## Timetable & Room Plan for MS

<table>
<thead>
<tr>
<th>Room No.</th>
<th>Aug. 24</th>
<th>25</th>
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<tbody>
<tr>
<td></td>
<td>am (9:55-12:30)</td>
<td>pm (14:45-17:20)</td>
<td>am (9:55-12:30)</td>
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<tr>
<td>A-05MH</td>
<td>MS 1</td>
<td>MS 8</td>
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<td>F-12CH</td>
<td>MS 2</td>
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<td>D-1003</td>
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<td>C-1001,2</td>
<td>MS 4</td>
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<td>G-1202</td>
<td>MS 5</td>
<td>MS 12</td>
<td>MS 19</td>
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<td>B-05SH</td>
<td>MS 6</td>
<td>MS 13</td>
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<tr>
<td>E-1009</td>
<td>MS 7</td>
<td>MS 14</td>
<td>MS 21</td>
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## Timetable & Room Plan for MS

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<td>am (9:55-12:30)</td>
<td>pm (14:45-17:20)</td>
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<td>pm (14:45-17:20)</td>
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<td>A-05MH</td>
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<td>C-1001,2</td>
<td>MS 46</td>
<td>MS 53</td>
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<td>G-1202</td>
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<td>E-1009</td>
<td>MS 49</td>
<td>MS 56</td>
<td>MS 63</td>
<td>MS 70</td>
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</table>
Sunday, August 24 - Morning - Microsymposia

**A-05MH (MS 1)**

9:55-10:00

Opening Remarks

Large macromolecular complexes: Chairs: L. Malinina, J. Diag

Advances in graging incidence, reflectivity and diffuse scattering: Chairs: A. Allen, M. Ree

New algorithms for single crystal and powder diffraction: Chairs: F. Izumi, R. Cooper

10:00-10:30

**MS.01(C15)**

M. G. Rossmann: The structural basis for the mechanism of influenza virus polymerase complex with a nucleotide analog

**MS.02(C14)**

P. Mueller-Buschbaum: Recent advances in understanding 2.8-A models of GISA/X and GISA/N - nanobeads and in-situ X-ray microscopy

**MS.03(C18)**

R. W. W. Hooff: Reliable determination of absolute structure using small Bovjett complexes

**MS.04(C19)**

J. L. Bourhis: Small molecule toolbox

11:00-11:30

**MS.05(C17)**

M. Yusupov: Structures of the ribosome on different functional states

**MS.06(C17)**

B. Lee: Structural characterization using the multiple scattering effect in GISA/X

**MS.07(C18)**

L. Palatinus: The charge-flipping algorithm and related dual-space structure solution methods

11:30-12:00

**MS.08(C15)**

M. G. Vasyutyn: Structural basis of transcription: Structures of the bacterial RNA polymerase elongation complex

**MS.09(C17)**

M. Yusupov: Neutron reflectivity study of chain conformation in polyelectrolyte brushes at the liquid interface

**MS.10(C19)**

H. Nishimori: Closing the gap between single crystal and powder diffraction

12:00-12:30

**MS.11(C16)**

N. Numoto: Ligand-induced structural changes of giant hemoglobin

**MS.05(C19)**

G. Iacovazzo: Advances in methods and algorithms in EXP02008

Sunday, August 24 - Morning - Microsymposia

**G-1202 (MS 5)**

Modelization of structure of molecular compounds and implications for reactivity: Chairs: M. J. Calabro, N. E. Ghermani

10:00-10:30

**MS.04(1C19)**

T. Adschiri: Superstructural synthesis of organic inorganic hybrid materials

**MS.05(1C21)**

K. Kirchner: Soluble-state vs solid-state activity of iron-sulfide complexes: Stereoscopic and reversible kinetic behavior

11:00-11:30

**MS.06(1C21)**

D. Ehrentraut: Adsorption and reaction of bulk TiN crystals

**MS.07(1C21)**

K. Tatsumi: New synthetic route to iron-sulfide clusters modeling the active site of nitrogenase

11:30-12:00

**MS.08(1C21)**

K. Kajiyoshi: Vapor-phase hydrothermal preparation of titane fibers and nanotubes

**MS.09(1C21)**

N. Boumida: Advances in electrochemistry and applications to molecular reactivity

12:00-12:30

**MS.10(1C21)**

M. Kakehina: Functional ZnO from solution or titanate fibers and nanotubes

**MS.11(1C21)**

K. Kajiyoshi: Hydrothermal growth of metallic TiO2 nano-particles

10:00-10:30

**MS.04(2C22)**

M. Kakihana: Selective synthesis of nano-crystalline TiO2 polymorphs from new water-soluble titanium complexes

**MS.05(2C22)**

T. Adschiri: Superstructural synthesis of organic inorganic hybrid materials

11:00-11:30

**MS.06(2C22)**

D. Ehrentraut: Adsorption and reaction of bulk TiN crystals

**MS.07(2C22)**

K. Tatsumi: New synthetic route to iron-sulfide clusters modeling the active site of nitrogenase

11:30-12:00

**MS.08(2C22)**

M. Kakehina: Functional ZnO from solution or titanate fibers and nanotubes

**MS.09(2C22)**

N. Boumida: Advances in electrochemistry and applications to molecular reactivity

12:00-12:30

**MS.10(2C22)**

M. Kakehina: Functional ZnO from solution or titanate fibers and nanotubes

**MS.11(2C22)**

K. Kajiyoshi: Hydrothermal growth of metallic TiO2 nano-particles

10:00-10:30

**MS.04(3C23)**

M. Kakihana: Selective synthesis of nano-crystalline TiO2 polymorphs from new water-soluble titanium complexes

**MS.05(3C23)**

T. Adschiri: Superstructural synthesis of organic inorganic hybrid materials

11:00-11:30

**MS.06(3C23)**

D. Ehrentraut: Adsorption and reaction of bulk TiN crystals

**MS.07(3C23)**

K. Tatsumi: New synthetic route to iron-sulfide clusters modeling the active site of nitrogenase

11:30-12:00

**MS.08(3C23)**

M. Kakehina: Functional ZnO from solution or titanate fibers and nanotubes

**MS.09(3C23)**

N. Boumida: Advances in electrochemistry and applications to molecular reactivity

12:00-12:30

**MS.10(3C23)**

M. Kakehina: Functional ZnO from solution or titanate fibers and nanotubes

**MS.11(3C23)**

K. Kajiyoshi: Hydrothermal growth of metallic TiO2 nano-particles

10:00-10:30

**MS.04(4C24)**

M. Kakihana: Selective synthesis of nano-crystalline TiO2 polymorphs from new water-soluble titanium complexes

**MS.05(4C24)**

T. Adschiri: Superstructural synthesis of organic inorganic hybrid materials

11:00-11:30

**MS.06(4C24)**

D. Ehrentraut: Adsorption and reaction of bulk TiN crystals

**MS.07(4C24)**

K. Tatsumi: New synthetic route to iron-sulfide clusters modeling the active site of nitrogenase

11:30-12:00

**MS.08(4C24)**

M. Kakehina: Functional ZnO from solution or titanate fibers and nanotubes

**MS.09(4C24)**

N. Boumida: Advances in electrochemistry and applications to molecular reactivity

12:00-12:30

**MS.10(4C24)**

M. Kakehina: Functional ZnO from solution or titanate fibers and nanotubes

**MS.11(4C24)**

K. Kajiyoshi: Hydrothermal growth of metallic TiO2 nano-particles

10:00-10:30

**MS.04(5C25)**

M. Kakihana: Selective synthesis of nano-crystalline TiO2 polymorphs from new water-soluble titanium complexes

**MS.05(5C25)**

T. Adschiri: Superstructural synthesis of organic inorganic hybrid materials

11:00-11:30

**MS.06(5C25)**

D. Ehrentraut: Adsorption and reaction of bulk TiN crystals

**MS.07(5C25)**

K. Tatsumi: New synthetic route to iron-sulfide clusters modeling the active site of nitrogenase

11:30-12:00

**MS.08(5C25)**

M. Kakehina: Functional ZnO from solution or titanate fibers and nanotubes

**MS.09(5C25)**

N. Boumida: Advances in electrochemistry and applications to molecular reactivity

12:00-12:30

**MS.10(5C25)**

M. Kakehina: Functional ZnO from solution or titanate fibers and nanotubes

**MS.11(5C25)**

K. Kajiyoshi: Hydrothermal growth of metallic TiO2 nano-particles
B6  Sunday, August 24 - Afternoon - Microsymposia  

14:45-14:50  Opening Remarks
- Protein-nucleic acid interactions  Chairs: N. Verdagarau, R. Sanarakanuranyan
- Macromolecular structural studies by diffraction, AFM, etc. Chairs: J. Hellwell, R. Thorne

14:50-15:20  MS.08.1(C25)  W. Yang: Stop action movie of viral helicase unwinding DNA
- MS.09.1(C27)  R. Von Dreele: Seeing the first stages of liquid-crystalline DNA nucleation through to a full powdered diffraction pattern
- MS.09.2(C27)  A. D. Shapiro: Serial crystallography by use of a microjet for diffusion of protein nano-crystals or molecules

15:20-15:50  MS.08.2(C26)  O. Nureki: Stop codon recoding by a tRNA synthetase revealed by the suppressor tRNA\textsubscript{Pyl}/Pyl\textsubscript{S} complex structure
- MS.09.3(C27)  Y. Hosokawa: Femtosecond laser etching of protein crystal to process and to isolate the single crystal

15:50-16:20  MS.08.3(C26)  M. Coli: DNA transfer machines
- MS.09.4(C27)  S. Basso: Dose on a sulfur sad experiment of wavelength, redundancy and dose on a sulfur sad experiment

16:20-16:50  MS.08.4(C26)  P. M. Alzari: Structural basis of biosynthesis regulation in Gram-positive bacteria
- MS.09.5(C28)  P. Bhat: Characterization of spider silks weaved by different species living in the Black sea region of Turkey

16:50-17:20  MS.08.5(C28)  I. D. Williams: Control of chirality by spontaneous crystallization and absolute asymmetric synthesis in fluid media
- MS.09.6(C28)  M. Cianci: Functional nanostructured liquid-crystalline assemblies

B7  Sunday, August 24 - Afternoon - Microsymposia  

14:00-14:30  Microsymposia  Chairs: A. Linden, I. D. Williams
- MS.10.1(C29)  M. Daniels: Successful robotic data collection - Bring your own crystals
- MS.10.2(C29)  J. Kaercher: True walk-away data acquisition
- MS.10.3(C29)  Y. Kato: Hands-on automation of data collection
- MS.10.4(C29)  T. Wagner: Automated high-throughput powder data collection
- MS.10.5(C29)  P. Davidso: Use of images in microcrystal detection

14:30-15:00  Microsymposia  Chairs: E. V. Pomjakushina, I. Hisaki
- MS.11.1(C30)  E. V. Pomjakushina: Symmetry, asymmetry and chirality in molecular aggregation
- MS.11.2(C30)  J. M. Tranquada: Exploring the phase diagram of the superconducting state of Cu-Ba-O superconductors
- MS.11.3(C30)  M. M. Julian: Inorganic and organic crystal growth of high-T\textsubscript{C} superconductors

15:00-15:30  Microsymposia  Chairs: H. Eisaki, I. Tanaka
- MS.12.1(C31)  H. Eisaki: Tailor-made single crystal growth of high-T\textsubscript{C} superconductors for neutron and X-ray diffraction studies of liquid-crystalline liquid-crystalline superconductors and cubic cobaltites grown by floating zone method
- MS.12.2(C31)  H. Koshima: Conquering the crystallographic structure of layered CuO\textsubscript{x} thin films
- MS.12.3(C31)  G. Ungar: Conquering the crystallographic structure of layered CuO\textsubscript{x} thin films
- MS.12.4(C31)  M. Saito: Characterization of supramolecular structure of exotic liquid crystals

15:30-16:00  Microsymposia  Chairs: B. Donini, A. Crispini
- MS.13.1(C32)  J. M. Tranquada: Exploring the phase diagram of La\textsubscript{2-x}Sr\textsubscript{x}CuO\textsubscript{4+\delta} and cubic cobaltites grown by floating zone method
- MS.13.2(C32)  Y. Shimizu: Tailor-made single crystal growth of high-T\textsubscript{C} superconductors for neutron and X-ray diffraction studies of liquid-crystalline liquid-crystalline superconductors and cubic cobaltites grown by floating zone method
- MS.13.3(C32)  G. Balakrishnan: High quality single crystals for neutron experiment
- MS.13.4(C32)  T. Kato: Automatic growth of single crystals

16:00-16:30  Microsymposia  Chairs: M. von Dreele, I. Hisaki
- MS.14.2(C33)  G. Holczer: Use of images to characterize by spectroscopy
- MS.14.3(C33)  I. D. Williams: A solution to the problem why crystal chiral pharmaceutical active forms crystals with Z = 2
- MS.14.4(C33)  G. Ungar: Conquering the crystallographic structure of layered CuO\textsubscript{x} thin films

16:30-17:00  Microsymposia  Chairs: E. V. Pomjakushina, I. Hisaki
- MS.15.1(C34)  J. M. Tranquada: Exploring the phase diagram of the superconducting state of Cu-Ba-O superconductors
- MS.15.2(C34)  J. M. Tranquada: Exploring the phase diagram of the superconducting state of Cu-Ba-O superconductors
- MS.15.3(C34)  J. M. Tranquada: Exploring the phase diagram of the superconducting state of Cu-Ba-O superconductors
<table>
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<tr>
<th>Time</th>
<th>A-05MH (MS 15)</th>
<th>F-12CH (MS 16)</th>
<th>D-1003 (MS 17)</th>
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<tr>
<td>09:55-10:00</td>
<td><strong>Opening Remarks</strong></td>
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<td>10:00-10:30</td>
<td><strong>MS.15.1/C33</strong> R. Sainsiavili: Small beams can make huge hits in macromolecular crystallography of insect virus polyhedra, determination of stoichiometry at 3rd generation crystals: Chair: J. Hoss, T. Tomizak</td>
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<td>10:30-11:00</td>
<td><strong>MS.15.2/C37</strong> J. Patel: Fragment-based drug discovery: From crystal to clinic: Chair: R. Hillgenfeld</td>
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<td>11:00-11:30</td>
<td><strong>MS.16.1/C37</strong> A. Metcalf: Microbeam studies of insect virus polyhedra, determination of stoichiometry at 3rd generation crystals at SPring-8: Chair: T. Matsuzaki</td>
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<td>11:30-12:00</td>
<td><strong>MS.16.2/C37</strong> K. Das: Role of structures in designing anti-AIDS drugs targeting viral transcripts: Chair: L. R. MacGillivray</td>
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<td>12:00-12:30</td>
<td><strong>MS.16.3/C37</strong> Q. Hao, T. Tomizaki (C37): Microcrystallography: Small beams can achieve protein microcrystallography at SPring-8</td>
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Monday, August 25 - Afternoon - Microsymposia

14:45-15:00 Opening Remarks

14:50-15:20

MS.22.1 (C46)
S. J. Ludcke: Protein backbone motion and macromolecular motion by cryo-EM and single particle analysis

MS.22.2 (C46)
W. Jiang: Backbone structure of the threonine tRNA synthetase of E. coli as identified by electron microscopy

15:20-15:50

MS.22.3 (C46)
A. Oshima: MS.22.2: N-terminus of Cx26 gap junction channel and functional significance of the gap junction N-terminus

MS.22.4 (C46)
E. Villa: MS.22.3: New approach to understanding the structure and functioning of helical polymers

15:50-16:20

MS.22.5 (C46)
H. N. Bordallo: Crystallographic studies of amino acids and pressure effects on the re-orientational dynamics of amino acids

16:20-16:50

MS.22.6 (C46)
E. Villasenor: Structural and functional significance of the N-terminus of Cx26 gap junction channel

16:50-17:20

MS.22.7 (C46)
E. Villa: Merging data from cryo-EM and X-ray crystallography to reveal biosensor function

MS.22.8 (C46)
C. Betzel: Dynamic light scattering in targeted optical data storage

17:00-17:25

C-1001, 2 (MS 25)
Crystallographic teaching using new computer and internet based approaches

G-1202 (MS 26)
Biological and soft condensed matter under pressure

B-05SH (MS 27)
Multitechnique approach for the determination of inorganic structures

E-1009 (MS 28)
Uncommon organic and organometallic structures and functions

Monday, August 25 - Afternoon - Microsymposia

14:45-15:20 Opening Remarks

15:30-16:00

MS.25.1 (C47)
G. Chupin: Web assisted cryo-EM and X-ray crystallography technology and learning

MS.25.2 (C47)
P. Turner: Learning to drive a diffractometer across the World Wide Web - virtually

16:00-16:30

MS.25.3 (C47)
S. J. Cole: High pressure and X-ray crystallography: Status, applications and prospects

MS.25.4 (C47)
J. Hallmann: Photoexcited state crystallography: Status, applications and prospects

16:30-17:00

MS.25.5 (C47)
E. Hitzer: Interactive 3D Space Group Visualizer

MS.25.6 (C47)
H. N. Bordallo: Temperature and pressure effects on the re-orientational dynamics of amino acids

MS.24.1 (C50)
G. Chupin: Web assisted cryo-EM and X-ray crystallography technology and learning

MS.24.2 (C50)
P. Turner: Learning to drive a diffractometer across the World Wide Web - virtually

17:00-17:25

C-1001, 2 (MS 25)
Crystallographic teaching using new computer and internet based approaches

G-1202 (MS 26)
Biological and soft condensed matter under pressure

B-05SH (MS 27)
Multitechnique approach for the determination of inorganic structures

E-1009 (MS 28)
Uncommon organic and organometallic structures and functions
Tuesday, August 26 - Microsymposia

C-1001, 2 (MS 32)  
Nanostructure refinement and solution  
Chairs: C. Giannini, F. Matteucci

G-1202 (MS 33)  
Liquids and amorphous systems at high pressure  
Chairs: M. Gutierrie, V. Katayama

B-05SH (MS 34)  
Advanced electron microscopy  
Chairs: K. Holmestad, A. Kirkland

E-1009 (MS 35)  
Combined XAFS and diffraction of inorganic structures  
Chairs: K. Asakura, A. Di Cicco

Tuesday, August 26 - Microsymposia

B50

Time  
9:55-10:00  
Opening Remarks  

A-05MH (MS 29)  
Virus structure and antiviral properties  
Chairs: J. Johnson, M. van Raaij

F-12CH (MS 30)  
From minerals to materials  
Chairs: R. Hock, G. Ferry

D-1003 (MS 31)  
Electric and magnetic properties of molecular crystals  
Chairs: M. Yamashita, A. Cornia

9:55-10:30  

MS.29.1(C57)  
P. F. Kwong: X-ray crystallography and HIV vaccine design

MS.30.1(C59)  
G. L. W. Hart: Where are Nature’s missing structures?

MS.31.1(C60)  
E. Coronado: Switching magnetic molecular materials

10:00-10:30  

MS.29.2(C57)  
N. Verdaguer: Proteins from a human survivor

MS.30.2(C59)  
N. Bmakut: High-voltage cathodes for Li-ion batteries

MS.31.2(C60)  
A. Kobayashi: Structures and physical properties of single-component molecular materials

10:30-11:00  

MS.29.3(C57)  
F. A. Rey: Evolutionary links among viruses of different categories revealed by dsRNA polymerases

MS.30.3(C59)  
J. Parsie: Towards a better understanding of atomic arrangements in nano-minerals

MS.31.3(C61)  
V. Marvaul: Photoswitchable high spin molecules

11:00-11:30  

MS.29.4(C57)  
E. E. Lee: Structure of the trimeric, prefusion Ebola virus GP complexed with an antibody from a human survivor

MS.30.4(C59)  
S. Schorr: Theoretical aspects of magnetic transitions and high conductivity in ionic crystals of fullerene complexes

MS.31.4(C64)  
K. Fuchizaki: Polyamorphism in tetraiodide Kesterite - an approach to the refinement of a new electron diffraction microscopy for diffractive imaging

11:30-12:00  

MS.29.5(C58)  
R. Hilgenfeld: Re-emerging viral diseases: How can structural biology support preparedness and response?

MS.30.5(C60)  
L. Bucio: Phase composition of amorphous trigonal aggregate and its role on properties as biomaterial cement

MS.31.5(C61)  
Y. Ohgo: The spin-crossover triangle in the iron(III) polyporphyrinidosts

12:00-12:30  

MS.29.6(C58)  
K. Suenaga: Development of advanced XAFS analysis techniques with FEL light sources

MS.30.6(C60)  
D. T. Bowon: Comprehensive structural characterization of local and bulk structure in disordered materials

MS.31.6(C64)  
A. Michalowicz: High pressure and high temperature EXAFS and diffraction study of AgI nanocrystals

MS.32.1(C62)  
F. Julaus: Nanostructure investigations using atomic pair distribution function and other direct-space methods

MS.33.1(C63)  
S. A. Bone: New liquid structures of alkali metals under pressure predicted from first principles theory

MS.34.1(C65)  
K. Suenaga: HR-TEM imaging of the carbon networks in high temperature EXAFS and diffraction studies of oxidation/water gas shift reactions of Cu doped ceria

MS.35.1(C66)  
J. C. Hanson: Combined XAFS and diffraction of inorganic structures
From bacteriophages, archaea and overall architecture of the giant capsids of phytoreoviruses, the nucleosome-like organization of the filamentous structure: The self-assembly of nucleosomes from nuclear to phasic and liquid protein 

self-assembly: From nucleation to crystal growth, from proteins to liquid and rigid tissues, and from theory to application: Chairs: D. Harada, F. Metzger.


MS.31.2 (C68) Chairs: M. Spackman, K. Tanaka

MS.31.3 (C69) Chairs: D. Jayatilaka

MS.31.4 (C70) Chairs: D. A. Keen

MS.31.5 (C71) Chairs: S. Shamoto

MS.31.6 (C72) Chairs: P. H. J. Mercereau, K. Hirose

MS.31.7 (C73) Chairs: S. Hovmöller

MS.31.8 (C74) Chairs: J. Nozawa

MS.31.9 (C75) Chairs: S. Panjikar

MS.31.10 (C76) Chairs: C. Vonrhein

MS.31.11 (C77) Chairs: N. Kunishima

MS.31.12 (C78) Chairs: Liang, Wang
<table>
<thead>
<tr>
<th>Time</th>
<th>Opening Remarks</th>
<th>A-05MH (MS 43)</th>
<th>F-12CH (MS 44)</th>
<th>D-1003 (MS 45)</th>
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<td>9:55-10:00</td>
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<td>10:00-10:30</td>
<td>Structural biology of the cell</td>
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<td>Chairs: P. Alzari, H. S. Yuan</td>
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<td>10:30-11:00</td>
<td>Teaching macromolecular crystallography</td>
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<td>Chairs: K. Kantardjeff, B. Santarsiero</td>
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<td>11:00-11:30</td>
<td>Crystallography</td>
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<td>Chairs: L. Armitage, M. Deisenhorn, T. Wolfson</td>
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<td>11:30-12:00</td>
<td>Crystallography</td>
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| Wednesday, August 27 - Morning - Microsymposia |

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<td>High pressure studies on hydrogen storage materials</td>
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<td>10:00-10:30</td>
<td>Powder diffraction studies of hydrogen storage materials</td>
<td>Chairs: M. O. Jones, P. Whitfield</td>
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<td>Structural biology of the cell</td>
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<td>Teaching macromolecular crystallography</td>
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<td>14:45-14:50</td>
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<td>Developments in structure solution and refinement from powders</td>
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<td>Chairs: Chai, Shav, S. Eon Ryu</td>
<td>Shape memory alloys&lt;br&gt;Chair: K. R. A. Ziekew, T. Kanamata</td>
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<td>Complementarity of SAXS and SANS with other structural methods in molecular biology</td>
<td>Surfaces&lt;br&gt;Chair: D. K. Saldin, F. Boscherini</td>
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<td>Chairs: J. Trewella, T. Fujisawa</td>
<td>Phase transitions and physical properties at high pressure&lt;br&gt;Chairs: L. Robin Benedetti, G. Shen</td>
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<td>15:00-15:50</td>
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<td>Phase transitions and physical properties at high pressure&lt;br&gt;Chairs: L. Robin Benedetti, G. Shen</td>
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<td>D-1003 (MS 52)</td>
<td>Chairs: S. A. Bourne, P. Bombize</td>
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<td>MS.51.1 (C91) D. L. Svergun: Joint use of SANS and SAXS with high resolution methods for macromolecular solutions</td>
<td>Surfaces&lt;br&gt;Chair: D. K. Saldin, F. Boscherini</td>
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<td>Phase transitions and physical properties at high pressure&lt;br&gt;Chairs: L. Robin Benedetti, G. Shen</td>
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<td>MS.52.2 (C92) L. Brammer: Porous material behaviour in non-porous crystals between structural information from NMR and SAXS data</td>
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<td>MS.53.1 (C93) E. J. Goldsmith: The structure of the MAP2K MEK6 is an auto-inhibitory domain in crystals and in solution</td>
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<td>MS.53.2 (C93) L. R. Nasmimbeni: Polymorphism, isostructurality and selectivity in inclusion compounds</td>
<td>Phase transitions and physical properties at high pressure&lt;br&gt;Chairs: L. Robin Benedetti, G. Shen</td>
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<td>16:20-17:00</td>
<td>MS.54.1 (C94) L. Tang: Structural studies of pre-β-NA3 β- and processing</td>
<td>Surfaces&lt;br&gt;Chair: D. K. Saldin, F. Boscherini</td>
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<td>MS.54.2 (C94) J. Trewhella, P. Bombize: Observation of assembly and disassembly dynamics of cyanobacterial clock proteins</td>
<td>Phase transitions and physical properties at high pressure&lt;br&gt;Chairs: L. Robin Benedetti, G. Shen</td>
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<td>MS.55.2 (C94) N. Dragoe: High pressure induced charge ordering in ionic vanadium nitride</td>
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<td>MS.55.3 (C94) A. R. B. M. Towles: Towards solution of the protein structure of the α-lactoglobulin</td>
<td>Phase transitions and physical properties at high pressure&lt;br&gt;Chairs: L. Robin Benedetti, G. Shen</td>
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<td>MS.55.4 (C94) M. A. Van Hove: Structure of biomacromolecules using X-ray scattering multiple scattering</td>
<td>Phase transitions and physical properties at high pressure&lt;br&gt;Chairs: L. Robin Benedetti, G. Shen</td>
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<td>MS.55.5 (C94) J. V. M. L. T. Ohba: Towards solution of the protein structure of the α-lactoglobulin</td>
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<td>17:00-17:20</td>
<td>MS.56.1 (C94) J. H. Wang: Decoding function and position specificity of Dscam, a neuronal receptor with thousands isoforms</td>
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### Wednesday, August 27 - Afternoon - Microsymposia

- **Hot structures**
  - **Chairs:** Chai, Shav, S. Eon Ryu
  - **Complementarity of SAXS and SANS with other structural methods in molecular biology**
    - **Chairs:** J. Trewella, T. Fujisawa
  - **Host-guest crystal chemistry**
    - **Chairs:** S. A. Bourne, P. Bombize

- **Development in structure solution and refinement from powders**
  - **Chair:** K. R. A. Ziekew, T. Kanamata

- **Surfaces**
  - **Chair:** D. K. Saldin, F. Boscherini

- **Phase transitions and physical properties at high pressure**
  - **Chairs:** L. Robin Benedetti, G. Shen
**Thursday, August 28 - Morning - Microsymposia**

**Microsymposia**

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<th>A-05MH (MS 57)</th>
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<tr>
<td>09:55-10:00</td>
<td>Opening Remarks</td>
<td>Structure-property correlations and phase transitions in inorganic materials</td>
<td>Chemical recognition and supramolecular architectures</td>
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</tbody>
</table>
| 10:00-10:30 | R. Kuroki: Structure of quadrilateral 
metal-containing protein domains determined by both X-ray and neutron diffraction | M. J. Hardie: Star-branched metallo-supramolecular prisms and coordination polymers with guest-accessible functional organic sites | M. Wais Hosseini: Vanadium coordination polymers having organic sites with carbonyl-stabilized 
metallic state of SmNiC |
| 10:30-11:00 | F. Meilleur: Neutron crystallographic analysis of unstructured and selectively CH-protonated deuterated rubredoxin | S. Van Smalend: Phase transition in the ferroelectric 
material GeOx (X = Cl, Br) | G. Resutul: A molecular 
Legoland through halogen bonding |
| 11:00-11:30 | M. P. Blaekley: Neutron macromolecular crystallography using the Laue diffractometer LADIII | J.-P. Itie: Local aspects of high-pressure phase transitions in ferroelectrics | R. Guinebretiere: High-resolution X-ray diffraction analysis of strain relaxation in epitaxial oxide thin films |
| 11:30-12:00 | N. Arakawa: Seeing hydrogen X-ray limitations and possibilities at 0.9 Â and synergy with neutron diffraction | K. Ogino: X-ray ray diffraction study on structures of vanadium dioxide films with metal- 
insulator transition | D. B. Livin: International-like tables for magnetic 
crystallography |
| 12:00-12:30 | J. P. Glauser: Locating hydrogen atoms in enzymes: A neutron structure of D-xylene isomerase with bound D-xylalose | S. Shimomura: Modulated metal and ferromagnetic metallic state of SmNi3 | R. Boer: Molecular recognition and supramolecular 
architectures of metallo-supramolecular helicates |

**Microscopy and structural imperfections**

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**Thursday, August 28 - Microscopy**

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<td>MS.65.1(C112) M.</td>
<td>MS.66.1(C114) G.</td>
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<td>MS.65.2(C113) S. M.</td>
<td>MS.66.2(C114) C.</td>
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<td>B. Aakeroy: From a molecular dating agency to successful</td>
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<td>MS.65.4(C113) A. Wagner:</td>
<td>MS.66.4(C115) G.</td>
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<td>Pedersen: Crystal structure of the</td>
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<td>the plasma membrane protein</td>
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<td>MS.65.5(C114) J. C.</td>
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<td>Use of coherence in life and physical sciences</td>
<td>Crystal chemistry and crystallography of apoplastic crystals</td>
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<td>MS.68.1(C116) A. Volkov: On the evaluation of energy densities with aspherical pseudopotentials: A model study</td>
<td>MS.69.1(C118) Y. Nishino: 3D view of energy densities with aspherical pseudopotentials: A model study</td>
<td>MS.70.1(C120) J. Hadermann: Applications of co-crystal synthesis to the preparation of incommensurately modulated compounds</td>
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<td>MS.67.2(C115) T. J. Sato: E/T-scaling behavior in the magnetic quasicrystal</td>
<td>MS.68.2(C117) G. R. N. Tayur: Exploring pathways of structural phase transitions via experimental charge density analysis</td>
<td>MS.69.2(C118) A. Barty: Femtosecond dynamic diffraction imaging: X-ray Speckle Interferometry with ultrafast nanoscale phenomena</td>
<td>MS.70.2(C120) O. Perez: Super spatial formation in crack complex codes in multicomponent modulated systems</td>
</tr>
<tr>
<td>14:50-15:20</td>
<td>MS.67.3(C118) S. A. Grigera: Quantum critical points and nematics: The archetype Sr$_3$Ru$_2$O$_8$</td>
<td>MS.68.3(C117) P. Luger: Intra and intermolecular electron density properties of fullerene</td>
<td>MS.69.3(C119) F. Pfeiffer: Coherent X-ray diffraction microscopy of extended objects</td>
<td>MS.70.3(C120) L. Elcoro: Long-period structures in the superspace formalism: From the rhombohedral to modular structures</td>
</tr>
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<td></td>
<td>MS.67.4(C118) Y. Yamauchi: Artificial superconductivity in crystals without metal inversion center</td>
<td>MS.68.4(C117) G. J. Williams: Feinstedt coherent diffraction imaging with X-rays</td>
<td>MS.69.4(C119) G. &amp; J. Williams: Feinstedt coherent diffraction imaging with X-rays</td>
<td>MS.70.4(C121) S. Lidin: Stipulate, an extension of the concept of solid solutions</td>
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<td>15:50-16:20</td>
<td>MS.68.1(C116)</td>
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Friday, August 29 - Morning - Microsymposia

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<tr>
<th>Time</th>
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<th>F-12CH (MS 72)</th>
<th>D-1003 (MS 73)</th>
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<tr>
<td>9:55-10:00</td>
<td>Opening Remarks</td>
<td>Biophysical techniques for detecting ligand binding to pharmaceutical targets Chairs: R. E. Hubbard, Y. Kawakami</td>
<td>Structure-function relationships of MoF Chairs: M. Eddaoudi, S. J. James</td>
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<tr>
<td>10:00-10:30</td>
<td>MS.71.(C121) A. Rafi: X-ray structural analysis of microbial enzymes: Progress and challenges</td>
<td>MS.72.(C123) T. Piloli: Combining microbial enzymes with micro-SAXS for studies of the dynamics of DNA replication</td>
<td>MS.73.(C124) R. Matsuoka: Guest-responsive structures and properties of porus coordination polymers</td>
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<td>11:30-12:00</td>
<td>MS.71.(C124) D. H. Harrison: Mechanism of the co-factor-less urate oxidase: X-ray structures with molecular oxygen or cyanide.</td>
<td>MS.72.(C129) D. Veremee: A mesoporous pattern created by nature: A SAXS and micro-SAXS study of the functionalization of a bionanocomposite</td>
<td>MS.73.(C129) G. Zhao: Elucidation of the structure of multifunctional metal-organic frameworks</td>
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<td>12:00-12:30</td>
<td>MS.71.(C122) L. N. Johnson: Flavopiridol binding to P-fib (CDK5) cyclin T1)</td>
<td>MS.72.(C127) Y. Nozue: Deformation behavior of field glasses studied using simultaneous micro-SAXS and WAXS</td>
<td>MS.73.(C125) N. Lock: Elucidating negative thermal expansion in metal-organic frameworks</td>
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Friday, August 29 - Morning - Microsymposia

<table>
<thead>
<tr>
<th>Time</th>
<th>C-1001 (MS 74)</th>
<th>G-1202 (MS 75)</th>
<th>B-05SH (MS 76)</th>
<th>E-1009 (MS 77)</th>
</tr>
</thead>
<tbody>
<tr>
<td>11:30-12:00</td>
<td>MS.74.(C129) D. N. Argyrion: Function from frustration in modern multiferroics</td>
<td>MS.75.(C129) P. Munshi: Estimation of optical properties from wavefunction fitting of X-ray diffraction data</td>
<td>MS.76.(C130) R. V. Dronyak: Electron diffusive imaging of the MgO nanoparticle: Towards atomic-resolution</td>
<td>MS.77.(C131) S. M. F. Francoan: Phason diffuse scattering in the coassembled quasicrystal</td>
</tr>
</tbody>
</table>
Friday, August 29 - Afternoon - Microsymposia

**14:45-14:50 Opening Remarks**

Chairs: E. Pehay-Peroula, S. Yoshikawa

**14:50-15:20**

**Microsymposia (MS 78)**

- J.L. Popot: Can amphipols be used to crystallize membrane proteins?
- C. Toyoshima: Crystallization of the calcium pump of skeletal muscle sarcoplasmic reticulum
- T. Kouyama: Crystallization of rhodopsins
- A. May: Diffraction-capable microfluidic crystallization chips for screening and structure determination

**15:20-15:50**

**Microsymposia (MS 78)**

- J. Lowe: DNA translocation by hexameric FtsK
- V. B. Rao: Mechanism of DNA packaging in bacteriophage T4
- J. Loew: DNA translocation by hexameric FtsK
- N. Sakamoto: Molecular motions of the bacterial flagellum and movement of the bacterial flagella filament

**15:50-16:20**

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**16:50-17:20**

**Microsymposia (MS 78)**

- E. Pebay-Peroula: Computed crystallography: Performance tests for iterative phase-retrieval methods in higher dimensions
- A. May: Diffraction-capable microfluidic crystallization chips for screening and structure determination
- D. Luo: Crystal structure of the NS1 protein-helicase from Dengue virus
- S. L. Price: Computed crystal energy landscapes as an aid to understanding polymorphism

**17:50-18:20**

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Friday, August 29 - Afternoon - Microsymposia

**14:00-14:50**

**Microsymposia (MS 80)**

- T. H. Kawata: New phenomena in epitaxial growth: Solid films on quasicrystalline substrates
- B. J. Kennedy: Crystallization of the cold neutron research facility project at HANARO
- J. Miao: Coherent diffraction microscopy: Present and future
- J. A. Duffy: Using magnetic Compton scattering to study Invar and spin-polarised materials

**15:10-16:00**

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**C-1001, 2 (MS 81)**

- New neutron sources
  - Chairs: S. J. Kennedy, Y. Noda

**C-1002, (MS 82)**

- Magnetic compton scattering
  - Chairs: Y. Sakurai, H. Kawata

**B-05SH (MS 83)**

- Femto-second diffraction: Time resolved studies
  - Chairs: S. Techert, R. Feldenhans

**E-1009 (MS 84)**

- Quasicrystals and related giant crystalline alloys
  - Chairs: E. Abe, R. McGrath
Satuday, August 30 - Morning - Microsymposia

B144

9:55-10:00 Opening Remarks

10:00-10:30

A05MH (MS 85)
Structural proteomics, focused structural protein synthesis systems

10:30-11:00

F12CH (MS 86)
Perovskites and related materials

11:00-11:30

A06MH (C143)
J. Weigelt: Structural genomics of protein families and patheways in human disease

11:30-12:00

B103 (MS 87)
Design and applications of nanoscale materials

12:00-12:30

C1001, 2 (MS 88)
Space groups and their generalizations: A tribute to E. Ascher and J.J. Burchhardt

12:30-13:00

D1003

E1009 (MS 91)
Spinel - geometrically frustrated system: Dedicated to Prof. Nishikawa

Saturday, August 30 - Morning - Microsymposia

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<th>Time</th>
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<th>F-12CH (MS 93)</th>
<th>D-1003 (MS 94)</th>
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<tr>
<td><strong>13:50-14:20</strong></td>
<td>MS.92.1(C14) A. M. Buckle: Federated repositories of X-ray diffraction data (25 min)</td>
<td>MS.93.1(C15) E. Westhof: The annotations of non-Water-Obs-Crack head groups and comparison between DNA structures and sequences</td>
<td>MS.94.1(C15) C. Sternemann: X-ray Raman scattering: A probe of soft X-ray absorption edges using hard X-rays</td>
</tr>
<tr>
<td><strong>14:20-14:50</strong></td>
<td>MS.92.2(C14) J. E. Johnson: Virus particle electron crystallography database for single-particle structures (25 min)</td>
<td>MS.93.2(C15) V. Li: Capturing hexagonal icosahedral virus structures (25 min)</td>
<td>MS.94.2(C15) S. K. Lee: Pressure-induced structural transition in oxides at high pressure: Inelastic X-ray scattering study</td>
</tr>
<tr>
<td><strong>14:50-15:20</strong></td>
<td>MS.92.3(C14) W. Minor: Metal and small molecule environment in macromolecules (25 min)</td>
<td>MS.93.3(C15) G. N. Parkinson: Ligand binding and the annotation of guaiphenes containing human telomeric sequences</td>
<td>MS.94.3(C15) S. T. Gerald: New applications of k-dependent XRS across the periodic table</td>
</tr>
<tr>
<td><strong>15:20-15:50</strong></td>
<td>MS.92.4(C14) M. S. Weiss: On atomic displacement parameters and coordinates in protein structures (25 min)</td>
<td>MS.93.4(C15) M. Georgiadis: Crystal structures of DNA-bound Cob(II)lumarins (25 min)</td>
<td>MS.94.4(C15) J. S. Tse: X-ray Raman of water in the condensed phases</td>
</tr>
<tr>
<td><strong>15:50-16:20</strong></td>
<td>MS.92.5(C15) J. Westbrook: Quality checks for carbohydrate structures in PDB entries (25 min)</td>
<td>MS.93.5(C15) M. Cardis: Molecular recognition and the DNA Holliday junction (25 min)</td>
<td>MS.94.5(C15) V. Cali: High-resolution X-ray Raman scattering and the study of ices under high pressure</td>
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<th>G-1206 (MS 96)</th>
<th>B-05SH (MS 97)</th>
<th>E-1009 (MS 98)</th>
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<tr>
<td>MS.95.2(C15) K. O. Yamahama: Scientific contribution to archaeology: Fingerprinting the ancient Egyptian objects</td>
<td>MS.96.2(C160) J. R. Hester: CIF software in a DDLm world</td>
<td>MS.97.2(C161) R. D. Burst: High speed readout of microgap X-ray detectors</td>
<td>MS.98.2(C163) J. M. Cole: Discovering the world’s best organic non-linear optical material</td>
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<tr>
<td>MS.95.3(C15) E. Kotulova: Salt corrosion of lead-based pigment: Laboratory experiments and analysis of ancient frescoes</td>
<td>MS.96.3(C160) H. J. Bernstein: Transition to object-oriented data representations: Interaction between CIF and other formats</td>
<td>MS.97.3(C162) C. Broennimann: The PILATUS detector: Hyperspectral detectors for synchrotron and industrial applications</td>
<td>MS.98.3(C163) S. Huth: The crystal structures of metal-organic frameworks: Towards materials synthesised systematically</td>
</tr>
<tr>
<td>MS.95.5(C15) C. Doury: Structural investigations of archaeological hybrid materials</td>
<td>MS.96.5(C161) T. C. McNab: pubCIF: A complete crystal structure publishing environment for authors</td>
<td>MS.97.5(C163) A. S. Schow: The 2D X-ray detector development program for the European XFEL</td>
<td>MS.98.5(C163) T. N. Bharti: Structural database using semantic Web concepts to support structure-based drug design for AIDS</td>
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Saturday, August 30 - Afternoon - Microsymposia

**Microsymposia**

- **Microanalysis of biological samples**
  - Chairs: Y. Terada, V. Kockelmann
  - Presentation by P. Pauller: Nanostructure of ancient Damascus blades
  - Presentation by K. O. Yamahama: Scientific contribution to archaeology: Fingerprinting the ancient Egyptian objects
  - Presentation by E. Kotulova: Salt corrosion of lead-based pigment: Laboratory experiments and analysis of ancient frescoes
  - Presentation by M. A. Arroyo: The bilbao crystallographic server

- **Programming for CIF and related structure databases**
  - Chairs: I. David Brown, I. Guzzell
  - Presentation by J. R. Hester: CIF software in a DDLm world
  - Presentation by R. D. Burst: High speed readout of microgap X-ray detectors

- **New X-ray detectors: Pixel detectors**
  - Chairs: M. Tate, P. Fajardo
  - Presentation by K. Hattori: Performance of micro pixel gas chamber in small angle X-ray scattering experiments

- **Knowledge-based applications in structural biology**
  - Chairs: M. Wain, J. van de Steek
  - Presentation by R. Subramanian: Quality of protein crystal structures in the protein data bank

**Database**

- **Database**
  - For icosahedral virus structures (25 min)
  - Presentation by M. S. Weiss
  - Presentation by W. Minor

**Microscopy**

- **Microscopy**
  - For icosahedral virus structures (25 min)
  - Presentation by M. S. Weiss
  - Presentation by W. Minor