

Supplementary information for:

Off-stoichiometry in I-III-VI₂ chalcopyrite absorbers: a comparative analysis of structures and stabilities

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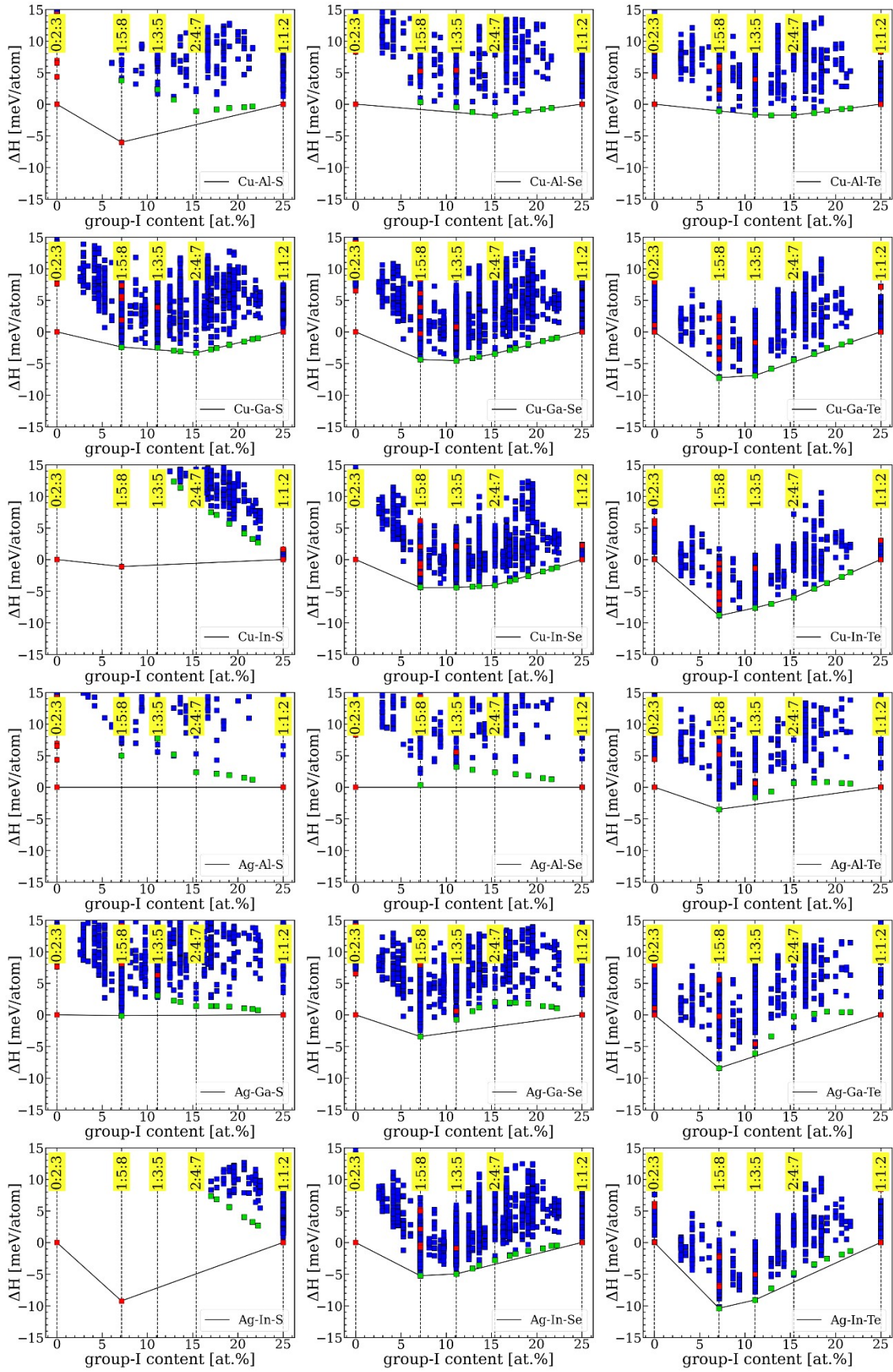


Figure S1. Convex hulls constructed for different I-III-VI systems. The ordinate axis (ΔH) is the formation enthalpy relative to a mixture of terminal phases (i.e. 1:1:2 and 0:2:3).

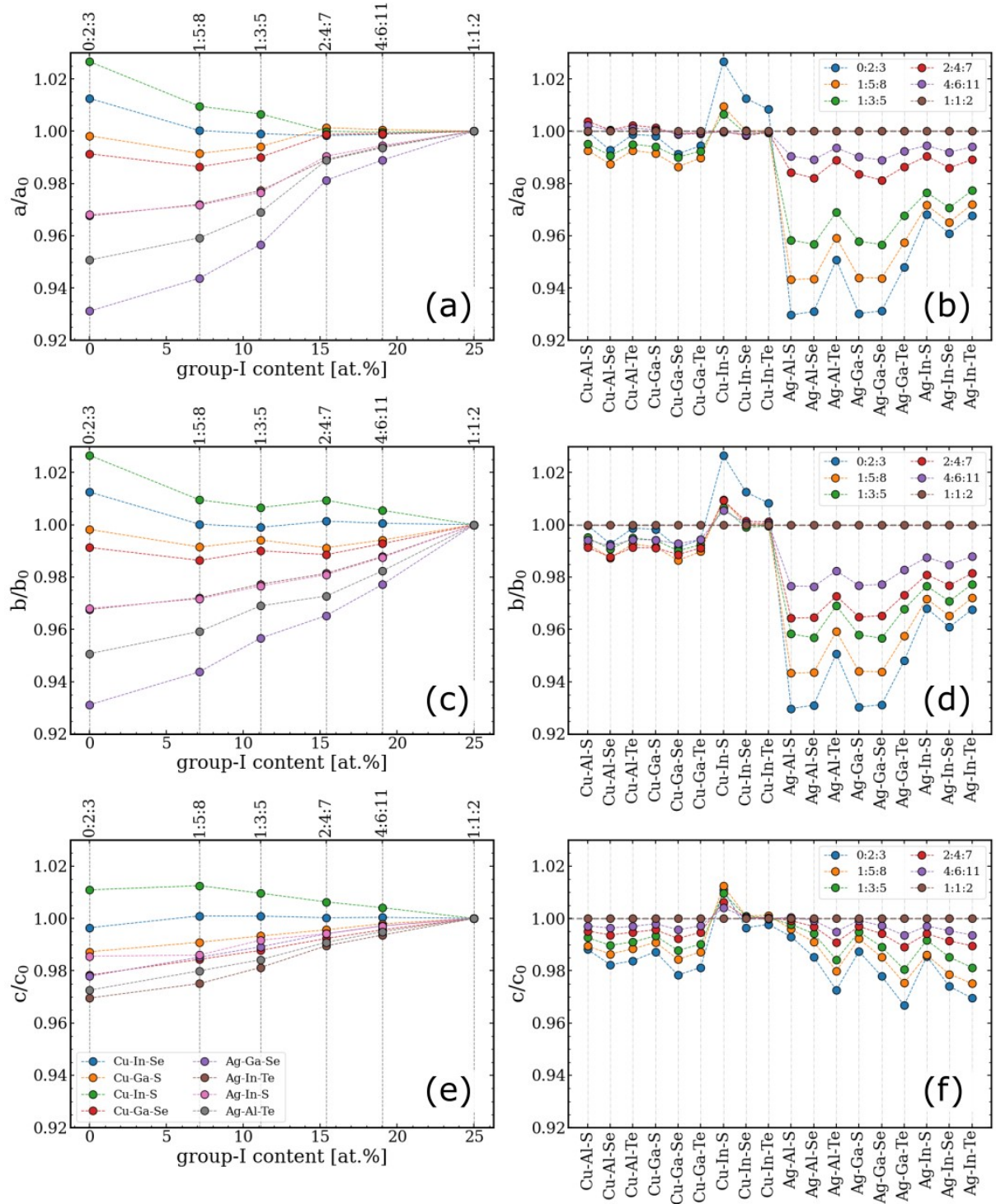


Figure S2. Ratios of the lattice parameters for ODCs related to the respective values for the corresponding chalcopyrite phase. The ratios are plotted versus (a,c,e) group-I content (for eight arbitrary systems) and (b,d,f) type of system for the entire I-III-VI family considered.

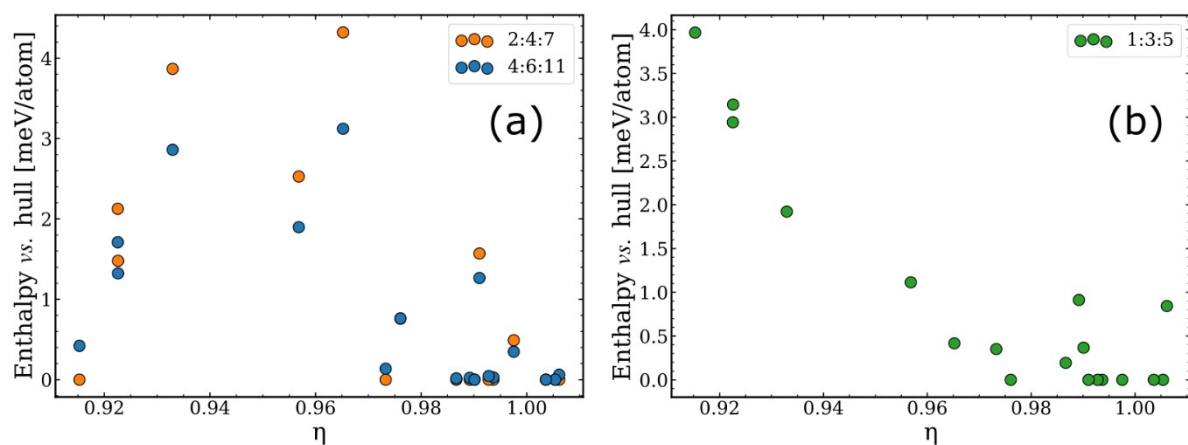


Figure S3. Enthalpies of (a) 2:4:7/4:6:11 ODCs and (b) 1:3:5 ODC related to convex hull versus tetragonal distortion in different I-III-VI systems.

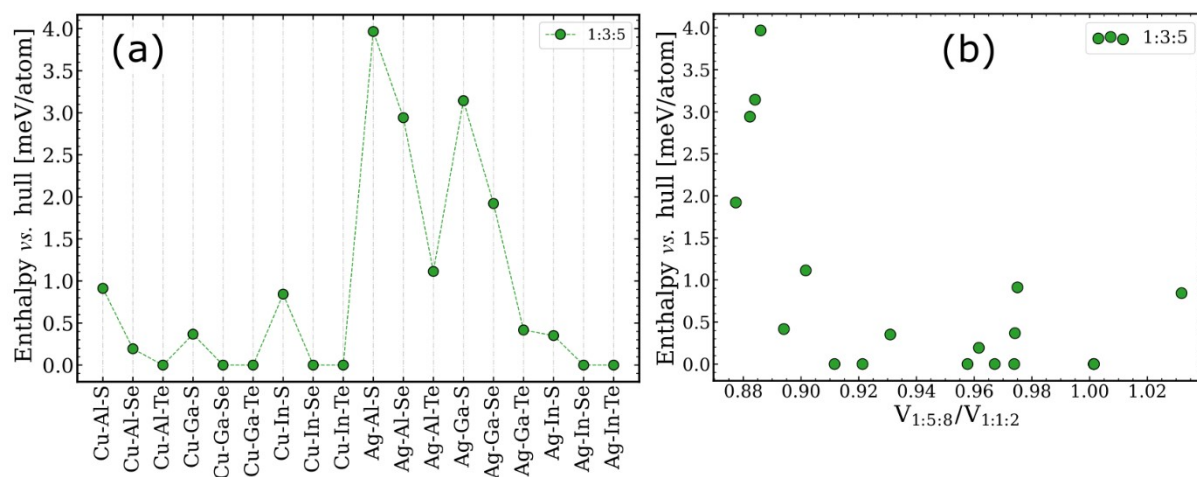


Figure S4. Enthalpies of 1:3:5 ODC above the simplified convex hull (consisting of five representative ZB-derived structures). The Enthalpies are presented (a) for different I-III-VI systems and (b) versus the ratio of the per-anion volume of 1:5:8 ODC to that of the 1:1:2 phase.