

$$\alpha_c \nu^{-1} + \beta_c = \text{eq}^{\text{lat}}(\text{cation nuclei})$$

Thus, the cation effect on the local Tc-99 EFGs manifests itself only in the lattice contributions. The valence contribution remains unchanged and reveals the distortion of the TcO_4 anion due to the site symmetry in the lattice. The valence term contains the unknown R-factor. To determine the R-factor, it is necessary to calculate a "pure" valence contribution eq^{val} . The eq^{val} to the Tc-99 EFG for TcO_4 with point symmetry C_{3v} was calculated by using the non-relativistic X_α discrete variation method with extended basis sets of atomic orbitals [3]. The calculated value is 34 MHz or $2813 \cdot 10^{18} \text{ V/m}^2$. Then, from the relation $(1 - R) \cdot 2813 \cdot 10^{18} = 1121 \cdot 10^{18}$, we obtain $R = 0.6$. The ratio between the lattice contributions to the EFGs at the anion and the cation positions in the pertechnetates is constant and has the value $\text{eq}^{\text{lat}}(\text{Tc-99})/\text{eq}^{\text{lat}}(\text{cation}) \cong 6$. It should be noted that the local EFGs at the cation positions in pertechnetates are approximately the same as in the corresponding perrhenates, perbromates, and perchlorates and are an order of magnitude higher than those in metaperiodates.

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