Open Commission Meetings

OCM01 Commission on Journals
R1008 (12:30-14:45)
Coordinator: G. Kostorz

OCM01.24.01(C167) / Gernot Kostorz:
Overview of IUCr journals

OCM01.24.02(C167) / Dieter Schwarzenbach:
Acta crystallographica section A: Foundations of crystallography

OCM01.24.03(C167) / Carolyn P. Brock:
Acta crystallographica section B: Structural science

OCM01.24.04(C167) / George Ferguson:
Acta crystallographica section C: Crystal structure communications

OCM01.24.05(C168) / E. N. Baker:
Acta crystallographica section D: Biological crystallography

OCM01.24.06(C168) / William Clegg:
Acta crystallographica section E: Structure reports online

OCM01.24.07(C168) / Howard M. Einspahr:
Acta crystallographica section F: Structural biology and crystallization communications

OCM01.24.08(C169) / Anke R. Pyzalla:
Journal of Applied Crystallography

OCM01.24.09(C169) / Dennis M. Mills:
Journal of Synchrotron Radiation

OCM02 Commission on Structural Chemistry
G1202 (12:40-13:40)

Luncheon Seminar
12:45-13:30
C-1001.2: Sponsored by Bruker AXS K.K. (200 seats)
E-1009: Sponsored by Rigaku Corp. (1) (200 seats)

Open Forum (1)
C-1001.2 (17:00-20:00)

Haruo Hosoya “Origami: Crystal model production with paper folding”

André Authier “History of X-ray diffraction-looking deeper and deeper into the structure of matter.”

Music Session (1)
B-05SH (18:30-21:00)

IUCr General Assembly
F-12CH (19:00-21:00)

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
24-25 August

Topics and Sub-topics

02 Methods for Structure Determination
1. Difficult Structures
2. Direct Methods of Phase Determination
3. Maximum Entropy Methods
4. Anomalous Dispersion/MAD/MIR Phasing
5. Laue Time-Resolved Methods
6. Incommensurate Structure Solution
7. EXAFS and XANES
8. High Resolution NMR and Macromolecules
9. Liquid Structure Determination
10. Structure Prediction: Computational Methods

03 Computers in Analysis, Molecular Modelling and Molecular Design
1. Programs for Refinement and Analysis
2. Atomic Displacement Analyses and Variable Temperature Analyses
3. Graphics and Virtual Reality
4. Rational Drug Design
5. Materials Design
6. Structure Simulations: Inorganic Crystals
7. Structure Simulations: Protein Folding Studies
8. Map Fitting and Modification
9. Image Reconstruction
10. Homology Modelling, Structural Families and Docking
11. Use of Genetic Algorithms and Other Optimization Methods

04 Crystallography of Biological Macromolecules
5. Nucleic Acids
6. Protein - DNA Interactions
7. Protein - RNA Interactions
8. Protein Design and Engineering
9. Protein Biosynthesis
10. Cryo-Crystallography: Applications to Macromolecules
12. Ab Initio Low Resolution Macromolecular Phasing
13. X-ray and Neutron Complementarity
14. Rietveld Refinement Methods
15. Computers in Analysis, Molecular Modelling and Molecular Design
16. Programs for Refinement and Analysis
17. Atomic Displacement Analyses and Variable Temperature Analyses
18. Graphics and Virtual Reality
19. Rational Drug Design
20. Materials Design
21. Structure Simulations: Inorganic Crystals
22. Structure Simulations: Protein Folding Studies
23. Map Fitting and Modification
24. Image Reconstruction
25. Homology Modelling, Structural Families and Docking
26. Use of Genetic Algorithms and Other Optimization Methods
27. Crystallography of Biological Macromolecules
28. Nucleic Acids
29. Protein - DNA Interactions
30. Protein - RNA Interactions
31. Protein Design and Engineering
32. Protein Biosynthesis
33. Cryo-Crystallography: Applications to Macromolecules

Sunday, August 24 - Monday, August 25 - Poster Sessions

Sunday, August 24 - Other Activities

Sunday, August 24 - Monday, August 25 - Poster Sessions
02. METHODS FOR STRUCTURE DETERMINATION

P02.01.01(C200) | S. Daoussis: Structural studies of urate oxidase via powder diffraction
P02.01.02(C200) | A. Van Der Lee: A new performing space group determination algorithm
P02.01.03(C201) | G. G. Langer: Tracing the protein main chain down to 5.5 Ångstroms
P02.01.04(C201) | J. Etheridge: Determination of structural phase in CBED patterns - applications to structure biologial systems
P02.01.05(C201) | RAELS: A program for crystal structure solutions that change across interfaces
P02.01.06(C202) | A. B. Smith: Direct space and simultaneous direct-reciprocal space optimization models for powder structures
P02.01.07(C202) | A. D. Ray: RAEELS: A program for crystal structures changing across interfaces
P02.01.08(C202) | J. Etheridge: Direct observation of structural phase in CBED patterns - applications to structure determination
P02.01.09(C202) | M. Kawamoto: Studies for S-SAD method using various wavelength at SPring-8 and SAGA-LS

P02.04.10(C203) | T. Hasagawa: Sulphur SAD (S-SAD) phasing using CoKα, radiation
P02.05.11(C203) | H. King: Development of computer software for general area detector diffraction systems (GADDS)
P02.05.12(C203) | A. W. Wrobel: Structural changes of reaction centre from Bl. viridis revealed by time-resolved Laue diffraction
P02.07.13(C204) | C. Numakaj: XAFS and XRF studies of anti-bacterial ceramics using synchrotron radiation
P02.07.14(C204) | M. T. Klepaka: Local atomic structure of iron in Fe-chitosan complexes, determined by XAFS
P02.07.15(C204) | T. Sata: 100-picosecond time-resolved X-ray absorption fine structure of Fe(1,10-phenanthroline)
P02.10.16(C205) | R. Ohashi: Indexing algorithm for powder diffraction pattern using topograph
P02.10.17(C205) | S. Ide: Structural characterization and developing a suitable SAXS model of diblock(DEAEMAn-PDMAEMAm) polymer
P02.10.18(C205) | S. Arapan: High-pressure phase transformations in aromatic, strotamite and withite
P02.10.19(C205) | M. A. Neumann: Crystal structures of moderately complex organic molecules are predictable

P02.10.20(C206) | D. M. Toebbens: Structure prediction of flexible small molecules - A case study
P02.10.21(C206) | A. L. Yakhov: Increasing the effectiveness of evolutionary crystal structure prediction using fingerprint function
P02.10.22(C206) | H. M. Paulenk: Inverse multislice calculations: A new method for solving complex structures
P02.10.23(C207) | V. P. Ting: Rapid and routine determination of hydrogen positions in inorganic and organometallic compounds
P02.10.24(C207) | N. Nakayama: Development of polarizable force field for the prediction of molecular crystal structures
P02.10.25(C207) | K. Lum: Drug virtual screen by GA/GP: Rapid and routine drug design
P02.10.26(C207) | J. R. Helliwell: Docking studies with tubulin inhibitors as anticancer agents
P02.10.27(C207) | H. M. L. Faulkner: Development of protein structure determination using fingerprint function
P02.10.28(C207) | T. Hasegawa: Validation of molecular crystal structures using dispersion-corrected DFT
P02.10.30(C208) | J. Van de Streek: Structure prediction of protein crystallography
P02.10.31(C208) | J. Rohlicek: Advanced strategy for ab initio structure determination of pharmaceutical compounds by powder data
P02.10.32(C208) | F. Kimura: Structure solution of low temperature simvastatin polymorphs from synchrotron powder diffraction

P02.11.29(C209) | S. H. Lapidus: A comparison of co-crystal structure solutions through powder and single crystal techniques
P02.11.30(C209) | A. J. Cowell: The co-crystalisation and thermal behaviour of oxamide, nicotineamide and isonicotinamide
P02.11.31(C210) | J. M. Cranwrick: The third structure determination by powder diffractionmetry round robin (SDPDR R.3)

P02.11.32(C210) | T. Kimura: Magnetic alignment to convert powder crystallites into a pseudo-single crystal
P02.11.33(C210) | F. Kimura: 3D alignment of LiCoPO4 microrods by modulated magnetic fields for X-ray single crystal analysis
P02.11.34(C210) | W. Oshima: Preparation of pseudo-single crystal of sucrose from powder by magnetic alignment
P02.11.35(C211) | J. Rohlicek: Crystal structure determination of captecinabine from X-ray synchrotron powder diffraction data
P02.11.36(C211) | M. Husak: Structure solution of low temperature simvastatin polymorphs from synchrotron powder diffraction
new structural type Bi3

diffraction data

magnetically prepared pseudo-single crystal of sucrose

oxotitanium phthalocyanine as charge generation materials

X evaluation of elec

structures

diffraction and electron microscopy to solve complex

data phasing method to the solution of inorganic structures from

assembly program using Monte Carlo si

- N method

electron density distribution of polymer by

atomic coordinates

solution scattering

First success in direct

powder diffraction, and Rietveld refinement

from powder data using a combination of real-space method

characterization of Bi

property of nanocrystalline La

Bacillus subtilis

site preference of Mn in Zn

by TEM, X-ray and neutron

Synthesis, microstructure and

crystal structure refinement

of waste magnesium by Rietveld analysis of X-ray diffraction

phosphor by combined Rietveld refinement

Inhibition of histidine

Site preference of Mn in Zn

effect of initial conformations of

A molecular dynamics

approach to equilibrium structures in crystals

Effects of initial conformations of

Trypanosoma cruzi

Density modification by

Validation and correction of

A molecular dynamics

approach to polymorphism of aspirin

Effects of initial conformations of small ligands on computational docking accuracies

Structure solution of

molecular graphics toolset for crystallography

structure-based design of 5-halogen and 5-alkyl orotate derivatives

Poster Sessions Sunday, August 24 - Monday, August 25
P03.06.18 | B16 | Magnetic neutron diffraction single crystal patterns of thiosemicarbazone complexes: Structural and theoretical simulations and diffuse scattering in BaTiO3 quasicrystals.


P03.06.20 | C224 | L. Boukli-Hacene, N(II) thiosuccinonitrile complexes: Structural and theoretical investigation.

P03.05.21 | C222 | A. K. Wolf: Prediction and experimental determination of the crystal structure of SrBi4.

P03.06.22 | C224 | M. J. Gutmann: Computation of diffuse neutron magnetic diffusion single crystal patterns.

P03.06.25 | C224 | M. Pasciak: Multi-resolution atomistic simulations and diffuse scattering in BaTiO3.

P03.01.24 | C225 | C. Tabti: Structural investigation of lithium niobate between 293 and 100K.

P03.05.16 | C222 | P03.05.17 | C223 | D. Kuroda, Y. Takahashi, T. Oroguchi, S. Mondal, K. Kudo, T. Chatake: Relationship between sequence and structure of CDR-H3 in antibodies.

P03.06.22 | C225 | E. V. Leonenko: Computer modeling of local structure, properties and stability of NaCl-KCl solid solution.

P03.07.26 | C226 | T. Zhou: Prediction of secondary structure and dihedral angles in proteins.

P03.11.27 | C226 | Y. Yakimov: Hybrid genetic algorithm for a full-profile analysis of XRD powder patterns.

P03.11.29 | C226 | Y. Volkov: Consistency of particle shape determination from small-angle scattering data: Computer modeling.

P03.10.30 | C227 | Y. Tschiya: Development of a scoring method for predicting protein complex structures.

P03.10.31 | C227 | L. R. Castillo: 3D homology structure model for a pyrazinamide susceptibility test in Mycobacterium tuberculosis.

P03.10.32 | C227 | L. Viitanen: Homology modeling of Arabidopsis thaliana glycerolipid transfer protein.

P03.10.33 | C228 | D. Kuroda: Relationship between sequence and structure of CDR-H3 in antibodies.

P03.10.34 | C228 | S. Mondal: Comparative analysis of putative NADPH- and NADH-dependent ketopantoate reductase.

P03.12.35 | C229 | J. Shen: A theoretical study of changes in the morphology of the diacylthiophen crystals.

P03.12.36 | C229 | S. Moriithu: Image reconstruction by a combination of diffractive imaging and selected area nano diffraction.

P03.10.40 | C229 | W. L. Daux: Universal tree of species evolution.


P03.09.39 | C230 | Y. Yakimov: Hybrid genetic algorithm for a full-profile analysis of XRD powder patterns.

P03.10.42 | C230 | T. Oroguchi, S. Mondal, K. Kudo, T. Chatake: Relationship between sequence and structure of CDR-H3 in antibodies.

P04.05.213 | C297 | J. Kondo: Crystal structures of the bacterial, mitochondrial and cytoplasmic A-site molecular switches.

P04.05.214 | C297 | T. Chatake: Crystal structure of Z-DNA dCGGCGG complexed with Ca2+ ion, and Mg2+ ion.

P04.05.215 | C297 | T. Haraguchi: X-Ray analyses of DNA duplexes stabilized by bicyclic C residues.

P04.05.216 | C297 | T. Prange: X-ray structure of A and B-DNA under high hydrostatic pressure (up to 2 GPa).

P04.05.218 | C297 | J. Van Meerweij: Conformational flexibility of cyclohexene residues.

P04.06.219 | C299 | D. Shahinas: Structural insight on the mechanism of regulation of the MarR family of proteins.

P04.06.220 | C299 | E. P. Lambe: Activity regulation of the transcription factor Fts-I by DNA-mediated homodimerization.

P04.06.221 | C300 | K. Tsai: Structure of the FOXO3a-DBD-DNA complex suggests the effects of post-translational modification.

P04.06.222 | C300 | Y. Lee: Structural basis for human mitochondrial DNA polymerase processivity.

P04.06.223 | C300 | K. Kitano: Crystal structure of the HRDC domain of human Werner syndrome protein, WRN.
P04.06.224(C301) | N. Yennawar: Macromolecular crystallography at the Penn State X-ray core facility

P04.06.225(C301) | J. Kim: Crystal structure of the Mus81-Eme1 complex

P04.06.226(C301) | D. Itagaki: Structural studies on the promoter recognition of transcription factor HIF-6

P04.06.227(C301) | J. Wang: Redesign a non-specific endonuclease

P04.06.228(C302) | P. Kug: Structural insights into TDP-43 in nucleic acid binding

P04.06.229(C302) | Y. Hsu: Crystal structure of CRN-4: Implications for domain function in apoptotic DNA degradation

P04.06.230(C302) | S. Sakurai: Structural studies of the C-terminal extension in the C-terminal domain of DNA gyrase

P04.06.231(C303) | E. Emes: Crystal structure of the Mus81-Eme1 complex

P04.06.232(C303) | M. Tanabe: Structural insights into TDP-43

P04.06.233(C303) | Y. Sawai: Structural basis for transcriptional regulation mechanisms by the transcription factor Ets2

P04.06.234(C303) | D. Huang: Comparison of crystal structures of NF-kB p50/ReIB DNA and p52/ReIB DNA complexes

P04.06.235(C303) | A. Nakamura: Structural basis for regulation of bifunctional roles of the F-plantamid replication initiator RepE

P04.06.236(C303) | C. Nei-Li: Structural study of the C-terminal domain of DNA gyrase

P04.06.237(C303) | K. Arita: Novel DNA-binding fold of TDP-43 proteins: Crystal structure of human DGC8 core

P04.06.238(C303) | H. Itou: Structural basis for hemi-methylated CpG DNA recognition by mouse Np95 SRA domain

P04.06.239(C303) | K. Arii: Structural basis for hemi-methylated CpG DNA recognition by mouse Np95 SRA domain

P04.06.240(C303) | M. J. Van Raaij: Structural basis for recognition and nuclear import of spliceosomal U2RNP complexes

P04.06.241(C306) | C. Merayevskii: A new nicking enzyme is developed from a modified type II restriction enzyme ScPvuII

P04.06.242(C306) | D. H. Welger: Structural characterization of ANAC019, a member of the NAC family of plant transcription factors

P04.06.243(C306) | J. Laposyov: Structure of the topoisomerase IV from S. pneumoniae with a DNA target and quinolone drug

P04.06.244(C306) | S. Shimizu: RNA splicing related proteins: Crystal structure of RNA 3'-terminal phosphate cyclase

P04.06.245(C306) | W. Hae: Crystal structure of human DNA gyrase

P04.06.246(C306) | M. I. Van Raaij: Structural basis for recognition of cognate tRNA by tyrosyl-tRNA synthetase

P04.06.247(C306) | D. Huang: Novel DNA-binding fold and DNA-recognition mode discovered in restriction enzyme PabI

P04.06.248(C306) | J. Kim: Structural basis for dsRNA recognition by nonstructural protein 1 of influenza A virus

P04.06.249(C306) | H. Yoshida: X-ray structure of a cysteine-less mutant galectin-1

P04.06.250(C306) | A. Cheng: Structural basis for dsDNA recognition by nonstructural protein 1 of influenza A virus

P04.06.251(C306) | H. Nishida: Structural basis for transcription factors

P04.06.252(C306) | A. Nakamura: Structural basis for transcription factors

P04.06.253(C306) | S. Chimnaronk: Structural basis for transcription factors

P04.06.254(C306) | A. C. W. Pike: Structural studies of the multidrug-responsible transcriptional repressor protein CgmR

P04.06.255(C306) | K. Yokoya: Structural studies of the multidrug-responsible transcriptional repressor protein CgmR

P04.06.256(C306) | S. Shimizu: Structural basis for transcription factors

P04.06.257(C307) | C. Nei-Li: Structural studies of the multidrug-responsible transcriptional repressor protein CgmR

P04.06.258(C307) | D. Huang: Structural basis for transcription factors

P04.06.259(C307) | K. Miyazono: Structural basis for transcription factors

P04.06.260(C307) | S. Chimnaronk: Structural basis for transcription factors

P04.06.261(C307) | H. Itou: Structural basis for transcription factors

P04.06.262(C307) | D. H. Welger: Structural basis for transcription factors

P04.06.263(C307) | J. Laposyov: Structure of the topoisomerase IV from S. pneumoniae with a DNA target and quinolone drug

P04.06.264(C307) | S. Shimizu: RNA splicing related proteins: Crystal structure of RNA 3'-terminal phosphate cyclase

P04.06.265(C307) | W. Hae: Crystal structure of human DNA gyrase

P04.06.266(C307) | M. I. Van Raaij: Structural basis for recognition of cognate tRNA by tyrosyl-tRNA synthetase

P04.06.267(C307) | D. Huang: Novel DNA-binding fold and DNA-recognition mode discovered in restriction enzyme PabI

P04.06.268(C307) | J. Kim: Structural basis for transcription factors

P04.06.269(C307) | H. Nishida: Structural basis for transcription factors

P04.07.244(C307) | H. Yoshida: X-ray structure of a cysteine-less mutant galectin-1

P04.07.245(C307) | A. Cheng: Structural basis for dsDNA recognition by nonstructural protein 1 of influenza A virus

P04.07.246(C307) | M. I. Van Raaij: Structural basis for recognition of cognate tRNA by tyrosyl-tRNA synthetase

P04.07.247(C307) | D. Huang: Novel DNA-binding fold and DNA-recognition mode discovered in restriction enzyme PabI

P04.07.248(C307) | S. Chimnaronk: Structural basis for transcription factors

P04.07.249(C307) | A. C. W. Pike: Structural studies of the multidrug-responsible transcriptional repressor protein CgmR

P04.07.250(C309) | H. Moon: Structural studies of human RIG-I in complex with double-stranded RNA

P04.07.251(C309) | A. Dickmanns: Structural requirements for recognition and nuclear import of spiloseicins UsnRNPs

P04.07.252(C309) | R. Fierer: Crystallographic studies on molecular motors and switches of the spliceosome

P04.07.253(C309) | Y. Kurasak: Molecular basis for recognition of cognate tRNA by tyrosyl-tRNA synthetase from three kingdoms

P04.07.254(C310) | A. Nakamura: High resolution structure of bacterial GaltAB reveals the C-tail domain structure in GaltAB

P04.07.255(C310) | C. Cheng: Structural basis for dsRNA recognition by nonstructural protein 1 of influenza A virus

P04.07.256(C311) | H. Yoshida: X-ray structure of a cysteine-less mutant galectin-1

P04.07.257(C311) | S. Pletnev: Far-red fluorescent protein mKate reveals pH-induced cis-trans isomerization of the chromophore

P04.07.258(C311) | A. Takenaka: Two threonyl-tRNA synthetases with complementary functions; Crystal structure of ThrRS-1

P04.07.259(C311) | A. Takenaka: Two threonyl-tRNA synthetases with complementary functions; Crystal structure of ThrRS-1

P04.09.258(C311) | A. Takenaka: Two threonyl-tRNA synthetases with complementary functions; Crystal structure of ThrRS-1
Manipulating protein radiation damage at cryogenic temperatures and the evolution of protein crystal disorder during slow cooling and the application of a novel mounting tool using adhesive for protein crystals.

Successful cryocooling of protein microcrystalline samples for powder diffraction and the use of a frozen buffer-free crystal mounting method for the longer wavelength SAD phasing probes.

The structure of archaeal ribosomal stalk complex and the temperature dependence of radiation damage to macromolecular crystals.

Characterization of the myomesin forms a 370 Å long two-chain, antiparallel filament across the muscle M-band region.

Atomic-level models of the Sec2p, the guanine nucleotide exchange factor for Sec4p on RNA polymerase function: Structure of the Gre-factor reveals its binding site explains D-staggered structure of collagen.

Application of a novel rearrangement in the baseplate of lactococcal phage Tuc2009 reveals the assembly of the tripartite bacterial efflux pump.

Coordination structure of the bacterial secretion ATPase revealed by X-ray crystallography and SAXS.

Successful cryocooling of protein microcrystalline samples for powder diffraction and the use of a frozen buffer-free crystal mounting method for the longer wavelength SAD phasing probes.

Structure of the Yersinia MacA pseudonarcissus lectin complex with mannobiose at 1.7 Å resolution, FORM II.

The structural analysis of Rpn14 as the molecular-chaperone for eukaryotic 26S proteasome assembly.

The structural analysis of Rpn14 as the molecular-chaperone for eukaryotic 26S proteasome assembly.

The temperature dependence of radiation damage at cryogenic temperatures.

Structural studies on the bacterial cellulose synthesis component A of a giant ab bacterial carboxysome shell.

A topological model of the octocoral hemidesmosomes.
Poster Sessions

Sunday, August 24 - Monday, August 25 - Poster Sessions

P04.19.402(C356) | H. Tsuchi: Structural basis of actin recognition and ADP-ribosylation by Clotstrium perfringens iota-toxin
P04.19.403(C356) | J. Brito: Okadaic acid, a conformational study in the solid state
P04.19.404(C356) | E. Sica: X-ray diffraction studies of two dimeric variants of human pancreatic ribonuclease
P04.19.405(C357) | M. Baker: Two staphylococcal staphlcalcid acid binding proteins from the superantigen family
P04.19.406(C357) | W. Weber: Crystal structure of the extracellular protease of the nosocomial pathogen Staphylococcus aureus
P04.19.407(C357) | T. Yokoyama: Crystal structure of a sigma28-regulated non-flagella virulence protein from Staphylococcus aureus
P04.19.408(C357) | H. Ihee: Time-resolved X-ray crystallography captures transition-state-like intermediate in the PYP photocycle crystallography
P04.19.409(C358) | B. Dittrich: Crystal structure of fully cold structure of lysozyme
P04.19.410(C358) | A. Tomita: Slow ligand migration dynamics in carbonmonoxy myoglobin at cryogenic temperature
P04.21.403(C355) | M. Abukhader: Crystal structure of quinone reductase 2 in complex with the selective inhibitor 5-hydroxyflavone
P04.23.433(C365) | S. Bong: A structural studies of free methionine-(R)-sulfoxide reductase from staphylococcus aureus
P04.23.434(C365) | J. Racynska: New insight into catalytic mechanism of serine proteases from ultra-high resolution X-ray studies
P04.23.435(C366) | A. Moren: Electrocatalytically assisted protein crystalization. Applications to protein crystallography
P04.23.436(C366) | B. Dritsch: Inversion refinement of 5 K 0.66 A data of the ethanol solvate of gramicidin A
P04.23.437(C367) | Z. Dauter: Ultra-high resolution and very cold structure of lysozyme
P04.23.438(C366) | L. Huang: Crystal structure of fully oxidized human thioredoxin I containing disulfide between Cys62 and Cys69
P04.23.439(C367) | A. Mitscher: Joint neutron and X-ray diffraction studies at 293 K of an antifeed protein
P04.24.440(C367) | E. Sica: X-ray induced perturbation in the high-resolution crystal structure of endopolygalacturonase determined by X-ray and neutron diffraction
P04.24.441(C367) | A. Higashita: The high-resolution X-ray crystallography of bovine H-protein of glycin cleavage system
P04.24.442(C368) | D. G. Liebschutz: Protein helix-dipole calculations based on experimental electron densities
P04.24.443(C368) | B. Guillot: Charge density analysis of human aldose reductase active site
P04.24.444(C368) | T. Shimizu: Ultra-high resolution structure of endopolygalacturonase determined by X-ray and neutron diffraction
P04.24.445(C369) | J. Raczynska: The high-resolution X-ray crystallography of bovine H-protein of glycin cleavage system
P05.03.03(C380) | F. P. A. Fabbiani: High-pressure crystallisation of antibioo molecules
P05.04.04(C381) | M. Botoshiyansky: Behaviour of the azido group in crystal structure of the intermediates of N-acetyl-L-cysteine antibacterial
P05.04.05(C381) | Y. K. Raini: Crystallography of steroids: A comparative analysis of geometrical features and hydrogen bonding
P05.05.06(C381) | J. H. Haller: Crystal and molecular structure of the diethyl ester of rhodoporphyrin
P05.05.07(C381) | A. S. Sloukina: Potassium salts of some ribonucleotides: AMP, IMP, CMP and UMP
P05.05.07(C381) | J. H. Haller: Crystal and molecular structure of the diethyl ester of rhodoporphyrin
P05.05.06(C382) | J. Delgado: Sesquiterpene lactones isolated from a medicinal plant of the Zizaniales Andes
P05.06.09(C382) | T. V. Timofeeva: Organic two-photon absorbing materials for technological applications and photodynamic therapy
P05.07.10(C382) | A. Wakahara: The structure of water nanowire, in crystal host
P05.08.11(C382) | C. H. Schwalbe: H-bonds in androgroplide and related molecules: Neutron diffraction, database and modeling studies

Poster Sessions

Sunday, August 24 - Monday, August 25 - Poster Sessions

P04.19.422(C356) | J. Pulchero: New insight into catalytic mechanism of serine proteases from ultra-high resolution X-ray studies
P04.19.404(C356) | E. Sica: X-ray diffraction studies of two dimeric variants of human pancreatic ribonuclease
P04.19.405(C357) | M. Baker: Two staphylococcal staphloccalcid acid binding proteins from the superantigen family
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P04.23.437(C367) | Z. Dauter: Ultra-high resolution and very cold structure of lysozyme
P04.23.438(C366) | L. Huang: Crystal structure of fully oxidized human thioredoxin I containing disulfide between Cys62 and Cys69
P04.23.439(C367) | A. Mitscher: Joint neutron and X-ray diffraction studies at 293 K of an antifeed protein
P04.24.440(C367) | E. Sica: X-ray induced perturbation in the high-resolution crystal structure of endopolygalacturonase determined by X-ray and neutron diffraction
P04.24.441(C367) | A. Higashita: The high-resolution X-ray crystallography of bovine H-protein of glycin cleavage system
P04.24.442(C368) | D. G. Liebschutz: Protein helix-dipole calculations based on experimental electron densities
P04.24.443(C368) | B. Guillot: Charge density analysis of human aldose reductase active site
P04.24.444(C368) | T. Shimizu: Ultra-high resolution structure of endopolygalacturonase determined by X-ray and neutron diffraction
P04.24.445(C369) | J. Raczynska: The high-resolution X-ray crystallography of bovine H-protein of glycin cleavage system
P05.03.03(C380) | F. P. A. Fabbiani: High-pressure crystallisation of antibioo molecules
P05.04.04(C381) | M. Botoshiyansky: Behaviour of the azido group in crystal structure of the intermediates of N-acetyl-L-cysteine antibacterial
P05.04.05(C381) | Y. K. Raini: Crystallography of steroids: A comparative analysis of geometrical features and hydrogen bonding
P05.05.06(C381) | J. H. Haller: Crystal and molecular structure of the diethyl ester of rhodoporphyrin
P05.05.07(C381) | A. S. Sloukina: Potassium salts of some ribonucleotides: AMP, IMP, CMP and UMP
06. CRYSTALLOGRAPHY OF ORGANIC COMPOUNDS

P06.01.01(C389) | K. Ohshima | Crystal structure of trehalose dihydrate by X-ray and neutron diffraction experiments

P06.01.03(C384) | K. Kataoka | Temperature-dependent structural change of trehalose dihydrate and anhydrate crystals

P06.01.04(C383) | S. V. Dhung | FTIRXD and XRD-DSC study of crystalline-noncrystalline phase transition of sucrose monohydrate

P06.04.08(C385) | M. Okulabouli | Structure of dihydroisoidolobenzoxazine-11-one and dibromo-cyclopenta[a]naphthalene-1-one

P06.04.09(C385) | K. Musui | Effects of substituents on the oxazaphosphorine heterocyclic compounds

P06.04.10(C385) | A. Gowda K.V. | Crystal and molecular structure of 4-7-dimethyl-2H-chromen-2-one

P06.04.11(C386) | Y. B. Rubayko | X-Ray data for novel tricyclic compounds based on indolizines

P06.04.12(C387) | H. Shimizu | Crystaline molecular assemblies of dehydrobenz[a]12]aunanes having carboxylic groups with amines

P06.04.13(C388) | R. K. Jadaprolu | Structures of benzo and dibenzo [d,f] [1,3,2] dioxaphosphepin 3-oxide (I, II) and 6-sulphide(III)

P06.04.14(C387) | A. Ozek | Crystal structure and quantum mechanical calculations of an oxime compound, C4H4(NO)

P06.05.16(C387) | K. Toyota | Crystal structure analysis of inclusion crystals with tetrapodal host molecules

P06.06.15(C388) | V. Thiruvenkatam | A detailed study of the supramolecular clusters of triphenylmethylammonium dibenzoate

P06.06.16(C387) | V. Thiruvenkatam | Designed supramolecular architectures by connecting of 4+4 supramolecular clusters

P06.06.17(C389) | T. Sasaki | Crystal structure analysis of intercalation with steroidal acids and cinchona sulfonates

P06.06.18(C389) | T. Shigemitsu | Crystal structure and quantum mechanical calculations of a simple alicyclic dialcohol

P06.06.19(C389) | J. Han | Designed supramolecular assembly of novel rosette layers

P06.06.20(C388) | A. Yamamoto | Functional porous crystals with supramolecular clusters of triphenylmethylammonium sulfonates

P06.06.21(C389) | J. H. N. | Guest-induced topological polymorphism of pseudo-cubic hydrogen bond networks

P06.06.22(C389) | T. Murai | Intercalation with steroidal alkaloids

P06.06.23(C389) | M. Dianez | Enantioselective inclusion crystals: Enantioresolution and layer inversion

P06.06.24(C388) | K. Toyota | Application of preferential enrichment to amino acids

P06.06.25(C388) | M. Estrada | Functional porous crystals

P06.06.26(C388) | K. Musui | Synthesis, structure and solid-state photochemistry of m-benzenediacrylic acid and its complexes

P06.06.27(C389) | H. Schenk | Enantioselective inclusion of methyl phenyl sulfonides by (S)-allylglycyl-(S)-phenylglycine

P06.07.28(C391) | T. Hirukawa | Structure and polymorphism of trans-mono-unsaturated tricyglycerols

P06.07.34(C393) | R. Bishop | H NMR application to inclusion chemistry: Selectivity profiles of a xanthone-related host

P06.07.35(C393) | A. Tamugi | Guest-dependent luminescence modulation in inclusion crystals of anthracene derivatives

P06.07.36(C393) | Y. A. | Synthesis, structure and solid state photochemistry of m-benzenediacrylic acid and its complexes

P06.08.27(C390) | J. Bruening | Five alternative crystal forms produced by crystallisation of a simple alicyclic dialcohol

P06.08.28(C390) | T. A. | Functional porous crystals

P06.08.29(C390) | H. Uekusa | Five alternative crystal forms produced by crystallisation of a simple alicyclic dialcohol
P06.07.38 | M. Dincer: An experimental and theoretical approach to the 2-chloro-1-(3-methyl-3-phenylcyclobutyl) ethanoic acid

P06.07.39 | M. J. Wojciechowski: Experimental versus theoretical electron density in the crystals of β -amino-phenolic acids

P06.10.47 | J. Svoboda: Lessons from a decade of X-ray crystallographic work on N-(hydroxy)thiazole-2(3H)-thione derivatives

P06.10.48 | K. Sakihata: Hydrogen-bonded network structures of cocrystals of some naphthalenediol with hexamethylenetetramine bis(mercaptopropionic acid) and phenylcyclobutyl) ethanone

P06.10.49 | M. Kokila: Molecular complexes of two homotetranuclear oxovanadium complexes

P06.10.50 | M. Jotani: Crystal structure of (4-(hydroxy)thiazole-2(3H))bis(thiophenyl)ethenes: Synthesis, structure and bonding

P06.10.51 | S. Ng: Experimental and theoretical electron density in the crystals of Ni(dmit)2 salt with di- and tri-alkylthiazole cations

P06.10.52 | S. Liu: Crystal structures of two homotetranuclear oxovanadium complexes

P06.10.53 | M. Arif: Two proton transfer compounds from benzene-1,2,4,5-tetracarboxylic acid and 1,10-phenanthroline

P06.10.54 | N. Hayashi: X-ray structures of quinone dimers linked either directly or through acetylene spacers

P06.10.55 | K. Ninomiya: Hydrogen-bonded network structures of cocrystals of some naphthalenediol with hexamethylenetetramine bis(mercaptopropionic acid) and phenylcyclobutyl) ethanone

P06.10.56 | L. Roces: Structural study of hydride and dihydrogen ligands ruthenium complexes: Reversible hydrogen release

P06.10.57 | L. Yamaoka: Synthesis, structure, and reactivity of ruthenium-zinc trinuclear hydrides with phosphine ligands

P07.01.02 | L. Tabatabae: Hydrothermal synthesis and crystal structure of a new copper coordination polymer

P07.01.03 | M. Dukovski: The isonicotinamide complexes of copper(II) with N3, SCN and SO4 as bridging ligands

P07.01.04 | G. Pelosi: Bis(trpp)copper(I): thiosuccinamates: Unexpected chemistry revealed by X-ray diffraction

P07.01.05 | H. Miyamae: Porous structure of bis(tris(bipyridine)ruthenium(II)) tris(oxoato)cobaltate(III) chloride

P07.01.06 | K. Tomono: Formation of alkylated dicopper by weak hydrogen bonds in the crystal of (N,dmit) salts

P07.01.07 | J. M. Wojciechowski: Experimental versus theoretical electron density in the crystals of β -amino-phenolic acids

P07.01.08 | K. C. Kumar: Inclusion properties of (Z)-Ethyl 4-chloro-2-[(4-phenyl-4-oxo-1,3-thiazolidin-2-yl)amino-4,5,6,7-tetrahydro-1-benzothiophene onohydrate clathrate
P07.01.17(C404) | N. Yoshikawa: Syntheses, characterization and DFT investigations of iridium complexes and digerminated terptidines

P07.01.18(C404) | M. Parvez: Iridium and zirconium formamidinates as precursors for novel stable carbenes

P07.01.19(C404) | H. Arslan: Synthesis and characterization of an N-heterocyclic carbene palladium-based complex

P07.01.20(C405) | P. Gomez-Sal: Structural studies on Ag(I) N-heterocyclic carbene complexes: From monomers to polymers

P07.01.21(C405) | N. Mizuno: Structural analysis of the rare earth metal hydride complexes

P07.01.22(C405) | E. V. Dikarev: Novel coordination polymers: From monomers to frameworks

P07.01.23(C405) | T. Kojima: Solvent driven association and structural analysis of the rare earth metal hydride complexes

P07.01.24(C405) | C. Cabreiro: Structural challenges of giant bisnuth oxo-diketenate clusters

P07.01.25(C405) | T. Kojima: Solvent driven association and dissociation of the hydrogen-bonded protonated decavanadate dimer

P07.01.26(C406) | C. Cabreiro: Structural challenges of giant bisnuth oxo-diketenate clusters

P07.02.26(C406) | L. Ditlovic: Anion directed self-assembly of a flexible ligand into highly porous and symmetrical organic solids

P07.04.27(C407) | Y. Yayimaru: Triple-stranded helical metal complexes of quatemoidazole and its highly-symmetrical network

P07.04.28(C407) | T. Akuagwa: Design of crystalline space for constructing ferrocenetric rotors in [Ni(dmit)]- salts

P07.04.29(C407) | L. McCorkind: The diabolomers: Some unexpected copper clusters

P07.04.30(C408) | K. Tanaka: A novel chiral metal-organic framework that calyses asymmetric reaction in the chiral open space

P07.04.31(C408) | S. Satihong: The 1-D polymeric dimorphism of copper(I) thiocyanato complexes containing MTAs ligand

P07.04.32(C408) | L. Bring: Novel coordination polymers generated from 2,2'-dipyridylidisulfide and CoCl2

P07.04.33(C409) | S. Krachonov: Concerted ary interaction in zinc-imidazole - Oxovanadate hybrid organic-inorganic materials

P07.04.34(C409) | C. Yang: Assemblies of three mixed-ligand coordination polymers with novel 3D metal-organic frameworks

P07.04.35(C409) | C. Liu: Structural characterization and thermal stability of three coordination polymers with 2D MOFs

P07.04.36(C409) | K. Chainok: Investigation structure and phase transitions of hybrids inorganic-organic metal vanadates

P07.04.37(C410) | C. Wang: Structural diversity of [M(Scn)] fragment with BPHD(2,5-bis(4-pyridyl)-3,4-diazao,2,4-hexadiene)

P07.04.39(C410) | E. Zangrando: Synthetic strategies and structural aspects of metal-mediated multi-porphyrin assemblies

P07.04.40(C410) | H. Ishida: Crystallographic structures of ruthenium tris(2,2'-bipiridine) having amid group at 5,5'-positions

P07.04.41(C410) | C. Habuta: Supramolecular assemblies of lanthanide clusters with chiral ligands in the crystalline state

P07.04.42(C410) | N. Matsunoto: A problem in the crystal structure of a two-step spin crossover complex: Rings and cages

P07.06.43(C411) | Y. Gunko: Metallassloxane complexes: Rings and cages

P07.08.45(C412) | S. Lee: Structures of tris([hydroxymethyl]aminomethane)-5-bromosaclylidenaminato)diaorganotin complexes

P07.05.44(C412) | Y. Uchigawa: Structural studies of 9,10-diheterotriphenylenes with group 15 elements and their halogen adducts

P07.05.45(C412) | V. N. Khrustalev: New stable lead(II) complexes with intramolecular coordination: Experimental and theoretical study

P07.07.46(C413) | H. Schneider: Annealing cattle tibiae: From nano-bio-apatite to geo-apatite

P07.07.47(C413) | J. P. Yennawar: Crystal structures of modified PNA analogues and of cationic dinode Pd(II)-alkyl porphyrin complexes

P07.07.49(C413) | Z. Travnicek: Coordination abilities of selected cytokinins and CDK inhibitors to transition metal ions

P07.07.50(C413) | M. Dhillon: Synthesis and spectroscopic characterization of high-spin iron(III) oxalato porphyrin complex

P07.07.52(C414) | A. A. Sarjeant: X-ray diffraction study of a low-temperature copper(I)/dioxygen adduct: A solid solution

P07.07.53(C414) | L. J. McCormick: Concerted aryl reaction in zinc-imidazole - Oxovanadate hybrid organic-inorganic materials

P07.07.54(C414) | Y. Gunko: Metallassloxane complexes: Rings and cages

P07.07.55(C414) | C. Cabreiro: Structural studies of methylammonium bis(citrato)borate
P07.10.54 (C414) | M. Mitsumi: Crystal structure, magnetic and dielectric property of linear chain rhodium(I)-semiquinonato complex
P07.02.55 (C415) | M. R. Silva: Magnetic and structural properties of some triazole metal complexes
P07.10.56 (C416) | B. Zhang: Construction molecular magnet with porosity, chirality from [Fe(C5P07.10.57)_2] with cation templpat
P07.10.57 (C418) | N. Tsyrulin: Quantum effects in S=1/2 two-dimensional Heisenberg antiferromagnet in applied magnetic field
P07.10.58 (C416) | T. Akitsu: Assembling strategy of magnetic Mn complexes to design solid state multifunctional hybrid materials
P07.10.59 (C410) | S. Ang: Studies on some manganese-containing single-molecule magnets
P07.10.60 (C416) | B. N. Arslan: Slow relaxation of the magnetization in rationally designed single chain magnets
P07.10.61 (C417) | A. Ueda: Synthesis, crystal structure, and magnetic properties of trioxotriangulene stable neutral radical
P07.11.62 (C417) | B. N. Aslan: Hemidirected novel lead(II) azide complex of 2,6-diacetylpyridine dihydrazine
P07.11.63 (C417) | H. Pfeftum: Novel route to synthesis copper halide with CuS2 core and its crystal packing
P07.11.64 (C417) | D. Ulku: Crystal structures of two new tetranuclear copper complexes based on Schiff-base ligands
P07.11.65 (C418) | F. Sis: Crystal structure of platinum 2-methyl- and palladium 2,4-dimethyl-8-hydroxolenquinoninate
P07.03.66 (C410) | M. A. Petrukhina: Indenocorannulene: Molecular geometry, solid state packing, and metal binding properties of some triazole metal complexes
P09.01.01 (C474) | A. Bacchi: Knowledge-based design of host-guest interactions in wheel-and-axe inorganic diols
P09.01.02 (C474) | M. Park: A designed metal-organic framework based on metal-organic polyhedral
P09.01.03 (C474) | S. A. Kumalah: Properties of metal-organometallic frameworks derived from facially metaled tetrapeptide
P09.01.04 (C475) | G. Diyar de Delgado: Cis-trans isomerizations and rearrangements during hydrothermal synthesis of metal carbonylates
P09.01.05 (C475) | M. Lusi: Real crystal engineering: Solid state reactions in metal-organic compounds
P09.02.06 (C475) | C. O. Toor: Design of supramolecular complexes: From concept to crystal structures
P09.04.07 (C476) | J. L. A. Ferrada da Silva: Supramolecular interactions in 3-ferrocenyl-methoxy-benzothiophenes, non stoichiometric drug precursors
P09.02.08 (C476) | M. Du: Cocrysallization of a pharmaceutical agent pamoic acid with piperazine or 4,4'-bipyridine
P09.02.09 (C476) | S. Aitipamula: Polymorphism of co-crystals: Co-crystal polymorphs of an antiseptic drug, ethamzamide
P09.01.10 (C477) | M. Duarte: New crystal forms of gabapentin
P09.01.11 (C477) | A. Tuibovy: Molecular cocrysallites of peganol with pegamine
P09.01.12 (C477) | R. Montis: Subtle relationships between the structures of some aspirin derivatives
P09.01.13 (C477) | E. K. Owusu-Marfo: The influence of hydrogen bonding on generation and stabilization of self-assembled layer structure
P09.01.14 (C478) | G. S. Nichol: Intermolecular interaction-directed conformations of bridged bis(1,4-piperazine-2,5-diones)
P09.02.15 (C478) | V. M. Fawcett: Polymorphism from a solution perspective: Rationalisation at the molecular level
P09.02.16 (C478) | J. King: Characteristic network structure constructed from various block-like molecules
P09.02.17 (C479) | J. King: Self assembled hierarchical nanostuctures: Controlling morphology and molecular arrangement
P09.02.18 (C479) | Y. Michishita: X-ray diffraction and small angle X-ray scattering study under high voltage in EHD application
P09.02.19 (C479) | A. Bacchi: Control of stoichiometry and structure: Mechanism of cocystal formation in mechanochemical synthesis
P09.02.20 (C480) | A. Delori: pKa directed host-guest assemblies of 2,4-diamino-6-methyl-triazine with various dicarboxylic acids
P09.02.21 (C480) | A. A. Kumalah: Cyclic transformation in novel shape and phase of Co nano/microcrystals
P09.02.22 (C480) | S. Sheshmani: Polymorphic complex obtained from a novel supramolecular proton transfer compound
P09.03.23 (C481) | M. Sari: Crystal phase analysis of by-products from NaBH4 production via high-low pressure process by XRD
P09.03.24 | C481 | O. Kaman | Acid phosphates of 1-(1-naphthyl)ethylamine - Importance of symmetry relation between enantiomers
P09.03.25 | C481 | R. Rodriguez-Miñano | A comparative study of two multiphasic alkali halide crystals: Quinary B34 magnet: K2 Fe2 (C481)
K III
P09.03.26 | C481 | M. Debbal | From dimeric tannalapotungsturate to monomeric organosilnyl Lindequist type polysiloxomelates
P09.03.27 | C481 | W. Loechel | Octamolybdates - promising materials for industry and medicine
P09.03.28 | C481 | K. Hayashi | Strongly and accurately shaped Ge crystal for non-scanning X-ray fluorescence spectrometer
P09.03.29 | C482 | O. Dere | Determination of thermal treatment effect of plating sludge by phase identification: XRD technique
P09.03.30 | C483 | Y. Zhang | Two binuclear molecular magnet: K2Fe2(C483)Cl2(H2O) and K2Fe(C483)Cl3(H2O)2
P09.03.31 | C483 | L. Sun | Structure diversity and reversible anion exchange properties of metal complexes with tripodal ligand
P09.03.32 | C483 | A. S. R. Chesman | Lanthanoid, transition metal and heterobimetallic complexes with polynitrile and derivative ligands
P09.03.33 | C483 | K. E. Knorr | Synthesis and characterization of mixed metal (UO2(NO3)2/TM3) inorganic organic framework materials
P09.03.34 | C483 | H. Ashhabozan | A nine-coordinated Zr VI complex obtained from a novel supramolecular proton transfer compound
P09.03.35 | C483 | J. Attar Gharanmaleki | Binuclear Sn(IV) complex obtained from benzene-1,3-diaminium bis(hydrogen pyridine-2,6-carboxylate)
P09.03.36 | C483 | J. Jokiniemi | A structural study of metal complexes of bisphosphate partial ester derivatives
P09.03.37 | C483 | V. Petrović | High pressure synthesis and analysis of new yellow emission Sr3Cu2Cl6: A visible-light driven phosphor
P09.04.38 | C483 | M. A. Fernandes | Designing Zn and Co based 1-D coordination polymers with possible magnetic and electronic properties
P09.04.39 | C483 | L. Dobrzańska | A single-crystal-to-single-crystal apical ligand exchange process in a 2D coordination network
P09.05.40 | C483 | M. R. J. Elsegood | Boronic acids as hydrogen-bond bridges between metal coordinated carboxylates
P09.05.41 | C483 | M. Rademeyer | Noncovalent interactions in a family of cyclic ammonium nitrates
P09.05.42 | C483 | U. Baisch | X-ray diffraction and microscopy study of supramolecular functionalized compounds
P09.05.44 | C483 | N. Kunishige | Systematic mutation study toward the engineering of protein crystals
P09.05.45 | C483 | M. Gryl | Crystal engineering of materials with potential NLO properties using barbituric acid as component
P09.05.46 | C483 | P. A. Wood | Energy versus 3D geometry - A study of intermolecular interactions using theory and experiment
P09.07.48 | C483 | H. Matsui | Crucible rotation dependence of oxygen concentration during solidification of multicitystrline Si
P16.01.01 | C580 | G. Juarez-Martinez | Portable thermal platform for optimising protein crystallisation
P16.01.02 | C580 | X. Xu | In situ proteolysis for protein crystallisation and structure determination
P16.02.03 | C580 | L. Ito | Co-crystallisation and crystal engineering
P16.03.05 | C581 | H. Matsui | Analysis of crystal growth of trigonal ribonuclease A from bovine pancreas
P16.05.05 | C581 | L. Ito | Protein crystallization in the presence of amino acids and their derivatives: (2) The mechanism
P16.03.06(C581): T. Shibano: Protein crystallization in the presence of amino acids and their derivatives: (1) The effect of surface-synthesized, micellar insulin on the nucleation of insulin nanocrystals.

P16.05.07(C581): S. Takahashi: Protein crystallization strategy in microgravity.

P16.05.08(C582): M. Sato: Protein crystallization under microgravity in JAXA New-GCF project.

P16.10.09(C582): M. Ootaki: Investigation of morphological and surface microtopography of cubic insulin nanocrystals.


P16.03.09(C583): M. Sato: Polymorphism in n-alkanes: Crystalization and hydroxyapatite growth kinetics.


P16.03.15(C583): K. Inaka: Optimization of a salt concentration in a PEG-based crystallization solution by a Gel-Tebe method.


P16.13.17(C583): M. Kujumaa: Polymorphism and crystal structure of BPT propyl ester in various solvents.


P16.03.21(C584): J. Martinez: Growth of large single crystals of high-Tc superconductor using a tilted-Lamé floating zone method.

P16.03.22(C584): S. Mahapatra: Influence of bath composition on the growth of KDP crystals in non-stoichiometric solutions.


P16.03.24(C584): K. Byrappa: Hydrothermal synthesis of doped ZnO and its application in photodegradation of toxic amaranth dye.


P16.01.25(C587): V. I. Voronova: Crystal growth peculiarities of new oxide conductor La₂M₀₉O₂₀₊ᵢ in the system La₂O₃-M₀₂O₃.


P16.03.27(C588): D. A. Vorontsov: Peculiarities of the growth of KDP crystals in non-stoichiometric solutions.

P16.03.28(C588): H. Jeon: Solvothermal synthesis of rare earth-iron mixed oxide.


P16.03.29(C588): S. Mahapatra: A novel approach to specifically crystallize anhydrox compounds: Crystal structure of adenine.


P16.03.33(C590): M. Maruyama: Chiral and achiral mechanisms of regulation of calcite crystallization.

P16.03.34(C590): H. Miura: Formation of barred olivine texture 4.6 billion years ago.

P16.11.35(C590): T. Adechar: Property and morphology of organo-Na₂CO₃ coated CeO₂ nanocrystals synthesized in supercritical water.


P16.04.40(C591): U. Pietsch: Initial state of VLS-growth of InAs nanorods on GaAs(111), probed by X-ray diffraction and TEM.


P16.04.43(C592): P. Cardoso: InGaP/GaAs(001) structural characterization by means of synchrotron radiation diffraction study of Al,Ga,Gasb alloys grown by liquid phase epitaxy.

P16.06.43(C593) | S. Emura: Crystal growth condition dependence of local structure around Gd in GaN nanotods

P16.08.44(C593) | T. Yamase: Photoinduced self-assembly to tube, chain, and other aggregate of molybdenum-blue nano-rings

P16.10.45(C593) | A. M. Askhabaj: On the nature of crystal growth units

P16.14.46(C593) | D. S. Yufit: Polymorphism below room temperature

P16.03.47(C594) | A. D. Handoko: Hydrothermal synthesis of (K,Na)NbO$_3$

P16.03.48(C594) | S. Feng: Perovskite-type LnFeO$_3$ (Ln= Y, Pr, Nd, Sm, Gd, Tb, Dy, Ho) prepared by mild hydrothermal method

P16.03.49(C594) | T. He: Effect of anion adsorption on the hydrothermal growth of boehmite

P16.10.50(C594) | S. Ghammamy: Using of Taguchi method for experimental design of crystallization processes of inorganic compounds

P16.03.51(C595) | Y. Suzuki: Hydrothermal synthesis of yttrium silicate based phosphors using new water soluble silicon compounds

P16.05.52(C595) | M. Wu: Morphological control of meso- and single- crystals of Perovskite under solvothermal conditions

P16.03.53(C595) | D. M. Sampady: Single crystal growth of nonlinear optical chalcogen derivative

P16.03.54(C595) | A. E. S. Van Driessche: In situ observation of the joint gel/impurity effect on protein crystal growth kinetics

P16.04.55(C596) | D. A. Pawlak: Self-organized eutectic microstructures towards photonic crystals and metamaterials

P16.15.56(C596) | J. Xu: Desktop Minstrel UV®: A novel protein crystal monitoring automation system using UV fluorescence

P16.02.57(C596) | C. Gerds: The microcapillary protein crystallization system

29. OTHER TOPICS

P29.01.01(C635) | J. R. Hester: Implementing DDLm: Rewriting dREL algorithms into other languages