

Poster Session I (Monday & Tuesday, 16.00 - 17.00)

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MS01-P01	A	Data Analysis Infrastructure for Serial Crystallography Experiments at the EuXFEL	Dall'Antonia F., et al.
MS01-P03	A	MicroMAX - New Possibilities for Serial Crystallography	Ursby T., et al.
MS01-P05	A	Serial Crystallography at the ESRF Extremely Brilliant Source: The ID29 Upgrade Project	de Sanctis D.
MS01-P07	A	Optimized Design for New Scientific Opportunities in Macro-Molecular Crystallography at the Future Microfocus XAIRA [...]	Juanhuix J., et al.
MS01-P09	A	P11 at PETRA III: A Versatile Beamline for Serial and High-Throughput Crystallography	Burkhardt A., et al.
MS02-P01	A	Structure-Based Drug Design to Tackle Disorders of Haem Biosynthesis	Arruda Bezerra G., et al.
MS02-P03	A	PanDDA: Extracting Ligand-Bound Protein States from Conventionally Uninterpretable Crystallographic Electron Density	Pearce N.
MS02-P05	A	New Fully Automatic Measurement MX Beamline BL45XU at SPring-8	Mizuno N., et al.
MS03-P01	A	Structural Basis of Inactivation of Human Counterpart of Mouse Motor Neuron Degeneration 2 Mutant in Serine Protease HtrA2	Wagh A.
MS03-P03	A	Molecular Investigation of Muscle Z-Disc Assembly Centered on the Complex Human A-actinin Isoform-2 and ZASP	Stefania V., et al.
MS03-P05	A	Invitation to Perform Experiments on High End Instruments: Centre of Molecular Structure in BIOCEV	Stránský J., et al.
MS03-P07	A	Structural and Biophysical Analysis of the Pyridoxal Phosphate Synthase from Plasmodium Vivax	Ullah N., et al.
MS03-P09	A	Crystal Structure of Human AMACR Provides Insight into Substrate Recognition and Catalytic Mechanism	Lin M.H., et al.
MS03-P11	A	A Reliable and Versatile Tool for High-End In-House Structural Studies	Smith V., et al.
MS03-P13	A	Profilins and the Quest for Structure-Based IgE-epitope Mapping	Gottstein N.A., et al.
MS03-P15	A	Novel Biochemical Bases for Nuclear Factor I X (NFI-X)	Lapi M.
MS03-P17	A	Crystal and Solution Structures of SH ₂ Domain of Signaling Molecule in Complex with the Co-stimulatory Receptor CD28	Inaba-Inoue S., et al.
MS03-P19	A	Structural Determinants of the Interaction Specificity at the G and NC Interfaces of Human Septins	Leonardo D., et al.
MS03-P21	A	The N-terminal Domain of Lactobacillus acidophilus SlpA promotes Self-Assembly of the S-Layer Array	Sagmeister T., et al.
MS03-P23	A	The Crystal Structure of the Major Olive Pollen Allergen Ole e 1	Hofer G., et al.
MS04-P01	A	CCP-EM: The Collaborative Computational Project for Electron Cryo-Microscopy	Winn M., et al.
MS04-P03	A	Efficient Real-Space Refinement for Cryo-EM and Crystallography	Urzhumtsev A., et al.
MS05-P01	A	The Critical Role of the Fourth Position of the VxGFL Motif of PP ₂ Cs from Oryza sativa in Regulation of ABA Responsiveness	Lee S., et al.
MS06-P01	A	Structural Insights in a Mitochondrial Nucleoid Maintenance Factor	Tarrés-Solé A.
MS06-P03	A	Structural Studies of Temperate Phage Genetic Switches	Varming A., et al.
MS06-P05	A	Molecular Basis of Self-Induced Genomic Degradation Inhibition by the Sub-Nanomolar Interaction of Nin with NucA and NucB [...]	Booth S., et al.
MS06-P07	A	Structural Study Two Different Forms of Smap From Halobacterium salinarum Which Have A Different [...]	Fando M., et al.
MS07-P01	A	Crystal Structure of the Cell Wall Binding Domain of a Novel Bacteriophage PBC5 Endolysin and its Peptidoglycan Interaction	Suh J.Y.
MS07-P03	A	Structural and Functional Characterization of Phosphoglucosyltransferase 5	Pühringer D.
MS07-P05	A	Studying the Structural Basis for Selectivity in Complexes of Peptide Inhibitors and Serine-Proteases of the Complement System	Dürvanger Z., et al.
MS07-P07	A	Beetle Luciferases and their Color Emission	Rabeh W.
MS07-P09	A	Active Site Evolution in Biomass Degrading Enzymes	Lo Leggio L., et al.
MS07-P11	A	Differences in Crystallization of Several Selected Haloalkane Dehalogenases and their Mutation Variants	Kuta Smatanova I., et al.
MS07-P13	A	Enzyme Activation by a Flavoprotein Redox Network	Hammerstad M., et al.

MS07-P15	A	Structural Insight in Peptidyl Substrate Binding to Cysteine Cathepsins	Loboda J., Tusar L.
MS07-P17	A	Porphyromonas Gingivalis Tpr Protease Zymogen Resembles Calpain-Calpastatin Complex	Staniec D.
MS07-P19	A	Neutron Protein Crystallography at the Heinz Maier-Leibnitz Zentrum (MLZ): New Developments and Recent Application	Schrader T.E., et al.
MS07-P21	A	Structure-Function Characterisation of Novel Galactosidases from Lactobacillus Plantarum: Exploring the Link Between Gut [...]	Feliciotti I., et al.
MS08-P01	A	Regulation of p97 ATPase Activity by Cofactor-Mediated Remodeling and Post-Translational Modification	Heinemann U., et al.
MS08-P03	A	TraF is an Essential Factor of the pIP501 Type IV Secretion System (T4SS) and Exhibits Structural Homology with the T7SS	Keller W., et al.
MS08-P05	A	Atomic Structure of Potato Virus X, the Prototype of the Alphaflexviridae Virus Family	Zanotti G., et al.
MS08-P07	A	Crystal Structures of Streptococcus Pyogenes Cas1 and Cas2 in the Type II-A CRISPR-Cas System	Ka D., et al.
MS08-P09	A	Structural Study for Recognition of Ubiquitylated Histone H3 by DNA Methyltransferase	Arita K., et al.
MS09-P01	A	Improving Density Histogram by Phase Optimisation Using a Genetic Algorithm	Kantamneni S.M., et al.
MS10-P01	A	A New 3D Reflection Data Viewer Based on NGL	Oeffner R., et al.
MS10-P03	A	Improving Identification and Validation of Water Molecules in Protein Crystal Structures with Molecular Dynamics Simulations	Caldararu O., et al.
MS10-P05	A	B-Factors Reflect the Local Dynamics of Proteins and Nucleic Acids	Schneider B., Cerný J.
MS11-P01	A	New ARP/wARP Web Service Integrated into Virtual Computation Frameworks	Sobolev E., et al.
MS11-P03	A	SIMBAD: Structure Based Search Model Identification for Molecular Replacement using the PDB Database	Simpkin A., et al.
MS11-P05	A	PReSTO Integrative Structure Biology Software for all Platforms	Unge J.
MS12-P01	A	Crystallization and Structure Determination of Aldo-keto Reductase 1C3 in Complex with Steroidal Inhibitors Using in situ Proteolysis	Petri E., Celic A.
MS12-P03	B	Symmetry in Structures of Protein Assemblies	Grudin S., Pages G.
MS12-P05	B	PDB Knowledge Base (PDB-KB) – Infrastructure for FAIR Structural and Functional Annotations	Velankar S.
MS12-P07	B	Structural Comparison and Evolutionary Relationships Between Ceruloplasmin, Hephaestin and Blood Coagulation Factor VIII	Zaitsev V., Lindley P.
MS13-P01	B	Brachiopod Shell Calcite Mineralization Occurs by Ion-by-Ion Transport Controlled by the Epithelial Cell Membranes	Schmahl W., et al.
MS13-P03	B	Structure and Microstructure Study of Charonia Lampas Lampas Shell	Salim O., et al.
MS13-P05	B	The Interaction Between Calcium Carbonate and Calcium Phosphate as the Driving Mechanism for [...]	Pastero L., et al.
MS14-P01	B	Reassessing Pauling's Rules	George J., et al.
MS14-P03	B	Electron Crystallography of Planetary Materials: Impactites and Micrometeorites	Gemmi M., et al.
MS14-P05	B	Synthesis and Crystal Structures of $Zr_2(OH)_2(XO_4)_3 \cdot 4H_2O$ (X=S,Se) and $Zr(SeO_3)_2$	Giestler G., et al.
MS14-P07	B	Steric Effect in Tetracoordinated Ni(II) Complexes with Enamino-Ketone Ligands and Their Reaction Products with Heterocyclic [...]	Zep A.
MS14-P09	B	Crystal Structure and Hirshfeld Surface Analyses of a new Organogold(III) with Thiosemicarbazone	Almeida C., et al.
MS14-P11	B	Synthesis of Calcium and Strontium Rare-Earth Aluminates and Its Use as Host Lattice for LEDs	Otgonbayar C., Poellmann H.
MS14-P13	B	Periodic Trend of Stereochemical Activity of Lone Electron Pairs	Murshed M.M., Gesing T.M.
MS14-P15	B	Crystal Structure and Thermodynamic Behavior of $Bi_6Te_2O_{15}$: the Likely Structure of the Rare Mineral Pingguite	Nenert G., et al.
MS14-P17	B	Preparation, Spectral, Structural, Hirshfeld Surface and Molecular Docking of Tetrakis(pyridine-'N)bis(thiocyanato-'N) [...]	El Hamdani H., et al.
MS14-P19	B	Synthesis, Spectroscopic Properties, Crystal Structure, Antimicrobial Properties and Molecular Docking Studies of [...]	El Hamdani H., et al.
MS14-P21	B	Inverse Crystal Structure Behaviour of $Ca_3Al_4ZnO_{10}$ at High Pressure and High Temperature	Hejny C., et al.
MS14-P23	B	Structural Ordering in the Pyrite-Related Phases: PtSnS, PtSnSe and PtSnTe	Laufek F., Vymazalová A.
MS14-P25	B	A New Polymorph of Trisodium Hexachlororhodate	Etter M.
MS14-P27	B	Doped Single Crystal TiO_2 Series Products by Molten Salt Method Used as Photocatalytic Materials	Zhao Z.

MS14-P29	B	Evidence of Anatase Intergrowths Formed During Slow Cooling of Reduced Ilmenite	D'Angelo A.
MS14-P31	B	Crystal Chemistry of Struvite and its Derivatives	Kiriukhina G., Yakubovich O.
MS14-P33	B	Crystal Structure and Biological Activities of a New Proton Transfer Material	Hamdi N., et al.
MS14-P35	B	The Crystal Structures of Natural Barium Beryll phosphates	Hatert F., et al.
MS14-P37	B	Crystal Structure of CaBaFe ₄ O ₇	Gutmann M.
MS14-P39	B	Stereochemistry of Tl(I) in Inorganic Oxysalts	Markovski M., Siidra O.
MS14-P41	B	Crystal structures of transition-metal halide complexes with cyanopyridine ligands: single chains, double chains, and networks.	Heine M.
MS15-P01	B	Reducing the Background of Ultra-Low Temperature X-Ray Diffraction Data	McMonagle C., Probert M.
MS15-P03	B	Pressure-Induced Spin Transitions in Garnets	Friedrich A., et al.
MS15-P05	B	Ab initio Simulation and X-Ray Diffraction Measurements of Deviatoric Stress in Mineral Inclusions	Morana M., et al.
MS15-P07	B	Toward One-Pot Green Synthesis of Nanoporous Carbon Nitrides	Dziubek K., et al.
MS15-P09	B	New Insights on the High Pressure Behaviour of the GeSe _x Te _{1-x} Solid Solution	Friese K., et al.
MS15-P11	B	Synthesis, Crystal Structures and Thermal Expansion of Novel Lutetium-Barium Borates	Biryukov Y., et al.
MS15-P13	B	High Pressure X-Ray Imaging and Diffraction on the Psiché Beamline: Recent Results and Developments Using Large Volume Presses	Itié J.P., et al.
MS15-P15	B	In-situ Single Crystal X-Ray Diffraction Studies of Proton Transfer Behaviour Under an Applied Electric Field on I19, Diamond [...]	Saunders L., et al.
MS16-P01	B	Short-Range Structure of Zr and Pd Bulk Metallic Glasses Prepared During the Melting and Cooling Process	Frison R., et al.
MS16-P03	B	Structure Design of Novel Ba _{3-x} Sr _x TeO ₆ Double Perovskites and the Effect of Temperature and Composition on Structure Stability	El Bachraoui F., et al.
MS16-P05	B	Environmental Effect on Titanium Alloy Ti6242S in Air Between 500 and 700°C	Kalienko M.
MS16-P07	B	Crystal Structure and Dehydration Behavior of Ag ⁺ -Exchanged Levyne	Cametti G., et al.
MS16-P09	B	Investigation of Physical Properties of Equiatomic Silver-Rare Earth Compounds Ag-Re (Re=Nd, Ce, Gd) from First [...]	Abdelhak F.
MS16-P11	B	Moringa Oleifera Waste as Dopants for S, N, C-TiO ₂ Photocatalysts Development	Agbahoungbata M.Y., Linden A.
MS17-P01	B	Symmetry Lowering in Natrochalcite NaCu ₂ (H ₃ O ₂)(SO ₄) ₂ Under Pressure	Miletich R., et al.
MS17-P03	B	Pressure-Induced Modification of Molecular Aggregation in Crystals of Benzocaine	Patyk-Kazmierczak E., et al.
MS17-P05	B	Ex-Situ Study of the Pressure Induced Decomposition of Iron Nitride Fe ₄ N	Wetzel M.H., et al.
MS17-P07	B	Phase Transitions of Copper(I) Iodide Compounds Under High Pressure	Gonzalez-Platas J., et al.
MS18-P01	B	Prussian Blue Analogues as Cathode Material in Low Cost Aqueous Batteries	Kjeldgaard S., et al.
MS18-P03	B	Phase Evolution During Perovskite Formation - Insight from PDF Analysis	Hua X.
MS18-P05	B	Combination of EXAFS and XRD for Studies of the Orthorhombic-Tetragonal Phase Transformation in MAPb _{1-3x} Cl _x	Schuck G., et al.
MS18-P07	B	First-Principles Study of Oxygen Adsorption Structure on Ni ₃ Al(210) Surface	Yamaguchi K., Nozawa K.
MS18-P09	B	Determination of Host and Dopant Ion Distribution in Mg ₂ Si _{1-x} Sn _x Thermoelectric Materials by Electron Channeling	Delimitis A., et al.
MS18-P11	B	Band Gap Depth Profile of Cu(In _{1-x} Ga _x)Se ₂ Absorbing Layer in Thin-Film Solar Cell by Glancing Incidence X-Ray Diffraction	Kim Y.I., Kim K.B.
MS18-P13	C	Local Structure of Glass-Ceramic Sodium Sulfidic Solid State Electrolytes	Fritsch C., et al.
MS18-P15	C	Thermochromic Lead-Free Halide Double Perovskites	Ning W., Gao F.
MS18-P17	C	The Influences of Mg Intercalation on the Structure and Supercapacitive Behaviors of MoS ₂	Liao L., et al.
MS18-P19	C	Combination of Data Mining and DFT Modeling of Ag ⁺ -Conductivity In S(Se)-Containing Inorganic Compound	Morkhova Y.
MS19-P01	C	High-Pressure Synthesis, Crystal Structure, and Magnetic Properties of Ba ₃ CuOs ₂ O ₉	Chen J., et al.

MS19-P03	C	Magnetism in Double Perovskites Ba ₂ CrMoO ₆	Bouadjemi B., et al.
MS20-P01	C	Discovery of Complex Metal Oxide Materials by Rapid Phase Identification and Structure Determination	Li J., Sun J.
MS20-P03	C	Raman and Surface Analysis Studies of (CuGaSe ₂) _{0.8} – (CuAlSe ₂) _{0.2} Single Crystals	Rywkin S., et al.
MS20-P05	C	Powder XRD Structure Determination of Nanostructured, Disordered MoS ₂ -Ethylenediamonium Layered Compound [...]	Goloveshkin A., et al.
MS21-P01	C	Structural Investigations on Bridging Stibinidene Complexes with Cu-K _β -radiation: A Comparison	Rummel L., et al.
MS21-P03	C	Accurate Experimental Charge Density Data: Tips & Tricks for Data Collection & Processing	Ott H., et al.
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MS22-P05	C	Charge Density Analysis of a Series of 4-methylthiostilbene Derivatives	Kubicki M., et al.
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MS23-P01	C	Correction for Phonons, Phasons and Multiple Scattering in Quasicrystals	Strzalka R.
MS23-P03	C	From a Single Slit to Periodic, Modulated and Quasiperiodic Crystals – a New Approach to the Diffraction Analysis of Aperiodic Systems	Wolny J.
MS23-P05	C	Crystal Structure of Incommensurately Modulated β-NaBrF ₄	Ivlev S., et al.
MS23-P07	C	Modulated Structure in Ni ₂ MnGa _{0.95} In _{0.05} Shape-Memory Alloy	Cejpek P., et al.
MS23-P09	C	Incommensurately Modulated Structures in the Series RETe _{2-d}	Doert T., Poddig H.
MS24-P01	C	Structural Disorder and Magnetic Correlations Driven by Oxygen Doping in Nd ₂ NiO _{4.11}	Keller L., et al.
MS24-P03	C	Revisiting the Magnetic Structure of R _{1/3} Sr _{2/3} FeO ₃ (R = La,Pr,Nd) by Neutron Powder and Single Crystal Diffraction Combined [...]	Pomjakushina E., et al.
MS24-P05	C	Understanding and Tuning Magnetism of Mesoscopic Hollow Oxide Sphere by Surface Engineering	Chen S., et al.
MS25-P01	C	Electron Crystallography for Studying MOF-Intercalated Guests	Samperisi I.
MS25-P03	C	Automated Electron Diffraction: 3D Structure Determination with Sub-Ångström Resolution	Roslova M., et al.
MS25-P05	C	Continuous Rotational Electron Diffraction Method for Structure Determination of Small Organic Molecules	Ge M., et al.
MS25-P07	C	Dynamical Structure Refinement from Data Obtained with a Dose of Less than 1 e ⁻ /Å ²	Klein H., Kodjikian S.
MS25-P09	C	Structure of a Novel R2-Like Ligand-Binding Oxidase Revealed by Electron Diffraction	Clabbers M., et al.
MS26-P01	C	Peculiarities of Solid Solutions with NaTl-Type Structure In Li-Zn-X (X=Al,Ga,In) Systems	Dmytriv G., et al.
MS26-P03	C	New Ca/Mg/Zn intermetallics of one intergrowth family.	Köhler K.
MS27-P01	C	Structural and Physical Properties of a 2,2',6',2''-terpyridine Derivative in the Solid State Phase Transition Behavior	Hsu I.J., et al.
MS27-P03	C	Local Order in Co and Mn Prussian Blue Analogues, the 3D-PDF analysis.	Simonov A., et al.
MS27-P05	C	Correlation of High-resolution X-Ray Diffraction with Mechanical Experiments and Finite Element Analysis	Dommann A., et al.
MS27-P07	C	Unique Properties of Geoinspired Nanotubes as Water Nanocontainer	Launois P., et al.
MS28-P01	C	Solving the Disordered Structure of beta-Cu ₂ Se Using the Three-Dimensional Difference Pair Distribution Function	Roth N.
MS28-P03	C	Understanding Structural Disorder in Nickel Cyanide Using 1D Statistical Mechanical Models	Wolpert E., et al.
MS29-P01	C	KOALA - Routine H-Atom Determinations by Laue Neutron Diffraction	Edwards A., Piltz R.
MS29-P03	C	Comparison of Different Strategies for Modelling Hydrogen Atoms in Charge-Density Analyses	Köhler C., et al.
MS29-P05	C	Comparison of X-Ray Wavefunction Refinement and Multipole Refinement Based on the Energetic Analysis of the [...]	Woinska M., et al.
MS30-P01	C	Features of Crystal Formation of Chiral Derivatives of 1,5-dihydro-2h-pyrrole-2-one	Saifina A., et al.
MS30-P03	C	Crystallization-Induced Stereoisomeric Recognition and Stereochemical Transformations of Chiral Organic Molecules: [...]	Lodochnikova O.
MS30-P05	C	Separation and Resolution of Methylcyclohexanones by Enclathration with Deoxycholic Acid	Bouanga Boudiombo J.S., et al.

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MS31-P03	C	Photocrystallographic Investigations of New Nickel(II) Nitro Complexes	Kutniewska S.E., et al.
MS31-P05	C	Structural and Computational Studies of a Series of New Photoswitchable Nickel Nitro Complexes	Borowski P., et al.
MS31-P07	C	Breathing Metal-Organic Frameworks Based On Flexible Inorganic Building Units	Inge A.K., et al.
MS31-P09	C	Wavelength-Selective Photoisomerisation of NO and NO ₂ Ligands	Schaniel D., et al.
MS31-P11	C	Molecular Switches in Nanocontainers	Diskin-Posner Y., et al.
MS31-P13	C	Exceptionally Flexible Coordination Polymers of Cd(II)	Pisacic M., Đakovic M.
MS31-P15	C	Separation of Isomers by Host-Guest Chemistry: Polymorphism, Resolutions and Templating	Nassimbeni L.
MS32-P01	C	In Situ PXRD Monitoring the Mechanochemistry of Metal-Organic Halogen-Bonded Cocrystals	Lisac K., et al.
MS32-P03	C	Influence of the Basicity of Halogen Bond Acceptors on Stoichiometry of Cocrystals with 1,3,5-triiodo-2,4,6-	Bedekovic N., et al.
MS32-P05	D	Insights into Weak C-H...F-C Interactions in C ₆ F ₆ :C ₆ H ₆ -nMen Co-Crystals Using Variable Temperature Crystallography to Follow [...]	Cockcroft J.
MS32-P07	D	Intermolecular Head-to-Head Interactions of Carbonyl and Thiocarbonyl Groups	Shteingolts S.A., Fayzullin R.R.
MS32-P09	D	Non-Covalent Bonding in Organic Crystals: a Combined X-Ray and DFT Study	Voronina J.
MS32-P11	D	Solid State Structure of Pharmaceutically Important Coumarin Derivatives from in House Collected XRPD Data	Bényei A., et al.
MS32-P13	D	Effect of Localized Non-Bonding/Repulsive Interactions on Distribution of Electron Density in Pi-Conjugated Systems	Lindeman S.
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MS33-P03	D	Heterocyclic Ligands for Water Sorption in Metal-Organic Frameworks: A Structural Study Using the Rietveld Method	Wharmby M., et al.
MS33-P05	D	Noble Gas Adsorption in MFU-4l Frameworks with Different Metal Atoms	Magdysyuk O.
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MS33-P09	D	Prior Evaluation of Guest Exchange in Crystalline Framework Using Preliminary Diffraction Data	Hoshino M., et al.
MS33-P11	D	Enhanced Selectivity for CO ₂ in Mixed-Ligand Bis(pyrazolate) Zn(II) MOFs Through Dilution of Functionalization: a Structural and [...]	Vismara R., et al.
MS33-P13	D	Crystal Engineering Meets Stereochemistry: Investigations of the Crystal Structures and Resulting Properties of Copper [...]	Kremer M., Englert U.
MS33-P15	D	Coordination Polymers and Solvatomorphs – Copper Complexes with Amino Acids and 2,2'-bipyridine	Vušak D., et al.
MS33-P17	D	Direct Structure Determination of Volatile Odor Compounds via Crystalline Sponge Method	Kikuchi T.
MS33-P19	D	Complexation Studies of Chiral Cyclohexylhemicucurbit[n]uril to Metalloporphyrins in Solid-State	Truong K.-N.
MS34-P01	D	Crystal Structure and Hirshfeld Surface Analysis of 1,3,4-thiadiazol Derivative	Tabti C.
MS34-P03	D	Polymorphism of R-Encenicline Hydrochloride: Access to the Highest Number of Structurally Characterized Polymorphs Using [...]	Kons A., et al.
MS34-P05	D	How to Correctly Sample Unit Cells in Computer Simulations of Crystal Structures	Kurlin V.
MS34-P07	D	Development of Accurate and Efficient Ab Initio Potentials for Effective Crystal Structure Prediction	Bowskill D., et al.
MS34-P09	D	Affinity Predictions for Cocrystals' Design: Computational vs. Experimental Results	Roca Paixao L., et al.
MS35-P01	D	Mononuclear Cobalt, Nickel and Copper Complexes with Glycinamide: Structural Properties and Biological Activity	Prugovecki B., et al.
MS35-P03	D	Luminescent [Os(Cl)(CO)(P^P)(pbi)] Complexes	Suwinska K., et al.
MS35-P05	D	Graph-Set Analysis and Non-Linear Optical Properties of Salts of L-Arginine Homologue	Rejnhardt P., Daszkiewicz M.
MS35-P07	D	Novel Schiff Base-Metal Complexes; Synthesis, Crystal Structure and Biological Activity	S. M. Abdelbaky M., et al.
MS35-P09	D	New Heterobimetallic Complexes of Cu(II) and Mn(II) with Cyclam Derivatives	Kuchár J., Samolová E.
MS35-P11	D	Structural and Computational Study of Quinoline-Based Chalcogenesemibazones	Klisuric O., et al.
MS35-P13	D	Exploring the Limits of Iodonium (I+) Formation	Ward J.

MS35-P15	D	Crystal Structures and Topological Analysis of Ag(I) Complexes with 1,4-heterodisubstituted Cyclohexanes	Marjanovic I., et al.
MS35-P17	D	Crystallographic Evidence for Aggregation Patterns of Two Cyclic Trimidazole Phosphors in Zn(II) and Cd(II) Complexes	Kravtsov V., et al.
MS35-P19	D	Cube Vs Dimer: Peculiarities of Crystal Structure of Cu ₂ I ₂ - and Cu ₄ I ₄ -Complexes of 10-(Aryl)Phenoxarsines and 10-[...]	Dobrynin A., et al.
MS35-P21	D	Filling the Gaps: What New Polymorphs of Acetylpyrene Tell us About the Fluorescence of Pyrene Derivatives	Tchon D., et al.
MS35-P23	D	Structural and Vibrational Study of New 2-ethylanilinium Phosphite (C ₈ H ₁₂ N)H ₂ PO ₃	Zerraf S.
MS35-P25	D	Revealing Mechanical Plastic Bending in Coordination Polymer Crystals	Bhattacharya B., et al.
MS35-P27	D	Engineering of Supramolecular Coordination Spheres for Selective Fullerene Binding and Functionalisation	Holstein J., et al.
MS35-P29	D	Insights into the Molecular Arrangements of Substituted Hydroxypyridine Carboxylic Acids	May N.V., et al.
MS35-P31	D	Design of Cocrystals Based on Essential Oils with a Palette of Different Properties	Bacchi A., et al.
MS35-P33	D	New Synthons in Supramolecular Chemistry of Short Biologically Active Peptides	Bojarska J., et al.
MS35-P35	D	Effect of Crystallization Conditions on Diuretic Clopamide and its Copper(II) Complexes	Gál G.T., et al.
MS35-P37	D	Structurally Diverse Manganese(III) - Salpn Complexes with Bridging Formate Ligand	Moncol J., Schoeller M.
MS36-P01	E	Four-Component Isomorphism in the Crystal Structure of [HL][Cd(HL)(NCS) ₂ XY]·H ₂ O, where L = 2-acetylpyridine-[...]	Rodic M., et al.
MS36-P03	E	Molecular Basis of Water Sorption Behavior of Rivaroxaban-Malonic Acid Cocrystal	Kale D.P., et al.
MS37-P01	E	Expanding Solid-State Landscape of Fluconazole: Combined Application of Solid-State NMR, X-Ray Diffraction and [...]	Nowak M., et al.
MS37-P03	E	{ ¹ H/ ¹⁹ F} -> ²⁹ Si/ ²⁷ Al CPMAS and HETCOR Spectroscopy of Synthetic Lepidolites: Connectivities Between F/OH and Si/Al [...]	Fechtelkord M., Sulcek L.
MS37-P05	E	Photoinitiated solid-state reactions of ketones with vinyl-acetylene fragments	Ushakov I.
MS38-P01	E	CdTe Based 2D Detectors for Hard Radiation	de Vries R., et al.
MS38-P03	E	The Potential Benefits of Using Higher X-Ray Energies for Macromolecular Crystallography	Dickerson J., Garman E.
MS38-P05	E	Resolution Function for 2D Pixel Detectors	Chernyshov D., Dyadkin V.
MS39-P01	E	Development of Data Processing Methods in Time-Resolved Laue Photocrystallography	Kaminski, R., et al.
MS39-P03	E	Development of Channel-Cut X-Ray Optics for Laboratory Small-Angle X-Ray Scattering Setups	Nádaždy P., et al.
MS39-P05	E	Structural Mechanisms Governing Redox-Linked Proton Pump in Cytochrome c Oxidase Studied by Time-Resolved X-Ray Methods	Ghosh, S.
MS40-P01	E	Structural Characterization of Exchange Biased Au-Fe ₃ O ₄ Dumbbell Nanoparticles	Feygenson M.
MS40-P03	E	Multiscale Structural Decoding of Electrospun Nanofibers: from Processing to Possibilities for Steering Functionality	Maurya O.F., et al.
MS40-P05	E	Possibilities of the X-Ray Diffraction Method for the Study of Ultradispersed Systems and Nanopowders	Yatsenko D.
MS40-P07	E	Diffraction Experiments Under Extreme Conditions on Single Crystals with Hot Neutrons on HEiDi	Meven M., et al.
MS40-P09	E	Quantification of the Strain Relaxation Processes in Silicon Nanowires Arrays Using Combined X-Ray Diffraction Analyses	Romanitan C., et al.
MS40-P11	E	Beam Damage of Single Semiconductor Nanowires During X-Ray Nano Beam Diffraction Experiments	Pietsch U., et al.
MS40-P13	E	Interplay between Crystal Structure, Shape and Functionality of Colloidal Nanocrystals and Supercrystals	Lechner R. T.
MS41-P01	E	Watching Nanodefects Grow in Si Crystals	Magerl A.
MS41-P03	E	Amine-imine Proton Tautomerism in Isomeric 2-phenylamino-1,3-thiazol-4(5H)- and 4-phenylamino-1,3-thiazol-2(5H)-one [...]	Pyrih A., et al.
MS41-P05	E	Phytochemical and Biological Studies of Anacyclus Pyrethrum L. from Ifrane-Morocco	Remok F., Zair T.
MS42-P01	E	Phase Diagram and Redox Behavior of (Nd/Pr) ₂ NiO _{4+d} Electrodes Explored by in situ Neutron Powder Diffraction During [...]	Ceretti M., et al.
MS42-P03	E	Formation Mechanism of Epitaxial Palladium-Platinum Core-Shell Nanocatalysts in a One-step Supercritical Synthesis	Broge N.N.L.
MS42-P05	E	Sequential SHELXL Refinement of Consecutive Datasets: a Tool to Probe Dynamically Evolving Single Crystal Structures	Törnroos K.W., et al.
MS42-P07	E	A New Concept for Sapphire Single-Crystal Cells to Study Solid-Gas Reactions via Real-Time in situ Neutron Scattering	Finger R., Kohlmann H.
MS42-P09	E	Space- and Time-Resolved Analysis of the Decomposition of Thermoelectric Materials with Mobile Atoms Under Working [...]	Oeckler O., et al.

Poster Session II (Wednesday & Thursday, 16.00 - 17.00)

Poster number	Area	Title	Author
MS01-P02	A	TREXX: a New Endstation for Serial Time-Resolved Crystallography at PETRA-III	von Stetten D., et al.
MS01-P04	A	MetalJet Source Enabling Advanced Protein Crystallography	Espes E., Hållstedt J.
MS01-P06	A	Better SAUC -- Improving the Identification of Nearby Cells	Bernstein H.J.
MS01-P08	A	Development of Serial Millisecond Crystallography at BioMAX Beamline	Shilova A., et al.
MS01-P10	A	Liquid Application Method for Time-Resolved Analyses (LAMA) by Serial Synchrotron Crystallography	Mehrabi P., et al.
MS02-P02	A	Getting the Most from Your Crystals Through the Full Automation of Complex Experiments	Bowler M.
MS02-P04	A	A Case Study of Fragment Screening: Protein Kinase A and PIM1-Kinase	Heine A., et al.
MS02-P06	A	Fragment Screening Project Management Web Application - FragMAX	Lima G.
MS03-P02	A	The MORPHEUS Protein Crystallisation Screens	Gorrec F.
MS03-P04	A	Crystal Structure of an Anti-Tumour Antibody in Complex with a Tumour-Specific Antigen	Johannesen H., et al.
MS03-P06	A	Crystal Production and Structure Solution Thanks to the Nucleating and Phasing Agent, Crystallophore	Girard E., et al.
MS03-P08	A	The Role of ODD in the Biosynthesis of Medically Important Alkaloids	Kot E., et al.
MS03-P10	A	SEC-SAXS Analysis of Oligomeric States of Human NKR-P1 with its Ligand LLT1 in Solution	Skalova T., et al.
MS03-P12	A	All-in-one Sample Holder for Macromolecular Crystallography	Feiler C., et al.
MS03-P14	A	One Step Co-purification and Crystallization of Three Soluble Proteins from Cyanobacteria, the Unique Crystallization [...]	Sarrou I., et al.
MS03-P16	A	Dynamic Formation and Internal Order of Liquid Dense Protein Clusters Beyond Crystallography	Falke S., et al.
MS03-P18	A	Surface Layer Proteins of Lactobacilli – Determining the Cell Wall Binding and their Antibacterial Effect	Eder M., et al.
MS03-P20	A	The SOD1-hCCS Mechanism Involved in Copper Homeostasis	Sala F.A., et al.
MS03-P22	A	Crystal Structure of Histone Chaperone Anti Silencing Function 1 (Asf1) from Plasmodium Falciparum and its Biochemical [...]	K. Srivastava D., et al.
MS03-P24	A	Preliminary Diffraction Experiments on the E.coli Toxin SAT	Meza D., et al.
MS04-P02	A	Tools for Validation of Maps and Atomic Model Fits in Single Particle Cryo-EM	Warshamanage R.
MS05-P02	A	Structural Studies of Type II TNF- α from Orange-spotted Grouper, <i>Epinephelus coioides</i>	Lin S.M., et al.
MS06-P02	A	Structural Basis for RNA Translocation and NTP Hydrolysis by the Zika Virus NS3 Helicase	Ge M., et al.
MS06-P04	A	Chromosome Partitioning System, ParABS	Sun Y.J.
MS06-P06	A	Structure and Function of <i>S. Aureus</i> YabJ as a Novel Chlorination-Induced Ribonuclease	Kwon A.R.
MS06-P08	A	Use of the Cocomaps Web Server to Analyze and Visualize the Interface of Biomolecular Complexes in Crystal Structures	Oliva R., Cavallo L.
MS07-P02	A	Oncogenic KRAS G12C Mutation Derived Inhibitor Development	Leveles I., et al.
MS07-P04	A	Regioselective Carboxylation by Prenylated Flavin and Mn-Dependent Decarboxylases	Pavkov-Keller T., et al.
MS07-P06	A	Covalent Bond Between Side Chains of Tryptophan and Histidine in Bilirubin Oxidase is Essential for Substrate Binding	Dohnálek J., et al.
MS07-P08	A	New Structural Insight into the Well Known Peptide Flip Observed in Flavodoxins	Hersleth H.P., et al.
MS07-P10	A	Interdomain Conformational Flexibility of the Peptidoglycan N-acetylglucosaminidases of <i>Staphylococcus Aureus</i>	Pintar S., et al.
MS07-P12	A	Enzymatic Control of O ₂ Reactivity and Functionalization of the Flavin Cofactor	Saleem Batcha B., Teufel R.
MS07-P14	A	Competitive Binding of Potential Drug Molecules at the Active Site of an Acylpeptide-Hydrolase	Kiss-Szemán A.
MS07-P16	A	Structural and Mutational Investigation of Psychrophilic Adenylate Kinase Reveals the Importance of Hydrophobic Packing in [...]	Koo J.
MS07-P18	A	High-Resolution Dimeric Crystal Structures of Wild-Type and Mutant <i>Aspergillus Niger</i> Glucose Oxidase	Pavlovic J., et al.
MS07-P20	A	Selective Inhibition of Astacin Metalloproteinases by Mammalian Fetuin-B	Gomis-Rüth F.X., et al.
MS07-P22	A	Structural Comparison of Two Mammalian Multicopper Oxidases, Hephaestin and Ceruloplasmin	Zaitsev V., Lindley P.

MS08-P02	A	Structure of the A-Actinin Actin-Binding Domain/F-Actin Complex	Vujin S., et al.
MS08-P04	A	Structural Basis of Ascorbate-Dependent Iron Reduction by Human Dcytb Involved in Intestinal Iron Absorption	Sugimoto H., et al.
MS08-P06	A	Crystal Structure of UHRF1:LIG1 Complex Revealed Structural Change of UHRF1 and the Key Residues for High Affinity Binding	Kori S., et al.
MS08-P08	A	Bacterial Nucleosidase is Regulated by the Alarmone (p)ppGpp	Bærentsen R.
MS10-P02	A	Analysis and Validation of B Values of Macromolecular Structures	Masmaliyeva R., Murshudov G.
MS10-P04	A	Validation in the PDB	Armstrong D., wwPDB consortium
MS11-P02	A	Harnessing the Data: Integrating Data Flows Across Home Laboratories, Facilities and Data Repositories [...]	Marquez J.A.
MS11-P04	A	Combining the Use of Libraries from Several Distant Homologs in ARCIMBOLDO_SHREDDER Spheres	Jiménez-Mellado E., et al.
MS12-P02	A	Enhancing Small Molecule Information in the Protein Data Bank in Europe	Pravda L., PDBe
MS12-P04	A	How Disease-Associated Mutations May Alter the Dynamic Motion of the N-terminal Domain of the Human Cardiac [...]	Bauer J., et al.
MS12-P06	A	Building the Protein Structure-Specific Side-Chain Rotamer Libraries	Grybauskas A., Gražulis S.
MS12-P08	A	New Covariance-Based Methods for Unconventional MR of Transmembrane Proteins	Sanchez Rodriguez F., et al.
MS13-P02	A	The Bone Mineral is Carbonato-Hydro-Apatite and it Transforms into Hydroxyapatite by Heating (Cremation) Beyond 700°C	Schmahl W., et al.
MS13-P04	A	Small-Angle X-ray Scattering Studies on the Interaction of Bicelles with Bovine Serum Albumin	Lin T.L.
MS14-P02	B	First-Principles Investigation of Structural, Electronic and Optical Properties of CsPb(I _{1-x} Br _x) ₃ (x = 0.0 - 1.0) Compounds	Ghaithan H.
MS14-P04	B	The Dependence of Yb Concentration on Lattice Parameters of YAG Single Crystals	Kodess B.
MS14-P06	B	Order-Disorder in the Arsenopalladinite, Pd ₈ As _{2.5} Sb _{0.5} , Crystal Structure	Karimova O., et al.
MS14-P08	B	Comparative Crystal Chemistry of the Solid Solution Systems Between Kieserite (MgSO ₄ ·H ₂ O) and Transition Metal [...]	Wildner M., Talla D.
MS14-P10	B	New Approaches for Rietveld Refinement in Size-Strain, Grain Size Distribution and Dislocation-Recrystallization Analysis	Kristály F., et al.
MS14-P12	B	Nickel(II) complexes with Dithiocarbazate Ligand: Crystal Structures and Spectroscopic Analysis	Lima F., Gatto C.
MS14-P14	B	Powder Diffraction Experiments on a Single Crystal Diffraction Instrument - How Far can we Push this?	Stuerzer T., et al.
MS14-P16	B	Isotope Effects in Recovered High-Pressure Phases of Ice	Fortes D., et al.
MS14-P18	B	Crystal Structures of the First Polymeric Cu(II) Complexes with Thiosemicarbazone Methyl Pyruvate	Radanovic M., et al.
MS14-P20	B	Modular Structures of Layered Uranyl Minerals and Synthetic Compounds	Nazarchuk E.
MS14-P22	B	Synthesis and Crystal Structure of New Alkali Chalcogenido Manganates/Indates	Langenmaier M.
MS14-P24	B	Pseudo-Symmetry and Order-Disorder Transitions in Metal Hydrides	Kohlmann H.
MS14-P26	B	Rare-Earth Pnictide Chalcogenides REBiTe and RESbS (RE = La-Nd): Structure Determination by Combination of Transmission [...]	Benndorf C., et al.
MS14-P28	B	New Cubic Borate Yb ₃ [BO ₃](OH) ₆ ·2.1H ₂ O with "Antizeolite" Framework and Isolated BO ₃ -Triangles in Cavities	Topnikova A., et al.
MS14-P30	B	Insight into the Crystallization and Structural Features of Cesium-Bearing Chain-Type Borophosphates	Shvanskaya L., et al.
MS14-P32	B	Layer Charge Influence on the Hydration Properties of Synthetic Na-Saturated Smectites	Vinci D.
MS14-P34	B	Hexagonal Bariumtitanate Stabilized as Ultra-Thin Film on Pt(111): An X-Ray Diffraction and Electron-Energy-Loss Spectroscopy Study	Meyerheim H., et al.
MS14-P36	B	The Crystal Structure of Koninckite	Bruni Y., et al.
MS14-P38	B	Preparation, Spectral, Structural, Thermal and Anticancer Molecular Docking Studies of Bis-(theophyllinato)- [...]	EL Hamdani H., et al.
MS14-P40	B	Calcium Oxalate Crystallization for a Non-Conventional CO ₂ Storage Method	Pastero L., et al.
MS15-P02	B	Xpress: Latest Results from the New Dedicated High Pressure Diffraction Beamline at Elettra	Lausi A., et al.
MS15-P04	B	Experimental Charge Density Distribution in Grossular Under High Pressure - a Feasibility Study	Wozniak K., et al.
MS15-P06	B	Structure, Crystal Chemistry, and Compressibility of Iron-Rich Silicate Perovskite at Pressures up to 95 GPa	Koemets I., et al.

MS15-P08	B	The Microscopic Origin of Axial Negative Thermal Expansion and Negative Linear Compressibility in Alpha- and Beta-PbAlBO ₄	Gogolin M., et al.
MS15-P10	B	Squeezing the Most Data out of Your High-Pressure Experiment	Graf J., et al.
MS15-P12	B	Antiferroelectric <i>Pnma</i> Phase: The Missing Element to Understand Morphotropic Phase Boundary Lead-Free Na _{1/2} Bi _{1/2} TiO ₃ [...]	Rouquette J., et al.
MS15-P14	B	The Influence of [2+2] Photodimerization and High Pressure on the Structural Transformations in Crystals	Galica T., Turowska-Tyrk I.
MS15-P16	B	Oxides Under Extreme Conditions: Pushing the Limits of Neutron Diffraction	Capone M., et al.
MS16-P02	B	Pure Gyrotropic Ferroelastic Phase Transitions in the Materials PbMXO ₄ (M = Ba, Sr; X=Si,Ge): a New Piezoelectric Family	Prugovecki S., et al.
MS16-P04	B	Perovskite BaTiO ₃ Doped with Pyrochlore Bismuth Zinc Niobate - a New Perovskite Relaxor Ferroelectric BZN-BT	Thomas P., et al.
MS16-P06	B	Forbidden/Non-Forbidden Bragg Reflections Study Under Phase Transitions and External Influences	Ovchinnikova E., et al.
MS16-P08	B	Lattice Constants Prediction and Thermochemistry of Hexahalometallate A ₂ MX ₆	Hadda K.
MS16-P10	B	LiTaO ₃ Defect Structures by Means of Forbidden Reflections	Nentwich M., et al.
MS16-P12	B	Morphological Analysis of the Migration-Induced Field-Stabilized Polar Phase in SrTiO ₃ with Scanning X-ray Diffraction Microscopy	Weigel T., et al.
MS17-P02	B	Structure–Magnetic Property Correlations in Metal–Formate Frameworks at High Pressure	Collings I., et al.
MS17-P04	B	Effect of Pressure on Slit Channels in Hydrate of Sodium Salt of Guanine: a Link to Nucleobase Intermolecular Interactions	Gaydamaka A., et al.
MS17-P06	B	Phase Transformations of (RS)-2-Chloromandelic Acid in the Solid State: From Racemic Compound to Conglomerate [...]	Liu J., et al.
MS18-P02	B	Tailored Exsolution of Metal Nanoparticles: Structural and Chemical Characterisation of Doped Perovskites by XPS and XRD	Raschhofer J., et al.
MS18-P04	B	Ab-initio Study of Oxygen Adsorption on PdZn(111) Surface	Otani Y., et al.
MS18-P06	B	Synthesis and Crystal Characterization of a New Layered Acidic Diphosphate Metallate	Hamdi N., et al.
MS18-P08	B	Structure and Thermoelectric Characterization of Lithium-substituted Bismuth Palladium Oxide	Nguyen H.H., et al.
MS18-P10	B	Structural Modification of Perovskites by Tailored Exsolution for Enhanced Catalytic Activity	Rameshan R., et al.
MS18-P12	B	In-situ Carbonation of SrO at 298 K and Controlled Humidity for Thermochemical Energy Storage	Gravogl G., et al.
MS18-P14	B	New Method for Electromechanical Losses Evaluation of the Electrostrictive Energy Efficiency: Experiments and Modeling	Farhan R.
MS18-P16	B	Influence of Fe Doping on the Crystal Structure, Electronic Structure and Supercapacitance Performance of Birnessite with High [...]	Liu H., et al.
MS18-P18	B	The Surface Phase Diagram of La _{0.8} Sr _{0.2} MnO ₃ in STM	Riva M., et al.
MS19-P02	B	Self-Assembly of Octanuclear Complexes Containing Tetra- and Pentacoordinate Co(II) Centers	Nemec I.
MS20-P02	B	Synthesis and Structure Determination of SCM-15: a 3D Large Pore Zeolite with Interconnected Straight 12×12×10-Ring Channels	Luo Y., et al.
MS20-P04	B	Universal Algorithm for Prediction of New Cleavage Planes in Single Crystals	Vaknin U., et al.
MS21-P02	B	Electron Densities of Molecular Crystals from Powder X-Ray Diffraction	Svane B., Iversen Brummerstedt B.
MS22-P02	B	Evaluation of Covalent Bond Density in Molecular Crystals Using Simplified Virtual Scattering centers	Nazarenko A.
MS22-P04	B	Assembly, Crystal Structures and (Non)Linear Optical Properties of Multicomponent Materials Containing Sulfonamides	Wojnarska J., et al.
MS22-P06	C	Insights into the Origin of Magnetic Anisotropy in Linear Iron Complexes from the Experimental Electron Density	Thomsen M.K., et al.
MS22-P08	C	Understanding of Chromic Phenomena: the Examples of Violuric Acid - Amino Acid Based Salts and Co-crystals	Rydz A., et al.
MS23-P02	C	The Real Space Refinement of the Icosahedral Quasicrystal	Buganski I., et al.
MS23-P04	C	Will PdPb Confirm the Prediction that its Structure is Modulated?	Folkers L., Lidin S.
MS23-P06	C	On the Puzzling Case of Sodium Saccharinate 1.875-Hydrate: Structure Description in (3+1)-Dimensional Superspace	Rekis T., et al.
MS23-P08	C	Novel Approach to Structure Determination of Complex Protein System Hyp-1/ANS	Smietanska J., et al.

MS24-P02	C	Oxygen Order Correlation to the Incommensurately Modulated Magnetic Stripes and their Interaction in 214-type Pr _{2-x} Sr _x NiO _{4+d}	Maity A., et al.
MS24-P04	C	MagStReX: Magnetic Structures Through Resonant X-Ray Scattering	Bereciartua P.J., et al.
MS24-P06	C	Probing the Magnetic Ground-States of Rare-Earth Compounds by Single Crystal Neutron Diffraction	Henriques M., et al.
MS25-P02	C	Data Processing of 3D Precession Electron Diffraction Data	Palatinus L., Brázda P.
MS25-P04	C	Dedicated Electron Source for Serial Electron Crystallography	Hogan-Lamarre P., et al.
MS25-P06	C	Low Dose Electron Diffraction Tomography (LD-EDT) Solves the Structure of a New (Na _{2/3} Mn _{1/3}) ₂ Mn ₃ Ge ₃ O ₁₂ phase [...]	Kodjikian S., et al.
MS25-P08	C	Refinement of Organic Crystal Structure with Multipolar Electron Scattering Factors	Dominiak P., et al.
MS25-P10	C	MicroED, Fast and Furious	Raaijmakers H.
MS26-P02	C	Chemical Bonding and Structural Complexity in Known Intermetallic Compounds o-Al ₁₃ Co ₄ and Al _{2.75} Ir ₂	Grin Y.
MS27-P02	C	New Radiation-Induced Phase of MAPbI ₃ - an Unexpected Surprise of Synchrotron Experiments	Minns J.
MS27-P04	C	Endohedral Metallofullerene Crystals: Playing with Disorders	Liu F., Popov A.A.
MS27-P06	C	The Benefits of Cu-K _α Radiation in Elucidating the Molecular Structure of Polypnictogen Cations	Riesinger C., et al.
MS28-P02	C	Local Dipole Formation in IV-VI Semiconductors	Holm K., et al.
MS29-P02	C	On Precision and Accuracy of X-Ray and Neutron Diffraction Results for Single Crystals of Glycine	Sutula S., et al.
MS29-P04	C	TAAM: A Reliable and User Friendly Tool for Hydrogen Atom Location Using X-Ray Diffraction Data	Chodkiewicz M., et al.
MS30-P02	C	Absolute Structure assignment Through Interplay of X-Ray Diffraction and EBSD	Borrmann H., et al.
MS30-P04	C	Unexpected Polymorphic Behavior of Four Racemic 3-Pyrrolin-2-One Derivatives	Gerasimova D., et al.
MS30-P06	C	Peculiarities of Supramolecular Organization in Centric, Acentric and Chiral Ketones with Vinylacetylene Fragments	Voronova E., et al.
MS31-P02	C	Triethylphosphine as a Molecular Gear — Phase Transitions in Ferrocenyl–Acetylide–Gold(I)	Makal A.
MS31-P04	C	Probing Spin Crossover in Novel Metal Organic Complexes	Musselle-Sexton J., et al.
MS31-P06	C	Pressure-Induced Polymerization and Electrical Conductivity of a Polyiodide	Poreba T.
MS31-P08	C	Conformational Switching in Single Crystals of a Calix[4]resorcinarene	Lindeman S., et al.
MS31-P10	C	Photoinitiated [2+2] Cycloaddition Reactions Observed in d-Metal(II) Malonates with N,N'-Containing Linkers	Vologzhanina A.V., et al.
MS31-P12	C	Dynamic, Breathing, Water-stable, Mixed-Ligand Zn(II) Metal-Organic Frameworks with Differing Water and Vapour Sorption [...]	Oliver C.L.
MS31-P14	C	Thermo- / Mechano- Mechanically Responsive Cocrystals During Single-Crystal-to-Single-Crystal Phase Transitions	Liu G., et al.
MS31-P16	C	Structure / Reactivity Relationships from Detailed Reaction Mechanisms	Roodt A., et al.
MS32-P02	C	Efficient Recognition of Steroids by Planar Aromatic Molecules: A Novel Biomolecular Recognition Motif and its Potential Applications	Topic F., Friscic T.
MS32-P04	C	Towards the Linear [S ₂ X] ⁺ Systems: Metal Complexes and Halogen Bonding	Valkonen A., et al.
MS32-P06	C	Identification of Non-Covalent Interactions by Hirshfeld Surface and Energy Frameworks in Chalcone-Flavanone Isomers	Checinska L., et al.
MS32-P08	C	Intermolecular Chalcogen...Halogen Interaction in Organic Molecular Crystals	Kazmierczak M., Katrusiak A.
MS32-P10	C	Structural Landscape of Cu(II) Coordination Compounds with Isomers and Derivatives of Cyclic Triimidazole	Fonari M., et al.
MS32-P12	C	Examination of the Intermolecular Auophilic Interactions in the Crystals of the (ArCOC=C)(PEt ₃)Au and [(ArCOC=C) ₂ Au [...]	Pawledzio S., et al.
MS32-P14	C	Hypervalent Chalcogen-Chalcogen Heteropentalenes and their Charge Transfer Adducts	Levendis D., et al.
MS32-P16	C	Interplay Between Occurrence Frequencies of Charged and Neutral Base Pairs in Small Molecule Crystals	Cabaj M., Dominiak P.
MS33-P02	C	Polarized Fluorescence Harvested from Fullerenes Loaded in Non-Centrosymmetric Ni-MOF	Vasylevskiy S., et al.
MS33-P04	C	Synthesis and Characterization of New Lanthanide MOFs Using a Semi-Flexible Bis-Imide Ligand	González Chávez F.
MS33-P06	C	Controlled Release of Natural Essential Oils from Microporous Metal-Organic Framework	Mazzeo P.P., et al.
MS33-P08	C	About the Polymorphism of Two Anti-Inflammatory Drugs within Thin Films	Kaltenegger M., et al.

MS33-P10	C	Mechanochemistry and Electron Crystallography: a Winning Combination for the Discovery of New Metal-Organic Materials	Lanza A., et al.
MS33-P12	C	Serial-MOF: Developing Serial Crystallography Methods for MOF Nano-crystals	De Zitter E., et al.
MS33-P14	C	Constructing Extended Bismuth(III) Structures Using Tridentate Organic Linkers	Senior L., Linden T.
MS33-P16	C	Giant Supramolecules as Molecular Containers	Virovets A., et al.
MS33-P20	C	Synthesis and crystal structure of a new bimetallic platinum complex [Pt ₂ (μ-H)(μ-PPh ₂) ₂ Br ₂ (PPh ₃) ₂]	Ouis, S.
MS34-P02	C	Use of Crystal Structure Prediction to Design Template Crystallization Experiments of Nitrobenzoic Acid Derivatives	Berzinš A., Actinš A.
MS34-P04	C	DFT Studies of Structural, Electronic and Magnetic Properties of InP and In _{0.75} X _{0.25} P (where X = Cr, Mn & Fe)	Kaur K., Sharma S.
MS34-P06	C	A Combined Theoretical and Experimental Investigation into the High Throughput Screening of Cocrystal Cofomers	Sugden I., et al.
MS34-P08	D	Understanding of Cholesterol Transport in NPC Family Protein: A Computational Study	Yoon H., et al.
MS35-P02	D	Phase Transitions Associated with Conformational Changes of Ligand and Anion Reorientation Trigger Normal and Reverse Spin [...]	Kusz J., et al.
MS35-P04	D	Structural Studies of the Host-Guest Complexes of Carboxylated Pillar[n]arenes	Butkiewicz H., et al.
MS35-P06	D	Novel Coordination Compounds for Biological Applications	Garcia-Granda S., et al.
MS35-P08	D	Two Composite Mn(II)-squarate-dpe Supramolecular Networks Showing Interesting Water Hysteresis Phenomenon in Water [...]	Wang C.C.
MS35-P10	D	Hydrothermal Synthesis, Crystal Structure and Luminescent Properties of a New Praseodymium Coordination Polymer of	Benmerad B., et al.
MS35-P12	D	New Titanium Calix[n]arene-based Scaffolds as Anti-tumour Agents	Elsegood M.
MS35-P14	D	Crystal Structure and Self-Assembly of Pillar[n]pyridiniums	Danylyuk O., et al.
MS35-P16	D	A Lamellar Structure Exhibiting Nano-Morphological Reversibility, Disassembly-and-Self-Assembly Crystallization into Novel [...]	Hung L.I., Chen P.
MS35-P18	D	Crystal Structures of Cholesterol Based Photo-Switchable Mesogenic Dimers. Strongly Bent Molecules Versus an [...]	Pruszkowska K., Zep A.
MS35-P20	D	Correlation Between Structural Studies and Third Order NLO Properties of Three New Semi-Organic Compounds	Benali-Cherif R., et al.
MS35-P22	D	Medium Chain Length (mcl)-PHA-based Nanocomposites for Biomedical Applications: System Evaluation Through XRD	Malagurski I., et al.
MS35-P24	D	Supramolecular Assemblies of Copper(II) Complexes: Supramolecular Synthron Transferability and Magnetic Properties	Penic N.
MS35-P26	D	Organic Cocrystals with Mechanically Interlocked Architectures: Unprecedentedly Stiff and Hard with Elastic Flexibility	Dey S., et al.
MS35-P28	D	Evaluation of Trends in a Series of Halogenated Isophthalamides	Gallagher J.F., Osman I.A.
MS35-P30	D	Halogenation Dictates Architectures and Properties of Amyloid Peptides	Terraneo G., et al.
MS35-P32	D	Hierarchical Design of Lipid-Polymer Composite Nanofibers: the Interplay of Multiscale Structures and Biofunctions	Sadeghpour A., et al.
MS35-P34	D	Controlling the Salt-Cocrystal Continuum and pKa rule: The Multi-Drug Ionic-Cocrystals of Lamatrigine and Valproic Acid	Lusi M., Kavanagh O.
MS35-P36	D	Multicomponent Crystal Formation of Baclofen with Acids and Bases	Malapile R., et al.
MS35-P38	D	The Photodimerization of Schiff Bases: Benzophenone Azine Crystals and their Weak C-H...pi Interactions	Smith M., Lemmerer A.
MS36-P02	D	Dynamical Disorder in the Solid State: Insights from Dielectric Relaxation Spectroscopies	Correia N., et al.
MS36-P04	D	Multicomponent Crystals of 2,2'-Bipyridine with Aliphatic Dicarboxylic Acids: Structure-Property Correlations	Batisai, E.
MS37-P02	D	Towards Understanding Phase Transitions of Confined Pharmaceuticals	Nartowski K., et al.
MS37-P04	D	The Drug Target Monoacylglycerol Lipase: Structure and Dynamics, Conservation and Divergence	Oberer M., et al.
MS38-P02	D	Pushing Data Quality for Laboratory Pair Distribution Function Experiments	Zobel M., et al.
MS38-P04	D	Measuring Accurate Single Crystal Diffraction Data Using a Pilatus3 CdTe Detector	Krause L., et al.
MS39-P02	D	A Novel X-Ray Diffraction Technique for in-situ Observations of Cathode/Anode Reaction in Electrolytes	Kubicek S.
MS39-P04	D	Silica Nanoparticle Agglomeration Studies Under Physiological Conditions Using Dynamical SAXS Methods	Iranpour N., et al.
MS39-P06	D	Recent Developments Towards High-Flux Time-Resolved and THz-SAXS-Experiments at the EMBL P12 BioSAXS Beamline	Schroer M.A., et al.
MS40-P02	D	Structural and Optical Properties of CuS Nanoparticles	Souici A., Chibani S.

MS40-P04	D	A Laboratory Rheo-SAXS Setup - Relating Nanostructure to Macroscopic Properties in one go	Jones A.O.F., et al.
MS40-P06	D	Study of Structural Polymorphism in Molecular Composites: Application to Energy Storage	Ouaaka E., et al.
MS40-P08	D	Morphology Characterization of Anatase TiO ₂ Nanocrystals by Advanced Rietveld Refinement of Powder X-Ray Diffraction Data [...]	Yu J.
MS40-P10	D	The Dynamic Structure of Au ₃₈ (SR) ₂₄ Nanoclusters Supported on CeO ₂ under CO Oxidation	Pollitt S., et al.
MS40-P12	D	Nanocrystalline Cd and (Cd,Mn)S Particles: Structure and Morphology	Cherepanova S., Evtushok B.
MS41-P02	D	Multiferroic Bi ₂ Fe ₄ O ₉ : Tuning of Crystallization Pathways and Kinetics	Kirsch A., Gesing T.
MS41-P04	D	Two New Polymorphs of CuCl ₂ ·2DMF Obtained via High-Temperature Crystallization	Goreshnik E.
MS41-P06	D	Dynamic Theory of Protein Crystallization	Hasek J., et al.
MS42-P02	E	Extracting Coherent Information About Phase Transformations in a Functional Material Studied by X-Ray Powder Diffraction	Gertenbach J., et al.
MS42-P04	E	SNBL's BM31 at ESRF Beyond 2020 - Combined XRD-PDF-XAS	van Beek W., et al.
MS42-P06	E	Testing a Home-Made Sample Holder with Flow-Through Capillary to Study in-situ Re-Solvation Process	Rohlicek J., et al.
MS42-P08	E	Latest Developments in Non-Ambient XRD Attachments from Anton Paar	Puhr B., et al.
MS42-P10	E	In-situ Wide-Angle X-Ray Scattering on Liquid Crystalline Elastomers for Orthopedic Applications	Dadivanyan N., et al.
MS42-P12	E	Operational Non-Uniformities of Lithium Distribution in Li-Ion Batteries Probed by Diffraction Techniques	Senyshyn A.
MS42-P14	E	Diffusion Mechanisms of Gas Adsorption by Porous Frameworks from Sub-Second Synchrotron Powder X-Ray Diffraction	Dovgaliuk I., et al.
MS43-P02	E	Instrumental Effects in Laboratory Pair Distribution Function (PDF) Analysis	Gateshki M., et al.
MS43-P04	E	Mapping Non-Crystalline Nanostructure With Low-dose Scanning Electron Pair Distribution Function Analysis	Laulainen J.E.I., et al.
MS43-P06	E	Investigation of the nanostructured materials by XRD method with use of simulation	Cherepanova, S
MS44-P02	E	Hydraulic, Structural and Photocatalytic Behavior of Cementitious Phases Incorporating Nanocomposite Mixed Zn-Al-Ti Oxydes	Amor F.
MS44-P04	E	Effects of X-Ray Irradiation and Thermal Annealing on the Co Dopant Location in Co-Doped TiO ₂ Nanocrystals	Soo Y.L., et al.
MS44-P06	E	Automated Serial Rotation Electron Diffraction Combined with Cluster Analysis as a Tool for Structure Determination	Smeets S., et al.
MS44-P08	E	Utilising MaXrd in the Study of Inclusion Compounds	Ramsnes S., et al.
MS44-P10	E	Indexing Grazing Incidence X-ray Diffraction Patterns of Thin Films	Salzmann I., et al.
MS45-P02	E	StructureFinder	Kratzert D.
MS46-P02	E	A Non-Ambient Single Crystal X-ray Diffraction Beamline at Taiwan Photon Source	Lee J-J., et al.
MS46-P04	E	The High Energy X-Ray Diffraction Beamline at the PETRA III Synchrotron Light Source at DESY	Noohinejad L., et al.
MS46-P06	E	Development of Microspectrophotometer for the Macromolecular Crystallography Beamline at the Photon Factory, Japan	Hikita M., et al.
MS46-P08	E	New Tricks for an Old Dog: The Powder Diffraction and Total Scattering Beamline P02.1 at PETRA III, DESY	Wharmby M., et al.
MS46-P10	E	Exploring New Data Collection Protocols with the Eiger2 Detector and SmarGon on the Variable and Microfocus Beamline I04 at [...]	Flaig R.
MS46-P12	E	FXE Status. Femtosecond X-Ray Experiments for Chemical Dynamics Research at the European Xfel	Rodriguez Fernandez A., et al.
MS46-P14	E	A New Single Crystal Diffractometer at BM20/ESRF	Hennig C., et al.
MS46-P16	E	Long-Wavelength Protein Crystallography at Diamond Light Source	Mykhalyyk V., et al.
MS46-P18	E	User Infrastructures at the Helmholtz-Zentrum Berlin für Materialien und Energie HZB	Wolter B.
MS48-P02	E	The HyPix-Arc 150°	White F., et al.
MS48-P04	E	CrysAlisPro 40: 64-bit, Synergy, HyPix-Arc 150°, AutoChem4.0, Ewald 3D	Meyer M.
MS48-P06	E	A Life with Crystallography...	Đakovic M.
MS48-P08	E	Olex2: Teaching New Software Old AND New Tricks	Puschmann H., Dolomanov O.

MS48-P10	E	Mathematical Justifications for Crystal Systems, Bravais Lattices and a New Continuous Classification	Kurlin V.
MS48-P12	E	Overcoming Ambiguous Tautomer Assignment in 1,2,4-triazole Crystal Structures	Schwalbe C.
MS48-P14	E	Teaching Old Tricks: Rotation Conventions in Crystallography and cryoEM	Urzhumtsev A., Urzhumtseva L.
MS48-P16	E	Absolute structure of (E)-2,2'-[3-(4-Fluorophenyl)prop-2-ene-1,1-diyl]bis(3-hydroxy-5,5-dimethylcyclohex-2-en-1-one)	Cha J. H.

Late Poster Session I (Monday & Tuesday, 16.00 - 17.00)

Poster number	Area	Title	Author
MS01-101	E	P14 TREXX: First Results From The Jurassic Beamline	Horrell. S., et al.
MS02-103	E	Long-Wavelength Native SAD Phasing at BL13-XALOC enabled by the presence of an Helium Cone	Calisto B., et al.
MS03-105	E	ContaMiner and ContaBase: Automated Identification of Unwantedly Crystallized Protein Contaminants	Arold S., et al.
MS03-107	E	Keeping muscle proteins in shape – UCS-proteins acting as myosin-specific quality control factors	Vogel A., et al.
MS03-109	E	How the pArg protein mark keeps the stress response kinase McsB under control	Hajdusits B., et al.
MS03-111	E	DNA Relaxase TraA of the G+ Plasmid pIP501 as Key Player in Bacterial Conjugation	Reisenbichler A.M.
MS04-113	E	Beam-Induced Movement Attenuation With Single Wall Carbon Nanotubes	Borsa C.
MS05-115	E	Structural studies of the atypical SLAMF3 receptor	Shaikh R., Burschowsky D.
MS05-117	E	The BEP1 Fic-domain: Unravelling the mechanism of narrow selectivity towards Rac GTPases	Huber M., et al.
MS07-119	E	Crystal structure of the crenarchaeal membrane family-2 glycosyltransferase reveals a minimal cellulose-synthase framework	Reichenbach T.
MS08-121	E	The ESCRT-III protein Vps24 forms double stranded filaments composed of domain-swapped dimers	Huber S., et al.
MS13-123	E	Halogenesis and biomineralization in the residual basins of the Aral Sea	Reykhard L., et al.
MS14-125	E	An occurrence of the acentric distortion due to Ag ⁺ /Bi ³⁺ ordering in the AgBi ₂ B ₅ O ₁₁ borate	Volkov S., et al.
MS14-127	E	Does the iota-alumina phase exist?	Lenz S., et al.
MS14-129	E	Multi-scale characterisation of the cationic disorder in the novel borate Sr ₆ Tb _{0.94} Fe _{1.06} (BO ₃) ₆	Péchev S., et al.
MS15-131	E	Thermal expansion of alluaudite group minerals (nickenichite and calciojohillerite)	Filatov S., et al.
MS15-133	E	Thermal Expansion of Alkaline-Earth Borates	Bubnova R., et al.
MS16-135	E	Synthesis and structural characterization of new salts containing 2-amino-3-methylpyridinium cations	Bednarchuk T.
MS16-137	E	Nanostructured flexible MOFs and related composite materials	Giménez Marqués M., et al.
MS05-139	E	Structural Characterization of the Linear Ubiquitin Chain Assembly Complex	Rodriguez a., et al.

Late Poster Session II (Wednesday & Thursday, 16.00 - 17.00)

Poster number	Area	Title	Author
MS20-100	E	Effect of the side-chain on the topology of coordination polymers of copper(II) with amino acids	Smokrovic K., et al.
MS21-102	E	Non-Spherical Form Factors and Crystallographic Refinement	Midgley L.
MS24-104	E	Magnetic textures in non-magnetic systems	Wolpert E., Goodwin A.
MS25-106	E	Exploration of Bragg in-line electron holography as a possible tool for crystal structure determination	Cassidy C., et al.
MS25-108	E	On the Design of a Dedicated Electron Diffractometer	Hovestreydt E., et al.
MS27-110	E	Towards phase transition in cocrystals of allylamine with aliphatic alcohols	Nowosielska B., et al.
MS30-112	E	Structural similarities of 2D and 3D water frameworks in 3,3-dimethyl-2-butylamine, tert-amylamine and azepane hydrates	Rzepinski P., et al.
MS32-114	E	2D Materials in Electron Microscope	Singh R.
MS32-116	E	Molecular interaction in hydrates of 4-methylpiperidine and 4-chloropiperidine	Socha P., et al.
MS33-118	E	Stability of non-toxic gamma-cyclodextrin-based metal-organic framework in various solvents	Kruk-Berzina K., et al.
MS33-120	E	The Crystalline Sponge Method for the Structural Determination of Non-Crystalline Compounds using Metal Organic Framework	Habib F.
MS33-122	E	Using Metal Organic Frameworks to Determine the Crystal Structures of Non-Crystalline Compounds	Lunn R., et al.
MS35-124	E	Structural chemistry of binary cocrystals of diamines and diols	Cichowicz G., et al.
MS35-126	E	Hybrid polyoxomolybdate systems based on rationally designed asymmetric carbohydrazones	Rubcic M., et al.
MS35-128	E	interactions in copper(II), nickel(II) and cobalt(II) complexes with N-methyl-, N-ethyl- and N-propylglycine: monomers, dimers and polymers	Matkovic-Calogovic D., et al.
MS36-130	E	Cocrystals of cyclopentylamine with alcohols. Synthesis and structural studies.	Sadocha A., et al.
MS36-132	E	Polymorphism in ionic co-crystals - structural characterization	Marek P., et al.
MS37-134	E	Configuration controlled crystal and/or gel formation of fully protected D-glucosamines	Harmat V., et al.
MS42-136	E	In Situ Crystallization of the Viscous Organosilicon Liquids	Volodin A., et al.
MS44-138	E	On phasing of oversampled diffraction data	Misnovs A., Mishnev A.
MS46-140	E	XALOC, the MX beamline at ALBA synchrotron: Current status and perspectives	Boer R., et al.