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Learning from structure solution: An enhanced solid-state Mg electrolyte

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All-solid-state batteries based on magnesium are considered for the use in mobile applications as well as to store energy from “renewable”intermittent energy sources. Recently, a solid state magnesium ion conductor, Mg(en)1(BH4)2 (en stands for ethylenediamine), obtained from Mg(BH4)2 : [Mg(en)3(BH4)2] 2:1 mixture, was reported to have an exceptionally high magnesium ion conductivity of up to 6·10−5 S·cm−1 at 70 ℃. Here we show that this synthesis actually yields a mixture of Mg(en)1.2(BH4)2 and amorphous Mg(BH4)2. The latter was often neglected in previous investigations, though it was shown recently that its dynamics have a positive influence on the conductivity. The structure of Mg(en)1.2(BH4)2 has been solved from single crystal X-ray diffraction in space group P-1 and confirmed by neutron powder diffraction on isotopically substituted Mg(en)1.2(11BD4)2. Its structure shows three Mg atoms with coordination numbers 4, 5 and 6, the BH4 groups behaving as terminal and bridging ligands, and en chelating and bridging Mg atoms. This complexity makes the structure solution virtually impossible from powder diffraction data. Thermal decomposition of Mg(en)1.2(BH4)2 goes through an intermediate formation of the previously unknown Mg(en)2(BH4)2, its structure was solved from synchrotron X-ray powder diffraction, complemented by DFT optimization.

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