Open Commission Meetings

OCM01 Commission on Journals

R1008 (12:30-14:45)

Coordinator: **G. Kostorz**

OCM.01.24.01*(C167)* | **Gernot Kostorz**:
Overview of IUCr journals

OCM.01.24.02*(C167)* | **Dieter Schwarzenbach**:
Acta crystallographica section A: Foundations of crystallography

OCM.01.24.03*(C167)* | **Carolyn P. Brock**:
Acta crystallographica section B: Structural science

OCM.01.24.04*(C167)* | **George Ferguson**:
Acta crystallographica section C: Crystal structure communications

OCM.01.24.05*(C168)* | **E. N. Baker**:
Acta crystallographica section D: Biological crystallography

OCM.01.24.06*(C168)* | **William Clegg**:
Acta crystallographica section E: Structure reports online

OCM.01.24.07*(C168)* | **Howard M. Einspahr**:
Acta crystallographica section F: Structural biology and crystallization communications

OCM.01.24.08*(C169)* | **Anke R. Pyzalla**:
Journal of Applied Crystallography

OCM.01.24.09*(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
11. *Ab Initio* Powder Diffraction Solutions:Molecular Compounds
12. *Ab Initio* Powder Diffraction Solutions:Inorganic Compounds
13. *Ab Initio* Powder Diffraction Solutions:Electron Diffraction
14. *Ab Initio* Low Resolution Macromolecular Phasing
15. X-ray and Neutron Complementarity
16. Rietveld Refinement 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

14. Macromolecular Assemblies
15. Macromolecular Based Drug Design
19. Diseases and Toxicity
21. Time Resolved Studies
23. High Resolution Protein Structures

05 Crystallography of Biological Small Molecules

1. Peptides
2. CNS Agents
3. Antibiotics
4. Steroids
5. Other Natural Products
6. Other Biosynthetic and Exotic Molecules
7. Hydrogen Bonding and Included Water Structure

06 Crystallography of Organic Compounds

1. Sugars
2. Lipids
3. Alkaloids
4. Fused Ring Systems
5. Fullerenes and Carbon Cages
6. Supramolecular Assemblies
7. Inclusion Compounds and Complexes
8. Intercalates
9. Clathrates

07 Crystallography of Organometallic, Coordination and Main Group Compounds

1. Metal Atom Complexes (N = 1-3) and Metal Clusters (N>3)
2. Molecular Recognition Complexes
3. Fullerene Metal Complexes
4. Supramolecular Coordination Complexes
5. Main Group Chemistry
6. Cage and Metallo-Cage Structures
7. Bio-Inorganic Structures
8. Bio-Mineralization and Modifications
9. Inclusion Compounds and Clathrates
10. Molecular Magnets

09 Crystal Engineering

1. General Applications and Strategy
2. Organic Compounds
3. Inorganic Compounds
4. Organometallic Complexes
5. Intermolecular Interactions: Exploitation
6. Noncentrosymmetric Systems: Creation and Applications

16 Crystal Growth: Techniques, Instrumentation and Applications

1. Systems that are Difficult to Crystallize
2. Industrial Mass Crystallization
3. Crystal Growth from Solution and Gels
4. Crystal Growth and Characterization from the Melt
5. Microgravity Crystallization
6. Epitaxial Growth
7. Crystal Doping and Imperfections
8. Self-Assembled Crystals
9. Exploitation of Chirality
10. Crystal Growth: Modelling, and Predicting Morphology
11. Morphology Modification: Theory and Experiment
12. Twinning: Acceptance and Avoidance
13. Polymorphism: Recognition and Applications
14. Low Temperature *in situ* Crystallization

29 Other Topics

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

02. Methods for Structure Determination

P02.01.01*(C200)* | S. Dagogo: 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 Angstroms

P02.01.04*(C201)* | N. P. Cowieson: SAXS, synchrotron CD and chemical cross-linking for structural study of complex biological systems

P02.01.05*(C201)* | A. D. Rae: RAELS: A program for crystal structures that change across interfaces

P02.02.06*(C202)* | A. B. Smith: Direct space and simultaneous direct-reciprocal space optimization models for phasing structures

P02.02.07*(C202)* | A. Van Der Lee: Macromolecular structure solution by charge flipping

P02.02.08*(C202)* | J. Etheridge: Direct observation of structural phase in CBED patterns - applications to structure determination

P02.04.09*(C202)* | M. Kawamoto: Studies for S-SAD method using various wavelength at SPring-8 and SAGA-LS

P02.04.10*(C203)* | T. Hasegawa: Sulphur SAD (S-SAD) phasing using CoK_α radiation

P02.05.11*(C203)* | H. Kim: Development of computer software for general area detector diffraction system(GADDS)

P02.05.12*(C203)* | A. B. Woehri: Structural changes of reaction centre from Bl. viridis revealed by time-resolved Laue diffraction

P02.07.13*(C204)* | C. Numako: XAFS and XRF studies of anti-bacterial ceramics using synchrotron radiation

P02.07.14*(C204)* | M. T. Klepka: Local atomic structure of iron in Fe-chitosan complexes, determined by XAFS

P02.07.15*(C204)* | T. Sato: 100-picosecond time-resolved X-ray absorption fine structure of $Fe^{II}(1,10\text{-phenanthroline})_3$

P02.10.16*(C205)* | R. Oishi: 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-DMAEMAm)polymers

P02.10.18*(C205)* | S. Arapan: High-pressure phase transformations in aragonite, strontianite and witherite

P02.10.19*(C205)* | M. A. Neumann: Crystal structures of moderately complex organic molecules are predictable

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

P02.10.20*(C206)* | D. M. Toebbens: Structure prediction of flexible small molecules - A case study

P02.10.21*(C206)* | A. O. Lyakhov: Increasing the effectiveness of evolutionary crystal structure prediction using fingerprint-function

P02.10.22*(C206)* | H. M. L. Faulkner: 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. Lou: Drug virtual screen by GA/GP: Docking studies with tubulin inhibitors as anticancer agents

P02.10.26*(C208)* | J. R. Helliwell: An investigation into protonation prediction implications for protein crystallography

P02.11.27*(C208)* | M. Sakata: Advanced strategy for *ab initio* structure determination of pharmaceutical compounds by powder data

P02.11.28*(C208)* | J. Van de Streek: Validation of molecular crystal structures using dispersion-corrected DFT

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-crystallisation and thermal behaviour of oxamic acid, nicotinamide and isonicotinamide

P02.11.31*(C209)* | L. M. Cranswick: The third structure determination by powder diffractometry round robin (SDPDRR-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 $LiCoPO_4$ 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 capecitabine from X-ray synchrotron powder diffraction data

P02.11.36*(C211)* | M. Husak: Structure solution of low temperature simvastatin polymorphs from synchrotron powder diffraction

P02.11.37*(C211)* | M. Ohno: *Ab-initio* structure determination of Pb-sulfonamide complexes from powder diffraction data

P02.11.38*(C212)* | Y. Kojima: Powder structure analysis of oxotitanium phthalocyanine as charge generation materials

P02.11.39*(C212)* | M. Maeyama: Single crystal analysis of magnetically prepared pseudo-single crystal of sucrose

P02.12.40*(C212)* | H. Miura: Crystal structure model assembly program using Monte Carlo simulation

P02.12.41*(C212)* | C. Miravitlles: Application of the S-FFT phasing method to the solution of inorganic structures from powder data

P02.12.42*(C213)* | D. Xie: Combining X-ray powder diffraction and electron microscopy to solve complex structures

P02.12.43*(C213)* | L. B. McCusker: Powder diffraction, electron microscopy, focus, charge flipping and zeolites

P02.15.44*(C213)* | K. Tashiro: First success in direct evaluation of electron density distribution of polymer by X- N method

P02.15.45*(C214)* | O. Smirnova: Multitechnique solution of a new structural type $Bi3^{Mn4}O11.22^{(NO3)0.93}$

P02.15.46*(C214)* | J. Y. H. Chow: The interaction between human rhinovirus 3C protease and stem loop D studied by solution scattering

P02.15.47*(C214)* | D. A. Jacques: Inhibition of histidine kinase A in *Bacillus subtilis*: A neutron contrast variation study

P02.15.48*(C214)* | D. B. Langley: The KipI-KipA complex and histidine kinase regulation in *Bacillus subtilis*

P02.16.49*(C215)* | L. D. Tran: Synthesis, microstructure and catalytic property of nanocrystalline $La_{1-x}Ce_xMnO_3$

P02.16.50*(C215)* | Y. Kim: Site preference of Mn in Zn_2SiO_4 phosphor by combined Rietveld refinement

P02.16.51*(C215)* | J. Hernandez-Velasco: *Ab initio* structural characterization of $Bi_{10}Mo_3O_{24}$ by TEM, X-ray and neutron powder diffraction

P02.16.52*(C216)* | S. N. Ivashevskaya: Structure solution from powder data using a combination of real-space method and Rietveld refinement

P02.16.53*(C216)* | A. Kanturk: Crystal structure refinement of waste magnesium by Rietveld analysis of X-ray diffraction data

P02.16.54*(C216)* | B. J. Campbell: Structural phase transitions: Refining distortion-mode amplitudes instead of atomic coordinates

P02.16.55*(C217)* | K. H. Stone: Structure solution of $Ag(pyz)_2S_2O_8$ in the presence of impurity phases using robust refinement

P02.17.56*(C217)* | H. Klein: Solving oxide structures by precession electron diffraction

P02.17.57*(C217)* | Z. Fu: Applying parallel computing for a faster and better structure solution

P02.07.58*(C217)* | K. Tokuda: Structure properties of AlCrN, GaCrN, and InCrN

P02.02.59*(C218)* | D. A. Langs: Efforts to improve the phase convergence of the shake-and-bake (SnB) algorithm towards solutions

03. Computers in Analysis, Molecular Modelling and Molecular Design

P03.01.01*(C218)* | P. S. White: NRCVAX revisited: Reusing existing software

P03.01.02*(C218)* | R. J. Gildea: Workflow and metadata in OLEX2

P03.01.03*(C219)* | O. V. Dolomanov: OLEX2: A portable molecular graphics toolset for crystallography

P03.01.04*(C219)* | F. Belaj: NORM - a program for performing normal probability plots and half-normal probability plots

P03.01.06*(C219)* | J. P. Bardhan: Computational challenges in wide-angle X-ray solution scattering (WAXS)

P03.01.07*(C220)* | J. Ilavsky: "Irena" software package for analysis and modeling of small-angle scattering data

P03.01.08*(C220)* | H. Doerksen: ARP/wARP: From noisy electron densities of proteins to complete structures

P03.08.09*(C220)* | P. Heuser: Density modification by directed evolution of electron density maps

P03.01.10*(C220)* | T. Lutteke: Validation and correction of carbohydrate 3D structures

P03.02.11*(C221)* | A. M. Reilly: A molecular dynamics approach to equilibrium structures in crystals

P03.02.12*(C221)* | A. Thorn: Restrained anisotropic refinement with SHELXL

P03.04.13*(C221)* | S. Obata: Computational chemistry approach to polymorphism of aspirin

P03.04.14*(C222)* | A. Oda: Effects of initial conformations of small ligands on computational docking accuracies

P03.04.15*(C222)* | D. K. Inaoka: *Trypanosoma cruzi* DHOD structure-based design of 5-halogen and 5-alkyl orotate derivatives

P03.05.16*(C222)* | K. Mukose: First principles study of composition fluctuation and residual strain in InGaN/GaN MQW

P03.05.17*(C223)* | S. Leoni: Simulation of the para to ferroelectric phase transition in $BaTiO_3$: The role of domains

P03.06.18*(C223)* | H. Nagara: Exploration of structures of phosphorus and calcium at high pressure using metadynamics simulation

P03.06.19*(C223)* | M. Inukai: Cluster models for decagonal quasicrystals

P03.06.20*(C224)* | L. Boukli-hacene: Ni(II) thiosemicarbazone complexes : Structural and theoretical investigation

P03.06.21*(C224)* | A. K. Wolf: Prediction and experimental determination of the crystal structure of $SiBr_4$

P03.06.22*(C224)* | M. J. Gutmann: Computation of diffuse magnetic neutron diffraction single crystal patterns

P03.06.23*(C225)* | M. Pasciak: Multi-resolution atomistic simulations and diffuse scattering in $BaTiO_3$

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

P03.06.25*(C225)* | E. V. Leonenko: Computer modelling 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)* | J. C. Facelli: Crystal structure prediction of flexible molecules with genetic algorithms and standard force field

P03.11.28*(C226)* | Y. Yakimov: Hybrid genetic algorithm for a full-profile analysis of XRD powder patterns

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

P03.10.30*(C227)* | Y. Tsuchiya: 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* glycolipid transfer protein

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

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

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

P03.12.35*(C228)* | T. Oroguchi: Dynamics of EcoO109I studied by small-angle X-ray scattering and molecular dynamics simulation

P03.12.36*(C229)* | N. Rademacher: Simulation on morphology controlling additives on Pigment Yellow 181, $C_{25}H_{21}N_7O_5$

P03.12.37*(C229)* | J. Shen: A theoretical study of changes in the morphology of the diarylethene crystals

P03.09.39*(C229)* | S. Morishita: Image reconstruction by a combination of diffractive imaging and selected area nano diffraction

P03.10.40*(C229)* | W. L. Duax: Universal tree of species evolution

P03.10.41*(C230)* | F. Xue: Structure of dengue virus - Implications for flaviviral assembly and opportunities for drug design

04. Crystallography of Biological Macromolecules

P04.05.213*(C297)* | A. Kiliszek: The effect of U-U mismatches on the RNA structure

P04.05.214*(C297)* | J. Kondo: Crystal structures of the bacterial, mitochondrial and cytoplasmic A-site molecular switches

P04.05.215*(C298)* | T. Chatake: Crystal structure of Z-DNA d(CGCGCG) complexed with Ca^{2+} ion , and Mg^{2+} ion

P04.05.216*(C298)* | T. Haraguchi: X-Ray analyses of DNA duplexes stabilized by bicyclic-C residues

P04.05.217*(C298)* | T. Prange: X-ray structure of A and B-DNA under high hydrostatic pressure (up to 2 GPa)

P04.05.218*(C299)* | L. Van Meervelt: 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. Lamber: Activity regulation of the transcription factor Ets-1 by DNA-mediated homo-dimerization

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. Iyaguchi: Structural studies on the promoter recognition of transcription factor HNF-6

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

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

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

P04.06.230*(C302)* | S. Sakurai: Crystallization and structure of human flap endonuclease 1, FEN1, in complex with a DNA product

P04.06.231*(C303)* | H. Itou: Structural studies of the multidrug-responsible transcriptional repressor protein CgmR

P04.06.232*(C303)* | M. Tanabe: The C-terminal extension in archaeal and eukaryotic DNA ligases modulates the DNA binding activity

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

P04.06.234*(C304)* | D. Huang: Comparison of crystal structures of NF-kB p50/RelB/DNA and p52/RelB/DNA complexes

P04.06.235*(C304)* | A. Nakamura: Structural basis for regulation of bifunctional roles of the F-plasmid replication initiator RepE

P04.06.236*(C304)* | C. Nei-Li: Structural study of the C-terminal domain of DNA gyrase

P04.06.237*(C305)* | K. Arita: Structural basis for hemi-methylated CpG DNA recognition by mouse Np95 SRA domain

P04.06.238*(C305)* | K. Miyazono: Novel DNA-binding fold and DNA-recognition mode discovered in restriction enzyme PabI

P04.06.239*(C305)* | K. Yokoya: X-ray crystal structure analysis of transcriptional regulator MobR

P04.06.240*(C306)* | A. C. W. Pike: Structure of human RECQ1 helicase: Identification of a putative DNA strand separation pin

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

P04.06.241*(C306)* | C. Meramveliotaki: A new nicking enzyme is developed from a mutant of the modified type II restriction enzyme scPvuII

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

P04.06.243*(C307)* | I. Laponogov: Structure of the topoisomerase IV from *S. pneumoniae* with a DNA target and quinolone drug

P04.07.244*(C307)* | S. Shimizu: RNA splicing related proteins; Crystal structure of RNA 3'-terminal phosphate cyclase

P04.07.245*(C307)* | W. Bae: Crystal structure of human DGCR8 core

P04.07.246*(C308)* | M. J. Van Raaij: Crystal structure of the avian reovirus inner capsid protein sigmaA

P04.06.247*(C308)* | H. Nishida: Structural basis for recruitment of replicative DNA polymerase to PCNA

P04.07.248*(C308)* | S. Chimnaronk: Mechanistic insight into isopentenylation of the anticodon of tRNA via a channel

P04.07.249*(C309)* | H. Matsumura: Crystal structure of RNA aptamer in complex with human immunoglobulin G

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 spliceosomal UsnRNPs

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

P04.07.253*(C310)* | Y. Kusakabe: 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 GatCAB reveals the C-tail domain structure in GatB

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

P04.08.256*(C311)* | H. Yoshida: X-ray structure of a cysteine-less mutant galectin-1

P04.08.257*(C311)* | S. Pletnev: Far-red fluorescent protein mKate reveals pH-induced *cis-trans* isomerization of the chromophore

P04.09.258*(C311)* | A. Takenaka: Two threonyl-tRNA synthetases with complementary functions; Crystal structure of ThrRS-1

P04.09.259*(C312)* | I. Tanaka: The structure of archaeal ribosomal stalk complex

P04.10.260*(C312)* | Y. Watier: Successful cryocooling of protein microcrystalline samples for powder diffraction

P04.10.261*(C312)* | N. Watanabe: New development of frozen buffer-free crystal mounting method for the longer wavelength SAD phasing

P04.10.262*(C313)* | T. Kitatani: Application of a novel mounting tool using adhesive for protein crystals

P04.10.263*(C313)* | M. A. Warkentin: Structural transitions and the evolution of protein crystal disorder during slow cooling

P04.10.264*(C313)* | R. E. Thorne: The temperature dependence of radiation damage to macromolecular crystals

P04.10.265*(C313)* | T. Hikima: Manipulating protein microcrystal with optical tweezers based on lensed fiber probes

P04.10.266*(C314)* | A. F. Meents: A new understanding of radiation damage at cryogenic temperatures

P04.14.315*(C329)* | A. Cabo Bilbao: New rearrangement in GroEL due to a 22 rotation between the heptameric rings

P04.14.316*(C329)* | M. P. Christie: Characterization of the Munc18-Syntaxin protein interaction

P04.14.317*(C330)* | S. Tanaka: Atomic-level models of the bacterial carboxysome shell

P04.14.318*(C330)* | K. Kawakami: Coordination structure of two Cl^--binding sites in oxygen-evolving photosystem II

P04.14.319*(C330)* | L. David: Crystallization and structure determination of the phycobilisome complex

P04.14.320*(C331)* | H. S. Lim: Crystal structure of the human GINS complex

P04.14.321*(C331)* | N. Pinotsis: Myomesin forms a 370 Å long two-chained, antiparallel filament across the muscle M-band region

P04.14.322*(C331)* | T. Kawaguchi: Electrostatic interaction explains D-staggered structure of collagen

P04.14.323*(C332)* | M. Vassylyeva: From Structure to function: Structure of the Gre-factor reveals its binding site on RNA polymerase

P04.14.324*(C332)* | M. Watanabe: Nature of the TRAP:Anti-TRAP complex revealed by symmetry remodeling

P04.14.325*(C332)* | K. Ihara: Vps9 assisted guanine nucleotide exchange intermediates of Rab5

P04.14.326*(C332)* | S. Fukai: Crystal structure of yeast Sec2p, the guanine nucleotide exchange factor for Sec4p

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P04.14.327*(C333)* | J. Cherfils: Structure and inhibition of Arf GTPases

P04.14.328*(C333)* | L. M. G. Chavas: Atomic model of Rab27a:Exophilin4/Slp2-a complex: Structural studies on vesicular transport

P04.14.329*(C333)* | S. Yum: Crystal structure of *E.coli* MacA reveals the assembly of the tripartite bacterial efflux pump

P04.14.330*(C334)* | Q. Xu: Structural basis of regulatory inactivation of DnaA

P04.14.331*(C334)* | N. Adir: Crystallographic analysis of the Phycobilisome antenna complex: Assembly and disassembly of a giant

P04.14.332*(C334)* | V. Campanacci: A topological model of the baseplate of lactococcal phage Tuc2009

P04.14.333*(C335)* | E. M. Juan: Structural studies on the active and inactive positive elongation factor b complexes

P04.14.334*(C335)* | D. S. Waugh: Structure of the Yersinia needle protein YscF in complex with its heterodimeric chaperone YscE/YscG

P04.14.335*(C335)* | S. Kim: The structural analysis of Rpn14 as the molecular-chaperone for eukaryotic 26S proteasome assembly

P04.14.336*(C336)* | M. W. Baumstark: 3D structure of small dense LDL; Application of low-resolution diffraction and *ab initio* methods

P04.14.338*(C336)* | A. Yamagata: The hexameric structures of the archeal secretion ATPase revealed by X-ray crystallography and SAXS

P04.14.339*(C336)* | K. Takagi: Crystal structure of a chaperone complex that contributes to the assembly of yeast 20S proteasomes

P04.14.340*(C337)* | J. M. De Pereda: Structural basis of the interaction between integrin β4 and plectin at the hemidesmosomes

P04.14.341*(C337)* | H. Matsunami: X-ray structural studies of Salmonella FlgA, a periplasmic chaperone for flagellar P-ring assembly

P04.14.342*(C337)* | T. Tamada: Structure determination of human cytokines and extracellular domains of receptors

P04.14.343*(C338)* | M. Yao: A novel octamer structure of bacterial cellulose synthesis component AxCesD

P04.14.344*(C338)* | S. Ozbey: Structure of Narcissus pseudonarcissus lectin complex with mannobiose at 1.7 Å resolution, FORM II

P04.14.345*(C338)* | A. Kita: Crystal structure of a lectin from the octocoral

P04.14.346*(C338)* | T. Itagaki: X-ray crystallographic analysis of galectin LEC-8 from *Caenorhabditis elegans*

P04.14.347*(C339)* | H. Kida: Structural and molecular characterization of the prefoldin beta subunit from *Thermococcus* strain

P04.14.348*(C339)* | S. Kanamaru: Domain interaction analyses of gp7, gp10 and gp11 of bacteriophage T4 for crystallization

P04.14.349*(C340)* | V. Samygina: X-ray crystallographic studies of the human ceruloplasmin-myeloperoxidase complex at low resolution

P04.14.350*(C340)* | E. Yamashita: IPR beamline for macromolecular assemblies at SPring-8

P04.14.351*(C340)* | K. Nagata: X-ray crystallographic and ultracentrifugal analyses of haloarchaeal nucleoside-diphosphate kinases

P04.14.352*(C341)* | K. Kato: Structure of vault purified from rat liver

P04.14.353*(C341)* | K. Miura: Macromolecular X-ray powder diffraction from the *in vivo* arm photophore of firefly squid

P04.15.354*(C341)* | M. D. Balcewich: Designing selective inhibitors to target NagZ a family 3 glycoside hydrolase

P04.15.355*(C342)* | U. Dhagat: The crystal structure of AKR1C1 in complex with an active-site inhibitor

P04.15.356*(C342)* | V. Fairweather: Eimeria tenella lactate dehydrogenase as a target for anti-parasitics

P04.15.357*(C342)* | R. Suryanarayanarao: Crystal structure and structure based drug design of HU (histone like protein) from *M.tuberculosis*

P04.15.358*(C342)* | X. Ji: Structure-based design of anticancer prodrug PABA/NO

P04.15.359*(C343)* | S. Kakuda: Structure of the LBD of rat VDR in complex with a non-seco-steroidal vitamin D3 analogue YR301

P04.15.360*(C343)* | L. J. Parker: Structural studies of glutathione S-transferase complexed to commonly used chemotherapy agents

P04.15.361*(C343)* | B. Hong: Crystal structure of human choline kinase in complex with hemicholinium

P04.15.362*(C344)* | J. L. Martin: Fragment screening and structure-based design of adrenaline synthesis inhibitors

P04.15.363*(C344)* | H. Kikuchi: Design of anti-allergic inhibitors for human hematopoietic prostaglandin D synthase

P04.15.364*(C344)* | A. Heine: Structure-based drug design in HIV protease- and tRNA-guanine transglycosylase inhibitor development

P04.15.365*(C345)* | P. Kaur: Crystal structure of complexes of peptidoglycan recognition protein with carbohydrates

P04.15.366*(C345)* | Y. Sekiguchi: Crystal structure of human CK2 alpha in complex with ellagic acid

P04.15.367*(C345)* | T. Matsuzaki: Rapid and precise protein 3D-model preparation for SBDD

P04.15.368*(C346)* | F. Kawai: Expression, purification and crystallization of LMW-PBP 4 and 5 from *Haemophilus influenzae*

P04.15.369*(C346)* | M. Wilmanns: The proteome of M. tuberculosis in 3D: Towards structure based drug discovery

P04.15.370*(C346)* | L. K. Williams: Inhibition of human pancreatic alpha-amylase by montbretin A: A new drug for diabetes and obesity?

P04.15.371*(C347)* | T. Nakaniwa: Structure of the catalytic subunit of human protein kinase CK2alpha prime with a potent inhibitor

P04.15.372*(C347)* | T. P. J. Garrett: Therepeutic antibodies target a locally misfolded region of tumour-specific EGFR

P04.15.373*(C347)* | A. L. Winther: Crystal structures of SERCA in complex with inhibitors with potential as prostate cancer drugs

P04.15.374*(C348)* | L. Lebioda: Human thymidylate synthase: Conformational stabilization and dimer asymmetry

P04.15.375*(C348)* | D. M. Himmel: Structure for an HIV-1 reverse transcriptase RNase H inhibitor bound at the active site

P04.15.376*(C348)* | K. L. Krause: Alanine racemase as a template for drug design against tuberculosis

P04.15.377*(C349)* | S. Gražulis: Novel thiadiazole inhibitors of human carbonic anhydrases

P04.15.378*(C349)* | C. L. Davies: Molecular basis for inhibition and resistance of glutamate racemase to a family of D-glu analogues

P04.19.399*(C355)* | D. Albesa-Jove: Advances in the structural elucidation of *Clostridium difficile* toxin B using SAXS and MX techniques

P04.19.400*(C355)* | M. J. Huseby: Activities and structure of beta toxin

P04.19.401*(C355)* | K. Kitadokoro: Structure and function of C-terminal catalytic region of *Pasteurella multocida* toxin

P04.19.402*(C356)* | H. Tsuge: Structural basis of actin recognition and ADP-ribosylation by *Clostridium perfringens* iota-toxin

P04.19.403*(C356)* | I. Brito: Okadaic acid,a conformational study in the solid state

P04.19.404*(C356)* | F. Sica: X-ray diffraction studies of two dimeric variants of human pancreatic ribonuclease

P04.19.405*(C357)* | H. M. Baker: Two staphylococcal sialic acid binding proteins from the superantigen superfamily

P04.19.406*(C357)* | W. Weber: Crystal structure of the extracellular protease of the nosocomial pathogen stenotrophomonas maltoph

P04.19.407*(C357)* | T. Yokoyama: Crystal structure of a sigma28-regulated non-flagella virulence protein *from campylobacter jejuni*

P04.21.409*(C358)* | H. Ihee: Time-resolved X-ray crystallography captures transition-state-like intermediate in PYP photocycle

P04.21.410*(C358)* | A. Tomita: Slow ligand migration dynamics in carbonmonoxy myoglobin at cryogenic temperature

P04.23.432*(C365)* | M. 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 staphylcoccus aureus

P04.23.434*(C365)* | J. Raczynska: New insight into catalytic mechanism of serine proteases from ultra-high resolution X-ray studies

P04.23.435*(C366)* | A. Moreno: Electrochemically assisted protein crystallization. Applications to protein crystallography

P04.23.436*(C366)* | B. Dittrich: Invariom refinement of 5 K 0.66 Å data of the ethanol solvate of gramicidin A

P04.23.437*(C366)* | Z. Dauter: Ultra-high resolution and very cold structure of lysozyme

P04.23.438*(C366)* | J. Hwang: Crystal structure of fully oxidized human thioredoxin1 containing disulfide between Cys62 and Cys69

P04.23.439*(C367)* | A. Mitschler: Joint neutron and X-ray diffraction studies at 293 K of antifreeze protein

P04.23.440*(C367)* | K. Takeda: X-ray induced perturbation in an ultra-high resolution protein structure

P04.23.441*(C367)* | H. Tanaka: High resolution crystals of human hematopoietic & lipocalin-type prostaglandin D synthases in space

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P04.23.443*(C368)* | B. Guillot: Charge density analysis of human aldose reductase active site

P04.23.444*(C368)* | T. Shimizu: Ultra-high resolution structure of endopolygalacturonase determined by X-ray and neutron diffraction

P04.23.445*(C369)* | A. Higashiura: The high-resolution X-ray crystallography of bovine H-protein of glycine cleavage system

P04.23.446*(C369)* | H. Kondo: Crystal structure of an antifreeze protein from snow mold fungi

P04.23.477*(C379)* | Q. Sun: Crystal structure of human cystathionine gamma lyase: A key enzyme in hydrogen sulfide production

05. Crystallography of Biological Small Molecules

P05.02.01*(C380)* | I. Fujii: Optical separation of rimantadine and *in silico* prediction of chiral selectivity of M2 protein

P05.03.02*(C380)* | J. J. Holstein: Validation of charge density refinements and application to molecules of biological interest

P05.03.03*(C380)* | F. P. A. Fabbiani: High-pressure crystallisation of antibiotic molecules

P05.03.04*(C381)* | M. Botoshansky: Behaviour of the azido group in crystal structure of the intermediates of aminoglycoside antibiotics

P05.04.05*(C381)* | V. K. Rajni: Crystallography of steroids: A comparative analysis of geometrical features and hydrogen bonding

P05.05.06*(C381)* | K. J. Haller: Crystal and molecular structure of the diethyl ester of rhodoporphyrin

P05.05.07*(C381)* | K. A. Slepokura: Potassium salts of some ribonucleotides: AMP, IMP, CMP and UMP

P05.05.08*(C382)* | J. Delgado: Sesquiterpene lactones isolated from a medicinal plant of the *Venezuelan* 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 nanopipe, a hollow-type water nanowire, in crystal host

P05.07.11*(C383)* | C. H. Schwalbe: H-bonds in andrographolide and related molecules: Neutron diffraction, database and modeling studies

06. Crystallography of Organic Compounds

P06.01.01*(C383)* | K. Ohshima: Crystal structure of trehalose dihydrate by X-ray and neutron diffraction experiments

P06.01.02*(C383)* | K. Kataoka: Temperature-dependent structural change of trehalose dihydrate and anhydrate crystals

P06.01.03*(C383)* | S. V. Phung: HTXRD and XRD-DSC study of crystalline-noncrystalline phase transition of sucrose crystals

P06.01.04*(C384)* | M. Estrada: Structure of sodium L-malate monohydrate

P06.01.05*(C384)* | M. Dianez: X-ray structure and hydrogen bonding study of taurine and N-(glucitol-1-yl)taurine

P06.03.06*(C384)* | K. L. Riechmann: Binary mixtures of a series of oxa-3,4-diazinan-2-ones

P06.03.07*(C385)* | I. Hisaki: Supramolecular tilt chirality in crystals of cholic acids

P06.04.08*(C385)* | M. Odabasoglu: Structure of dihydro-isoindolo benzoxazine-11-one and dibromo-cyclopenta[a] naphthalene-1-one

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

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

P06.04.11*(C386)* | V. B. Rybakov: X-Ray data for novel tricyclic compounds based on indolizines

P06.04.12*(C386)* | H. Shigemitsu: Crystalline molecular assemblies of dehydrobenzo[12]annulenes having carboxylic groups with amines

P06.04.13*(C386)* | R. K. Jadaprolu: Structures of benzo and dibenzo [d,f] [1,3,2] dioxaphosphepine 3-oxide (I, II) and 6-sulphide(III)

P06.04.14*(C387)* | A. Ozek: Crystal structure and quantum mechanical calculations of an oxime compound, $C_9H_{11}N_3O_2$

P06.06.15*(C387)* | K. Toyota: Crystal structure analysis of inclusion crystals with tetrapodal host molecules

P06.06.16*(C387)* | V. Thiruvenkatam: A detailed study of the helical conformation in 2-aminothiazole derivatives

P06.06.17*(C388)* | T. Sasaki: Guest-induced topological polymorphism of pseudo-cubic hydrogen bond networks

P06.06.18*(C388)* | T. Hirukawa: Supramolecular clusters composed of triphenylmethylamine and various sulfonic acids

P06.10.19*(C388)* | O. Buyukgungor: Crystal structure and *ab initio* calculations of three 4-methoxy salisylaldehyde derivatives

P06.06.20*(C388)* | N. Tohnai: Constructions of higher order architectures by connecting of 4+4 supramolecular clusters

P06.06.21*(C389)* | N. Shizuki: Supramolecular structures in co-crystals composed of steroidal acids and cinchona alkaloids

P06.06.22*(C389)* | A. Yamamoto: Functional porous crystals with supramolecular clusters of triphenylmethylammonium sulfonates

P06.06.23*(C389)* | J. Han: Designed supramolecular assembly of novel rosette layers

P06.06.24*(C390)* | R. Tamura: Control of polymorphic transition inducing preferential enrichment

P06.06.25*(C390)* | P. A. Bombicz: Supramolecular symmetries in the Piedfort units

P06.06.26*(C390)* | S. Iwama: Application of preferential enrichment to amino acids

P06.08.27*(C390)* | T. Murai: Intercalation with steroidal inclusion crystals: Enantioresolution and layer inversion

P06.07.28*(C391)* | M. Akazome: Enantioselective inclusion of methyl phenyl sulfoxides by (*S*)-alkylglycyl-(*S*)-phenylglycine

P06.02.29*(C391)* | H. Schenk: Structure and polymorphism of trans mono-unsaturated triacylglycerols

P06.10.31*(C391)* | J. Bruening: Polymorphism and structure solution from powder data of *N,N'*-1,4-phenylene-bis(3-oxobutanamide)

P06.10.32*(C392)* | A. Fitch: Crystal structures of two insect recognition pheremones

P06.09.33*(C392)* | R. Bishop: Five alternative crystal forms produced by crystallisation of a simple alicyclic dialcohol

P06.07.34*(C392)* | G. Ramon: ^{1}H NMR application to inclusion chemistry: Selectivity profiles of a xanthenol-related host

P06.09.35*(C393)* | A. Tamugi: Guest-dependent luminescence modulation in inclusion crystals of anthracene derivatives

P06.07.36*(C393)* | S. Yang: Synthesis, structure and solid-state photochemistry of *m*-benzenediacrylic acid and its complexes

P06.07.37*(C393)* | H. Uekusa: Vapor induced reversible guest exchange of organic inclusion crystal

P06.07.38*(C393)* | U. Rychlewska: Inclusion properties of trianglamines

P06.07.39*(C394)* | P. H. Van Rooyen: Molecular complexes of 4,4'-dinitrobiphenyl

P06.07.40*(C394)* | A. Erdonmez: (*Z*)-Ethyl 4-chloro-2-[(4-chlorophenyl)-hydrazino]-3-oxobutanoate

P06.08.41*(C394)* | J. L. Pinto: Synthesis and structural characterization of 1,4-bis-(2-phenyl-4-oxo-1,3-thiazolidin-3-yl)butane

P06.09.42*(C395)* | S. Ng: Hexamethylenetetramine bis(*p*-nitrophenol) monohydrate clathrate

P06.09.43*(C395)* | A. Mamadrakhimov: Structure of the anhydrous form of gossypol - Dianhydrogossypol

P06.10.44*(C395)* | M. Kokila: A study on the effect of substitutions and intermolecular interactions in thiophene 3-carboxamides

P06.10.45*(C396)* | G. N. A. Kumar: Crystal and molecular structure of biologically active thiophene 3 -furfuryl carboxamide derivative

P06.10.47*(C396)* | K. C. Kumar: Crystal structure of 2-amino-4,5,6,7-tetrahydro-1-benzothiophene -3-carboxamide

P06.10.48*(C396)* | M. Dincer: An experimental and theoretical approach to the 2-chloro-1-(3-methyl-3-phenylcyclobutyl) ethanone

P06.10.49*(C397)* | J. M. Wojciechowski: Experimental *versus* theoretical electron density in the crystals of β -aminophosphonic acids

P06.10.50*(C397)* | I. Svoboda: Lessons from a decade of X-ray crystallographic work on *N*-(hydroxy)thiazole-2(3*H*)-thione derivatives

P06.10.51*(C397)* | H. Saitoh: Hydrogen-bonded network structures of cocrystals of some naphthalenediol with pyrazine

P06.10.52*(C398)* | M. M. Jotani: Crystal structure of (4*Z*)-2-phenyl-4-(3,4,5-trimethoxybenzylidene)-1,3-oxazol-5(4*H*)-one

P06.10.53*(C398)* | M. A. Sharif: Two proton transfer compounds from benzene-1,2,4,5-tetracarboxylic acid and 1,10-phenanthroline

P06.10.54*(C398)* | N. Hayashi: X-ray structures of quinone dimers linked either directly or through acetylene spacers

P06.10.55*(C398)* | K. Ninomiya: Homogeneous and heterogeneous mixed crystals composed of phenoxyl radical and phenol

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07. Crystallography of Organometallic, Co-ordination and Main Group Compounds

P07.01.01*(C399)* | S. K. Brayshaw: Metal complexes of di(thiophenyl)ethenes: Synthesis, structure and bonding

P07.01.02*(C399)* | L. Russo: Recent results from a long-term academic collaboration

P07.01.03*(C399)* | R. Haruki: Structural study of an iron oxalate and a copper rubeanate layer on an ultra-smooth sapphire *c*-face

P07.01.04*(C400)* | S. Liu: Crystal structures of two homotetranuclear oxovanadium complexes

P07.01.05*(C400)* | A. Martin: Cleavage of Ti_3E_3 (E= O, N) rings by aluminum derivatives

P07.01.06*(C400)* | K. Tomono: Formation of alkylated di-cation by weak hydrogen bonds in the crystal of $Ni(dmit)_2$ salts

P07.01.07*(C401)* | E. Tomiyama: Honeycomb-like structures in the crystals of $Ni(dmit)_2$ salts with di- and tri-alkylthiazole cations

P07.01.08*(C401)* | H. Görls: Structural investigations of the nickel mediated coupling products of CO_2 and isoprene

P07.01.09*(C401)* | M. Tabatabaee: Hydrothermal synthesis and crystal structure of a new copper coordination polymer

P07.01.10*(C402)* | B. Kukovec: Copper(II) complexes with derivatives of picolinic acid. Synthesis, structural and magnetic study

P07.01.11*(C402)* | L. Roces: Structural and oxidation state study of two novel mixed-valence binuclear copper complexes

P07.01.12*(C402)* | M. Đaković: The isonicotinamide complexes of copper(II) with N_3^-, SCN^- and SO_4^{2-} as bridging ligands

P07.01.13*(C403)* | G. Pelosi: Bis(tpp)copper(I) thiosemicarbazonates: Unexpected chemistry revealed by X-ray diffraction

P07.01.14*(C403)* | H. Miyamae: Porous structure of bis{tris(bipyridine)ruthenium(II)} tris(oxalato)cobaltate(III) chloride

P07.01.15*(C403)* | L. Vendier: Structural study of hydride and dihydrogen ligands ruthenium complexes: Reversible hydrogen release

P07.01.16*(C403)* | T. Yamagata: Synthesis, structure, and reactivity of ruthenium-zinc trinuclear hydrides with phosphine ligands

P07.01.17*(C404)* | N. Yoshikawa: Syntheses,characterization and DFT investigations of iridium complexes and diprotonated terpyridines

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: Structural challenges of giant bismuth oxo-diketonate clusters

P07.01.23*(C406)* | T. Kojima: Solvent driven association and dissociation of the hydrogen-bonded protonated decavanadate dimer

P07.01.24*(C406)* | C. Mealli: Is 2.07 Å the record for the shortest Pt-S distance? Two questionable experimental structures

P07.02.25*(C406)* | A. Roodt: Solid state packing behaviour in pseudo Vaska-type complexes

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

P07.04.27*(C407)* | Y. Yakiyama: Triple-stranded helical metal complex of quaterimidazole and its highly-symmetrical network

P07.04.28*(C407)* | T. Akutagawa: Design of crystalline space for constructing ferroelectric rotators in $[Ni(dmit)_2]$- salts

P07.04.29*(C407)* | L. J. McCormick: The diabolecules: Some unexpected copper clusters

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

P07.04.31*(C408)* | S. Saithong: The 1-D polymeric dimorphism of copper(I) thiocyanate complexes containing MTA ligand

P07.04.32*(C408)* | I. Brito: Novel coordination polymers generated from 2,2-dipyridyldisulfide and $CuCl_2$

P07.04.33*(C409)* | S. Krachodnok: Concerted aryl interactions in zinc-imidazole − Oxovanadate hybrid organic-inorganic materials

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

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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 $[M(SCN)_2]$ fragment with BPHD(2,5-bis(4-pyridyl)-3,4-diaza-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 amide groups at 5,5'-positions

P07.04.41*(C411)* | C. Kabuto: Supramolecular assemblies of lanthanide clusters with chiral ligands in the crystalline state

P07.04.42*(C411)* | N. Matsumoto: A problem in the crystal structure of a two-step spin crossover complex

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

P07.05.45*(C412)* | S. Lee: Structures of tris{[(hydroxymethyl)aminomethane]5-bromosalicylideneaminato}diorganotin complexes

P07.05.46*(C412)* | Y. Uchiyama: Structural studies of 9,10-diheteratriptycenes with group 15 elements and their halogen adducts

P07.05.47*(C412)* | V. N. Khrustalev: New stable lead(II) complexes with intramolecular coordination: Experimental and theoretical study

P07.07.48*(C413)* | J. Schneider: Annealing cattle tibiae: From nano-bio-apatite to geo-apatite

P07.07.49*(C413)* | H. P. Yennawar: Crystal structures of modified PNA analogues and of cationic diimine Pd(II)-alkyl complex

P07.07.50*(C413)* | Z. Travnicek: Coordination abilities of selected cytokinins and CDK inhibitors to transition metal ions

P07.07.51*(C414)* | M. M. Dhifet: 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)* | I. Zviedre: Synthesis and crystal structure 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*(C415)* | B. Zhang: Construction molecular magnet with porosity, chirality from $[Fe(C_2O_4)Cl_2^-]_n$ with cation templet

P07.10.57*(C416)* | 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*(C416)* | S. Ang: Studies on some manganese-containing single-molecule magnets

P07.10.60*(C416)* | L. Bogani: 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. Arslan: Hemidirected novel lead(II) azide complex of 2,6-diacetylpyridine dihydrazone

P07.11.63*(C417)* | H. Phetmung: Novel route to synthesis copper halide with Cu_2S_2 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)* | E. Silina: Crystal structure of platinum 2-methyl- and palladium 2,4-dimethyl-8-hydroselenoquinolinate

P07.03.66*(C418)* | M. A. Petrukhina: Indenocorannulene: Molecular geometry, solid state packing, and metal binding

09. Crystal Engineering

P09.01.01*(C474)* | A. Bacchi: Knowledge-based design of host-guest interactions in wheel-and-axle inorganic diols

P09.01.02*(C474)* | M. Park: A designed metal-organic framework based on a metal-organic polyhedron

P09.01.03*(C474)* | S. A. Kumalah: Properties of metal-organometallic frameworks derived from facially η^6 metalated terephtalates

P09.01.04*(C475)* | G. Diaz de Delgado: *Cis-trans* isomerizations and rearrangements during hydrothermal synthesis of metal carboxylates

P09.01.05*(C475)* | M. Lusi: Real crystal engineering: Solid state reactions in metal-organic compounds

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P09.02.08*(C476)* | M. Du: Cocrystallization of a pharmaceutical agent pamoic acid with piperazine or 4,4' -bipyridyl

P09.02.09*(C476)* | S. Aitipamula: Polymorphism of co-crystals: Co-crystal polymorphs of an analgesic drug, ethenzamide

P09.01.10*(C477)* | M. Duarte: New crystal forms of gabapentin

P09.02.11*(C477)* | A. Tojiboev: Molecular cocrystals of peganole with peganine

P09.02.12*(C477)* | R. Montis: Subtle relationships between the structures of some aspirin derivatives

P09.02.13*(C477)* | E. K. Owusu-Marfo: The influence of hydrogen bonding on generation and stabilization of self-assembled layer structure

P09.02.14*(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)* | H. Masu: Characteristic network structure constructed from various block-like molecules

P09.02.17*(C479)* | J. Kim: Self assembled hierarchical nanostructures: 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

P09.02.19*(C479)* | S. Karki: Control of stoichiometry and structure: Mechanism of cocrystal 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. Masuhara: Cyclic transformation in novel shape and phase of C_{60} nano/microcrystals

P09.03.22*(C480)* | S. Sheshmani: Polymeric complex obtained from a novel supramolecular proton transfer compound

P09.03.23*(C481)* | M. Sari: Crystal phase analysis of by-products from $NaBH_4$ 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-Mijangos: A comparative study of two multiphasic alkali halide crystals: Quinary vs.exenary

P09.03.26*(C481)* | M. Debbabi: From dimeric tantalopentatungstate to monomeric organosilyl Lindqvist type polyoxometalates

P09.03.27*(C482)* | W. Lasocha: Octamolybdates - promising materials for industry and medicine

P09.03.28*(C482)* | 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 molecualr magnet: $K_2Fe_2(C_2O_4)Cl_6(H_2O)_2$ and $K_6Fe_6(C_2O_4)_3Cl_{14}(H_2O)_{10}$

P09.03.31*(C483)* | W. 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*(C484)* | K. E. Knope: Synthesis and characterization of mixed metal (UO_2^{2+}/TM^{2+}) inorganic/organic framework materials

P09.03.34*(C484)* | H. Aghabozorg: A nine-coordinated Zr^{IV} complex obtained from a novel supramolecular proton transfer compound

P09.03.35*(C484)* | J. Attar Gharamaleki: Binuclear Sn(VI) complex obtained from benzene-1,3-diaminium bis(hydrogen pyridine-2,6-carboxylate)

P09.03.36*(C485)* | J. Jokiniemi: A structural study of metal complexes of bisphosphonate partial ester derivatives

P09.03.37*(C485)* | V. Petrykin: High pressure synthesis and analysis of new yellow emission Sr_2ZnS_3: Eu visible-light driven phosphor

P09.04.38*(C485)* | M. A. Fernandes: Designing Zn and Co based 1-D coordination polymers with possible magnetic and electronic properties

P09.04.39*(C486)* | L. Dobrzańska: A single-crystal-to-single-crystal apical ligand exchange process in a 2D coordination network

P09.05.40*(C486)* | M. R. J. Elsegood: Boronic acids as hydrogen-bond bridges between metal coordinated carboxylates

P09.05.41*(C486)* | M. Rademeyer: Noncovalent interactions in a family of cyclic ammonium nitrates

P09.05.42*(C487)* | U. Baisch: X-ray diffraction and microscopy study of supramolecular networks of amido functionalized compounds

P09.05.44*(C487)* | N. Kunishima: Systematic mutation study toward the engineering of protein crystals

P09.05.45*(C487)* | M. Gryl: Crystal engineering of materials with potential NLO properties using barbituric acid as component

P09.05.46*(C487)* | P. A. Wood: Energy versus 3D geometry - A study of intermolecular interactions using theory and experiment

P09.07.47*(C488)* | C. R. Martin: Controlling the formation of co-crystal polymorphs

P09.07.48*(C488)* | A. Parkin: Comparing entire crystal structures: Structural genetic fingerprinting

P09.06.49*(C488)* | M. Y. Antipin: Mixed crystal of bidentate and tridentate perfluoro-phenylmercury Lewis acids with organic molecules

P09.07.50*(C489)* | H. Matsuo: Crucible rotation dependence of oxygen concentration during solidification of multicrystalline Si

P09.04.51*(C489)* | G. Resnati: Supramolecular anion coordination networks with (6.3) cation-templated topologies

P09.02.52*(C489)* | G. Sadiq: Co-crystallisation and crystal engineering

P09.05.53*(C490)* | E. Zaini: Cocrystal formation between trimethoprim and sulfamethoxazole by sealed-heating method

16. Crystal Growth: Techniques, Instrumentation and Applications

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 crystallization and structure determination

P16.02.03*(C580)* | A. Dong: *In situ* proteolysis for protein crystallization and structure determination

P16.03.04*(C581)* | H. Takusagawa: Analysis of crystal growth of trigonal ribonuclease A from bovine pancreas

P16.03.05*(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

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 morphology and surface microtopograph of cubic insulin

P16.15.10*(C583)* | L. C. Johansson: Development of a lipidic-sponge phase screen for membrane protein crystallization

P16.15.11*(C583)* | K. Tomoyori: Crystal growth of multicopper oxidase CueO Δ α 5-7 mutant

P16.03.12*(C583)* | F. Kaneko: Influence of polytypism on polymorphism in n-alkanes: Cryatallization and thermodynamic stability

P16.03.13*(C584)* | O. Dogan: Effect of biopolymers on hydroxyapatite growth kinetics

P16.03.14*(C584)* | K. Hasegawa: Crystal morphology and surface microtopograph of disodium inosine 5' -monophosphate octahydrate

P16.03.15*(C584)* | K. Inaka: Optimization of a salt concentration in a PEG-based crystallization solution by a Gel-Tube method

P16.04.16*(C585)* | S. Mahapatra: A novel approach to specifically crystallize anhydrous compounds: Crystal structure of adenine

P16.13.17*(C585)* | M. Kitamura: Polymorphism and crystal structure of BPT propyl ester in various solvents

P16.13.18*(C585)* | S. Kobatake: Photoinduced phase transition between polymorphic crystals of a photochromic diarylethene

P16.14.19*(C585)* | A. Hoshikawa: *In situ* observation of CH_4 hydrate growth by neutron powder diffraction

P16.15.20*(C586)* | K. R. Etzel: Abiotic growth and biological dissolution of pyrite surfaces

P16.03.21*(C586)* | G. Juarez: Synthesis and structural characterization of ZnO deposited by chemical bath

P16.03.22*(C586)* | J. Martinez: Influence of bath composition in structure of ZnO deposited by microwave activated chemical bath

P16.03.23*(C587)* | K. Byrappa: Hydrothermal synthesis of doped ZnO and its application in photodegradation of toxic amaranth dye

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

P16.08.24*(C587)* | E. H. Otal: Structural characterization of nanostructures hierarchical rare earth doped ZnO colloids

P16.01.25*(C587)* | V. I. Voronkova: Crystal growth peculiarities of new oxide conductor $La_2Mo_2O_9$ in the system La_2O_3 - MoO_3

P16.03.26*(C588)* | S. Hosokawa: Glycothermal growth of yttrium aluminium garnet nanocrystals

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

P16.04.29*(C588)* | A. A. Babaryk: Langbeinite-type phosphates $K_2Ln_{1.5-x}Nb_{0.5+x}(PO_4)_3$ (*Ln* = Sc, Y, In, Ho-Lu): Synthesis and structure

P16.04.30*(C589)* | A. Islam: Growth of large single crystals of high-Tc superconductor using a tilted-Lamp floating zone furnace

P16.04.31*(C589)* | M. A. Sarker: Solid-liquid interface in floating zone growth of rutile crystal with variation of focusing angle

P16.04.32*(C589)* | D. Kwon: Growth of Nd-doped YVO_4 single crystals by anisotropic heating floating zone method

P16.09.33*(C590)* | M. Maruyama: Chiral and achiral mechanisms of regulation of calcite crystallization

P16.10.34*(C590)* | H. Miura: Formation of barred olivine texture 4.6 billion years ago

P16.11.35*(C590)* | T. Adschiri: Property and morphology of organic modified CeO_2 nanocrystals synthesized in supercritical water

P16.12.36*(C591)* | K. Momma: The role of Japanese twin boundary in quartz as a source of Brazil twin

P16.04.38*(C591)* | N. A. Shah: Preparation and characterization of cadmium telluride thin films by vacuum evaporation

P16.04.39*(C591)* | S. Niefeng: Synthesis large-scale high purity InP crystal by P-injection method

P16.06.40*(C591)* | U. Pietsch: Initial state of VLS-growth of InAs nanorods on GaAs(111), probed by X-ray diffraction and TEM

P16.06.41*(C592)* | L. P. Cardoso: InGaP/GaAs(001) structural characterization by means of synchrotron radiation Renninger Scan

P16.06.42*(C592)* | M. Rojas: High resolution X-ray diffraction study of $Al_xGa_{1-x}Sb$ 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. Askhabov: 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

P16.03.52*(C595)* | M. Wu: Morphological control of meso- and single- crystals of Perovskite under solvothermal conditions

P16.03.53*(C595)* | D. M. Sampyady: Single crystal growth of nonlinear optical chalcone 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. Gerdts: The microcapillary protein crystallization system

29. Other Topics

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

Memo