Crystal Structures of $BaSrRTaO_6$ (R = Tm, Lu)

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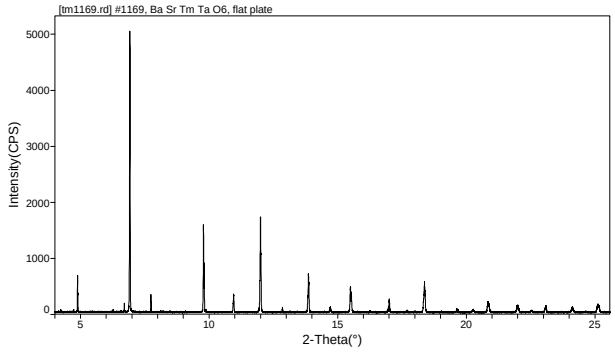
Introduction

An emphasis in laser research has been the effort to find new materials which can be used as hosts for rare earth ions that have desirable fluorescent characteristics. The symmetry of a series of $BaSrRTaO_6$ compounds (R = Nd, Sm, Gd, Tm, and Lu) is quite clearly lower than the cubic of the ideal perovskite structure [1]. High-resolution powder diffraction studies at the MRCAT ID10 beamline at the Advaced Photon Source have permitted unambiguous determination of the nature of the distortion in the R = Tm and Lu materials.

Methods and Materials

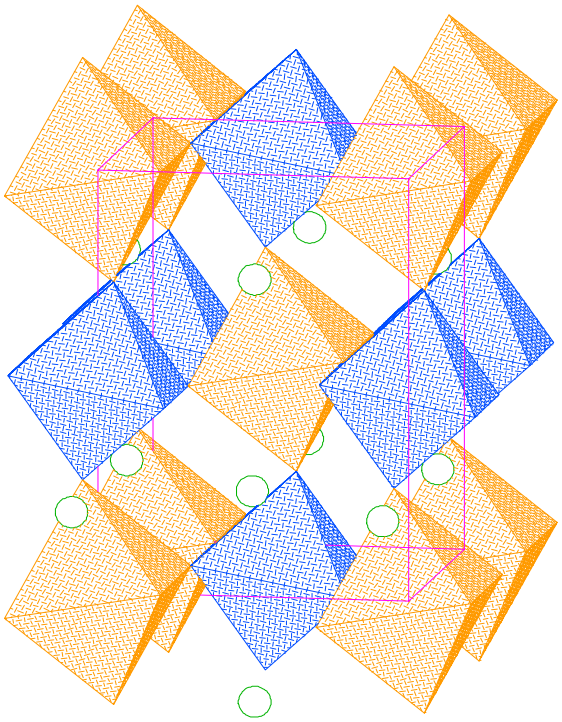
Powder diffraction patterns were measured from flat plate specimens at an energy of 35 keV (λ = 0.353973(10) Å, calibrated using NIST SRM 1976), using a Si(333) monochromator and Si(111) analyzer crystal.
The pattern could be indexed on a body-centered monoclinic



unit cell having a = 5.86792(10), b = 5.87983(10), c = 8.28161(11) Å, β = 90.016(13)°, and V = 285.735(8) Å^3. The observed peak splittings rule out tetragonal or rhombohedral distortions of the ideal cubic structure. No orthorhombic space group yielded a chemically-reasonable refinement. The true symmetry appears to be *I2/m*, analogous to the structure of $Ba_2Bi_2O_6$ [2]. A combined refinement using synchrotron and laboratory data yielded the residuals wRp = 0.1054, Rp = 0.1141, R(F^2) = 0.11, and χ^2 = 2.630.

Discussion

The occupation of the two independent *B* sites By Tm and Ta is completely ordered. The average Tm-O and Ta-O bond distances are 2.218(5) and 1.975(3) Å, respectively. The largest deviations from the ideal octahedral angles are 5.7 and 8.3° for Tm and Ta, respectively. The Tm and Ta octahedra are tilted 7.6 and 8.5° from the *c*-axis. The *A* site is randomly occupied by Ba and Sr; this site is 12-coordinate, with bond distances ranging from 2.64-3.23 Å.



Acknowledgments

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References

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