

unit-cell volume \mathcal{V} should be expected for the compounds with the same structure. The experimental value of eq^{exp} is related to the quadrupole coupling constant C_Q by the expression

$$eq^{\text{exp}} (\text{V/m}^2) = 41,37 \cdot 10^{18} C_Q (\text{MHz})/Q(\text{barn}) \quad (3)$$

The following numerical values of the quadrupole moment $Q(\text{barn})$ and Sternheimer antishielding factor $(1 - \gamma)$ were used in the calculation: 0.5 and 6, for TcO_4 ; 0.15 and 6.1, for Na-23; 0.06 and 20.2, for K-39; 0.14 and 56, for Rb-87; and 0.003 and 111, for Cs [2]. Table presents the experimental values of QCC, the unit-cell volumes \mathcal{V} , and calculated values eq^{lat} at the anion and cation positions.

Table. Values of the unit-cell volumes, QCCs, and local EFGs at the cation and anion positions of the pertechnetates.

Compound	$\mathcal{V} \cdot 10^{-30}$ m^3	Cation positions		Anion positions		
		C_Q (MHz)	$eq^{\text{lat}} 10^{-18}$ V/m^2	C_Q (MHz)	$eq^{\text{exp}} 10^{-18}$ V/m^2	$eq^{\text{lat}} 10^{-18}$ V/m^2
$^{23}\text{NaTcO}_4$	338.32	0.95(3)	42.9	9.36(1)	774.5	305.7
$^{39}\text{KTcO}_4$	416.54	1.22(2)	41.6	5.19(1)	429.4	248.3
NH_4TcO_4	441.96	-	-	3.3(1)	273.0	222.2
$^{87}\text{RbTcO}_4$	448.92	7.0(1)	39.9	3.78(1)	312.7	228.8
$^{133}\text{CsTcO}_4^*$	500.22	0.25(1)	31.1	2.00(5)	165.5	204.2
AgTcO_4	347.2	-	-	8.59(2)	710.7	295.1

* Measured at 430 K.

An examination of the $eq^{\text{exp}}(\text{Tc-99})$ and $eq^{\text{exp}}(\text{cation})/(1 - \gamma)$ as a function of the unit-cell volume \mathcal{V} revealed the linear dependences

$$eq^{\text{exp}}(\text{Tc-99}) = \alpha_a \mathcal{V}^{-1} + \beta_a \quad (4)$$

$$eq^{\text{exp}}(\text{cation nuclei})/(1 - \gamma) = \alpha_c \mathcal{V}^{-1} + \beta_c$$

where $\alpha_a = 6.4 \cdot 10^{-7} \text{ V m}$, $\beta_a = -1121 \cdot 10^{18} \text{ V/m}^2$, $\alpha_c = 0.1 \cdot 10^{-7} \text{ V} \cdot \text{m}$, $\beta_c \cong 14 \cdot 10^{18} \text{ V/m}^2$. It is assumed that the observed changes in C_Q (Tc-99) and $C_Q(\text{cation})$ along the series of similar compounds with the same lattice structures are only caused by the changes in the lattice constants and that the structure and the symmetry of the TcO_4 anion remain unaltered. A comparison of eqs.(1), (2) and (4) makes it possible to assign the following meanings to the parameters α and β :

$$\alpha_a \mathcal{V}^{-1} = (1 - \gamma) eq^{\text{lat}} (\text{Tc-99}), \beta_a = (1 - R) eq^{\text{val}}(\text{Tc-99})$$