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Substitution sites for 3+ defects in LiNbO₃ FRANK BRIDGES, CAMERON MACKEEN, Physics Dept. UC Santa Cruz, LASZLO KOVACS, Hungarian Academy of Sciences, Budapest, Hungary — The photorefractive response of LiNbO₃ can be suppressed by substitution of both 2+ and 3+ dopants, which is very important for harmonic generation applications. An issue that has not been completely resolved is the substitution site – on Li with compensating Li vacancies, or self compensating clusters with the defect atom substituting on both Li and Nb sites. For Zn(2+) we have found that Zn primarily substitutes on the Li site with very little Zn on a Nb site. Here we consider the 3+ dopants, In and Er, and present EXAFS data for both defects. The signature for substitution on a Li site is a large peak near 2.9 Å in an EXAFS r-space plot, while for Nb substitution the main In-Nb or Er-Nb peak would occur near 3.5 Å. For In there is a large peak at 2.9 Å, and most of the substitution appears to be on the Li site but the In-Nb distances are substantially increased (.1-.15 Å) and the local environment about In is more distorted than around Zn. For Er, both congruent and stoichiometric crystals were studied; the EXAFS plots are nearly identical except for a range near 3 Å where the amplitude is lower for the stoichiometric sample. Possible models for the local environment about each defect will be discussed.

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