24th Congress and General Assembly of the International Union of Crystallography

Hyderabad International Convention Centre
21 - 28 August 2017, Hyderabad, India

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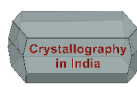
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www.iucr2017.org

Hyderabad will host the 24th Congress and General Assembly of the International Union of Crystallography (IUCr) between 21 - 28 August 20I7. This is a huge meeting held once every three years and top experts, scientists and students from all five continents will converge into India for this unique occasion. Details of the Congress are given on our website (www.iucr2017.org).

Crystallography is a subject of immense importance to those of us in drug design and drug development activities. Macromolecular crystallography finds immediate application in the design of New Chemical Entities (NCEs) and in elucidating mechanisms of various diseases. Small molecule crystallography is of vital importance in the study of pharmaceutical solid forms such as polymorphs, solvates, cocrystals and hydrates. The three important techniques of powder diffraction, single crystal diffraction and electron diffraction will be highlighted in the 24th Congress. To facilitate the participation of scientists and research managers from the Indian pharmaceutical industries, we have concentrated the pharma part of the program on 21, 22, 23 and 24 August 2017. The highlights include a choice of workshops on 21 August 2017 one of which may be selected by every registered participant. Keynote lectures by Dario Braga, David Bryce, Matteo Leoni, Ashwini Nangia and Neil Champness are of direct relevance to the pharma industry. A microsymposium on 23 August on terminology issues in crystal engineering will highlight the implications of correctly defining terms such as polymorph, cocrystal and hydrate. Solid state NMR makes its appearance in an IUCr Congress for the first time. The highlight of the program is a special session on collaboration between Academia, Industry and Government in drug design and drug development. This session will be chaired by Girish Sahni, DG CSIR, Government of India and will include as speakers Gautam R. Desiraju, Stephen R. Byrn, Girish Sahni, Rakesh K. Khandal and A. Venkateswarlu. The discussion will stress that very serious collaborations between these three domain expert groups is vital for the structured progress of drug development in India.

Considering the topical relevance of the 24th IUCr Congress to the day-to-day and long term activities of the pharma industry in India, the Local Organizing Committee (LOC) is pleased to offer a special 2-day registration package for Rs. 15,000 (21 to 22 August) and a 4-day registration package for Rs. 30,000 (21 to 24 August) to scientists and managers in the Indian pharmaceutical industry.

To avail of these special offers, please contact registrations@iucr20l7.org as soon as possible.

Day 1 (Monday, 21 August 2017)

Full and half-day workshops will be held on 21 August 2017 in Hyderabad International Conventional Center and should conclude in time for participants to be able to attend the opening ceremony of the Congress. You may select any one of the following, which will be covered within your registration payment (includes lunch).

Workshop 1	X-Ray Absorption Spectroscopy for the Crystallographer
Workshop 3	Rigaku Oxford Diffraction: CrysAlis^{Pro} and Olex^2 Workshop
Workshop 4	Cambridge Structural Database Workshop: Communication, Education and Research
Workshop 5	COMCIFS Dictionary Writing Workshop
Workshop 6	Electron Diffraction for Materials Science and Pharmaceutical Applications

W1 X-Ray Absorption Spectroscopy for the Crystallographer
Hyderabad, 21 August 2017

This one-day, free tutorial workshop will provide an overview of the physics and chemistry of X-ray Absorption Spectroscopy with a particular emphasis on its complementarity with diffraction techniques. The curriculum will include introductions to beamline instrumentation, measurement methods, and methods of data processing and analysis.

This workshop, which is organized by the IUCr XAFS Commission and the International X-ray Absorption Society, with the local support from the Board of Research in Nuclear Science (India), will be held on 21 August 2017 in HICC.

Chairs:

Christopher Chantler	University of Melbourne, Australia	e-mail: chantler@unimelb.edu.au
Farideh Jalilehvand	University of Calgary, Canada	e-mail: faridehj@ucalgary.ca

Local organizer:

Dibyendu Bhattacharyya	Bhabha Atomic Research Centre, India	e-mail: dibyendu@barc.gov.in

W3 Rigaku Oxford Diffraction: CrysAlis^{Pro} and Olex^2 Workshop
Hyderabad, 21 August 2017

This workshop will be split into two sections. The first will cover how best to collect and process your data within CrysAlis^{Pro}. The second half is dedicated to solving and refining your structures in Olex^2.

SESSION 1:

CrysAlis^{Pro} is a powerful and freely available data processing program that is able to read images from most commercially available detectors, whether or not the data was collected with CrysAlis^{Pro}. The software is capable of handling complex crystals, including twinned, multiphase, and incommensurate samples. Using a range of examples, the aim is to teach both standard and non-standard data processing workflow. Specifically, data integration (software strategies and settings; frame scaling; empirical absorption correction), data reduction (face-indexed absorptions corrections, beam profile corrections), and space group determination, will be covered. This session is ideal for participants either collecting or just processing data with CrysAlis^{Pro}.

SESSION 2:

Olex^2 handles very complex crystallographic tasks through an intuitive GUI. The graphical user interface is the result of 10 years of striving to provide the best possible experience to modelling even the most challenging structures with ease. The workshop will begin by hands-on routine structure solution and refinements within Olex^2, highlighting the general workflow of the program. This is ideal for novices in crystallography or those new to Olex^2. Following on from this, more in-depth samples will be tackled, for example those with disorder. Finally there will be some time spent on preparing your structure for publication. Participants will generate comprehensive CIF based on all experimental information available from the start of the experiment to the final stages of the refinement. They will also be generating reports and include molecular graphics suitable for publication submission.

Note: In order to ensure efficient use of the workshop time, participants will be asked to download, install, and test the software on their personal Windows laptop prior to the workshop. Datasets and documentation will also be made available for download.

Chairs:

Alexandra Griffin	Rigaku Oxford Diffraction	e-mail: alex.griffin@rigaku.com
Fraser White	Rigaku Oxford Diffraction	e-mail: fraser.white@rigaku.com
Takashi Sato	Rigaku Oxford Diffraction	e-mail: takashi.sato@rigaku.com
Horst Puschmann	OlexSys	e-mail: horst@olexsys.org

W4 CSD Workshop: Communication, Education and Research
Hyderabad, 21 August 2017

The Cambridge Structural Database (CSD) is the world's repository for small-molecule organic and metal-organic crystal structures, containing more than 8,50,000 entries. The Cambridge Crystallographic Data Centre (CCDC) not only distributes the CSD but also provides a comprehensive set of software tools that enable the valuable structural data to be searched, analysed, visualised and explored. This full-day workshop on the CSD and its associated software is split into two half-day sessions.

SESSION 1: Deposit, access, visualise, educate
This first session of the workshop will highlight how free services available through CSD-Community can exploit the knowledge contained in the CSD to aid both education and research.
Topics covered will include:
- CSD Deposition tools including validation and integrity checks
- Sharing and accessing structures
- Educational resources and tutorials
- The production of high impact graphics and movies

SESSION 2: Advanced research applications
The second session of the workshop will take attendees through a range of fundamental, intermediate and advanced research applications of the CSD Python API. The CSD Python API is a powerful platform, now installed automatically alongside the CSD desktop software, which provides programmatic access to the complete range of CSD data and functionality. We will help you put together bespoke analysis as well as tailored application scripts to address common challenges in a diverse range of structural research applications, from fundamental crystallography to drug discovery and development.

Note: Attendees should already have access to the CSD (including the CSD Python API) through their institution's CSD licence,but for any attendees without an existing license, we will provide workshop licences in advance. Participants will be expected to bring along their own laptops and to have already installed the CSD software on their laptop prior to the workshop.

Chairs:

Amy Sarjeant	Cambridge Crystallographic Data Centre, Piscataway, NJ, USA
Peter Wood	Cambridge Crystallographic Data Centre, Cambridge, UK
Suzanna Ward	Cambridge Crystallographic Data Centre, Cambridge, UK
Andrew Maloney	Cambridge Crystallographic Data Centre, Cambridge, UK
	For questions, email: teaching@ccdc.cam.ac.uk

W5 COMCIFS Dictionary Writing Workshop
Hyderabad, 21 August 2017

The Dictionary Writing Workshop will provide participants with the skills to create high-quality dictionary definitions and complete data dictionaries suitable either for inclusion within the CIF/mmCIF framework or as standalone dictionaries for use within other data frameworks, such as NeXus. Participants will be guided during practical sessions towards the goal of producing a complete dictionary or set of additional definitions in a scientific domain of interest to them.

Aims:

At the end of the workshop, participants will be able to:

- Understand the role that dictionaries play in data specifications
- Understand how data names are stored in a variety of data formats (including "3-column ASCII"/ CIF/ NeXus)
- Construct a high-quality data name definition
- Construct a DDL2/m domain dictionary potentially building on previously-existing dictionaries and/or previously-existing data standards

Participants wishing to construct a dictionary for a particular domain are encouraged to bring a wish list of the items for inclusion in the dictionary to the workshop, and will be guided throughout the workshop in constructing their particular dictionary.

Prerequisites: There are no specific requirements. In particular, no programming or CIF experience is assumed.

Chairs:

James Hester   ACNS, ANSTO, Australia   email: jamesrhester@gmail.com

W6: Electron Diffraction for Materials Science and Pharmaceutical Applications
Hyderabad, 21 August 2017

This workshop will focus on applications of electron diffraction in materials science and pharmaceuticals. After a basic introduction to transmission electron microscopy (TEM) and electron diffraction (ED) there will be an in depth analysis of the latest state-of-the-art applications in materials science and crystal structure analysis using electron diffraction. This will give a unique opportunity for young and senior scientists from industry and academia to learn about exciting latest results in this area. There will be useful case studies for solving pharmaceutical crystal structures with ED along with amorphous and nanomaterials characterization, orientation, phase, texture maps at the nanometer scale for alloys, metals, semiconductors and organics.

NanoMEGAS SPRL, Belgium (http://www.nanomegas.com/pharma) is the workshop organizer working in close collaboration with leading Indian academics and scientists from the materials science and pharmaceutical industry communities.

http://www.nanomegas.com/IUCR2017EDWorkshop

Chairs:

Stavros Nicolopoulos   email: info@nanomegas.com
Partha Pratim Das   email: partha@nanomegas.com

Local organizer:

Partha Ghosal   DMRL   email: dr.parthaghosal@gmail.com
Ram K. R. Jetti   Mylan Laboratories Ltd   email: jetti@iucr2017.org
Vishweshwar Peddy   Dr. Reddy's Laboratories   email: vishweshwarp@drreddys.com

Day 2 (Tuesday, 22 August 2017)

KEYNOTE:

KN-01: X-ray Absorption Spectroscopy and Chemical Speciation: from Archaeology to Biology
Speaker: Farideh Jalilehvand
Tuesday, 22 Aug 0900 hrs

KN-02: Making crystals with a purpose
Speaker: Dario Braga
Tuesday, 22 Aug 0900 hrs

KN-03: Soft quasicrystals
Speaker: Ron Lifshitz
Tuesday, 22 Aug 0900 hrs

KN-04: Structure and mechanism of respiratory complex I
Speaker: Leonid Sazanov
Tuesday, 22 Aug 1800 hrs

KN-05: Structure and properties of materials by solid-state nuclear magnetic resonance (SSNMR) observables
Speaker: David Bryce
Tuesday, 22 Aug 1800 hrs

KN-06: Total scattering study of chaotic/statistical microstructure with traditional crystallographic tools
Speaker: Matteo Leoni
Tuesday, 22 Aug 1800 hrs
(Sponsored by Anton Paar)

MICROSYMPOSIA:

Tuesday, 22 August 2017 1030 - 1305 hrs

Title	Chairs	Speakers
Biological Macromolecules (Structure) MS-001: Analysis and validation of protein ligand structures	Bohdan Schneider, Andreas Heine	Genji Kurisu, Sivakumar Sekharan, Orly Dym, Dorothee Claudia Liebschner, Kurt L Krause
Crystal Engineering of MOFs & Open Framework Compounds MS-002: Crystallographic approach for designing new metal organic frameworks	Qiaowei Li, Felipe Gandara	Mohamed Eddaoudi, Shane Telfer, Bu Xian-He, Stuart Robert Batten, Peter Andrew Wood, Santiago Garcia-Granda
Crystal Engineering of Organic & Pharmaceutical Compounds MS-003: Crystal engineering solutions to improve pharmaceutical tableting	Thomas Hartman, Changun Calvin Sun	Arvind Bansal, Venu R. Vangala, Lewis L. Stevens, Srinivasulu Aitipamula, Siti Fatimah Ibrahim, Sandeep S. Zode
Instrumentation techniques and/or Computation MS-004: Novel direct methods for electron diffraction and imaging	Stavros Nicolopoulos, Partha Ghosal	Fu-Rong Chen, Yasar Krysiak, Enrico Mugnaioli, Igor Nederlof, Jonas Angstrom
Instrumentation techniques and/or Computation MS-005: Total scattering	Eduardo Granado, Katherine Page	Despina Louca, Philip Anthony Chater, Nalini Ganapathy Sundaram, Anthony Phillips, Akihiko Machida
Instrumentation techniques and/or Computation MS-006: Computational materials design	Samrath Lal Chaplot, Artem Oganov	Eugeny V. Alexandrov, Matthew Dunstan, Sandro Scandolo, Ivan Kruglov, Jonathan Michael Skelton, John Rodgers
Materials and Minerals MS-007: Topology and symmetry of modular structures	Isabella Pignatelli, Sergey V. Krivovichev	Berthold Stöger, Marie Colmont, Oleg Siidra, Stuart James Mills, Vadim M. Kovrugin, Diana Olegovna Nekrasova, Anastasiya Igorevna Zadoya

Title	Chairs	Speakers
Physical and/or Fundamental MS-008: Magnetic order and its consequences	Arsene Goukassov, Takashi Kamiyama	Arsene Goukassov, Takashi Kamiyama, Sanjay Singh, Javier Campo, Giuditta Perversi, Ryszard Zach
Biological Macromolecules (Function) MS-009: Enzymes, mechanism and drug design	Marjolein Thunnissen, Anthony Addlagatta	S Ramaswamy, Minoru Kubo, Andreas Heine, Yasufumi Umena, Shamayeeta Ray, Alice Parnell, Jacinthe Gagnon

Tuesday, 22 August 2017 1455 - 1730 hrs

Title	Chairs	Speakers
Biological Macromolecules (Structure) MS-010: Membrane proteins, lipid-protein interactions and membrane fusion	Arun Shukla, Margarida Archer	So Iwata, Kallol Gupta, Isabel Moraes, Diana R Tomchick, Peter Czabotar, Sarah Hannah, Anne Waldie
Crystal Engineering of MOFs & Open Framework Compounds MS-011: Applications of post-synthesis modified metal-organic frameworks	Myoung Soo Lah, Praveen Thallapally	Vaidhyanathan Ramanathan, Hoi Ri Moon, Guilllaume Maurin, Shalisa Malane Oburn, Bikash Garai, Margaret Damilola Olawale
Crystal Engineering of Organic & Pharmaceutical Compounds MS-012: Structure-property correlation in pharmaceutical solids	Javier Ellena, Christian W. Lehmann	Krunoslav Uzarevic, Jayprakash Amarpal Yadav, Alejandro Pedro Ayala, Changquan Calvin Sun, Andrew Gerrard, Patrick Maloney, Poonam Singh Thakur
Instrumentation techniques and/or Computation MS-013: Quantitative electron imaging and tomography	Andreas Rosenauer, Eric Van Cappellen	Ivan Lazic, Knut Müller-Caspary, Georg Haberfehlner, Peter Nellist, Duncan N. Johnstone
Instrumentation techniques and/or Computation MS-014: Advanced neutron sources in biological and materials sciences	Despina Louca	Ken Holst Andersen, Toshiji Kanaya, Werner Schweika, Estelle Mossou
Instrumentation techniques and/or Computation MS-015: In-situ and in-operando characterization of energy materials	Diego Lamas, Yang Ren	Valeri Petkov, Jose Antonio Alonso, Matthias Zschornak, Ivan Bobrikov, David Gordon Billing, Thomas Degen, Víctor Antonio De La Peña O'Shea, Meriem Medjani
Special Activities MS-016: New approaches in crystallographic teaching	Louise Dawe, Peter Moeck	Robert Mark Hanson, Gemma De La Flor Martin, Saulius Grazulis, Helen Elizabeth Maynard-Casely, Amy A. Sarjeant, Bill Duax
Physical and/or Fundamental MS-017: Extending the boundaries of crystallography	Manuel Loquias, Mois I Aroyo	Walter Steurer, Stephen Timothy Hyde, Tomonari Dotera, Espen Drath Boejesen, Alistair Overy, Lorraine Andrade Malaspina
Biological Macromolecules (Function) MS-018: Ion transport	Nakagawa Atsushi, Daniel Minor	Rachelle Gaudet, Jeff Abramson, Alexandru Radu Aricescu, Osamu Nureki

PARALLEL PROGRAM:

Academia/Industry/Government Collaborations in Drug Design and Drug Development

(22 August 1455 to 1730 hrs)

150 minutes session on academia/industry/government interaction in the area of solid state pharma and novel crystal forms for innovator and generic companies. Speakers represent academic, industrial and government agencies both in India and abroad.

Chair : Girish Sahni, Director-General, CSIR India.

Speakers :

Gautam R. Desiraju (IISc, Bangalore) will present a survey of solid forms that are of significance in the development of new drugs and why they are expected to show promise in the near future. Salts, cocrystals, solvates and amorphous forms are different solid state variations of a drug. Any of these forms is capable of existing in polymorphic modifications. All this greatly increases the structural landscape which the drug inhabits: this in turn is expected to be the key to property modulation. Notable among the properties that can be modified are solubility and permeability, thereby affecting bioavailability. The core inputs for this and related activity arises from the field of crystal engineering and the possibilities for logic driven solid state synthesis through supramolecular heterosynthons.

His talk title, "API solid forms and the crystal structure landscape".

Stephen R. Byrn (Purdue, USA), will summarize the regulatory science of solid-state chemistry. The FDA defines regulatory science as the science of developing new tools, standards, and approaches to address safety, efficacy, and quality. The role of solid-state chemistry will be outlined. The Q1/Q2/Q3 approach to determine equivalence will be used: Q1 - same ingredients, Q2 - same amounts of ingredients, and Q3 has a broader meaning related to same structure, microstructure, and physical/chemical properties. From the perspective of solid-state chemistry, Q3 would mean same solid-state structure. The determination of Q3 involves a range of crystallographic studies including powder diffraction, single crystal studies, and pair distribution function analysis.

His talk title, "Regulatory Science and the Solid State Chemistry of Drugs".

Girish Sahni (CSIR Headquarters) will describe his experiences with drug design based on macromolecular crystallography. Critical and intricate structural details associated with streptokinase, a bacterial thrombolytic protein, were gleaned from X-ray and solution studies to design newer drug candidates with smarter and clinically useful functions. Crystallography is important in drug design and redesign, as well as in gaining deep mechanistic insights but when the resolution is limited, the available structures do not represent the full complement of polypeptide partners relevant to the biology of the multi-component system. Streptokinase represents one such example.

His talk title, "Quasi-structural studies in the redesign of a clot-buster protein drug".

Rakesh K. Khandal (India Glycols) will talk on success factors for drug processing and manufacture. Drug discovery involves a large number of steps before a desired drug molecule is introduced in the market. Continuous research and development efforts must come up with novel and innovative molecules for the purpose. One of the key aspects of drug discovery pertains to the development and validation of chemical processes to manufacture the desired molecule. Often, industry units keep a watch on the molecules that are going off-patent. By the time they are allowed to manufacture products that are already off-patent, they must be ready before-hand with a cost effective process. India is already in a leadership position as far as generics are concerned. In the present era of competition, Indian industry would need technical support from organisations like CSIR.

His talk title, "Success factors for drug processing and manufacture".

A. Venkateswarlu (DRILS, Hyderabad), will present a high level SWOT analysis of pharmaceutical cocrystals and their potential role in design and development of therapeutics. The emerging impact of cocrystals as alternate solid forms with pharmaceutical applications, both in the drug substance and the drug product, presents itself as a powerful opportunity to address unmet medical needs. Typically, the landscape of new chemical entities (NCEs) and active pharmaceutical ingredients (APIs) has been dominated by solid forms, involving either the native chemical forms or salts, solvates and corresponding polymorphs thereof. Cocrystal forms of such NCEs or APIs as novel compositions of matter offer not only IP potential but also non-obvious therapeutic profile coupled with means to favorably impact the life cycle management.

His talk title, "Pharmaceutical Cocrystals: a SWOT Perspective".

Day 3 (Wednesday, 23 August 2017)

KEYNOTE:

KN-07: Virulence factors and host defenses to viral infection
Speaker:
Janet Smith
Wednesday, 23 Aug 0900 hrs

KN-08: Pharmaceutical solids in crystal engineering
Speaker:
Ashwini Nangia
Wednesday, 23 Aug 0900 hrs

KN-09: Magnetic degrees of freedom in emerging materials
Speaker:
Dmitry Khalyavin
Wednesday, 23 Aug 0900 hrs

KN-10: Taking Snapshots of Photosynthetic Water Oxidation with an X-ray Laser
Speaker: Vittal Yachandra
Wednesday, 23 Aug 1800 hrs

KN-11: Stochastic polarity formation: Molecular crystals, composite materials and natural tissues
Speaker: Jurg Hulliger
Wednesday, 23 Aug 1800 hrs

KN-12: Charge density as a powerful tool to predict reactivity
Speaker:
Dietmar Stalke
Wednesday, 23 Aug 1800 hrs

MICROSYMPOSIA:

Wednesday, 23 August 2017 1030 - 1305 hrs

Title	Chairs	Speakers
Biological Macromolecules (Structure) MS-019: Interactions between proteins and nucleic acids	Markus Wahl, Barnali Chaudhuri	Wei Yang, Michal Hammel, Osamu Nureki, Udo Heinemann, Ruchi Anand, Xiao-Dong Su
Crystal Engineering of MOFs & Open Framework Compounds MS-020: Controlling dimensions of porous crystalline polymers	Wei Wang, P S Mukherjee	Xin Zhao, Tapas Kumar Maji, Wei Wang, Debajyoti Ghoshal, Tatiana Timofeeva, Boomishankar Ramamoorthy, Katherine Chulvi-Iborra
Special Activities MS-021: Terminology issues in crystal engineering	Christer Aakeröy, Carolyn P. Brock	Gautam R. Desiraju, Pierangelo Metrangolo, Jagadese J Vittal, Leonard Richard MacGillivray, Christer Bjorn Aakeroy
Instrumentation techniques and/or Computation MS-023: Synchrotron and XFEL for materials at ambient and extreme conditions	John Tse, Yasuo Ohishi	Luke Fletcher, Valery Nosik, Michael Hanke, Norimasa Ozaki, Irimpan Mathews, Ahmed S. A. Mohammed
Instrumentation techniques and/or Computation MS-024: NMR Crystallography and related methods	Manish Mehta	James Harper, Gerd Buntkowsky, Perunthiruthy Madhu, Sachin Rama Chaudhari, Brijith Thomas, Yusuke Nishiyama
Materials and Minerals MS-025: Crystallography of battery materials	Prabeer Barpanda	Michal Leskes, Karena W. Chapman, Maria Diaz-Lopez, Toru Ishigaki, Falk Meutzner, Hamdi Ben Yahia

Title	Chairs	Speakers
Physical and/or Fundamental MS-026: A bridge between two worlds: Graphs as structural descriptors	Hamilton Barbosa Napolitano, Bernd Souvignier	Jean Guillaume Eon, Eduard Camangian Taganap, Olga Sidorova
Instrumentation techniques and/or Computation MS-027: Synchrotron-based X-ray techniques and the environment	Richard Garrett, Hugh Harris	Bhoopesh Mishra, Marine Cotte, Yang Ren

Wednesday, 23 August 2017 1455 - 1730 hrs

Title	Chairs	Speakers
Biological Macromolecules (Structure) MS-028: Long wavelength applications in macromolecular crystallography	Christoph Mueller-Dieckmann, Dorothee Liebschner	Gordon Leonard, Vincent Olieric, Armin Wagner, Naohiro Matsugaki, James Parkhurst, Guillaume Pompidor
Crystal Engineering of MOFs & Open Framework Compounds MS-029: Porous framework materials for gas adsorption	Hoi Ri Moon	Nak Cheon Jeong, Haiqing Li, Christian James Doonan, Tanay Kundu, Carlotta Giacobbe, Sandeep Singh Dhankhar
Crystal Engineering of Organic & Pharmaceutical Compounds MS-030: Crystallization mechanisms of small molecule organic materials	Jaime Gomez Morales, Raj Suryanarayana	Tonglei Li, Ian Rosbottom, Isaac Rodriguez-Ruiz, Abdul Ajees Abdul Salam, Ilia Guzei
Instrumentation techniques and/or Computation MS-031: Nanoparticles / nanostructures	N. Ravishankar	Bo Brummerstedt Iversen, Matthew Cliffe, Tom Willhammar, Oleg Prymak, Alison Jeanine Edwards, Katharine Lynn Page, Kullaiah Byrappa
Special Activities MS-032: Crystallography courses around the world	Annalisa Guerri, Juan Manuel Garcia Ruiz	Amy A. Sarjeant, Alessia Bacchi, Diego Germán Lamas, Michele Zema, Fermín Otálora, Andreas Roodt, Ivana Kuta Smatanova, Dubravka Sisak Jung
Instrumentation techniques and/or Computation MS-033: Magnetic diffuse scattering and magnetic PDF analysis	Werner Schweika, Branton Campbell	Benjamin Allen Frandsen, Joseph Paddison, Shang Gao, Nikolaj Roth
Materials and Minerals MS-034: Synthesis and properties of multi ferroics and multi-functional materials	La-Sheng Long, Francesco Mezzadri	Nami Matsubara, Jorge Hernández-Velasco, Maria Paula Seabra, T Vijayakanth, Roksana Parvin
Physical and/or Fundamental MS-035: Crystal structure relationships and their applications	Wolfgang Schmahl, V. M. Talanov	Gervais Chapuis, Sergey V. Krivovichev, Branton Campbell, Dhananjai Pandey, Stefan Adams, Swastik Mondal
Biological Macromolecules (Function) MS-036: Structural immunology and receptor signalling	Mike Lawrence, Yvonne Jones	Ian Andrew Wilson, Stephanie Gras, Kerry Marie Goodman, Yibin Xu, Michael William Parker, Arvind Sharma

Day 4 (Thursday, 24 August 2017)

KEYNOTE:

KN-13: Two decades of proteasome research: From structure to application
Speaker: Michael Groll
Thursday, 24 Aug 0900 hrs

KN-14: Molecular Organisation: Working with Molecules on the Nanoscale
Speaker:
Neil Champness
Thursday, 24 Aug 0900 hrs

KN-15: Indian geometric patterns, compared to Persian and Moroccan styles
Speaker:
Jean Marc Castera
Thursday, 24 Aug 0900 hrs

KN-16: Small-angle x-ray scattering for biological macromolecules
Speaker:
Dmitri Svergun
Thursday, 24 Aug 1800 hrs
(Sponsored by Rigaku)

KN-17: Topological approach for the design of new materials
Speaker:
Vladislav Blatov
Thursday, 24 Aug 1800 hrs

KN-18: The science is in the data
Speaker:
John Helliwell
Thursday, 24 Aug 1800 hrs
(Sponsored by Rigaku)

MICROSYMPOSIA:

Thursday, 24 August 2017 1030 - 1305 hrs

Title	Chairs	Speakers
Biological Macromolecules (Structure) MS-037: Macromolecular structures by hybrid methods	Jill Trewhella, Amit Sharma	Jonathan Grimes, Frank Richard Gabel, Madhanagopal Anandapadamanaban, Jennifer Anne Channell, Yujung Jeon, Brinda Vallat
Crystal Engineering of MOFs & Open Framework Compounds MS-038: Porous framework materials for separation	Jie-Peng Zhang	Praveen Thallapally, Wei Shi, Guangshan Zhu, Satoshi Horike, Kaushik Dey, Renjith S. Pillai
Crystal Engineering of Organic & Pharmaceutical Compounds MS-039: Structural chemistry in 2-D: Crystal growth, surface structure and morphology	Matthew Hill, Bo Wang	Matthew Hill, Jayanth Channagiri, Jie-Peng Zhang, Bo Wang, Arjun Halder
Instrumentation techniques and/or Computation MS-040: Microstructure, defects, stress and strain determination and modelling with powder diffraction data	Takashi Ida, Davor Balzar	Radomir Kuzel, Rene Guinebretiere, Alexander Ulyanenkov, Bob He, Roman Svetogorov, Hantaro Ozawa
Instrumentation techniques and/or Computation MS-041: Advances in computational methods for powder diffraction	Basab Chattopadhyay, Andy Fitch	Alan Anthony Coelho, Roland Resel, James William Lewis, Paolo Bosetti, Akito Sasaki, Manju V V
Instrumentation techniques and/or Computation MS-042: High-resolution spectroscopy	Dimosthenis Sokaras, Dennis Nordlund	John Thomas Vinson, Christoph J. Sahle, Ratibor Chumakov
Physical and/or Fundamental MS-043: Models for refining the electron density from elastic scattering. Bob Stewart's legacy	T. N. Guru Row, Paulina Dominiak	Simon Grabowsky, Christian Jelsch, Kiyoaki Tanaka, Birger Dittrich, Kasper Tolborg, Suman Kumar Mandal

Title	Chairs	Speakers
Special Activities MS-044: Structural databases as teaching tools - Part A (macromolecules)	Joel Sussman, Christine Zardecki	Jaime Prilusky, Shuchisimta Dutta, Urmila Kulkarni-Kale, Matthew J Conroy, Alexey Kikhney, Hirofumi Suzuki
Special Activities MS-045: Structural data bases as teaching tools - Part B (organics, minerals)	Amy Sarjeant, Graciela Delgado	Louise Nicole Dawe, Simon John Coles, José Miguel Delgado, Edgar Eduardo Villalobos

Thursday, 24 August 2017 1455 - 1730 hrs

Title	Chairs	Speakers
Biological Macromolecules (Structure) MS-046: Macromolecular structure determination at XFEL sources	Arwen Pearson, Makina Yabashi	Junko Yano, Eriko Nango, Ruslan Kurta, Allen Milster Orville, Johanna Hakanpää
Crystal Engineering of MOFs & Open Framework Compounds MS-047: Crystalline materials characterization with combined techniques	Koen Janssens, Alejandro Ayala	Izumi Nakai, Marc Walton, Eric Dooryhee, Magdalena Ola Cichocka, Marcelo B Andrade, Laura Cañadillas-Delgado, Peter Moeck
Crystal Engineering of Organic & Pharmaceutical Compounds MS-048: Supramolecular synthons at the confluence of theory and practice	P Venugopalan, Catharine Esterhuysen	Lee Brammer, Narasimha Moorthy Jarugu, Susan Ann Bourne, Edward R.T. Tiekink, Ivan Fedyanin, Izabela D. Madura
Instrumentation techniques and/or Computation MS-049: In-situ and in-operando characterization of catalytic and functional materials	Antonio F. Moreira Dos Santos, Miguel Delgado	Peter Chupas, Daniel Olds, Jonathan Hanson, Olga Bulavchenko, Masao Yonemura, Daniel Shoemaker
Instrumentation techniques and/or Computation MS-050: Small-Angle Scattering studies of biomacromolecular kinetics	Pau Bernado, Clement Blanchet	Hironari Kamikubo, Lise Arleth, Martha Elisabeth Brennich, Sébastien Teychené, Andrey Gruzinov, Antonia Neels
Instrumentation techniques and/or Computation MS-051: Recent developments in XAFS spectroscopy: Theory, instrumentation and data analysis	Konstantin Klementiev	Edmund Welter, Christopher Thomas Chantler, Keisuke Hatada, James Reginald Hester, Konstantin Klementiev, Christopher Thomas Chantler
Materials and Minerals MS-052: Minerals/gems in industrial applications	Patrick Mercier, Fermin Otalora	Jaime Gomez Morales, Matthew Ryan Rowles, Camelia Veronica Stan, Meenakshi Pokhriyal, Luis Guillermo Romero-Esquivel, Imane Bouali
Special Activities MS-053: Scientific value of raw data	Loes Kroon-Batenburg, Brian McMahon	George Phillips, Marek Piotr Grabowski, James Parkhurst, Christopher Thomas Chantler, Andreas Foerster, Kamil Filip Dziubek
Biological Macromolecules (Function) MS-054: Mechanisms of bacterial resistance	Natalie Strynadka, Miquel Coll	Albert Marinus Berghuis, Mark Rutherford Sanderson, Juan A. Hermoso, Aravindan Ilangovan, Dilip Badgujar, Chun-Jung Chen

Registration

There are two registration packages that will be of high interest to the pharmaceutical industry.

The first is a 2-day package for Rs. 15,000 on 21 - 22 August.

The second is a four day package for Rs. 30,000 on 21 - 24 August.

S. No.	Package	Amount	Dates
1	2 day package	INR 15,000	21 - 22 August
2	4 day package	INR 30,000	21 - 24 August

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- Lunch, AM and PM coffee breaks
- Congress bag containing program and other material
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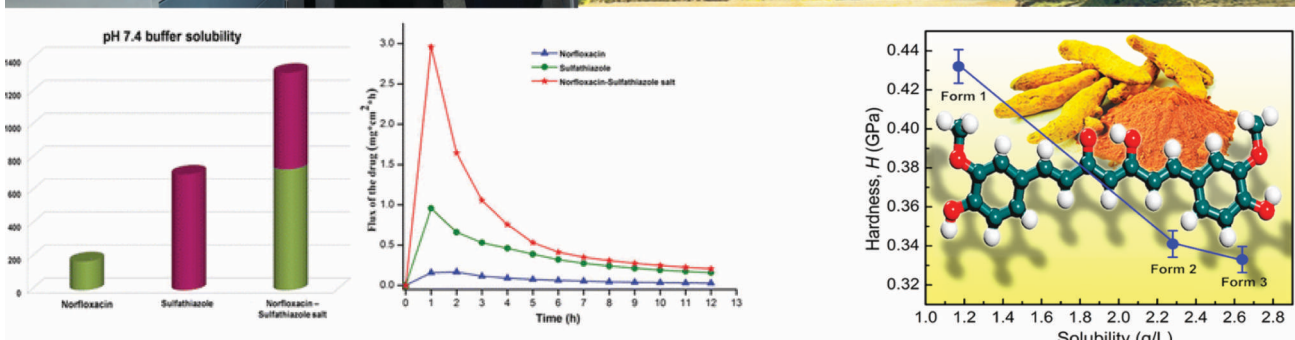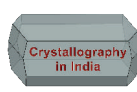
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