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Mn-rich fluorapatite from Austria: Crystal structure, chemical analysis, and spectroscopic investigations

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ABSTRACT

The crystal structure of a pale blue transparent Mn-rich fluorapatite (MnO: 9.79 wt%) with the optimized formula ~$(Ca_{8.56}Mn^{2+}_{1.41}Fe^{2+}_{0.01})P_6O_{24}F_{2.00}$ and space group $P6_3/m$, $a = 9.3429(3)$, $c = 6.8110(2)$ Å, $Z = 2$ has been refined to $R = 2.05\%$ for 609 unique reflections (Mo$K\alpha$). The Mn in the Eibenstein an der Thaya, Austria apatite is strongly ordered at the Ca1 site: Ca1: $Ca_{0.72(1)}Mn_{0.28}$, Ca2: $Ca_{0.96(1)}Mn_{0.04}$. There is a linear variation in <Ca1-O> as a function of Mn content ($r^2 = 1.00$). The dominant band in the optical absorption spectrum of fluorapatite from Eibenstein is in the 640 nm region with **E** ∥ **c** > **E** ⊥ **c**. The 640 nm band is attributed to Mn^{5+} at the P site by analogy with previous studies. This interpretation is consistent with studies of well-characterized synthetic materials of the apatite structure that contain Mn^{5+}. Because Mn^{5+} has intense absorption in the visible region of the spectrum, if a small proportion of the total Mn is Mn^{5+} at the P site, that substituent dominates the spectrum and the color of the mineral. To determine if the pale blue color is due to radiation effects, a fragment of the fluorapatite crystal was heated at 400° C for 1 hour, and the change in color was slight. All of these observations are consistent with the origin of color from Mn^{5+}. Assuming that all the intensity of the 640 nm (**E** ∥ **c**) absorption is from Mn^{5+}, the concentration of Mn^{5+} in this fluorapatite sample was calculated as 2.6% of the total manganese content (~$P_{5.96}Mn^{5+}_{0.04}$). The calibration was estimated from the spectrum of the related compound $Sr_5(P_{0.99}Mn^{5+}_{0.01})_3Cl$. The weak band at about 404 nm in the **E** ∥ **c** spectrum may be the corresponding band for Mn^{2+} in octahedral coordination.