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COVER ILLUSTRATION *Front cover* with the friendly assistance of Rainer Pöttgen and Václav Petříček. Crystallographic Computing System JANA2006: General features (cf. Graphical Abstract Figure of Petříček, Dušek & Palatinus, pp. 345–352, this issue).

Graphical Synopsis

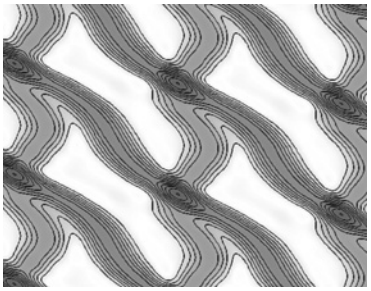
Review Article

Václav Petříček, Michal Dušek and Lukáš Palatinus

Crystallographic Computing System JANA2006: General features

DOI 10.1515/zkri-2014-1737
Z. Kristallogr. 2014; 229(5): 345–352

Synopsis: JANA2006 is a crystallographic software for calculation of standard, modulated and magnetic structures from X-ray, neutron or electron diffraction data. The article summarizes features and possibilities of its latest version.



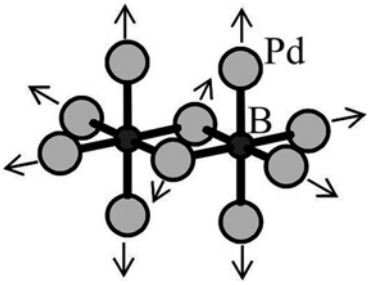
Inorganic Crystal Structures

Andreas Leineweber, Tilmann Georg Berger, Alexander Udyansky, Volodymyr N. Bugaev and Viola Duppel

The incommensurate crystal structure of the Pd_5B_{1-z} phase; B ordering driven by elastic interaction between B atoms

DOI 10.1515/zkri-2013-1710
Z. Kristallogr. 2014; 229(5): 353–367

Synopsis: The incommensurately modulated crystal structure of Pd_5B_{1-z} is characterised by B ordering in volving occurrence of B_2Pd_{10} double octahedra due to the predominance of elastic interaction between the B atoms.



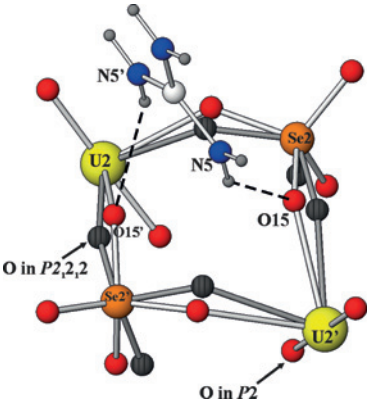
Organic and Metalorganic Crystal Structures

Vladislav V. Gurzhiy, Darya V. Tyshchenko, Sergey V. Krivovichev and Ivan G. Tananaev

Symmetry reduction in uranyl compounds with $[(UO_2)_2(TO_4)_3]^{2-}$ (T = Se, S, Mo) layers: crystal structures of the new guanidinium uranyl selenate and methylammonium uranyl sulfate

DOI 10.1515/zkri-2013-1651
Z. Kristallogr. 2014; 229(5): 368–377

Synopsis: The symmetry reduction of the new guanidinium uranyl selenate and methylammonium uranyl sulfate is induced by the hydrogen-bond interactions of amine groups emanated from organic substructure with the oxygen atoms from the inorganic layered complexes.

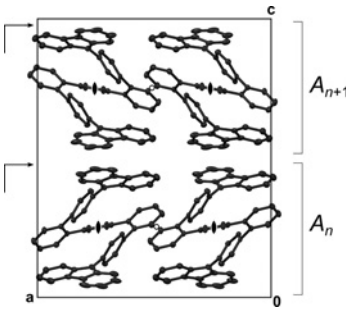


Berthold Stöger, Paul Kautny, Daniel Lumpi, Erich Zobetz and Johannes Fröhlich

The pseudo-inversion symmetry of 9,9′-(1,3,4-oxadiazole-2,5-diyldi(1,1′-biphenyl)-2′,4-diyl)bis[9*H*-carbazole] in the light of OD theory

DOI 10.1515/zkri-2014-0001
Z. Kristallogr. 2014; 229(5): 378–384

Synopsis: The crystal structure of the title compound features pseudo-inversion strictly valid only for distinct layers. A parameter quantifying the deviation from perfect centrosymmetry is obtained by application of the order-disorder theory.

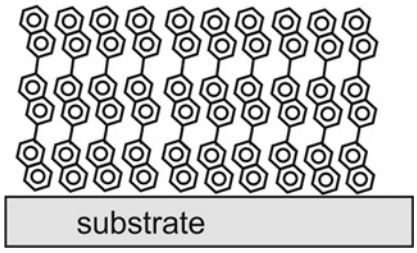


Alexander Pichler, Roland Resel, Alfred Neuhold, Theo Dingemans, Günther Schwabegger, Massimo Moret, Clemens Simbrunner and Ingo Salzmann

Crystal structure determination of organic thin-films: the example of 2,2′:6′,2″-ternaphthalene

DOI 10.1515/zkri-2013-1704
Z. Kristallogr. 2014; 229(5): 385–393

Synopsis: The solution of a crystal structure from a thin film is exemplarily shown for the molecule ternaphthalene using grazing incidence X-ray diffraction. The introduced method allows the study of specific polymorphs which are present only within thin films.

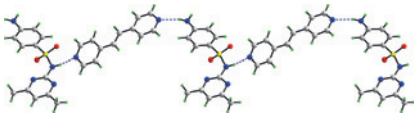


Hadi D. Arman, Trupta Kaulgud and Edward R. T. Tiekink

1:1 Co-crystals of sulfadimidine with three bipyridine-type molecules: Persistence of N–H…N hydrogen bonded supramolecular chains

DOI 10.1515/zkri-2013-1706
Z. Kristallogr. 2014; 229(5): 394–404

Synopsis: Non-linear supramolecular chains sustained by amino- and amide-H…N(pyridyl) hydrogen bonds feature in the co-crystals formed between sulfadimidine and pyridyl donors [4,4′-bipyridine, 4-[(E)-2-(pyridin-4-yl) ethenyl]pyridine and 4-[2-(pyridin-4-yl) ethyl]pyridine].



Crystallographic Computing

Ross J. Angel, Javier Gonzalez-Platas and Matteo Alvaro

EosFit7c and a Fortran module (library) for equation of state calculations

DOI 10.1515/zkri-2013-1711
Z. Kristallogr. 2014; 229(5): 405–419

Synopsis: EosFit7c is a new program to perform EoS calculations and fitting for both volume and linear (unit-cell parameter) data in P, T and P-T. A new module for EoS calculations is provided in the CrysFML library.