

Keplerite, $\text{Ca}_9(\text{Ca}_{0.5}\square_{0.5})\text{Mg}(\text{PO}_4)_7$, a new meteoritic and terrestrial phosphate isomorphous with merrillite, $\text{Ca}_9\text{NaMg}(\text{PO}_4)_7$

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ABSTRACT

Keplerite is a new mineral, the Ca-dominant counterpart of the most abundant meteoritic phosphate, which is merrillite. The isomorphous series merrillite-keplerite, $\text{Ca}_9\text{NaMg}(\text{PO}_4)_7$ – $\text{Ca}_9(\text{Ca}_{0.5}\square_{0.5})\text{Mg}(\text{PO}_4)_7$, 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) \rightarrow $\text{Ca}^{2+} + \square$ (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 (–), $\omega = 1.622(1)$, $\varepsilon = 1.619(1)$. 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 $\text{Ca}_{9.00}(\text{Ca}_{0.33}\text{Fe}_{0.20}\square_{0.47})_{1.00}\text{Mg}_{1.04}\text{P}_{6.97}\text{O}_{28}$. The ideal formula is $\text{Ca}_9(\text{Ca}_{0.5}\square_{0.5})\text{Mg}(\text{PO}_4)_7$. Keplerite is trigonal, space group $R\bar{3}c$, unit-cell parameters refined from single-crystal data are: $a = 10.3330(4)$, $c = 37.0668(24)$ Å, $V = 3427.4(3)$ Å³, $Z = 6$. The calculated density is 3.122 g/cm³. 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, $100 \times \text{Na}/(\text{Na} + \text{Ca})$ (apfu), is herein proposed for the characterization of solid solutions between merrillite and keplerite. The merrillite end-member, $\text{Ca}_9\text{NaMg}(\text{PO}_4)_7$, has the Na-number = 10, whereas keplerite, $\text{Ca}_9(\text{Ca}_{0.5}\square_{0.5})\text{Mg}(\text{PO}_4)_7$, 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