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Paulišite, $Ca_2Zn(CO_3)_3 \cdot 2H_2O$, a new mineral with a novel crystal structure

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Abstract

Paulišite, $Ca_2Zn(CO_3)_3 \cdot 2H_2O$, is a new mineral species discovered in the underground workings at the abandoned mine adit of the first level of the Staročeské Lode, near the historical shaft Šafary, Kaňk near Kutná Hora, central Bohemia, Czech Republic. Paulišite is associated with hydrozincite and aragonite (holotype sample) or calcite, aragonite, hydrozincite, and monohydrocalcite (other samples). The new mineral occurs as crusts, up to 1 cm thick, formed by parallel or radial aggregates of acicular crystals, elongated on [100], up to 5 mm long. Paulišite is colorless to white, with a white streak. It is transparent and has a vitreous luster. Mohs hardness is ca. 4; the calculated density is 2.756 g/cm^3. Paulišite is optically biaxial positive, with $\alpha = 1.554(1)$, $\beta = 1.569(2)$, $\gamma = 1.605(1)$ (589 nm), and $2V_{(meas)} = 68(2)°$. The empirical formula, based on electron-microprobe analyses ($n = 11$), is $Ca_{2.00}(Zn_{0.97}Mg_{0.02}Cu_{0.01}Al_{0.01})_{\Sigma 1.01}(CO_3)_3 \cdot 2H_2O$ based on three cations (excluding C) per formula unit. The ideal formula is $Ca_2Zn(CO_3)_3 \cdot 2H_2O$, which requires (in wt%) CaO 31.02, ZnO 22.50, CO_2 36.51, H_2O 9.97, total 100.00. The strongest reflections of the powder X-ray diffraction pattern [d (Å)/(I_{rel})/hkl] are: 8.226/(100)/011, 6.492/(100)/002, 4.112/(18)/022, 3.246/(35)/004, 3.085/(19)/130, and 2.458/(21)/042. According to single-crystal X-ray diffraction data, paulišite is monoclinic, space group Ia, $Z = 4$ with $a = 6.3007(6)$, $b = 10.6236(11)$, $c = 12.9837(12)$ Å, $\beta = 90.840(5)°$, $V = 868.99(15)$ Å^3. The crystal structure was refined to $R_1 = 0.0229$ for 2330 unique reflections with $F_o > 4\sigma(F_o)$ and 164 refined parameters. It is characterized by Zn(1)-centered tetrahedra, two independent Ca(1)- and Ca(2)-centered polyhedra, and CO_3 groups. Heteropolyhedral Ca-Zn-CO_3 {001} layers occur in paulišite and are connected along **c** through CO_3 groups and Ca(2)-centered polyhedra, as well as H-bonds. Along with minrecordite, skorpionite, and znucalite, paulišite is the fourth mineral containing Ca, Zn, and (CO_3) groups as species-defining elements. Its origin is related to the supergene alteration of ore deposits following the mining activity, probably at low T and basic pH conditions. The mineral and its name, honoring the Czech mineralogist and geologist Petr Pauliš (b. 1956), have been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (no. 2023-031).

Keywords: Paulišite, new mineral, zinc, carbonate, crystal structure, Kaňk near Kutná Hora, Czech Republic