Memo

Morning Session 8:30-9:30

A-05MH *(KN 22)*

KN22*(C8)* | **Nobuo Niimura**:
Neutron protein crystallography, beyond the folding structure of biological macromolecules

Chair: **Ryota Kuroki**

F-12CH *(KN 23)*

KN23*(C9)* | **J. Manuel Perez-Mato**:
Crystallography and mechanisms of structural phase transitions: The use of symmetry-adapted modes

Chair: **Anthony M. Glazer**

D-1003 *(KN 24)*

KN24*(C9)* | **Cristian Mocuta**:
X-ray scattering on nanostructures: From ensemble average to single object properties

Chair: **Sol M. Gruner**

Afternoon Session 17:30-18:30

A-05MH *(KN 25)*

KN25*(C9)* | **Gervais Chapuis**:
Incommensurate, composite modulated structures and beyond

Chair: **Sander van Smaalen**

F-12CH *(KN 26)*

KN26*(C10)* | **Peter Fratzl**:
Materials research with scanning microfocus small-angle X-ray scattering

Chair: **Dmitri Svergun**

D-1003 *(KN 27)*

KN27*(C10)* | **Alan Tennant**:
Using neutrons and synchrotron X-rays together: Looking at the full picture in condensed matter

Chair: **Michael Steiner**

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-insulater 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

Thursday, August 28 - Morning - **Microsymposia**

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. Schafler**: 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**: *Ab initio* 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 *Bacillus subtilis*
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

Thursday, August 28 - Afternoon - **Microsymposia**

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 *R. sphaeroides*	**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 *E. coli*	**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**: *In-situ* 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**: *E*/*T*-scaling behavior in the magnetic quasicrystal Zn-Mg-Ho	**MS.68.2**(C117) **G. R. N. Tayur**: Exploring pathways of structural phase transitions *via* 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 $Sr_3Ru_2O_7$	**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 $(NH_4)_2PtCl_6$	**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 $KNbOB_2O_5$ and $RbNbOB_2O_5$