Supplementary Information

Order-Disorder and Displacive Components in the Ferroelectric- Paraelectric Phase Transition of Potassium Titanyl Phosphate $KTiOPO_4$

by Masatomo Yashima and Takafumi Komatsu

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)=c*(4*z(Ti1)+4*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*(4*z(Ti1)+4*z(Ti2)-1)*C*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

$$distP := \frac{c}{2} \cdot (zP1 + zP2 - 0.75)$$

where zP1 and zP2 are z coordinates of P1 and zP2 atoms, respectively. Contribution of P atoms to the polarization was calculated by

$$pP := \frac{c}{Vol} \cdot 5(4 \cdot zP1 - 1 + 4 \cdot zP2 - 2) \cdot Coulum \left(10^8\right)^2 \cdot 10^6$$

where the Vol and Coulum are unit-cell volume and elementary charge = 1.60218*10^-19 (C).

Average value of the displacement of K atoms is estimated by

$$distK := \frac{c}{8} \cdot [gK1 \cdot (4 \cdot zK1 - 1) + gK2 \cdot (4 \cdot zK2 - 1) + (1 - gK1) \cdot (4 \cdot zK1a - 1) + (1 - gK2) \cdot (4 \cdot zK2a - 1)]$$

where gK1 is occupancy factor of K atom at the K1 site, zK1 is the z coordinate of K1 atom, 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

$$pK := \frac{c}{Vol} \cdot 1[gK1 \cdot (4zK1 - 1) + gK2 \cdot (4 \cdot zK2 - 1) + (1 - gK1) \cdot (4 \cdot zK1a - 1) + (1 - gK2) \cdot (4 \cdot zK2a - 1)] \cdot Coulum \left(10^8\right)^2 \cdot 10^6$$

Average value of the displacement of O atoms is estimated by

$$distO := c \cdot \frac{[4 \cdot (zO1 + zO2 + zO3 + zO4 + zO5 + zO6 + zO7 + zO8 + zO9 + zO10 - 3)]}{40}$$

where zOi is the z coordinate of Oi atom.
Average value of the displacement of O atoms is estimated by

$$pO := \frac{c \cdot 2}{Vol} \cdot [4 \cdot (zO1 + zO2 + zO3 + zO4 + zO5 + zO6 + zO7 + zO8 + zO9 + zO10 - 3)] \cdot Coulum \left(10^8\right)^2 \cdot 10^6$$