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# Bradleyite, $Na_3Mg(PO_4)(CO_3)$, inclusion in diamond: Structure and significance

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## Abstract

Bradleyite, a sodium phosphate-magnesium carbonate, $Na_3Mg(PO_4)(CO_3)$, occurs in sedimentary salt rocks and in igneous, carbonatitic, and kimberlitic rocks. In this paper, we present the characteristics of a bradleyite sample found in a new geological environment as an inclusion in a diamond from the Córigo Sorriso placer deposit in Mato Grosso State, Brazil, where other unusual mineral inclusions in diamond were earlier identified. Bradleyite is part of a polymineral inclusion, comprising a porous aggregate of grains <150 nm in size, hosted within a dolomite crystal. The studied bradleyite is characterized by the highest MgO+FeO concentrations and the lowest Na content among bradleyites from other localities. It demonstrates significant variability in composition, particularly Na (28.75–37.84 mass % $Na_2O$). Nitrogen was also detected by EDS analysis. We report for the first time the ab initio crystal structure of natural bradleyite. It has monoclinic symmetry, with cell parameters $a = 8.684$ Å, $b = 6.804$ Å, $c = 5.074$ Å, and $\beta = 90.34°$. The structure was solved ab initio and refined using dynamical scattering theory in space group $P2_1/m$, confirming the model obtained from powder XRD analysis of synthetic analogs. The final structure model converged to a formula $Na_3(Mg_{0.86}Fe_{0.14})(PO_4)(CO_3)$, $Z = 2$. Bradleyite is a polygenetic mineral. In continental salt deposits, it forms under atmospheric pressure during sedimentation. In deep-formed igneous rocks, such as kimberlites and carbonatites, bradleyite occurs as a product of late-stage crystallization of carbonatitic melt and as a primary-crystallized phase in deep-seated minerals, such as olivine, ilmenite, chrome spinel, and magnetite. Our findings demonstrate its stability in diamond and diamond-forming environments and that it may be considered a product of crystallization from a primary melt inclusion.

**Keywords:** Bradleyite, phosphate-magnesium carbonate, diamond, inclusion, dolomite, Juina area