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The site and high field β NMR properties of ⁸Li⁺ implanted into α -Al₂O₃

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We present high magnetic field β NMR measurements of ⁸Li⁺ implanted in single crystals of sapphire, a commonly used backing material for other samples. From the well-resolved quadrupolar splitting, we extract the electric field gradient (EFG) at the implanted ⁸Li⁺ site. Comparison with supercell density functional theory calculations of the EFG allows us to identify the octahedral interstitial site as the most likely candidate. In contrast to the zero field β NQR spectra, only a single site is evident at high field. We discuss possible explanations for this discrepancy. The high field spin lattice relaxation is extremely slow ($1/T_1 < 0.02 \text{ s}^{-1}$) from 4 to 300 K. This regime, where cross relaxation to the ²⁷Al nuclear spins is quenched, extends down to at least 2.2 Tesla.

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