

Thursday, August 28 - Other Activities

Crystallographic Software Faire (3)

R-1102 (9:00-17:00)

Organizer: L. Cranswick

Luncheon Seminar

12:45-13:30

C-1001.2 : Sponsored by Sysmex Corp. (200 seats)

C-1003 : Sponsored by SPring-8 (200 seats)

Commission on Small-Angle Scattering

R-1101 (12:30-14:45)

Programm Committee of European Crystallographic Association

R-1008 (12:30-14:45)

Commission on Aperiodic Crystals

R-0805 (13:00-14:30)

Music Session (3)

B-05SH (18:30-21:00)

IUCr General Assembly

F-12CH (19:00-21:00)

Thursday, August 28 - Friday, August 29 - Poster Sessions

Poster Numbers:

Poster number indicates Topic, Sub-topic and serial number, for example :

P01.01.01 → Topic 01. *Instrumentation and Experimental Techniques* / Sub-Topic 01. *Conventional Sources of X-rays* / Serial Number within the main topic.

Poster Presentation

28-29 August

Topics and Sub-topics

01 Instrumentation and Experimental Techniques

1. Conventional Sources of X-rays
2. Synchrotron Radiation I:Instrumentation and Techniques
3. Synchrotron Radiation II: Applications
4. New X-ray Sources
5. Electron Diffraction (LEED, RHEED, PED, AED)
6. Cryo-Electron Microscopy
7. X-ray Imaging
8. Neutron Scattering I:Techniques and Instrumentation
9. Neutron Scattering II: Applications
10. Area Detectors(Multi-wire, Image Plate, CCD)
11. Data Accuracy and Detectors
12. Cryo-Crystallography:Techniques and Instrumentation
13. Fast (pico-second) Crystallography
14. Free Electron Lasers for X-rays

04 Crystallography of Biological Macromolecules

1. Peptide and Protein Crystallization
2. Enzymes and Enzyme Catalysis
4. Muscle and Motor Proteins
20. NMR Applications to Macromolecules

08 Structure/Property Relationships

1. Molecular Recognition
10. Polymorphism and Isomorphism: Identification and Characterization
11. Polymorphism: Applications
14. Structure-Property Relationships

11 Crystallography in Material Science

2. Catalysis: *In situ* Studies
5. Noncrystalline Materials
8. Polymers
9. Liquid Crystals
13. Battery and Fuel Cell Materials
14. Residual Stress Measurements
15. Pore Framework Materials

15 Diffraction Physics and Optics

1. Interferometry
2. Inelastic Scattering
3. Neutron Optics
4. X-ray Optics: Lenses, Guides and Focusing
5. Resonant Magnetic X-ray Diffraction
6. Anisotropic Resonant Scattering

Thursday, August 28 - Friday, August 29 - Poster Sessions

- 7. Polarization: Generation and Exploitation
- 8. Dynamical Diffraction
- 9. Extinction and Absorption
- 10. N-beam Diffraction
- 11. Grazing Angle Incidence

21 Symmetry and its Generalizations

- 1. General Symmetry: Theory
- 2. Designer Symmetry: Theory and Practice
- 3. Pseudo-Symmetry: Recognition and Applications

22 Aperiodic and Incommensurate Structures

- 1. Data Collection and Structure Solution
- 2. Identification and Refinement
- 3. Results and Applications

23 Crystallographic Topology

- 1. Group Theory and Topology
- 2. Tiling
- 3. Quasicrystals
- 4. Networks
- 5. Critical Points

24 Databases

- 1. Creation and Exploitation
- 2. Coping with Rapid Expansions of Data: The Next Generation of Databases
- 3. Research Applications of the CSD
- 4. Research Applications of the PBD/ NADB

- 5. Research Applications of the ICSD
- 6. Research Applications of the PDF
- 7. Data Mining and Knowledge Generation
- 8. Bioinformatics: The Future

25 Industrial Crystallography

- 1. Instrumentation and Techniques
- 2. Stress-Strain Analysis
- 3. On Line Diffraction Analysis
- 4. Line Broadening
- 5. Amorphous and SAS
- 6. Microporous Materials
- 7. Nanomaterials
- 8. High Temperature Crystallography
- 9. Thick Coatings
- 10. Pharmaceutical Crystallography

29 Other Topics

Thursday, August 28 - Friday, August 29 - Poster Sessions

01. INSTRUMENTATION AND EXPERIMENTAL TECHNIQUES

P01.01.01(CI71) | H. Okuda: Two-dimensionally curved Ge for focusing crystals prepared by a hot plastic deformation

P01.01.02(CI71) | J. D. Ferrara: New optics for molecular macromolecular crystallography

P01.01.03(CI71) | C. Michaelsen: X-ray diffractometry with a microfocus source

P01.04.04(CI71) | J. Graf: Small X-ray beams for small crystals: Pushing the limits of home-lab X-ray sources

P01.04.05(CI72) | D. C. Frankel: Optimizing signal-to-noise on a home X-ray source for the analysis of microcrystals

P01.04.06(CI72) | H. Kawata: Present status of energy recovery linac project in Japan

P01.04.07(CI72) | Z. Amirkhanyan: Transition radiation of relativistic electron from the superlattice of dielectric permittivity

P01.02.08(CI73) | A. Douangamath: A monochromatic station for macromolecular crystallography at diamond light source

P01.02.09(CI73) | R. Flraig: Experience from operation and commissioning of the phase 1 MX beamlines at diamond light source

P01.02.10(CI73) | J. Jeyaraman: Installation of high throughput protein crystallography data collection at SPring-8 BL12B2

P01.02.11(CI74) | K. Larsson: Crystallography at MAX-lab

P01.02.12(CI74) | D. Hall: Macromolecular crystallography at Diamond Light Source: Automation and pathogenic sample environment

P01.02.13(CI74) | M. Hiraki: Approach for automated data collection at the photon factory protein crystallography beamlines

P01.02.14(CI75) | L. E. Berman: A proposed suite of macromolecular crystallography facilities for NSLS-II

P01.02.15(CI75) | N. Matsugaki: A new macromolecular crystallography beamline for softer X-ray at the Photon Factory

P01.02.16(CI75) | Y. Yamada: AR-NE3A, a new pharmaceutical beamline for macromolecular crystallography at the Photon Factory

P01.02.17(CI76) | N. Igarashi: Beamline developments for structural biology at the Photon Factory

P01.03.18(CI76) | C. B. Trame: Experiences with automated crystal screening at the JCSG

Thursday, August 28 - Friday, August 29 - Poster Sessions

P01.03.19(CI76) | M. Wang: Automation of the protein crystallography beamline X06DA at the swiss light source

P01.03.20(CI77) | G. Ueno: Beamline automation and mail-in data collection at SPring-8 structural biology beamlines

P01.02.21(CI77) | C. Chao: Beamline automation and remote access at NSRRC BL-13

P01.03.22(CI77) | M. Aslantas: New aproaches to room-temperature synchrotron data collection in macromolecular crystallography

P01.03.23(CI77) | D. K. Schneider: The PXRR integrates six beamlines for macromolecular crystallography at the NSLS into one resource

P01.02.24(CI78) | S. Classen: SAXS and macromolecular crystallography at the SIBYLS beamline (12.3.1) of the Advanced Light Source

P01.02.25(CI78) | G. L. Card: The new micro-focus beamline at SSRL: Current capabilities and future possibilities

P01.02.26(CI78) | K. Igor: NorthEastern Collaborative Access Team (NE-CAT) beam lines at the advanced photon source

P01.02.27(CI79) | R. Fourme: A beamline for anomalous diffraction at SOLEIL : Proxima 1

P01.03.28(CI79) | J. P. Rose: Pushing the envelop of sulfur SAS structure determination at UGA/SER-CAT

P01.03.29(CI79) | R. F. Fischetti: Probing radiation damage with a 1-micron beam

P01.03.30(CI80) | S. W. Wilkins: Towards protein structure determination using two-dimensional crystals and powders

P01.02.31(CI80) | D. Ahn: 8C2 high resolution powder diffraction beamline at Pohang Light Source and its recent results

P01.02.32(CI80) | N. A. Rae: Accurate powder diffraction standards: Determination of the lattice parameter of LaB₆ SRM(660)

P01.02.33(CI80) | J. M. Sasaki: A halogen lamp furnace to synthesize nanoparticles: *In situ* X-ray absorption spectroscopy

P01.03.34(CI81) | M. Tanaka: Vacuum-ultraviolet circular dichroism of amino acid films by polarizing-undulator based system

P01.03.35(CI81) | W. Clegg: Bringing the power of synchrotron crystallography to the chemical community

P01.02.36(CI81) | Y. Ohishi: X-ray focusing by using compound refractive lens optimized for high-pressure XRD at SPring-8

Thursday, August 28 - Friday, August 29 - Poster Sessions

P01.02.37(CI82) | J. Wiesmann: Total reflection and multilayer optics for synchrotrons and free-electron lasers

P01.02.38(CI82) | J. P. Wright: Center of mass grain maps in 3D

P01.07.39(CI82) | H. P. Bezirganyan: Grazing-angle incidence hard X-ray nanoscope

P01.07.40(CI83) | M. M. Murshed: Application of synchrotron X-ray micro tomographic microscopy at low temperature

P01.07.41(CI83) | J. Hodeau: Imaging and structural analysis of heterogeneous diluted materials by diffraction tomography

P01.07.42(CI83) | K. Sakurai: Realtime imaging in X-ray fluorescence and X-ray diffraction

P01.07.43(CI84) | P. Maj: Low noise multichannel ASIC for readout of SSD used in diffraction for powder and multilayer samples

P01.08.44(CI84) | I. Tanaka: A new biological neutron diffractometer (iBIX) in J-PARC

P01.08.45(CI84) | K. Kusaka: Optimization of design parameters of IBARAKI Biological Crystal Diffractometer (iBIX) in J-PARC

P01.08.46(CI85) | K. Kurihara: Optics and shielding of IBARAKI Biological Crystal Diffractometer (iBIX) in J-PARC

P01.10.47(CI85) | T. Hosoya: Development of a new detector and DAQ systems for iBIX

P01.08.48(CI85) | T. Ohhara: Development of data processing software for a TOF single crystal neutron diffractometer at J-PARC

P01.08.49(CI86) | T. Ishigaki: The current status of iMATERIA - Versatile neutron diffractometer at J-PARC

P01.09.50(CI86) | P. F. Henry: Impact of modern neutron powder diffraction instrumentation on the study of hydrogenous materials

P01.08.51(CI86) | C. Hoffmann: TOPAZ: A new time-of-flight laue diffractometer for new science

P01.08.52(CI87) | R. O. Piltz: First results from the KOALA neutron Laue instrument

P01.08.53(CI87) | M. Christensen: Mismatch cobaltite lattices investigated by white beam neutron diffraction

P01.09.54(CI87) | M. Meven: Unconventional single crystal diffraction studies with hot neutrons on HEiDi at FRM II

P01.08.55(CI88) | B. Deme: New design for D16 at the ILL

Thursday, August 28 - Friday, August 29 - Poster Sessions

P01.08.56(C188) | K. C. Littrell: CG2 general-purpose high-flux SANS instrument at HFIR at Oak Ridge National Laboratory

P01.08.57(C188) | S. Zhang: Neutron transmission strain tomography

P01.08.58(C188) | M. Strobl: BioRef - a time-of-flight reflectometer at Hahn-Meitner Institute Berlin

P01.08.59(C189) | V. M. Hutana: The new polarised hot neutron single crystal diffractometer POLI-HEiDi at FRM II

P01.09.60(C189) | C. Pappas: Polarimetric neutron spin echo spectroscopy

P01.08.61(C189) | K. Shibata: The study of thermal diffuse scattering measured by pulsed neutron diffraction

P01.09.62(C190) | M. M. Jones: Simultaneous thermogravimetric and neutron diffraction characterization of hydrogen stores

P01.08.63(C190) | P. Mikula: Boost of multiple reflection effects - a new challenge for high-resolution neutron experiments

P01.08.64(C190) | M. B. Tamaki: Transmission neutron monochromator and coherent neutron scattering images

P01.08.65(C191) | A. M. Filhol: Anniversary - 10 years of McStas for instrument design and science

P01.10.66(C191) | M. Moon: Development of curved position-sensitive neutron detectors for FCD at HANARO

P01.10.67(C191) | Y. Ishikawa: Single crystal structure analysis by neutron 2D-PSD

P01.10.68(C191) | M. W. Tate: Pixel array detectors for high count rate X-ray imaging

P01.11.69(C192) | K. Hasegawa: Shutter-less continuous rotation data collection from protein crystals with the X-ray CMOS detector

P01.10.70(C192) | T. Taguchi: Novel pixel detector for in-house XRD applications

P01.10.71(C192) | J. Dohnalek: Protein diffraction experiments with Atlas CCD detector

P01.11.72(C192) | N. Boudet: The XPAD3 hybrid pixel detector applications

P01.11.73(C193) | A. J. Schierbeek: More signal, less noise : Making good use of bright sources & fast detectors

P01.11.74(C193) | M. R. Probert: DATAVIEW: A new post processing analysis tool

P01.12.75(C193) | A. Yamano: A hyperquenching tool

P01.12.76(C193) | S. K. Nayak: *In situ* crystallizations of Cl and Br substituted anilines and its intermolecular interactions

Thursday, August 28 - Friday, August 29 - Poster Sessions

P01.15.77(C194) | K. Shiba: Relation of DLS distribution of protein samples with thermal stability

P01.15.78(C194) | J. N. Poulsen: Microseed matrix screening: A modified version

P01.12.79(C194) | B. Rupp: An open and flexible robotic system designed towards autonomous protein crystal harvesting

P01.15.80(C195) | J. M. Jenkins: Facilitating low volume protein crystallography set-ups using the mosquito® liquid handler

P01.02.81(C195) | H. J. Bernstein: A simplified unified approach for animations and movies using SBEVSL

P01.02.82(C195) | J. C. Nix: Remote data collection and rapid scheduling at the Molecular Biology Consortium beamline ALS 4.2.2

P01.13.83(C196) | S. L. Johnson: Femtosecond X-ray science at the Swiss Light Source

P01.02.84(C196) | D. J. Rodi: WAXS as a novel tool in drug discovery

P01.13.85(C196) | M. R. Warren: Time-resolved photocrystallographic investigation of metastable species

P01.13.86(C197) | J. Hallmann: Picosecond crystallography of homogeneous [2+2] photodimerisation reactions

P01.14.87(C197) | G. Faigel: Modeling of single molecule imaging by X-ray free electron laser

P01.11.88(C197) | B. B. He: Geometry and resolution of area detectors for X-ray powder diffraction

P01.15.89(C197) | T. K. Mondal: Effect of pressure and temperature on the crystallization behavior of As Te glasses with selenium

P01.11.90(C198) | V. Y. Lunin: The modelling of experimental errors improves statistical description of merohedrally twinned data

P01.11.91(C198) | T. Ida: Statistical properties of measured X-ray intensities affected by counting loss of detection system

P01.15.92(C198) | E. Brostrom: The XtalFinder imaging system

P01.15.93(C199) | H. te Nijenhuis: Possibilities and limitations of X-ray diffraction using high energy X-rays on a laboratory system

P01.08.94(C199) | S. Torii: Super high resolution powder diffractometer at J-PARC

P01.08.95(C199) | R. Kajimoto: 4SEASONS: A high-intensity chopper spectrometer for inelastic neutron scattering at J-PARC/MLF

Thursday, August 28 - Friday, August 29 - Poster Sessions

P01.15.96(C200) | P. Nollert: Preparation and imaging of lipidic cubic phase based protein crystallization experiments

P01.15.97(C200) | F. P. M. Gorrec: Protein crystallization at the laboratory of molecular biology: Robotics, procedures and developments

04. CRYSTALLOGRAPHY OF BIOLOGICAL MACROMOLECULES

P04.01.01(C230) | K. Furuta: Photochemical neutral radical induced nucleation of proteins

P04.01.02(C230) | N. V. Pletneva: The three dimensional structure of red, yellow and green fluorescent proteins from Zoanthus

P04.01.03(C231) | P. Sledz: The role of protein methylation rescue method for protein crystallization

P04.01.04(C231) | A. Shahar: Progress in structure determination of the 18kDa TSPO and the outer matrix Matrilin 3 protein

P04.01.05(C231) | C. L. Rush: The role of chilectins in rheumatoid arthritis

P04.01.06(C232) | S. E. Broughton: A structural investigation in to the basis of Celiac disease

P04.01.07(C232) | H. Adachi: Purification, crystallization and preliminary X-ray analysis of photosystem II dimer from a red alga

P04.01.08(C232) | A. Park: Structural analysis of ATP:Cob(I) alamin adenosyltransferase

P04.01.09(C233) | G. Petreanu: Expression, purification and crystallization of phosphoketolase from *Lactococcus lactis*

P04.01.10(C233) | Y. Li: Try to solve abscisic acid (ABA) receptor's structure and learn how ABA signal is transduced

P04.01.11(C233) | J. Hasek: Polymer and co-polymer surface modifying effects in the protein crystallization

P04.01.12(C233) | T. Mori: Structural basis for CD44 recognition by ERM proteins

P04.01.13(C234) | M. Isogai: Expression, purification and crystallization of Aurora kinase C

P04.01.14(C234) | S. Hu: Structural insights into the SM protein-syntaxin interactions

P04.01.15(C234) | M. Sugahara: Nucleant-mediated protein crystallization with microporous zeolite showing heteroepitaxial growth

Thursday, August 28 - Friday, August 29 - Poster Sessions

P04.01.16(C235) | K. Tomoo: Crystallization and preliminary X-ray analysis of Ca²⁺-free primary Ca²⁺-sensor of Na⁺/Ca²⁺ exchanger

P04.01.17(C235) | H. Wang: The crystal structure of villin domain 6

P04.01.18(C235) | H. Shimizu: Crystallization and X-ray structure analysis of Complex II from adult *Ascaris suum* mitochondria

P04.01.19(C235) | F. L. Imai: The crystal structure at 1.8 Å resolution of the calcium-bound human S100A13 at pH 7.5

P04.01.20(C236) | T. Ibuki: X-ray analysis of FliJ, a cytoplasmic component of the flagellar type III protein export apparatus

P04.01.21(C236) | K. Hara: Crystallographic study of zinc finger domain of Eco1 involved in sister chromatid cohesion

P04.01.22(C236) | J. Duskova: Crystallization of carbohydrate oxidase from *Microdochium nivale*

P04.01.23(C237) | M. Tsunoda: Crystal structure of actinohivin; A novel anti-human immunodeficiency virus protein

P04.01.24(C237) | S. R. Shouldice: Structural and functional analysis of an important *Pseudomonas aeruginosa* redox protein

P04.01.25(C237) | T. Yamada: Crystallization of serine proteases for neutron single crystal structure determination

P04.01.26(C238) | M. Horiuchi: Structural basis for the antiproliferative activity of the Tob-hCafl complex

P04.01.27(C238) | O. B. Clarke: Towards the structure of the β 4 subunit of the human BK channel

P04.01.28(C238) | T. Yoshizawa: Crystallographic study of extracellular dermal glycoprotein of carrot

P04.01.29(C239) | A. Mikami: Crystallization of *Clostridium botulinum* serotype D neurotoxin complex

P04.01.30(C239) | S. Kamachi: Expression and crystallization of *Drosophila* EcR/USP

P04.01.31(C239) | L. G. Munoz: Molecular basis of histone H3K4ME3 recognition by ING4

P04.01.32(C240) | A. Suzuki: A new type of precipitant, metal cyanide complex

P04.01.33(C240) | C. Sauter: Crystallization and crystallographic analysis in a microfluidic chip

P04.01.34(C240) | Y. Kim: Improving protein crystallization: A large-scale evaluation of protein reductive methylation

P04.01.35(C241) | A. D. Clark: Many are called but few are chosen: 20 years of crystallizing HIV-1 reverse transcriptase

Thursday, August 28 - Friday, August 29 - Poster Sessions

P04.01.36(C241) | S. T. Partanen: Studies on enzymes belonging to the crotonase superfamily

P04.01.37(C241) | J. Yoo: Structure analysis of ligand-independent activation of Fushi tarazu factor-1 ligand binding domain

P04.01.38(C242) | K. Kawamura: X-ray diffuse scattering from protein crystals caused by the lattice defects

P04.01.39(C242) | M. Goto: Structure of membrane-bound quiohemoprotein alcohol dehydrogenase

P04.01.40(C242) | C. Chen: Rational crystallization of β -lactoglobulin and vitamin D₃ complex reveal a secondary binding site

P04.01.41(C243) | Y. Ohnishi: Large single crystal growth and preliminary neutron diffraction analysis of *Achromobacter* protease I

P04.01.42(C243) | C. Ishida: Purification and crystallization of a C-terminal domain of a human single-pass transmembrane protein

P04.01.43(C243) | S. Sugiyama: Crystallization and preliminary X-ray analysis of RNA aptamer in complex with human immunoglobulin G

P04.01.44(C244) | M. Yamakami: Growth of high-quality and large crystals of HIV protease for neutron crystallography

P04.01.45(C244) | J. Tsai: X-ray crystallographic study of the C-terminal domain of Tic110 protein from *Cyanidioschyzon merolae*

P04.01.46(C244) | D. Choquesillo-Lazarte: Protein crystallization through screening of pH and precipitants using counterdiffusion technique

P04.01.47(C244) | Y. Hagiwara: Snapshots in the reaction pathway of bilin reductase PcyA

P04.01.48(C245) | A. Brandt: The crystal structure of lipase a from *Candida Antarctica*

P04.01.49(C245) | L. Li: Novel approaches in protein crystallization

P04.01.50(C245) | B. Jeong: A preliminary crystallographic study of CDCP2 from *Arabidopsis thaliana*

P04.01.51(C246) | J. Otani: Crystal structure of DNMT3A ADD domain

P04.01.52(C246) | H. Kawahara: The observation of individual protein molecules on a protein crystal under forced solution-flow

P04.01.53(C246) | R. Murai: Study on femtosecond laser-induced nucleation dynamics of proteins

P04.01.54(C247) | G. Sasaki: Single-molecule visualization on a protein crystal surface

Thursday, August 28 - Friday, August 29 - Poster Sessions

P04.01.55(C247) | H. Hasenaka: Wavelength dependence of the crystallization by the laser irradiation

P04.01.56(C247) | N. Shimizu: Growth of large protein crystals for neutron crystallography by hanging a seed crystal

P04.01.57(C248) | B. R. Jeong: Crystallization and biochemical analysis of eIF4A protein

P04.01.58(C248) | S. Cameron: The scottish structural proteomics facility

P04.01.59(C248) | N. Furubayashi: A dynamic light scattering system combined with a conventional chromatography for sample preparation

P04.01.60(C249) | H. Lee: SAXS and crystal structural analysis of *Helicobacter pylori* GroES

P04.01.61(C249) | Y. Zhai: Crystallographic study of the bacterial prolipoprotein posttranslational lipid modification system

P04.01.62(C249) | X. Pang: Preliminary crystallographic studies on ACAP1 BAR-PH and GAP-ANK domains

P04.02.63(C249) | C. Chakrabarti: A comparative study on substrate specificity, activity and thermal stability of some plant proteases

P04.02.64(C250) | H. Koskineni: Aromatic hydroxylases in polyketide antibiotic biosynthesis

P04.02.65(C250) | N. Watanabe: Mechanism of stereospecific substrate recognition by LL-diaminopimelate aminotransferase

P04.02.66(C250) | A. Bowyer: L-Threonine dehydrogenase (TDH) from *T. kodakaraensis*, an enzyme involved in amino acid metabolism

P04.02.67(C251) | A. S. Thakur: Structural studies of acyl-CoA thioesterase 7 and its role in inflammation

P04.02.68(C251) | W. Wong: Structural proteomics of secreted proteases from the ovine footrot pathogen, *Dichelobacter nodosus*

P04.02.69(C251) | J. Zheng: Structure determination of *E. coli* isocitrate dehydrogenase kinase/phosphatase

P04.02.70(C252) | J. Andrell: Structure of decameric PLP-dependent acid induced arginine decarboxylase from *Escherichia coli*

P04.02.71(C252) | M. Hoque: The substrate recognition and the catalytic reaction mechanisms of D-3-hydroxybutyrate dehydrogenase

P04.02.72(C252) | J. Peek: Using natural variations among shikimate dehydrogenases to study modes of substrate selectivity

Thursday, August 28 - Friday, August 29 - Poster Sessions

P04.02.73(C253) | M. Pascaaru: Structure-function analysis of Eyes absent protein, aspartate dependent protein tyrosine phosphatase

P04.02.74(C253) | K. Banaszak: First crystallographic structure of mammalian phosphofructokinase from rabbit skeletal muscle

P04.02.75(C253) | C. Angkawidjaja: Crystal structure of a family I.3 lipase from *Pseudomonas* sp. MIS38 in a closed conformation

P04.02.76(C254) | T. Nakamura: Hypervalent intermediate of archaeal peroxiredoxin

P04.02.77(C254) | K. Matoba: Crystal structures of alkaline protease from *Pseudomonas aeruginosa* complexed with peptides

P04.02.78(C254) | S. Suh: Crystal structure of YlqF, a circularly permuted GTPase

P04.02.79(C255) | K. Kubota: Crystal structure of L-sorbose reductase from *Gluconobacter frateurii* at 2.4 Å resolution

P04.02.80(C255) | M. R. N. Murthy: Structural studies by X-ray on enzymes involved in propionate metabolism from membrane integrated protein leukotriene C₄ synthase

P04.02.81(C255) | T. Fujii: Crystal structure of tetrameric malate dehydrogenase from *Antarctic psychrophile*

P04.02.82(C256) | S. Kawano: Crystallographic analysis of complexes of bovine trypsin and Schiff base metal chelate

P04.02.83(C256) | Y. Higuchi: Evolution of nylon-oligomer-degrading enzyme based on high resolution crystal structure analysis

P04.02.84(C256) | X. Wang: Structural biology study in biosynthesis of plant natural products

P04.02.85(C257) | B. Ha: Structural basis for Ufm1 processing by UfSP1

P04.02.86(C257) | Y. Kikuchi: Crystal structure of the muramidase domain of FlgJ, a putative flagellar rod cap protein

P04.02.87(C257) | R. Bott: The three dimensional structure of an intact glucoamylase

P04.02.88(C257) | G. D. Brayer: Allostery and functional refolding in the Gram-negative hexameric Type II citrate synthases

P04.02.89(C258) | H. Ago: Crystal structure analysis of human membrane integrated protein leukotriene C₄ synthase

P04.02.90(C258) | K. Yamamoto: Structural insights into substrate specificity of isomaltase from *Saccharomyces cerevisiae*

P04.02.91(C258) | M. Konno: Mechanism for formation of Arg-AMP in help of tRNA on the basis of structure of ArgRS, tRNA and ATP

P04.02.92(C259) | S. Okazaki: Crystal structures of α -amino- ϵ -caprolactam racemase from *Achromobacter obae*

P04.02.93(C259) | A. Ruf: FBPase allosteric transition: Crystal structures of liver and muscle isoforms from rodents and human

P04.02.94(C259) | M. Fujihashi: Catalytic promiscuity and mechanistic determinants of ODCase - A high-resolution investigation

P04.02.95(C260) | R. Obata: Crystal structures of arylmalonate decarboxylase -Implications for enantioselective reaction

P04.02.96(C260) | S. Tanaka: Study on the Ca²⁺-dependent maturation mechanism of subtilisin from a hyperthermophilic archaeon

P04.02.97(C260) | H. Ishikawa: Structural and functional analysis of TTHA0252, a novel RNase of the β -CASP family

P04.02.98(C261) | T. Wakamatsu: Structural basis for different substrate specificities of two ADP-ribose pyrophosphatase

Thursday, August 28 - Friday, August 29 - Poster Sessions

P04.02.99(C261) | S. Chern: Dimerization is important for the GTPase activity of chloroplast translocon components

P04.02.100(C261) | H. Tamura: Crystal structure of RuBisCO-like protein from *Bacillus subtilis*

P04.02.101(C262) | M. Senda: Molecular mechanism of the redox-dependent interaction between ferredoxin reductase and ferredoxin

P04.02.102(C262) | G. Kawai: Crystal structures of GAR transformylase 1 (PurN) from *A. aeolicus*, *S. toebii* and *G. kaustophilus*

P04.02.103(C262) | M. Elias: Structural basis for natural lactonase and promiscuous phosphotriesterase activities

P04.02.104(C263) | K. Suzuki: Crystal structure of α -carbonic anhydrase from *Chlamydomonas reinhardtii*

P04.02.105(C263) | C. Li: Mechanistic role of the catalytic residue D300 in human pancreatic alpha-amylase

P04.02.106(C264) | S. Baba: Crystal structures of GAR synthetase (PurD) from *A. aeolicus*, *G. kaustophilus* and *T. thermophilus*

P04.02.107(C264) | G. Sampei: Structural genomics on the purine nucleotides biosynthetic pathway

P04.02.108(C264) | B. Heras: Redox catalysis and protein folding in bacterial virulence

Thursday, August 28 - Friday, August 29 - Poster Sessions

P04.02.109(C265) | K. Endo: Crystal structure of Dxp reductoisomerase from *Geobacillus stearothermophilus*

P04.02.110(C265) | S. Yajima: Crystal structure of the thermostable mutant of hygromycin phosphotransferase from *Escherichia coli*

P04.02.111(C265) | H. Taka: Crystal structures of N^5 -CAIR synthetase (PurK) from *A. aeolicus*, *T. thermophilus* and *S. tokodaii*

P04.02.112(C266) | B. Mikami: Structural titration of two mobile loops in trigonal soybean β -amylase crystal with maltose

P04.02.113(C266) | Y. Sogabe: The structure of the exo-arabinanase complex with arabinobiose

P04.02.114(C266) | K. Takeda: Crystallization and preliminary X-ray analysis of D-arabinose isomerase from *Bacillus pallidus*

P04.02.115(C267) | S. Nakamura: Structures of NADH and NAD $^+$ bound 3 α -hydroxysteroid dehydrogenase from *Pseudomonas* sp. B-0831

P04.02.116(C267) | T. Nakamura: High-resolution X-ray diffraction study of the hMTH1 mutant

P04.02.117(C267) | K. Uegaki: Tertiary structure of the catalytic and chitin-binding domains of hyperthermophilic chitinase

P04.02.118(C268) | M. Igura: Successful expression of archaeal STT3/AglB membrane protein in *E.coli* cells

P04.02.119(C268) | V. Prashar: X-ray structure of HIV-1 protease-product peptides complex: Insights into the reaction mechanism

P04.02.120(C268) | Y. Sun: Crystal structure of *Helicobacter pylori* spermidine synthase suggests a distinct active site

P04.02.121(C269) | T. Shiba: Crystallographic studies of ferredoxin-NAD(P) $^+$ reductase from *Chlorobium tepidum*

P04.02.122(C269) | S. Zoll: The crystal structure of the staphylococcal amidase AmiE reveals the active site of a metalloenzyme

P04.02.123(C269) | S. Fukuoka: Structure of the inactive mutant of arabinanase complexed with oligosaccharides

P04.02.124(C269) | M. Akiyoshi: Structure of endo-1,5- α -L-arabinanase from *Penicillium chrysogenum*

P04.02.125(C270) | M. Kanagawa: Crystal structure of GMP synthetase (GuaA) from *T. thermophilus*

P04.02.126(C270) | T. Hisano: Crystal structures of the oxygenase component of an aromatic monooxygenase in ligand-bound forms

Thursday, August 28 - Friday, August 29 - Poster Sessions

P04.02.127(C270) | J. Cavarelli: Functional insights from structures of coactivator-associated arginine methyltransferase 1 domains

P04.02.128(C271) | A. Gustchina: Crystal structure of Histo-aspartic protease from *Plasmodium falciparum*

P04.02.129(C271) | H. Unno: Structural and mutational studies of anthocyanin malonyltransferases

P04.02.130(C271) | N. Kamiya: Reaction pathway of ADP-ribose pyrophosphatase, revealed by time-resolved X-ray crystallography

P04.02.131(C272) | Y. Kitamura: Ligand-induced conformational change of D-alanine:D-alanine ligase from *Thermus thermophilus* HB8

P04.02.132(C272) | M. A. Carrondo: Structure of wild type Plk1 kinase domain in complex with a selective DARPin

P04.02.133(C272) | S. Pengthaisong: Crystallization of rice BGlu1 β -glucosidase E176Q mutant with oligosaccharide substrates

P04.02.134(C273) | A. Henriksen: Barley alkenal hydrogenase, a trans-2-nonenal processing enzyme

P04.02.135(C273) | T. Maeda: Crystallization and preliminary X-ray analysis of phosphoribulokinase from *Synechococcus* sp.PCC 7942 cycle

P04.02.136(C273) | A. S. Gardberg: Toward a joint X-ray/neutron refinement of the cysteine peptidase papain: The 300K X-ray structure

P04.02.137(C274) | M. Yamada: Crystal structures of *Streptococcus pneumoniae* penicillin-binding proteins acyl-enzyme complexes

P04.02.138(C274) | N. Yang: Crystal structure of a serine protease defines a novel family of secreted bacterial proteases

P04.02.139(C274) | M. Irie: Crystal structures of *Escherichia coli* γ -glutamyltranspeptidase in complex with glutamine antagonists

P04.02.140(C275) | Y. Kido: Crystallization and preliminary crystallographic analysis of *Trypanosome alternative oxidase*

P04.02.141(C275) | K. Kim: Structural and functional basis for (S)-allantoin formation in the ureide pathway

P04.02.142(C275) | T. Arimori: Structural basis of the substrate recognition and hydrolysis reaction mechanisms of 8-oxo-dGDPase

P04.02.143(C276) | M. Akutsu: Crystal structure of Otubain1

P04.02.145(C276) | S. Du: Catalysis and electron transfer in glycerol-3-phosphate dehydrogenase

Thursday, August 28 - Friday, August 29 - Poster Sessions

P04.02.146(C276) | Y. D. Lobsanov: Mechanism of retaining glycosyltransferases: Structure of Kre2p/Mnt1p in complex with a donor analog

P04.02.147(C277) | X. Su: Solving enzyme structures by metabolic pathways

P04.02.148(C277) | M. Kataoka: X-ray crystal structure analysis of reaction intermediates of bacterial copper amine oxidase

P04.02.149(C277) | E. Park: Structural comparison of 5'-methylthioadenosine nucleosidases from *Arabidopsis thaliana*

P04.02.150(C278) | B. Lee: Structural and biochemical characterization of ClpP from *Bacillus subtilis*

P04.02.151(C278) | S. Sekine: Implications for selenophosphate generation by crystal structure of selenophosphate synthetase

P04.02.152(C278) | K. Nishio: The crystallographic study of the deubiquitinating enzyme UCH37 N-terminal domain

P04.02.153(C278) | M. L. Hackert: Flexibility in active site of *cis*-3-chloroacrylic acid dehalogenase revealed by multiple structures

P04.02.154(C279) | J. Noguchi: Crystal structure of the covalent intermediate of human cytosolic β -glucosidase

P04.02.155(C279) | N. Sakai: Crystal structure analysis of the oligo-peptide binding protein OppA complexed with peptides

P04.02.156(C279) | S. Konishi: Structural basis for the enzymes in de novo pathway of Human Malaria Parasite *Plasmodium falciparum*

P04.02.157(C280) | T. Ozaki: Structural study of enzyme inhibitor complexes of eukaryotic glutamine synthetase from *Zea mays*

P04.02.158(C280) | M. Blum: H/D-exchange and water structure in diisopropylfluorophosphatase as revealed by neutron diffraction

P04.02.159(C280) | I. Miyahara: Structural study of putative aminotransferase from *Thermus thermophilus* HB8

P04.02.160(C281) | T. Nishio: Crystal structure of mouse sulfotransferase 2A4 (SULT2A4)

P04.02.161(C281) | H. Chan: Unusual conformational pathways of mismatched dNTP incorporation by DNA Pol β

P04.02.162(C281) | Y. Shoyama: Crystal structure of Delta1-tetrahydrocannabinolic acid synthase from *Cannabis sativa*

P04.02.163(C282) | K. Wong: Structure determination of hydrogenase maturation factor HypB from *Archaeoglobus fulgidus*

Thursday, August 28 - Friday, August 29 - Poster Sessions

P04.02.164(C282) | M. Eda: Production and crystallization of tomato β -galactosidase 4

P04.02.165(C282) | O. Kristensen: Crystal structure of *Aquifex aeolicus* PPX/GPPA in complex with ppGpp

P04.02.166(C282) | P. H. Harris: Inhibition by dTTP of the bifunctional dCTP deaminase:dUTPase from *Mycobacterium tuberculosis*

P04.02.167(C283) | M. Tanokura: Expansion of substrate specificity and the structural basis of AzoR from *Escherichia coli*

P04.02.168(C283) | M. Gajhede: The complex between a branched pentasaccharide and *Thermobacillus xylanilyticus* arabinofuranosidase

P04.02.169(C283) | J. I. Yeh: Structure of glycerol-3-phosphate dehydrogenase, an essential monotopic membrane enzyme

P04.02.170(C284) | R. Zhang: The crystal structure of capsule synthesis protein CapD, a major virulence factor in *B. anthracis*

P04.02.171(C284) | R. Li: Crystal structure of adenosine kinase from *M. tuberculosis* in complex with nucleoside analogs

P04.02.172(C284) | H. Otten: Structure and mechanism of rhamnogalacturonan lyases

P04.01.173(C285) | M. Lee: Crystal structure to functional correlation of WhiE aromatase/cyclase from *Streptomyces coelicolor*

P04.01.174(C285) | H. Wu: Structural study of laminarinpentose-producing β -1,3-glucanase from *Streptomyces matensis* DIC-108

P04.02.175(C285) | T. Oda: The crystal structure of N-terminal domain of plant NADPH oxidase

P04.02.176(C286) | Y. C. Hsieh: Crystal structure and functional study of wild type and mutated *Bacillus cereus* NCTU2 chitinase

P04.04.207(C295) | A. P. T. Salmazo: Crystallization and SAXS of α -Actinin 2

P04.04.208(C296) | M. Muthu: Structural and biochemical characterization of actin binding by dystrophin and utrophin

P04.04.209(C296) | Y. Shirakihara: Crystallization and crystal analysis of ATP synthase

P04.04.210(C296) | P. Llinas: Structural view of the ATPase cycle of a myosin that moves backward

P04.04.211(C297) | C. M. Jeffries: Small angle scattering: The regulatory domains of cardiac C-protein and their complex with F-actin

Thursday, August 28 - Friday, August 29 - Poster Sessions

P04.04.212(C297) | A. E. Whitten: A small-angle neutron contrast variation study of the complex of actin and myosin binding protein C

P04.20.408(C357) | R. Akella: Allostery in p38-docking-peptide interaction-an NMR study

P04.26.470(C377) | H. Yoon: Crystal structure of L-CKS from *Haemophilus influenzae* in complex with KDO

P04.26.471(C377) | H. Yeo: Towards the structural basis for bacterial two-partner secretion

P04.26.472(C377) | Y. Akai: Structure and function of the human histone chaperone CIA complexed with the bromodomain from TFIID

P04.26.473(C378) | A. Hishiki: Structural studies of human PCNA mutant, REV6-1

P04.26.474(C378) | A. Dahlstroem: Uranyl mediated photocleavage in proteins

P04.26.475(C378) | A. Uchida: Water-soluble chlorophyll-binding protein from *Chenopodium album*

P04.26.476(C379) | L. Mazzarella: Multiple coordination and quaternary states of fish hemoglobin re-open the root effect question

P04.02.478(C379) | D. Ruiz Carrillo: Structural characterization of the bacterial glutaminyl cyclase from *Zymomonas mobilis*.

08. STRUCTURE/PROPERTY RELATIONSHIP

P08.01.86(C444) | Y. Kin: Chiral recognition for inclusion compounds of 3-epicholic and 3-epideoxycholic acids with alcohols

P08.01.87(C445) | J. Liu: Glycosphingolipid-facilitated membrane insertion and pore formation of cobra cardiotoxin

P08.01.88(C445) | V. R. Pedireddi: Crystals, cocrystals & supramolecular synthesis

P08.01.89(C445) | M. Eisenstein: Anchoring spots mapping on protein surfaces: Application in docking and peptide inhibitor design

P08.01.90(C445) | H. Arslan: Crystal structure and theoretical calculations of *N*-(2,2-diphenylacetyl)-*N'*-(naphthalen-1-yl)thiourea

P08.01.91(C446) | N. Iimura: Molecular complex formation of medicinal cationic surfactants with aromatic compounds

P08.01.92(C446) | M. Miyata: Chiral recognition in cholamide crystals: Four-location model for hydrogen and stereogenic carbon

Thursday, August 28 - Friday, August 29 - Poster Sessions

P08.01.93(C446) | U. H. Sauer: Protein intrinsic disorder predicted with conditional random fields

P08.10.94(C447) | A. D. Bond: The remarkable "polymorphism" of aspirin

P08.10.95(C447) | S. Wishkerman: Polymorphism and structural mechanism of the phase transformation of phenyl carbamate (PC)

P08.10.96(C447) | K. Fucke: Polymorphic study of the model system hexamidine diethione

P08.10.97(C448) | V. V. Chernaya: Order and disorder in the $\text{Sr}_2\text{VO}(\text{XO}_4)_2$ ($\text{X}=\text{V,P}$) phases

P08.10.98(C448) | P. P. Neves: Powder X-ray diffraction study of polymorphic drugs: fluconazole and mebendazole

P08.10.99(C448) | C. Van Blerk: Low temperature and ambient phases of decane-1,10-diammonium dichloride monohydrate

P08.10.100(C449) | B. Sarma: Synthon polymorphism in dihydroxybenzoic acids

P08.10.101(C449) | B. N. Jagadeesh: Conformational polymorphs of temozolomide and furosemide

P08.10.102(C449) | Y. Abe: Crystal structures and pseudo polymorphism of anionic surfactants

P08.10.103(C450) | H. Su: Polymorphism, isomorphism and variability in the inclusion chemistry of a diol host compound

P08.10.104(C450) | D. C. Levendis: New crystal forms of gabapentin

P08.10.105(C450) | H. Gontani: The effect of substituents on the occurrence of polymorphism in diaminodicyanopyrazine dyes

P08.10.106(C450) | J. Galcera: Isomorphous pharmaceutical salts of lamotrigine with counterion dependence on water solubility

P08.10.107(C451) | S. Yamamura: Polymorphs and humidity-induced transition of a serotonin receptor antagonist, $\text{C}_{29}\text{H}_{33}\text{N}_3\text{O}_2\text{.HCl.xH}_2\text{O}$

P08.10.108(C451) | R. V. Shpanchenko: Order-disorder transitions in sodium vanadylphosphate $\text{Na}_4\text{VO}(\text{PO}_4)_2$

P08.10.109(C451) | D. A. Parrish: Polymorphs of picryl bromide

P08.10.110(C452) | D. A. Mikhailova: New $\text{M}_{1/3}\text{Re}_{2/3}\text{O}_2$ ($\text{M} = \text{Fe, Co, Ni}$) oxides with rutile-like structures

P08.10.111(C452) | G. Shen: Compression and thermal behavior of GeO_2 glass

P08.10.112(C452) | I. Barsky: Disappearing and reappearing polymorphism in *p*-methylchalcone

Thursday, August 28 - Friday, August 29 - Poster Sessions

P08.11.113(C452) | T. Mutai: Switchable polymorph-dependent luminescence of terpyridine

P08.11.114(C453) | T. N. Drebushchak: Polymorphism of chlorpropamide: Structure and transitions

P08.14.115(C453) | T. Bezrodna: Structure formation effects on electro-optics of montmorillonite clay-5CB liquid crystal composites

P08.14.116(C453) | O. A. Alekseeva: Crystal structure of metastable cubic B₁-phase of the La₂Mo₂O₉ single crystal

P08.14.117(C454) | D. Sonu: Pulse laser deposition of AgInSe₂ films

P08.14.118(C454) | T. Teerawatananond: Modified 6-deoxyclitoriacetal and their crystal structures as anticancer agents

P08.14.119(C454) | H. T. Luu: Using electron microscopy techniques studies in microstructure of NdFeCoAl-(B,C) based alloys

P08.14.120(C455) | R. P. Forbes: Negative and low positive thermal expansion behaviour of niobate based ceramics and solid solutions

P08.14.121(C455) | K. Kihira: The crystal structure analysis of release factor 3 from sulfate-reducing bacterium

P08.14.122(C455) | R. S. Black: The structure and photoluminescence of chiral tin and lead inorganic-organic hybrid perovskites

P08.14.123(C456) | K. Yubuta: Boron ordering in CeRh₃B_x and ScRh₃B_x alloys

P08.14.124(C456) | S. A. Barannikova: The effect of extension axis orientation on the localized plasticity in FCC single crystals

P08.14.125(C456) | L. Torre-Fernandez: Structural studies of a new series of ester derivatives in cyclopropanol chemistry

P08.14.126(C457) | R. Puntharod: Crystal structure and resonance Raman spectra of chloro[tetra(*p*-methoxyphenyl)porphyrinatoiron(III)]

P08.14.127(C457) | S. Son: Human monoamine oxidase A: Structure and control of opening the entry for substrates/inhibitors

P08.14.128(C457) | J. R. Deschamps: Relationship between nitrogen conformation and spectral properties in nitric oxide prodrugs

P08.14.129(C458) | R. L. Withers: Structured diffuse scattering and polar nano-regions in BaTiO₃ doped relaxor ferroelectric systems

P08.14.130(C458) | A. Elmali: Crystal structure and nonlinear optical behavior of N-(2 or 3-nitrobenzalidene)2,4-dimethylaniline

P08.14.131(C458) | H. Unver: Crystal structure and nonlinear optical properties of n-(3-hydroxybenzalidene)4-bromoaniline

P08.14.132(C458) | D. Brown: Virtual chemistry - The game we all play

P08.14.133(C459) | N. E. Novikova: Structure of KTP crystals grown by top-seeded solution and spontaneous flux crystallization methods

P08.14.134(C459) | U-S. Jeng: Anomalous SAXS for the morphology and metal content of a metallothionein in a metal-atom replacement

P08.14.135(C459) | E. V. Shtykova: Synchrotron SAXS reveals structural organization of iron oxide nanoparticles in aqueous solutions

P08.14.136(C460) | T. Hinoue: Drastic modulation of solid-state luminescence derived from molecular arrangement of organic salts

P08.14.137(C460) | Y. Takano: Electronic structures of heme a of cytochrome c oxidase in the redox states

P08.14.138(C460) | D. M. Standley: Functional annotation by sequence-weighted structural alignments

Thursday, August 28 - Friday, August 29 - Poster Sessions

P08.14.139(C460) | P. Liu: Formation of ϵ -martensite (ϵ -Fe) in stainless steels

P08.14.140(C461) | T. Moriga: Structure of homologous series Zn_k(In,Ga)₂O_{k+3} of as thermoelectric materials

P08.14.141(C461) | S. Djordjevic: X-ray crystallography and NMR spectroscopy in unrevealing the catalytic mechanism of a peroxiredoxin

P08.14.142(C462) | G. Jovanovski: Jahn-Teller distortions in mixed crystals, [Cu_xMn_{1-x}(H₂O)₄(C₇H₄NO₃S)₂](H₂O)₂

P08.14.143(C462) | K. H. Michel: Evolution of phonon spectra and elastic constants from graphene to graphite

P08.14.144(C462) | A. A. Levin: Lattice strain tuning in SrTiO₃/La_{0.7}Sr_{0.3}MnO₃ films by inverse piezoelectric effect of PMN-PT wafer

P08.14.145(C462) | K. Kimura: Coupling between magnetic and dielectric properties in a triangular lattice antiferromagnet CuCrO₂

P08.14.146(C463) | H. Kawaji: Location of proton in proton conducting perovskite oxides Ba₃Ca_{1.18}Nb_{1.82}O_{8.73} and BaZr_{0.8}Sc_{0.2}O_{2.9}

P08.14.147(C463) | Y. Huang: Solution SAXS and NMR on the domain orientation and binding of the components of human BCKD complex

Thursday, August 28 - Friday, August 29 - Poster Sessions

P08.14.148(C463) | D. S. Adipranoto: Crystal and local structural studies of superionic conductor cubic CuI

P08.14.149(C464) | S. Danjoh: Hysteretic magnetic and dielectric properties in $\text{Eu}_{1-x}\text{Y}_x\text{MnO}_3$

P08.14.150(C464) | F. Werner: Subtle structural differences in the system $[\text{Ln}(\text{phen}/\text{phen-d}_8)_2(\text{NO}_3)_3]$ ($\text{Ln}=\text{Eu}^{3+}, \text{Tb}^{3+}$)

P08.14.151(C464) | S. Matsumoto: Structure-colour relationship of diaminodicyanopyrazine derivatives having azomethine groups

P08.14.152(C465) | A. Matsumoto: Solid-state thermochromism of polydiacetylenes containing robust 2D hydrogen bond network

P08.14.153(C465) | Y. Ito: Relation between X-ray emission mechanism and crystal structure in LiTaO_3

P08.14.154(C465) | H. Stoecker: Reversible structural changes by electrostatic fields in strontium titanate at room temperature

P08.14.155(C465) | S. Sato: The crystal structure of a metachromatic dye toluidine blue

P08.14.156(C466) | O. Kazheva: Structure of new organic semiconductors with cobalt bis(dicarbollide) bromine anion

P08.14.157(C466) | K. Kato: Optical activity of *N*-benzoylglycine crystals

P08.14.158(C466) | S-L. Wang: New photoluminescent microporous metal phosphate as a hybrid intrinsic yellow phosphor

P08.14.159(C467) | V. Langer: New 1D, 2D and 3D azido Mn, Cd and Zn complexes with magnetic and non-linear optical properties

P08.14.160(C467) | N. Igawa: Motion of inclusion gas molecules in clathrate hydrate observed by neutron powder diffraction

P08.14.161(C467) | V. M. Sanchez Fajardo: Possible non-centrosymmetric structure of vaterite type yttrium orthoborate

P08.14.162(C468) | M. E. Torres: Effects of Er^{3+} and Yb^{3+} doping on non linear properties of double lithium sulphates

P08.14.163(C468) | I. I. Leonidov: $\text{Ln}_2(\text{Ca,Mn})\text{Ge}_4\text{O}_{12}$ - New materials for photonics

P08.14.164(C468) | A. D. Lozano-Gorrin: Different ordered defect scheelite type in $\text{RE}_2(\text{MoO}_4)_3$ crystal structures

P08.14.165(C469) | S. B. Carnaby: Application of statistical methods for the prediction of properties of organic solid forms

P08.14.166(C469) | G. Krauss: High hardness and incompressibility in transition metal borides

Thursday, August 28 - Friday, August 29 - Poster Sessions

P08.14.167(C469) | C. Sheu: Structure and magnetic study of solvated and non-solvated spin crossover complex $[\text{Fe}(\text{SalEen})_2]\text{ClO}_4$

P08.14.168(C469) | K. M. EL-Sayed: Structural-microstructural & magnetic properties relationships of $\text{In}_{1.0}\text{Fe}_{0.1}\text{Te}_{0.9}$, $\text{In}_{1.0}\text{Co}_{0.1}\text{Te}_{0.9}$

P08.14.169(C470) | K. Murai: Properties and local structure analysis of N or Nb doped TiO_2

P08.14.170(C470) | P. Huang: Crystal structural determination and SAXS/SANS structural analysis of human thrombomodulin domains

P08.14.171(C470) | Y. M. Abbas: Structural and magnetic investigations of nanocrystalline nickel ferrite NiFe_2O_4

P08.14.172(C471) | G. Li: Synthesis and intense blue luminescence of sodium yttrium fluoride microcrystals

P08.15.173(C471) | H. Nakajima: Solid-state optical properties of CT complexes with ammonium anthracene-2,6-disulfonate and TCNB

P08.15.174(C471) | V. Y. Pomjakushin: Crystal and magnetic structure of quantum spin-trimer compounds $\text{Ca}_3\text{Cu}_3\text{xNix}(\text{PO}_4)_4$

P08.15.175(C472) | S. Nishikawa: Temperature-dependent disordered structure of $(\text{BEDT-TTF})_3\text{Cl}_2\cdot 5\text{H}_2\text{O}$

P08.15.176(C472) | S. Ravy: Observation of micrometric correlations in sliding incommensurate charge density waves

P08.15.177(C472) | M. Brunelli: Pair distribution function analysis of nanosized materials

P08.15.178(C473) | M. H. Sorby: Structural studies and thermal decomposition of light complex hydride

P08.14.179(C473) | W. Jung: Structures of Li_2MnO_3 for lithium battery electrode materials

P08.14.180(C473) | V. T. Nguyen: Studies of the nanostructure of natural vegetable fibers

P08.10.181(C473) | L. Guzei: Concomitant polymorphism and twinning of dichloro-bis(η 5-tert-butylcyclopentadienyl) titanium(IV)

11. CRYSTALLOGRAPHY IN MATERIAL SCIENCE

P11.05.69(C528) | F. M. Neto: SAXS investigation of SBA-15 vacuum calcination process

P11.09.70(C529) | Y. Abe: Crystal structures and mesomorphism of metal-salen complexes with 4-substituted long alkoxy chains

P11.08.71(C529) | Y. P. Mascarenhas: Profile analysis of chemically prepared emeraldine-salt and emeraldine-base forms of polyaniline

Thursday, August 28 - Friday, August 29 - Poster Sessions

P11.08.73(C529) | A. R. Esterman: Coordination polymers towards applications: Chirality by design

P11.08.74(C530) | W. Chuang: Crystals orientation of polybutylene adipate/polyvinyl chloride blend under uniaxial drawing

P11.02.75(C530) | E. H. Figen: Crystallographic structure of LiCoO₂ based ruthenium catalyst for sodium borohydride hydrolysis

P11.02.76(C530) | T. Wakita: Structural disorder in the Ce_{0.5}Zr_{0.5}O₂ catalyst: A possible factor of the high catalytic activity

P11.02.77(C531) | K. Ito: Electron density distribution in anatase (TiO₂) under UV-irradiation: Observation and calculation

P11.02.78(C531) | S. Takeda: Structure determination of metallic nanoparticle catalysts by atomic scale *in-situ* environmental TEM

P11.05.79(C531) | T. U. Kardash: Nanocrystalline structure of an active phase in V-Mo-Nb-O catalysts for ethane (amm) oxidation

P11.13.80(C531) | M. Yashima: Structure and ionic conduction in inorganic materials through nuclear/electron density analysis

P11.13.81(C532) | Y. Yoneda: Short-range to long-range order structure change of Mg-Fe alloys

P11.13.82(C532) | S. Park: Development of a new type of Li-battery materials based on the milarite-family

P11.13.83(C532) | M. B. Piskin: Optimization of energy parameters indemnification of impurity levels in lead and bismuth

P11.13.84(C533) | T. Ohta: Structural investigation of the cubic perovskite-type doped lanthanum cobaltite La_{0.4}Ba_{0.6}CoO_{3-x}

P11.13.85(C533) | I. O. Fabregas: Synchrotron XRD and EXAFS studies on nanocrystalline ZrO₂-CaO solid solutions

P11.13.87(C533) | R. Ishikawa: Novel long period structures in hydrogen storage La_xY_{1-x}Ni_{3.8} compounds

P11.13.88(C533) | P. HyunMin: Structural investigation of the Ba doped LaInO₃

P11.13.89(C534) | K. Nomura: High temperature crystallographic study of perovskite-type mixed conductor, (La_{0.5}Sr_{0.5})CoO_{3-δ}

P11.13.90(C534) | M. Yonemura: Synthesis and crystal structure of novel proton-conductor, RbMg(PO₃)₃·3(H₂O)

Thursday, August 28 - Friday, August 29 - Poster Sessions

P11.13.91(C534) | M. Nagao: Structural studies on lithiation process of nano-size γ-Fe₂O₃ using neutron scattering technique

P11.13.92(C535) | R. Kiyanagi: Free oxygen ions in nanoporous material 12CaO·7Al₂O₃ and cage deformation at high temperature

P11.14.93(C535) | R. V. Martins: Residual stress investigation of dissimilar overlap-friction stir welds made from Al and steel

P11.14.94(C535) | A. M. Venter: Residual stresses associated with laser bending of mild steel plates

P11.15.95(C536) | P. J. Byrne: Charge density and *in-situ* studies of ionic and ionothermally prepared materials

P11.15.96(C536) | S. Garcia-Granda: Hydrothermal synthesis and structural features of metal phosphates in the presence of amines

P11.15.97(C536) | M. C.A. Fantini: Iron incorporated in cubic mesoporous silica: Synthesis, composition and structure

P11.15.98(C536) | C. Ferraris: Cation exchange mechanism for natural apatite with a simulated Cd-polluted solution TEM-AEM and XPS

P11.15.99(C537) | R. P. Nikolova: Crystal structure of a new small – pore zirconosilicate Na₂ZrSi₂O₇·H₂O

P11.15.100(C537) | F. Gandara: A rare-earth MOF series: Fascinating structure, efficient light emitters and promising catalysts

P11.15.101(C537) | N. Snejko: Same connector, same linker, different dimensionality

P11.15.102(C538) | E. Gutierrez-Puebla: A new 2D germanate formed by selective coordination of the *trans* 1,2-diaminocyclohexane to Ge atoms

P11.15.103(C538) | S. Huh: Structural characterizations of nanoporous In(III)-MOFs

P11.15.104(C538) | G. J. Halder: *In situ* X-ray diffraction studies of host-guest properties in nanoporous spin crossover frameworks

P11.15.105(C539) | S. J. Kennedy: Insight into the mechanisms of metal ion binding in hexagonal tungsten bronze

P11.15.106(C539) | M. Tadokoro: Dynamics phase transition of water nanotube cluster stabilized in molecular nanoporous crystal

P11.15.107(C539) | S. Park: A fluorescent two-dimensional Zn(II) framework containing 2,2'-bipyridine-5,5'-dicarboxylic acid

P11.15.108(C540) | L-H. Huang: Hydrothermal synthesis and characterization of transition metal gallophosphates

P11.15.109(C540) | Y.-T. Huang: Elastic layered zincophosphate intercalated with ice-like water cluster or superamolecular chains

P11.15.110(C540) | Y. Kubota: Gas adsorption process on silica mesoporous crystals obtained by *in-situ* SR powder diffraction

P11.15.111(C541) | Y. Yang: Nanoporous metal phosphates with photoluminescence property

P11.16.112(C541) | J. Y. Cho: Crystal growth, structure and physical properties of $Ln(\text{CuGa})_{13}$ compounds ($Ln = \text{La-Nd, Eu}$)

P11.16.113(C541) | C. Wei: Structure and magnetic properties of a iron(III) spin crossover complex

P11.16.114(C541) | B. H. Nguyen: The local structure & dielectric properties of the cubic pyrochlore $\text{Bi}_{1.67}\text{M}_{0.75}\text{Nb}_{1.5}\text{O}_7$ ($\text{M}=\text{Mg and Ni}$)

P11.16.115(C542) | J. Popovic: Structural study of Co-doped zinc aluminate

P11.16.116(C542) | B. Grzeta: Effect of tin level on microstructure of tin-doped indium oxide

P11.16.117(C542) | S. Sakai: Crystal structure and site occupancy of boron in synthetic high-pressure spinel $\text{MgAl}_{2-x}\text{B}_x\text{O}_4$

P11.16.118(C543) | A. Adam: Magnetic and structural investigations of nanocrystalline nickel ferrite NiFe_2O_4

P11.16.119(C543) | T. Kawasaki: X-ray structural study of intercalation compound M_xTiS_2 ($\text{M}=\text{Ni, Co}$)

P11.16.120(C543) | N. Shin: A synchrotron powder diffraction study for luminescent materials

P11.16.121(C544) | H. Fujiwara: X-ray crystallographic analysis of by-products produced in photochromism of dithienylcyclopentenes

P11.16.122(C544) | L. Benedetti: X-ray diffraction of laser-heated silicon at high pressures

P11.16.123(C544) | A. O. Dos Santos: Rochelle salt thermal expansion coefficients determined by synchrotron radiation renninger scan

P11.16.124(C544) | G. B. M. Vaughan: Monocrystal like structural, stochastic and microstructural information from polycrystalline samples

P11.16.125(C545) | J. Madarász: Structural and thermal analytical study on *trans*-diammine-bis(nitrito) complex of Pd(II) and Pt(II)

P11.16.126(C545) | J. A. Kaduk: Crystal structure of synthetic hydrotungstate, $\text{WO}_2(\text{OH})_2(\text{H}_2\text{O})$

P11.16.127(C545) | J. C. A. Boeyens: Periodic properties of atomic matter

P11.05.128(C546) | G. Gao: Preparation of cuprous oxide microspheres via HTAB-assisted glucose reduction approach

15. DIFFRACTION PHYSICS AND OPTICS

P15.06.01(C574) | E. K. Mukhamedzhanov: Absolute intensity and phase of the resonant X-ray scattering from a germanium crystal

P15.06.02(C574) | J. Kokubun: Quantitative evaluation of quadrupole transition effect in ATS scattering from magnetite, Fe_3O_4

P15.10.03(C574) | S. Chang: Twenty-four beam X-ray diffraction in a two-plate Fabry-Perot silicon crystal cavity

P15.06.04(C575) | M. Zschornak: Site-selective determination of coordination symmetries by anisotropic anomalous X-ray scattering

P15.06.05(C575) | S. R. Bland: Resonant X-ray diffraction study of low temperature magnetite

P15.06.06(C575) | Y. Murakami: Orbital ordering and the impurity effect in layered manganites

P15.07.07(C576) | T. Morita: Flipping ratio in circularly polarized X-ray diffraction

P15.07.08(C576) | H. Ohsumi: Development of a polarization rotator for X-ray magnetic diffraction

P15.10.09(C576) | S. Weng: Multiple-wave X-ray resonant diffraction using iterative Born approximation

P15.04.10(C577) | S. Y. Chen: Beam suppression and focusing in multi-plate crystal cavity with compound refractive lenses

P15.04.11(C577) | P. Miklik: Beam conditioning by diffractive-refractive crystal monochromators in Bragg and Laue geometries

P15.08.12(C577) | A. Movsisyan: Study of complete transfer phenomenon for media with various thermal conductivity

P15.08.13(C577) | M. Yoshizawa: Observation of rocking curves in Bragg-Laue case

P15.08.14(C578) | K. Hirano: Interference fringe in Bragg-(Bragg)^m-Laue case

P15.08.15(C578) | R. Negishi: Observation of in-phase interference fringes

P15.08.16(C578) | T. Fukamachi: Anomalously large dispersion angle of refracted wave in Bragg case

P15.08.17(C579) | T. Nakajima: New mechanism of anomalous transmission, absorption and their additional unusually curious feature

Thursday, August 28 - Friday, August 29 - Poster Sessions

P15.09.19(C579) | H. Hu: The influence of mosaic distribution upon the extinction factors in real crystals

P15.09.20(C579) | V. Kocharyan: Absorption coefficient of X-rays in crystals in presence of temperature gradient

21. SYMMETRY AND ITS GENERALISATIONS

P21.01.01(C617) | T. F. Veremeichik: Crystallographic model of an atom and the dimension of real Euclidean space in Mendeleev's Table

P21.01.02(C617) | A. S. Wills: Application of corepresentations to magnetic structures and displacive crystallographic transitions

P21.01.03(C618) | M. Nespolo: Point groups in crystallography

P21.02.04(C618) | K. Sakaguchi: Hierarchical structural analysis of supramolecular isomers of organic crystalline host compounds

P21.02.05(C618) | A. Arakcheeva: The (3+1)-dimensional scheelite structure type

P21.04.06(C618) | Z. D. Papadopolos: A model of decagonal Al-Cu-Co

P21.03.07(C619) | N. V. Somov: The pseudosymmetry of atomic structures in crystals of organic and organoelemental compounds

22. APERIODIC AND INCOMMENSURATE STRUCTURES

P22.01.01(C619) | H. Abe: Local structure study in decagonal quasicrystals

P22.02.02(C619) | K. Saitoh: Structure refinement of a decagonal $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$ quasicrystal by convergent-beam electron diffraction

P22.01.03(C620) | A. Strutz: Superstructure solution of decagonal Al-Co-Ni using 5D and 3D approaches

P22.01.04(C620) | H. J. M. Orsini-Rosenberg: New boron-based decagonal approximants

P22.01.05(C620) | K. Yamamoto: X-ray analysis of phason strains for one-dimensional Al-Ni-Co quasicrystals

P22.04.06(C620) | H. Grimmer: Elastic properties of 2-dimensionally quasiperiodic and 1-dimensionally periodic quasicrystals

P22.04.07(C621) | T. Watanuki: Successive phase transition of a Cd-Yb 1/1 crystalline approximant under high pressure

P22.01.08(C621) | Y. Miyazaki: Aperiodic tiling structure with ten-fold symmetry in B-Ti-Ru rapidly solidified alloy

P22.04.09(C621) | Y. So: HRTEM observation of displacement fields around dislocations in quasicrystals

P22.03.10(C622) | A. Schoenleber: Incommensurately modulated structure of malayamycin A

Thursday, August 28 - Friday, August 29 - Poster Sessions

P22.03.11(C622) | W. Steurer: Distinct band gaps and isotropy combined in icosahedral band gap materials

P22.02.12(C622) | K. Takada: Structure analysis of layered sodium cobalt oxide hydrates based on composite crystal models

P22.01.13(C623) | B. Lake: Nuclear and magnetic structure of CaCu_3O_6

P22.03.14(C623) | N. K. Mukhopadhyay: An analysis on the synthesis of icosahedral quasicrystal based on AlMgMn complex metallic alloys

23. CRYSTALLOGRAPHY TOPOLOGY

P23.03.01(C623) | J. Yuhara: Atomic arrangement of Al-Co-Ni Co-rich quasicrystal and W(AlCoNi) crystalline approximant

P23.03.02(C624) | K. Yamaguchi: Quasicrystals and approximants in the Ag-In- M and Au-Sn- M (M :Ca or rare earth metals) systems

P23.03.03(C624) | S. Ohhashi: Formation of quasicrystal and approximant phases and their structures in Zn-Mg-(Ti, Zr, Hf) alloys

P23.03.04(C624) | N. Kamiyama: The role of Mg in the stable Cd-Mg-RE (RE: rare earth metals) quasicrystals

P23.03.05(C624) | M. Shimoda: Surface studies on quasicrystals

P23.04.06(C625) | A. Monge: Influence of the additional ligands dimensionality on the topology of Zn MOFs

P23.02.07(C625) | S. Deloudi: The periodic average structure of 7-, 8-, 10-, and 12-fold quasiperiodic tilings

P23.05.08(C625) | I. Kanazawa: The breaking of duality symmetry, melting, and glass transition

24. DATABASES

P24.01.01(C626) | A. Le Bail: The predicted powder diffraction database (P2D2)

P24.01.02(C626) | C. T. Chantler: Databases for absorption, XAFS and XANES, and future opportunities for research and investigation

P24.02.03(C626) | H. J. Feldman: Modernization of protein crystallography data formats: PDBML as a replacement for PDB?

P24.02.04(C626) | S. J. Coles: The eCrystals Federation: Management and publication of small molecule structure data for all

P24.04.05(C627) | N. Okazaki: Development of hydrogen and hydration database for biomolecules (HHDB)

Thursday, August 28 - Friday, August 29 - Poster Sessions

P24.04.06(C627) | P. Chakrabarti: Protein-protein interactions: Structural features and empirical estimation of free energy of binding

P24.07.07(C627) | B. Stec: Defining a protein: Mining the protein structure database

P24.06.08(C628) | F. Needham: Analysis of the organic X-ray powder diffraction database and its use with pharmaceutical substances

P24.07.09(C628) | A. J. Hamilton: Studying conformational preferences for mechanistic purposes: Using database mining and computation

P24.07.10(C628) | J. E. Debreczeni: Ligand substructure validation in macromolecular crystallography using the CSD

P24.09.11(C629) | H. Schmidt: Nucleation of heat storage materials - search algorithms for similarities of crystal surfaces

25. INDUSTRIAL CRYSTALLOGRAPHY

P25.01.01(C629) | M. A. G. Aranda: Hydration of activated belite cements studied by synchrotron X-ray powder diffraction

P25.03.02(C629) | I. Yakimov: Bath quantitative XRD control at Russia aluminum smelters

P25.08.03(C630) | R. C. Hock: Diffraction experiments with high-energy X-rays during PVT growth of SiC

P25.04.04(C630) | P. Dasgupta: Dislocation assisted intermetallic layer formation at the interface of Sn-Pb solder and Cu

P25.02.05(C630) | R. Yokoyama: Characterization of strain in cubic thin film with $\langle hkl \rangle$ fiber texture in anisotropic stress state

P25.07.06(C631) | D. G. Lamas: Local structure of the tetragonal phase in nanostructured zirconia-based solid solutions

P25.07.07(C631) | H. Sheu: Phase separation inside the CdTe-CdSe type II quantum dots revealed by synchrotron PXRD and SAXS

P25.06.08(C631) | M. D. Eddleston: Teaching an old molecule new tricks: A novel tubular morphology of caffeine

P25.10.09(C632) | C. A. Reiss: X-ray non-ambient powder diffraction of paracetamol polymorph form III

P25.10.10(C632) | G. Petrushevski: Crystal structure of sodium valproate - a hint in understanding the valproate physiological action?

P25.10.11(C632) | N. Chirgadze: Identification of novel fragment-based hits for *P. berghei* orotidine 5'-monophosphate decarboxylase

Thursday, August 28 - Friday, August 29 - Poster Sessions

P25.01.12(C632) | I. Hatta: SAXD/WAXD study on structural change of intercellular lipid matrix in skin by applying chemicals

P25.10.13(C633) | T. Degen: XRPD lab instrument measurements and crystallographic analysis on insulin and insulin derivatives