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Pretulite, $ScPO_4$, a new scandium mineral from the Styrian and Lower Austrian lazulite occurrences, Austria

Franz Bernhard,[1,*] Franz Walter,[1] Karl Ettinger,[1] Josef Taucher,[2] and Kurt Mereiter[3]

[1]Institut für Mineralogie-Kristallographie und Petrologie, Karl-Franzens-Universität Graz, Universitätsplatz 2, A-8010 Graz, Austria
[2]Referat für Mineralogie, Landesmuseum Joanneum, Raubergasse 10, A-8010 Graz, Austria
[3]Institut für Mineralogie, Kristallographie und Strukturchemie, Technische Universität Wien, Getreidemarkt 9, A-1060 Wien, Austria

Abstract

Pretulite is a new Sc phosphate with zircon-type structure from the phyllite-micaschist hosted hydrothermal lazulite-quartz veins in the Lower Austroalpine Grobgneis complex, eastern Austria. The new species is the Sc-dominant analogue of xenotime-(Y) and occurs as an accessory mineral in all investigated lazulite specimens, forming anhedral to euhedral crystals up to 200 μm long with the dominant form {211}. It is associated with lazulite, fluorapatite, chlorapatite, quartz, muscovite, clinochlore, paragonite, kyanite, pyrophyllite, augelite, wardite, hydroxylherderite, goyazite, florencite-(Ce), xenotime-(Y), bearthite, rutile, pyrite, corundum, and an AlO(OH)-phase. Pretulite is translucent to transparent with an adamantine luster, colorless to pale pink, uniaxial positive with $\omega = 1.790$ (5), $\epsilon = 1.86$ (1) and shows a weak orange fluorescence at 254 nm as well as a bright blue cathodoluminescence. Mohs hardness is about 5. The empirical formula for pretulite (based on four O atoms) is $(Sc_{0.98}Y_{0.02})_{1.00}P_{1.00}O_{4.00}$. It contains variable amounts of Y with Y/(Y + Sc) = 0.5 − 3.2 mol% and traces of Yb, Er, and Dy. The space group is $I4_1/amd$ with $a = 6.589$ (1) Å, $c = 5.806$ (1) Å, $V = 252.1$ (1) Å^3, $d_{calc} = 3.71$ g/cm^3, $Z = 4$. The four strongest lines in the X-ray powder pattern are $d_{200} = 3.293$ (100), $d_{112} = 2.4636$ (42), $d_{312} = 1.6927$ (45), $d_{332} = 1.3697$ (15) Å. The crystal structure was refined using 108 reflections to $R(F_o) = 0.018$. Cell parameters and average M-O distances confirm a small amount of Y substituting Sc in the eightfold-coordinated M-position. The formation of pretulite is attributed to a moderate enrichment of Sc in lazulite-rich domains of the veins (about 180 ppm) and the inability of the accompanying minerals to incorporate larger quantities of Sc in their crystal structure. The name is after the mountain Pretul, Fischbacher Alpen, Styria, Austria.