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A quasielastic and inelastic neutron scattering study of the alkaline and alkaline-earth borohydrides LiBH4, Mg(BH4)2 and the mixture LiBH4+Mg(BH4)2

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Quasielastic neutron scattering was used to investigate the low energy transfer dynamics of the complex borohydrides Mg(BH₄)₂ in the α - and β -modifications, LiBH₄ in the low and high temperature crystal structure, and the 1:1 molar mixture of LiBH₄+ α -Mg(BH₄)₂. All investigated compounds show a rich dynamic behavior below an energy range of $\Delta E=10$ meV with the superposition of rotational dynamics of the constituent [BH₄]⁻ anions and low lying lattice modes. For Mg(BH₄)₂, the rotational diffusion of the [BH₄] units was found to be much more activated in the metastable β -polymorph compared to the α -phase, and the low lying lattice modes are even softer in the former crystal structure. In Mg(BH₄)₂, the structural phase transition is mainly governed by the lattice dynamics, while alkaline LiBH₄ exhibits a transition of the [BH₄] rotations around the phase transition temperature. Ball milled LiBH₄+ α -Mg(BH₄)₂ remains a physical mixture of the parent compounds and each component retains its characteristic dynamic signature up to the melting temperature.

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