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Rotational Motion in LiBH4/LiI Solid Solutions

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Lithium borohydride (LiBH4) is an ionic crystal, consisting of (Li)+ cations and (BH4)- anions. It undergoes an order/disorder transition at 380 K. The dynamic disorder of the HT phase originates from rotational jumps of the (BH4)- anions. The transition is accompanied by an increase of Li ionic conductivity by more than 3 orders of magnitude.
The HT phase of LiBH4 can be stabilized by addition of lithium halides, resulting in the enhanced conductivity at room temperature.
We investigated the localized rotational diffusion
of the (BH4)- anions in LiBH4/LiI solid solutions by means of quasielastic and inelastic neutron scattering. The (BH4)- motions are thermally activated and characterized by activation energies in the order of 40 meV. Typical dwell times between jumps are in the picosecond range at temperatures of about 200
K. The motion is dominated by 90° reorientations around the 4-fold symmetry axis of the tetrahedraly shaped (BH4)- ions.
The presence of iodide
markedly reduces activation energies and increases the rotational frequencies by more than a factor of 100. The addition of
iodide lowers the transition temperature, stabilizing the disordered HT phase well below RT.

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