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The Crystal Structure and Nonstoichiometry of Rare Earth Oxyfluoride*

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Abstract

Oxyfluoride phases for the rare earth Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, and Y have been prepared by heating a mixture of lanthanon fluorides, LnF_3 , and lanthanon oxides, Ln_2O_3 . Three phases were identified. The rhombohedral phases, LnOF , have a stoichiometric composition, and the tetragonal phases, $\text{Ln}_4\text{O}_3\text{F}_6$, have a comparatively large nonstoichiometric composition range. The third cubic phase, with a fluorite-type structure, was observed in the $\text{SmOF-Sm}_4\text{O}_3\text{F}_6$ region after quenching from a high temperature. This establishes that both the rhombohedral SmOF and the tetragonal $\text{Sm}_4\text{O}_3\text{F}_6$ transform to the cubic phase and form a complete solid solution in the high-temperature range. It is postulated that the rhombohedral and tetragonal phases are pseudocubic from the fact that the diffraction patterns of these two phases are closely similar to that of the fluorite type.

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