

Timetable & Room Plan for MS

Room No.	Aug. 24		25		26	
	am (9:55-12:30)	pm (14:45-17:20)	am (9:55-12:30)	pm (14:45-17:20)	am (9:55-12:30)	pm (14:45-17:20)
A-05MH	MS 1	MS 8	MS 15	MS 22	MS 29	MS 36
F-12CH	MS 2	MS 9	MS 16	MS 23	MS 30	MS 37
D-1003	MS 3	MS 10	MS 17	MS 24	MS 31	MS 38
C-1001,2	MS 4	MS 11	MS 18	MS 25	MS 32	MS 39
G-1202	MS 5	MS 12	MS 19	MS 26	MS 33	MS 40
B-05SH	MS 6	MS 13	MS 20	MS 27	MS 34	MS 41
E-1009	MS 7	MS 14	MS 21	MS 28	MS 35	MS 42

Timetable & Room Plan for MS

27		28		29		30	
am (9:55-12:30)	pm (14:45-17:20)	am (9:55-12:30)	pm (14:45-17:20)	am (9:55-12:30)	pm (14:45-17:20)	am (9:55-12:30)	pm (13:45-16:20)
MS 43	MS 50	MS 57	MS 64	MS 71	MS 78	MS 85	MS 92
MS 44	MS 51	MS 58	MS 65	MS 72	MS 79	MS 86	MS 93
MS 45	MS 52	MS 59	MS 66	MS 73	MS 80	MS 87	MS 94
MS 46	MS 53	MS 60	MS 67	MS 74	MS 81	MS 88	MS 95
MS 47	MS 54	MS 61	MS 68	MS 75	MS 82	MS 89	MS 96
MS 48	MS 55	MS 62	MS 69	MS 76	MS 83	MS 90	MS 97
MS 49	MS 56	MS 63	MS 70	MS 77	MS 84	MS 91	MS 98

Time	A-05MH (MS 1)	F-12CH (MS 2)	D-1003 (MS 3)
9:55-10:00 Opening Remarks	Large macromolecular complexes Chairs: L. Malinina, J. Ding	Advances in grazing 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.01.1(C15) M. G. Rossmann: The maturation pathway of flaviviruses studied by crystallography and electron microscopy	MS.02.1(C16) P. Muller-Buschbaum: Recent developments in GISAXS and GISANS - nanobeams and <i>in-situ</i> kinetic investigations	MS.03.1(C18) R. W. W. Hoof: Reliable determination of absolute structure using small Bijvoet differences
10:30-11:00	MS.01.2(C15) W. A. Hendrickson: Structural insights into molecular chaperone activity	MS.02.2(C16) T. Matsushita: Quick X-ray reflectometry in simultaneous multiwavelength dispersive mode	MS.03.2(C18) L. J. Bourhis: Small molecule toolbox
11:00-11:30	MS.01.3(C15) M. Yusupov: Structures of the ribosome on different functional states	MS.02.3(C17) B. Lee: Structural characterization using the multiple scattering effects in GISAXS	MS.03.3(C18) L. Palatinus: The charge-flipping algorithm and related dual-space structure solution methods
11:30-12:00	MS.01.4(C15) D. G. Vassilyev: Structural basis of transcription: Structures of the bacterial RNA polymerase elongation complexes	MS.02.4(C17) A. Takahara: Neutron reflectively study of chain conformation in polyelectrolyte brushes at the liquid interface	MS.03.4(C19) H. O. Sorensen: Closing the gap between single crystal and powder diffraction
12:00-12:30	MS.01.5(C16) N. Numoto: Ligand-induced structural changes of giant hemoglobin	MS.02.5(C17) R. Lazzari: Following growth and catalytic reaction of oxide supported metal nanoparticles with GISAXS	MS.03.5(C19) C. Giacovazzo: Advances in methods and algorithms in EXPO2008

C-1001, 2 (MS 4)	G-1202 (MS 5)	B-05SH (MS 6)	E-1009 (MS 7)
Hydrothermal growth of crystals Chairs: K. Byrappa, S. Feng	Modelization of structure of molecular compounds and implications for reactivity Chairs: M. J. Calhorda, N. E. Ghermani	Computational methods Chairs: G. Murshdov, V. Lunin	Water clusters in molecular crystals, coordination polymers and biological macromolecule Chairs: K. Biradha, L. Infantes
MS.04.1(C19) T. Adschiri: Supercritical hydrothermal synthesis of organic inorganic hybrid nanoparticles	MS.05.1(C21) K. Kirchner: Solid-state vs solution reactivity of iron complexes: Stereospecific and reversible CO binding	MS.06.1(C22) P. D. Adams: Macromolecular refinement at subatomic resolution with interatomic scatterers	MS.07.1(C24) J. L. Atwood: Supramolecular stabilization of well-ordered water clusters
MS.04.2(C19) D. Ehrentraut: Acidic ammonothermal growth of bulk GaN crystals	MS.05.2(C21) K. Tatsumi: A new synthetic route to iron-sulfide clusters modeling the active site of nitrogenase	MS.06.2(C23) P. Emsley: Macromolecular model-building and validation using Coot	MS.07.2(C24) M. Nakasako: Hydration structure changes around proteins at work
MS.04.3(C20) K. Kajiyoshi: Vapor-phase hydrothermal preparation of titanate fibers and nanotubes	MS.05.3(C21) N. Bouhaida: Advances in electrostatics and application to molecular reactivity	MS.06.3(C23) S. X. Cohen: Advances in automatic model building and structure completion in the context of ARP/wARP	MS.07.3(C24) C. Ruiz-Pérez: Water embedded in metal-polycarboxylate crystal host
MS.04.4(C20) M. Kakihana: Selective synthesis of nano-crystalline TiO ₂ polymorphs from new water-soluble titanium complexes	MS.05.4(C22) M. M. Kubicki: Structural chemistry of 2-aza-1,3-dienes	MS.06.4(C23) D. Turk: MAIN 2008: Real space model fitting - as good as it gets	MS.07.4(C25) Y. Sugawara: Diffused scattering and dynamic disorder observed nucleotide hydrates
MS.04.5(C20) J. Riegler: Simple processing of functional ZnO from solution - route towards designed nano-hybridmaterials	MS.05.5(C22) J-C. Daran: Iridium catalyzed hydrogenation with chiral ferrocenyl P-S ligands. X-ray structure of precatalysts	MS.06.5(C23) E. A. Merritt: Beyond crystallographic refinement: Broader application of TLSMD to model protein dynamics	MS.07.5(C25) T. Ozeki: Incompatible host-guest strategy to enclathrate water clusters into polyoxometalate crystals

Time	A-05MH (MS 8)	F-12CH (MS 9)	D-1003 (MS 10)
14:45-14:50 Opening Remarks	Protein-nucleic acid interactions Chairs: N. Verdagner, R. Sankaranarayanan	Macromolecular structural studies by powder diffraction, AFM, etc. Chairs: J. Helliwell, R. Thorne	Decision making and algorithms for automation of data acquisition Chairs: J. Wang, J. F. Britten
14:50-15:20	MS.08.1(C25) W. Yang: Stop-action movie of UvrD helicase unwinding DNA	MS.09.1(C27) R. Von Dreele: Seeing the first stages of protein crystal nucleation through to a full powder pattern	MS.10.1(C28) B. H. Toby: Automation of the APS 11-BM high-resolution and high-throughput powder diffractometer
15:20-15:50	MS.08.2(C25) O. Nureki: Stop codon recoding mechanism revealed by the suppressor tRNAPyl/PyIS complex structure	MS.09.2(C27) D. A. Shapiro: Serial crystallography: Use of a micro-jet for diffraction of protein nano-crystals or molecules	MS.10.2(C28) L. M. Daniels: Start to finish: Algorithms and parameters for successful robotic data collection
15:50-16:20	MS.08.3(C26) M. Coll: DNA transfer machines	MS.09.3(C27) Y. Hosokawa: Femtosecond laser etching of protein crystal to process and to isolate the single crystal	MS.10.3(C29) J. Kaercher: True walk-away automation in chemical crystallography
16:20-16:50	MS.08.4(C26) J. Li: RNA-protein interactions in the U4 snRNP core domain	MS.09.4(C27) S. Basso: Features of the secondary structure of protein molecules from powder diffraction data	MS.10.4(C29) S. K. Burley: Rapid synchrotron X-ray crystallography for drug discovery using the SGX-CAT beamline at the APS
16:50-17:20	MS.08.5(C26) P. M. Alzari: Structural basis of lipid biosynthesis regulation in Gram-positive bacteria	MS.09.5(C28) P. Batat: Characterization of spider silks weaved by different species living in the Black sea region of Turkey	MS.10.5(C29) M. Cianci: The interdependence of wavelength, redundancy and dose on a sulfur sad experiment

C-1001, 2 (MS 11)	G-1202 (MS 12)	B-05SH (MS 13)	E-1009 (MS 14)
Pitfalls and successes in crystallographic teaching Chairs: D. Watkin, P. Spadon	Liquid crystals and crystallography: A tribute to Pierre-Gilles de Gennes (1932.10.24-2007.5.18) Chairs: B. Donnio, A. Crispini	Growth of single crystals for neutron and X-ray investigation by the floating zone and other techniques Chairs: H. Dabkowska, I. Tanaka	Symmetry, asymmetry and chirality in molecular aggregation Chairs: W. Kaminsky, I. Hisaki
MS.11.1(C30) A. Linden: Hands-on crystallographic teaching: The Zurich School of Crystallography - Bring your own crystals	MS.12.1(C31) P. Davidson: X-ray scattering studies of liquid-crystalline suspensions of anisotropic mineral nanoparticles	MS.13.1(C33) J. M. Tranquada: Exploring the phase diagram of $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$: Spins, stripes, and superconductivity	MS.14.1(C34) R. Kuroda: Chirality realized only in the crystalline state: Inorganic and organic compounds
MS.11.2(C30) T. Wagner: Conquering superspace - A beginner's guide to modulated structures	MS.12.2(C31) G. Ungar: Crystallography of 2D and 3D structures in liquid crystal amphiphiles and nanocomposites	MS.13.2(C33) G. Balakrishnan: High quality single crystals for neutron experiments	MS.14.2(C34) V. S. Minkov: Structure-property relationship in the crystals of chiral amino acids and their racemic counterparts
MS.11.3(C30) K. A. Kantardjiev: Sustaining crystallography in the 21st century: Education policies and use of cyberinfrastructure	MS.12.3(C32) K. Saito: Molecular aggregation structure of exotic liquid crystals formed by thermotropic mesogen BABH(n)	MS.13.3(C33) H. Eisaki: Tailor-made single crystal growth of high-Tc superconductors for characterization by spectroscopy	MS.14.3(C35) H. Koshima: Chiroptical properties of N-benzoylglycine crystals
MS.11.4(C31) M. M. Julian: Use of images from neolithic art, clip art, digital cameras, and MATLAB® in teaching crystallography	MS.12.4(C32) Y. Shimizu: Mesophase semiconductors: Design for 3D-mesophases with effective paths for electronic charge hopping	MS.13.4(C33) E. V. Pomjakushina: Layered and cubic cobaltites grown by floating zone, structural and magnetic properties study	MS.14.4(C35) C. H. Görbitz: A solution to the problem why chiral hydrophobic amino acids form crystals with $Z' = 2$
MS.11.5(C31) I. D. Williams: Teaching crystallography: Approaches for non-crystallographers and non-native speakers in Asia	MS.12.5(C32) T. Kato: Functional nanostructured liquid-crystalline assemblies	MS.13.5(C34) R. Fittipaldi: Micro-crystallographic structure of $\text{Sr}_2\text{RuO}_4/\text{Sr}_3\text{Ru}_2\text{O}_7$ eutectic crystals grown by floating zone method	MS.14.5(C35) M. Sakamoto: Control of chirality by spontaneous crystallization and absolute asymmetric synthesis in fluid media

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

C-1001, 2 (MS 18)	G-1202 (MS 19)	B-05SH (MS 20)	E-1009 (MS 21)
<i>In-situ</i> & 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 <i>in-situ</i> 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: <i>In situ</i> 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: <i>In situ</i> 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. Milanese: <i>In situ</i> 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

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. Sasaki	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: <i>In situ</i> 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 ⁺ 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 patterns in co-crystals of small molecules

Time	A-05MH (MS 29)	F-12CH (MS 30)	D-1003 (MS 31)
9:55-10:00 Opening Remarks	Virus structure and antiviral strategies Chairs: J. Johnson, M. J. van Raaij	From minerals to materials Chairs: R. Hock, G. Ferey	Electric and magnetic properties of molecular crystals Chairs: M. Yamashita, A. Cornia
10:00-10:30	MS.29.1(C57) P. D. 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
10:30-11:00	MS.29.2(C57) N. Verdagner: What we can learn from the structure of viral RNA-dependent RNA polymerases	MS.30.2(C59) N. N. Bramnik: High-voltage cathodes for Li-ion batteries: Metallophosphoolivines and manganese-based spinels	MS.31.2(C60) A. Kobayashi: Structures and physical properties of single-component molecular metals
11:00-11:30	MS.29.3(C58) F. A. Rey: Evolutionary links among viruses of different categories revealed by dsRNA virus capsid structures	MS.30.3(C59) J. B. Parise: Towards a better understanding of atomic arrangements in nano-minerals	MS.31.3(C61) V. Marvaud: Photoswitchable high spin molecules
11:30-12:00	MS.29.4(C58) J. E. Lee: Structure of the trimeric, prefusion Ebola virus GP complexed with an antibody from a human survivor	MS.30.4(C59) S. Schorr: Kesterite - an alternative absorber material for thin film solar cells	MS.31.4(C61) S. S. Khasanov: Structural aspects of magnetic transitions and high conductivity in ionic complexes of fullerenes
12:00-12:30	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 mineral trioxide aggregate and its role on properties as biomaterial cement	MS.31.5(C61) Y. Ohgo: The spin-crossover triangle in the iron(III) porphyrinoids

C-1001, 2 (MS 32)	G-1202 (MS 33)	B-05SH (MS 34)	E-1009 (MS 35)
Nanostructure refinement and solution Chairs: C. Giannini, F. Matteucci	Liquids and amorphous systems at high pressure Chairs: M. Guthrie, Y. Katayama	Advanced electron microscopy Chairs: R. Holmestad, A. Kirkland	Combined XAFS and diffraction of inorganic structures Chairs: K. Asakura, A. Di Cicco
MS.32.1(C62) P. Juhas: Nanostructure investigations using atomic pair distribution function and other direct-space methods	MS.33.1(C63) S. A. Bonev: 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	MS.35.1(C66) D. T. Bowron: Comprehensive structural characterisation of local and bulk structure in disordered systems
MS.32.2(C62) A. Cervellino: Analysis of partially ordered (nano)materials through the Debye function method	MS.33.2(C63) M. G. Tucker: Total scattering studies of pressure induced amorphization	MS.34.2(C65) S. Stemmer: Image contrast in atomic resolution high-angle annular dark-field images	MS.35.2(C66) M. G. Newville: Developments of advanced XAFS analysis techniques with Ifeffit
MS.32.3(C62) Y. Andreev: Atomic arrangement in a nanotube from powder X-ray diffraction	MS.33.3(C64) K. Fuchizaki: Polyamorphism in tin tetraiodide	MS.34.3(C65) A. L. Bleloch: In aberration corrected STEM, shrinking some dimensions expands others	MS.35.3(C67) A. Michalowicz: Apparent mismatch between XAFS and XRD structure of crystalline and amorphous electrochromic WO ₃
MS.32.4(C63) C. F. Campana: The application of a molecular replacement approach to the refinement of a copper nanoball complex	MS.33.4(C64) K. Matsuda: Structural studies of expanded fluid alkali metals	MS.34.4(C65) O. Kamimura: Development of new electron diffraction microscope for diffractive imaging	MS.35.4(C67) A. Yoshiasa: High pressure and high temperature EXAFS and diffraction study of AgI
MS.32.5(C63) I. A. Vartanians: Coherent diffractive imaging of nanostructures at synchrotron and FEL sources	MS.33.5(C64) C. Sanloup: Structural transition in amorphous sulfur compressed up to 100 GPa	MS.34.5(C66) G. Botton: Applications of aberration-corrected TEM-STEM and high-resolution EELS in materials research	MS.35.5(C67) J. C. Hanson: <i>In situ</i> XRD and XAFS studies of oxidation/reduction and water gas shift reactions of Cu doped ceria

Time	A-05MH (MS 36)	F-12CH (MS 37)	D-1003 (MS 38)
14:45-14:50 Opening Remarks	Biological interests and biological electron microscopy Chairs: M. R. N. Murthy, K. Iwasaki	Crystal properties and bonding: What we really learn from accurate charge density studies and quantum calculations? Chairs: M. Spackman, K. Tanaka	Self-organization and self-assembly: From nucleation to crystal growth, from eutectics to photonic and liquid crystals, and from theory to application Chairs: D. Pawlak, P. Metrangolo
14:50-15:20	MS.36.1(C67) M. Wilmanns: Zooming into the overall architecture of the giant muscle protein titin	MS.37.1(C69) D. Stalke: Charge density based ligand design	MS.38.1(C71) L. Granasy: Phase field modeling of self-organized polycrystalline structures: Denrites, spherulites, eutectics
15:20-15:50	MS.36.2(C68) C. Sato: Ion channel structures by single particle analysis using EM: Sodium and TRP channels, IP3 receptor	MS.37.2(C69) D. Jayatilaka: Non-linear optical properties & structure determination by combining X-ray data and QM wavefunctions	MS.38.2(C71) Y. Waku: High temperature characteristics of unidirectionally solidified ceramic eutectics
15:50-16:20	MS.36.3(C68) T. Omura: The assembly process of the double-layered capsids of phytoreoviruses	MS.37.3(C70) D. Hashizume: Characterization of weak chemical bonds in highly strained and hypervalent compounds	MS.38.3(C71) G. G. Long: Nanoparticle halo formation around colloids in binary solutions
16:20-16:50	MS.36.4(C68) A. Goulet: A new virus structure: The nucleosome-like organization of the filamentous archaeal virus AFV1	MS.37.4(C70) C. Gatti: How and why elemental boron undergoes self charge transfer between 19 and 89 GPa	MS.38.4(C72) K. Itaya: Perfect single crystals of organic semiconductors prepared by crystallization from solutions
16:50-17:20	MS.36.5(C69) D. Suck: Structural studies of Holliday junction resolvases from bacteriophages, archaea and yeast	MS.37.5(C70) R. Orlando: Advances in quantum <i>ab initio</i> calculations with the CRYSTAL code	MS.38.5(C72) J. Nozawa: Self-assembled magnetite particles formed 4.6 billion years ago

C-1001, 2 (MS 39)	G-1202 (MS 40)	B-05SH (MS 41)	E-1009 (MS 42)
PDF/RDF analysis from pulsed-neutron and X-ray scattering Chairs: T. Egami, M. Tucker	Crystallography of planetary materials at extreme conditions Chairs: T. Yagi, J. Parise	Precession electron diffraction and electron crystallography Chairs: S. Nicolopoulos, J. Gjornes	Decision making and algorithms for automation in macromolecular structure solution Chairs: H. Powell, R. Hoofft
MS.39.1(C72) T. Proffen: Total scattering: The key to the local and medium range structure of complex materials	MS.40.1(C74) J. S. Loveday: High pressure studies of planetary ices	MS.41.1(C75) C. J. Gilmore: Solving zeolite structures using electron crystallography	MS.42.1(C77) N. Kunishima: High-throughput crystallization-to-structure pipeline at RIKEN SPring-8 Center
MS.39.2(C72) T. Otomo: New opportunity to explore noncrystalline materials by neutron total diffractometer (NOVA) at J-PARC	MS.40.2(C74) H. Fukazawa: Nucleation and growth of ice XI -Study suggests the existence of ferroelectric ice in the Universe-	MS.41.2(C75) J. P. Abrahams: Prospects for structure solution by electron diffraction of three-dimensional protein crystals	MS.42.2(C77) J. M. Holton: There and back again: Using simulated diffraction images to optimize data processing by Elves
MS.39.3(C73) D. A. Keen: Negative thermal expansion and local crystal structure	MS.40.3(C74) K. Hirose: High-pressure phase transitions of deep Earth materials	MS.41.3(C76) J-P. Morniroli: Symmetry determinations from electron precession: Comparison and advantages with CBED	MS.42.3(C77) B-C. Wang: Signal-based data collection: A novel approach to on-site auto-structure determination at SER-CAT
MS.39.4(C73) V. Petkov: High-resolution structure of disordered materials by high-energy X-ray diffraction	MS.40.4(C75) M. Avdeev: Perovskites ABX ₃ under pressure: Transition to post-perovskite CaIrO ₃ type and other scenarios	MS.41.4(C76) S. Hovmöller: Quantitative 3D electron diffraction data by precession and electron rotation methods	MS.42.4(C78) S. Panjekar: Auto-Rickshaw: An online tool for validation of an X-ray diffraction experiment
MS.39.5(C73) S. Shamoto: Atomic pair distribution function analysis on nanomaterials	MS.40.5(C75) P. H.J. Mercier: <i>Ab-initio</i> crystallography of kaolin minerals: Synthesis, diagenesis and mantle pressures	MS.41.5(C76) W. Sinkler: Models for simplified treatment of precession electron diffraction	MS.42.5(C78) C. Vonrhein: AutoPROC - A framework for automated data processing

Time	A-05MH (MS 43)	F-12CH (MS 44)	D-1003 (MS 45)
9:55-10:00 Opening Remarks	Structural biology of the cell Chairs: P. Alzari, H. S. Yuan	Teaching macromolecular crystallography Chairs: K. Kantardijeff, B. Santarsiero	Crystal design from hydrogen bond to halogen bond and beyond Chairs: A. Beatty, M. Bhadbhade
10:00-10:30	MS.43.1(C78) K. Diederichs: Structure of AcrB: A novel mechanism for multidrug resistance	MS.44.1(C80) M. Ruf: Is there a steep learning curve in crystallography?	MS.45.1(C81) G. Minguez: Metal-organic networks designed by combination of hydrogen bonds and halogen bonds
10:30-11:00	MS.43.2(C78) A. M. Houdusse: Structural description of the ATPase cycle of a myosin that moves backward	MS.44.2(C80) A. Faust: A tutorial for learning and teaching macromolecular crystallography	MS.45.2(C81) P. Metrangolo: A journey through the rational design of molecular solids with halogen bonding
11:00-11:30	MS.43.3(C79) P. E. Czabotar: How programmed cell death is regulated: Insights from structures of Bel-2 family protein complexes	MS.44.3(C80) S. Djordjevic: The web-based teaching in the Institute of Structural and Molecular Biology, University of London	MS.45.3(C82) J. F. Gallagher: Structural systematic studies of fluoro(pyridinyl) benzamide derivatives
11:30-12:00	MS.43.4(C79) M. Machius: Structural basis of spindle checkpoint activation and inactivation by Mad2 and p31comet	MS.44.4(C81) C. Yang: Sulfur-SAD phasing becomes a routine approach to solve <i>de novo</i> structures	MS.45.4(C82) S. A. Bourne: Crystal engineering using the thiourea moiety
12:00-12:30	MS.43.5(C79) S. B. Gabelli: Structural basis for the effects of PI3Kalpha oncogenic mutations	MS.44.5(C81) B. Rupp: Scientific inquiry and inference in macromolecular crystallography	MS.45.5(C82) M. A. Spackman: Electrostatic complementarity: A universal theme in molecular crystal structures?

C-1001, 2 (MS 46)	G-1202 (MS 47)	B-05SH (MS 48)	E-1009 (MS 49)
Powder diffraction studies of hydrogen storage materials Chairs: M. O. Jones, P. Whitfield	High pressure studies on advanced and nano-materials Chairs: N. Dubrovinskaia, V. Solozhenko	Physical properties from integrated electron diffraction and X-ray diffraction Chairs: A. Avilov, K. Tsuda	Wide-gap semiconductors for health, energy and environment Chairs: K. Kakimoto, D. Bliss
MS.46.1(C83) B. David: Structure and properties of ammonia borane based hydrogen storage materials	MS.47.1(C84) E. Takayama-Muromachi: High pressure synthesis and physical property measurements of perovskite transition-metal oxides	MS.48.1(C85) Y. Zhu: Quantitative electron and X-ray diffraction study of charge density in complex oxides	MS.49.1(C87) K. Stanislaw: The structure and dynamics of GaN(0001) surface during HVPE GaN growth – <i>Ab initio</i> study
MS.46.2(C83) Y. Filinchuk: Light metal borohydrides: Going beyond crystal structures	MS.47.2(C84) E. Gregoryanz: Synthesis and characterization of metal nitrides	MS.48.2(C86) K. Kato: Bonding electrons visualization in photo-excited state using synchrotron X-ray powder diffractometry	MS.49.2(C87) A. Koukitu: Hydride vapor phase epitaxy of AlN and AlGaIn
MS.46.3(C83) T. Sato: Structural investigation of metal borohydrides by X-ray/neutron diffraction and computational study	MS.47.3(C85) L. S. Dubrovinsky: High pressure synthesis of nanocrystalline superhard materials	MS.48.3(C86) B. B. Iversen: Structure based design of new thermoelectric materials	MS.49.3(C88) S. Naritsuka: Fabrication of InN dot structures by droplet epitaxy using NH ₃
MS.46.4(C83) C. Weidenthaler: Powder diffraction investigations of a new class of rare-earth aluminum hydrides	MS.47.4(C85) S. Quartieri: Pressure-induced over-hydration of zeolites: New insights from the elastic behavior of gismondine	MS.48.4(C86) J. Ciston: Experimental measurements of bond density at the Si(111)-7x7 surface	MS.49.4(C88) X. Chen: Dislocation density in silicon ingot during a unidirectional solidification process
MS.46.5(C84) J-H. Her: Neutron scattering studies on deuterium adsorbed pore framework compound, K ₂ Zn ₃ [Fe(CN) ₆] ₂	MS.47.5(C85) J-P. Itie: Pressure induced transition in nano-TiO ₂ : An X-ray absorption spectroscopy study	MS.48.5(C87) V. E. Dmitrienko: Phonon and electronic properties of crystals and chirality studied with resonant X-ray diffraction	MS.49.5(C88) T. Ohachi: AlN and GaN hetero epitaxy on Si substrate using activity modulation migration enhanced MBE (15 min)
			MS.49.6(C89) H. Matsuhata: Contrast of dislocations in 4H-SiC by SR topography in grazing-incidence geometry (15 min)

Time	A-05MH (MS 50)	F-12CH (MS 51)	D-1003 (MS 52)
14:45-14:50 Opening Remarks	Hot structures Chairs: P. Chui Shaw, S. Eon Ryu	Complementarity of SAXS and SANS with other structural methods in molecular biology Chairs: J. Trehella, T. Fujisawa	Host-guest crystal chemistry Chairs: S. A. Bourne, P. Bombizc
14:50-15:20	MS.50.1(C89) J-H. Wang: Decoding homophilic recognition specificity of Dscam, a neuronal receptor with thousands isoforms	MS.51.1(C91) D. I. Svergun: Joint use of SAXS and SANS with high resolution methods for macromolecular solutions	MS.52.1(C92) K. Tanaka: Novel cyclic salicylide derivatives: Guest inclusion and organo-gellation
15:20-15:50	MS.50.2(C89) K. Miki: Crystal structure of the [2Fe-2S] transcriptional activator SoxR bound to DNA	MS.51.2(C91) M. Kojima: Additivity, redundancy, and complementarity between structural information from NMR and SAXS data	MS.52.2(C92) L. Brammer: Porous material behaviour in non-porous crystals: A route to chemical reactions
15:50-16:20	MS.50.3(C89) J-O. Lee: Hybrid LRR technique and crystal structures of the toll-like receptor complexes	MS.51.3(C91) E. J. Goldsmith: The structure of the MAP2K MEK6 is an autoinhibitory dimer both in crystals and in solution	MS.52.3(C93) L. R. Nassimbeni: Polymorphism, isostructurality and selectivity in inclusion compounds
16:20-16:50	MS.50.4(C90) J. P. Morth: Crystal structure of the sodium pump at 3.5 Å	MS.51.4(C91) H. Tsuruta: Time-resolved X-ray scattering studies on bacteriophage assemblies	MS.52.4(C93) L. Fabian: What are the molecular properties that influence the formation of methanol solvates?
16:50-17:20	MS.50.5(C90) L. Tong: Structural studies of pre-mRNA 3'-end processing	MS.51.5(C92) S. Akiyama: Real-time SAXS observation of assembly and disassembly dynamics of cyanobacterial clock proteins	MS.52.5(C93) X. Wang: Framework deformation and guest packing in a microporous vanadium benzenedicarboxylate

C-1001, 2 (MS 53)	G-1202 (MS 54)	B-05SH (MS 55)	E-1009 (MS 56)
Developments in structure solution and refinement from powders Chairs: H. Toraya, P. W. Stephens	Shape memory alloys Chairs: K. R. A. Ziebeck, T. Kanomata	Surfaces Chairs: D. K. Saldin, F. Boscherini	Phase transitions and physical properties at high pressure Chairs: L. Robin Benedetti, G. Shen
MS.53.1(C94) M. Takata: Electrostatic potential and electric field imaging by MEM powder diffraction data analysis	MS.54.1(C95) R. Kainuma: Martensitic transformations in the Ni-based ferromagnetic shape memory alloys	MS.55.1(C97) M. A. Van Hove: Structure of nanomaterials via electron multiple scattering	MS.56.1(C98) Y. Feng: Quantum phase transitions using non-resonant X-ray magnetic scattering at high pressures
MS.53.2(C94) M. C. Burla: MAD techniques applied to powder data: The method of the joint probability distribution functions	MS.54.2(C96) T. Ohba: Martensitic transformation and phonon softening behavior in TiNi alloy system	MS.55.2(C97) C. J. Hirschmugl: Distinguishing chirality using electron diffraction	MS.56.2(C99) N. Dragoe: High pressure induced charge ordering in lithium vanadate spinel
MS.53.3(C94) C. C. Wilson: Towards routine refinement of hydrogenous materials by neutron powder diffraction	MS.54.3(C96) T. Hickel: First principles determination of phase transitions in magnetic shape memory alloys	MS.55.3(C97) A. Diethert: Surface enrichment layers in pressure sensitive adhesive films	MS.56.3(C99) Y. Lee: Pressure-induced hydration and order-disorder transition in a synthetic gismondine zeolite
MS.53.4(C95) V. V. Chernyshev: Powder diffraction and DFT optimization in structural characterization of macrocyclic compounds	MS.54.4(C96) W. Hu: X-ray fluorescence holography of Ti-Ni-Fe alloy single crystal	MS.55.4(C98) C. Carbone: Coordination effects in magnetic nanostructures	MS.56.4(C99) I. Loa: Lattice dynamics in incommensurate elemental crystals at high pressure
MS.53.5(C95) K. Shankland: SDPD: A key component in populating the carbamazepine crystal structure landscape	MS.54.5(C96) K. Rolfs: Co-doped Ni-Mn-Ga - A new smart material for industry	MS.55.5(C98) E. Holub-Krappe: Structural effects and the spin reorientation in Au/Co/Au films	MS.56.5(C100) M. Eremets: Phase transformations in silane - Hydrogen-dominant material

Time	A-05MH (MS 57)	F-12CH (MS 58)	D-1003 (MS 59)
9:55-10:00 Opening Remarks	Recent and future advances in neutron structural biology Chairs: D. Myles, I. Tanaka	Structure-property correlations and phase transition in inorganics Chairs: J. Kreisel, W. Kleemann	Chemical recognition and supramolecular architectures Chairs: M. Wais Hosseini, P. Paoli
10:00-10:30	MS.57.1(C100) R. Kuroki: Structure of drug-target proteins determined by both X-ray and neutron diffraction	MS.58.1(C102) H. Fuess: Nature of the morphotropic phase boundary (MPB) in lead zirconate titanate (PZT)	MS.59.1(C103) M. J. Hardie: Star-burst metallo-supramolecular prisms and coordination polymers with pyramidal ligands
10:30-11:00	MS.57.2(C100) F. Meilleur: Neutron crystallographic analysis of deuterated and selectively CH ₃ -protonated deuterated rubredoxin	MS.58.2(C102) S. Van Smaalen: Phase transitions in MOX (M = Ti, V, Cr; X = Cl, Br)	MS.59.2(C104) S. Kitagawa: Porous coordination polymers having guest accessible functional organic sites
11:00-11:30	MS.57.3(C101) M. P. Blakeley: Neutron macromolecular crystallography using the Laue diffractometer LADI-III	MS.58.3(C102) J-P. Itie: Local aspects of high-pressure phase transitions in ferroelectrics	MS.59.3(C104) G. Resnati: A molecular Legoland through halogen bonding
11:30-12:00	MS.57.4(C101) S. Antonyuk: Seeing hydrogens: X-ray limitations and possibilities at 0.9 Å and synergy with neutron diffraction	MS.58.4(C103) K. Okimura: X-ray diffraction study on structures of vanadium dioxide films with metal-insulator transition	MS.59.4(C104) T. C. W. Mak: Coordination network assembly with carbonyl-bridged nitrogen heterocycles
12:00-12:30	MS.57.5(C101) J. P. Glusker: Locating hydrogen atoms in enzymes: A neutron structure of D-xylose isomerase with bound D-xylulose	MS.58.5(C103) S. Shimomura: Modulated structure and ferromagnetic metallic state of SmNiC ₂	MS.59.5(C105) R. Boer: Molecular recognition and self-organization of three-way DNA junctions and supramolecular helicates

C-1001, 2 (MS 60)	G-1202 (MS 61)	B-05SH (MS 62)	E-1009 (MS 63)
Microstructure and structural imperfections Chairs: A. Leineweber, T. Ungar	New algorithms for magnetic crystallography and understanding magnetic structures Chairs: S. Cadogan, M. Avdeev	Real space direct methods Chairs: P. Combettes, J. Zuo	XAFS in biocrystallography Chairs: I. Ascone, T. Prangé
MS.60.1(C105) C. Genzel: Analysis of residual stresses induced by surface processing: Angle vs. energy dispersive diffraction	MS.61.1(C107) A. S. Wills: Application of representation theory and SARAh to magnetic structure determination	MS.62.1(C108) D. K. Saldin: Keeping a promise of the XFEL: Crystallography without crystals	MS.63.1(C109) B. Hedman: Photoreduction of metalloprotein active sites by synchrotron radiation
MS.60.2(C105) E. Schaffer: X-ray line profile analysis for the characterization of nanostructured materials	MS.61.2(C107) J. Rodriguez-Carvajal: The determination of magnetic structures by simulated annealing using the FullProf Suite	MS.62.2(C108) S. Marchesini: Hybrid thresholding-projection algorithms for the crystallographic phase problem	MS.63.2(C110) S. Hasnain: Crystallography with X-ray and optical spectroscopies for metalloproteins structural studies
MS.60.3(C106) R. Guinebretiere: High-resolution X-ray diffraction analysis of strain relaxation in epitaxial oxide thin films	MS.61.3(C107) D. B. Litvin: International-like tables for magnetic crystallography	MS.62.3(C109) R. Luke: Relaxed averaged alternating reflections for diffraction imaging	MS.63.3(C110) S. Mangani: X-ray absorption spectroscopy for the structure determination of copper transport proteins
MS.60.4(C106) P. Imperia: Paramagnetism and ferromagnetism of TiO ₂ and ZnO as seen by XMCD: A way to study defects in oxides	MS.61.4(C107) A. L. Goodwin: <i>Ab initio</i> magnetic structure refinement: Total scattering and RMCProfile	MS.62.4(C109) I. Yamada: Reduced-rank extension of BLUE and deep lipschitzian gradient projector for inverse problems	MS.63.4(C110) P. Fons: Structure in the local environment of Zn ²⁺ ion in the anti-termination protein of <i>Bacillus subtilis</i>
MS.60.5(C106) K. Lawniczak-Jablonska: Mn atoms in GaAs: First evidence for Ga interstitial site occupation	MS.61.5(C108) C-H. Lee: An ion sputtering epitaxial FePt ultra-thin film studied by magnetic circular dichorism	MS.62.5(C109) P. F. Lyman: Solution to the phase problem for surface X-ray diffraction	MS.63.5(C111) V. A. Streltsov: The structure of the Amyloid β -peptide high affinity copper II binding site in Alzheimer's disease

Time	A-05MH (MS 64)	F-12CH (MS 65)	D-1003 (MS 66)
14:45-14:50 Opening Remarks	New membrane protein structures Chairs: R. Stroud, A. Yamashita	Recent progress in synchrotron data collection Chairs: R. Sanishvili, C. Schulze-Briesse	Co-crystals: Theory, synthesis and use Chairs: M. Du, A. Bond
14:50-15:20	MS.64.1(C111) A. Amunts: Structural basis of a plant photosystem I sunlight conversion	MS.65.1(C112) M. Kobas: Synchrotrons data collection with PILATUS detectors - Perspectives for today and tomorrow	MS.66.1(C114) G. R. Desiraju: Multi-component solids in crystal engineering
15:20-15:50	MS.64.2(C111) D. Xia: Inhibitor complexed structures of the Cyt bc1 from the photosynthetic bacterium <i>R. sphaeroides</i>	MS.65.2(C113) S. M. Soltis: Remote access to the SSRL protein crystallography beam lines	MS.66.2(C114) C. B. Aakeroy: From a molecular dating agency to successful co-crystal synthesis
15:50-16:20	MS.64.3(C111) K. Inaba: Structure and mechanism of the DsbB-DsbA protein disulfide generation system in <i>E. coli</i>	MS.65.3(C113) M. Schiltz: Exploiting the anisotropy of anomalous scattering boosts the phasing power of SAD/MAD experiments	MS.66.3(C114) W. Jones: Multicomponent crystals; Their formation, characterisation and application
16:20-16:50	MS.64.4(C112) B. P. Pedersen: Crystal structure of the plasma membrane proton pump	MS.65.4(C113) A. Wagner: Microcrystal manipulation with laser tweezers	MS.66.4(C115) C. P. Brock: An unexpected molecular co-crystal with a variable degree of order
16:50-17:20	MS.64.5(C112) S. Murakami: Bacterial multi drug efflux transporter AcrB, - The pumping mechanism	MS.65.5(C114) J. C. Spence: Serial crystallography using protein beams	MS.66.5(C115) M. T. Kirchner: <i>In-situ</i> cocrystallisation combined with Raman spectroscopy

C-1001, 2 (MS 67)	G-1202 (MS 68)	B-05SH (MS 69)	E-1009 (MS 70)
Quantum phase transitions Chairs: B. Lake, M. Kenzelmann	Extraction of physical and chemical properties from charge density maps Chairs: U. Pietsch, W. Scherer	Use of coherence in life and physical sciences Chairs: I. Vartaniants, H. Chapman	Crystal chemistry and crystallography of aperiodic crystals Chairs: Y. Michiue, A. Monge
MS.67.1(C115) S-H. Lee: Magnetic and structural transitions in frustrated magnets	MS.68.1(C116) A. Volkov: On the evaluation of energy densities with aspherical pseudoatoms: A model study	MS.69.1(C118) Y. Nishino: 3D view of mesoscopic internal structure by coherent hard X-ray diffraction	MS.70.1(C120) J. Hadermann: Applications of TEM in the study of incommensurately modulated compounds
MS.67.2(C115) T. J. Sato: <i>E/T</i> -scaling behavior in the magnetic quasicrystal Zn-Mg-Ho	MS.68.2(C117) G. R. N. Tayur: Exploring pathways of structural phase transitions <i>via</i> experimental charge density analysis	MS.69.2(C118) A. Barty: Femtosecond dynamic diffraction imaging: X-ray snapshots of ultra-fast nanoscale phenomena	MS.70.2(C120) O. Perez: Super space formalism to crack complex codes in material chemistry
MS.67.3(C116) S. A. Grigera: Quantum critical points and nematics: The ruthenate Sr ₃ Ru ₂ O ₇	MS.68.3(C117) P. Luger: Intra and intermolecular electron density properties of fullerene derivatives: First C ₇₀ examples	MS.69.3(C119) F. Pfeiffer: Coherent X-ray diffraction microscopy of extended objects	MS.70.3(C120) L. Elcoro: Long-period structures in the superspace formalism: From pyrrhotite to modular structures
MS.67.4(C116) Y. Yanase: Exotic superconductivity in crystals without inversion center	MS.68.4(C117) P. Macchi: Effects of crystal packing on the electron density of metal carbonyl complexes	MS.69.4(C119) G. J. Williams: Fresnel coherent diffractive imaging with X-rays	MS.70.4(C121) S. Lidin: Stistaite, an extension of the concept of solid solutions
MS.67.5(C116) T. Matsuo: Quantum mechanical delocalization of hydrogen atoms in (NH ₄) ₂ PtCl ₆	MS.68.5(C118) K. Tanaka: XAO analysis of the 5d-occupation in rare-earth complexes with high potential as quantum	MS.69.5(C119) J. K. Basu: Coherent small angle scattering from polymer nanocomposites	MS.70.5(C121) S. Schmid: Temperature dependence of the modulations in KNbOB ₂ O ₅ and RbNbOB ₂ O ₅

Time	A-05MH (MS 71)	F-12CH (MS 72)	D-1003 (MS 73)
9:55-10:00 Opening Remarks	Biophysical techniques for detecting ligand binding to pharmaceutical targets Chairs: R. E. Hubbard, Y. Kawakami	Micro-SAXS for nanoscience and medicine Chairs: P. Fratzl, J. Doucet	Structure-functions relationships of MOF Chairs: M. Eddaoudi, S. L. James
10:00-10:30	MS.71.1(C121) A. Ruf: X-ray structural analysis and biophysical assays in drug discovery	MS.72.1(C123) T. Pfohl: Combining microfluidics with micro-SAXS for studies of the dynamics of DNA compaction	MS.73.1(C124) R. Matsuda: Guest-responsive structures and properties of porous coordination polymers
10:30-11:00	MS.71.2(C121) S. Akashi: Studies of protein-protein and protein-RNA complexes by mass spectrometry	MS.72.2(C123) M. Foldvari: Application of SWAXS in nanomedicine: Characterizing nanoparticles and their interaction with skin	MS.73.2(C125) M. J. Rosseinsky: <i>In-situ</i> reactivity and selective chiral sorption in metal-organic frameworks
11:00-11:30	MS.71.3(C122) J. Murray: Characterising protein-ligand binding in support of structure-based drug discovery	MS.72.3(C123) F. Artzner: Peptidic nanotubes: From drug release to glass nanowires	MS.73.3(C125) L. J. Barbour: Porosity in flexible metal-organic systems
11:30-12:00	MS.71.4(C122) L. Gabison: Mechanism of the cofactor-less urate oxidase: X-ray structures with molecular oxygen or cyanide.	MS.72.4(C124) D. Viterbo: A mesoporous pattern created by nature: A SAXS and micro-SAXS study	MS.73.4(C125) G. Zhu: The synthesis and structure of multifunctional metal-organic frameworks
12:00-12:30	MS.71.5(C122) L. N. Johnson: Flavopiridol binding to P-TEFb (CDK9/cyclin T1)	MS.72.5(C124) Y. Nozue: Deformation behavior of drawn polymer spherulite studied by simultaneous micro SAXS-WAXS and POM	MS.73.5(C125) N. Lock: Elucidating negative thermal expansion in metal-organic frameworks

C-1001, 2 (MS 74)	G-1202 (MS 75)	B-05SH (MS 76)	E-1009 (MS 77)
Multiferroic materials Chairs: T. Kimura, L. Pinsard-Gaudart	Charge, spin and momentum density studies in material science Chairs: B. Gillon, P. Macchi	Diffraction imaging Chairs: F. Chen, H. Faulkner	Diffuse scattering in partially ordered/disordered systems Chairs: H. Abe, C. Branton
MS.74.1(C126) Y. Noda: Magnetic and crystal structure in connection with ferroelectric properties of multiferroic RMn_2O_5	MS.75.1(C127) W. Scherer: Electron localization phenomena in complex carbides of rare earth and transition metals	MS.76.1(C129) K. A. Nugent: Coherent diffraction imaging: A new tool for high resolution X-ray imaging	MS.77.1(C131) R. Welberry: Diffuse scattering as a probe of local structure
MS.74.2(C126) M. Kenzelmann: Ferroelectricity from magnetic order	MS.75.2(C128) J. Kozisek: Study of electronic structure of tetrakis(μ_2 -Acetato)-diaqua-di-copper(II) complex	MS.76.2(C129) U. J. Weierstall: Diffraction imaging and serial crystallography	MS.77.2(C131) M. Takahashi: Magnetic short-range order in Pt-rich Pt-Mn alloys
MS.74.3(C126) D. N. Argyriou: Function from frustration in modern multiferroics	MS.75.3(C128) P. Munshi: Estimation of optical properties from wavefunction fitting of X-ray diffraction data	MS.76.3(C130) R. V. Dronyak: Electron diffraction imaging of the MgO nanoparticle: Towards atomic-resolution	MS.77.3(C131) S. M. P. Francoual: Phason diffuse scattering in the icosahedral quasicrystalline phases Zn-X-Sc, X = Co, Ag, Mg
MS.74.4(C127) F. H. Damay: Crystal and magnetic structures of frustrated antiferromagnet CuCrO_2	MS.75.4(C128) J. Campo: Magnetic interactions in thiazyl-based magnets: The role of the charge and spin densities	MS.76.4(C130) C. Giannini: Coherent X-ray diffraction imaging of non periodic single objects	MS.77.4(C131) T. Weber: 3D-PDF analysis of single crystal diffuse scattering on the example of disordered quasicrystals
MS.74.5(C127) J. B. Claridge: Frustration of magnetic and ferroelectric long-range order in $\text{Bi}_2\text{Mn}_{4/3}\text{Ni}_{2/3}\text{O}_6$	MS.75.5(C129) M. Ito: Observation of spin densities by the X-ray magnetic diffraction	MS.76.5(C130) K. Kawahara: Beam divergence in electron diffraction imaging	MS.77.5(C132) S. Haas: Nanostructure of silver-free photochromic glasses studied by anomalous small angle X-ray scattering

Time	A-05MH (MS 78)	F-12CH (MS 79)	D-1003 (MS 80)
14:45-14:50 Opening Remarks	Crystallization of membrane proteins Chairs: E. Pebay-Peroula, S. Yoshikawa	Motion in macromolecular machines Chairs: M. Rossmann, H. Wu	Understanding and controlling polymorphism Chairs: S. M. Reutzel-Edens, U. Rychlewska
14:50-15:20	MS.78.1(C132) J.-L. Popot: Can amphipols be used to crystallize membrane proteins?	MS.79.1(C134) K. Namba: Molecular mechanisms of self-assembly and motion of the bacterial flagellum	MS.80.1(C135) J. Bernstein: Understanding and controlling polymorphism
15:20-15:50	MS.78.2(C132) C. Toyoshima: Crystallisation of the calcium pump of skeletal muscle sarcoplasmic reticulum	MS.79.2(C134) V. B. Rao: Mechanism of DNA packaging in bacteriophage T4	MS.80.2(C135) K. Fujii: Dehydration process of lisinopril, investigated by <i>ab initio</i> powder crystal structure analysis
15:50-16:20	MS.78.3(C133) T. Kouyama: Crystallization of visual pigments and archaeal rhodopsins	MS.79.3(C134) J. Lowe: DNA translocation by hexameric FtsK	MS.80.3(C136) L. Yu: What do polymorphs teach us about crystal nucleation and growth?
16:20-16:50	MS.78.4(C133) S. Maeda: X-ray structure of human gap junction channel	MS.79.4(C134) C. V. Stauffacher: Crystallographic snapshots of the enzyme mechanisms of HMG-CoA reductase and HMG-CoA synthase	MS.80.4(C136) E. J. Chan: Modeling single crystal diffuse scattering on polymorphs of the drug benzocaine
16:50-17:20	MS.78.5(C133) A. May: Diffraction-capable microfluidic crystallization chips for screening and structure determination	MS.79.5(C135) D. Luo: Crystal structure of the NS3 protease-helicase from Dengue virus	MS.80.5(C136) S. L. Price: Computed crystal energy landscapes as an aid to understanding polymorphism

C-1001, 2 (MS 81)	G-1202 (MS 82)	B-05SH (MS 83)	E-1009 (MS 84)
New neutron sources Chairs: S. J. Kennedy, Y. Noda	Magnetic Compton scattering Chairs: Y. Sakurai, H. Kawata	Femto-second diffraction: Time resolved studies Chairs: S. Techert, R. Feidenhans'l	Quasicrystals and related giant crystalline alloys Chairs: E. Abe, R. McGrath
MS.81.1(C137) B. J. Kennedy: Crystallography at the new Australian research reactor OPAL	MS.82.1(C138) N. Sakai: Momentum density of uncompensated electron spins measured by magnetic Compton scattering	MS.83.1(C140) J. Miao: Coherent diffraction microscopy: Present and future	MS.84.1(C141) F. Fleischer: Performance tests on iterative phase-retrieval methods in higher dimensions
MS.81.2(C137) C-H. Lee: Current situation of the cold neutron research facility project at HANARO	MS.82.2(C138) A. Bansil: Inelastic X-ray scattering as a powerful probe of correlation effects in materials	MS.83.2(C140) M. M. Nielsen: Time-resolved X-ray scattering of an electronically excited state in metal complexes in solution	MS.84.2(C141) K. Sugiyama: Approximant structures for the AlCo based decagonal phases
MS.81.3(C137) I. S. Anderson: SNS and HFIR: Breaking new ground	MS.82.3(C139) J. A. Duffy: Using magnetic Compton scattering to study Invar and spin-polarised materials	MS.83.3(C140) S. L. Johnson: Femtosecond X-ray crystallography of elemental solids: Coherent dynamics in bismuth and tellurium	MS.84.3(C142) V. Fournee: New phenomena in epitaxial growth: Solid films on quasicrystalline substrates
MS.81.4(C137) Y. Ikeda: An advanced pulse neutron source and scientific challenges at J-PARC	MS.82.4(C139) H. Kobayashi: Magnetic Compton scattering under high pressure	MS.83.4(C140) J. Cao: Electronic Grüneisen parameter and thermal expansion in ferromagnetic transition metals	MS.84.4(C142) T. Dotera: Mesoscopic quasicrystalline and Archimedean tilings in polymer alloys
MS.81.5(C138) C. Vettier: Progress for the European spallation source	MS.82.5(C139) N. Qureshi: Spin and magnetization density in the kagome staircase system $\text{Co}_3\text{V}_2\text{O}_8$	MS.83.5(C141) A. Foehlich: Ultrafast electron dynamics excited and probed with X-rays	MS.84.5(C142) M. De Boissieu: Atomic simulation and lattice dynamics of the ZnMgSc icosahedral quasicrystal

Time	A-05MH (MS 85)	F-12CH (MS 86)	D-1003 (MS 87)
9:55-10:00 Opening Remarks	Structural proteomics, focused structural proteomics Chairs: M. Tanokura, R. Page	Perovskites and related materials Chairs: D. Pandey, C. J. Howard	Design and applications of nanoscale materials Chairs: S. Takamizawa, J. J. Vittal
10:00-10:30	MS.85.1(C143) J. Weigelt: Structural genomic of protein families and pathways in human disease	MS.86.1(C144) P. M. Woodward: Complex perovskites: Chemical order, crystallographic distortions and physical properties	MS.87.1(C146) M. Kawano: Crystallographic direct observation of chemical reactions in a pore
10:30-11:00	MS.85.2(C143) I. A. Wilson: Structural genomics and the expanding protein universe	MS.86.2(C144) M. Catti: Local and long-range structure in LLTO perovskites with Li ⁺ superionic mobility	MS.87.2(C146) P. Thiyagarajan: Phase behavior of block copolymer/inorganic nanocomposites
11:00-11:30	MS.85.3(C143) R. Page: Using focused structural proteomics to elucidate the molecular basis of MAPK regulation in T cells	MS.86.3(C144) J-M. Kiat: Size and strain effects in nanostructured relaxor and morphotropic compounds	MS.87.3(C146) K. P. Loh: From molecular clusters to nanocrystals - Optical and magnetic properties of metal sulfides
11:30-12:00	MS.85.4	MS.86.4(C145) Y. Kuroiwa: Thermal motion of atoms in cubic structure of perovskites and ferroelectric phase transitions	MS.87.4(C147) R. Theissmann: <i>In-situ</i> transmission electron microscopy and theoretical studies on the coalescence of nanoparticles
12:00-12:30	MS.85.5(C144) S. Yokoyama: Focused structural proteomics of protein synthesis systems	MS.86.5(C145) R. Schierholz: The system of PbZr _{1-x} Ti _x O ₃ studied by convergent-beam electron diffraction (15 min)	MS.87.5(C147) J. Bak-Misiuk: Structural and magnetic properties of MBE grown MnSb layers
		MS.86.6(C145) J. Bezjak: The synthesis, crystal structural study and microwave dielectric properties of Ba ₆ WNB ₂ O ₁₄ (15 min)	

C-1001, 2 (MS 88)	G-1202 (MS 89)	B-05SH (MS 90)	E-1009 (MS 91)
Algorithmic developments for solving and refining periodic and aperiodic structures Chairs: H. Fan, M. Lutz	Space groups and their generalizations: A tribute to E. Ascher and J.J. Burckhardt Chairs: H. Grimmer, M. Nespola	New X-ray sources: ERLs, table top SR, (X)FELs Chairs: G. Materlik, T. Matsushita	Spinel - geometrically frustrated system: Dedicated to Prof. Nishikawa Chairs: K. Kakurai, B. Chakoumakos
MS.88.1(C147) M. Merli: Leverage analysis: A statistical tool to enhance the control on the crystal structure refinement	MS.89.1(C149) A. Janner: Experiencing space groups	MS.90.1(C150) L. N. Johnson: Life sciences at Diamond Light Source and prospects with new light sources	MS.91.1(C152) H. Takagi: Liquid state of spins and charges in geometrically frustrated spinel oxides
MS.88.2(C148) H. Puschmann: Small-molecule refinement using the computational crystallography toolbox (cctbx) with Olex2	MS.89.2(C149) I. Orlov: Space groups resulting from 3D sections of (3+1)D superspace groups. Can all 3D groups be generated?	MS.90.2(C151) T. Ishikawa: A compact X-ray free electron laser at SPring-8	MS.91.2(C152) D. Louca: Local order and frustration in vanadate spinels
MS.88.3(C148) A. O. Madsen: Anisotropic displacement parameters for molecular crystals from periodic HF and DFT calculations	MS.89.3(C149) P. Zeiner: Space groups, subgroups and a lot more	MS.90.3(C151) S. M. Gruner: Status of the Energy Recovery Linac (ERL) project at Cornell University	MS.91.3(C152) A. S. Wills: Controlling spin glass entropy - Frustrated magnetism in the spinels
MS.88.4(C148) M. Dusek: Joint refinement of single crystal and powder data from X-ray and neutron sources	MS.89.4(C150) B. Souvignier: J.J. Burckhardt's contributions to crystallography	MS.90.4(C151) H. Yamada: Electron storage ring based tabletop light source named MIRRORCLE for protein crystallography	MS.91.4(C153) N. Ishizawa: Polaronic behavior of Mn ₄ O ₄ heterocubane clusters in LiMn ₂ O ₄ spinel
MS.88.5(C149) R. De Gelder: FIDDLE: A method for simultaneous indexing and structure solution from powder diffraction data	MS.89.5(C150) Y. Teshima: Heterogeneous cylinder packing: Space group on periodic structures with <110> six directions	MS.90.5(C152) W. S. Graves: Integrating laser and linac technology for next generation X-ray sources	MS.91.5(C153) O. Pieper: Magnetic structure of the quasi-one-dimensional, frustrated, spin-1 antiferromagnet CaV ₂ O ₄

Time	A-05MH (MS 92)	F-12CH (MS 93)	D-1003 (MS 94)
13:45-13:50 Opening Remarks	Structural informatics and database Chairs: Z. Dauter, J. Richardson	RNA and DNA structures Chairs: A. Takenaka, A. Dock-Bregeon	Complementary low-Z element absorption spectroscopy by X-ray Raman scattering Chairs: U. Bergmann, E. Holub-Krappe
13:50-14:20	MS.92.1 (C153) A. M. Buckle: Federated repositories of X-ray diffraction images (25 min)	MS.93.1 (C155) E. Westhof: The annotations of non-Watson-Crick base pairs and comparisons between RNA structures and sequences	MS.94.1 (C157) C. Sternemann: X-ray Raman scattering: A probe of soft X-ray absorption edges using hard X-rays
14:20-14:50	MS.92.2 (C154) J. E. Johnson: Virus particle explorer: An X-ray and electron microscopy database for icosahedral virus structures (25 min)	MS.93.2 (C156) Y-I. Chi: Capturing hammerhead ribozyme structures in action by modulating the rate of general base catalysis	MS.94.2 (C157) S. K. Lee: Pressure-induced structural transition in oxides at high pressure: Inelastic X-ray scattering study
14:50-15:20	MS.92.3 (C154) W. Minor: Metal and small molecule agent environment in macromolecules (25 min)	MS.93.3 (C156) G. N. Parkinson: Ligand binding and structural rearrangements of quadruplexes containing human telomeric sequences	MS.94.3 (C157) S. T. Gerald: New applications of q-dependent XRS across the periodic table
15:20-15:50	MS.92.4 (C154) M. S. Weiss: On atomic displacement parameters and coordinates in protein structures (25 min)	MS.93.4 (C156) M. M. Georgiadis: Crystal structures of DNA-bound Co(III)-bleomycins	MS.94.4 (C158) J. S. Tse: X-ray Raman of water in the condensed phases
15:50-16:20	MS.92.5 (C155) T. Lutteke: Quality checks for carbohydrate structures in PDB entries (25 min)	MS.93.5 (C156) C. J. Cardin: Molecular recognition and the DNA Holliday junction	MS.94.5 (C158) Y. Cai: High-resolution X-ray Raman scattering and the study of ices under high pressure
	MS.92.6 (C155) J. Westbrook: Data quality in the PDB archive (30 min)		

C-1001, 2 (MS 95)	G-1202 (MS 96)	B-05SH (MS 97)	E-1009 (MS 98)
Microanalysis of cultural heritage Chairs: Y. Terada, W. Kockelmann	Programming for CIF and related file structures Chairs: I. David Brown, I. Guzei	New X-ray detectors : Pixel detectors Chairs: M. Tate, P. Fajardo	Knowledge-based applications in structural chemistry Chairs: M. Winn, J. van de Streek
MS.95.1 (C158) P. Paufler: Nanostructure of ancient Damascus blades	MS.96.1 (C159) N. Spadaccini: CIF and a new DDL – What it can do; How it is done	MS.97.1 (C161) K. Hattori: Performance of micro pixel gas chamber in small angle X-ray scattering experiments	MS.98.1 (C163) R. Subramanian: Quality of protein crystal structures in the protein data bank
MS.95.2 (C158) K. O. Yamahana: Scientific contribution to archaeology: Fingerprinting the ancient Egyptian objects	MS.96.2 (C160) J. R. Hester: CIF software in a DDLm world	MS.97.2 (C161) R. D. Durst: High speed readout of microgap X-ray detectors	MS.98.2 (C163) J. M. Cole: Discovering the world's best organic non-linear optical materials
MS.95.3 (C159) E. Kotulanova: Salt corrosion of lead-based pigments: Laboratory experiments and analysis of ancient frescoes	MS.96.3 (C160) H. J. Bernstein: Transition to object-oriented data representations: Interconversion between CIF and other formats	MS.97.3 (C162) C. Broennimann: The PILATUS detectors: Hybrid pixel detectors for synchrotron and industrial applications	MS.98.3 (C163) S. Huth: The crystal structures of para-acetanilides analysed systematically
MS.95.4	MS.96.4 (C160) M. I. Aroyo: The Bilbao crystallographic server	MS.97.4 (C162) G. A. Carini: Monolithic active-matrix silicon X-ray detectors	MS.98.4 (C163) S. J. Fisher: An investigation into deuteration effects: Implications for protein crystallography
MS.95.5 (C159) E. Dooryhée: Structural investigations of archaeological hybrid materials	MS.96.5 (C161) B. McMahon: publCIF: A complete crystal structure publishing environment for authors	MS.97.5 (C162) A. S. Schwarz: The 2D X-ray detector development program for the European XFEL	MS.98.5 (C164) T. N. Bhat: Structural database using semantic Web concepts to support structure-Based drug design for AIDS