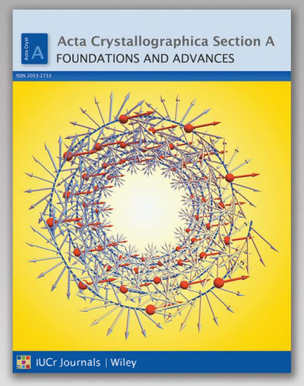

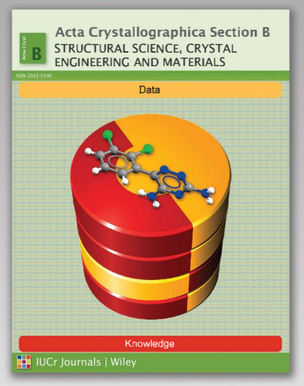

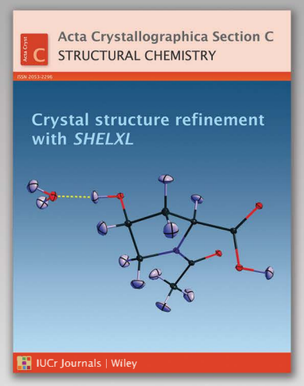

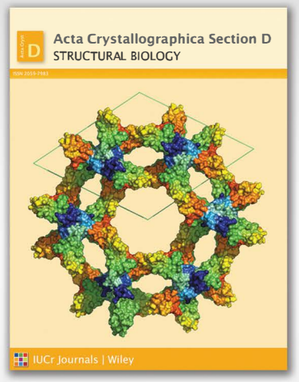

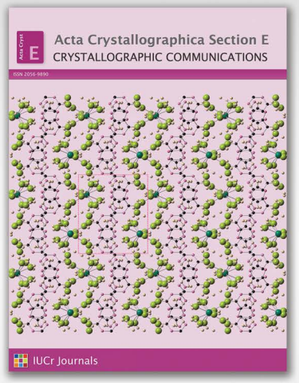

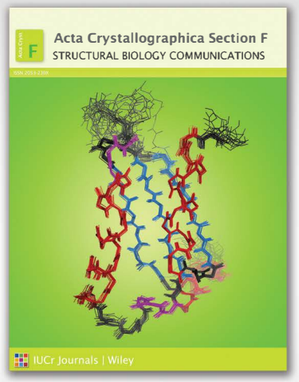

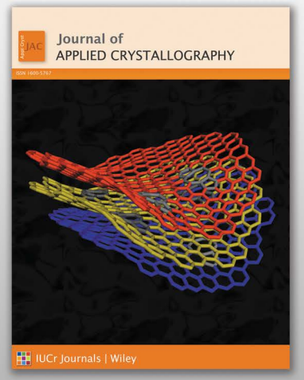

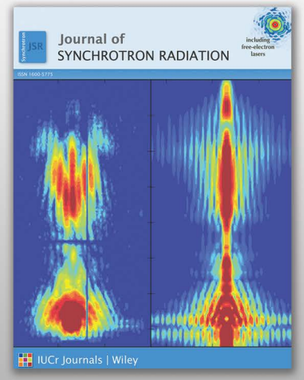

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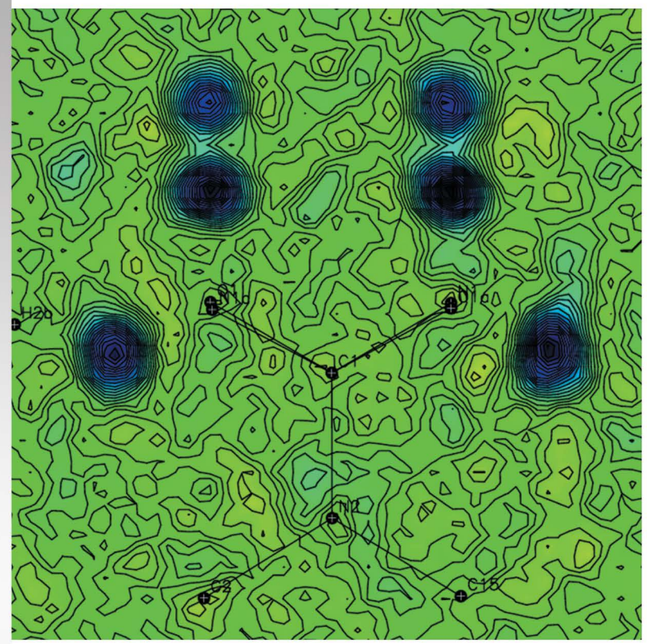
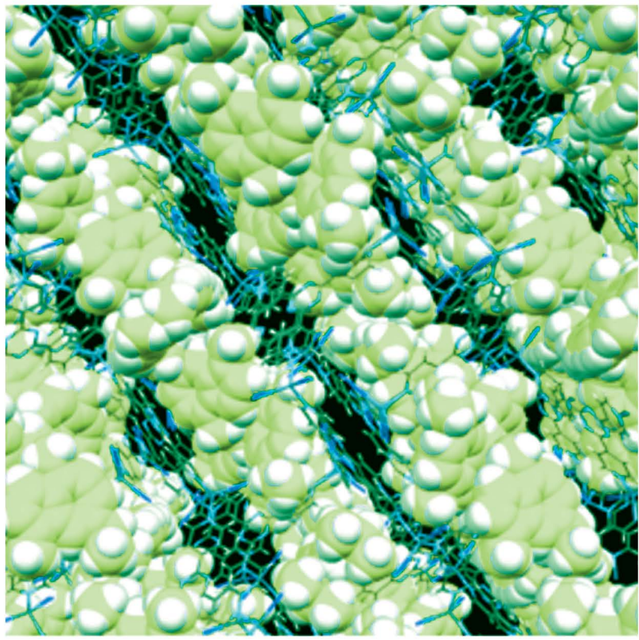
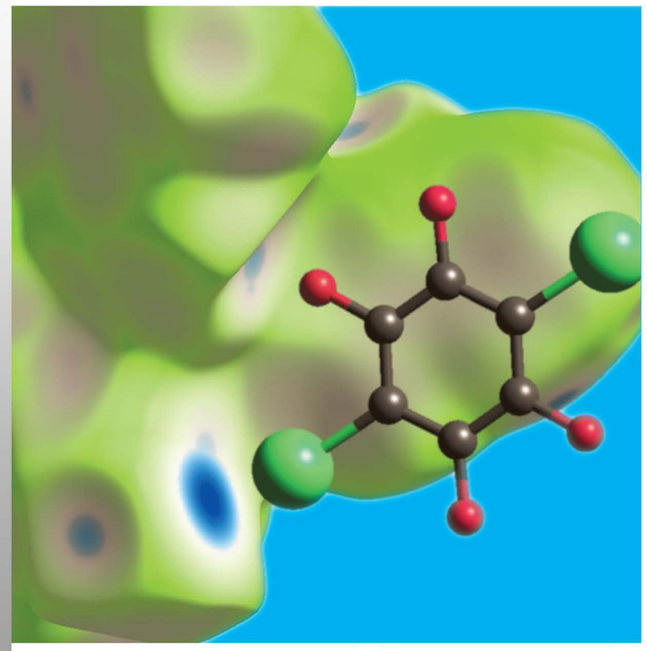
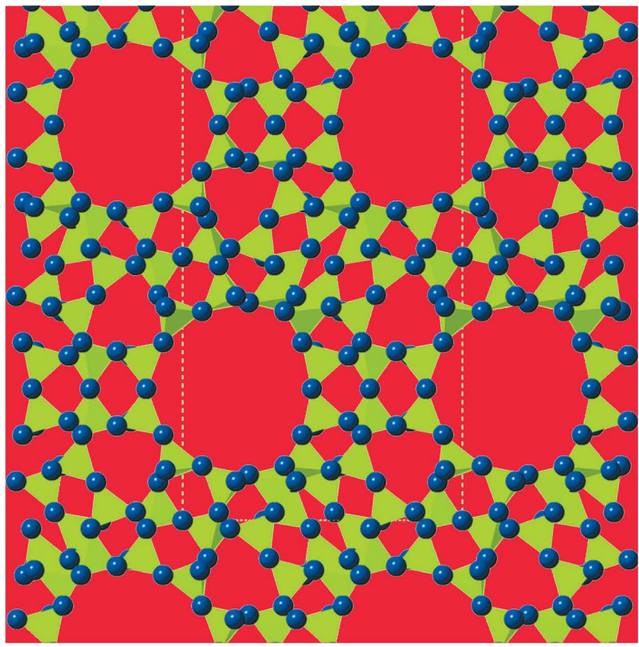
Chemistry from IUCr journals









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Bonding

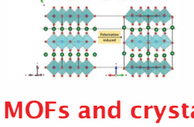
IUCrJ (2015). **2**, 157–158
http://dx.doi.org/10.1107/S2052252515002006

Intermolecular atom–atom bonds in crystals?

J. D. Dunitz

Some questions are raised concerning the interpretation of distances between atoms of neighbouring molecules in crystals.

Acta Cryst. (2015). C**71**, 991–995
http://dx.doi.org/10.1107/S2053229615019002

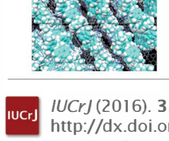


Halogen bonds on demand: I···S contacts in cocrystals of *trans*-bis(thiocyanato-κ*N*)tetrakis(4-vinylpyridine-κ*N*)nickel(II) and 2,3,5,6-tetrafluoro-1,4-diiodobenzene

M.-D. Serb, C. Merkens, I. Kalf and U. Englert

A short S···I halogen bond occurs in the cocrystal formed by dithiocyanatotetrakis(4-vinylpyridine)-nickel(II) and 2,3,5,6-tetrafluoro-1,4-diiodobenzene. Such halogen bonds to sulfur are significantly less common than to smaller electronegative atoms.

IUCrJ (2015). **2**, 675–690
http://dx.doi.org/10.1107/S2052252515014608



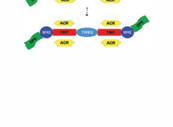
Supramolecular interactions in the solid state

G. Resnati, E. Boldyreva, P. Bombicz and M. Kawano

Supramolecular interactions in the solid state are discussed in the context of crystal engineering. Specific topics include halogen bonding, ambient and non-ambient conditions, isostructurality and polymorphism, and kinetic assembly of coordination polymers.

Biochemistry

Acta Cryst. (2016). C**72**, 35–47
http://dx.doi.org/10.1107/S2053229615022536



3':5'-Cyclic nucleotides: two sodium salts of cdTMP

K. A. Slepokura

Two salts of thymidine 3':5'-cyclic phosphate (cdTMP), namely Na(cdTMP)·7H2O, with *Z'* = 1, and Na(cdTMP)·3.7H2O, with *Z'* = 8, are compared in terms of cyclic nucleotide conformation, inter-nucleotide interactions and nucleotide–sodium interactions.

Hydrogen storage materials

Acta Cryst. (2016). B**72**, 232–240
http://dx.doi.org/10.1107/S2052520616000093

Molecular structure of diethylaminoalane in the solid state: an X-ray powder diffraction, DFT calculation and Raman spectroscopy study

T. Bernert, M. B. Ley, J. Ruiz-Fuertes, M. Fischer, M. Felderhoff and C. Weidenthaler

The density functional theory (DFT) calculations were validated by calculating the ground state structures of two known aminoalanes while the Raman spectrum of diethylaminoalane was measured and compared to the simulated ones.

Magnetic materials

Acta Cryst. (2016). B**72**, 3–19
http://dx.doi.org/10.1107/S2052520615022106

Hexagonal RMnO$_3$: a model system for two-dimensional triangular lattice antiferromagnets

H. Sim, J. Oh, J. Jeong, M. Le and J.-G. Park

A review of the crystal and magnetic structure as well as the spin dynamics of two-dimensional triangular lattice multiferroic hexagonal manganite RMnO$_3$ is presented.

MOFs and crystal engineering

IUCrJ (2016). **3**, 139–151
http://dx.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**, 96–101
http://dx.doi.org/10.1107/S2052252515023945

Four- and five-component molecular solids: crystal engineering strategies based on structural inequivalence

N. A. Mir, R. Dubey and G. R. Desiraju

A logic driven synthetic approach is used in this first report of the isolation of stoichiometric four-component molecular solids. A possible extension to a five-component solid is also described.

Acta Cryst. (2015). B**71**, 587–607
http://dx.doi.org/10.1107/S2052520615018168

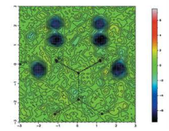
Structural studies of metal–organic frameworks under high pressure

S. McKellar and S. Moggach

A review on the effect of high pressure on metal–organic framework materials is presented.

Pharmaceuticals

Acta Cryst. (2016). B**72**, 39–50
http://dx.doi.org/10.1107/S2052520615019538

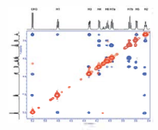


Electron density, disorder and polymorphism: high-resolution diffraction studies of the highly polymorphic neuralgic drug carbamazepine

I. Sovago, M. Gutmann, H. Senn, L. Thomas, C. Wilson and L. Farrugia

An experimental charge density study on polymorph (III) of carbamazepine is in excellent agreement with theory and a Hirshfeld atom refinement based on the X-ray data provides positional and anisotropic displacement parameters for the H atoms closely similar to those obtained from the neutron diffraction data.

Acta Cryst. (2016). C**72**, 14–20
http://dx.doi.org/10.1107/S2053229615022305

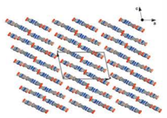


Structural corroboration of two important building blocks of the anticancer drug eribulin mesylate through 2D NMR and single-crystal X-ray diffraction studies

S. V. Pullela, V. Acharya, N. Reddy, J. Harlikar, A. Kulkarni, R. Chavan, A. Yadav, S. Manna and A. Ghosh

Two building blocks having a major influence on the stereochemical orchestration of the drug molecule eribulin mesylate were prepared and their 2D-NMR spectra generated. These data were corroborated by the single-crystal X-ray diffraction data generated for these molecules.

Acta Cryst. (2016). B**72**, 263–273
http://dx.doi.org/10.1107/S2052520615024956



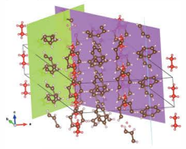
New polymorphs of an old drug: conformational and synthon polymorphism of 5-nitrofurazone

D. Pogoda, J. Janczak and V. Videnova-Adrabinska

Two new polymorphic forms of 5-nitrofurazone have been synthesized and structurally characterized by single-crystal and powder X-ray diffraction methods, vibrational spectroscopy, thermal and Hirshfeld surface analysis.

Planetary chemistry

IUCrJ (2016). **3**, 192–199
http://dx.doi.org/10.1107/S2052252516002815



A co-crystal between benzene and ethane: a potential evaporite material for Saturn's moon Titan

H. E. Maynard-Casely, R. Hodyss, M. L. Cable, T. H. Vu and M. Rahm

A 3:1 stoichiometric co-crystal of benzene and ethane has been structurally characterized at 90 K using synchrotron powder X-ray diffraction following *in situ* crystal growth at 130 K. The conditions under which the co-crystal forms identify it as a potential evaporite material on the surface of Saturn's moon Titan.

Structure determination and crystallographic databases

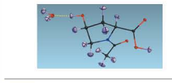
Acta Cryst. (2015). A**71**, 3–8
http://dx.doi.org/10.1107/S2053273314026370

SHELXT – Integrated space-group and crystal-structure determination

G. M. Sheldrick

SHELXT automates routine small-molecule structure determination starting from single-crystal reflection data, the Laue group and a reasonable guess as to which elements might be present.

Acta Cryst. (2015). C**71**, 3–8
http://dx.doi.org/10.1107/S2053229614024218

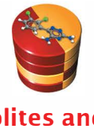


Crystal structure refinement with *SHELXL*

G. M. Sheldrick

New features added to the refinement program *SHELXL* since 2008 are described and explained.

Acta Cryst. (2016). B**72**, 171–179
http://dx.doi.org/10.1107/S2052520616003954



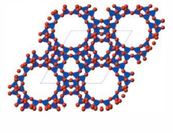
The Cambridge Structural Database

C. R. Groom, I. J. Bruno, M. P. Lightfoot and S. C. Ward

This paper is the definitive article describing the creation, maintenance, information content and availability of the Cambridge Structural Database (CSD), the world's repository of small molecule crystal structures.

Zeolites and frameworks

Acta Cryst. (2015). B**71**, 641–647
http://dx.doi.org/10.1107/S2052520615018739



Intrinsic flexibility of porous materials; theory, modelling and the flexibility window of the EMT zeolite framework

R. E. Fletcher, S. A. Wells, K. M. Leung, P. P. Edwards and A. Sartbaeva

Framework flexibility properties in energy materials are reviewed and novel results on the flexibility window of the EMT zeolite framework containing 18-crown-6 ether as a structure directing agent are presented.