Quadrupole Moments of the ⁴⁰Ca Core Plus One Nuclein ⁴¹Sc and ⁴¹Ca

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The electric-field-gradient (EFG) and anisotropic chemical shift of 45 Sc($I^{\pi}=7/2^{-}$, stable) in TiO₂ crystal were determined by detecting the FT-NMR of 45 Sc(0.5 atm% of Ti in TiO₂) doped in TiO₂ crystal at a high field of 7.0 T and 9.4 T. Using the EFG, an old β -NQR spectrum of 41 Sc was reanalyzed to obtain $eq Q(^{41}$ Sc)/h which was combined with the renewed $Q(^{45}$ Sc) = $-(23.6 \pm 0.2)$ fm² to obtain $|Q(^{41}$ Sc; $|I^{\pi}=7/2^{-}$, $|I_{1/2}=0.596$ s)| = (15.6 ± 0.3) fm². Also the atomic EFG in Ca was recalculated, using a finite-element multi configuration Hartree-Fock method to renew $Q(^{43}$ Ca). Finally using the known hyperfine constants of 41 Ca, the $Q(^{41}$ Ca) value has been renewed.

Key words: Quadrupole Moments of Sc and Ca Isotopes; Electric Field Gradients; Ca and Sc Atoms; TiO₂.