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A new intermetallic prototype? Verifying new structure predictions in CdPt and PtPd[1] GUS HART, Brigham Young University — A recent data-mining approach to predicting the structure of intermetallic compounds has suggested that the CdPt and PtPd systems harbor a new crystal structure. Unlike other such predictions, this one is unique. The structure, never seen in any other fcc- based intermetallic, contains only four atoms per unit cell. Furthermore, this structure is the only one of this small size, except $L1_2$, that cannot be characterized as a sequential stacking of planes containing only A or B atoms. The stability of such a structure is tested using an exhaustive search of a cluster-expansion Hamiltonian.

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