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SYNTHESIS, STRUCTURE AND PROPERTIES OF NEW BARIUM DECATUNGSTATE

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A new material with fascinating properties was obtained. For the first time crystalline decatungstate with barium cation (+2) Ba(H2O)2C3H7NO3]2[W10O32]·2C3H7NO was synthesized from aqueous dimethylformamide medium.
The composition was confirmed by chemical analysis, IR- and Raman spectroscopy, electron absorption spectroscopy and scanning electron microscopy.
The first barium decatungstate was characterized X-ray diffraction analysis. The centrosymmetric W10O32 anion in the composition has a typical structure (two “square pyramids”, which consist of five distorted WO6octahedra, connected by “bases” through the common vertices of the four octahedra). The coordination polyhedron of the barium is a monocapped square antiprism. The main crystallographic characteristics of the structure of barium decatungstate: triclinic, P-1space group, a = 11.899 (3), b = 12.1313 (11), c = 13.341 (2) Å, α = 70.417 (11), β = 64.254 (18), γ = 87.185 (12) °, V = 1623.7 (5) Å3 at T = 293K, Z=1, ρ = 3.356 g/cm3.
It was determined that thermal decomposition of the salt occurs in four stages of successive loss of solvent molecules with heat absorption and final crystallization of BaWO4 and WO3.
The reversible photochromic propertiy of the synthesized barium decatungstate has been discovered –the substance turns blue under the influence of daylight or a UV-irradiation and returns white color when the excitation source is eliminated.

Summary

A new material with fascinating properties was obtained. For the first time crystalline decatungstate with barium cation (+2) Ba(H2O)2C3H7NO3]2[W10O32]·2C3H7NO was synthesized from aqueous dimethylformamide medium. The thermodynamic aspects of synthesis, chemical composition, crystal structure, surface morphology, thermal decomposition were investigated by mathematical modeling, chemical, UV-vis., FTIR- and Raman-spectroscopy, X-ray, DTA analysis. Due to photochromic properties this substrate is going to be used in catalysis, biomedicine, molecular electronics, energy and optical application.

Author: Ms KRETOVA, Elena (Donetsk National University)

Co-author: Mrs POIMANOVA, Elena (Donetsk National University)

Presenter: Ms KRETOVA, Elena (Donetsk National University)

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