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Finding one of Nature's missing crystal structures

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There are an infinite number of ways atoms can be arranged on a lattice. But, like the integers, the arrangements can be counted and some are “smaller” than others. These small crystal structures are popular in common alloys. But mother Nature refuses to use some other small crystal structures. Why? Maybe she really uses them and we just haven't looked in the right places. We have developed an algorithm for generating a complete list of the possible structures. Using a combination of computation and experiment, we are closing in on a never-before-observed crystal structure.