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Jianmuite, $ZrTi^{4+}Ti^{3+}_5Al_3O_{16}$, a new mineral from the Allende meteorite and from chromitite near Kangjinla, Tibet, China

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Abstract

The new mineral jianmuite, $ZrTi^{4+}Ti^{3+}_5Al_3O_{16}$ (IMA No. 2023-057) was found: (1) as an inclusion in a corundum grain from the Cr-11 orebody near Kangjinla (29°11′N, 92°18′E), Tibet, China, with wenjiite, $Ti_{10}(Si,P,\square)_7$, Al-rich spinel, osbornite, TiN, a Ca-amphibole particularly enriched in Ti, a Sr-rich dmisteinbergite, $CaAl_2Si_2O_8$, and amorphous phases (probably residual melt) (holotype and first cotype), and (2) as several grains with corundum, mullite, $Al_6Si_2O_{13}$, tistarite, Ti_2O_3, and kaitianite, $Ti^{3+}_2Ti^{4+}O_5$, in the matrix of the CV3 carbonaceous chondrite Allende (second cotype). Eight energy-dispersive spectroscopic analyses of the holotype normalized to 100% gave SiO_2 1.83, ZrO_2 23.17, Al_2O_3 18.41, Ti_2O_3 54.32, Sc_2O_3 1.25, MgO 1.03, total 100.00 wt%. The empirical formula calculated on the basis of 10 cations and 16 O atoms is $^{VIII}Zr\ ^{VII}(Ti^{3+}_{3.034}Ti^{4+}_{0.602}Zr_{0.364})_{\Sigma 4.000}\ ^{VI}(Ti^{3+}_{1.845}Al_{1.838}Mg_{0.186}Sc_{0.131})_{\Sigma 4.000}\ ^{IV}(Al_{0.780}Si_{0.220})_{\Sigma 1.000}O_{16}$. The simplified formula is $Zr(Ti^{3+},Ti^{4+},Zr)_4(Ti^{3+},Al)_4(Al,Si)O_{16}$ and the ideal chemical formula is $ZrTi^{4+}Ti^{3+}_5Al_3O_{16}$, which requires calculated contents of ZrO_2 17.23 wt%, TiO_2 11.16 wt%, Ti_2O_3 50.23 wt%, and Al_2O_3 21.38 wt%, total 100 wt%. Six energy-dispersive spectroscopic analyses of the first cotype normalized to 100% gave SiO_2 2.86, ZrO_2 23.06, Al_2O_3 18.10, Ti_2O_3 53.78, Sc_2O_3 1.17, MgO 1.04, total 100.00 wt%. Three-dimensional electron diffraction of the holotype determined jianmuite as *I*-centered tetragonal, space group: ($I\bar{4}$) (#82), with $a = 10.3675(10)$ Å, $b = 10.3675(10)$ Å, $c = 9.8125(10)$ Å, $V = 1054.70(18)$ Å^3, and $Z = 4$. Wavelength-dispersive spectroscopic electron probe microanalyses of Allende jianmuite (second cotype) gave for the two grains (5 analyses each) SiO_2 2.32, 3.02, ZrO_2 13.95, 10.79, Al_2O_3 26.82, 21.83, Ti_2O_3 44.68, 49.47, TiO_2 12.62, 14.75, Sc_2O_3 0.12, 0.04, MgO 0.19, 0.80, FeO, 0.52, 0.55, CaO 0.17, 0.08, total 101.40, 101.34 wt%. TiO_2 (wt%) and Ti_2O_3 (wt%) were calculated from formula units Ti^{4+} and Ti^{3+}, which were determined assuming a stoichiometry of 10 cations and 16 O atoms. Electron backscatter diffraction (EBSD) patterns on the Allende jianmuite (second cotype) can be indexed by the tetragonal $I\bar{4}$ structure obtained on the holotype, with a mean angular deviation of ~0.7°, thereby confirming identification of the Allende mineral as jianmuite. The structure of jianmuite consists of cations packed in a distorted *I*-centered lattice. There are eight independent cation sites: two inside distorted cubes with tetragonal ridged faces (CN = 8), two inside capped trigonal prisms (CN = 7), two inside distorted octahedra (CN = 6), and two inside tetrahedra (CN = 4). All coordination polyhedra are connected by edges, except for the tetrahedra, which are connected by vertexes with other polyhedra. Despite the similarity in composition with carmeltazite, $ZrTi^{3+}_4Al_2O_{11}$, the structures of the two minerals bear little resemblance to one another, most notably in the number and type of cation-oxygen polyhedra. Instead, the jianmuite structure has several features in common with structures of pyrochlore-supergroup minerals, including similarity in unit-cell parameters, cubic $a \approx 10$ Å and tetragonal $a \approx c \approx 10$ Å in pyrochlore and jianmuite, respectively, and cation packing being cubic *I*-centered in both structures.

Keywords: Jianmuite, Luobusa chromitite, Allende meteorite, carmeltazite, pyrochlore supergroup, crystal structure, transmission electron microscopy, three-dimensional electron diffraction, electron backscatter diffraction