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A new anhydrous amphibole from the Eifel region, Germany: Description and crystal structure of obertiite, $NaNa_2(Mg_3Fe^{3+}Ti^{4+})Si_8O_{22}O_2$

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ABSTRACT

Obertiite is a new amphibole species from Bellerberg, Laccher See district, Eifel, Germany. It occurs with tridymite, fluororichterite, hematite, rutile, aegirine-augite, kinoshitalite, and fluor-apatite in vugs in volcanic rocks, and crystallized from late-stage hydrothermal fluids associated with recent volcanism. Obertiite occurs as pale-pink elongated blades and divergent aggregates. It is brittle, $H = 5$, $D_{calc} = 3.16$ g/cm^3, has a colorless streak, vitreous luster, and does not fluoresce; it has perfect cleavage on {110} and conchoidal fracture. In plane-polarized light, obertiite is slightly pleochroic in shades of pink to red-orange; $X \wedge a = 2°$ (in β obtuse), $Z = b$, $Y \wedge c = 12°$ (in β obtuse) with absorption $X \sim Y \sim Z$. It is biaxial negative, $\alpha = 1.643(1)$, $\beta = 1.657(1)$, $\gamma = 1.670(3)$, $2V_x = 81(1)°$, no dispersion visible. Obertiite is monoclinic, space group $C2/m$, $a = 9.776(2)$, $b = 17.919(3)$, $c = 5.292(1)$ Å, $\beta = 104.05(2)°$, $V = 899.3(3)$ Å^3, $Z = 2$. The strongest ten X-ray diffraction lines in the powder pattern are [d(*I*,*hkl*)]: 8.414(10,110), 2.705(7,331,151), 3.390(6,131), 4.467(5,040), 3.117(5,310), 2.531(5,202), 3.255(3,240), 2.577(3,061), 2.163(3,171,261), 4.013(2,111). Analysis by a combination of electron microprobe, SIMS, and crystal-structure refinement gives SiO_2 54.53, Al_2O_3 0.15, TiO_2 7.75, Fe_2O_3 2.61, Mn_2O_3 3.27, FeO 3.36, ZnO 0.08, MgO 14.13, Li_2O 0.05, CaO 0.52, Na_2O 9.51, K_2O 0.98, F 0.55, H_2O 0.20, O ≡ F –0.23, Ni, Cr, V, Cl not detected, sum 97.46 wt%. The formula unit, calculated on the basis of 24(O,OH,F) is $(K_{0.18}Na_{0.84})(Na_{1.86}Ca_{0.08}Fe^{2+}_{0.06})(Mg_{3.09}Zn_{0.01}Li_{0.03}Fe^{3+}_{0.29}Mn^{3+}_{0.37}Fe^{2+}_{0.41}Ti^{4+}_{0.86}Al_{0.03})Si_{8.00}O_{22}[(OH)_{0.20}F_{0.26}O_{1.54}]$, and is close to the ideal end-member composition $Na\ Na_2\ (Mg_3Fe^{3+}Ti^{4+})\ Si_8\ O_{22}\ O_2$.

The crystal structure of obertiite was refined to an *R* index of 2.6% using Mo*K*α X-ray intensity data. The M1 site is split into two subsites along the **b** axis, M1 and M1A; the M1 site is occupied by Mg, and M1A is occupied predominantly by Ti^{4+} and Mn^{3+}; M2 is occupied by Mg, Fe^{2+}, and Fe^{3+}, and M3 is occupied by Mg. Local bond-valence considerations suggest that O^{2-} at O3 is linked to $Ti^{4+}Mg$ or $Mn^{3+}Mn^{3+}$ at the adjacent M1 and/or M1A sites, and that OH or F at O3 is linked to MgMg at the adjacent M1 sites.