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Analysis of the disordered crystal structure of LiBH4 by 3D-Δ-PDF

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LibH4 shows strong diffuse scattering in layers normal to c* at integer l, predominantly at odd l. The diffuse scattering within the layers is circular around the Bragg reflections and stronger close to the reciprocal origin. This observation tits to columnar defects with a negative correlation in the a-b-plane and preserved correlation along c. The 3D-DELTA-PDF shows an intricate pattern of positive and negative peaks, which were interpreted with by manual Patterson search.

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