Goldschmidtite, (K,REE,Sr)(Nb,Cr)O₃: A new perovskite supergroup mineral found in diamond from Koffiefontein, South Africa

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ABSTRACT

Goldschmidtite is a new perovskite-group mineral (IMA No. 2018-034) with the ideal formula (K,REE,Sr)(Nb,Cr)O₃. A single grain of goldschmidtite with a maximum dimension of ~100 µm was found as an inclusion in a diamond from the Koffiefontein pipe in South Africa. In addition to the dark green and opaque goldschmidtite, the diamond contained a Cr-rich augite (websteritic paragenesis) and an intergrowth of chromite, Mg-silicate, and unidentified K-Sr-REE-Nb-oxide. Geothermobarometry of the augite indicates that the depth of formation was ~170 km. The chemical composition of goldschmidtite determined by electron microprobe analysis (n = 11, WDS, wt%) is: Nb₂O₅ 44.82, TiO₂ 0.44, ThO₂ 0.10, Al₂O₃ 0.35, Cr₂O₃ 7.07, La₂O₃ 11.85, Ce₂O₃ 6.18, Fe₂O₃ 1.96, MgO 0.70, CaO 0.04, SrO 6.67, BaO 6.82, K₂O 11.53, total 98.53. The empirical formula (expressed to two decimal places) is (K₂O 0.55La₂O₃ 0.11SrO 0.13BaO 0.09CeO₂ 0.08)Σ2.09(Nb₂O₇ 0.73Cr₂O₃ 0.19Fe₂O₅ 0.05Al₂O₃ 0.01MgO 0.04TiO₂ 0.01)Σ1.00O₃. Goldschmidtite is cubic, space group Pm̅3m, with unit-cell parameters: a = 3.9876(1) Å, V = 63.40(4) Å³, Z = 1, resulting in a calculated density of 5.32(3) g/cm³. Goldschmidtite is the K-analog of isolueshite, (Na,La)NbO₃. Raman spectra of goldschmidtite exhibit many second-order broad bands at 100 to 700 cm⁻¹ as well as a pronounced peak at 815 cm⁻¹, which is possibly a result of local ordering of Nb and Cr at the B site. The name goldschmidtite is in honor of the eminent geochemist Victor Moritz Goldschmidt (1888–1947), who formalized perovskite crystal chemistry and identified KNbO₃ as a perovskite-structured compound.

Keywords: Perovskite, niobium, mantle, diamond inclusion, new mineral, Koffiefontein, Kaapvaal

INTRODUCTION

Diamonds are carriers of minerals from the lithospheric mantle underpinning cratons (Harris and Gurney 1979; Meyer 1987; Helmstaedt et al. 2010), the mantle transition zone (Pearson et al. 2014; Kiseeva et al. 2016; Tschauner et al. 2018), and the lower mantle (Harte et al. 1999; Tschauner et al. 2014; Palot et al. 2016; Nestola et al. 2018). As a chemically inert and rigid host, diamond can preserve included minerals for billions of years, and thus provide a snapshot of ancient chemical conditions in cratonic keels or deep-mantle regions.

The Kaapvaal craton in South Africa is host to many diamondiferous kimberlites that have been intensively mined and studied since the 1970s (e.g., the International Kimberlite Conferences held since 1973). Large-scale mining, large inclusion-bearing diamonds, and the efforts of geochemists globally have made it the most studied craton from the perspective of diamond formation.

We report the first natural occurrence of (K,REE,Sr)(Nb,Cr)O₃, now named goldschmidtite (IMA No. 2018-034), included in a websteritic diamond from the Koffiefontein kimberlite, Kaapvaal craton, South Africa. The holotype specimen is deposited in the Royal Ontario Museum, accession number M58208. It is the fifth perovskite-structured mineral to occur in Earth’s mantle, along with perovskite sensu stricto (CaTiO₃), bridgmanite (Harte et al. 1999; Tschauner et al. 2014), CaSiO₃-perovskite (Nestola et al. 2018), and K-REE-Cr-rich tausonite, which previously recorded the highest Nb- and K-content in a perovskite mineral-inclusion from diamond (Kopylova et al. 1997).

Goldschmidtite is the natural analog of the well-known ferroelectric material KNbO₃, which has the perovskite structure type with orthorhombic symmetry at room temperature (coexisting with a metastable monoclinic phase: Lummen et al. 2017), and whose symmetry increases to cubic above ~400 °C (Skjærvø et al. 2018). Solid solution of LaFeO₃ in KNbO₃, at molar amounts of 20% or more, also has the effect of increasing the symmetry to cubic at room temperature (Kakimoto et al. 2003).

End-member KNbO₃ was first synthesized by Joly (1877), as discussed by Holmquist (1896). Thomas F.W. Barth, a member of Victor Moritz Goldschmidt’s research group, was the first to determine the crystal structure of perovskite, CaTiO₃ (Barth 1925). In the following year, Goldschmidt and his group reported that KNbO₃ was effectively isosctructural, and simultaneously introduced the famous tolerance factor for prediction of the