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# Pressure-induced effects on the spectroscopic properties of Nd<sup>3+</sup> in MgO:LiNbO<sub>3</sub> single crystal. A crystal field approach

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## Abstract

The effects of pressure on the Nd<sup>3+</sup>-doped MgO:LiNbO<sub>3</sub> single crystal have been studied by luminescence spectroscopy at low temperature and high pressures from ambient conditions up to 33 GPa. Specifically, the pressure-induced evolution of the emission spectra, corresponding to the  $^4F_{3/2} \rightarrow ^4I_{9/2}$ ,  $^4I_{11/2}$  transitions, and the excitation spectra, corresponding to the  $^4I_{9/2} \rightarrow ^4F_{5/2} + ^2H_{9/2}$ , and  $^4I_{9/2} \rightarrow ^4F_{7/2} + ^4S_{3/2}$  transitions, show a gradual red-shift that follows a linear pressure dependence and a decrease in the intensity of the spectra with increasing pressure. The initial effect of increasing pressure on the MgO:LiNbO<sub>3</sub> crystal is the modification of the relative amount of the several centers in the sample. At pressures around 20 GPa the characteristic multicenter Nd<sup>3+</sup> structure eventually disappears indicating that all the centers have very similar environments near this pressure. At higher pressures, observed changes seem to have a different origin. The evolution of Nd<sup>3+</sup> luminescence is studied in the frame of crystal-field theory in order to evaluate its capability of monitoring the pressure-induced structural changes. Crystal-field analysis, under approximated C<sub>3v</sub> symmetry, shows a smooth increase of the overall crystal-field strength on the luminescent ion, which can be related to the volume reduction as pressure increases. Crystal-field parameters also show a general monotonic behavior with pressure that indicates a structural modification of the local structure that, maintaining the trigonal symmetry around the impurity ion, evolves towards a lower axial character. No evidences of a phase transition have been observed in the studied pressure range.

## Keywords

High Pressure; Lithium Niobate; Rare Earth ions; Nd; Photoluminescence; Energy levels; Crystal-Field

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