A possible analog to MgB$_2$: Discovery of a predicted layered LiB via cold compression$^1$ ALEKSEY KOLMOGOROV, SAMAD HAJINAZAR, CHRIS ANGYAL, Binghamton University, VLADIMIR KUZNETZOV, University of Oxford, ANDREW JEPHCOAT, Okayama University — Stoichiometric LiB has been previously predicted $^{[1,2]}$ to be a new synthesizable layered material with electronic and vibrational properties desired for MgB$_2$-type superconductivity. However, previous experiments showed no signs of the proposed compound forming under high pressures. We report on the synthesis of the LiB via cold compression in the diamond anvil cell $^{[3]}$. Remarkably, the signature powder XRD peak from the new layered compound appeared above 21 GPa and remained visible down to ambient pressure upon sample quenching. Apparent stacking disorder in LiB and a stoichiometry shift in the starting LiB$_y$ (from $y \approx 0.90$ down to $y \approx 0.75$) made material characterization a challenge. Ab initio modeling allowed us to establish the pressure-dependent composition of LiB$_y$ and predict related stable structures overlooked in previous studies. 


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