

Supporting information

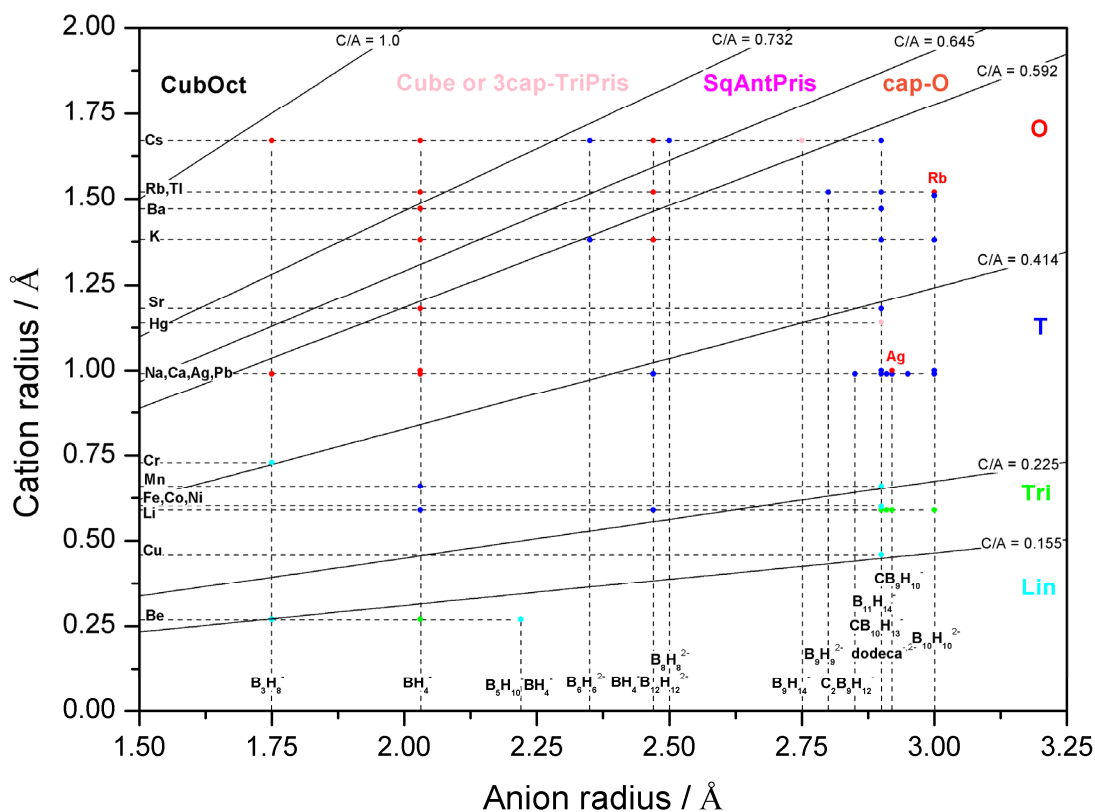


Figure S1: Cation coordination in single metal hydroborates as a function of cation/anion radius ratio C/A . The regions of various coordination polyhedra are calculated according to the first Pauling rule: linear (Lin), triangular (Tri), tetrahedral (T), octahedral (O), mono-capped octahedral (cap-O), square anti-prismatic (SqAntPris), cubic (Cube), tri-capped trigonal prismatic (3cap-TriPris), cuboctahedral (CubOct). The color code of the observed coordination (data point) is the same as for the predicted regions.

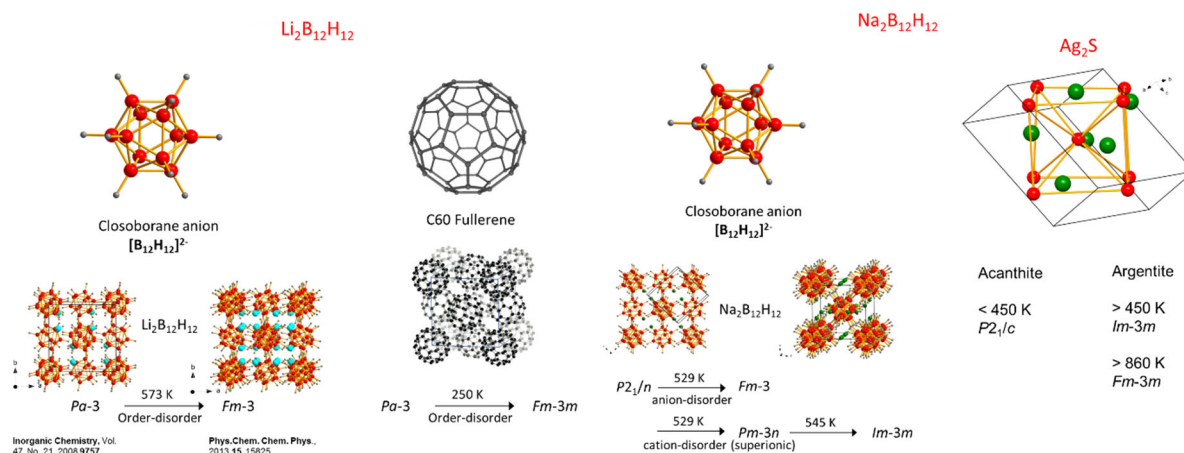


Figure S2: Analogy between temperature polymorphs of Li₂B₁₂H₁₂ and C60, and between Na₂B₁₂H₁₂ and Ag₂S.