

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

N. Bendjellal, C. Trifa, H. Anana, C. Boudaren

Unité de Recherche de Chimie de l'Environnement et Moléculaire
Structurale, CHEMS, Université Mentouri–Constantine, 25000
Algeria nassimabendjellal@gmail.com

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 titanate 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

References

- [1] M. Louër, D. Louër, F.J. Gotor, J.M. Criado, *J. Solid State Chem.* 92 (1991) 565-572. [2] C. Boudaren, J.P. Auffrédic, M. Louër, D. Louër, *Chem. Mater.* 12 (2000) 2324-2333.
- [3] C. Sterling, *Nature* 205 (1965) 588-589.
- [4] N. Gérard, G. Watelle-Marion, A. Thierri-Sorel, *Bull. Soc. Chim. Fr.* 11(1968) 4367-4378. [5] T. Bataille, J.P. Auffrédic, D. Louër, *Chem. Mater.* 11 (1999) 1559-1567.
- [6] T.M. Reineke, M. Eddaoudi, M. Fehr, D. Kelley, O.M. Yaghi, *J. Am. Ceram. Soc.* 121 (1999) 1651- 1657.
- [7] F. Serpaggi, T. Luxbacher, A.K. Cheetham, G. Férey, *J. Solid State Chem.* 145(1999) 580-586.