

Abstract Submitted
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Local and distant charge compensation of iron ions in ABO₃ ferroelectrics¹ GALINA MALOVICHKO, ROBERT PETERSEN, VALENTIN GRACHEV, Montana State University — The determination of the lattice sites and charge compensators of non-isovalent impurities are vitally important for both fundamental science and tailoring material properties for various applications. Results of our study of Fe³⁺ centers in LiNbO₃, LiTaO₃ and KTaO₃ (LN, LT and KT) with the help of Electron Paramagnetic Resonance (EPR) and Electron Nuclear Double Resonance (ENDOR) have shown significant difference in spectroscopic characteristics and, correspondingly, structures of these centers. Two Fe³⁺ dominant centers in cubic KT crystals have axial <100> symmetry caused by the presence of local charge compensators (oxygen vacancy for Ta⁵⁺ substitution and interstitial oxygen for K⁺ substitution). In Li-deficient congruent LT and LN crystals the Fe³⁺ ions substitute only for Li⁺. Since no disorder in the nearest surrounding was found, the distant charge compensation by intrinsic defects in cation sublattice is supposed. In stoichiometric samples of LT and LN the iron ions randomly substitute for both Li⁺ and Ta⁵⁺ (Nb⁵⁺) having average self-compensation of excess charges.

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Galina Malovichko
Montana State University

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