

## Unified lattice dynamics model for hydrogen-bonded crystals

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Contribution presents a semi-phenomenological atomistic model applicable for lattice dynamics simulation of hydrogen-bonded dielectric crystals. The model potential function takes into account the long-range Coulomb, short-range Born-Mayer-type and covalent interatomic interactions. "Oxygen-hydrogen" interactions within the  $O - H(D) \cdots O$  hydrogen bonds were simulated like the weak covalent interactions. The lattice dynamics both of monoclinic KDP-type crystals, namely  $CsH_2PO_4$ ,  $CsD_2PO_4$ ,  $RbD_2PO_4$ ,  $PbHPO_4$ ,  $PbDPO_4$ ,  $TlH_2PO_4$ ,  $TlD_2PO_4$  compounds and betaine phosphite  $(CH_3)_3NCH_2COO^*H_3PO_3$  crystals was simulated using this atomistic model. The phonon frequencies in the centre of Brillouin zone, phonon dispersion relations, density of phonon states, partial density of states, dispersion of atomic mean-square displacements and structure factors were calculated in various structural phases of the crystals mentioned above. The good agreement between the calculated and experimental data reveals reliability of the current simulation. Based on this model we simulated the conditions of some structural phase transitions occurred in these compounds. The phase transition mechanism involves the phonon anharmonicity and proton-phonon interactions.