Analysis
3. On Line Diffraction Analysis
4. Line Broadening
5. Amorphous and SAS
6. Microporous Materials
7. Nanomaterials
8. High Temperature Crystallography
9. Thick Coatings
10. Pharmaceutical Crystallography

26 Crystallographic Teaching

1. Changes in Teaching Methods for the Future
2. Maintaining Standards Despite Automation
3. Cheap Computer Programs for Developing Countries
4. Preparation for Publication; CIF Files; How Much?
5. Crystallography on the World Wide Web

27 The History of Crystallography

1. History of Crystallography

28 Art, Cultural Heritage and Crystallography

1. Art, Cultural Heritage and Crystallography
2. Crystallography and Art

29 Other Topics

1. Crystallography and Forensic Science
2. Crystallography and Environment
3. Other

ABSTRACT SUBMISSION

Deadline for the submission of Bursary Applications: February 10, 2005

Deadline for Submission of Abstracts: February 28, 2005

Abstracts must be submitted on-line by connecting to the Web site www.iucr2005.it.

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 the 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 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 1, 2005.

ABSTRACT PREPARATION INSTRUCTIONS

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.iucr2005.it/image/documents/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

250 words (1800 characters) of text in Times New Roman, font size 9 in a maximum area of 9 x 11.5 cm Do NOT use a smaller font size. Use single spacing. Include graphics (minimum resolution 300 dpi) only if they will necessary, and if they will reproduce well in black and white. Note that 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 and in gray scale (or at a great reduced color depth) before including them in your abstract.

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 documentation section.

(<http://www.iucr2005.it/image/documents/keywords.pdf>)

ABSTRACT SUBMISSION

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

1) Access the Web site www.iucr2005.it within the period January 10-February 28, 2005.

Click on "Abstract Submission" and log in with your Username and Password. If you do not have Username and Password, click on the "Registration" button and enter the required information. Immediately after confirmation, you will automatically receive Username and Password by e-mail.

2) Select the type of contribution.

a) Invited speaker: your name will be recognized by the system and you will be automatically directed in the appropriate KN or MS or OCM area (please contact the congress secretariat by e-mail iucr2005@iucr2005.it for any incongruence). You will be asked to complete a form containing the following four different fields where you must insert your data.

I) "Title": write the abstract title (< 80 characters).

II) "Co-authors": write fullnames (first, middle, last) separated by commas (e.g. Paola Paoli, Carlo Mealli, Patrizia Rossi, Andrea Ienco).

III) "Keywords": enter the three keywords already present in the abstract and separated by commas (use small letters).

IV) "Abstract File": use the "Browse" button to locate the prepared abstract file in your computer.

b) Poster presentation and requested oral contribution: Please fill all the fields in the form.

The first group of four fields (namely, "Title", "Co-authors", "Keywords", and "Abstract File") is the same as above for the invited speakers.

The other fields are:

Contribution Category: please indicate topic and sub-topic, chosen from the supplied list of Main Topics

(also reported at pages 15-17 of this circular).

Request for Oral Presentation: authors, who apply for MS presentation, must check the checkbox and quote the corresponding number of the MS (see the tables on pages 6-11 of this circular).

After submission, the presenting author has only a 10 day period to modify the abstract by repeating the above procedure. After this time (or at the abstract deadline, if this comes first), the abstract is automatically finalized and cannot be further changed.

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 Congress Secretariat at iucr@iucr2005.it.

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 8, 2005**.

Acceptance of the poster contribution will be notified to the presenting authors by **April 8, 2005**. Final scheduling of the poster presentation will be communicated to the submitting author after payment of the registration fee (deadline: **June 1, 2005**). The accepted contributions will be printed in the Book of Abstracts and included in the congress Web site as well as in a CD-ROM. The abstracts

will also be made available online in a special issue of Acta Crystallographica Section A, published at the end of the year 2005.

POSTER PRIZE AWARDS

CCDC

Cambridge Crystallographic Data Centre will be awarding three poster prizes each comprising a commemorative item and a monetary prize. Candidates should not be more than 35 years of age on the January 1, 2005. Posters should report original research in:

* Chemical crystallography, including advances in instrumental, experimental or computational techniques.

* Applications of small-molecule crystallographic information in, e.g., structural chemistry, molecular modelling, materials design, structural biology or chemical informatics.

RCSB PDB

The RCSB PDB Poster Prize is awarded for the best student poster presentation.

Information about the poster prize is at:

http://www.rcsb.org/pdb/poster_prize.html

MOLECULAR DIMENSIONS

Molecular Dimensions Ltd. will be awarding a monetary prize for one poster within the subject of Protein Crystal Growth. More details will be available at a later stage.

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 **February 10, 2005** 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) waiving of the 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.

GENERAL INFORMATION

HOW TO GET TO FLORENCE

BY AIR

Florence airport is only 4 km from the city centre. Bus and taxi are available between the airport and downtown Florence. A taxi ride from the airport to the city centre costs about € 20,00.

Pisa Galileo Galilei airport and Florence Amerigo Vespucci airport are served by several international airlines. Pisa airport is about 90 km far from Florence, and a shuttle train operates every hour between the airport and the main railway station in Florence. The trip lasts approximately 1 hour.

BY TRAIN

Eurostar trains connect Florence with Milan (approximately 2h. and 45 min.) and Rome (approximately 1h. and 30 min.). The main railway station in Florence is Santa Maria Novella and it is located at walking distance from the congress centre (Fortezza da Basso).

BY CAR

The A1 (Autostrada del Sole) is the main motorway linking Florence to both northern and southern Italy. The A1 leads west to the coast and then to Genoa and the French border: both are toll motorways. The use of seat belts is mandatory. Car lights are compulsory in motorways. All road distances and speed limits are indicated in kilometres.

CITY TRANSPORTATION

The historical area of Florence is relatively compact, and all major sites are within walking distance from the city centre. Florence has a fairly comprehensive network of local bus routes, and many have a stop at the main railway station. Bus tickets may be purchased at most coffee-bars and tobacconists. Two bus companies serving several cities around Florence have their terminal next to the main railway station.

VENUE

The site of the XX IUCr Congress and General Assembly is Fortezza da Basso, Viale Strozzi 1, Florence, Italy. This congress centre hosts international congresses, fairs and exhibitions and it is equipped with all the modern facilities. The site is within walking distance from the main railway station and the downtown area of Florence.

OPENING HOURS OF THE REGISTRATION DESK ON-SITE

From Tuesday 23 to Tuesday 30, August 2005

08.00 - 19.00

OFFICIAL WEB SITE

The official Web site of the congress is: www.iucr2005.it

In the Web site participants will be able to submit abstracts, to register at the congress, to make reservations for hotels and tours and could find the updated version of the Scientific Program.

Any news on the congress will be published in the official Web site.

LANGUAGE

The official language of the congress is English. Sessions and posters will be presented in this language.

LUNCHES

Buffet lunches will be provided at the congress venue (included in the registration fee of congress delegates and accompanying persons) from Wednesday 24 to Tuesday 30, August 2005.

COFFEE POINTS

Coffee points will be available at any time during congress hours.

BADGES

Each participant will receive a name badge upon registration. Participants are kindly requested to wear their badge during all congress activities and social events.

EXHIBITION

A professional exhibition is scheduled to take place in conjunction with the congress, from Tuesday 23 to Saturday 27, August 2005. For more information please visit the Web page www.iucr2005.it/exhibition.htm or contact the Fund Raising Manager:

Annalisa Guerri

Dept. of Energy Engineering "Sergio Stecco"

University of Florence

Fund Raising Manager of IUCr2005

tel: +39 055 4796240, fax: +39 055 4796342

guerri@iucr2005.it

CLIMATE

The temperature in Florence during August is typical of an Italian summer, being the average temperature around 28°C. All the rooms in the congress centre are provided by air conditioning.

CLOTHING

Informal for all the occasions.

BANKS

Money can be easily exchanged at all main banks and exchange offices downtown Florence. Traditional banking hours are: Monday through Friday 8.30-13.20 and 14.30-15.30. Banks are closed on Saturday and Sunday. Some automatic cash machines are located outside the major banks to provide 24-hour service.

ELECTRICITY

Electrical current in Italy is 220V, 50-cycle AC. Italian outlets take only round-prong plugs. Appliances designed to operate on 110/120 V need a voltage converter and a plug adapter.

TIME

The time in Florence is the Central European Time (Summer Time GMT +1).

MEDICAL SERVICE

The number for the medical emergency service in Italy is 118. Chemists are open from 9.00 to 13.00 and from 16.00 to 20.00, Monday to Friday.

The main chemist is located in Santa Maria Novella railway station and it is open 24 hours a day.

POST OFFICE

The Post Office is located next to Santa Maria Novella railway station and it is open from 8.15 to 19.00, Monday to Friday.

VISAS

Entry visas are not required for citizens of most European countries, the USA and Canada. Citizens of other countries can obtain a visa at the Italian Embassy or Consulate in their country. A valid passport is required. A letter of invitation will be provided for those who need it.

For more information about visas, please check the Web site of the Italian Ministry of Foreign Affairs:

http://www.esteri.it/eng/5_32_183.asp

SOCIAL PROGRAM

The following program will be organized for participants and accompanying persons

WELCOME RECEPTION

Tuesday, August 23, 2005

(Included in the registration fee)

The Welcome Cocktail will take place immediately after the Open Ceremony. Participants registered at the congress and accompanying persons are invited to come and share in the celebration and festivities, after having checked in at the Registration Desk.

EVENING CONCERT

Saturday, August 27, 2005

(Included in the registration fee)

A concert will take place in one of the most famous churches of Florence. Further details will be given in the Final Program.

SOCIAL BANQUET

Monday, August 29, 2005

(Included in the registration with a booking fee of € 20,00.

See the registration form)

Further details will be given in the Final Program.

REGISTRATION

Payment received

	Before April 15, 2005	After April 15, 2005
CONGRESS		
Participant	€ 540,00	€ 630,00
Student*	€ 270,00	€ 320,00
Accompanying Person	€ 230,00	€ 230,00
Social Banquet booking fee for registered persons	€ 20,00	€ 20,00
Social Banquet booking fee for NOT registered persons	€ 75,00	€ 75,00

WORKSHOPS ON AUGUST 23 *(inclusive of coffee break and lunch)*

(for some workshops, registration bursaries may be provided. Please check the Web site for the latest news).

Participant	€ 100,00
Student*	€ 60,00

* *under 35 years old and with proof of student status (a copy of a valid student card or a letter of the supervisor should be sent to Newtours by fax or mail).*

HOW TO REGISTER

Registration should be made through the congress Web site (www.iucr2005.it) or by sending the attached Registration Form to the Organizing Secretariat.

FEE INCLUDES

Participant or student: participation at the congress scientific sessions, congress program, Book of Abstracts and CD ROM. Lunches for seven working days (from Wednesday, August 24 to Tuesday, August 30), invitation to the following social events: opening ceremony and welcome cocktail, concert and social banquet (with a booking charge of € 20,00).

Accompanying persons: Two half day tours (tour 2 and tour 9) scheduled to take place during session hours (tours have to be booked in advance), opening ceremony and welcome cocktail, lunches for seven working days (from Wednesday, August 24 to Tuesday, August 30), concert and social banquet (with a booking charge of € 20,00). Social Banquet for those who are not registered has a fee of € 75,00.

METHODS OF PAYMENT

Payment of fees must accompany all registrations. No registration will be confirmed until payment is received. Payment can be made by the following methods: credit cards (Visa, Master Card, American Express and Diners Club), cheque or bank transfer in favour of:

Newtours S.p.A.

BANCA INTESA / Bci S.p.A. - Div. Cariplo

Florence branch, Viale Gramsci 39/41

Account number: 000000078158

SWIFT: BIC: B C I T I T 3 3 4 5 7

IBAN: IT30 Y030 6902 8200 0000 0078 158

These two latter methods apply to those who prefer to send the registration form via mail or fax.

Please send the copy of the bank transfer and cheque with the registration form.

Those planning to register are strongly recommended to complete and submit the registration forms online, using the electronic form at: <http://www.iucr2005.it>. In this case they will be free to pay via credit cards or bank transfer. Should you prefer to pay by bank transfer, you must send via fax a copy of the receipt within 5 working days or the registration and all other services required will not be confirmed.

Newtours will send a written confirmation to all the participants.

CANCELLATION AND REFUND POLICY

Cancellations of registrations shall be notified by sending a written and signed document to Newtours.

100 % refund cancellation by: **January 31, 2005**

70% refund cancellation by: **April 15, 2005**

50% refund cancellation by: **June 30, 2005**

No refund after: **July 1, 2005**

In any case an administrative charge of € 15,00 applies. Refunds will be made using the same method chosen for the payment (i.e. payment by credit card will be refunded to the same credit card).

For cancellations **after April 15, 2005** refunds will be made by Newtours after the end of the congress.

Newtours SpA

Via A Righi 8 - 50019 Sesto Fiorentino, Florence, Italy

Phone +39 055 33611

Fax +39-055-3361350

newtours@iucr2005.it

HOTEL ACCOMMODATION

Deadline for hotel reservation: April 15, 2005

Newtours has reserved rooms in Florence and advises all congress registrants to make reservations as soon as possible to guarantee accommodation in Florence. Please send the enclosed hotel accommodation form and specify the hotel category and type of room (single or double) desired as well as arrival and departure dates.

All requests must be accompanied by a deposit, as specified in the table below plus € 15,00 for agency fees and mailed directly to:

Newtours SpA

Via A Righi 8 - 50019 Sesto Fiorentino, Florence, Italy

Phone: +39 055 33611 - Fax +39 055 3361350

newtours@iucr2005.it

Payment can be made by the following methods:

Credit cards (Visa, Master Card, American Express and Diners Club), cheque or bank transfer in favour of:

Newtours S.p.A.

BANCA INTESA / Bci S.p.A. - Div. Cariplo

Florence branch, Viale Gramsci 39/41

Account number : 000000078158

SWIFT: BIC: B C I T I T 3 3 4 5 7

IBAN: IT30Y030 6902 8200 0000 0078 158

- Newtours will send a voucher, which must be presented at the check-in at the hotel, specifying the name and address of the hotel and confirming the reservation and receipt of the deposit.
- The deposit must be paid within **April 15, 2005**, and the balance will be paid directly to the hotel.
- The hotel will issue receipt of payment (inclusive of deposit).
- Single rooms are available in a very limited number and will be assigned on a first-come, first-served basis. If not available, the Secretariat will assign double rooms for single use.
- Please be aware that only 2 persons can stay in a double room.
- If you need to accommodate 3 persons you will need to require a triple room and if more a family room.
- Air conditioning is not always provided in ** and * star hotels. Before booking be sure to check if available.
- Reserved rooms will be held for participants for the night covered by their booking deposit. Should participants fail to arrive, the hotel will then be free to use the rooms from 12.00 (noon) on the next day, unless otherwise notified by the participants.

Hotel reservation forms without the first night's deposit will not be considered.

HOTEL CATEGORY	SINGLE	DOUBLE FOR SINGLE USE	DOUBLE
	min / max	min / max	min / max
5-star	€ 165,00 / € 190,00	€ 190,00 / € 225,00	€ 210,00 / € 275,00
4-star	€ 115,00 / € 150,00	€ 130,00 / € 150,00	€ 130,00 / € 150,00
3-star	€ 70,00 / € 95,00	€ 95,00	€ 95,00
2-star	€ 60,00 / € 80,00	€ 73,00 / € 95,00	€ 100,00 / € 120,00
1-star	€ 40,00 / € 73,00	€ 65,00 / € 85,00	€ 75,00 / € 95,00
Low Cost Accommodation*	€ 25,00 / € 37,00	€ 35,00 / € 47,00	€ 40,00 / € 54,00

* Low cost accommodations are available in a very limited number and will be assigned on a first-come, first-served basis.

The indicated rates, in Euro, are valid for the period of the congress and include one overnight stay, continental breakfast, taxes, V.A.T.

Breakfast is not included for * star and low-cost accommodation.

The first night deposit (Max. rate) must be mailed to Newtours within **April 15, 2005**.

CANCELLATION

All cancellations must be addressed to Newtours. Newtours will refund:

- 100% of the deposit for cancellation postmarked: **before April 15, 2005**
- 50% of the deposit for cancellation postmarked: **before June 30, 2005**
- No refund will be made for cancellations **after this date**.

In case of partial reduction of room nights received after **June 30, 2005**, the hotel will decide if a penalty will be applied.

CONGRESS TOURS**Deadline****for tours reservation: 30 June 2005**

The following tours are based on the participation of minimum 15 maximum 25 people for the walking and museum tours, minimum 20 and maximum 40 people for the bus tours. All tours are organised for delegates and accompanying persons. Each tour can be reserved with the Congress Tours form. If a minimum number of participants is not obtained by 30 June, 2005 Newtours will suggest alternative tours. The descriptions of the tours are available on the web site.

Wednesday, August 24, 2005

- TOUR 1** **SIENA AND SAN GIMIGNANO**
09.00-18.00 / full day, by bus
Euro 95,00 per person
- TOUR 2** **CITY CENTRE**
09.15-12.00 / half day
Euro 30,00 per person (free of charge for accompanying person)
- TOUR 3** **UFFIZI GALLERY**
16.30-18.45 / half day
Euro 35,00 per person

Thursday, August 25, 2005

- TOUR 4** **PISA AND LUCCA**
09.00-18.00 / full day, by bus
Euro 95,00 per person
- TOUR 5** **THE MEDICI FAMILY**
09.15-12.00 / half day
Euro 38,00 per person
- TOUR 6** **THE PITTI PALACE**
16.30-18.45 / half day
Euro 35,00 per person

Friday, August 26, 2005

- TOUR 7** **SANTA CROCE, ITS MONASTERY AND ITS DISTRICT**
09.15-12.00 / half day
Euro 35,00 per person
- TOUR 8** **BARGELLO MUSEUM AND PALAZZO VECCHIO**
12.45-15.00 / half day
Euro 35,00 per person
- TOUR 9** **GALLERY OF THE ACCADEMIA AND SS. ANNUNZIATA SQUARE**
16.30-18.30 / half day
Euro 35,00 per person (free of charge for accompanying person)

Saturday, August 27, 2005

- TOUR 10** **CHIANTI AREA**
09.00-17.00 / full day, by bus
Euro 95,00 per person
- TOUR 11** **SANTA MARIA NOVELLA, ITS CLOISTERS AND THE PHARMACY**
09.15-12.00 / half day
Euro 35,00 per person
- TOUR 12** **UFFIZI GALLERY**
16.30-18.45 / half day
Euro 35,00 per person

Sunday, August 28, 2005

- TOUR 13** **MEDICI VILLAS**
09.00-17.00 / full day, by bus
Euro 95,00 per person
- TOUR 14** **FLORENTINE HILLS**
09.15-12.00 / half day, by bus
Euro 40,00 per person
- TOUR 15** **THE PITTI PALACE**
16.30-18.45 / half day
Euro 35,00 per person

Monday, August 29, 2005

- TOUR 16** **SIENA AND SAN GIMIGNANO**
09.00-18.00 / full day, by bus
Euro 95,00 per person
- TOUR 17** **MASACCIO AND CHURCHES IN THE OLTRARNO AREA**
09.15-12.00 / half day
Euro 35,00 per person
- TOUR 18** **THE RESTORATION LABORATORY AND THE MUSEUM OF THE CATHEDRAL**
16.30-18.30 / half day
Euro 45,00 per person

Tuesday, August 30, 2005

- TOUR 19** **PISA AND LUCCA**
09.00-18.00 / full day, by bus
Euro 95,00 per person
- TOUR 20** **SAN MARCO AND SANTA APOLLONIA MUSEUMS**
09.15-12.00 / half day
Euro 35,00 per person
- TOUR 21** **GALLERY OF THE ACCADEMIA AND SS. ANNUNZIATA SQUARE**
16.30-18.30 / half day
Euro 35,00 per person

Wednesday, August 31, 2005

- TOUR 22** **MEDICI VILLAS**
09.00-17.00 / full day, by bus
Euro 95,00 per person
- TOUR 23** **THE GREAT WINES OF TUSCANY**
08.30-19.00 / full day, by bus
Euro 115,00 per person
- TOUR 24** **UFFIZI GALLERY**
09.15-11.30 / half day
- TOUR 25** **GALLERY OF THE ACCADEMIA AND SS. ANNUNZIATA SQUARE**
09.15-11.30 / half day
Euro 35,00 per person
- TOUR 26** **THE PITTI PALACE**
09.15-11.30 / half day
Euro 35,00 per person

CANCELLATION POLICY

All the cancellations must be addressed to Newtours S.p.A. The following penalties will be applied for cancellations:

no penalties by:	June 30, 2005
50% penalties between:	June 30 and July 30, 2005
no refund after:	July 30, 2005



XX Congress of the International Union of Crystallography

Congress and General Assembly

REGISTRATION FORM

Please PRINT in BLOCK LETTERS and FAX, EMAIL or AIRMAIL to:

Newtours S.p.A.

Via A. Righi, 8 - 50019 Sesto Fiorentino, Florence, Italy

Personal Data

Prof. Dr. Mr Mrs Ms

Family Name _____

First Name _____

Male Female Date of Birth _____

Organization or Institution _____

Department _____

Institution Address _____ State _____

Zip/Postal Code _____ City _____ Country _____

Phone _____ Fax _____

Email _____

Accompanying Member(s)

1. Family name _____ First Name _____

2. Family name _____ First Name _____

3. Family name _____ First Name _____

Registration Fees (in Euro)

	Before April 15, 2005	After April 15, 2005
Participant	€ 540,00	€ 630,00
Student	€ 270,00	€ 320,00
Accompanying Person	n. _____ x € 230,00	

Workshop on August 23

Please check the appropriate box/es:

Workshop n. **Participant € 100,00** **Student € 60,00**

Social Program

Free of charge, included in the registration fee for members, accompanying members and students. Please indicate the number of persons attending the Social Program events.

Opening Ceremony and Welcome Cocktail n. of participants _____

Concert n. of participants _____

Social Banquet n. _____ x € 20,00 for registered participant

Social Banquet n. _____ x € 75,00 for **NOT** registered participant

REGISTRATION FORM



XX Congress of the International Union of Crystallography

Congress and General Assembly

Tours for Accompanying Persons

Half Day tour n. 2 n. of participants _____
 Half Day tour n. 9 n. of participants _____

Payment

Please indicate the total amount and the preferred mode of payment. Ensure that you send your fully completed registration form together with your payment:

Registration fee: _____
 Workshop: _____
Total amount _____

Method of payment

Credit Card

Visa MasterCard Diners American Express

Number _____ Expiry Date _____ (Month/Year)

Name as shown on Card _____

Signature _____

Bank Transfer

With your name and address indicated. If payment is made for more than one person or by a company, please make sure all names are indicated. Please forward bank transfer to:

Newtours S.p.A.

BANCA INTESA / Bci S.p.A. – Div. Cariplo

Florence branch, Viale Gramsci 39/41

Account number : 000000078158

SWIFT: BIC: B C I T I T 3 3 4 5 7

IBAN: IT30 Y030 6902 8200 0000 0078 158

Bank charges are the responsibility of the payee and should be paid at source in addition to the registration fee.

Cheque - Payable to Newtours S.p.A.

For cancellation policy, see the Program

For Italian participants only

According to art. 10/law 675/96, Newtours S.p.A. is authorized to use personal data for purposes connected to the Congress Management.

I agree

Yes

Not

Date _____

Signature _____



XX Congress of the International Union of Crystallography

Congress and General Assembly

ACCOMMODATION AND TOURS FORM

Please PRINT in BLOCK LETTERS and FAX, EMAIL or AIRMAIL to:

Newtours S.p.A.

Via A. Righi, 8 - 50019 Sesto Fiorentino, Florence, Italy

The FORM must be received by **April 15, 2005** for accommodation and by **June 30, 2005** for tours reservation

Personal Data

Prof. Dr. Mr Mrs Ms

Family Name _____

First Name _____

Male Female Date of Birth _____

Organization or Institution _____

Department _____

Institution Address _____ State _____

Zip/Postal Code _____ City _____ Country _____

Phone _____ Fax _____

Email _____

Accommodation in Florence Hotel

All requests must be accompanied by a deposit (Max rate), as specified in the table below, plus € 15,00 as agency fees.

Hotel category	Single	Double for Single Use	Double
	min / max	min / max	min / max
5-star	€ 165,00 / € 190,00	€ 190,00 / € 225,00	€ 210,00 / € 275,00
4-star	€ 115,00 / € 150,00	€ 130,00 / € 150,00	€ 130,00 / € 150,00
3-star	€ 70,00 / € 95,00	€ 95,00	€ 95,00
2-star	€ 60,00 / € 80,00	€ 73,00 / € 95,00	€ 100,00 / € 120,00
1-star	€ 40,00 / € 73,00	€ 65,00 / € 85,00	€ 75,00 / € 95,00
Low Cost Accommodation*	€ 25,00 / € 37,00	€ 35,00 / € 47,00	€ 40,00 / € 54,00

*Please note that only a limited number of low cost accommodations are available.

The indicated rates, in Euro, are valid for the period of the congress and include one overnight stay, continental breakfast, taxes, V.A.T. Breakfast is not included for one star and low cost accommodation. The deposit must be paid by April 15, 2005 and the balance will be paid directly to the hotel. The hotel will issue a receipt of payment inclusive of deposit. Single rooms are available in a very limited number and they will be assigned on a first-come first-served basis. If not available, the Organizing Secretariat will assign double rooms for single use.

I reserve:

n. _____ single room/s or double for single occupancy room/s

n. _____ double room/s

I wish to share the room with _____

n. _____ triple room/s

I wish to share the room with _____

I wish to share the room with _____

Hotel **** Hotel *** Hotel ** Hotel * Low Cost Accommodation

Arrival Date _____ Departure Date _____ N. of nights _____

Deposit € _____ per n. _____ of rooms € _____

Agency fee € _____ 15,00

Total Reservation Deposit € _____

ACCOMMODATION AND TOURS FORM



Further Information

- Smoking Room Room for disabled person Difficulty in moving Food restriction
- Other comments

Optional Tours

					Total
<input type="checkbox"/>	Tour n. _____	€ _____	per n. of participants _____	€ _____	_____
<input type="checkbox"/>	Tour n. _____	€ _____	per n. of participants _____	€ _____	_____
<input type="checkbox"/>	Tour n. _____	€ _____	per n. of participants _____	€ _____	_____
<input type="checkbox"/>	Tour n. _____	€ _____	per n. of participants _____	€ _____	_____
<input type="checkbox"/>	Tour n. _____	€ _____	per n. of participants _____	€ _____	_____
<input type="checkbox"/>	Tour n. _____	€ _____	per n. of participants _____	€ _____	_____

Total € _____

Payment

Payments in Euro should be made in favour of **Newtours S.p.A.**

Hotel reservation deposit: _____

Optional tours: _____

Total amount: _____

Method of payment

- Credit Card
 - Visa MasterCard Diners American Express

Number _____ Expiry Date _____ (Month/Year)
 Name as shown on Card _____

Signature _____

- Bank Transfer

With your name and address indicated. If payment is made for more than one person or by a company, please make sure all names are indicated. Please forward bank transfer to:

Newtours S.p.A.
 BANCA INTESA / Bci S.p.A. – Div. Cariplo
 Florence branch, Viale Gramsci 39/41
 Account number : 000000078158
 SWIFT: BIC: B C I T I T 3 3 4 5 7
 IBAN: IT30 Y030 6902 8200 0000 0078 158

Bank charges are the responsibility of the payee and should be paid at source in addition to the registration fee.

- Cheque - Payable to Newtours S.p.A.

For cancellation policy, see the Program

For Italian participants only

According to art. 10/law 675/96, Newtours S.p.A. is authorized to use personal data for purposes connected to the Congress Management.

I agree

- Yes Not

Date _____

Signature _____