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Wenjiite, $Ti_{10}(Si,P,\square)_7$, and kangjinlaite, $Ti_{11}(Si,P)_{10}$, new minerals in the ternary Ti-P-Si system from the Luobusa ophiolite, Tibet, China

Fahui Xiong[1,2,*,†], Xiangzhen Xu[1,2], Enrico Mugnaioli[3], Mauro Gemmi[3], Richard Wirth[4], Jingsui Yang[1,5], and Edward S. Grew[6]

[1]Center for Advanced Research on the Mantle (CARMA), Key Laboratory of Deep-Earth Dynamics of Ministry of Land and Resources, Institute of Geology, Chinese Academy of Geological Sciences, Beijing 100037, China
[2]Southern Marine Science and Engineering Guangdong Laboratory, Guangzhou 511458, China
[3]Center for Nanotechnology Innovation@NEST, Istituto Italiano di Tecnologia (IIT), Piazza San Silvestro 12, 56127 Pisa, Italy
[4]Helmholtz Centre Potsdam, GFZ (German Research Centre for Geosciences), 3.5 Surface Geochemistry, Telegrafenberg, C 120, D-14473 Potsdam, Germany
[5]School of Earth Sciences and Engineering, Nanjing University, Nanjing, 210023, China
[6]School of Earth and Climate Sciences, University of Maine, Orono, Maine 04469, U.S.A.

Abstract

The new minerals wenjiite, $Ti_{10}(Si,P,\square)_7$ (IMA2019-107c) and kangjinlaite, $Ti_{11}(Si,P)_{10}$ (IMA2019-112b) occur with badengzhuite, zhiqinite, and a K-bearing dmisteinbergite-like mineral in a spheroid 20 µm across enclosed in corundum from the Cr-11 podiform chromitite orebody near the Kangjinla, Luobusa ophiolite, Tibet, China. In addition, wenjiite occurs with deltalumite, jingsuiite, osbornite-khambaraevite, and the K-bearing dmisteinbergite-like mineral in a lamellar intergrowth 100 µm long, also enclosed in corundum from the same locality. The new minerals were characterized by energy-dispersive spectroscopy and three-dimensional electron diffraction, which enabled us to obtain an ab initio structure solution and dynamical refinement from grains a few micrometers across hosted in a FIB lamella. Four analyses of wenjiite from the spheroid gave in wt% Si 21.67, P 6.24, Ti 66.39, V 1.37, Cr 2.20, Mn 0.97, and Fe 1.17 (normalized to 100), which corresponds to $(Ti_{0.93}Cr_{0.03}Mn_{0.01}Fe_{0.01}V_{0.02})_{10}(Si_{0.79}P_{0.21})_{6.51}$ on the basis of 10 cations excluding Si and P. The simplified formula is $Ti_{10}(Si,P)_{6.5}$, or more generally $Ti_{10}Si_xP_y$, where $x > y$ and $6 \leq (x + y) \leq 7$, i.e., $Ti_{10}(Si,P,\square)_7$. Wenjiite has hexagonal symmetry, space group: $P6_3/mcm$ (no. 193), with $a = 7.30(10)$ Å, $c = 5.09(10)$ Å, $V = 235(6)$ Å^3, $Z = 1$, and is isostructural with xifengite, mavlyanovite, synthetic Ti_5Si_3, and synthetic $Ti_5P_{3.15}$. Four analyses of kangjinlaite gave in wt% Si 25.56, P 9.68, Ti 62.35, V 0.21, Cr 0.83, Mn 0.42, and Fe 0.95 (normalized to 100), which corresponds to $(Ti_{10.65}V_{0.03}Cr_{0.13}Mn_{0.06}Fe_{0.14})_{\Sigma 11.01}(Si_{7.43}P_{2.55})_{\Sigma 9.99}$. The simplified formula is $Ti_{11}(Si,P)_{10}$. Kangjinlaite is tetragonal, with space group: $I4/mmm$ (no. 139), $a = 9.4(2)$ Å, $c = 13.5(3)$ Å, $V = 1210(50)$ Å^3, $Z = 4$, and is isostructural with synthetic compounds of the $Ho_{11}Ge_{10}$ type, being the most compact of these phases. Despite there now being over 70 compounds containing 38 elements isostructural with $Ho_{11}Ge_{10}$, synthesis of an analog of kangjinlaite has not been previously reported in either the Ti-P or Ti-Si binary systems or in a multicomponent system. The previously deduced crystallization sequence with decreasing temperature of the four minerals in the spheroid is wenjiite → kangjinlaite → zhiqinite + badengzhuite. This sequence is consistent with relationships reported in 9 binary systems containing intermetallic compounds of Ge and Sn isostructural with Mn_5Si_3 and $Ho_{11}Ge_{10}$. In eight of these systems the Mn_5Si_3 analog melts congruently, whereas the $Ho_{11}Ge_{10}$ analog never does. Instead, the $Ho_{11}Ge_{10}$ analog melts peritectically, generally to an Mn_5Si_3 analog and less commonly to compounds with 5:4 stoichiometry. Final crystallization of the spheroid to zhiqinite + badengzhuite is expected to be well below the temperature of 1500 °C for the congruent melting of zhiqinite in the Ti-Si system, i.e., in the range of ~1100–1300 °C.

Keywords: Luobusa chromitite, wenjiite, kangjinlaite, intermetallic melts, crystal structure, transmitting electron microscopy, three-dimensional electron diffraction