

BaC₄O₄ — An Alkaline-Earth Squarate Free from Water of Crystallization with Three-dimensional Framework Structure Featuring a Layer-like Separation of Cations and Anions

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Abstract

Colourless single crystals of BaC₄O₄ have been obtained from aqueous solution at 80 °C. BaC₄O₄ is stable in air up to 490 °C. BaCO₃ is formed by further increase of temperature. BaC₄O₄ crystallizes in the tetragonal space group I4/mcm (nr. 140) with a=635.95(5), c=1240.77(13) pm, Z=4. Ba²⁺ is coordinated by eight oxygen atoms of the squarate dianions; Ba—O 276.1(1) pm. The coordination polyhedron is a distorted, square anti-prism. The squarate dianions occupy crystallographic mirror planes and possess approximately 4/mmm symmetry; C—C 145.7(5) and 146.5(5) pm, C—O 125.9(3) pm. A layer-like separation between the cations and anions exists with respect to the [001] direction.

