Graphical Synopsis

Micro Review

Theresa Block, Stefan Seidel and Rainer Pöttgen
BÄRNIGHAUSEN TREES – A group-subgroup reference database

Synopsis: A group-subgroup reference database.

https://doi.org/10.1515/zkri-2022-0021

Inorganic Crystal Structures

Volker Kahlenberg and Hannes Krüger
High-temperature behavior and structural studies on Ca_{14}Al_{10}Zn_{6}O_{35}

Synopsis: Natural tiling of the tetrahedral framework compound Ca_{14}Al_{10}Zn_{6}O_{35} that has been studied between ambient temperature and 790 °C by in-situ single-crystal diffraction. The four fundamental cages of the 3D-net are indicated with different colors.

https://doi.org/10.1515/zkri-2022-0014
Nilanjan Roy, Biplab Koley, Harshit and Partha P. Jana

**Formation and stability of Rh\(_2\)Cd\(_5\) and its structural correlation with RhCd and Rh\(_3\)Cd\(_5\)-\(\delta\) (\(\delta\sim 0.56\))**

https://doi.org/10.1515/zkri-2022-0008
Z. Kristallogr. 2022; 237(6–7): 233–238

**Synopsis:** Three structurally related intermetallic compounds Rh\(_2\)Cd\(_5\), Rh\(_3\)Cd\(_5\)-\(\delta\) and RhCd are compared in terms of electronic structure calculations and chemical bonding analysis. The significance of the 2:5 stoichiometry in Rh\(_2\)Cd\(_5\) has been explored by means of formation energy calculations and crystal orbital Hamilton population analysis on several atomic configurations. The contribution of Cd–Cd and Rh–Cd interactions in these crystal structures are unveiled.

Nataliya L. Gulay, Jutta Kösters, Yaroslav M. Kalychak, Samir F. Matar, Alfred Rabenbauer, Tom Nilges and Rainer Pöttgen

**Peierls distortion of the cobalt chain in the low-temperature structure of CoIn\(_2\)**

https://doi.org/10.1515/zkri-2022-0020
Z. Kristallogr. 2022; 237(6–7): 239–248

**Synopsis:** The intermetallic compound CoIn\(_2\) shows a Peierls type distortion of the cobalt chains at 195(1) K with shorter (252.4 pm) and longer (284.1 pm) Co–Co distances in LT-CoIn\(_2\).

Mohd Mustaqim Rosli, Nuridayanti Che Khalib, Kaliyaperumal Thanigaimani, Suhana Arshad and Ibrahim Abdul Razak

**Structural, Hirshfeld Surface and HOMO-LUMO gap analysis of five co-crystals of 2-amino-5-chloropyridine or 2-amino-bromopyridine with isomeric methylbenzoic acids**

https://doi.org/10.1515/zkri-2021-2061
Z. Kristallogr. 2022; 237(6–7): 249–258

**Synopsis:** Five co-crystals featuring 2-amino-5-halopyridine and n-methyl-benzoic acids are described.
Crystallographic Computing

Raffaele Sentiero and Francesc Gispert-Guirado
Direct determination of thermal expansion coefficients from the profile fitting of a diffractogram

https://doi.org/10.1515/zkri-2022-0016
Z. Kristallogr. 2022; 237(6–7): 259–269

Synopsis: All the structural classes (SCs) of molecular crystals, which are possible to be formed by a sole intermolecular bearing contact, are derived from 1,1- and 2,1-transitive nets. There are 160 (167 including enantiomorphic pairs) monosystemic SCs (in which the molecules occupy one crystallographic orbit) and 244 (248) bisystemic SCs (in which the molecules occupy two crystallographic orbits), i.e. 404 (411) SCs in all. These are the only SCs which can correspond to a homodesmic crystal structure, either organic, or inorganic, in which the structural units are bonded in a single way. Statistical investigation of the Cambridge Structural Database (CSD) shows that ~1% of monosystemic molecular crystals can be formed by a sole intermolecular bearing contact.