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Ophirite, $Ca_2Mg_4[Zn_2Mn^{3+}_2(H_2O)_2(Fe^{3+}W_9O_{34})_2]\cdot 46H_2O$, a new mineral with a heteropolytungstate tri-lacunary Keggin anion

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Abstract

Ophirite, $Ca_2Mg_4[Zn_2Mn^{3+}_2(H_2O)_2(Fe^{3+}W_9O_{34})_2]\cdot 46H_2O$, is a new mineral species from the Ophir Hill Consolidated mine, Ophir district, Oquirrh Mountains, Tooele County, Utah, U.S.A. Crystals of ophirite are orange-brown tablets on {001} with irregular {100} and {110} bounding forms; individual crystals are up to about 1 mm in maximum dimension and possess a pale orange streak. The mineral is transparent, with a vitreous luster; it does not fluoresce in short- or long-wave ultraviolet radiation. Ophirite has a Mohs hardness of approximately 2 and brittle tenacity. No cleavage or parting was observed in the mineral. The fracture is irregular. The density calculated from the empirical formula using the single-crystal cell data is 4.060 g/cm^3. Ophirite is biaxial (+) with a $2V$ angle of 43(2)°. Indices of refraction for ophirite are $\alpha = 1.730(3)$, $\beta = 1.735(3)$, $\gamma = 1.770(3)$°. The optic orientation (incompletely determined) is $Y \angle \mathbf{b} \approx 9°$ and one optic axis is approximately perpendicular to {001}. Dispersion $r > v$, strong; pleochroism is X = light orange brown, Y = light orange brown, Z = orange brown; $X < Y << Z$. Chemical analyses of ophirite were obtained by electron probe microanalysis; optimization of that analysis using the results of the crystal-structure analysis yielded the formula

$$(Ca_{1.46}Mg_{0.50}Zn_{0.04})_{\Sigma 2.00}(Mg_{3.96}Mn^{3+}_{0.04})_{\Sigma 4.00}[(Zn_{1.16}Fe^{3+}_{0.68}Ca_{0.14}Sb^{5+}_{0.02})_{\Sigma 2.00}(Mn^{3+}_{1.42}Sb^{5+}_{0.32}Fe^{3+}_{0.24}W_{0.02})_{\Sigma 2.00}$$
$$\{(H_2O)_2[(Fe^{3+}_{0.80}Sb^{5+}_{0.11}Ca_{0.07}Mg_{0.02})_{\Sigma 1.00}(W_{8.71}Mn^{3+}_{0.29})_{\Sigma 1.00}]_2\}]\cdot 46H_2O;$$

the simplified formula of ophirite is $Ca_2Mg_4[Zn_2Mn^{3+}_2(H_2O)_2(Fe^{3+}W_9O_{34})_2]\cdot 46H_2O$. Ophirite is triclinic, $P\bar{1}$, with $a = 11.9860(2)$, $b = 13.2073(2)$, $c = 17.689(1)$ Å, $\alpha = 69.690(5)$, $\beta = 85.364(6)$, $\gamma = 64.875(5)$°, $V = 2370.35(18)$ Å^3, and $Z = 1$. The strongest four lines in the diffraction pattern are [d in Å (I)(hkl)]: 10.169(100)(100,110), 11.33(91)(011,010), 2.992(75)(334,341,$\bar{1}\,\bar{1}$ 5), and 2.760(55)(412,006,$\bar{1}$ 3 5). The atomic arrangement of ophirite was solved and refined to $R_1 = 0.0298$ for 9230 independent reflections. The structural unit, ideally $\{^{[6]}Zn_2{}^{[6]}Mn^{3+}_2(H_2O)_2(^{[4]}Fe^{3+}{}^{[6]}W^{6+}_9O_{34})_2\}^{12-}$, consists of a $[Zn_2Mn^{3+}_2(H_2O)_2]$ octahedral layer sandwiched between opposing heteropolytungstate tri-lacunary ($^{[4]}Fe^{3+}{}^{[6]}W^{6+}_9O_{34}$) Keggin anions. Similar structures with an octahedral layer between two tri-lacunary Keggin anions are known in synthetic phases. Charge balance in the ophirite structure is maintained by the $\{[Mg(H_2O)_6]_4[Ca(H_2O)_6]_2\cdot 10H_2O\}^{12+}$ interstitial unit. The interstitial unit in the structure of ophirite is formed of two distinct $Mg(H_2O)_6$ octahedra and a $Ca(H_2O)_6O_1$ polyhedron, as well as five isolated water molecules. The linkage between the structural unit and the interstitial unit results principally from hydrogen bonding between oxygen atoms of the structural unit with hydrogen atoms of the interstitial unit. Ophirite is the first known mineral to contain a lacunary defect derivative of the Keggin anion, a heteropolyanion that is well known in synthetic phases. The new mineral is named ophirite to recognize its discovery at the Ophir Hill Consolidated mine, Ophir District, Oquirrh Mountains, Tooele County, Utah, U.S.A.

Keywords: Ophirite; new mineral species; heteropolytungstate lacunary Keggin anion; crystal structure; Ophir Hill Consolidated mine, Tooele County, Utah