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

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The two new silicates, Cd$_2$Er$_8$(SiO$_4$)$_6$O$_2$ and Cd$_2$Tb$_8$(SiO$_4$)$_6$O$_2$, 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.

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The title compounds are free of any such anions; because they were synthesized from melts lacking water, fluoride or chlorine: colourless Cd$_2$Er$_8$(SiO$_4$)$_6$O$_2$ and pink Cd$_2$Tb$_8$(SiO$_4$)$_6$O$_2$ crystallise in small prisms from a high-temperature flux (MoO$_3$-based flux mixtures in Pt crucibles in air; $T_{\text{max}} = 1150^\circ\text{C}$, cooling rate 2 K/h, $T_{\text{min}} = 900^\circ\text{C}$).

The crystal structures have been determined from single-crystal X-ray diffraction data (MoKα, 293 K; Bruker APEX II diffractometer).

The two isotypic compounds crystallise in the hexagonal space group P6$_3$/m (176), with $a = 9.3175(13)/9.3802(13)$, $c = 6.7030(13)/6.7983(14)$ Å, $V = 503.96(14)/518.03(15)$ Å$^3$, $R(F) = 0.019/0.021$, 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.

Keywords: silicates, oxyapatite, crystal structure