High Pressure Structures and Compressibilities of YF_3 and LaF_3

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Many studies have been devoted to the study of laser-hosting *Ln* (*Ln* = REE, Y, Sc) fluorides; particularly $ALnF_4$ phases crystallizing in the scheelite structure. Yet, for many *Ln* chemistries the scheelite form is unknown and, in the case of those known compositions, e.g. $LiGdF_4$, decomposition, to LiF + LnF_3, occurs at high-*p* [1]. We have investigated how the LnF_3 structure controls both the synthesis and the decomposition of the binary fluoride phase at high *p* conditions.

YF_3 crystallizes in the β-YF_3-type structure at ambient *p*. It has been proposed [2], though not observed, that the high-*p*, RT structure is the same as that of LaF_3, tysonite-type. This conjecture we can confirm, in addition to obtaining compressibilities of high- and low-*p* forms. These data allow calculation of molar volumes at high-*p*, e.g. $LiYF_4$ cf. LiF + YF_3 and judge the effect of increase in REE-coordination at phase transitions on phase stability.

LaF_3 has no known binary fluoride scheelite forms and undergoes a phase transition at $p > 12$ GPa to a structure previously described in *Cmma* and *I4/mmm* symmetries (subgroups of CaF_2 structure) [3,4]. We will present our determination of the high-*p* structure of this phase that extends the currently known transition sequence for LnF_3, thus:

δ-UO_3 (ReO_3) *to* dist-ReO_3 *to* α-UO_3 *to* β-YF_3 *to* LaF_3 *to* *Pmmn*.

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