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The roscherite group and its new representative member atencioite,



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A new mineral atencioite, triclinic member of the roscherite group, occurs in granite pegmatite at Linópolis, Divino das Laranjeiras, Minas Gerais State, Brazil, in association with albite, quartz, lepidolite, beryllonite, moraesite and ushkovite. The mineral forms groups of greenish-brown sub-parallel individuals and spherules up to 8 mm. Atencioite is transparent, with vitreous lustre; streak is white. Mohs' hardness is 4½, brittle, cleavage is none observed.  $D_{\text{meas}} = 2.84(1) \text{ g/cm}^3$  (volumetric method) and  $2.86(1) \text{ g/cm}^3$  (equilibration in heavy liquids).  $D_{\text{calc}} = 2.832 \text{ g/cm}^3$ . Weight loss on heating (vacuum, 23.7 mg, 20°/min, up to 1000°C) is 13.5%. Compared with monoclinic members of the roscherite group, atencioite shows in the IR spectrum splitting of the bands of P-O stretching (1031+1019  $\text{cm}^{-1}$ ) and Be-O stretching (721+709  $\text{cm}^{-1}$ ) vibrations, and presence of three maxima at 522, 491 and 449  $\text{cm}^{-1}$  (stretching vibrations of octahedra). Optical data were obtained by A.E. Zadov. Atencioite is biaxial, negative;  $\alpha = 1.613(2)$ ,  $\beta = 1.620(2)$ ,  $\gamma = 1.626(2)$ ,  $2V$  (meas.) = 60(10)°,  $2V$  (calc.) = 85°. Dispersion is not observed. Pleochroism:  $\beta$  (greenish-brown) >  $\alpha$  (brown) >  $\gamma$  (brown). The chemical composition is (wt. %, ranges are indicated in brackets; EDS mode electron microprobe, 15.7 kV, 1.5 nA, 8  $\mu\text{m}$  beam diameter; Be – by wet-chemical analysis; H<sub>2</sub>O – by the Penfield method; Fe<sup>2+</sup>:Fe<sup>3+</sup> - from the Mössbauer spectrum): CaO 9.91 (9.78-9.99); MgO 8.54 (8.35-8.75); MnO 1.30 (1.22-1.41); FeO 13.44, Fe<sub>2</sub>O<sub>3</sub> 3.92 (for total Fe as FeO the ranges are 16.70-17.29); Al<sub>2</sub>O<sub>3</sub> 0.41 (0.33-0.51); BeO 9.30; P<sub>2</sub>O<sub>5</sub> 40.28 (40.11-40.52); H<sub>2</sub>O 13.20, total 100.30. Empirical formula:  $\text{Ca}_{1.87}\text{Mg}_{2.24}\text{Mn}_{0.19}\text{Fe}^{2+}_{1.98}\text{Fe}^{3+}_{0.52}\text{Al}_{0.08}\text{Be}_{3.93}(\text{PO}_4)_6(\text{OH})_{4.22}\cdot 5.63\text{H}_2\text{O}$ . The crystal structure is solved,  $R = 0.051$ . Atencioite is triclinic,  $P-1$ ;  $a = 6.668(1)$ ,  $b = 9.879(2)$ ,  $c = 9.883(1) \text{ \AA}$ ;  $\alpha = 73.53(1)$ ,  $\beta = 85.60(1)$ ,  $\gamma = 86.93(1)^\circ$ ;  $V = 622.8(4) \text{ \AA}^3$ ;  $Z = 1$ . The crystal-chemical formula based on single-crystal and Mössbauer data is:  $\text{Ca}_2[\text{Fe}_{0.5}^{2+}\text{Mn}_{0.2}\text{Al}_{0.1}\square_{0.2}][\text{Mg}_{0.2}\square_{0.8}][\text{Mg}_{1.1}\text{Fe}^{3+}_{0.5}\text{Fe}^{2+}_{0.4}][\text{Fe}^{2+}_{1.1}\text{Mg}_{0.9}]\text{Be}_4(\text{PO}_4)_6(\text{OH})_4(\text{OH}, \text{H}_2\text{O})_2\cdot 4\text{H}_2\text{O}$ . Strong lines of X-ray powder diffraction pattern,  $d \text{ \AA}(I; hkl)$ , are: 9.47(41; 010), 5.92(100; 0-11), 3.31 (34; -1-21, 1-21), 3.17(53; 210), 2.784(86; -103), 2.639(30; -202), 2.202(32; -1-32, -124).  $1-K_p/K_c=0.001$  (for  $D_{\text{calc}}$ );  $1-K_p/K_c=0.008$  (for  $D_{\text{meas}}$ ). The name is for Dr. Daniel Atencio, professor of mineralogy at the Geoscience Institute of the University of São Paulo, Brazil. Type material is deposited in the Mineralogical Museum of the Technische Universität Bergakademie, Freiberg, Germany, inventory number 80905.