American Mineralogist, Volume 106, pages 1917–1927, 2021

Keplerite, $Ca_9(Ca_{0.5}\square_{0.5})Mg(PO_4)_7$, a new meteoritic and terrestrial phosphate isomorphous with merrillite, $Ca_9NaMg(PO_4)_7$

Sergey N. Britvin[1,2,*], Irina O. Galuskina[3], Natalia S. Vlasenko[4], Oleg S. Vereshchagin[1,†], Vladimir N. Bocharov[4], Maria G. Krzhizhanovskaya[1], Vladimir V. Shilovskikh[4,5,‡], Evgeny V. Galuskin[3], Yevgeny Vapnik[6], and Edita V. Obolonskaya[7]

[1]Institue of Earth Sciences, St. Petersburg State University, Universitetskaya Nab. 7/9, 199034 St. Petersburg, Russia
[2]Kola Science Center, Russian Academy of Sciences, Fersman Str. 14, 184209 Apatity, Russia
[3]Faculty of Natural Sciences, Institute of Earth Sciences, University of Silesia, Bedzińska 60, 41-200 Sosnowiec, Poland
[4]Centre for Geo-Environmental Research and Modelling, St. Petersburg State University, Ulyanovskaya str. 1, 198504 St. Petersburg, Russia
[5]Institute of Mineralogy, Urals Branch of Russian Academy of Science, Miass 456317, Russia
[6]Department of Geological and Environmental Sciences, Ben-Gurion University of the Negev, POB 653, Beer-Sheva 84105, Israel
[7]The Mining Museum, St. Petersburg Mining University, 2, 21st Line, 199106 St. Petersburg, Russia

Abstract

Keplerite is a new mineral, the Ca-dominant counterpart of the most abundant meteoritic phosphate, which is merrillite. The isomorphous series merrillite-keplerite, $Ca_9NaMg(PO_4)_7$-$Ca_9(Ca_{0.5}\square_{0.5})Mg(PO_4)_7$, represents the main reservoir of phosphate phosphorus in the solar system. Both minerals are related by the heterovalent substitution at the *B*-site of the crystal structure: $2Na^+$ (merrillite) → $Ca^{2+} + \square$ (keplerite). The near-end-member keplerite of meteoritic origin occurs in the main-group pallasites and angrites. The detailed description of the mineral is made based on the Na-free type material from the Marjalahti meteorite (the main group pallasite). Terrestrial keplerite was discovered in the pyrometamorphic rocks of the Hatrurim Basin in the northern part of Negev desert, Israel. Keplerite grains in Marjalahti have an ovoidal to cloudy shape and reach 50 μm in size. The mineral is colorless, transparent with a vitreous luster. Cleavage was not observed. In transmitted light, keplerite is colorless and non-pleochroic. Uniaxial (−), ω = 1.622(1), ε = 1.619(1). Chemical composition (electron microprobe, wt%): CaO 48.84; MgO 3.90; FeO 1.33; P_2O_5 46.34, total 100.34. The empirical formula (O = 28 apfu) is $Ca_{9.00}(Ca_{0.33}Fe^{2+}_{0.20}\square_{0.47})_{1.00}Mg_{1.04}P_{6.97}O_{28}$. The ideal formula is $Ca_9(Ca_{0.5}\square_{0.5})Mg(PO_4)_7$. Keplerite is trigonal, space group *R*3*c*, unit-cell parameters refined from single-crystal data are: a = 10.3330(4), c = 37.0668(24) Å, V = 3427.4(3) Å^3, Z = 6. The calculated density is 3.122 g/cm^{-3}. The crystal structure has been solved and refined to R_1 = 0.039 based on 1577 unique observed reflections [$I>2\sigma(I)$]. A characteristic structural feature of keplerite is a partial (half-vacant) occupancy of the sixfold-coordinated *B*-site (denoted as CaIIA in the earlier works). The disorder caused by this cation vacancy is the most likely reason for the visually resolved splitting of the ν_1 (symmetric stretching) (PO_4) vibration mode in the Raman spectrum of keplerite. The mineral is an indicator of high-temperature environments characterized by extreme depletion of Na. The association of keplerite with "*REE*-merrillite" and stanfieldite provides evidence for the similarity of temperature conditions that occurred in the Mottled Zone to those expected during the formation of pallasite meteorites and lunar rocks. Because of the cosmochemical significance of the merrillite-keplerite series and by analogy to plagioclases, the Na-number measure, 100×Na/(Na+Ca) (apfu), is herein proposed for the characterization of solid solutions between merrillite and keplerite. The merrillite end-member, $Ca_9NaMg(PO_4)_7$, has the Na-number = 10, whereas keplerite, $Ca_9(Ca_{0.5}\square_{0.5})Mg(PO_4)_7$, has Na-number = 0. Keplerite (IMA 2019-108) is named in honor of Johannes Kepler (1571–1630), a prominent German naturalist, for his contributions to astronomy and crystallography.

Keywords: Keplerite, merrillite, whitlockite, phosphate, meteorite, pallasite, angrite, pyrometamorphism