

Oral Contributions

[MS19-04] Novel silicates with apatite crystal structure type. Maria Wierzbicka-Wieczorek,^a Gerald Giester^b

^aInstitute for Geosciences, Friedrich-Schiller University Jena, Carl-Zeiss Promenade 10, 07745 Jena, Germany, ^bInstitut für Mineralogie und Kristallographie, Universität Wien, Althanstr. 14, 1090 Wien, Austria.

E-mail: maria.wierzbicka-wieczorek@uni-jena.de

The two new silicates, $\text{Cd}_2\text{Er}_8(\text{SiO}_4)_6\text{O}_2$ and $\text{Cd}_2\text{Tb}_8(\text{SiO}_4)_6\text{O}_2$, 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. [1-4] The first REE silicates with apatite structure were described by Felsche in 1972. [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 $\text{Cd}_2\text{Tb}_8(\text{SiO}_4)_6\text{O}_2$ and pink $\text{Cd}_2\text{Er}_8(\text{SiO}_4)_6\text{O}_2$ 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 ($\text{MoK}\alpha$, 293 K; Bruker APEX II diffractometer). The two isotopic compounds crystallise in the hexagonal space group $\text{P6}_3/m$ (176), with $a = 9.3175(13)/9.3802(13)$, $c = 6.7030(13)/6.7983(14)$ Å, $V = 503.96(14)/518.03(15)$ 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.

[1] Wakabayashi, T., Kato, S., Nakahara, Y., Ogasawara, M. & Nakata, S. (2011). *Catal. Today* **164**, 575-579.

[2] Leon-Reina, L., Losila, E.R., Martinez-Lara, M., Bruque, S. & Aranda, M.A.G. (2004). *J. Mater. Chem.* **14**, 1142-1149.

[3] Ferdov, S., Sa Ferreira, R.A. & Lin, Z. (2006). *Mater. Chem.* **18**, 5958-5964.

[4] Ewing, R.C. & Weber W.J. (2010). in *The Chemistry of the Actinides and Transactinide Elements*, edited by L. R. Morss, N.M. Edelstein & J. Fuger (Springer, New York) 6, p. 3813.

[5] Felsche, J. (1972). *J. Solid State Chem.* **5**, 266-275.

Keywords: silicates, oxyapatite, crystal structure