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New Solid Solutions Based on Barium Borates Incorporating Bismuth and Rare Earth Elements: Thermal Expansion, Crystal Structures, and Photoluminescence

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INTRODUCTION & AIM

Seven new series of solid solutions (42 compositions total), doped with REE^{3+} ions, were synthesized based on two barium borate matrices: $BaBi_2B_2O_7$ and $Ba_3REE_2(BO_3)_4$ (*REE* = Y, Eu). Nine crystal structures were refined using single-crystal X-ray diffraction. Additional characterization included Raman spectroscopy, IR spectroscopy, thermal analysis (DSC + TG), and high-temperature powder X-ray diffraction. Photoluminescence spectra were recorded for all series, and the temperature dependence of photoluminescence intensity was examined.

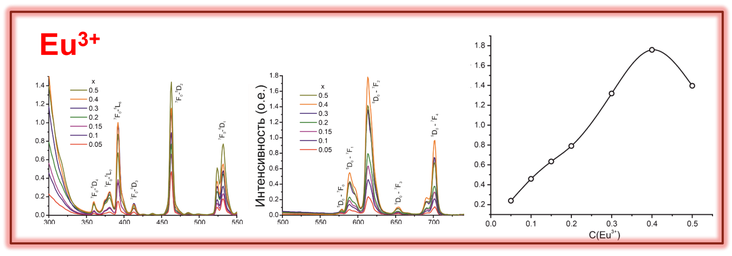
For the $BaBi_2B_2O_7$ matrix, solid solutions doped with REE^{3+} were obtained. The compositional ranges of continuous solid solutions were determined.

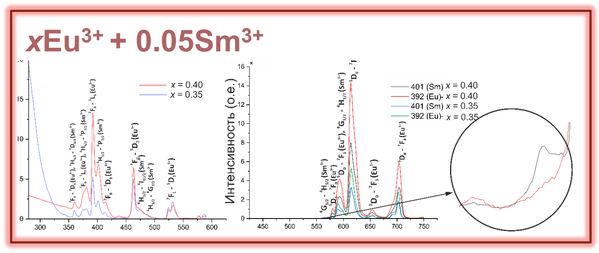
METHOD

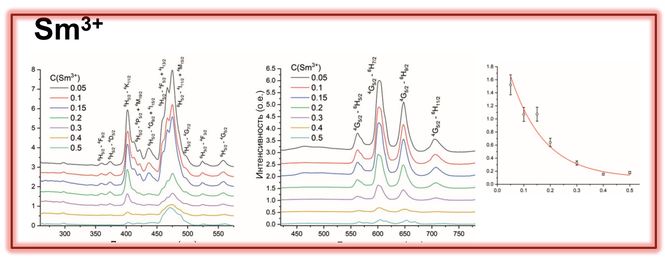
- X-ray Powder diffraction (XRD)
- Single crystal X-ray diffraction
- High-temperature powder X-ray diffraction
- Thermal Analysis: Thermogravimetry (TG) and Differential Scanning Calorimetry (DSC)
- Light Scattering Spectroscopy (LSS)
- Infrared Spectroscopy (IR Spectroscopy)
- Luminescent Spectroscopy

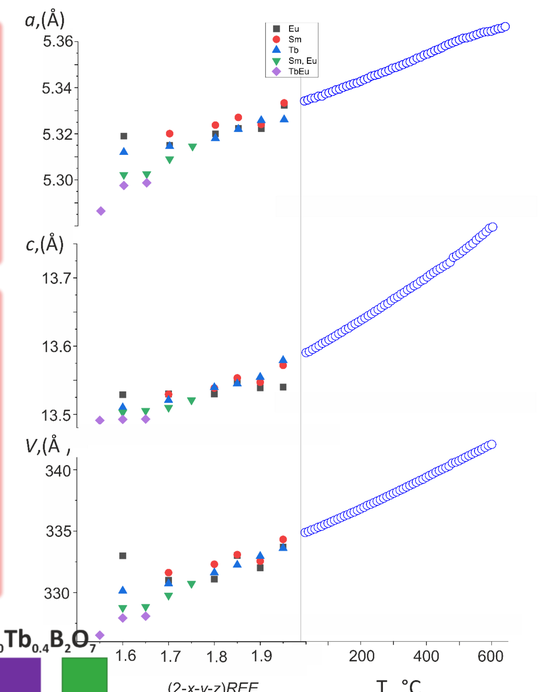
RESULTS & DISCUSSION

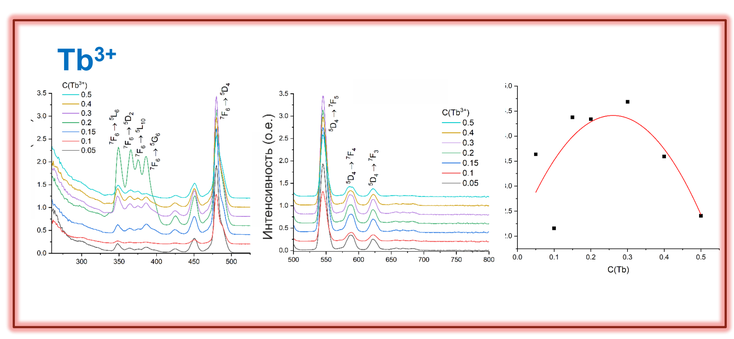
Co-doping of the $BaBi_2B_2O_7$ lattice was found to expand the miscibility regions of the solid solutions. Eight crystal structures were refined from single-crystal data for $BaBi_{2-x}Eu_xB_2O_7$ (x = 0.1, 0.2, 0.4), $BaBi_{2-x}Sm_xB_2O_7$ (x = 0.05, 0.3), $BaBi_{2-x}Tb_xB_2O_7$ (x = 0.1, 0.3, 0.4). All compounds crystallize in the $BaBi_2B_2O_7$ structure type (hexagonal system, space group $P6_3$). The structure contains three independent crystallographic sites for large cations, each split into Ba and Bi subsites. REE^{3+} ions occupy the Bi subsites. Upon REE^{3+}activation, the larger Sm and Eu ions preferentially occupy the *M*1 and *M*2 sites (largest coordination polyhedra volumes), whereas Tb^{3+}, with the smallest ionic radius, occupies the *M*3 site (smallest polyhedral volume)

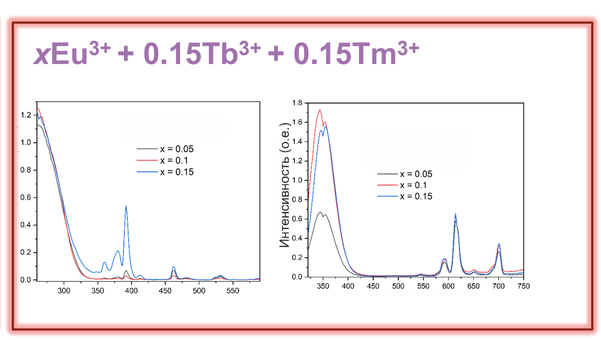


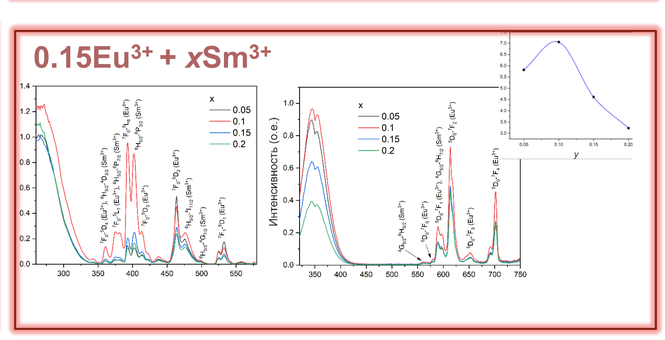


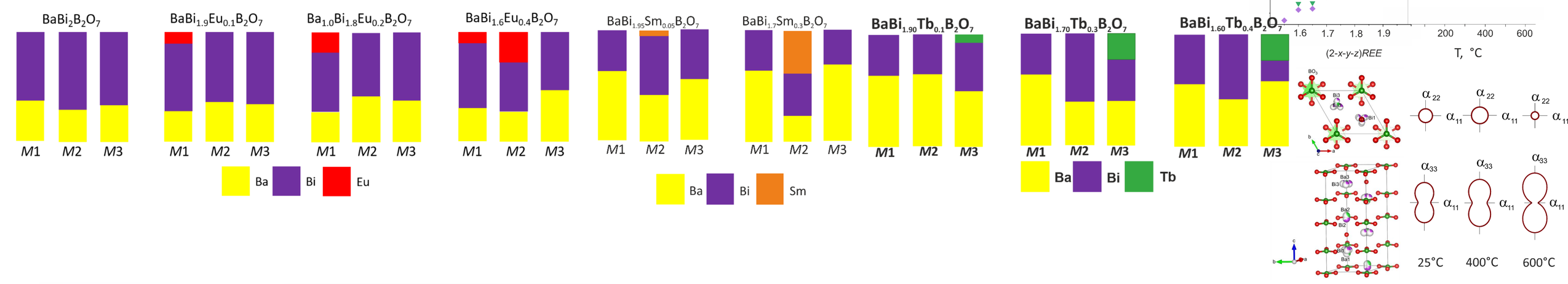


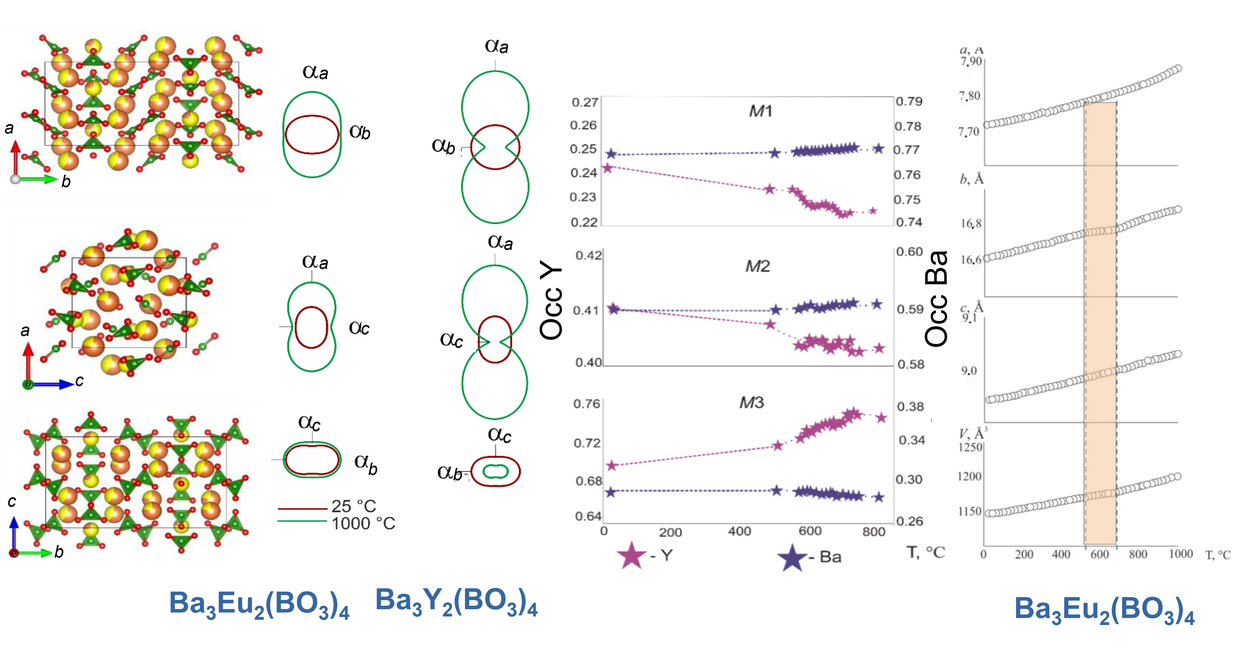


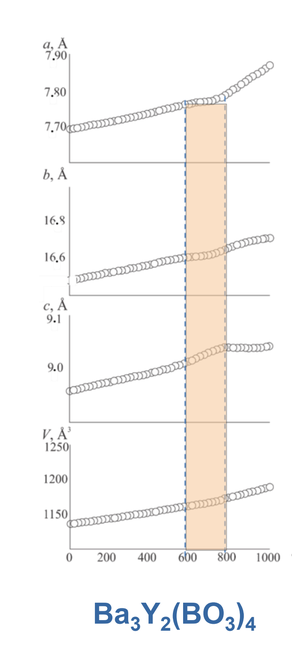


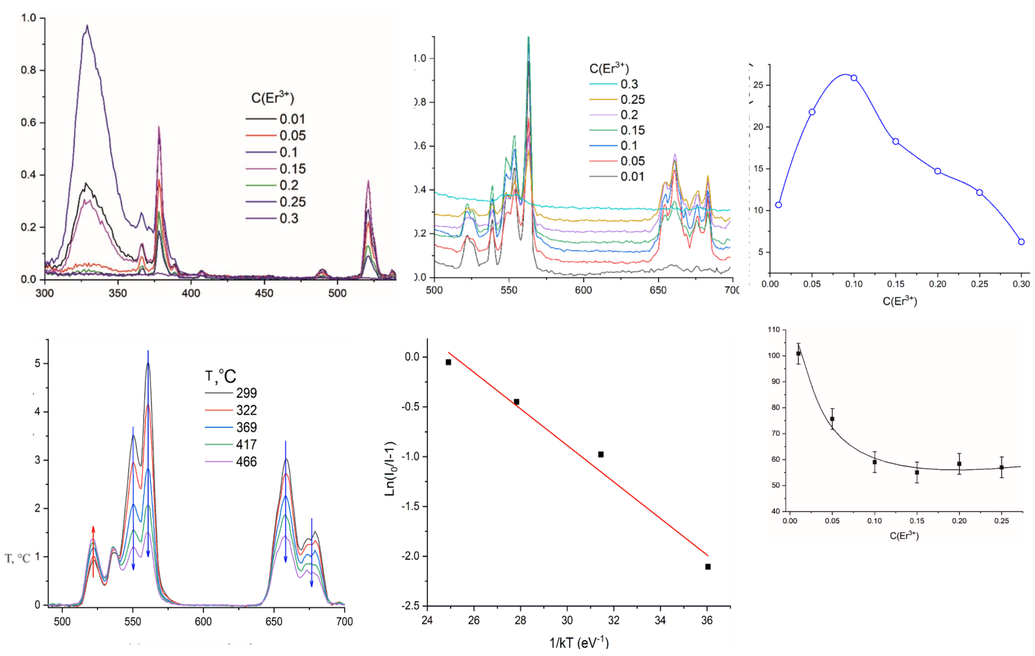












CONCLUSIONS

A new solid-solution series $Ba_3Y_{2-x}Er_x(BO_3)_4$ (x = 0.01—0.3), along with end-member borates $Ba_3Y_2(BO_3)_4$, $Ba_3Eu_2(BO_3)$, was synthesized via melt crystallization. Thermal expansion was studied for $Ba_3Eu_2(BO_3)$ and $Ba_3Y_2(BO_3)_4$, and the crystal structure of $Ba_3Y_2(BO_3)_4$ was refined across a wide temperature range (40 data points). Photoluminescence spectra and their temperature dependence were investigated for the $Ba_3Y_{2-x}Er_x(BO_3)_4$ series. The optimal activator concentration was determined to be x = 0.1]

FUTURE WORK/ REFERENCES/ACKNOWLEDGMENT

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