Graphical Synopsis

Special Issue: Dedicated to Professor Dr. Ulrich Müller on the occasion of his 80th birthday

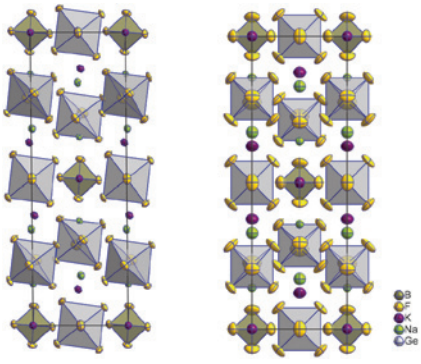
Laudatio/Preface

Jascha Bandemehr, Josefin Klippstein, Sergei I. Ivlev, Malte Sachs and Florian Kraus

Laboratory synthesis and characterization of Knasibfite $K_3Na_4[SiF_6]_3[BF_4]$ and the homologous Ge compound $K_3Na_4[GeF_6]_3[BF_4]$

https://doi.org/10.1515/zkri-2019-0068
Z. Kristallogr. 2020; 235(8–9): 247–254

Synopsis: Knasibfite occurs in nature as the only mineral containing $[BF_4]^-$ and $[SiF_6]^{2-}$ anions. We present a laboratory synthesis, the crystal structure, and its IR and Raman spectra. The homologous compound $K_3Na_4[GeF_6]_3[BF_4]$ is reported as well. Phase transition temperatures of the compounds were determined by heat capacity measurements. The crystal structures of the monoclinic low-temperature (space group *I*121) and the orthorhombic higher-temperature polymorphs (space group *Im*2*m*) are related by a *translationengleiche* step of index 2.

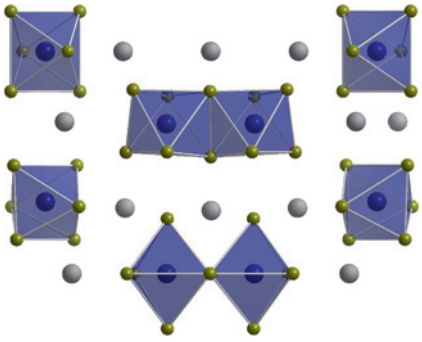


Jen-Hui Chang, Thomas Doert and Michael Ruck

The crystal structures of α-$Rb_7Sb_3Br_{16}$, α- and β-$Tl_7Bi_3Br_{16}$ and their relationship to close packings of spheres

https://doi.org/10.1515/zkri-2020-0013
Z. Kristallogr. 2020; 235(8–9): 255–261

Synopsis: α-$Tl_7Bi_3Br_{16}$ and α-$Rb_7Sb_3Br_{16}$ (both adopting the $Tl_7Bi_3I_{16}$ structure type) and β-$Tl_7Bi_3Br_{16}$ (new structure type) comprise slabs of isolated $[EX_6]^{3-}$-octahedra and $[E_2X_{10}]^{4-}$ octahedra pairs, which can topologically be described as sphere close packing.

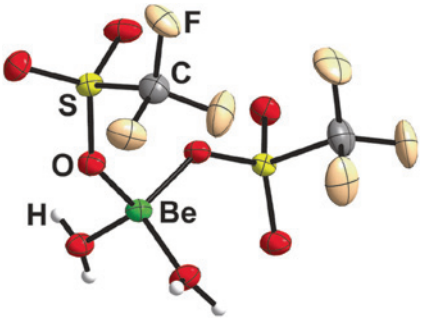


Matthias Müller and Magnus R. Buchner

Beryllium triflates: synthesis and structure of $BeL_2(OTf)_2$ (L=H_2O, THF, $^nBu_2O$)

https://doi.org/10.1515/zkri-2020-0016
Z. Kristallogr. 2020; 235(8–9): 263–268

Synopsis: The beryllium triflates $Be(H_2O)_2(OTf)_2$, $Be(OTf)_2(THF)_2$ and $Be(^nBu_2O)_2(OTf)_2$ were synthesized and characterized *via* single crystal X-ray diffraction. The observed Be–O atomic distances between Be^{2+} and the triflate anions in solid state are the shortest known distances of this kind found in a metal triflate yet.

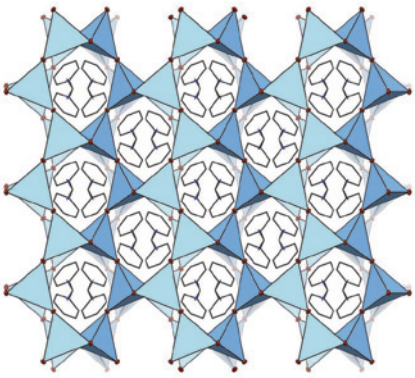


Natalie Dehnhardt, Chantsalmaa Berthold, Kevin Dollberg, Frank Tambornino and Johanna Heine

Synthesis and crystal structures of two layered Cu(I) and Ag(I) iodidometalates

https://doi.org/10.1515/zkri-2020-0021
Z. Kristallogr. 2020; 235(8–9): 269–273

Synopsis: Two new layered Cu(I) and Ag(I) iodidometalates have been prepared using benzylammonium as a counterion.

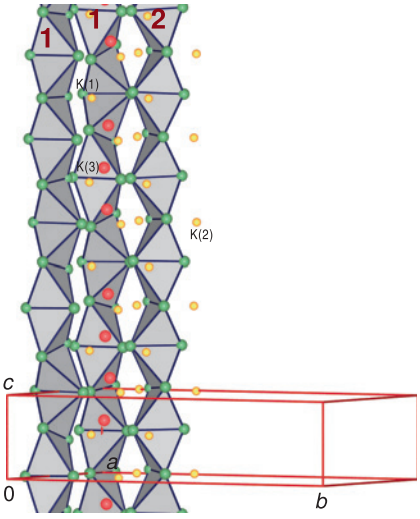


Michael Schwarz, Pirmin Stüble, Katharina Köhler and Caroline Röhr

New mixed-valent alkali chain sulfido ferrates $A_{1+x}[FeS_2]$ (A = K, Rb, Cs; x = 0.333–0.787)

https://doi.org/10.1515/zkri-2020-0023
Z. Kristallogr. 2020; 235(8–9): 275–290

Synopsis: Undulated tetrahedra chains in the (3+1)D modulated crystal structure of the mixed-valent sulfido ferrate salt $K_{7.15}[FeS_2]_4$.

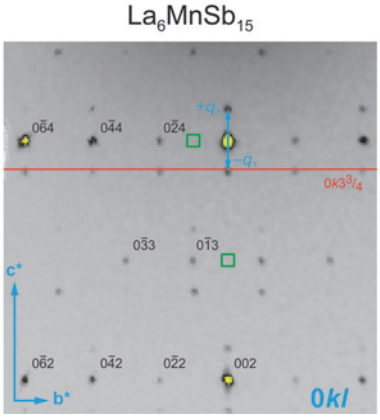


Mathis Radzieowski, Steffen Klenner, Rolf-Dieter Hoffmann and Oliver Janka

Structure solution of incommensurately modulated La_6MnSb_{15}

https://doi.org/10.1515/zkri-2020-0034
Z. Kristallogr. 2020; 235(8–9): 291–301

Synopsis: La_6MnSb_{15} was synthesized from elements in quartz ampoules, the crystal structure was investigated *via* single-crystal X-ray diffraction experiments leading to the observation of superstructure reflections. The structure could be solved and refined in superspace group *Immm*(00*γ*)000. Additionally, the temperature dependence of the electrical resistivity was investigated and ^{121}Sb *Mößbauer*-spectroscopic measurements at 78 K were conducted.

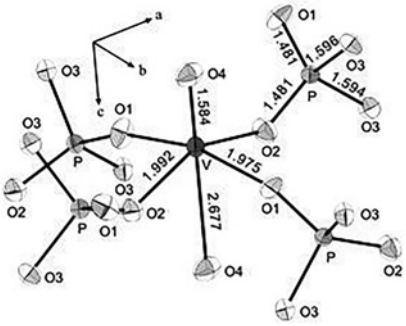


Sven Umlauf, Markus Weber and Robert Glaum

Polymorphs of $VO(PO_3)_2$: synthesis and crystal structure refinement revisited

https://doi.org/10.1515/zkri-2020-0037
Z. Kristallogr. 2020; 235(8–9): 303–309

Synopsis: Single crystals of β-$(V^{IV}O)(PO_3)_2$ were grown in a sealed silica ampoule with chlorine as mineralizer. The crystal structure of the orthorhombic (pseudo-tetragonal) β-polymorph was refined from X-ray single-crystal data [pseudo-merohedral twin, *Fdd*2, Z = 8, a = 15.536(2) Å, b = 15.586(2) Å, c = 4.2611(5) Å, R_1 = 0.0322, wR_2 = 0.068 for 1072 unique reflections with $F_o > 4sig(F_o)$, 50 variables]. Earlier reports on a tetragonal polymorph with unusual geometric structure of the $[(V{\equiv}O)O_5]$ polyhedron are corrected.

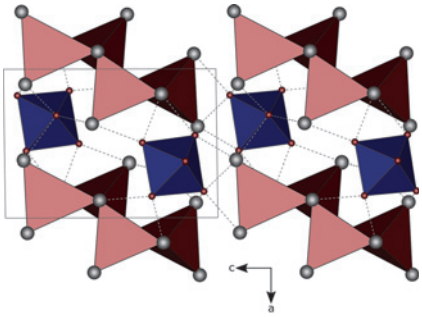


Stephan G. Jantz, Florian Pielnhofer and Henning A. Höppe

On tungstates of divalent cations (III) – $Pb_5O_2[WO_6]$

https://doi.org/10.1515/zkri-2020-0041
Z. Kristallogr. 2020; 235(8–9): 311–317

Synopsis: The new lead tungstate $Pb_5O_2[WO_6]$ comprises $[Pb_{10}O_4]^{12+}$ oligomers and non-condensed WO_6 octahedra and is obtained as yellowish powder in accordance with a band-gap of 2.8 eV (calculated by DFT: 2.9 eV).

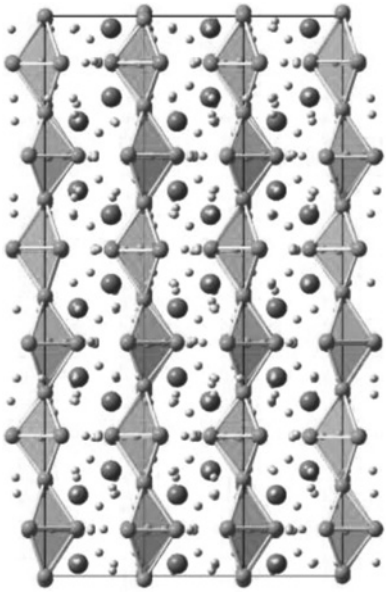


Holger Kohlmann

Hydrogen order in Laves phases hydrides

https://doi.org/10.1515/zkri-2020-0043
Z. Kristallogr. 2020; 235(8–9): 319–332

Synopsis: Order-disorder phase transitions in Laves phase hydrides are described concisely using *Bärnighausen* trees.

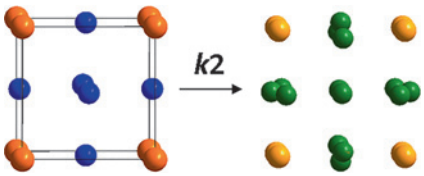


Julia-Maria Hübner, Wilder Carrillo-Cabrera, Raul Cardoso-Gil, Primož Koželj, Ulrich Burkhardt, Martin Etter, Lev Akselrud, Yuri Grin and Ulrich Schwarz

High-pressure synthesis of $SmGe_3$

https://doi.org/10.1515/zkri-2020-0058
Z. Kristallogr. 2020; 235(8–9): 333–339

Synopsis: The high-pressure phase $SmGe_3$ adopts a new $2 \times 2 \times 2$ superstructure of the Cu_3Au motif, thus representing a distorted binary variant of *fcc*.

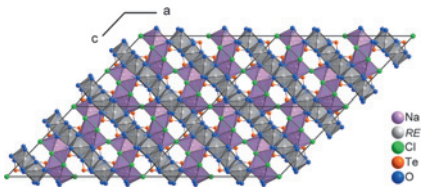


Stefan Greiner, Sabine Zitzer, Sabine Strobel, Peter S. Berdonosov and Thomas Schleid

The complete series of sodium rare-earth metal(III) chloride oxotellurates(IV) $Na_2RE_3Cl_3[TeO_3]_4$ (*RE* = Y, La–Nd, Sm–Lu)

https://doi.org/10.1515/zkri-2020-0051
Z. Kristallogr. 2020; 235(8–9): 341–352

Synopsis: The oxotellurates $Na_2RE_3Cl_3[TeO_3]_4$ crystallize in the monoclinic space group no. 15, but their structure was described in different settings ($C2/c$ and $A2/n$) with almost the same metrics. Now the complete series (*RE* = Y, La–Nd, Sm–Lu) is uniformly available with the *Pearson* symbol mC96 and the *Wyckoff* sequence $f^{11}ea$.

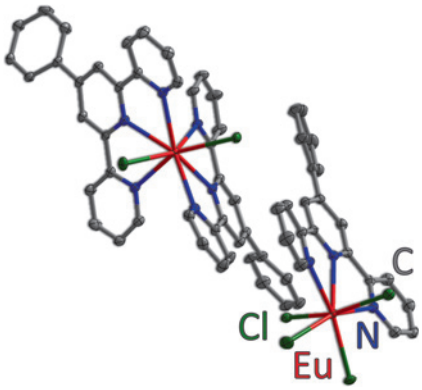


Alexander E. Sedykh, Robin Bissert, Dirk G. Kurth and Klaus Müller-Buschbaum

Structural diversity of salts of terpyridine derivatives with europium(III) located in both, cation and anion, in comparison to molecular complexes

https://doi.org/10.1515/zkri-2020-0053
Z. Kristallogr. 2020; 235(8–9): 353–363

Synopsis: Variation of the backside of terpyridyl-ligands gives salt-like Eu-compounds with the Ln-cation present in both, cation and anion, whereas additional dipyridyl ligands function as a linker that result in the crystallization of dimeric complexes.

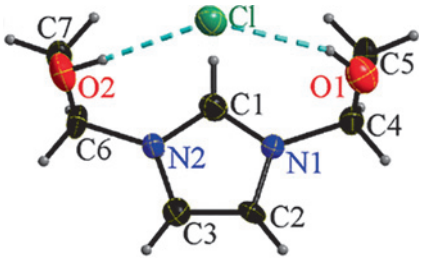


Kai Richter, Katharina V. Dorn, Volodymyr Smetana and Anja-Verena Mudring

Elucidating structure–property relationships in imidazolium-based halide ionic liquids: crystal structures and thermal behavior

https://doi.org/10.1515/zkri-2020-0046
Z. Kristallogr. 2020; 235(8–9): 365–374

Synopsis: Endowing ionic liquid forming ions with an enhanced hydrogen bonding capacity leads to hydrogen bond frustration and is an additional, effective design tool to suppress the melting point of salts

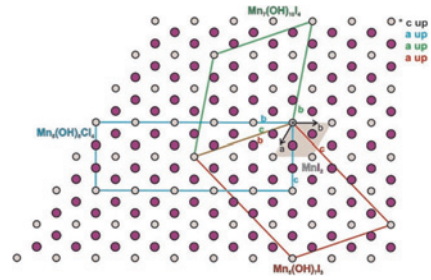


Viktoria Falkowski, Alexander Zeugner, Stefan Seidel, Rainer Pöttgen, Klaus Wurst, Michael Ruck and Hubert Huppertz

Syntheses and crystal structures of the manganese hydroxide halides $Mn_5(OH)_6Cl_4$, $Mn_5(OH)_7I_3$, and $Mn_7(OH)_{10}I_4$

https://doi.org/10.1515/zkri-2020-0040
Z. Kristallogr. 2020; 235(8–9): 375–389

Synopsis: Syntheses and crystal chemical relationships of the new manganese hydroxide halides $Mn_5(OH)_6Cl_4$, $Mn_5(OH)_7I_3$, and $Mn_7(OH)_{10}I_4$ with respect to the aristotype $Mg(OH)_2$ (brucite).

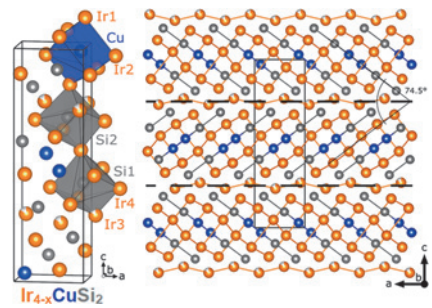


Jan P. Scheifers and Boniface P. T. Fokwa

Site-preferential copper substitution for silicon leads to Cu-chains in the new ternary silicide $Ir_{4-x}CuSi_2$

https://doi.org/10.1515/zkri-2020-0061
Z. Kristallogr. 2020; 235(8–9): 391–399

Synopsis: $Ir_{4-x}CuSi_2$, the first ternary silicide in the Ru_4Si_3-type structure is discover-ed. Its structure contains Ir vacancies along the twin boundary (see Figure) and exhibits a distorted structure compared to Ru_4Si_3, as the larger Cu selectively replaces Si on one of three possible sites, leading to zigzag chains with short Cu–Cu distances.

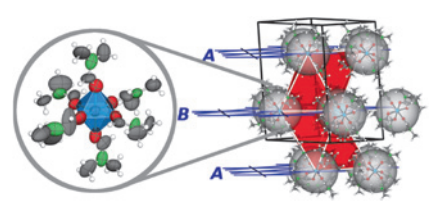


Constantin Hoch

Syntheses and crystal structures of solvate complexes of alkaline earth and lanthanoid metal iodides with *N*,*N*-dimethylformamide

https://doi.org/10.1515/zkri-2020-0071
Z. Kristallogr. 2020; 235(8–9): 401–411

Synopsis: The crystal structures of solvate complexes of earth alkaline and lanthanoid metal iodides with *N*,*N*-dimethylformamide (DMF) are described on the basis of single-crystal structures. DMF acts as monodentate ligand with very low sterical demands. The DMF complexes $[M(DMF)_x]I_y$ can be taken as starting materials for a number of reactions and are much easier to prepare than the binary metal iodides themselves. The plethora of crystal structures can be compared on the basis of the packing topology of the almost spherical cationic complex units.



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