Xocolatlite, Ca$_2$Mn$_{4+}$Te$_2$O$_{12}$·H$_2$O, 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-Dorgny, 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$_2$Mn$_{4+}$Te$_2$O$_{12}$·H$_2$O, 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 greater 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 $P2_1$, $P2_1/m$, or $P2_1$, 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, $\beta = 102.39(3)^\circ$, $V = 463.0(3)$ 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 [in Å ($I$ $hkl$): 3.267(100)(012), 2.52(71)(305), 4.361(51)(002), 1.762(39)(323), 4.924 (34)(010), 2.244(32)(317), 1.455(24)(006), 1.996(21)(014), 1.565(20) (611), and 2.353(18)(41T)].

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$^{IV}$ 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

INTRODUCTION

Despite low crustal abundances (1 ppb, compared to 3.1 ppb for Au), the semi-metal tellurium (Te) is found in relatively high concentrations (tens to thousands of ppm) in several ore deposits. In particular, Te is closely associated with Au in many epithermal-type deposits such as Cripple Creek, Colorado (Kelley et al. 1998), Emperor, Fiji (Pals and Spry 2003), and Săcărîmb, Romania (Ciobanu et al. 2004), as well as in some “orogenic” world-class Sunrise Dam deposit in Western Australia (Bateman and Hagemann 2004; Shackleton et al. 2003; Sung et al. 2007). Tellurium mineralogy tends to be relatively complex, with more than 140 minerals containing Te as an essential element known worldwide. This complexity is linked primarily to the rich redox chemistry of Te, where many oxidation states are available for this element: Te$^{VI}$, Te$^{IV}$, Te$^{V}$, Te$^{I}$ as well as intermediate states such as in polytellurides (e.g., Te$^{II}$).

The Moctezuma deposit in Sonora, Mexico, can be considered as the “World Capital” of tellurium mineralogy. Moctezuma is the type locality for 22 known minerals, all containing Te (Braith et al. 2001). Three of those minerals are tellurides (bambollaite, benleonardite, cervelleite), corresponding to primary hydrothermal minerals. The rest are tellurites (Te$^{IV}$) and tellurates (Te$^{VI}$) that developed during weathering of the deposit. In this