Memo

Morning Session 8:30-9:30

A-05MH *(KN 4)*

KN04*(C3)* | **Sine Y Larsen**:
The role of micrometer sized synchrotron radiation beams in the development of structural biology

Chair: **Soichi Wakatsuki**

F-12CH *(KN 5)*

KN05*(C4)* | **Masahiro Irie**:
Photochromism of diarylethene single crystals-reversible color and shape changes on photoirradiation

Chair: **Sergey M. Aldoshin**

D-1003 *(KN 6)*

KN06*(C4)* | **Giulia A Galli**:
Quantum simulations of liquids and solids under pressure: Synergy between theory and experiment

Chair: **Artem R. Oganov**

Afternoon Session 17:30-18:30

A-05MH *(KN 7)*

KN07*(C4)* | **Wolfgang Baumeister**:
Cryoelectron tomography: From molecules to systems

Chair: **Keiichi Namba**

F-12CH *(KN 8)*

KN08*(C4)* | **Kenneth D. M. Harris**:
Advances in direct-space structure determination of molecular materials from powder diffraction data

Chair: **René de Gelder**

D-1003 *(KN 9)*

KN09*(C5)* | **Irene Margiolaki**:
Powder diffraction studies of proteins

Chair: **Robert von Dreele**

Time	A-05MH **(MS 15)**	F-12CH **(MS 16)**	D-1003 **(MS 17)**
9:55–10:00 Opening Remarks	**Protein "microcrystallography": Methods and results for tiny crystals at 3rd generation sources** Chairs: **Q. Hao, T. Tomizaki**	**Structure-based drug design** Chairs: **J. Wouters, R. Hilgenfeld**	**Photochemistry and solid-state transformations of molecular solids** Chairs: **H. Uekusa, M. Kaftory**
10:00–10:30	**MS.15.1**(C35) **R. Sanishvili**: Small beams can play big roles in macromolecular crystallography	**MS.16.1**(C37) **J. Patel**: Fragment-based drug discovery: From crystal to clinic	**MS.17.1**(C38) **P. Coppens**: Time-resolved diffraction at atomic resolution: What's here now and what's next?
10:30–11:00	**MS.15.2**(C36) **D. Flot**: Recent developments and success on ID23-2, at the ESRF	**MS.16.2**(C37) **K. Das**: Role of structures in designing anti-AIDS drugs targeting reverse transcriptase	**MS.17.2**(C39) **L. R. MacGillivray**: Reactive crystalline molecular assemblies
11:00–11:30	**MS.15.3**(C36) **P. Metcalf**: Microbeam studies of insect virus polyhedra, infectious protein crystals containing virus particles	**MS.16.3**(C37) **A. Mattevi**: Monoamine oxidases and LSD1: Similar chemistry for neurotransmitter and chromatin modification	**MS.17.3**(C39) **M. Kato**: Vapor-induced transformation followed by luminescence switching for a dinuclear platinum(II) complex
11:30–12:00	**MS.15.4**(C36) **K. Hirata**: A new beamline to achieve protein micro-crystallography at SPring-8	**MS.16.4**(C38) **T. Matsuzaki**: CPADD(Closest Packing Approach for denovo Drug Design) to inhibit VEGF/R and Notch/RBP/MAM systems	**MS.17.4**(C39) **J. Harada**: Photochromism and thermochromism of crystalline salicylideneanilines
12:00–12:30	**MS.15.5**(C37) **G. Evans**: Microcrystallography at Diamond: Facilities for crystal optimization and structure determination	**MS.16.5**(C38) **A. K. Roos**: A family wide approach to structure-based inhibitor design for protein tyrosine phosphatases	**MS.17.5**(C40) **S. L. James**: Mechanochemical solvent-free synthesis of metal-organic frameworks

Monday, August 25 - Morning - **Microsymposia**

C-1001, 2 **(MS 18)**	G-1202 **(MS 19)**	B-05SH **(MS 20)**	E-1009 **(MS 21)**
***In-situ* & time-resolved powder diffraction studies** Chairs: **C. Weidenthaler, J. Hanson**	**Structure simulation under extreme condition** Chairs: **R. Ahuja, J. Tse**	**Time resolved and coherent X-ray scattering** Chairs: **P. Thiyagarajan, S. Akiyama**	**Crystallographic algorithm libraries: In honor of P. Jane Brown** Chairs: **J. Wright, L. Palatinus**
MS.18.1(C40) **P. J. Chupas**: Application of the pair-distribution-function method to *in-situ* studies in catalysis	**MS.19.1**(C41) **A. R. Oganov**: Evolutionary crystal structure prediction and its applications to materials at extreme conditions	**MS.20.1**(C43) **S. Takahashi**: Protein folding dynamics by time resolved SAXS and single molecule fluorescence spectroscopy	**MS.21.1**(C44) **R. W. Grosse-Kunstleve**: Cctbx architecture and algorithms
MS.18.2(C40) **K. Stahl**: *In situ* studies on hydrogen/ammonia storage materials	**MS.19.2**(C42) **D. D. Klug**: Theoretical prediction and characterization of high pressure structures and properties of calcium	**MS.20.2**(C43) **R. L. Leheny**: XPCS studies of slow, non-diffusive dynamics in glassy soft materials	**MS.21.2**(C45) **G. G. Darakev**: Identifying residues using 3D coordinates: An application of multiple APIs
MS.18.3(C40) **P. Norby**: *In situ* synchrotron powder X-ray diffraction studies of catalytic materials	**MS.19.3**(C42) **R. Martonak**: Polymorphism and structural phase transitions in crystals: Computer simulations by metadynamics	**MS.20.3**(C44) **Q. Shen**: Studies of material structure and process with coherent diffraction and time-resolved X-ray imaging	**MS.21.3**(C45) **O. Zaharko**: Magnetic structure determination combining nonpolarised and polarised neutron diffraction
MS.18.4(C41) **M. Milanesio**: *In situ* simultaneous Raman/XRPD study of solid-state reactions at non-ambient conditions	**MS.19.4**(C42) **W. Luo**: First-principles calculations of pressure induced magnetic transition in siderite $FeCO_3$	**MS.20.4**(C44) **Y. Shinohara**: Studies of silica aggregate structure and its dynamics in rubber using time-resolved USAXS and XPCS	**MS.21.4**(C45) **S. Schmidt**: An algorithm for determining crystal lattices in unknown polycrystalline compounds
MS.18.5(C41) **P. S. Whitfield**: Application of a high-pressure CO_2 cell to time-resolved studies with a lab powder diffractometer	**MS.19.5**(C43) **C. J. Pickard**: Predicting crystal structures by random searching	**MS.20.5**(C44) **S. V. Roth**: Time-resolved monitoring of nanocomposite growth using grazing incidence small-angle scattering	**MS.21.5**(C46) **J. Rodriguez-Carvajal**: New developments on CrysFML: Global and local optimization methods

Monday, August 25 - Afternoon - **Microsymposia**

Time	A-05MH **(MS 22)**	F-12CH **(MS 23)**	D-1003 **(MS 24)**
14:45–14:50 Opening Remarks	**Interface between cryo-EM and crystallography** Chairs: **W. Chiu, C. Lawson**	**Crystallizing macromolecular complexes and engineering crystallization** Chairs: **C. Sauter, G. Sazaki**	**Photo-excited state crystallography** Chairs: **S. Pillet, Y. Ozawa**
14:50–15:20	**MS.22.1**(C46) **S. J. Ludtke**: Protein backbone tracing and macromolecular motion by cryo-EM and single particle analysis	**MS.23.1**(C47) **T. M. Bergfors**: The search for good crystals: How far have we come?	**MS.24.1**(C49) **S. Adachi**: Watching photo-induced dynamics with picosecond time-resolved X-ray diffraction
15:20–15:50	**MS.22.2**(C46) **W. Jiang**: Backbone structure of the infectious Epsilon15 virus capsid revealed by electron cryomicroscopy	**MS.23.2**(C48) **T. Okutsu**: Photochemically induced nucleation of protein	**MS.24.2**(C49) **J. Hallmann**: Photo-crystallographic studies of dimerisation processes: From picoseconds to hours transformation
15:50–16:20	**MS.22.3**(C46) **E. H. Egelman**: A new approach to understanding the structure and dynamics of helical polymers	**MS.23.3**(C48) **M. G. Gruetter**: Applications of designed ankyrin repeat proteins as chaperones in structural biology	**MS.24.3**(C49) **M. Chergui**: Picosecond and femtosecond X-ray absorption studies of the photoinduced spin change in Fe-complexes
16:20–16:50	**MS.22.4**(C47) **A. Oshima**: Structural and functional significance of the N-terminus of Cx26 gap junction channels	**MS.23.4**(C48) **J. Jean**: A simple method to introduce anomalous scatterers in a wide number of proteins	**MS.24.4**(C50) **P. R. Raithby**: Photocrystallographic studies on metastable linkage isomers of transition metal complexes
16:50–17:20	**MS.22.5**(C47) **E. Villa**: Merging data from Cryo-EM and X-ray crystallography to reveal biomolecular function	**MS.23.5**(C48) **C. Betzel**: Dynamic light scattering in protein crystallization: Analysis and optimization	**MS.24.5**(C50) **A. E. Phillips**: Metastable photoisomerism in materials targeted for optical data storage

C-1001, 2 **(MS 25)**	G-1202 **(MS 26)**	B-05SH **(MS 27)**	E-1009 **(MS 28)**
Crystallographic teaching using new computer and Internet based approaches Chairs: **T. N.Guru Row, A. Le Bail**	**Biological and soft condensed matter under pressure** Chairs: **F. P. A. Fabbiani, R. Winter**	**Multitechnique approach for the determination of inorganic structures** Chairs: **H. Fuess, C. Ferraris**	**Uncommon organic and organometallic structures and functions** Chairs: **J. Ellena, H. Arslan**
MS.25.1(C50) **G. Chapuis**: Web assisted crystallography teaching and learning	**MS.26.1**(C52) **I. Daniel**: *In situ* measurement of microorganisms metabolism under high hydrostatic pressure	**MS.27.1**(C54) **D. Pandey**: Structure of ferroic phases in mixed perovskites: Role of multitechnique approach	**MS.28.1**(C55) **A. E. Goeta**: Induced structural diversity in magnetic molecular materials
MS.25.2(C51) **P. Turner**: Learning to drive a diffractometer across the World Wide Web - virtually!	**MS.26.2**(C52) **C. R. Pulham**: High-pressure studies of pharmaceutical compounds	**MS.27.2**(C54) **J-L. Hodeau**: Probing the structure of heterogeneous diluted materials by diffraction tomography	**MS.28.2**(C56) **F. Adhami**: Crystal structure of 6PicTubenzo thiourea derivative, oxidative cyclization and coordinated with Cu^{2+}
MS.25.3(C51) **S. J. Coles**: Open repositories and web services for teaching and outreach in chemical crystallography	**MS.26.3**(C53) **O. Ces**: Time resolved studies of lyotropic phase transitions using the pressure jump technique	**MS.27.3**(C54) **P. J. Becker**: Electronic behaviour of materials from combined X-Ray, neutron diffraction and Compton scattering	**MS.28.3**(C56) **M. K. Lo**: Synthesis and crystal structures of diorganotin schiff base complexes
MS.25.4(C51) **M. M. Julian**: Use of MATLAB® in teaching crystallography	**MS.26.4**(C53) **R. Fourme**: High-pressure macromolecular crystallography:Status, applications and prospects	**MS.27.4**(C55) **Y. Miura**: Complex texture and structure of shocked quartz mineral with graphite grains	**MS.28.4**(C56) **J. Simpson**: Unusual C-Br$^{\cdots}$ π interactions in ferrocenyl systems
MS.25.5(C51) **E. Hitzer**: Interactive 3D Space Group Visualizer	**MS.26.5**(C53) **H. N. Bordallo**: Temperature and pressure effects on the re-orientational dynamics of amino acids	**MS.27.5**(C55) **H. Ehrenberg**: The effect of structural and compositional details on physical properties of new double-perovskites	**MS.28.5**(C57) **R. Boese**: Unexpected patters in co-crystals of small molecules