IUCrJ (2017). **4**, 87–99
https://doi.org/10.1107/S2052252516018315

Raw diffraction data preservation and reuse: overview, update on practicalities and metadata requirements

L. M. J. Kroon-Batenburg, J. R. Helliwell, B. McMahon and T. C. Terwilliger

There are rapid developments in storage options for the preservation and reuse of raw data within the scientific domain of the IUCr and its Commissions. Formulation of improved metadata descriptors for the raw data is under way. Science policy makers strive towards an 'Open Science' model within which crystallographers will increasingly work in the future. Case studies are described that show the community's progress.

IUCrJ (2016). **3**, 319–325
https://doi.org/10.1107/S2052252516010514

Neutron structure of human carbonic anhydrase II in complex with methazolamide: mapping the solvent and hydrogen-bonding patterns of an effective clinical drug

M. Aggarwal, A. Y. Kovalevsky, H. Velazquez, S. Z. Fisher, J. C. Smith and R. McKenna

The room-temperature X-ray/neutron structure of human carbonic anhydrase II in complex with methazolamide has been determined. The study provides new insights into the hydrogen-bonding changes that take place within the active site of an enzyme upon drug binding.

IUCrJ (2016). **3**, 296–297
https://doi.org/10.1107/S2052252516013439

Neutron crystallography aids in drug design

M. P. Blakeley

Because drugs bind to their targets through directional H bonding and non-directional hydrophobic and electrostatic interactions, neutron crystallography can help guide structure-based drug design. A commentary is given on the Aggarwal article listed above.

Physics and free electron laser science and technology

IUCrJ (2017). **4**, 322–339
https://doi.org/10.1107/S2052252517005760

XFELs for structure and dynamics in biology

J. C. H. Spence

The use of X-ray lasers to obtain structures and molecular movies in biology is reviewed. Methods include single-particle imaging, serial crystallography and fast solution scattering at room temperature.

IUCrJ (2016). **3**, 127–138
https://doi.org/10.1107/S2052252516001238

Whole-pattern fitting technique in serial femtosecond nanocrystallography

R. A. Dilanian, S. R. Williams, A. V. Martin, V. A. Streltsov and H. M. Quiney

The whole-pattern fitting technique, originally designed for one-dimensional powder diffraction crystallography, is reconsidered and applied to the analysis of higher-dimensional serial femtosecond X-ray crystallography data. For nanocrystals with a small number of unit cells, the whole-pattern fitting approach is shown to be more accurate than integration-based Monte Carlo methods.

IUCrJ (2017). **4**, 24–36
https://doi.org/10.1107/S2052252516016730

Orientational order of liquids and glasses *via* fluctuation diffraction

A. V. Martin

A new method of extracting distributions of orientational order, like bond angles, from fluctuation diffraction data is presented. It has potential applications to the study of liquids, glasses and other systems that lack long-range order.

IUCrJ (2016). **3**, 420–429
https://doi.org/10.1107/S2052252516013956

Angular correlations of photons from solution diffraction at a free-electron laser encode molecular structure

D. Mendez *et al.*

An atomic twinning structure is observed by averaging intensity correlations from many snapshots of gold nanoparticles in solution.

IUCrJ (2016). **3**, 180–191
https://doi.org/10.1107/S2052252516002980

Protein structure determination by single-wavelength anomalous diffraction phasing of X-ray free-electron laser data

K. Nass *et al.*

A systematic analysis of anomalous diffraction data obtained by serial femtosecond crystallography at an XFEL is presented and sulfur SAD phasing of SFX data from thaumatin microcrystals is demonstrated.

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Selected articles from the IUCr's flagship open-access journal

journals.iucr.org

One hundred years after the first Nobel Prize to crystallography to Laue in 1914, the IUCr celebrated the impact and influence of crystallography by launching a comprehensive, all-inclusive open-access journal *IUCrJ* with the aim of it becoming the '*PNAS* of the IUCr'. Here, we highlight some of the key papers that have been published in 2016 and 2017 covering the whole range of sciences and technology. We encourage you all to consider the journal alongside other notable journals such as *PNAS*, *JACS*, *Nature Communications* and *Nature Materials*. – Samar Hasnain

Biology and medicine

IUCrJ (2017). **4**, 308–321
https://doi.org/10.1107/S2052252517009241

Protein crystallography and drug discovery: recollections of knowledge exchange between academia and industry

T. L. Blundell

Structure-guided drug discovery is a story of applications of protein crystallography and knowledge exchange between academia and industry. It has led to new drug approvals by the FDA in the USA and hope for treatment of rare genetic diseases and infectious diseases in the developing world.

IUCrJ (2016). **3**, 3–7
http://dx.doi.org/10.1107/S2052252515023738

CryoEM at IUCrJ: a new era

S. Subramaniam, W. Kühlbrandt and R. Henderson

In this overview, the authors briefly outline recent advances in electron cryomicroscopy (cryoEM) and explain why the journal **IUCrJ** can provide a natural home for publications covering many present and future developments in the cryoEM field.

IUCrJ (2017). **4**, 393–399
https://doi.org/10.1107/S2052252517005243

Segregation of lipids near acetylcholine-receptor channels imaged by cryo-EM

N. Unwin

A single-particle helical reconstruction from cryo-EM images reveals a segregated distribution of lipids around acetylcholine-receptor channels in the outer leaflet of the bilayer. The existence of a cholesterol-rich microdomain next to the receptor suggests how this lipid ensures a productive conformational change when acetylcholine binds, triggering the channel to open.

IUCrJ (2016). **3**, 271–281
https://doi.org/10.1107/S205225151600823X

Serial crystallography captures enzyme catalysis in copper nitrite reductase at atomic resolution from one crystal

S. Horrell, S. V. Antonyuk, R. R. Eady, S. S. Hasnain, M. A. Hough and R. W. Strange

Serial crystallography has been used to drive copper nitrite reductase through its enzymatic cycle while sampling the same volume of a single cryogenically maintained crystal. A movie of X-ray-driven enzyme catalysis reveals the structural changes that occur during the catalytic reaction in unprecedented detail.

IUCrJ (2016). **3**, 88–95
http://dx.doi.org/10.1107/S2052252515022927

In cellulo serial crystallography of alcohol oxidase crystals inside yeast cells

A. J. Jakobi *et al.*

The application of serial femtosecond crystallography to naturally occurring peroxisomal protein crystals within yeast cells is described. The concept of utilizing peroxisomes for the production of protein nanocrystals is outlined.

IUCrJ (2016). **3**, 10–19
http://dx.doi.org/10.1107/S2052252515019971

Peptide binding to a bacterial signal peptidase visualized by peptide tethering and carrier-driven crystallization

Y. T. Ting, P. W. R. Harris, G. Batot, M. A. Brimble, E. N. Baker and P. G. Young

Utilizing a peptide-anchoring strategy, transient signal-peptide complexes of a Gram-positive bacterial signal peptidase were trapped, revealing the atomic details of their interaction.

IUCrJ (2016). **3**, 440–447
https://doi.org/10.1107/S2052252516016018

Resolution of *ab initio* shapes determined from small-angle scattering

A. T. Tuukkanen, G. J. Kleywegt and D. I. Svergun

A quantitative resolution measure of the *ab initio* shapes restored from small-angle scattering data is introduced based on the variability of multiple reconstructions. The new measure is validated in simulated examples and its efficiency has been demonstrated in applications to experimental data.

IUCrJ (2017). **4**, 50–64
https://doi.org/10.1107/S2052252516018017

CADEE: Computer-Aided Directed Evolution of Enzymes

B. A. Amrein, F. Steffen-Munsberg, I. Szeler, M. Purg, Y. Kulkarni and S. C. L. Kamerlin

A new computational tool, *CADEE* (Computer-Aided Directed Evolution of Enzymes), is presented.

IUCrJ (2016). **3**, 115–126
https://doi.org/10.1107/S2052252515024161

High-resolution neutron and X-ray diffraction room-temperature studies of an H-FABP–oleic acid complex: study of the internal water cluster and ligand binding by a transferred multipolar electron-density distribution

E. I. Howard *et al.*

Neutron and high-resolution X-ray crystallography were used to determine fully the structure of the internal water cluster in H-FABP. Analysis of the orientation and electrostatic properties of the water molecules showed significant alignment of the permanent dipoles of the water molecules with the protein electrostatic field.

Chemistry and crystal engineering

IUCrJ (2016). **3**, 139–151
https://doi.org/10.1107/S2052252515024379

The crystalline sponge method updated

M. Hoshino, A. Khutia, H. Xing, Y. Inokuma and M. Fujita

The protocols of the crystalline sponge method, particularly those in the soaking, data collection and refinement processes, are considerably improved to give reliable structural information.

IUCrJ (2016). **3**, 402–407
https://doi.org/10.1107/S2052252516013762

Constructing covalent organic frameworks in water *via* dynamic covalent bonding

J. Thote *et al.*

The present work effectively highlights the utilization of Dynamic Covalent Chemistry (DCC) principles in conjunction with the keto-enol tautomerism to synthesize useful, stable, crystalline and porous Covalent Organic Frameworks (COFs) in water, which thereby merits over the conventional solvothermal COF synthesis protocol with its simpler and greener appeal.

IUCrJ (2016). **3**, 354–366
https://doi.org/10.1107/S2052252516012574

Cooperative Jahn–Teller effect and the role of strain in the tetragonal-to-cubic phase transition in $Mg_xCu_{1-x}Cr_2O_4$

S. C. Tarantino, M. Giannini, M. A. Carpenter and M. Zema

In the $Mg_xCu_{1-x}Cr_2O_4$ solid solution, progressive substitution of the Jahn–Teller and d^9 Cu^{2+} cation with the spherical and closed-shell Mg^{2+} cation results in a gradual reduction of the splitting of *a* and *c* unit-cell parameters, until transformation occurs from the tetragonal $I4_1/amd$ to the cubic $Fd\bar{3}m$ archetype spinel structure.

IUCrJ (2016). **3**, 341–353
https://doi.org/10.1107/S2052252516010472

An exceptional series of phase transitions in hydrophobic amino acids with linear side chains

C. H. Görbitz, P. Karen, M. Dusek and V. Petrícek

Four amino acids with linear, hydrophobic side chains display an unprecedented series of solid-state phase transitions between 100 and 470 K. These involve hydrogen-bond rearrangements, sliding of molecular bilayers in one or two dimensions and development of side-chain disorder.

IUCrJ (2016). **3**, 367–376
https://doi.org/10.1107/S2052252516013129

Observation of a re-entrant phase transition in the molecular complex tris(μ_2-3,5-diisopropyl-1,2,4-triazolato-κ^2N^1:N^2)trigold(I) under high pressure

C. H. Woodall *et al.*

Single-crystal crystallography shows that one polytype of the Au^I trimer tris(μ_2-3,5-diisopropyl-1,2,4-triazolato-κ^2N^1:N^2)trigold(I), $[Au_3(N_3C_8H_{14})_3]$, undergoes four successive phase transitions between 1 and 3.5 GPa, driven by aurophilic interactions, and that the ambient-pressure structure re-emerges at high pressure.

IUCrJ (2017). **4**, 411–419
https://doi.org/10.1107/S2052252517004262

Halogen bonding in hypervalent iodine and bromine derivatives: halonium salts

G. Cavallo, J. S. Murray, P. Politzer, T. Pilati, M. Ursini and G. Resnati

The presence of halogen bonds in some hypervalent iodine and bromine derivatives is demonstrated. Hypervalent atoms in polyatomic cations and anions do have σ-holes on the extensions of their covalent bonds and the cation holes are influential on the crystal lattice structures of halonium salts.

IUCrJ (2017). **4**, 350–359
https://doi.org/10.1107/S2052252517006042

NMR crystallography: structure and properties of materials from solid-state nuclear magnetic resonance observables

D. L. Bryce

This topical review provides a brief overview of recent developments in NMR crystallography and related NMR approaches to studying the properties of molecular and ionic solids.

IUCrJ (2017). **4**, 369–379
https://doi.org/10.1107/S2052252517005917

Making crystals with a purpose; a journey in crystal engineering at the University of Bologna

D. Braga, F. Grepioni, L. Maini and S. d'Agostino

The bottom-up preparation of mixed crystals, co-crystals and photoreactive materials starting from molecular building blocks across the borders of organic, organometallic and metal–organic chemistry is described in this topical review.

Materials and computation

IUCrJ (2016). **3**, 237–246
https://doi.org/10.1107/S2052252516006242

Quantum crystallographic charge density of urea

M. E. Wall

A charge-density model of urea was calculated using quantum theory and was refined against publicly available ultra-high-resolution X-ray diffraction data. The quantum model differs from a multipole model but agrees comparably with the data; quantum crystallography therefore can provide unique and accurate charge-density models.

IUCrJ (2016). **3**, 71–83
https://doi.org/10.1107/S2052252515019727

Advanced electron crystallography through model-based imaging

S. Van Aert, A. De Backer, G. T. Martinez, A. J. den Dekker, D. Van Dyck, S. Bals and G. Van Tendeloo

An overview of statistical parameter estimation methods is presented and applied to analyse transmission electron microscopy images in a quantitative manner.

IUCrJ (2016). **3**, 20–31
https://doi.org/10.1107/S2052252515018722

Total scattering and pair distribution function analysis in modelling disorder in PZN ($PbZn_{1/3}Nb_{2/3}O_3$)

R. E. Whitfield, D. J. Goossens and T. R. Welberry

The ability of the pair distribution function analysis of total scattering from a powder to determine the local ordering in ferroelectric PZN ($PbZn_{1/3}Nb_{2/3}O_3$) is explored by comparing it with a model established using single-crystal diffuse scattering.

IUCrJ (2016). **3**, 377–388
https://doi.org/10.1107/S2052252516012707

Carrier concentration dependence of structural disorder in thermoelectric $Sn_{1-x}Te$

M. Sist *et al.*

The crystal structure of SnTe is investigated from 20 to 800 K in two samples with different carrier concentrations by single-crystal and powder synchrotron X-ray diffraction, coupled with maximum entropy analysis.

IUCrJ (2016). **3**, 108–114
https://doi.org/10.1107/S205225151502271X

Real-time direct and diffraction X-ray imaging of irregular silicon wafer breakage

A. Rack, M. Scheel and A. N. Danilewsky

Crack propagation in an Si wafer under thermal stress is depicted by combining diffraction and transmission X-ray imaging. The use of synchrotron radiation allows for the high imaging frame rates required to follow the crack dynamics in real time.

IUCrJ (2016). **3**, 8–9
https://doi.org/10.1107/S2052252515024033

Perovskites take the lead in local structure analysis

D. A. Keen

Materials with the much-loved perovskite structure are being used to develop and test new methods for interpreting local structural arrangements in crystals, and these methods are in turn uncovering unexpected new structural insight.

Neutron and synchrotron science and technology

IUCrJ (2016). **3**, 43–50
https://doi.org/10.1107/S2052252515018795

Protein crystal structure from non-oriented, single-axis sparse X-ray data

J. L. Wierman, T.-Y. Lan, M. W. Tate, H. T. Philipp, V. Elser and S. M. Gruner

Using the *EMC* algorithm, the three-dimensional intensity was successfully reconstructed from millions of non-oriented, sparse data frames collected from a hen egg-white lysozyme crystal rotating about a single axis. The protein structure was solved from the reconstructed intensity. This result is encouraging for the development of synchrotron-based serial microcrystallography.