

Commission	President	Members	Indications for the Scientific Program of XX IUCr
Aperiodic Crystals	Sander van Smaalen	M. de Boissieu, S. Lidin, R. Lifshitz, M. Onoda, V. Petricek, K. Saitoh, N. L. Speziali, R. Withers	<p>Two microsymposia,</p> <p>1. The structure of quasicrystals. (dedicated to the newest structure refinements, but also reports on diffuse scattering, electron microscopy and high-pressure studies.</p> <p>2) Incommensurate aspects of crystal structures. (dedicated to the reports on structural studies on important classes of incommensurately modulated and incommensurate composite crystals, e.g. Charge-density, wave compounds and Composite perovskites. Furthermore it should include reports on new methods of structural analysis of incommensurate crystals, e.g. the Maximum Entropy Method, Direct Methods and Rietveld refinements, as well as diffuse scattering and scattering studies on phase transitions as a function of temperature or pressure.</p> <p>Keynote lectures:</p> <p>1. Quasicrystals.</p> <p>2. Incommensurate crystallography.</p>
Biological Macro-molecules	Jules Mitchell Guss	E. Arnold, J. L. Dattagupta, B. W. Dijkstra, M. Hackert, G. Oliva, T. Tsukihara, D. Turk, L. Van Meervelt	No indication
Charge, Spin and Momentum Densities	Prof. Claude Lecomte	C. Gatti, K. Hämäläinen, B. Iversen, P. Montano, F. Sacchetti, N. Sakai, J. C. H. Spence, V.G. Tsirelson, Y. Wang	<p>1) Charge Spin and Momentum density and Quantum Chemistry (bonding , interactions , properties)</p> <p>2) New methodologies: combine density, charge spin and momentum methods, combined X-Ray and electron diffraction methods , diffraction and spectroscopic methods ,time resolved diffraction and frontiers results (proteins , heavy atoms etc..)</p>
Powder Diffraction	Prof. Robert Dinnebier	D. Balzar, W. I. F: David, M. Delgado, R. Delhez, A. N. Fitch, C. Hubbard, G. J. Kruger, N. Masciocchi, I. Madsen, R. L. Snyder	<p>1) Microstructural Properties from Powder Diffraction Data</p> <p>2) Powder Diffraction on Nano- and Mesoporous Materials</p> <p>3) Synchrotron and Neutron Powder Diffraction</p> <p>4) High Energy X-Ray Powder Diffraction</p> <p>5) Non-Ambient Powder Diffraction and Kinetics Studies</p> <p>6) High Pressure Powder Diffraction</p> <p>7) Structure Determination from Powder Diffraction Data (Organics)</p> <p>8) Structure Determination from Powder Diffraction Data (Inorganics)</p> <p>9) Industrial Applications of Powder Diffraction and Standardization</p> <p>10) Powder Diffraction as an Educational Tool</p> <p>11) Powder Diffraction in Drug Design and Manufacture</p> <p>12) Powder Diffraction in Mining and Mineral Processing</p> <p>13) Powder Diffraction in Forensic Science</p> <p>14) Powder Diffraction in Earth and Environmental Sciences</p> <p>15) Powder Diffraction in Astro- and Planetary Studies</p> <p>16) Time-resolved powder diffraction for materials production and processing</p> <p>17) Diffraction from thin films</p>

Small-Angle Scattering	Jan Skov Pedersen	A. Allen, Y. Amemiya, P. Fratzl, T. M. Sabine, D. Svergun, P. Thiyagarajan, I. Torriani	One-day tutorial workshop on SAS the day before the start of the conference. Four symposia: (1) Methods for structure determination of macromolecules and macromolecular assemblies for solution small-angle scattering (Dr. Disvergun would be the ideal chairman for such a symposium). (2) Analysis of two-dimension small-angle scattering data from anisotropic materials (e.g. polymers, alloys) (suggested chair: Dr. P. Fratzl). (3) Contrast variation by combining SANS and SAXS. (4) High resolution tomography or 3D visualization methods using small-angle scattering (suggested chair: Dr. A. Allen from NIST)
Structural Chemistry	Lee Brammer	A. Bacchi, V. K. Belsky, D. Braga, G. R. Desiraju, T. W. Hambley, D. C. Levendis, G. Punte, D. Rice, H. Uekusa	speakers and audience would find more attractive if Symposia lasted longer than the traditional IUCr half-day. This could even be done by grouping 3-4 related microsymposia under a central theme.
Synchrotron Radiation	Prof. Ian Robinson	L. T. J. Delbaere, H. Graafsma, S. M. Gruner, H. Kitamura, G. N. Kulipanov, T. Matsushita, D. McMorrow, J. Schneider	Microdiffraction, Inelastic X-ray Scattering in Biology <i>Louis Delbaere</i> writes: A suggested speaker is Zbigniew Dauter from Brookhaven National Laboratory and a possible topic is, "Data Collection Strategies for Protein Crystals with Synchrotron Radiation". Dr. Dauter had extensive experience at the EMBL Outstation in Hamburg and he has been at Brookhaven for the past several years
High Pressure	Martin Kunz	I. N. Goncharenko, N. Hamaya, R. J. Hemley, W. F. Kuhs, J. S. Loveday, M. Mezouar, J. B. Parise, S. Tolbert, J. Tse, R. Winter	6 microsymposia on 6 successive sessions (3-days) plus 3 keynotes. MS 1) Novel Materials under HP (interest for the material science) 2) Liquids- and amorphous systems at HP 3) Structures, phase transitions and properties at HP 4) Biological and organic soft condensed material under pressure (interest Bio) 5) Crystallography at conditions of Earth- and Planetary Interiors (interest Mineralogy) 6) Computational crystallography applied to extreme conditions Speakers: 1) Malcolm McMahon (UK): on complex materials at HP 2) John Tse (Can): on theory and experiments in HP crystallography 3) Richard Templer (UK): on biological membranes at HP Alternative speakers: 1) Paul Loubeyre (F): crystallography of molecular solids at extreme conditions 2) Guillaume Fiquet (F): HP crystallography in geophysics 3) Giulia Galli (USA): computational crystallography at HP 4) T. Yagi (Japan): Advances in the study of Earth and Planetary Materials 5) John Loveday (UK) neutron diffraction at non-ambient conditions 6) Paul McMillan (UK): the search for novel material under pressure.
Electron Diffraction	John C. H. Spence	A. Eades, J. Gjønnes, F.-h. Li, C. Roussouw, N. Tanaka, D. Van Dyck, X.-D. Zou	1) Cryomicroscopy (Biology). 2) Diffractive imaging with electrons and Xrays. (Joint session with free-electron laser group). 3) Precession cameras and nanoprobes for nanostructures One of these is a joint session with those doing pulsed synchrotron. Diffraction from nanostructures and proteins. Electron crystallography on minerals and nanosized materials

Inorganic and Mineral Structures	Prof. Giovanni Ferraris	I. D. Brown, G. Calestani, W. Depmeier, M. Jansen, A. M. Glazer, M. Matsui, D. Yu Pushcharovsky J. Rius, E. Tillmanns	1) Crystal chemistry of inorganic and mineral compounds; 2) Structure/properties relationships in inorganic and mineral structures of technological interest; 3) Inorganic and mineral structures at high pressure (Joint Session with the Commission on High Pressure); 4) Peculiar results on inorganic and mineral structures by neutron diffraction (JS with the Commission on Neutron diffraction); 5) Solution and refinement of inorganic and mineral structures by powder diffraction data (JS with the Commission on Powder Diffraction); 6) Electron crystallography applied to inorganic and mineral structures (JS with the Commission on Electron diffraction); 7) Impact of synchrotron radiation on the study of inorganic and mineral structures (JS with the Commission on Synchrotron radiation). 8) Modularity and modulation in inorganic and mineral structures (JS with the Commissions on Aperiodic crystal); 9) Peculiar computational aspects of inorganic and mineral structures (Joint Symp with the Commission on Computing).
Neutron Scattering	Prof. Michael Steiner	Y. Fujii, S. Harkema, A. W. Hewatt, J. D. Jorgensen, S. J. Kennedy, R. I. McGreevy, J. S. Pedersen, V. C. Rakhecha, S. K. Satija	4 microsymposia + Open Commission meeting. + 1 Satellite 1. Perspective of neutron crystallogr. at high power spallation sources 2. Stress and strain analysis in neutron scattering and synchrotron radiation – from basics to industrial application 3. Advanced functional materials (including molecular, biological, fuel cell, battery and other materials) 4. Neutron scattering in geo-science Satellite meeting requested " Novel superconductors, orbital and charge ordering in transition metal oxides: the impact of neutron and synchrotron experiments under extreme conditions". Furthermore, the Commission on Neutron Scattering favours an Open Commission meeting.
Crystal Growth and Characterization Materials	Prof. Roberto Fornari	D. F. Bliss, K. Byrappa, T. Duffar, T. Ohachi, R. Rudolph, G. Svensson, E. Vlieg, A. Voloshin, P. M. Dryburgh, G. Kostorz	1) polymorphism, 2) materials for energy storage and energy conversion, 3) in situ characterisation during crystal growth,
Crystallographic Computing	Prof. Antony Spek	I. D. Brown, L. M. D. Cranswick, V. Favre-Nicolin, R. W. Grosse-Kunstleve, A. Gualtieri, E. Merritt, S. Parsons, B. Vincent	1) Advances in computational methods for protein crystallography 2) Advances in computational methods for powder diffraction 3) Advances in computational methods for small molecule crystallography 4) Problems and solutions in programming robust CIF and XML into crystallographic software 5) Computational problems and solutions for quasi-crystal crystallography 6) Advances in computational methods incommensurate structures 7) Computational solutions for high-throughput service crystallography 8) Applying non-crystallographic algorithms to crystallography 9) Advances in computational methods for charge density studies 10) New Algorithms for Crystal structure prediction

Crystallographic Teaching	Prof. Reinhard B. Neder	J. D. Barnes, G. Chapuis, L. M. D. Cranswick, K. Crennel, M. E. Kastner, K. Ogawa, S. Parthasarathy, P. Spadon, V. S. Urusov	No Indications
XAES	Prof. D. Arvanitis	K. Asakura, K. Baberschke, B. Hedman, A. Michalowicz, S. Mobilio, A. Molenbroek, R. F. Pettifer	<p>Suggestions by S. Mobilio:</p> <p>Plenary lecture on the x-ray absorption to illustrate the systems for which the information on classic absorption (EXAFS) has been complementary on the information from diffraction. Amongst the speakers, prestigious names are those of G.N. Greaves, F. Boscherini, K. Hodgson, G.E. Brown who could give general overviews in the areas of Material Science, Semiconductors, Biology, and Environment. It is suggested a MS with the participation of them all or one or more on their specific topics.</p> <p>A session on the applications of the multiple scattering methods in the extended regions or in the threshold region can be useful to illustrate the evolution of the modern applications and their perspectives. In the first area, potential speakers are P. D'Angelo (Universita' di Roma) or A. Filippini (Universita' de L'Aquila). In the second area, very good results have been obtained from M. Benfatto (Frascati Labs). An American speaker, who can cover both aspects is J.J. Rehr (Washington University). If not covered already by other sectors, a space must be dedicated to the resonant diffraction (magnetic and non-magnetic). Here, we have some Italian speakers such as M. Altarelli sincrotrone Trieste), C.R. Natoli (Laboratori Nazionali di Frascati), L. Paolasini (European Synchrotron Radiation Facility). The magnetic aspects can be described from Vettier (Istituto Laue Langevin of Grenoble), who is an excellent speaker.</p>
Crystallographic Nomenclature	Prof. André Authier	E. Arnold, C. Pratt Brock, D.I. Brown, W. Clegg, G. Ferguson, J. P. Glusker, T. Hahn, S. R. Hall, J. R. Helliwell, V. Kopsky, G. Kostorz, Å. Kvick, D. B. Litvin, B. McMahon, D. M. Mills, U. Mueller, T. Ohta, E. Prince, M. G. Rossmann, R. B. Neder, H. Schenk, D. Schwarzenbach, U. Shmueli, D.G. Watson, H. Wondratschek	<p>1) "n-dimensional crystallography".</p> <p>No plan for an Open Commission Meeting</p> <p>Suggestion received by Theo Hahn about the "Commission on International Tables":</p> <p>i) Since the whole series of the International Tables is published, I have resigned from the chairmanship. I act as caretaker until the new chair arrives. I cannot speak for the Commission as far ahead as 2005 but I will advise my successor. (ii) Since the interests and expertises of the various volume editors are quite different, there has never been a single person to represent the I.T. Commission in the SPT. As a personal suggestion, I propose Prof. Uri Shmueli of Tel-Aviv University (editor of Volume B), who has great experience with International Tables, including its homepage. (iii) The major task for the new chairperson should be the organisation of an "Open Commission Meeting on International Tables", in which the new team and the new projects are illustrated. I organized such meetings at Seattle (1996) and Glasgow (1999).</p>