American Mineralogist, Volume 96, pages 983–991, 2011

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

Jakub Plášil,[1,2,*] Michal Dušek,[3] Milan Novák,[2] Jiří Čejka,[4] Ivana Císařová,[5] and Radek Škoda[2]

[1]Department of Mineralogy and Petrology, National Museum, Václavské náměstí 68, CZ-115 79, Prague 1, Czech Republic
[2]Department of Geological Sciences, Faculty of Science, Masaryk University, Kotlářská 2, CZ-611 37, Brno, Czech Republic
[3]Institute of Physics ASCR, v.v.i., Na Slovance 2, CZ-182 21 Prague, Czech Republic
[4]Natural History Museum, National Museum, Václavské náměstí 68, CZ-115 79, Prague 1, Czech Republic
[5]Department of Inorganic Chemistry, Faculty of Science, Charles University, Hlavova 6, CZ-128 43, Prague 2, Czech Republic

Abstract

Sejkoraite-(Y), the triclinic $(Y_{1.98}Dy_{0.24})_{\Sigma 2.22}H^{+}_{0.34}[(UO_2)_8O_{88}O_7OH(SO_4)_4](OH)(H_2O)_{26}$, 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 to 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 $\alpha' = 1.62(2)$, $\beta' = 1.662(3)$, $\gamma' = 1.73(1)$, $2V_{calc} = 79°$. The empirical chemical formula (mean of 8 electron microprobe point analyses) was calculated on the basis of 12 (S + U) atoms: $(Y_{1.49}Dy_{0.17}Gd_{0.11}Er_{0.07}Yb_{0.05}Sm_{0.02})_{\Sigma 1.90}H^{+}_{0.54}[(UO_2)_{8.19}O_7OH(SO_4)_{3.81}](H_2O)_{26.00}$. Sejkoraite-(Y) is triclinic, space group $P\bar{1}$, $a = 14.0743(6)$, $b = 17.4174(7)$, $c = 17.7062(8)$ Å, $\alpha = 75.933(4)$, $\beta = 128.001(5)$, $\gamma = 74.419(4)°$, $V = 2777.00(19)$ Å^3, $Z = 2$, $D_{calc} = 4.04$ g/cm^3. The seven strongest reflections in the X-ray powder diffraction pattern are [d_{obs} in Å (I) (*hkl*)]: 9.28 (100) (100), 4.64 (39) (200), 3.631 (6) ($\bar{1}42$), 3.451 (13) ($\bar{1}44$), 3.385 (10) ($\bar{2}\bar{4}2$), 3.292 (9) (044), 3.904(7) (300), 2.984 (10) ($\bar{1}\bar{4}2$). 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 $Y^{3+}(H_2O)_n$ polyhedra and uncoordinated H_2O 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^{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