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Synthesis, crystal chemistry and topology of $BaYb_6(Si_2O_7)_2(Si_3O_{10})$, the first silicate containing both $(Si_2O_7)_2$ and Si_3O_{10} groups

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The novel compound $BaYb_6(Si_2O_7)_2(Si_3O_{10})$, simplified $BaYb_6Si_7O_{24}$, represents the first silicate containing both $(Si_2O_7)_2$ and (Si_3O_{10}) groups. It is also the first silicate that is isotypic with $(NH_4)Cd_6(P_2O_7)_2(P_3O_{10})$ (Ivanov et al., 1978; space group incorrectly given as $P11m$ and also incorrectly adopted in the corresponding ICSD entry), the structure type of which is adopted by a small number of phosphates and arsenates with $(T_2O_7)_2$ and T_3O_{10} groups (T = P, As) (Bennazha et al., 2001, 2002; Ayed et al., 2004; Frigui et al., 2010). The title compound crystallised as a by-product from a high-temperature flux-growth experiment in air in the system Cs-Ba-Yb-Co-Si-O (molybdate-carbonate-based flux solvent; T_{max} = 1150°C, followed by cooling at 2 K/h down to 750°C) aimed at the synthesis of new mixed framework silicates containing heavy metals (e.g. Pb, Cd, Hg, Cr, Co, Ni, Sb). The crystal structure of the new silicate was determined from single-crystal X-ray intensity data (Mo$K\alpha$, 293 K; Nonius Kappa APEX II diffractometer). $BaYb_6(Si_2O_7)_2(Si_3O_{10})$ is monoclinic, space group $P2_1/m$, with a = 5.5173(11), b = 27.260(6), c = 6.8150(14) Å, β = 106.73(3)°, V = 981.6(3) Å^3; $R(F)$ = 2.50%. The asymmetric unit of $BaYb_6(Si_2O_7)_2(Si_3O_{10})$ contains one Ba, three Yb, four Si and thirteen O atoms. The architecture of the new silicate is characterised by one isolated, horseshoe-shaped Si_3O_{10} group and two symmetrically equivalent Si_2O_7 groups (Si_3O_{10}:Si_2O_7 ratio = 1:2). Edge-sharing YbO_6 octahedra with the sequence Yb1-Yb2-Yb3-Yb3-Yb2-Yb1 form the backbone of zigzag chains, with a backbone length of ~18 Å. The zigzag chains run approximately along [0 -0.25 -1] and [0 0.25 -1] and are linked along the a-axis by sharing one further edge with an YbO_6 octahedra from an adjacent chain.

Three structurally related silicates [isotypic $BaY_4(Si_2O_7)(Si_3O_{10})$, $SrYb_4(Si_2O_7)(Si_3O_{10})$ and $SrSc_4(Si_2O_7)(Si_3O_{10})$; Wierzbicka-Wieczorek 2008] with similar zigzag chains are characterised by a Si_3O_{10}:Si_2O_7 ratio of 1:1 and the length of the chain backbone amounts to only ~13 Å. The eight-coordinated Ba atom is located in [100] channels of the framework. The average Ba–O bond length is 2.90 Å and the average Yb–O bond length in each of the three YbO_6 octahedra measures 2.24 Å. The Si-Si-Si angle in the horseshoe-shaped Si_3O_{10} unit is 93.5° and the Si-O-Si angle is 135.5° (2x), whereas the Si-O-Si angle of the Si_2O_7 group is 165.3°.

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