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Predicting new structures in B-cation ordering perovskites MATTHEW LORDS, GUS HART<sup>1</sup>, Brigham Young University — Material properties are intimately tied to crystal structure. Many materials, alloys in particular, share a common, underlying "motif", such as an fcc/bcc/hcp "parent lattice," but have different chemical orderings. Among the infinite possibilities for chemical orderings, why does nature choose the few it does? We answer this question generally by using a method that only looks at the geometry of the structure. Using this structure-analysis method we examine possible new ordering for a class of simple cubic structures, the ever-important perovskites.

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