

Synthesis, spectroscopic characterization, and X-ray crystal structure of a novel 3D barium strontium oxalate

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Abstract

Oxalate-based compounds have attracted much attention in many areas. Due to their low thermal stability they can be used as precursors of nanocrystalline oxides, e.g., pure BaTiO₃ can be produced from the decomposition of barium titanyl oxalate hydrate [1] and, recently, PbZrO₃ has been prepared from a new lead zirconium oxalate [2]. Moreover, the presence of cavities in the structures of a number

of them is at the origin of zeolitic properties, arising from weakly bonded water molecules, reported long ago [3-4] and thoroughly studied recently in a few oxalate- and, also, carboxylate-based materials for instance [5-7]. A novel 3D crystal structure of the title compound (Ba_{0.741}Sr_{0.259})C₂O₄ has been synthesized from precipitation methods at room temperature. Its molecular structure was determined by single X-ray diffraction analysis. The compound crystallizes with space group C2/c and the cell parameters are $a = 10.348 (5) \text{ \AA}$, $b = 5.489 (5) \text{ \AA}$, $c = 8.218 (5) \text{ \AA}$, $\beta = 125.09 (5)^\circ$, $V = 382.0 (5) \text{ \AA}^3$, and $Z = 4$ ($R_1 = 0.026$). The crystal structure can be described as double parallel zigzag chains running along the c axis and linked together by additional monodentate oxalate-metal bonding. The distance between two chains is $b/2$. Each metal ion has six O-atom neighbours and they are linked together via the different coordination modes of the oxalate groups, resulting in the formation of a three-dimensional network.

Key words: barium strontium oxalate, single crystal diffraction

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