Sejkoraite-(Y), a new member of the zippeite group containing trivalent cations from Jáchymov (St. Joachimsthal), Czech Republic: Description and crystal structure refinement

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ABSTRACT

Sejkoraite-(Y), the triclinic \((Y_{0.58}Dy_{0.42})_{2}K_{2.22}H_{2.34}[(UO_{2})_{3}O_{38}O_{6}OH(SO_{4})_{3}](OH)(H_{2}O)_{26}\) is a new member of the zippeite group from the Červená vein, Jáchymov (Street Joachimsthal) ore district, Western Bohemia, Czech Republic. It grows on altered surface of relics of primary minerals: uraninite, chalcopyrite, and tennantite, and is associated with pseudojohannite, rabejacite, uranopilite, zippeite, and gypsum. Sejkoraite-(Y) forms crystalline aggregates consisting of yellow-orange crystals, rarely up to 1 mm in diameter. The crystals have a strong vitreous luster and a pale yellow-to-yellow streak. The crystals are very brittle with perfect \(\{100\}\) cleavage and uneven fracture. The Mohs hardness is about 2. The mineral is not fluorescent either in short- or long-wavelength UV radiation. Sejkoraite-(Y) is yellow, with no visible pleochroism, biaxial negative with \(\alpha' = 1.62(2), \beta' = 1.662(3), \gamma' = 1.73(1), 2V_{\text{calc}} = 79^\circ\). The empirical chemical formula (mean of 8 electron microprobe point analyses) was calculated on the basis of 12 \((S + U)\) atoms: \((Y_{1.06}Dy_{0.78}Gd_{0.33}Er_{0.07}Yb_{0.05}Sm_{0.02})_{2}K_{2.22}H_{2.34}[(UO_{2})_{3}O_{38}O_{6}OH(SO_{4})_{3}](OH)(H_{2}O)_{26}\). Sejkoraite-(Y) is triclinic, space group \(P\bar{1}, a = 14.0743(6), b = 17.4174(7), c = 17.7062(8)\ Å, \alpha = 75.933(4), \beta = 128.001(5), \gamma = 74.4194(5)^\circ, V = 2777.00(19)\ Å³, Z = 2, D_{calc} = 4.04 g/cm³. The seven strongest reflections in the X-ray powder diffraction pattern are \([d_{obs} \text{ in } Å (1) (hkℓ)]: 9.28 (100), 4.64 (39) (200), 3.63 (6) (T42), 3.45 (13) (T44), 3.385 (10) (T42), 3.292 (9) (044), 3.904 (7) (300), 2.984 (10) (T42). The crystal structure of sejkoraite-(Y) has been solved by the charge flipping method from single-crystal X-ray diffraction data and refined to \(R_{obs} = 0.060\) with \(GOF_{obs} = 2.38\), based on 6511 observed reflections. The crystal structure consists of uranyl sulfate sheets of zippeite anion topology, which alternate with an interlayer containing \(Y^{3+}(H_{2}O)\), polyhedra and uncoordinated \(H_{2}O\) groups. Two yttrium atoms are linked to the sheet directly via uranyl oxygen atom, and the remaining one is bonded by hydrogen bonds only. In the Raman and infrared spectrum of sejkoraite-(Y) there are dominating stretching vibrations of \(SO_{4}\) tetrahedra (\(1200–1100\) cm\(^{-1}\)), \(UO_{2}\) stretching vibrations (\(900–800\) cm\(^{-1}\)), and O-H stretching (\(3500–3200\) cm\(^{-1}\)) and H-O-H bending modes (\(1640\) cm\(^{-1}\)). The new mineral is named to honor Jiří Sejkora, a Czech mineralogist of the National Museum in Prague.

Keywords: Sejkoraite-(Y), new mineral, uranyl, zippeite group, crystal structure, vibration spectroscopy, Jáchymov

INTRODUCTION

Uranyl sulfates are typical products of uraninite alteration in the acidic oxidizing environment (Ondruš et al. 1997a; Finch and Murakami 1999; Meisser et al. 2002; Brugger et al. 2003, 2006). The sulfate-rich solutions, resulting from the decomposition of primary sulfide minerals by oxidizing descending waters, are responsible for migration of the uranyl ion \((UO_{2})^{2+}\) under low pH conditions (Fernandes et al. 1995; Brugger et al. 2003, 2006). Precipitation of uranyl sulfate minerals is connected with evaporation/precipitation from acid mine drainage waters (Finch and Murakami 1999). Zippeite-group minerals are typical products of supergene alteration processes of U-rich ores. Up to date, the minerals of the zippeite group include (1) “zippeites” sensu stricto—zippeite, natrozippeite, magnesiozippeite, cobaltzippeite, nickelzippeite, and zinczippeite (Frondel et al. 1976; Burns et al. 2003); (2) triclinic members: marécottite (Brugger et al. 2003) and pseudojohannite (Brugger et al. 2006). Moreover, rabejacite (Deliens and Pier 1993) should be considered as an additional member of the zippeite group, based on many similar characteristics. Minerals of the zippeite group typically occur as powdery coatings and mixtures growing on the surface of uranium-bearing specimens. Gypsum usually covers the samples in rich crystalline coatings, and it is present as a fine-grained admixture in the aggregates of zippeite-group minerals; hence, the structural characterization of these minerals often becomes difficult. As a result, only structures of two minerals adhering to the zippeite-group have been reported up to date: marécottite...