# Investigation of the Spin Hamiltonian Parameters and the Local Structure of Two $Ni^{3+}$ Centers in $KTaO_3$

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The spin Hamiltonian anisotropic $g$ factors $g_{\|}$ and $g_{\perp}$ and the local structures of the $Ni^{3+}$ centers I and II in $KTaO_3$ are theoretically investigated by using the perturbation formulas of the spin Hamiltonian parameters for $3d^7$ ions in tetragonally distorted octahedrons and dodecahedrons. By analyzing the electron paramagnetic resonance data of the studied systems, the centers I and II can be attributed to $Ni^{3+}$ ions occupying octahedral $Ta^{5+}$ (associated with a nearest-neighbour oxygen vacancy $V_O$ along the $C_4$ axis) and the dodecahedral $K^+$ (associated with a nearest-neighbour interstitial oxygen $O_I$ along the $C_4$ axis) sites, respectively. Based on these studies, it is found that at the center I the impurity $Ni^{3+}$ is displaced away from $V_O$ by $\Delta Z_I \approx -0.31(2)$ Å along the $C_4$ axis. At the center II a large off-center displacement, $\Delta Z_{II} \approx 1.12(2)$ Å, towards the $O_I$ along the $C_4$ axis is obtained, due to $Ni^{3+}$-$O_I$ covalent bonding.

*Key words:* Electron Paramagnetic Resonance; Defect Structures; Crystal- and Ligand-field Theory; $Ni^{3+}$; $KTaO_3$.