Poster Presentations

[MS19-P02] Novel silicates with apatite crystal structure type.

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The two new silicates, $Cd_2Er_8(SiO_4)_6O_2$ and $Cd_2Tb_8(SiO_4)_6O_2$, were obtained as byproducts during a project focusing on the incorporation of heavy metals within the crystal structures of mixed-framework silicates. They crystallise in the apatite structure type and represent the first silicates housing the rare earths elements (Er/Tb) and a transition metal. Silicates with apatite structure containing lanthanides have been widely studied due to their potential use as catalysts, fast oxygen ion conductors, luminescent materials, and actinide waste forms. [1-4] The first REE silicates with apatite structure were described by Felsche in1972.[5] Since then 33 further silicates were reported in the Inorganic Crystal Structure Database (ICSD). However, most of them contain OH- groups, F- or even Cl- anions in the structure. The title compounds are free of any such anions; because they were synthesized from melts lacking water, fluorine or chlorine: colourless $Cd_2Tb_8(SiO_4)_6O_2$ and pink $Cd_2Er_8(SiO_4)_6O_2$ crystallise in small prisms from a high-temperature flux (MoO_3–based flux mixtures in Pt crucibles in air; T_{max} = 1150°C, cooling rate 2 K/h, T_{min} = 900°C).
The crystal structures have been determined from single-crystal X-ray diffraction data (Mo$K\alpha$, 293 K; Bruker APEX II diffractometer). The two isotypic compounds crystallise in the hexagonal space group P63/*m* (176), with *a* = 9.3175(13)/9.3802(13),*c*=6.7030(13)/6.7983(14) Å, *V* = 503.96(14)/518.03(15) Å3, *R(F)* = 0.019/0.021, respectively (Er/Tb). The crystal structures are built from an isolated SiO_4 tetrahedron and two further polyhedra: a seven-coordinated one (on Wyckoff position 6h) is dominantly occupied by REE and only 3-4% Cd. The nine-coordinated polyhedron on 4f shows a mixed occupancy with about 55% REE and 45% Cd.

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