Lattice dynamical study of phase transitions in TlH_2PO_4 and TlD_2PO_4 crystals

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The contribution presents the results of the lattice dynamical simulation of TlH_2PO_4 and TlD_2PO_4 crystals in different temperature phases. At high temperature TlH_2PO_4 and TlD_2PO_4 crystallize with the same orthorhombic *Pbcn* structure (Z=4). However, TlH_2PO_4 exhibits the transition to ferrodistorsive ferroelastic $P2_111/b$ phase (Z=4), whereas the TlD_2PO_4 demonstrates the antiferroelectric phase transition to $P1121/b$ phase which is accompanied with the unit cell doubling along the *a*-axis (Z=8).

The aim of our study was to explain the microscopic mechanism leading to the phase transitions of different character in TlH_2PO_4 and TlD_2PO_4. The lattice dynamics of these crystals was simulated within the semi-empirical approach assuming the Coulomb, short range Born-Mayer type, covalent and hydrogen bonded interatomic interactions. The phonon dispersion relations, partial density of phonon states, dispersion of atomic mean square displacements and temperature factors were calculated in various structural phases.

As follows from our simulation, the protons placed on the shorter $O-H_1\cdots O$ hydrogen bonds play the crucial role at the para – ferroelastic transition in TlH_2PO_4. The 2 % variation of the interatomic interaction within the $O-H_1\cdots O$ bonds leads to the softening of the lowest frequency B_{3g} optic mode in Γ point. However, the proper ferroelastic phase appears as the result of the bilinear interaction between the soft B_{3g} and B_{1u} acoustic V_{YZ} (C_{44}) mode.

The $O-D_2\cdots O$ longer bonds play more significant role at the para – antiferroelectric phase transition in TlD_2PO_4. The slight variation of the interatomic interaction within the $O-D_2\cdots O$ hydrogen bonds of TlD_2PO_4 results in falling down of the S^{1+} phonon branch in $(1/2, 1/2, 0)$ point and evokes the antiferroelectric phase transition.