American Mineralogist, Volume 93, pages 1911–1920, 2008

Xocolatlite, $Ca_2Mn_2^{4+}Te_2O_{12}\cdot H_2O$, a new tellurate related to kuranakhite: Description and measurement of Te oxidation state by XANES spectroscopy

Pascal V. Grundler,[1,*] Joël Brugger,[1] Nicolas Meisser,[2] Stefan Ansermet,[2] Stacey Borg,[3] Barbara Etschmann,[3] Denis Testemale,[4] and Trudy Bolin[5]

[1]Department of Geology and Geophysics, University of Adelaide, North Terrace, SA-5005 Adelaide, Australia and South Australian Museum, North Terrace, SA-5000 Adelaide, Australia

[2]Musée Cantonal de Géologie and Laboratoire des Rayons-X, Institut de Minéralogie and Géochimie, UNIL-Anthropole, CH-1015 Lausanne-Dorigny, Switzerland

[3]CSIRO Exploration and Mining, Clayton, VIC-3800, Australia

[4]CNRS Institut Néel, département MCMF, 25 Avenue des Martyrs, 38042 Grenoble Cedex 9, France and SNBL/ESRF, 6 Rue Jules Horowitz, 38043 Grenoble, France

[5]Advanced Photon Source, Sector 9 BM, Argonne, Illinois 60439, U.S.A.

Abstract

Xocolatlite, $Ca_2Mn_2^{4+}Te_2^{6+}O_{12}\cdot H_2O$, is a rare new mineral from the Moctezuma deposit in Sonora, Mexico. It occurs as chocolate-brown crystalline crusts on a quartz matrix. Xocolatlite has a copper-brown streak, vitreous luster, and is transparent. Individual crystals show a micaceous habit. Refractive indices were found to be higher than 2.0. Density calculated from the empirical formula is 4.97 g/cm^3, and immersion in Clerici solution indicated a density higher than 4.1 g/cm^3. The mineral is named after the word used by the Aztecs for chocolate, in reference to its brown color and provenance.

The crystallographic characteristics of this monoclinic mineral are space group *P*2, *P*2/*m*, or *Pm*, with the following unit-cell parameters refined from synchrotron X-ray powder diffraction data: a = 10.757(3) Å, b = 4.928(3) Å, c = 8.942(2) Å, β = 102.39(3)°, V = 463.0(3) Å^3, and Z = 2. The unavailability of a suitable crystal prevented single-crystal X-ray studies. The strongest 10 lines of the X-ray powder diffraction pattern are [d in Å (I) (hkl)]: 3.267(100)(012), 2.52(71)(30$\overline{3}$), 4.361(51)(002), 1.762(39)(32$\overline{3}$), 4.924 (34)(010), 2.244(32)(31$\overline{3}$), 1.455(24)(006), 1.996(21)(014), 1.565(20)(611), and 2.353(18)(41$\overline{1}$).

XANES Te L_{III}-edge spectra of a selection of Te minerals (including xocolatlite) and inorganic compounds showed that the position of the absorption edge can be reliably related to the oxidation state of Te. XANES demonstrated that xocolatlite contains Te^{6+} as a tellurate group. Water has been tentatively included in the formula based on IR spectroscopy that indicated the presence of a small amount of water. Raman, IR, XANES, and X-ray diffraction data together with the chemical composition show a similarity of xocolatlite to kuranakhite. A possible series may exist between these two species, xocolatlite being the Ca-rich end-member and kuranakhite the Pb-rich one.

Keywords: Xocolatlite, Kuranakhite, new mineral, XANES spectroscopy, tellurium oxidation state, Moctezuma, Sonora, Mexico