**Workshops**

**IUCr 2011 XAFS Tutorial for Crystallographers and Beginners**  
Time: 9:30-18:25 - Room: Madrid  
Organizers: Isabella Ascone & Joaquín García Ruiz

**Current Research on Molecular Structures and Chemical Properties – A Young Perspective**  
Time: 9:30-18:25 - Room: Amsterdam  
Organizers: Teresa Duarte, Fernando J. Lahoz & Peter Wood

**Opening Ceremony**

Time: 18:30-19:20 - Room: Auditorium A

**Ewald Prize Lectures**

Time: 19:30-20:30 - Room: Auditorium A

- **EL - (CI) - Carmelo Giacovazzo:**  
  About the VLD phasing approach and the variance of electron density maps

- **Eleanor Dodson:**  
  Fifty Years on; a personal view of progress in large molecule crystallography.

- **George M. Sheldrick:**  
  A very short history of SHELX

**Welcome reception**

Time: 20:30-22:00 - Place: Hall Auditorium A
Morning Session 09:00-09:50

Auditorium A (PL 1)

PL01 (C1) – Thomas A. Steitz (Nobel Laureate):
FBBVA Conferences
From the Structure and Function of the Ribosome to New Antibiotics
Chair: Sine Larsen

Afternoon Session 17:40-18:30

Auditorium A (KN 1)

KN01 (C5) - Tomitake Tsukihara:
Structural studies of macromolecular assemblies playing roles in transportation
Chair: Yasushi Kai

Roma (KN 2)

KN02 (C5) - John C.H. Spence:
Time-resolved nanocrystallography with X-ray lasers
Chair: Keith Hodgson

Auditorium B (KN 3)

KN03 - Davide Proserpio:
Topological characterization of coordination networks & metalorganic frameworks
Chair: Omar M. Yaghi
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<thead>
<tr>
<th>Time</th>
<th>Auditorium A (MS01)</th>
<th>Auditorium B (MS02)</th>
<th>Roma (MS03)</th>
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<tbody>
<tr>
<td>10:15-10:20</td>
<td><strong>Opening Remarks</strong></td>
<td><strong>Opening Remarks</strong></td>
<td><strong>Polymer and Gel Structure:</strong></td>
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<td></td>
<td><strong>Hot Structures in Biology I</strong></td>
<td><strong>Hybrid Methods: the EM-Crystallography Interface</strong></td>
<td><strong>Arriving at a Structural Model</strong></td>
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<tr>
<td>10:20-10:50</td>
<td><strong>MS.01.1 (C23)</strong> <strong>O. Daumke:</strong> Structure, oligomerization and mechanism of dynamin superfamily proteins</td>
<td><strong>RS.02.1 (C24)</strong> <strong>R. Beckmann:</strong> Cryo–EM of the ribosome–SecYEG complex in nanodiscs</td>
<td><strong>MS.03.1 (C26)</strong> <strong>I. W Hamley:</strong> Structure and self-assembly of amyloid peptide-based hydrogelators</td>
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<tr>
<td>10:50-11:20</td>
<td><strong>MS.01.2 (C23)</strong> <strong>E. Skordalakes:</strong> Telomerase structure function</td>
<td><strong>MS.02.2 (C25)</strong> <strong>J. E. Johnson:</strong> Dynamics and stability in virus maturation: mechanisms of a molecular machine</td>
<td><strong>MS.03.2 (C26)</strong> <strong>S. R. Raghavan:</strong> Crystalline vs Amorphous molecular gels: two distinct classes of self-assembled structures with unique biological connections</td>
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<tr>
<td>11:20-11:50</td>
<td><strong>MS.01.3 (C23)</strong> <strong>D. Barford:</strong> Structural basis of the anaphase promoting complex</td>
<td><strong>MS.02.3 (C25)</strong> <strong>Z. Hong Zhou:</strong> Lessons learned from the cryoEM and x-ray structures of the human adenovirus</td>
<td><strong>MS.03.3 (C27)</strong> <strong>J.H. van Esch:</strong> Dynamic covalent molecular gelators: in control of soft matter properties by dynamic covalent chemistry</td>
</tr>
<tr>
<td>11:50-12:20</td>
<td><strong>MS.01.4 (C23)</strong> <strong>F. Forneris:</strong> Complement convertase formation based on the structures of C3b in complex with factors B and D</td>
<td><strong>MS.02.4 (C25)</strong> <strong>I. G. Muñoz:</strong> Crystal structure of the open conformation of the mammalian chaperonin CCT in complex with tubulin</td>
<td><strong>MS.03.4 (C27)</strong> <strong>G. O. Lloyd:</strong> The relationship between crystallisation and gel formation in low molecular weight gelators</td>
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<td>12:20-12:50</td>
<td><strong>MS.01.5 (C24)</strong> <strong>G. Phan:</strong> Crystal structure of the Usher:Chaperone:Adhesin subunit complex - insights into pilus assembly mechanism</td>
<td><strong>MS.02.5 (C26)</strong> <strong>P. Heuser:</strong> Pattern recognition for modeling in very low resolution density maps</td>
<td><strong>MS.03.5 (C27)</strong> <strong>B. Bagautdinov:</strong> New insights into the polymerization and structural mechanisms of the polydiacetylene DCHD: an X-ray/MEM study</td>
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<tr>
<td>Paris (MS04)</td>
<td>Berlin (MS06)</td>
<td>Londres (MS05)</td>
<td>Madrid (MS07)</td>
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<td><strong>MS.04.1 (C28)</strong>&lt;br&gt;M. Shibayama: Small-angle neutron scattering studies on catalyst ink of fuel cell</td>
<td><strong>MS.06.1 (C32)</strong>&lt;br&gt;A. R. Oganov: Evolutionary crystal structure prediction: method and results</td>
<td><strong>MS.05.1 (C30)</strong>&lt;br&gt;R. Dinnebier: New tools for the analysis of in-situ XRPD data: symmetry mode analysis, parametric rietveld refinement and MEM</td>
<td><strong>MS.07.1 (C32)</strong>&lt;br&gt;R. McGreevy: Pulsed neutron sources for neutron crystallography: new and future capabilities</td>
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<td><strong>MS.04.2 (C28)</strong>&lt;br&gt;J. Doucet: Industrial SAS activities at European facilities ESRF and ILL</td>
<td><strong>MS.06.2 (C32)</strong>&lt;br&gt;A. J. Cruz-Cabeza: In silico crystallisations of organic molecules: what have we learnt?</td>
<td><strong>MS.05.2 (C30)</strong>&lt;br&gt;A.P. Wilkinson: A high energy view of structure in negative thermal expansion materials</td>
<td><strong>MS.07.2 (C34)</strong>&lt;br&gt;J. Feldhaus: Investigation of nanometer structures with soft X-ray FEL radiation at FLASH</td>
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<td><strong>MS.04.3 (C29)</strong>&lt;br&gt;J D Londono: SAXS in support of industrial research at DuPont</td>
<td><strong>MS.06.3 (C33)</strong>&lt;br&gt;M. Habgood: Disorder in organic crystals: modelling and prediction</td>
<td><strong>MS.05.3 (C31)</strong>&lt;br&gt;T. Yagi: Behavior of SiO2 in helium pressure medium</td>
<td><strong>MS.07.3 (C34)</strong>&lt;br&gt;J. N. Galayda: Linac Coherent Light Source: Status and Plans for Expansion†</td>
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<td><strong>MS.04.4 (C29)</strong>&lt;br&gt;A. Allen: SAXS and SANS for industrial materials-by-design</td>
<td><strong>MS.06.4 (C33)</strong>&lt;br&gt;J. van de Streek: Validating Multiple DFT-D methods for crystal-structure prediction</td>
<td><strong>MS.05.4 (C31)</strong>&lt;br&gt;A. D. Fortes: High-pressure polymorphism of ammonia hydrates</td>
<td><strong>MS.07.4 (C34)</strong>&lt;br&gt;T. Tschentscher: X-ray layout and radiation properties of the European XFEL</td>
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<tr>
<td><strong>MS.04.5 (C30)</strong>&lt;br&gt;H. E. A. Brand: In Situ SAXS studies of Jarosite formation</td>
<td><strong>MS.06.5 (C33)</strong>&lt;br&gt;R. de Gelder: IsoQuestCSP: analyzing sets of predicted crystal structures and selecting the true structure</td>
<td><strong>MS.05.5 (C31)</strong>&lt;br&gt;T.-Yee Tan: Structural Evolution of Ca$<em>{0.4}$Sr$</em>{0.4}$Nd$<em>{0.2}$Mn$</em>{1-x}$Cr$_x$O$_3$; 0 ≤ x ≤ 0.2 perovskites</td>
<td><strong>MS.07.5 (C35)</strong>&lt;br&gt;S. C. Capelli: A multi-purpose neutron diffractometer at the ILL: the state-of-the-art of D19</td>
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<td>Time</td>
<td>Auditorium A (MS08)</td>
<td>Auditorium B (MS09)</td>
<td>Roma (MS10)</td>
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<td>15:00-15:05</td>
<td><strong>Opening Remarks</strong></td>
<td><strong>Time</strong></td>
<td><strong>Determination of Ab-Initio Crystal Structures from Powder Diffraction and their Applications in Pharmaceutical Industry</strong></td>
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<td><strong>Large Biological Assemblies</strong></td>
<td><strong>Topological Correlations and Crystal Structure Interconnections</strong></td>
<td><strong>Chairs</strong>: F. Gozzo, M. Tremayne</td>
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<td><strong>Chairs</strong>: A. Leslie, K. Namba, T. Tsukihara</td>
<td><strong>Chairs</strong>: J.G. Eon, H.J. Klein</td>
<td><strong>Chairs</strong>: F. Gozzo, M. Tremayne</td>
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<td><strong>MS.08.1</strong> (C35)</td>
<td><strong>MS.09.1</strong> (C37)</td>
<td><strong>MS.10.1</strong> (C40)</td>
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<td><strong>D. Stock: Molecular basis for rotational switching in the bacterial flagellar motor</strong></td>
<td><strong>MS.09.2</strong> (C38)</td>
<td><strong>C. Gilmore: Solving Structures from Powder Data Using Maximum Entropy and Charge Flipping</strong></td>
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<td>15:35-16:05</td>
<td><strong>MS.08.2</strong> (C36)</td>
<td><strong>MS.09.3</strong> (see MS09.P01, C268)</td>
<td><strong>I. Margiolaki: Macromolecular Powder Diffraction: From Structure to drug</strong></td>
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<td><strong>T. Yeates: Structure and function of protein-based metabolic organelles in bacteria</strong></td>
<td><strong>E. V. Alexandrov: Underlying nets in three-periodic coordination polymers</strong></td>
<td><strong>MS.10.3</strong> (C40)</td>
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<td>16:05-16:35</td>
<td><strong>MS.08.3</strong> (C36)</td>
<td><strong>MS.09.4</strong> (see MS09.P01, C268)</td>
<td><strong>H. Uekusa: Pseudo-polymorphic transition of pharmaceutical crystals revealed by SDPD method</strong></td>
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<td><strong>F. Coulibaly: Unlikely crystals: poxivirus spheroids in vivo crystallization</strong></td>
<td><strong>E. Gobechiya: The role of metal cations as template species in zeolite framework formation</strong></td>
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<td>16:35-17:05</td>
<td><strong>MS.08.4</strong> (C36)</td>
<td><strong>MS.09.4</strong> (C39)</td>
<td><strong>MS.10.4</strong> (C41)</td>
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<td><strong>G. Kurisu: X-ray structure of a functional full-length dynein motor domain</strong></td>
<td><strong>E. Gobechiya: The role of metal cations as template species in zeolite framework formation</strong></td>
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<td>17:05-17:35</td>
<td><strong>MS.08.5</strong> (C37)</td>
<td><strong>MS.09.5</strong> (C39)</td>
<td><strong>A. Mohamed Moustafa: Structure Determination of Barbiturate Derivative Using X-Ray Powder Diffraction</strong></td>
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<tr>
<td>Paris (MS11)</td>
<td>Berlin (MS12)</td>
<td>Londres (MS13)</td>
<td>Madrid (MS14)</td>
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| **Standardization, Validation, and Automation in Modern Biological Small-Angle Scattering**  
*Chairs:* J. Pérez, M. de Oliveira Neto | **Non-Covalent Interactions in Molecular Crystals and Biomolecular Systems under Pressure**  
*Chairs:* S. Parsons, K. Dziubek | **Automation of Data Collection and Remote Control of Experiments**  
*Chairs:* O. Svensson, M. Yamamoto | **Biominerilization and Biomimetic Materials**  
*Chairs:* D. Aquilano, J. Gómez-Morales |
| MS.11.3 (C42) S. Akiyama: Quality Control of Protein Standards for Molecular Mass Determinations by SAXS | MS.12.3 (C44) H. L. S. Wong: Study of Palladium Thioether Complexes at High Pressure | MS.13.3 (C46) K. Hasegawa: Automation and remote access at SPRing-8 MX beamlines | MS.14.3 (C48) B. Pokroy: Intracrystalline-molecule-induced changes in the crystal structure of biogenic and biomimetic calcium carbonates |
| MS.11.5 (C43) N. P Cowieson: The role of conformational change in HIV maturation revealed by SAXS | MS.12.5 (C45) D. Paliwoda: NH···N hydrogen bonds in high-pressure phase of imidazole | MS.13.5 (C47) R. Cooper: Optimising X-ray experiment strategy on-the-fly based on feedback from automated structure solution | MS.14.5 (C48) W. W. Schmahl: Biodiversity of hierarchical architectures and texture in calcite biomaterials |
Crystallography Software Fayre

Time: 10:45-12:15, 13:00-17:00 - Room: Amsterdam
Organizer: Martin Lutz (Utrecht University, The Netherland)

10:45-11:30h Gianluca Cascaraono
“New algorithms and new tools in the suite Il Milione”

11:30-12:15h Patrick McArdle
“Using Oscaill to solve crystal structures and to analyse and present the results”

13:00-14:00h Install Session
Users can contact software authors for help and support with the installation:
  • Il Milione
  • Oscaill
  • ShelXle
  • MoProSuite & MoProViever
  • Olex2

14:00-14:45h Christian B. Hübschle, George M. Sheldrick
“ShelXle - A Qt GUI for SHELXL”

14:45-15:30h Christian Jelsch, Guillot Benoit
“MoProSuite & MoProViever software for charge density refinement or database transfer”

16:15-17:00h Horst Puschmann
“Olex2: Making Crystallography Accessible”

Open Commission Meetings

Time: 13:00-14:50
Commission on Crystal Growth and Characterization of Materials
Room: Berlín
Coordinator: Hanna A. Dabkowska
Commission on Journals
Room: Paris
Coordinators: Gernot Kostorz, Peter Strickland

ECA - Executive Committee

Time: 13:00-14:50 - Room: Buenos Aires

GE3C Executive Committee
(Crystallographic Spanish Association)

Time: 13:00-14:50 - Room: Oslo
ALBA Meeting
Time: 13:00-14:50 - Room: Londres
Opportunities in Macromolecular Crystallography at ALBA Synchrotron
Speakers: Jordi Juanhuix & Jordi Benach

Commercial Meeting
Bruker
Time: 13:30-14:50 - Room: Caracas, Bogotá, La Paz
“Bruker Seminar: Integrated solutions - as individual as your research”

ECA – Special Interest Group Meetings
SIG1
Time: 18:30-19:30 - Room: La Habana
Chair: Keith Wilson

SIG2
Time: 18:30-19:30 - Room: Mónaco
Chair: Bo Brummerstedt Iversen

SIG5 MIC
Time: 18:30-19:30 - Room: Reijkiavik
Chair: Frédéric Hatert

SIG7 MIR
Time: 18:30-19:30 - Room: Dublin
Chair: Susan Bourne

IUCr General Assembly
Time: 19:30-21:30 - Room: Madrid

ECA - General Interest Group – Young Crystallographers
Time: 19:30-21:30 - Room: Paris
Chairs: Laura Roces & Susanne Coles
Morning Session 09:00-09:50

Auditorium A (KN 4)

KN04 (C6) – Peter D. Kwong: Crystallography and HIV-1 Vaccine Design
Chair: David Stuart

Roma (KN 5)

KN05 (C6) – Iris L. Torriani: Structural characterization of applied organic materials and soft matter
Chair: Araceli Flores

Auditorium B (KN 6)

KN06 (C7) – Makoto Fujita: Crystalline Molecular Flasks
Chair: Kumar Biradha

Afternoon Session 17:40-18:30

Auditorium A (KN 7)

KN07 (C7) – Eva Nogales: Microtubule-Kinetochoore Interactions
Chair: Michael Rossmann

Roma (KN 8)

KN08 (C7) – Roberto Fornari: Use of external fields in the melt growth of semiconductors
Chair: Jiyang Wang

Auditorium B (KN 9)

KN09 (C8) – Kei Hirose: Discovery of Post-Perovskite at High Pressure and Its Geophysical Implications
Chair: Przemek Dera

Afternoon Session 18:35-19:25

Auditorium A (PL 2)

PL02 (C1) - Omar M. Yaghi: Heterogeneity within Order in Metal-Organic Frameworks
Chair: M. Angeles Monge
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<th>Auditorium B (MS15)</th>
<th>Roma (MS17)</th>
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<td><strong>Opening Remarks</strong></td>
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<td></td>
<td><strong>Crystallography in Disease and Therapy</strong></td>
<td><strong>Nucleosome Processing and Epigenetics</strong></td>
<td><strong>Synthons: from Small to Macromolecules</strong></td>
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<td><em>Chairs:</em> H. L. Monaco, C. Groom</td>
<td><em>Chairs:</em> D. Rhodes, K. Morikawa</td>
<td><em>Chairs:</em> P. Chakrabarti, C. Abad-Zapatero</td>
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<td>10:50-11:20</td>
<td><strong>MS.16.2 (C51)</strong> E. Sauer-Eriksson: The multiple personalities of transthyretin</td>
<td><strong>MS.15.2 (C49)</strong> S. Eustermann: Combinatorial readout of histone H3 modifications specifies localization of ATRX to heterochromatin</td>
<td><strong>MS.17.2 (C53)</strong> A. Heine: Molecular probes as starting point for structure-based lead development</td>
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<td>11:20-11:50</td>
<td><strong>MS.16.3 (C51)</strong> G. Oliva: Structural biology and medicinal chemistry in neglected diseases of poverty</td>
<td><strong>MS.15.3 (C49)</strong> A. Mattevi: Molecular mimicry in the assembly of chromatin protein complexes</td>
<td><strong>MS.17.3 (C53)</strong> K. Biradha: Supramolecular synthons in crystal engineering</td>
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<td>12:20-12:50</td>
<td><strong>MS.16.5 (C52)</strong> C. Naylor: Insights into the Food-Poisoning toxin, <em>Clostridium perfringens</em> enterotoxin</td>
<td><strong>MS.15.5 (C50)</strong> N. Yang: Structure of a CENP-A-histone H4 heterodimer in complex with chaperone HJURP</td>
<td><strong>MS.17.5 (C54)</strong> T. Gelbrich: The $XPac$ dissimilarity index as a quantitative descriptor of isostructurality</td>
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<td>Paris (MS18)</td>
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<td>Londres (MS20)</td>
<td>Madrid (MS21)</td>
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<td><strong>Powder Diffraction at the Nanoscale</strong></td>
<td><strong>Synthesis, Structure and Properties of Novel Materials at High Pressure</strong></td>
<td><strong>Beyond Space-Group Symmetry in Periodic Structures</strong></td>
<td><strong>Surfaces &amp; Interfaces</strong></td>
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<td><strong>Chairs:</strong> A. Guagliardi, Y. Andreev</td>
<td><strong>Chairs:</strong> O. Degtyareva, V. García Baonza</td>
<td><strong>Chairs:</strong> M. Pasero, B. Souvignier</td>
<td><strong>Chairs:</strong> U. Pietsch, M. Varela del Arco</td>
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<td>MS.18.1 (C54)</td>
<td>MS.19.1 (C56)</td>
<td>MS.20.1 (C58)</td>
<td>MS.21.1 (C60)</td>
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<td>V. Petkov: Structure of nanosized crystals by total x-ray diffraction</td>
<td>V. L. Solozhenko: High-pressure synthesis, structure and properties of novel superhard phases</td>
<td>C. Ferraris: Disordered and incommensurate crystal structures by transmission electron microscopy - some examples</td>
<td>A. B. Shah: Interfaces of lanthanum and strontium manganite superlattices</td>
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<tr>
<td>MS.18.2 (C54)</td>
<td>MS.19.2 (C56)</td>
<td>MS.20.2 (C59)</td>
<td>MS.21.2 (C60)</td>
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<tr>
<td>D. A. Keen: Contrasting $p$ and $T$-induced amorphization using ZrW$_2$O$_8$ and ZIF-4 as case studies</td>
<td>J. Haines: Amorphization, insertion and reactions in microporous materials at high pressure</td>
<td>J.M. Pérez-Mato: Symmetry considerations in commensurate and incommensurate multiferroic materials</td>
<td>S. Grenier: Interfacial magnetism by resonant X-ray reflectivity</td>
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<td>MS.18.3 (C55)</td>
<td>MS.19.3 (C57)</td>
<td>MS.20.3 (C59)</td>
<td>MS.21.3 (C61)</td>
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<td>MS.18.4 (see MS18.P02, C321)</td>
<td>MS.19.4 (C57)</td>
<td>MS.20.4 (C59)</td>
<td>MS.21.4 (C61)</td>
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<tr>
<td>D. Schaniel: Identification of single photoswitchable molecules in nanopores of silica xerogels using neutron powder diffraction</td>
<td>C. Sanloup: Xe-H$_2$O compound synthesized at extreme conditions</td>
<td>P. Kocian: The Lie group of translations: a unified way for describing structures, modulated or not</td>
<td>A. Vasiliev: High resolution STEM study of InGaAs/InAlAs and Si/Ge heterostructures</td>
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<td>MS.18.5 (C55)</td>
<td>MS.19.5 (C58)</td>
<td>MS.20.5 (C60)</td>
<td>MS.21.5 (C61)</td>
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<td>A. Cervellino: Debye function analysis on disordered metal-organic compounds: the pathfinder $[Ru/(CO)]_{10}$</td>
<td>N. Hirao: Structural, magnetic and electrical properties of iron-hydride</td>
<td>M.L. N. de las Penas: On subgroups of hyperbolic crystallographic groups</td>
<td>K. H. Stone: Spatial resolution of electronic structure through modeling reflectivity spectra</td>
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<td>Time</td>
<td>Auditorium A (MS22)</td>
<td>Auditorium B (MS23)</td>
<td>Roma (MS24)</td>
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<td>15:00-15:05</td>
<td><strong>Opening Remarks</strong></td>
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<td>New Challenges in Crystal Engineering: Correlating Structure and Properties</td>
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<td>15:05-15:35</td>
<td><em>Cell Signalling and Protein-Protein Interactions</em></td>
<td><em>Difficult Phasing and Difficult Structures</em></td>
<td><em>M. Wais Hosseini: Molecular tectonics: Design of enantiomerically pure tubular crystals</em></td>
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<td><em>Chairs:</em> M. Parker, M.V. Hosur</td>
<td><em>Chairs:</em> P. Evans, M. Weiss</td>
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<td></td>
<td>MS.22.1 (C62) S. A. Teichmann: Evolution and dynamics of protein complexes</td>
<td>MS.23.1 (C64) B.C. Wang: Recent efforts on phase determination by S-SAD</td>
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<td>MS.23.2 (C64) A. Lebedev: Macromolecular OD-structures</td>
<td>MS.24.2 (C66) G. Resnati: Fluorocarbon control of crystal structures: NLO materials and supramolecular LCs</td>
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<tr>
<td>15:35-16:05</td>
<td>MS.22.2 (C62) J. W. Wu: Structural insight into the regulation of AMP-activated protein kinase</td>
<td>MS.23.3 (C64) R. J. Read: Extending the limits in solving and rebuilding molecular replacement structures</td>
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<td>16:05-16:35</td>
<td>MS.22.3 (C62) C. L. Gee: A pseudokinase mediates cell wall integrity in <em>Mycobacterium Tuberculosis</em></td>
<td>MS.23.4 (C65) B. Franke: Phasing of an unpredicted palindromic coiled-coil motif</td>
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<td></td>
<td>MS.22.4 (C63) C. B. Folsted Andersen: Structural basis for vitamin B&lt;sub&gt;12&lt;/sub&gt; uptake</td>
<td>MS.23.5 (C65) S. Panjikar: S-SAD phasing of protein α-fucosyltransferase-1 at a resolution of 2.6 Å in the monoclinic space group C2</td>
<td></td>
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<tr>
<td>16:35-17:05</td>
<td>MS.22.5 (C63) Y. Hirano: Structural basis of cargo recognition by the myosin-X MyTH4-FERM domain</td>
<td>MS.24.4 (C66) C. B. Aakerøy: From molecules, via supramolecular assembly, to tunable physical properties</td>
<td></td>
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<tr>
<td></td>
<td>MS.22.6 (C63) Y. Hirano: Structural basis of cargo recognition by the myosin-X MyTH4-FERM domain</td>
<td>MS.24.5 (C67) S. Varughese: Probing mechanical anisotropy in molecular crystals using nanoindentation methods</td>
<td></td>
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<tr>
<td>Paris (MS25)</td>
<td>Berlin (MS26)</td>
<td>Londres (MS27)</td>
<td>Madrid (MS28)</td>
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<tr>
<td><strong>Crystallography of Materials with Exchange, Sequestration and Storage Properties</strong>&lt;br&gt;<em>Chairs:</em> T. Albrecht-Schmitt, E. Bonaccorsi&lt;br&gt;<em>In memoriam of Prof. F. Liebau</em></td>
<td><strong>SAXS/SANS, Total Scattering and the Nanostructure Problem</strong>&lt;br&gt;<em>Chairs:</em> S. Billinge, M.V. Avdeev</td>
<td><strong>Developments and Directions for Crystallographic Databases</strong>&lt;br&gt;<em>Chairs:</em> S. Gražulis, J. Westbrook</td>
<td><strong>Wide Band Semiconductor and Other Crystals Used in Optoelectronics</strong>&lt;br&gt;<em>Chairs:</em> E. Talik, E. Calleja</td>
</tr>
<tr>
<td>MS.25.2 (C68) A. M. Fogg: Synthesis and structures of new layered and framework anion exchangeable hydroxides</td>
<td>MS.26.2 (C70) D. I. Svergun: Analysis of isotropic nanostructured systems using SAS</td>
<td>MS.27.2 (C72) H. M. Berman: The wwPDB and Future perspectives in sharing macromolecular data</td>
<td>MS.28.2 (C73) V. Holý: Diffuse x-ray scattering from defects in GaN epitaxial layers</td>
</tr>
<tr>
<td>MS.25.3 (C68) W. Depmeier: LHT-9: layered nano-material with reductive adsorption and exchange properties</td>
<td>MS.26.3 (C70) U. Jeng: Competition between PCBM Aggregation and P3HT crystallization in thin films upon annealing</td>
<td>MS.27.3 (C72) C. R Groom: Possible futures for small molecule crystal structure archives?</td>
<td>MS.28.3 (C74) M. D Fontana: Lithium niobate: a smart material for various applications in optoelectronics</td>
</tr>
</tbody>
</table>
Crystallography Software Fayre

Time: 10:00-12:15, 13:00-17:00
Room: Amsterdam
Organizer: Martin Lutz (Utrecht University, The Netherlands)

10:00-10:45h Simonov Arkadiy
“Presentation of (yet unnamed) program for diffuse scattering solution with 3D PDF method”

10:45-11:30h Michal Chodkiewicz
“ZODS: a software for modeling diffuse scattering”

11:30-12:15h Loes Kroon-Batenburg
“Using EVAL to solve complicated diffraction problems”

13:00-14:00h Install Session
Users can contact software authors for help and support with the installation:
- Arkadiy's software
- ZODS
- EVAL
- ISODISTORT
- SIR2011
- XRD2Dscan

14:00-14:45h Branton J. Campbell, Harold T. Stokes
“ISODISTORT”

14:45-15:30h Carmelo Giacovazzo
“The VLD (Vive La Difference) algorithm: a new tool in SIR2011 for phasing, from small structures up to proteins”

15:30-16:15h Alejandro Rodriguez Navarro
“Use of XRD2Dscan software for the characterization of polycrystalline materials from 2D X-ray diffraction patterns”

Open Commission Meetings

Time: 13:00-14:50

Commission on Mathematical and Theoretical Crystallography
Room: Berlin
Coordinator: Massimo Nespolo

Commission on Structural Chemistry
Room: Madrid
Coordinator: Alessia Bacchi

Commission on Inorganic & Mineral Structures
Room: Paris
Coordinator: Wulf Depmeier

Commission on Crystallography in Art and Cultural heritage
Room: Roma
Coordinator: Eric Dooryhee
ECM28-Warwick Programme Committee Meeting
Time: 13:00-14:00 - Room: Oslo
Organizers: Alexander Blake

ECA Individual Members Meeting
Time: 13:00-14:50 - Room: Londres

ECA - Executive Committee
Time: 13:00-14:50 - Room: Buenos Aires

ECA – Special Interest Group Meetings
SIG4
Time: 13:00-14:50 - Room: Mónaco
Chair: Louisa Meshi

SIG6 IET
Time: 13:00-14:50 - Room: Reijkiavik
Chair: Jean-Louis Hodeau

SIG8
Time: 13:00-14:50 - Room: Dublin
Chair: Paolo Scardi

CCDC/CSD Forum
Time: 13:00-14:50 - Room: Bratislava
“Cambridge Structural Database Discussion Forum”

Commercial Meeting
Agilent
Time: 13:50-14:45 - Room: Caracas, Bogotá, La Paz
“Agilent Technologies Single Crystal Seminar”

IUCr General Assembly
Time: 19:30-21:30 - Room: Madrid

Evening Session 1
Time: 19:30-21:30 - Room: Auditorium A
Film: The Mystery of the Giant Crystals
Speaker: Juan Manuel García-Ruiz
**Morning Session 09:00-09:50**

**Auditorium A (KN 10)**

**KN10 (C8) – Ian A. Wilson:**
Exploration of the Protein Universe with High Throughput Structural Biology

Chair: **Helen Berman**

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**Roma (KN 11)**

**KN11 (C9) - Yaroslav Filinchuk:**
Energy related materials: borohydrides

Chair: **Bjorn Hauback**

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**Auditorium B (KN 12)**

**KN12 (C9) - Alessia Bacchi:**
Crystal engineering of flexible metallorganic networks

Chair: **Guy Orpen**

**Afternoon Session 17:40-18:30**

**Auditorium A (KN 13)**

**KN13 (C10) - Juan A. Hermoso:**
Bacterial pathogenesis and peptidoglycan degradation machines

Chair: **Rita Berisio**

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**Roma (KN 14)**

**KN14 (C10) - Ian Robinson:**
Coherence in crystallography for imaging materials and biology

Chair: **Laurence Marks**

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**Auditorium B (KN 15)**

**KN15 (C10) - Len Barbour:**
Structure-Property Relationships of Inclusion Compounds

Chair: **Santiago García-Granda**
<table>
<thead>
<tr>
<th>Time</th>
<th>Auditorium A (MS29)</th>
<th>Auditorium B (MS30)</th>
<th>Roma (MS31)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10:15-10:20</td>
<td>Viruses and Viral Proteins</td>
<td>Diffuse Scattering in Partially Ordered/Disordered Systems</td>
<td>Structural Implications in Catalytic Processes</td>
</tr>
<tr>
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<td><em>Chairs</em>: Fasseli Coulibaly, Ying-Fang Liu</td>
<td><em>Chairs</em>: Thomas Weber, Ernesto Estevez Rams</td>
<td><em>Chairs</em>: María José Calhorda, Jorge Rodríguez-Navarro</td>
</tr>
<tr>
<td>11:20-11:50</td>
<td>MS.29.3 (C76) F. A. Rey: The cell fusion proteins of the “FF” family are homologous to class II viral fusion proteins</td>
<td>MS.30.3 (C78) D. J. Goossens: Diffuse scattering from molecular crystals</td>
<td>MS.31.3 (C80) B. Stec: Trapping and visualization of catalytic intermediates</td>
</tr>
<tr>
<td>11:50-12:20</td>
<td>MS.29.4 (C76) M. Kvansakul: Structural basis for the inhibition of apoptosis by Epstein-Barr virus BHRF1</td>
<td>MS.30.4 (C78) D. Chernyshov: A new model of correlated disorder in relaxor ferroelectrics</td>
<td>MS.31.4 (C80) C. Weidenthaler: Catalytic decomposition of ammonia monitored by in situ X-ray diffraction studies</td>
</tr>
<tr>
<td>12:20-12:50</td>
<td>MS.29.5 (C76) L. Castillo: Crystal structure of the N-terminal domain of HIV-1 capsid in complex with an assembly-inhibiting nanobody</td>
<td>MS.30.5 (C78) L. Guérin: Diffuse scattering in one dimensional “liquid-like” aperiodic composites</td>
<td>MS.31.5 (C80) N. Kamiya: Mechanism of PSII oxygen evolution predicted from its 1.9 Å resolution structure</td>
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<tr>
<td>Paris (MS32)</td>
<td>Berlin (MS33)</td>
<td>Londres (MS34)</td>
<td>Madrid (MS35)</td>
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</table>
| **Crystallography in Industrial Process Control**  
*Chairs:* J. Kaduk, N. Scarlett | **Coherent Diffraction and Imaging**  
*Chairs:* V. Favre-Nicolin, J. Rodenburg | **Descriptors of Electronic Structure and Chemical Bonding**  
*Chairs:* L. J. Farrugia, A. Martín Pendás | **The Growth and Morphology of Crystals**  
*Chairs:* A. Glikin, S. López-Andrés |
| **MS.32.1** (C81)  
J. Neubauer: Rietveld refinement using G-Faktor applied on early OPC hydration | **MS.33.1** (C83)  
O. Kamimura: Low-voltage electron diffractive imaging | **MS.34.1** (C85)  
E. Matito: An account on multicenter bonding and its relationship with aromaticity | **MS.35.1** (C87)  
S. Bocharov: Kinetic anomalies of crystal growth: object, novelty and implication |
| **MS.32.2** (C81)  
D. P. Riley: Materials development; novel applications of time-resolved diffraction | **MS.33.2** (C84)  
M. Allain: Strain at the nanoscale revealed by 3D lensless x-ray microscopy | **MS.34.2** (C85)  
P. Bultinck: The hirshfeld-i method: atoms in molecules and chemical bonding perspective | **MS.35.2** (C88)  
P. Gille: Growth of Al-based quasicrystals and other complex metallic phases |
| **MS.32.3** (C82)  
P. Liu: Nonlinearity in residual stress measurements using X-ray powder diffraction | **MS.33.3** (C85)  
T.B.A: The limits of information content in Ptychographic diffractive imaging | **MS.34.3** (C86)  
G. Eickerling: Relativistic effects on the topology of the electron density | **MS.35.3** (C88)  
A. Fernández-González: Influence of SO$_4^{2-}$ and SeO$_4^{2-}$ on the crystallization of CaCO$_3$; structural and morphological aspects |
| **MS.32.4** (C82)  
R. J. Cernik: The development of rapid tomographic energy dispersive diffraction imaging TEDDI | **MS.33.4** (C84)  
G. Beutier: Coherent x-ray diffraction of copper islands under in situ loading | **MS.34.4** (C86)  
S. Mondal: Electron Deficient and Polycenetric Bonds in $\gamma$-B$_{28}$ | **MS.35.4** (C88)  
E. Griesshaber: Biomimetic calcite crystal nucleation and growth from ACC and PILP amorphous precursors, |
| **MS.32.5** (C83)  
C. P. Buioli: Crystalline texture in Zr based alloys tubes | **MS.33.5** (C85)  
M. B. Luu: Quantitative phase imaging with polychromatic sources | **MS.34.5** (C86)  
J. Overgaard: Core and valence electron density distribution in a Ga$^1$ NHC-analogue | **MS.35.5** (C89)  
L.A. González-Ramírez: Crystallization in gels and microgravity: a comparative study |
<table>
<thead>
<tr>
<th>Time</th>
<th>Auditorium A (MS36)</th>
<th>Auditorium B (MS37)</th>
<th>Roma (MS38)</th>
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<tbody>
<tr>
<td>15:00-15:05</td>
<td><strong>Opening Remarks</strong></td>
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<td></td>
<td>Understanding Bacterial Pathogenesis</td>
<td>X-Ray Lasers and Other New Frontiers in Synchrotron Applications to Structural Science</td>
<td>Fabrication and Macroscopic Properties of Flexible Frameworks</td>
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<tr>
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<td><em>Chairs:</em> J. Chai, D. Heinz, A. Albert</td>
<td><em>Chairs:</em> S. Wakatsuki, J. L. Smith</td>
<td><em>Chairs:</em> M. Hardie, C. Ruiz-Pérez</td>
</tr>
<tr>
<td></td>
<td>MS.36.2 (C90) T. Stehle: Bacterial cell wall degradation by a staphylococcal autolysin</td>
<td>MS.37.2 (C92) C. Song: 3D imaging with coherent X-rays at nano-scale resolution and beyond</td>
<td>MS.38.2 (C93) R. Matsuda: Unusual porous functions of stimuli responsive porous coordination polymers</td>
</tr>
<tr>
<td>16:05-16:35</td>
<td>MS.36.3 (C90) H. J. Kang: Gram-positive bacterial pili: structures, assembly and function</td>
<td>MS.37.3 (C92) A. Ourmazd: Structure and dynamics from random snapshots of heterogeneous ensembles</td>
<td>MS.38.3 (C94) L. J. Cameron: Negative thermal expansion in porous framework materials</td>
</tr>
<tr>
<td>17:05-17:35</td>
<td>MS.36.5 (C91) B. L. Brown: Toxicity and neutralization mechanism of the mqsRA toxin:antitoxin module</td>
<td>MS.37.5 (C93) T. R.M. Barends: Imaging biological molecules using X-FELs</td>
<td>MS.38.5 (C95) A. E. Platero-Prats: The role of synthesis conditions on SBU condensation of Mg polymeric frameworks</td>
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<tr>
<td>Paris (MS39)</td>
<td>Berlin (MS40)</td>
<td>Londres (MS41)</td>
<td>Madrid (MS42)</td>
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</tbody>
</table>
| **Energy-Related Materials**  
*Chairs:* W. I.F. David,  
R. Palacín | **Pressure-Induced Phase Transitions**  
*Chairs:* V. Brazhkin,  
K. Friese | **Advanced Approaches in Charge Density Analysis and Derived Properties**  
*Chairs:* N. Bouhmaida,  
C. Jelsch | **XAFS Studies in Biology Coupled to Crystallography**  
*Chairs:* F. Jalilehvand,  
S. Díaz-Moreno |
| **MS.39.1** (C95)  
M. Bowden: The structure and dynamics of hydrogen storage materials based on boron and nitrogen | **MS.40.1** (C97)  
K. Takemura: Pressure-induced phase transitions in Na-Au intermetallic compounds | **MS.41.1** (C99)  
A. Martín Pendás: Is a more predictable QTAIM possible? | **MS.42.1** (C101)  
V. K. Yachandra: Polarized XAS of photosystem II and relevant Mn model complexes |
| **MS.39.2** (C95)  
C. Masquelier: Synchrotron x-rays and neutrons as essential tools in Li battery research: new structures and new properties of LiFePO4-based cathodes | **MS.40.2** (C98)  
W. A. Crichton: Making use of topological similarities in HP structures | **MS.41.2** (C99)  
E. Espinosa: Halogen bonding from charge density analysis | **MS.42.2** (C101)  
W. Meyer-Klaucke: The synergism of XAS and crystallography |
| **MS.39.3** (C96)  
L. Suescun: A new homologous series of oxygen vacancy ordered strontium manganese perovskite | **MS.40.3** (C98)  
E. Kudrenko: The origin of memory glass effect in pressure amorphized rare earth molybdates | **MS.41.3** (C100)  
P. Becker: Joint densities and density matrices refinements: First attempts and first results | **MS.42.3** (C102)  
B. Hedman: Single Crystal XAS Studies on Transient Metalloprotein Intermediates |
| **MS.39.4** (C96)  
D. Viterbo: Polyene-diphenylaniline D5 dyes and their role in the efficiency of DSSC solar cells | **MS.40.4** (C99)  
J. Ruiz-Fuertes: Multiferroic CuWO4 under pressure: Comparison of PXRD and SXRD studies | **MS.41.4** (C100)  
J. M. Bąk: Quantitative information on polarization of ED from multipolar model – possible? | **MS.42.4** (C102)  
V. A. Streltsov: Structural studies of Amyloid-β oligomerization and metal binding in Alzheimer’s disease |
| **MS.39.5** (C97)  
C. Stephan: The cation distribution in off stoichiometric CuInSe2 and CuGaSe2 | **MS.40.5** (C99)  
B. Boates: Phase transitions in carbon dioxide at high pressures and temperatures | **MS.41.5** (C101)  
P. N. H. Nakashima: Chemical bonds in aluminium | **MS.42.5** (C103)  
A. Díaz-Quintana: Metal-protein interplay in protein function and stability |
Crystallography Software Fayre

Time: 10:00-12:15, 13:00-17:00 - Room: Amsterdam
Organizer: Martin Lutz (Utrecht University, The Netherland)

10:00-10:45h Reinhard Neder, Thomas Proffen
“DISCUS: program to simulate crystals, especially disordered crystals and nanoparticles and to calculate the corresponding diffraction pattern”

10:45-11:30h Richard Cooper
“CRYSTALS: An Introduction and Some Recent Enhancements”

11:30-12:15h Stuart McNicholas
“The CCP4 Molecular Graphics Program: CCP4MG”

13:00-14:00h Install Session
Users can contact software authors for help and support with the installation:
- DISCUS
- CRYSTALS
- CCP4MG
- DRAWxtl
- Python for Crystallographers
- MAX3D
- XPac

14:00-14:45h Martin Kröker, Brian Toby
“DRAWxtl”

14:45-15:30h Ralf W. Grosse-Kunstleve
“Python for Crystallographers”

15:30-16:15h Jim Britten
“Tutorial on MAX3D”

16:15-17:00h Thomas Gelbrich
“XPac - Comparison of molecular crystal structures”

Open Commission Meetings

Time: 13:00-14:50
Commission on International Tables
Room: Berlin
Coordinators: Carolyn P. Brock, Peter Strickland

Commission on Crystallography in Art and Cultural heritage
Room: Roma
Coordinator: Eric Dooryhee

ECA Meetings

ECA - Council Meeting
Time: 13:00-14:50 - Room: Bratislava
Thursday, August, 25 - Other Activities

Commercial Meeting
Dectris
Time: 13:00-14:45 - Room: Caracas, Bogotá, La Paz
“DECTRIS Seminars”

PDB Forum
Time: 13:40-14:40 - Room: Paris
Organizer: Christine Zardecki
“Protein Data Bank Q & A: Learn about the latest developments and projects from the wwPDB directors”

ECA – Special Interest Group Meetings
SIG9
Time: 18:30-19:30 - Room: La Habana
Chair: Harry Powell

SIG11
Time: 18:30-19:30 - Room: Mónaco
Chair: Leonid Dubrovinsky

SIG12
Time: 18:30-19:30 - Room: Reijkiavik
Chair: Helmut Ehrenberg

SIG13
Time: 18:30-19:30 - Room: Dublin
Chair: Fernando J. Lahoz

Musical Event
Time: 19:30-19:30 - Room: Auditorium A
Ballet Folclórico de Madrid
### Morning Session 09:00-09:50

**Auditorium A (KN 16)**

**KN16 (C11) – Gerard J. Kleywegt:**
Validation and errors in protein structures  
Chair: **Gert Vriend**

**Roma (KN 17)**

**KN17 (C11) - Helmut Cölfen:**
Prenucleation clusters and crystallization control by additives  
Chair: **Juan Manuel García Ruiz**

**Auditorium B (KN 18)**

**KN18 (C12) - Stephen J. Pennycook:**
Atomic-resolution Real-space Imaging and Aberration Corrected Electron Microscopy  
Chair: **Carlos Otero**

### Afternoon Session 17:40-18:30

**Auditorium A (KN 19)**

**KN19 (C12) - Xiaoliang Sunney Xie:**
Life at the single molecule level  
Chair: **Ignacio Tinoco**

**Roma (KN20)**

**KN20 (125) - Emil Makovicky:**
From plane groups to quasilattices: Hispano-Islamic art of the Alhambra, Cordoba and Sevilla  
Chair: **Henk Schenk**

**Auditorium B (KN 21)**

**KN21 (C13) - Bo Brummerstedt Iversen:**
Charge densities and materials crystallography  
Chair: **Carlo Gatti**
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<thead>
<tr>
<th>Time</th>
<th>Auditorium A (MS43)</th>
<th>Auditorium B (MS45)</th>
<th>Roma (MS44)</th>
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</thead>
<tbody>
<tr>
<td>10:15-10:20</td>
<td>Validation, Error Detection and Fraud Prevention</td>
<td>Dynamical Structural Science</td>
<td>Quantitative Real Space Electron Imaging</td>
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<td></td>
<td><em>Chairs:</em> E. Dodson, I. Bruno</td>
<td><em>Chairs:</em> P. Naumov, E. Collet</td>
<td><em>Chairs:</em> S. Van Aert, A. Landa</td>
</tr>
<tr>
<td>10:50-11:20</td>
<td>MS.43.2 (C104) S. Gore: Validation of small- and macro-molecular X-ray structures: PDB and CCDC collaborations</td>
<td>MS.45.2 (C108) D. M. Fritz: Measuring femtosecond structural dynamics at a hard X-ray laser: challenges and successes</td>
<td>MS.44.2 (C106) M. Hýtch: Measuring lattice distortions from HR(S)TEM images</td>
</tr>
<tr>
<td>11:20-11:50</td>
<td>MS.43.3 (C104) B. Rupp: The most powerful crystallographic validation tool: Common sense</td>
<td>MS.45.3 (C108) S. Techert: Structural dynamics of proteins conformers and conformer selection in chemical reactions</td>
<td>MS.44.3 (C106) H. Y. Jeong: Structures of catalytically important nano-structured materials revealed by TEM</td>
</tr>
<tr>
<td>11:50-12:20</td>
<td>MS.43.4 (C104) O. V. Sobolev: Unrestrained reciprocal space refinement can indicate alternative conformations</td>
<td>MS.45.4 (C108) P. Coppens: Single-pulse laue TR diffraction: Methods, results and use of QM/MM theory</td>
<td>MS.44.4 (C106) J. Etheridge: Imaging a sub-Ångström electron beam after scattering in a crystal</td>
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<tr>
<td>Paris (MS46)</td>
<td>Berlin (MS47)</td>
<td>Londres (MS48)</td>
<td>Madrid (MS49)</td>
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<tr>
<td><strong>Powder Diffraction</strong>&lt;br&gt;<strong>Methods in Archaeometry</strong>&lt;br&gt;<strong>Chairs:</strong> G. Artioli, P. Bezdicka</td>
<td><strong>Advances in High Pressure Techniques and Instrumentation</strong>&lt;br&gt;<strong>Chairs:</strong> C. Tulk, G. Aquilanti</td>
<td><strong>Electron Momentum and Spin Densities in Correlated Electron Systems</strong>&lt;br&gt;<strong>Chairs:</strong> B. Barbiellini, M. Ito</td>
<td><strong>Crystal Growth and Interface Phenomena at Nanoscale</strong>&lt;br&gt;<strong>Chairs:</strong> K. Tsukamoto, J. De Yoreo</td>
</tr>
<tr>
<td><strong>MS.46.1</strong> (C109)&lt;br&gt;C. Cardell: X-ray diffraction methods as a complementary tool for analyses of historical objects</td>
<td><strong>MS.47.1</strong> (C111)&lt;br&gt;F. Decremps: Structure and elasticity of single-crystals by phonon imaging at high pressure</td>
<td><strong>MS.48.1</strong> (C113)&lt;br&gt;S. B Dugdale: Probing the electronic structure of correlated electron systems with synchrotron light</td>
<td><strong>MS.49.1</strong> (C115)&lt;br&gt;H. Yamada: Molecular-scale 3D visualization of solid-liquid interfaces by FM-AFM</td>
</tr>
<tr>
<td><strong>MS.46.2</strong> (C110)&lt;br&gt;P. Martinetto: Synthetic or manufactured ancient pigments studied by means of synchrotron radiation–based methods</td>
<td><strong>MS.47.2</strong> (C112)&lt;br&gt;M. Guthrie: High-pressure neutron diffraction at the SNS</td>
<td><strong>MS.48.2</strong> (C114)&lt;br&gt;M. Okube: Resonant X-Ray Magnetic Scattering for transition-metal ferrites</td>
<td><strong>MS.49.2</strong> (C116)&lt;br&gt;F. M. Ross: Step flow and interface structure during the growth of semiconductor nanowires</td>
</tr>
<tr>
<td><strong>MS.46.3</strong> (C110)&lt;br&gt;F. Grazzi: Quantitative characterization of Japanese ancient swords through time of flight neutron diffraction and energy resolved neutron imaging</td>
<td><strong>MS.47.3</strong> (C112)&lt;br&gt;C. Dejoie: Towards the use of Laue microdiffraction intensities for structural studies at extreme conditions</td>
<td><strong>MS.48.3</strong> (C114)&lt;br&gt;A. Bansil: High resolution compton scattering as a new tool for imaging dopants and probing metal-insulator transitions</td>
<td><strong>MS.49.3</strong> (C116)&lt;br&gt;N. A. J. M. Sommerdijk: Transient phases and prenucleation clusters in biomimetic calcium phosphate mineralization</td>
</tr>
<tr>
<td><strong>MS.46.4</strong> (C111)&lt;br&gt;C. Gervais: Estimation of iron valencies of Prussian blue pigment by anomalous X-ray diffraction</td>
<td><strong>MS.47.4</strong> (C113)&lt;br&gt;A. Burkhardt: High pressure freezing of protein crystals</td>
<td><strong>MS.48.4</strong> (C115)&lt;br&gt;A. I. Baranov: Metal-insulator transitions: a real space picture</td>
<td><strong>MS.49.4</strong> (C117)&lt;br&gt;J. Morales: Nanoscopic characteristics of anhydrite (100) surface growth under mild hydrothermal conditions</td>
</tr>
<tr>
<td><strong>MS.46.5</strong> (C111)&lt;br&gt;A. Rafalska-Lasocha: XRPD studies of the objects of cultural heritage made of copper or its alloys</td>
<td><strong>MS.47.5</strong> (C113)&lt;br&gt;H. Liu: Synchrotron X-ray diffraction tomography technique using diamond anvil cell</td>
<td><strong>MS.48.5</strong> (C115)&lt;br&gt;Y Sakurai: Spin-wise decomposed compton profiles</td>
<td><strong>MS.49.5</strong> (C117)&lt;br&gt;Y. Kimura: Double wavelength interferometry for direct observation of homogeneous nucleation in vapor phase</td>
</tr>
<tr>
<td>Time</td>
<td>Auditorium A (MS50)</td>
<td>Auditorium B (MS51)</td>
<td>Roma (MS53)</td>
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<tr>
<td>15:00-15:05</td>
<td><strong>Opening Remarks</strong></td>
<td><strong>Complementary Biophysical Methods: Adding Value to Protein Structures</strong></td>
<td><strong>High-Throughput Crystallization and Polymorphic Search in Pharmaceuticals</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Chairs:</strong> D. M. Salunke, Y. Jones</td>
<td><strong>Chairs:</strong> N. Cowieson, D. Beckett</td>
<td><strong>Chairs:</strong> U. Griesser, S. M. Reutzel-Edens</td>
</tr>
<tr>
<td>15:05-15:35</td>
<td><strong>MS.50.1 (C118)</strong> D. M. Zajonc: Microbial glycolipid antigen recognition by invariant natural killer T cells</td>
<td><strong>MS.51.1 (C120)</strong> R. Loris: Mechanism of transcription regulation by conditional co-operativity</td>
<td><strong>MS.53.1 (C124)</strong> J. Rantanen: High-throughput crystallization as a part of streamlined drug development</td>
</tr>
<tr>
<td>15:35-16:05</td>
<td><strong>MS.50.3 (C118)</strong> P. Gros: Mechanistic insights into the complement system</td>
<td><strong>MS.51.3 (C120)</strong> J. Cherfils: What makes homologous small GTPases specific? A combined X-ray, SAXS &amp; NMR study</td>
<td><strong>MS.53.3 (C125)</strong> D E. Braun: Does computational work help in solid form screening?</td>
</tr>
<tr>
<td>16:35-17:05</td>
<td><strong>MS.50.5 (C120)</strong> A. E. Aleshin: Structure of Complement C6 Suggests a Universal Model for Pore Formation by Cytolysins</td>
<td><strong>MS.51.5 (C121)</strong> N. LaRonde-LeBlanc: The Effect of Ligand-Stabilized Oligomerization on Rio1 Kinase Activity</td>
<td><strong>MS.53.5 (C126)</strong> G. J. Simpson: Crystal screening by second order nonlinear optical imaging of chiral crystals (SONICC)</td>
</tr>
<tr>
<td>Paris (MS52)</td>
<td>Berlin (MS56)</td>
<td>Londres (MS54)</td>
<td>Madrid (MS55)</td>
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<td><strong>Graphitic Materials</strong>&lt;br&gt;<strong>Chairs:</strong> K. Suenaga, P. Launois</td>
<td><strong>Spectroscopic Approaches (XAFS, NMR, …) in Crystallography</strong>&lt;br&gt;<strong>Chairs:</strong> M. C. Asensio, C. Castellano</td>
<td><strong>Minerals as Advanced Materials</strong>&lt;br&gt;<strong>Chairs:</strong> V. Kahlenberg, C. Weidenthaler</td>
<td><strong>Atomic Dynamics Using X-Ray and Neutrons</strong>&lt;br&gt;<strong>Chairs:</strong> A. Baron, H. Schober</td>
</tr>
<tr>
<td><strong>MS.52.2: T.B.A.</strong></td>
<td><strong>MS.56.2 (C130)</strong>&lt;br&gt;A. V. Soldatov: XANES spectroscopy for determination of the 3D nanoscale atomic structure</td>
<td><strong>MS.54.2 (C126)</strong>&lt;br&gt;H. Dittrich: Crystallography, physical properties and applications of sulfosalts</td>
<td><strong>MS.55.2 (C128)</strong>&lt;br&gt;M. Johnson: Structure and dynamics of hydrogen bonded systems from inelastic scattering</td>
</tr>
<tr>
<td><strong>MS.52.3 (C122)</strong>&lt;br&gt;J. C. Meyer: The physics of nano-carbons explored by high-resolution transmission electron microscopy</td>
<td><strong>MS.56.3 (C131)</strong>&lt;br&gt;F. J. Gacia de Abajo: Graphene, electrons, plasmons, and quantum: A perfect match</td>
<td><strong>MS.54.3 (C127)</strong>&lt;br&gt;O. Yakubovich: Genetic aspects of borophosphate crystal chemistry</td>
<td><strong>MS.55.3 (C129)</strong>&lt;br&gt;D. Reznik: Using phonon measurements to study electrons in superconductors</td>
</tr>
<tr>
<td><strong>MS.52.4 (C123)</strong>&lt;br&gt;J. L. Hodeau: Carbon polymorphs in pressure-crushed C60 analyzed by scattering tomography</td>
<td><strong>MS.56.4 (C131)</strong>&lt;br&gt;A. Comotti: Amphiphatic and amphidynamic crystalline materials: an XRD and MAS NMR study</td>
<td><strong>MS.54.4 (C127)</strong>&lt;br&gt;A. Guagliardi: Debye function analysis and 2D imaging of nanoscale bioapatite in bone tissue</td>
<td><strong>MS.55.4 (C129)</strong>&lt;br&gt;R. Grifone: Time-resolved X-ray diffraction study of LiNbO3 under pulsed external electric field</td>
</tr>
<tr>
<td><strong>MS.52.5 (C123)</strong>&lt;br&gt;C. Baehzt: In-situ characterization of the carbon nanotube growth process by X-ray diffraction</td>
<td><strong>MS.56.5 (C131)</strong>&lt;br&gt;J. Avila: Metal-semiconductor surface phase transitions: A photoelectron – diffraction study</td>
<td><strong>MS.54.5 (C128)</strong>&lt;br&gt;S. Yudintsev: Radiation induced disordering in crystalline actinide hosts</td>
<td><strong>MS.55.5 (C129)</strong>&lt;br&gt;G. J. McIntyre: Phonons observed by Laue diffraction on a continuous neutron source</td>
</tr>
</tbody>
</table>
Friday, August, 26 - Other Activities

Crystallography Software Fayre

Time: 10:00-12:15, 13:00-17:00 - Room: Amsterdam
Organizer: Martin Lutz (Utrecht University, The Netherland)

10:45-11:30h Mois Ilia Aroyo
“The Bilbao Crystallographic Server”

11:30-12:15h Isabel Usón
“ARCIMBOLDO”

13:00-14:00h Install Session
Users can contact software authors for help and support with the installation:
• Bilbao Crystallographic Server
• ARCIMBOLDO
• HKL2MAP
• ESCET
• ANODE
• ARP/wARP

14:00-14:45h Thomas R. Schneider
“HKL2MAP - SHELX-phasing for macromolecules”

14:45-15:30h Fabio Dall’Antonia
“ESCET - Analysis of ensembles of macromolecular structures”

15:30-16:15h Andrea Thorn, George M. Sheldrick
“ANODE - ANOmalous electron DEnsity analysis”

16:15-17:00h Tim Wiegels
“ARP/wARP for building models of proteins and their binding partners”

ECM27-Bergen Programme Committee Meeting

Time: 13:00-14:50 - Room: Buenos Aires

Open Commission Meetings

Time: 13:00-14:50

Commission on Crystallographic Computing
Room: Berlín
Coordinator: Harry Powell

Commission on Synchrotron Radiation
Room: París
Coordinator: Soichi Wakatsuki

Commission on Neutron Scattering
Room: Madrid
Coordinator: M. Teresa Fernández-Díaz
Commission on Electron Crystallography
Room: Roma
Coordinator: Lian-Mao Peng

AsCA Council Meeting
Time: 13:00-14:50 - Room: Bratislava

GE3C Executive Committee
(Crystallographic Spanish Association)
Time: 13:00-14:50 - Room: Oslo

Commercial Meetings
Molecular Dimensions
Time: 13:30-14:30 - Room: Londres
Molecular Dimensions Seminar: In situ X-ray diffraction Screening

PANalytical
Time: 14:00-14:40 - Room: Caracas
PANalytical Seminar: Cutting-edge diffraction solutions for powders, thin films, nanomaterials and solid objects

Gjønnes Medal Conference
Time: 18:30-20:00 - Room: Auditorium A
Archie Howie:
Fifty Years of Defect Imaging – Focusing on Dislocation Core Structure
Organizers: Laurence Marks

Remembering Lodovico Riva
Time: 18:30-20:00 - Room: Auditorium B
Organizers: Paola Spadon, Frank Allen and Keiichiro Ogawa

Congress Dinner
Time: 21:00-1.00
Congress Dinner will take place at the Botanical Garden of the Universidad Complutense de Madrid (UCM).
Metro: Metropolitano or Ciudad Universitaria (Line 6)
Morning Session 09:00-09:50
Auditorium A (KN 22)
KN22 (C13) – George M. Sheldrick:  
The SHELX approach to experimental phasing of macromolecules  
Chair: David Brown

Roma (KN 23)
KN23 (C14) - Ute Kolb:  
Ab-initio structure solution by automated electron diffraction tomography (ADT)  
Chair: Christian Baerlocher

Auditorium B (KN 32)
KN32 (C17) - Ronan McGrath:  
Structure of quasicrystalline surfaces  
Chair: Ron Lifshitz

Afternoon Session 17:40-18:30
Auditorium A (KN 25)
KN25 (C15) - Christiane Schaffitzel:  
*E. coli* co-translational targeting complexes studied by cryo-EM  
Chair: Daniela Stock

Roma (KN26)
KN26 (C15) - Sergey V. Krivovichev:  
Topological variations in inorganic oxocompounds: origin of structural diversity  
Chair: Massimo Nespolo

Auditorium B (KN 27)
KN27 (C15) - S. Samar Hasnain:  
XAFS Contribution to Protein Structure-Function Investigations  
Chair: Britt Hedman

Afternoon Session 18:35-19:25
Auditorium A (PL 3)
PL03 (C3) - Venki Ramakrishnan (Nobel Laureate):  
*FBBVA Conferences*  
Unraveling the structure of the ribosome and its role in decoding the genetic message  
Chair: Ted Baker
<table>
<thead>
<tr>
<th>Time</th>
<th>Auditorium A (MS57)</th>
<th>Auditorium B (MS58)</th>
<th>Roma (MS59)</th>
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<tbody>
<tr>
<td>10:15-10:20</td>
<td><strong>Opening Remarks</strong></td>
<td><strong>Opening Remarks</strong></td>
<td><strong>Opening Remarks</strong></td>
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</table>
| 10:20-10:50     | MS.57.1 (C132) *Y. Endo:* An attempt to prepare membrane proteins using the wheat cell-free protein production system | MS.58.1 (C133)  
T. Burnley: Ensemble refinement of protein crystal structures in PHENIX                                        | MS.59.1 (C135)  
P. Metrangolo: Halogen vs. Hydrogen bonding in the design of anion receptors                           |
| 10:50-11:20     | MS.57.2 (C132)  
V. Cherezov: Structural biology of G protein-coupled receptors                                                  | MS.58.2 (C134)  
G. N. Murshudov: Low resolution refinement in the program – REFMAC                                                                 | MS.59.2 (C136)  
Sarah L Price: Ionic, hydrogen or halogen bonds? Relevance for predicting crystal structures             |
| 11:20-11:50     | MS.57.3 (C132)  
P. Listwan: Application of split fluorescent proteins to challenges in crystallography: present and future | MS.58.3 (C134)  
O. S. Smart: Better ligand representation in BUSTER protein-complex structure determination C135        | MS.59.3 (C136)  
L. Brammer: Halogen bonding involving metallate ions and anionic ligands C137                           |
| 11:50-12:20     | MS.57.4 (C133)  
W. L. Duax: Immutable glycine based perfect alignment of protein families                                    | MS.58.4 (C134)  
D. Rigden: Structure solution by molecular replacement using *ab initio* protein models                  | MS.59.4 (C136)  
G. Manca: Electronic factors affecting the I-I bonds in the simplest polyiodides                           |
| 12:20-12:50     | MS.57.5 (C133)  
Y. Thielmann: Differential scanning fluorimetry at the ESFRI-Instruct Core Centre Frankfurt                  | MS.58.5 (C135)  
S. Hazledine: Release 7.2 of ARP/wARP software suite                                                       | MS.59.5 (C137)  
C. Esterhuysen: Computational and CSD analysis of I₃⋯I₃⁻ halogen bonds                                     |
<table>
<thead>
<tr>
<th>Paris (MS60)</th>
<th>Berlin (MS62)</th>
<th>Londres (MS61)</th>
<th>Madrid (MS63)</th>
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</thead>
<tbody>
<tr>
<td><strong>Solid State Reactivity</strong>&lt;br&gt;<strong>Chairs:</strong> S. Galli, J. B. Parise</td>
<td><strong>Crystallographic Software: the Library Approach</strong>&lt;br&gt;<strong>Chairs:</strong> R. Grosse-Kunstleve, L. Bourhis</td>
<td><strong>Hot Structures in Chemical Crystallography</strong>&lt;br&gt;<strong>Chairs:</strong> S.-Ming Peng, D. Stalke</td>
<td><strong>Quasicrystals and Their Approximants: Structure and Physical Properties</strong>&lt;br&gt;<strong>Chairs:</strong> H. Takakura, N.K. Mukhopadhyay</td>
</tr>
<tr>
<td><strong>MS.60.1</strong> (C137)&lt;br&gt;A. Fuertes: Perovskite oxynitride materials: anion order, Valence States and physical properties</td>
<td><strong>MS.62.1</strong> (C142)&lt;br&gt;V. Favre-Nicolin: Crystallography On-A-Chip: using GPU for fast scattering computing</td>
<td><strong>MS.61.1</strong> (C140)&lt;br&gt;T. C. W. Mak: Supramolecular assembly based on multinuclear silver(i) ethynide synthons</td>
<td><strong>MS.63.1</strong> (C143)&lt;br&gt;R. Tamura: Structural and magnetic transitions of Cd₆R₉ approximants</td>
</tr>
<tr>
<td><strong>MS.60.2</strong> (see MS60.P03, C602): A. Tumanov: Controlled mechanochemical synthesis. Relating chemistry to crystal structures</td>
<td><strong>MS.62.5</strong> (C143)&lt;br&gt;S. Androulakis: MyTARDIS: Managing the Lifecycle of Crystallography Data</td>
<td><strong>MS.61.5</strong> (C142)&lt;br&gt;B. Gabidullin: Two different types of supramolecular architectures of p-sulphonated thiacalix[4]arene with Zn(dipy): Structure and stability</td>
<td><strong>MS.63.5</strong> (C145)&lt;br&gt;Y. K. Vekilov: Variable-Range-Hopping Conductivity in Quasicrystals</td>
</tr>
<tr>
<td><strong>MS.60.3</strong> (C138)&lt;br&gt;K. W. Chapman: Insights into reactions of functional materials using pair distribution function analysis</td>
<td><strong>MS.62.2</strong> (C142)&lt;br&gt;E. Krissinel: Software libraries in CCP4 Program Suite</td>
<td><strong>MS.61.2</strong> (C140)&lt;br&gt;A. J. Edwards: Polycoordinate hydride inside a Cu₇ cluster authenticated by neutron diffraction</td>
<td><strong>MS.63.2</strong> (C144)&lt;br&gt;M. Engel: A dense quasicrystalline phase of hard tetrahedra</td>
</tr>
<tr>
<td><strong>MS.60.4</strong> (C139)&lt;br&gt;S. Pagola: Structural analysis of mechanochemical reaction products from powder diffraction</td>
<td><strong>MS.62.3</strong> (C143)&lt;br&gt;L. M. Daniels: Libraries and software development at rigaku</td>
<td><strong>MS.61.3</strong> (C141)&lt;br&gt;D. Kratzert: Germynenes: high resolution X-ray data for unambiguous ligand identification</td>
<td><strong>MS.63.3</strong> (C144)&lt;br&gt;M Mihalkovič: Prediction of low-temperature phase transition in Al₁₁Ir₄ compound</td>
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<tr>
<td><strong>MS.60.5</strong> (C139)&lt;br&gt;L. Barrio: In-situ XRD study of the reduction of copper spinel with H₂ and CO</td>
<td><strong>MS.62.4</strong> (C143)&lt;br&gt;P. Juhas: DiffPy - an opensource library for powder crystallography</td>
<td><strong>MS.61.4</strong> (C141)&lt;br&gt;J. E. Van der Maelen Uría: Theoretical QTAIM study on S- and Se-bridged polynuclear Mn complexes</td>
<td><strong>MS.63.4</strong> (C144)&lt;br&gt;P. Kuczera: The structure of Al-Cu-Me (Me =Co, Rh, Ir) quasicrystals</td>
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<td>Time</td>
<td>Auditorium A (MS64)</td>
<td>Auditorium B (MS66)</td>
<td>Roma (MS65)</td>
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<td>15:00-15:05</td>
<td><strong>Opening Remarks</strong></td>
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<td></td>
<td>Hot Structures in Biology II</td>
<td>Electric, Magnetic and other Physical Properties of Molecular Crystals</td>
<td>Atomistic and Electronic Structures of Nanomaterials</td>
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<tr>
<td></td>
<td><em>Chairs:</em> T. Inoue, S. Won Suh</td>
<td><em>Chairs:</em> S. Gao, A. Kobayashi</td>
<td><em>Chairs:</em> M. Malac, Q. Li</td>
</tr>
<tr>
<td>15:05-15:35</td>
<td><strong>MS.64.1</strong> <em>(C145)</em> H. Matsumura: Structural basis for the sequential assembly of photosynthetic multienzyme complex</td>
<td><strong>MS.66.1</strong> <em>(C149)</em> E. Coronado: Molecular design of multifunctional magnetic materials</td>
<td><strong>MS.65.1</strong> <em>(C147)</em> V. J. Keast: Atomic structure, electronic structure and optical response of metal nanoparticles</td>
</tr>
<tr>
<td>15:35-16:05</td>
<td><strong>MS.64.2</strong> <em>(C146)</em> S. Yokoyama: Structural basis for specific aminoacyl-tRNA synthesis</td>
<td><strong>MS.66.2</strong> <em>(C149)</em> H. Kobayashi: Development of molecular materials with electric and/or magnetic functions</td>
<td><strong>MS.65.2</strong> <em>(C148)</em> C. H. Chen: Chemical mapping at atomic-column resolution by STEM-EDX</td>
</tr>
<tr>
<td>16:05-16:35</td>
<td><strong>MS.64.3</strong> <em>(C146)</em> M. Lawrence: First view of insulin bound to its primary binding site on the insulin receptor</td>
<td><strong>MS.66.3</strong> <em>(C150)</em> Ren-Gen Xiong: Jahn-teller effect and ferroelectric phase transition in a metal-organic complex</td>
<td><strong>MS.65.3</strong> <em>(C148)</em> S. Van Aert: Three-dimensional atomic imaging of crystalline nanoparticles</td>
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<tr>
<td>16:35-17:05</td>
<td><strong>MS.64.4</strong> <em>(C147)</em> A. Athanasiadis: The structure of conformational junctions in DNA and genomic instability</td>
<td><strong>MS.66.4</strong> <em>(C150)</em> B. Gillon: Finite size effects in a quantum chain of antiferromagnetically coupled spins 3/2</td>
<td><strong>MS.65.4</strong> <em>(C148)</em> G.A. Botton: Bonding and electronic structure of nanomaterials and interfaces with electron energy loss spectroscopy</td>
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<tr>
<td>17:05-17:35</td>
<td><strong>MS.64.5</strong> <em>(C147)</em> H Wu: Crystal structures of key components in toll-like receptor signaling</td>
<td><strong>MS.66.5</strong> <em>(C151)</em> N. F. Sciortino: Interplay between structure and functional properties in spin crossover frameworks</td>
<td><strong>MS.65.5</strong> <em>(C149)</em> W. F. Pong: Photo-conductivity and electronic structures of Au-nanoparticle embedded silica-nanowires</td>
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<td>Paris (MS67)</td>
<td>Berlin (MS68)</td>
<td>Londres (MS69)</td>
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<td><strong>Layered Inorganic Materials and Layered Precursors of 3D Structures</strong></td>
<td><strong>Chairs:</strong> B. Marler, H. Pastore</td>
<td><strong>Data Reduction of Area Detector Measurements</strong></td>
<td><strong>Crystallographic Methods and Software for Periodic and Aperiodic Crystals</strong></td>
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<tr>
<td><strong>MS.67.1</strong></td>
<td><strong>C151</strong> R. Millini: News from the world of eni carbon silicate (ECS) materials</td>
<td><strong>C154</strong> C. Hoffmann: Data reduction of area detector measurements</td>
<td><strong>C155</strong> L. J. Allen: Modelling thermal scattering and solving structures using Z-contrast imaging</td>
</tr>
<tr>
<td><strong>MS.67.2</strong></td>
<td><strong>C152</strong> E. Sokolova: Revision of the crystal chemistry of the astrophyllite group</td>
<td><strong>C154</strong> D. Chateigner: Applications of area detectors to texture measurements</td>
<td><strong>C156</strong> L. D Marks: SrTiO₃ surface structures from diffraction &amp; DFT: Homologous Series &amp; Glasses</td>
</tr>
<tr>
<td><strong>MS.67.3</strong></td>
<td><strong>C152</strong> P. A. Guńka: Ammonium polyoxoarsenates(III) – from columns to 3D structure</td>
<td><strong>C154</strong> A. Gukasov: Modern trends in area detectors for single-crystal neutron diffraction</td>
<td><strong>C156</strong> O. Gourdon: JANA2006 as a unique tool to refine nuclear and/or magnetic structures using ToF data</td>
</tr>
<tr>
<td><strong>MS.67.4</strong></td>
<td><strong>C153</strong> E. V. Alekseev: Complex topologies as a result of simple relationships between 2D and 3D actinide borates</td>
<td><strong>C155</strong> R. Piltz: Accurate data analysis for the koala and VIVALDI neutron Laue diffractometers</td>
<td><strong>C157</strong> J. J. Lovelace: Fitting a square peg into a round hole: Simulating a modulated protein crystal</td>
</tr>
<tr>
<td><strong>MS.67.5</strong></td>
<td><strong>C153</strong> V. Kahlenberg: Temperature and moisture dependent studies on kanemite (NaSi₂O₄(OH)*3H₂O)</td>
<td><strong>C155</strong> L.M.J. Kroon-Batenburg: Diffraction data quality analysis of EVAL15 integration</td>
<td><strong>C157</strong> S. Deloudi: Higher-dimensional crystallography of n-fold quasiperiodic tilings (n=7-15)</td>
</tr>
</tbody>
</table>
Crystallography Software Fayre

Time: 10:00-12:15, 13:00-17:00 - Room: Amsterdam
Organizer: Martin Lutz (Utrecht University, The Netherland)

10:00-10:45h Valeri Petkov
“RAD” for XRD data processing into atomic pair distribution functions” “ISAACS” suits of programs for analysis of 3D structure models of periodic (e.g. crystals) and non periodic (e.g. glasses) systems “

10:45-11:30h Anna Moliterni
“Crystal structure solution by EXPO2011”

13:00-14:00h Install Session
Users can contact software authors for help and support with the installation:

- RAD, ISAACS
- EXPO2011
- EXPGUI
- DiffPy
- FOX
- Smirnova's software

14:00-14:45h Brian Toby
“EXPGUI”

14:45-15:30h Pavol Juhas
“DiffPy - a software suite for structure analysis from powder diffraction”

15:30-16:15h Vincent Favre-Nicolin
“Solving crystal structures from powder diffraction using FOX”

16:15-17:00h Olga Smirnova
“Advanced mathematical models for the development of the automated SDPD software”
Open Commission Meetings
Time: 13:00-14:50
Commission on Charge, Spin and Momentum Densities
Room: Paris
Coordinator: Carlo Gatti
Commission on Crystallographic Teaching
Room: Berlín
Coordinator: Paola Spadon

ECA Meetings
ECA - Council Meeting
Time: 13:00-14:50 - Room: Bratislava

ECA Special Interest Group Meeting
SIG3
Time: 13:00-14:30 - Room: Monaco
Chair: Sander van Smaalen

IUCr General Assembly
Time: 19:30-21:30 - Room: Madrid

Evening Session 2
Time: 19:30-21:30 - Room: Paris
Talk: The making of Bernal’s Picasso: a documentary where Art meets Sciences
Speaker: Celerino Abad-Zapatero
Morning Session 09:00-09:50

Auditorium A (KN 28)

KN28 (C16) - Leemor Joshua Tor:
Structural Basis of Cell Regulatory Processes
Chair: María Armenia Carrondo

Roma (KN 29)

KN29 (C16) - Elena Boldyreva:
High-pressure studies of molecular crystals
Chair: Andrzej Katrusiak

Auditorium B (KN 30)

KN30 (C16) - Reinhard B. Neder:
Powder diffraction at the nanoscale: structure and defects
Chair: David Keen

Afternoon Session 17:40-18:30

Auditorium A (KN 31)

KN31 (C17) – So Iwata:
Molecular basis of antihistamine specificity against Human Histamine H1 receptor
Chair: Mitchell Guss

Roma (KN 24)

KN24 (C14) - José Elguero:
Conflicts and complicities between crystallography, solid state NMR and vibrational circular dichroism (VCD)
Chair: Andre Roodt

Auditorium B (KN 33)

KN33 (C18) - Anatoly M. Balagurov:
Magnetic neutron crystallography - commensurate and incommensurate structures
Chair: Emmanuelle Suard
<table>
<thead>
<tr>
<th>Time</th>
<th>Auditorium A (MS71)</th>
<th>Auditorium B (MS72)</th>
<th>Roma (MS73)</th>
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<tbody>
<tr>
<td></td>
<td>Chairs: B. Luisi, M. Glover</td>
<td>Throughput Crystallography</td>
<td>Interaction for Molecular Recognition</td>
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<td>Chairs: F. Von Delft, R. Caliandro</td>
<td>Chairs: P. Gilli, A. Bond</td>
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<td>RNA recognition by RIG-I</td>
<td>determination and refinement in PHENIX</td>
<td>Toolkit</td>
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<tr>
<td>10:50-11:20</td>
<td>MS.71.2 (C160) C. Oubridge: Crystallographic insights into the</td>
<td>MS.72.3 (C162) C. Giacovazzo: New phasing methods for high</td>
<td>MS.73.2 (C163) P. Macchi: Strong Hydrogen bonds</td>
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<td>structure of spliceosomal snRNPs</td>
<td>throughput crystallography</td>
<td>in crystals under high pressure</td>
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<td>11:20-11:50</td>
<td>MS.71.3 (C160) H. Li: Structural studies of a CRISPR RNA</td>
<td>MS.72.2 (C162) A. W. Ashton: More speed, more data, more</td>
<td>MS.73.3 (C164) M. Lusi: Determining Hydrogen</td>
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<tr>
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<td>processing endonuclease</td>
<td>automation, less work!</td>
<td>Positions in Hydrogen Bonded Structures: A CSD</td>
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<td>Survey</td>
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<td>suppression</td>
<td>merging of multiple datasets in macromolecular crystallography</td>
<td>cocryostals model drug-receptor interactions</td>
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<td>12:20-12:50</td>
<td>MS.71.5 (C161) W. Galej: Biochemical studies of the snRNPs</td>
<td>MS.72.5 (C163) K. Yamashita: LAFIRE: Automated refinement</td>
<td>MS.73.5 (C164) C. H. Görbitz: Hydrogen bonding in</td>
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<td>core domain formation in Saccharomyces cerevisiae</td>
<td>software for biomacromolecular crystallography</td>
<td>amino acid racemates and a game of side-chain</td>
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<td>Paris (MS74)</td>
<td>Berlin (MS75)</td>
<td>Londres (MS76)</td>
<td>Madrid (MS77)</td>
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| **Powder Diffraction and Complementary Techniques**  
*Chairs:* P. Chupas, M. Milanesio | **Liquids, Amorphous and Nanocrystalline Solids at High Pressure**  
*Chairs:* C. Sanloup, S. Bonev | **Density Functional Methods for Electronic Structure Calculations**  
*Chairs:* A. Rubio, R. Nieminen | **XAFS Instrumentation: Automation, Standardization and Validation of XAFS Experiments**  
*Chairs:* C. Chantler, K. Asakura |
| MS.74.1 (C165)  
**J. Hanson:** Combined X-ray Diffraction and Absorption Measurements of Active Catalysts | MS.75.1 (C167)  
**L. Stixrude:** Structure of silicate liquids in the deep Earth | MS.76.1 (C169)  
**M. Walter:** Structure and electronic properties of free, supported and protected clusters | MS.77.1 (C171)  
**R. Frahm:** Advances in instrumentation, automation and validation of fast XAFS experiments |
| **MS.74.2 (C165)**  
**W. van Beek:** Modulation Enhanced Diffraction: a new tool for solving crystal structures and study solid-state kinetics | MS.75.2 (C167)  
**Y. Katayama:** Structure of water under high temperature and pressure | MS.76.2: T.B.A. | **MS.77.2 (C171)**  
**M. Newville:** Standardizing Data Formats for X-ray Absorption Spectra and Libraries |
| **MS.74.3 (C166)**  
**H.O. Sørensen:** Non-destructive determination of minerals and their locations within chalk | MS.75.3 (C168)  
**L. Spanu:** Stability of hydrocarbons at deep Earth pressures and temperatures | MS.76.3 (C170)  
**A. Castro:** Optimization of materials with time dependent density functional theory | **MS.77.3 (C172)**  
**M. Nomura:** Revisit the basics to optimize detection systems and time-resolved XAFS |
| **MS.74.4 (C166)**  
**N. Huber:** Combining μ-XRD² and DTA: deeper insights in temperature-dependent processes | MS.75.4 (C168)  
**C. A. Tulk:** High pressure amorphization processes in water – methane clathrates | MS.76.4 (C170)  
**J. D Bourke:** Density functional calculations of electron energy loss data and inelastic mean free paths in elemental and binary materials | **MS.77.4 (C172)**  
**J. Hester:** Development and adoption of scientific data exchange frameworks: a CIF perspective |
| **MS.74.5 (C167)**  
**P. Sozzani:** Powder X-ray diffraction combined with solid state and ¹²⁹Xe NMR to study supramolecular crystalline materials | MS.75.5 (C168)  
**S. Petitgirard:** In-situ chemical partitioning of trace elements between silicate and iron rich liquids at extreme conditions | MS.76.5 (C170)  
**A. A. Korlyukov:** Topological analysis of charge densities obtained from experiment and plane-wave calculations | **MS.77.5 (see MS77.P02, C687)**  
**J. Wang:** Industrial applications at the national synchrotron light source |
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<th>Time</th>
<th>Auditorium A (MS78)</th>
<th>Auditorium B (MS81)</th>
<th>Roma (MS80)</th>
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</table>
| 15:00-15:05       | **Opening Remarks**  
Chairs: A. Liljas, D. Vassylyev                                                   | **Time**  
Chairs: D. Pandey, Y. Kuroiwa                                                   | **Solid State Photochemistry**  
Chairs: M. Kaftory, P. Gómez Sal                                                     |
| 15:05-15:35       | **MS.78.1 (C172)**  
P. Cramer: Structural biology of eukaryotic gene transcription  | **MS.81.1 (C178)**  
Y. Shimakawa: A-site ordered perovskite-structure oxides with functional properties  | **MS.80.2 (C176)**  
P. R. Raithby: Structural Studies on Photoactivated Transition Metal Complexes  |
|                   | **MS.78.2 (C173)**  
M. Yusupov: Crystal structures of bacterial and yeast ribosomes  | **MS.81.2 (C178)**  
J. Hadermann: Electron crystallography for Li-based battery materials  | **MS.80.3 (C177)**  
M. Scholz: Real Time Dynamics of Solid Molecular Switches and “Machines” Investigated with Ultrafast Pulsed X-ray Radiation |
| 15:35-16:05       | **MS.78.3 (C173)**  
T. Lavy: The GAL regulon in *S. CEREVISIAE*: the Gal3p/Gal80p interaction  | **MS.81.3 (C179)**  
B. Dkhil: Oxygen tilts against polar shifts in the multiferroic BiFeO$_3$  | **MS.80.5 (C178)**  
Y. Ozawa: Photoexcited state crystallography of luminescent hexanuclear d$^{10}$ metal complexes |
| 16:05-16:35       | **MS.78.4 (C173)**  
Z. Wang: Structure and function of human BMAL1-CLOCK-DNA complex  | **MS.81.4 (C179)**  
A. E. Phillips: Photorefractivity via linkage isomerism: from detecting small responses to engineering large ones  | **MS.80.4 (C177)**  
J. M. Cole: Time-resolved photo-crystallography of ruthenium sulfur-dioxide complexes  |
| 16:35-17:05       | **MS.78.5 (C174)**  
Kiyohito Kihira: Crystal structure analysis of release factor 3  | **MS.81.5 (see MS81.P09,C703)**  
C. Howard: Predicting switchable multiferroic ruddlesden-popper phases & phase transitions.  | **MS 80.1 (see MS80.P02, C699)**  
A. Sekine: Control of photochromic reactivity in hybrid type cobaloxime complex  |
<p>| 17:05-17:35       |                                                                                   |                                                                                   |                                                                                                |</p>
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<th>Paris (MS79)</th>
<th>Berlin (MS82)</th>
<th>Londres (MS83)</th>
<th>Madrid (MS84)</th>
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</thead>
</table>
| **Electron Diffraction and Crystallography**  
*Chairs: P. Nakashima, C. Koch* | **Biological Neutron Scattering and Deuteration**  
*Chairs: T. Forsyth, J. Krueger* | **Application of Crystal Structure Information in Chemical Education**  
*Chairs: G. M. Battle, L. Infantes* | **What is order, and how can one describe it? (Which kinds of matter diffract?)**  
*Chairs: M. Senechal, U. Grimm* |
| **MS.79.1** (C174)  
A. Stewart: Electron crystallography: harder, better, faster, stronger | **MS.82.1** (C180)  
A. Podjarny: Neutron structure of type-III antifreeze protein leads to ice interface model | **MS.83.1** (C182)  
K. A. Kantardjieff: Cyber-enabled learning and practice in crystallography: educating the next generation | **MS.84.1** (C184)  
W. Steurer: Measures of complexity |
| **MS.79.2** (C174)  
R. Withers: Modulated structures and TEM’s: from relaxor ferroelectrics to nano-chessboards | **MS.82.2** (C180)  
O. Byron: Neutron scattering reveals human pyruvate dehydrogenase complex organisation | **MS.83.2** (C182)  
F. H. Allen: Promoting crystallography: using crystal structures in chemical education | **MS.84.2** (C184)  
R. Mosseri: Frustrated Order |
| **MS.79.3** (C175)  
A. W S Johnson: Bonding charge density in srtio, under an electric field measured by electron diffraction | **MS.82.3** (C181)  
M. G. Cuyper: Neutron high resolution crystallographic study of perdeuterated *P.f.* rubredoxin | **MS.83.3** (C183)  
D. H. Johnston: Experimental determination of chemical structure in the undergraduate curriculum | **MS.84.3** (C184)  
N. Dolbilin: Local Rules and Global Order |
| **MS.79.4** (C175)  
P. Oleynikov: Automated quantitative 3d electron diffraction rotation tomography | **MS.82.4** (C181)  
L. Coates: Active site protonation states of perdeuterated Toho-1 beta lactamase | **MS.83.4** (C183)  
J. M. Tanski: Writing crystal structure reports in collaboration with undergraduate students | **MS.84.4** (C185)  
S. I. Ben-Abraham: Aperiodic structures, order and disorder, complexity and entropy |
| **MS.79.5** (C176)  
K Tsuda: Electrostatic potential analysis of the rhombohedral phase of ferroelectric BaTiO₃ using CBED | **MS.82.5** (C182)  
T. Darwish: Deuteration of oleic acid, lipids and other molecules for neutron studies | **MS.83.5** (C183)  
E. V. Boldyreva: “Applied crystal chemistry” for chemists and materials scientists | |

**Sunday, August, 28 - Afternoon - Microsymposia**
Crystallography Software Fayre

Time: 10:00-12:15, 13:00-17:00 - Room: Amsterdam
Organizer: Martin Lutz (Utrecht University, The Netherlands)

10:00-10:45h Andrew Stewart
“ADT3D: Electron crystallography using diffraction tomography data.”

10:45-11:30h Luis Fuentes-Montero
“ANAELU for X-ray diffraction analysis using two-dimensional patterns”

11:30-12:15h Silvina Pagola
“Crystal structure solution of molecular solids using the computer program PSSP (Powder Structure Solution Program)”

13:00-14:00h Install Session
Users can contact software authors for help and support with the installation:
- ADT3D
- ANAELU
- PSSP
- 3Dtomo

14:00-14:45h Peter Oleynikov
“3Dtomo a program for 3D reciprocal space reconstruction from electron diffraction rotation data”

Open Commission Meetings

Time: 13:00-14:50

Commission on XAFS
Room: Madrid
Coordinator: Isabella Ascone

Commission on Aperiodic Crystals
Room: Berlín
Coordinator: Marc de Boissieu

GE3C - Xavier Solans Prize Lecture

Time: 13:15-14:00 - Room: Londres
Talk: Mechanistic Insights into a Gas-Solid Reaction in Molecular Crystals: The Role of Hydrogen Bonding
Speaker: Guillermo Mínguez Espallargas
Chair: Fernando J. Lahoz
Sunday, August, 28  -  Other Activities

**ECA - Executive Committee**

Time: 13:00-14:50 - Room: Buenos Aires

**GE3C General Assembly**  
(*Crystallographic Spanish Association*)

Time: 14:00-14:50 - Room: Londres

**IUCr General Assembly**

Time: 19:30-21:30 - Room: Madrid

**Evening Session 3**

Time: 19:30-21:30 - Room: Paris  
Talk: *Nonius 1970-2000, a view from inside*  
Speaker: Frank Van Meurs  
Talk: *Choosing a single crystal diffraction system: an insider’s view*  
Speaker: Anita Coetzee
Morning Session 09:00-09:50

Auditorium A (KN 34)

KN34 (C18) - Janet Newman:
XDX - An initial solution to crystallization

Chair: Joseph Ng

Roma (KN 36)

KN36 (C19) - Isabelle Mirebeau:
Frustration and spin lattice coupling in pyrochlores magnets and multiferroics

Chair: J. L. García Muñoz

Auditorium B (KN 35)

KN35 (C18) – Gautam R. Desiraju:
Crystal engineering. From molecules to crystals

Chair: Carlo Mealli

Afternoon Session 17:10-18:00

Auditorium A (PL 4)

PL04 (C4) - Ada E. Yonath (Nobel Laureate):
FBBVA Conferences
The Spectacular Architecture of the Ribosome and Clues about its Origin

Chair: Peter Colman
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<th>Time</th>
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<th>Auditorium B (MS86)</th>
<th>Roma (MS87)</th>
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<tr>
<td>10:15-10:20</td>
<td><strong>Opening Remarks</strong>&lt;br&gt;Membrane Protein Structures&lt;br&gt;&lt;br&gt;<em>Chairs:</em> S. Iwata, M.J. Sánchez-Barrena</td>
<td>Challenges of Low-Resolution Crystallography&lt;br&gt;&lt;br&gt;<em>Chairs:</em> J. Sussman, I. Margiolaki</td>
<td>Chirality in the Solid State, from Organic Molecules to Chiral MOF and Helical Materials&lt;br&gt;&lt;br&gt;<em>Chairs:</em> S. Bourne, B. Gómez Lor</td>
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<td>10:20-10:50</td>
<td>MS.85.1 (C185)&lt;br&gt;I. B. Schäfer: Inhibition of SNARE-mediated membrane fusion by VARP</td>
<td>MS.86.1 (C187)&lt;br&gt;A. T. Brunger: Challenges for refinement at low resolution</td>
<td>MS.87.1 (C189)&lt;br&gt;M. Miyata: Handedness of two-fold helices and chiral space-groups</td>
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<td>10:50-11:20</td>
<td>MS.85.2 (C185)&lt;br&gt;T. Shimamura: Structure of the human histamine H1 receptor with doxepin</td>
<td>MS.86.2 (C187)&lt;br&gt;John R Helliwell: Lessons of diffraction resolution and the crustacyanin structures</td>
<td>MS.87.2 (189)&lt;br&gt;I. Justyniak: Molecular building block approach to chiral coordination polymers and noncovalent porous materials</td>
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<td>11:20-11:50</td>
<td>MS.85.3 (C186)&lt;br&gt;S. Newstead: Towards a structural understanding of drug and peptide transport within the proton dependent oligopeptide transporter (POT) family</td>
<td>MS.86.3 (C187)&lt;br&gt;T. Zeev-Ben-Mordehai: Studying membrane fusion at molecular resolution</td>
<td>MS.87.3 (C190)&lt;br&gt;N. B. Báthori: Chiral discrimination in the solid state</td>
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<td>11:50-12:20</td>
<td>MS.85.4 (C186)&lt;br&gt;M. Palacín: Molecular basis of substrate-induced permeation by an amino acid antiporter</td>
<td>MS.86.4 (C188)&lt;br&gt;S. Nicolopoulos: Low resolution electron crystallography challenges in organic and inorganic crystals with transmission electron microscope (TEM)</td>
<td>MS.87.4 (C190)&lt;br&gt;G. Terraneo: Chirality in halogen-bonded supramolecular architectures</td>
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<td>12:20-12:50</td>
<td>MS.85.5 (C186)&lt;br&gt;X.-Yu Liu: Crystal structure of the copper pump</td>
<td>MS.86.5 (C188)&lt;br&gt;S. C. M. Teixeira: Low resolution neutron crystallography of biological macromolecules</td>
<td>MS.87.5 (C191)&lt;br&gt;S. Parsons: Precise absolute structure determination for light-atom structures</td>
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<td>Paris (MS88)</td>
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<td>Londres (MS89)</td>
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<td><strong>Crystal Chemistry and Physics of Modulated and Composite Crystals</strong>&lt;br&gt; <em>Chairs:</em> J. Haderman, A. Schönleber</td>
<td><strong>Hydrogen Bonding: from the Solid State to Solution</strong>&lt;br&gt; <em>Chairs:</em> A. Soper, M. E. Tuckerman</td>
<td><strong>Archiving, Exchange and Retrieval of Scientific Data in the 21st Century</strong>&lt;br&gt; <em>Chairs:</em> J. Hester, D. Brown</td>
<td><strong>X-Ray Absorption, Diffraction and Imaging in Forensic Science and Ancient Materials</strong>&lt;br&gt; <em>Chairs:</em> S. Quartieri, J. Susini</td>
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<td>Time</td>
<td>Auditorium A (MS93)</td>
<td>Auditorium B (MS92)</td>
<td>Roma (MS94)</td>
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<td>14:25-14:30</td>
<td>Opening Remarks</td>
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<td>14:35-15:05</td>
<td>MS.93.1 (C201) A. Vrielink: Structural studies of an endotoxin biosynthesis enzyme from neisseria meningitidis</td>
<td>MS.92.1 (C199) A. Rodríguez-Romero: Strategies in the crystallization of a glycoallergen and a F1-ATPase complex</td>
<td>MS.94.1 (C202) J. M. Ribo: Metastability in supersaturated solution and transition towards chirality in the Crystallization of NaClO₃</td>
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<td>15:35-16:05</td>
<td>MS.93.3 (C201) H. Luecke: Dissecting Enzyme Mechanisms</td>
<td>MS.92.3 (C200) L. David: Crystallization of a giant photosynthetic antenna complex – the phycobilisome</td>
<td>MS.94.3 (C203) T. R. Walsh: Facet-specific binding of amino-acid analogues on quartz</td>
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<td>16:05-16:35</td>
<td>MS.93.4 (C201) F. J. Medrano: Structure of lysine oxidase with a cysteine tryptophylquinone in the active site</td>
<td>MS.92.4 (C200) J. A. Márquez: Crystal direct : A new system for automated crystal harvesting</td>
<td>MS.94.4 (C203) S. D. Zarić: Noncovalent interactions of aromatic molecules</td>
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<td>16:35-17:05</td>
<td>MS.93.5 (C202) S. Watanabe: Crystal structures of [NiFe] hydrogenase maturase complexes</td>
<td>MS.92.5 (C200) C. Abad-Zapatero: Humidity control can compensate the damage induced in protein crystals by alien solvents.</td>
<td>MS.94.5 (C204) E. Kováts: Formation and structure of fullerene and cubane based cocrystals</td>
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<td>Paris (MS95)</td>
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<td>Londres (MS97)</td>
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| Automated Data Processing and Structural Solution for Powder Crystallography  
*Chairs:* Rosanna Rizzi, Anton Meden | Complementary Use of Neutrons and Photons in Magnetism  
*Chairs:* Robert Cywinski, Valeria Lauter M. Teresa Fernández-Díaz | Web Based Crystallography Teaching: the Use of Modern Communication Methods to Teach Crystallography  
*Chairs:* Katherine Kantardjieff, Gervais Chapuis | Complex Structure and Frustrated Systems: Simulation and Experiments  
*Chairs:* Olivier Perez, Guido Kreiner |
| **MS.95.1 (C204)**  
B. H. Toby: Automating mail-in data collection at 11-BM at the APS | **MS.96.1 (C206)**  
B. P. Toperverg: Polarized Neutron and Light Scattering from Magnetic Nano-structures under AC-field | **MS.97.1 (C208)**  
R. Resel: Harnessing students to advance e-learning | **MS.98.1 (C210)**  
G. E. O. Borgstahl: Solving the incommensurately modulated structure in profilin:actin crystals |
| **MS.95.2 (C204)**  
A. Altomare: Automation and efficiency in the powder structure solution by EXPO package | **MS.96.2 (C207)**  
Y. Liu: Understanding the Interface Properties of Magnetic Heterostructures | **MS.97.2 (C209)**  
G. M. Battle: WebCSD: bringing the Cambridge Structural Database to undergraduate teaching | **MS.98.2 (C210)**  
R. Lifshitz: Soft Quasicrystals Thermodynamic stability of complex structures |
| **MS.95.3 (C205)**  
L. B. McCusker: Pushing the limits of powder charge flipping | **MS.96.3 (C207)**  
J.-P. Wang: Structural and Polarized Neutron Reflectometry Characterization of Fe$_{16}$N$_2$ Thin Films with Giant Saturation Magnetization | **MS.97.3 (C209)**  
C. Smith: Remote access to SSRL crystallography beamlines: Tools for education and training | **MS.98.3 (C211)**  
L. Palatinus: Incommensurate Tiling in $\eta'$-Cu$_{3+x}$(Si,Ge)$_2$ Determined by Electron Diffraction |
| **MS.95.4 (C205)**  
R. Oishi-Tomiyasu: Algorithm and performance of a new powder indexing software Conograph | **MS.96.4 (C208)**  
V. Y. Pomjakushin: Iron vacancy superstructure and room temperature antiferromagnetic order in superconducting X$_2$Fe$_{24}$Sc$_2$(X=K, Cs, Rb) | **MS.97.4 (C209)**  
Mois I. Aroyo: Structure utilities hosted by the Bilbao crystallographic server | **MS.98.4 (C211)**  
M. de Boissieu: Dynamics of the inner tetrahedron in the ZnSc$_{1/1}$ quasicrystal approximant: experiment and simulation |
| **MS.95.5 (C206)**  
M. Milanesio: Chemical selectivity in structure determination by modulation enhanced X-ray diffraction | **MS96.5 (see MS96.P02, C800)**  
A. Schönelle: Structure and magnetic order in CrOCl at low temperatures | **MS.97.5 (C210)**  
A. J. Markvardsen: Jpowder: a Web/Java based program for the display of powder diffraction data | **MS.98.5 (C212)**  
M. C. Menard: Exotic Ground States: A Study in the Structural Effects of Frustration and Dimensionality |
ECA - Council Meeting
Time: 13:00-14:50 - Room: Bratislava

GE3C General Assembly
(Crystallographic Spanish Association)
Time: 13:00-14:15 - Room: Londres

“International School on Charge Density”
Organization Meeting
Time: 13:15-14:15 - Room: Paris

Closing Ceremony
Time: 18:30-20.00 - Room: Auditorium A
Chair: E. Gutiérrez-Puebla

1. Review of IUCr 2011
2. Presentation of Poster Prizes
3. Speech by the ex – President of IUCr
4. Speech by the new President of IUCr
5. Invitation to XXIII IUCr, Montreal 2014
Developers of academic and/or open-source crystallographic software are invited to present their new developments at the 2011 Madrid Crystallographic Software Fayre.

<table>
<thead>
<tr>
<th>Time</th>
<th>Tuesday August, 23</th>
<th>Wednesday August, 24</th>
<th>Thursday August, 25</th>
</tr>
</thead>
<tbody>
<tr>
<td>10:00-10:45</td>
<td>Simonov Arkadiy: “Diffuse scattering”</td>
<td>Reinhard Neder, Thomas Proffen: DISCUS</td>
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<tr>
<td>10:45-11:30</td>
<td>Gianluca Cascaraono: Il Milione</td>
<td>Michal Chodkiewicz: ZODS</td>
<td>Richard Cooper: CRYSTALS</td>
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<tr>
<td>13:00-14:00</td>
<td>Il Milione / Oscail / ShelXle / MoProSuite &amp; MoProViewer / Olex2</td>
<td>Arkadiy’s software / ZODS / EVAL / ISODISTORT / SIR2011 / XRD2Dscan</td>
<td>DISCUS / CRYSTALS / CCP4MG / DRAWxtl / Python for Crystallographers / MAX3D / XPac</td>
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<tr>
<td>Install Session</td>
<td>Il Milione / Oscail / ShelXle / MoProSuite &amp; MoProViewer / Olex2</td>
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<tr>
<td>14:00-14:45</td>
<td>Christian B. Hübschle, George M. Sheldrick: ShelXle</td>
<td>Branton J. Campbell, Harold T. Stokes: ISODISTORT</td>
<td>Martin Kröker, Brian Toby: DRAWxtl</td>
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<tr>
<td>15:30-16:15</td>
<td>Alejandro Rodriguez Navarro: XRD2Dscan</td>
<td>Jim Britten: MAX3D</td>
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<tr>
<td>16:15-17:00</td>
<td>Horst Puschmann: Olex2</td>
<td>Tomás Galbrich: XPac</td>
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<tr>
<td>Time</td>
<td>Friday August, 26</td>
<td>Saturday August, 27</td>
<td>Sunday August, 28</td>
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<tr>
<td>10:00-10:45</td>
<td>Valeri Petkov: RAD, ISAACS</td>
<td>Andrew Stewart: ADT3D</td>
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<tr>
<td>11:30-12:15</td>
<td>Isabel Usón: ARCIMBOLDO</td>
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<td>Silvina Pagola: PSSP</td>
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<tr>
<td>13:00-14:00</td>
<td>Bilbao Crystallographic Server / ARCIMBOLDO / HKL2MAP / ESCET / ANODE / ARP/wARP</td>
<td>RAD, ISAACS / EXPO2011 / EXPGUI / DiffPy / FOX / Smirnova's software</td>
<td>ADT3D / ANAELU / PSSP / 3Dctomo</td>
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<tr>
<td>14:00-14:45</td>
<td>Thomas R. Schneider: HKL2MAP - SHELX</td>
<td>Brian Toby: EXPGUI</td>
<td>Peter Oleynikov: 3Dctomo</td>
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<tr>
<td>14:45-15:30</td>
<td>Fabio Dall’Antonia: ESCET</td>
<td>Pavol Juhas: DiffPy</td>
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<tr>
<td>15:30-16:15</td>
<td>Andrea Thorn, George M. Sheldrick: ANODE</td>
<td>Vincent Favre-Nicolin: FOX</td>
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<tr>
<td>16:15-17:00</td>
<td>Tim Wiegels: ARP/wARP</td>
<td>Olga Smirnova: SDPD</td>
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