Supplementary Information

Order-Disorder and Displacive Components in the Ferroelectric-Paraelectric Phase Transition of Potassium Titanyl Phosphate KTiOPO$_4$
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For the high-temperature Pnna KTP there exist no displacements and polarization. For the low-temperature Pna21 KTP the average value of the displacements of each atomic species and polarization were calculated as follows.

Average value of the displacement of Ti atoms was estimated by
\[ d(Ti) = \frac{c \cdot (4 \cdot z(Ti1) + 4 \cdot z(Ti2) - 1)}{8} \]
where \( c \), \( z(Ti1) \) and \( z(Ti2) \) are c-axis value, z coordinate of Ti1 atom and z coordinate of Ti2 atom, respectively. Contribution of Ti atoms to the polarization was calculated by
\[ p(Ti) = c \cdot (4 \cdot z(Ti1) + 4 \cdot z(Ti2) - 1) \cdot C \cdot 10^{22}/V \]
where the \( C \) and \( V \) are the elementary charge=1.60218*10^-19 (C) and unit-cell volume, respectively.

Average value of the displacement of P atoms is estimated by
\[ \text{distP} = \frac{c}{2} \cdot (zP1 + zP2 - 0.75) \]
where \( zP1 \) and \( zP2 \) are z coordinates of P1 and P2 atoms, respectively. Contribution of P atoms to the polarization was calculated by
\[ pP = \frac{c}{\text{Vol}} \cdot 5(4 \cdot zP1 - 1 + 4 \cdot zP2 - 2) \cdot \text{Coulum} \cdot (10^8)^2 \cdot 10^6 \]
where the \( \text{Vol} \) and \( \text{Coulum} \) are unit-cell volume and elementary charge = 1.60218*10^-19 (C).

Average value of the displacement of K atoms is estimated by
\[ \text{distK} = \frac{c}{8} \cdot \left[ \text{gK1} \cdot (4 \cdot zK1 - 1) + \text{gK2} \cdot (4 \cdot zK2 - 1) + (1 - \text{gK0}) \cdot (4 \cdot zK1a - 1) + (1 - \text{gK2}) \cdot (4 \cdot zK2a - 1) \right] \]
where \( \text{gK1} \) is occupancy factor of K atom at the K1 site, \( zK1 \) is the z coordinate of K1 atom, \( \text{gK2} \) is occupancy factor of K atom at the K2 site, \( zK2 \) is the z coordinate of K2 atom, \( zK1a \) is the z coordinate of K1s atom, and \( zK2a \) is the z coordinates of K2a atom. Contribution of P atoms to the polarization was calculated by
\[ pK = \frac{c}{\text{Vol}} \cdot \left[ \text{gK1} \cdot (4zK1 - 1) + \text{gK2} \cdot (4 \cdot zK2 - 1) + (1 - \text{gK0}) \cdot (4 \cdot zK1a - 1) + (1 - \text{gK2}) \cdot (4 \cdot zK2a - 1) \right] \cdot \text{Coulum} \cdot (10^8)^2 \cdot 10^6 \]

Average value of the displacement of O atoms is estimated by
\[ \text{distO} = c \cdot \left[ \frac{14 \cdot (zO1 + zO2 + zO3 + zO4 + zO5 + zO6 + zO7 + zO8 + zO9 + zO10 - 3)}{40} \right] \]
where \( zOi \) is the z coordinate of Oi atom.
Average value of the displacement of O atoms is estimated by
\[ pO = \frac{c}{\text{Vol}} \cdot \left[ 4 \cdot (zO1 + zO2 + zO3 + zO4 + zO5 + zO6 + zO7 + zO8 + zO9 + zO10 - 3) \right] \cdot \text{Coulum} \cdot (10^8)^2 \cdot 10^6 \]