Graphical Synopsis

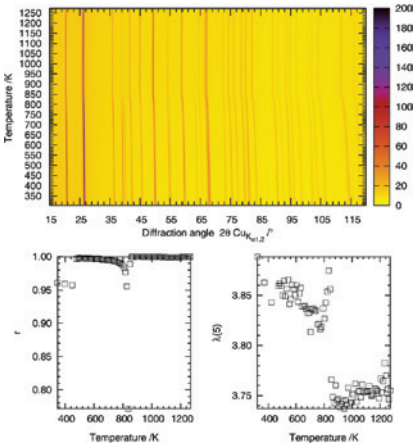
Inorganic Crystal Structures

Lars Robben

On the autocorrelation method of external parameter depending data-sets

DOI 10.1515/zkri-2016-2000
Z. Kristallogr. 2017; 232(4): 267–277

Synopsis: The autocorrelation method is applied on spectroscopic and diffraction data sets depending on an external parameter. A single parameter is presented, which characterizes each single data file. For FTIR data the calculation effort is reduced in comparison to the known Δcorr parameter. In the case of X-ray powder diffraction data, the usefulness of the parameter and the advantages over Pearson's *r*-value are discussed.

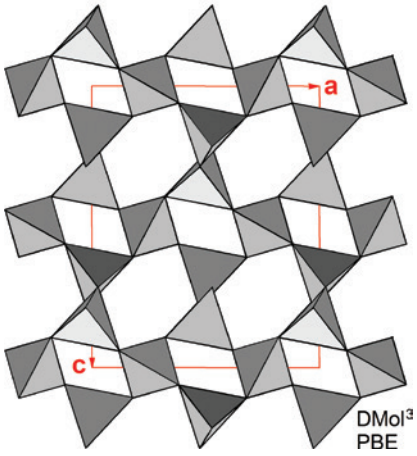


Hans Grimmer and Bernard Delley

Comparison of experimental and theoretical results for the structure and elastic properties of moganite

DOI 10.1515/zkri-2016-1997
Z. Kristallogr. 2017; 232(4): 279–286

Synopsis: The shape of the oxygen tetrahedra in monoclinic moganite has been determined more reliably by density functional theory (DFT) calculations than by experiment. The most convincing DFT results for the binding angles in moganite have been obtained for the DMol^3 code with functional PBE.



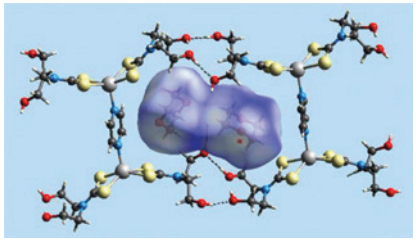
Organic and Metalorganic Crystal Structures

Mukesh M. Jotani, Pavel Poplaukhin, Hadi D. Arman and Edward R.T. Tiekink

Supramolecular association in (μ_2-pyrazine)-tetrakis(N,N-bis(2-hydroxyethyl)dithiocarbamato) dizinc(II) and its di-dioxane solvate

DOI 10.1515/zkri-2016-2014
Z. Kristallogr. 2017; 232(4): 287–298

Synopsis: Three-dimensional molecular packing based on hydroxyl-O–H···O(hydroxyl) is found in {Zn[$S_2CN(CH_2CH_2OH)_2$]$_2$}$_2$(pyrazine) and its dioxane solvate.

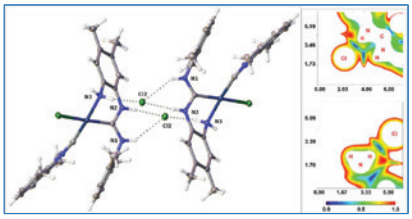


Mikhail A. Kinzhalov, Alexander S. Novikov, Alexander N. Chernyshev and Vitalii V. Suslonov

Intermolecular hydrogen bonding H···Cl⁻ in the solid palladium(II)-diaminocarbene complexes

DOI 10.1515/zkri-2016-2018
Z. Kristallogr. 2017; 232(4): 299–305

Synopsis: Weak intermolecular non-covalent H···Cl⁻ interactions in the solid chelated palladium(II)-diaminocarbene complex *cis*-[PdCl(CNXyl){C(NHXyl) = $NHC_6H_2Me_2NH_2$}]Cl (**3**; Xyl = 2,6-$Me_2C_6H_3$) were studied by XRD followed by appropriate DFT calculations.

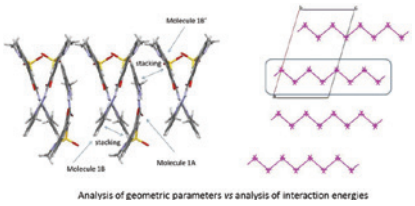


Svitlana V. Shishkina, Igor V. Ukrainets and Lidiya A. Petrushova

Competition between intermolecular hydrogen bonding and stacking in the crystals of 4-Hydroxy-*N*-(pyridin-2-yl)-2,2-dioxo-1*H*-2λ⁶,1-benzothiazine-3-carboxamides

DOI 10.1515/zkri-2016-2011
Z. Kristallogr. 2017; 232(4): 307–316

Synopsis: In contrast to the usual study of geometric characteristics of intermolecular interactions, the analysis of the pairwise interaction energies between molecules in crystal phase by quantum-chemical calculations has revealed the dominating role of stacking interactions in spite of the presence of N-H...O intermolecular hydrogen bonds.

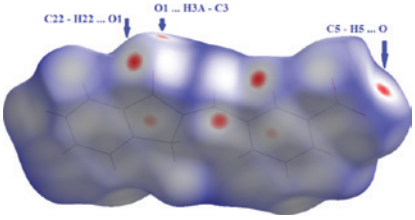


Thomas C. Baddeley, Ligia R. Gomes, John N. Low, Janet M.S. Skakle, Alan B. Turner, James L. Wardell and Graeme J.R. Watson

Structural studies of (*E*)-2-(benzylidene)-2,3-dihydro-1H-inden-1-one derivatives: crystal structures and Hirshfeld surface analysis

DOI 10.1515/zkri-2016-2020
Z. Kristallogr. 2017; 232(4): 317–333

Synopsis: The PLATON and Hirshfeld surface analyses gave consistent and complementary results although the Hirshfeld surface analysis indicated the significance of weak C–H–O interactions beyond the cutoff parameters given by PLATON.



Corrigendum
Formulae Index