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Predictions of the Pt_8Ti phase in unexpected systems[1] RICHARD TAYLOR, Brigham Young University, STEFANO CURTAROLO, Duke University, GUS HART, Brigham Young University — The binary phase with 8:1 stoichiometry (prototype Pt_8Ti) has been observed in 11 systems. In every case, the elemental phase of A is face centered cubic (fcc) and is one of the group 10 (IUPAC nomenclature) elements (Pt, Pd, or Ni). High-throughput quantum mechanical energy calculations indicate, however, that the fcc group 9 elements Rh and Ir may also form the A_8B phase with W. Extending the high-throughput search to the entire transition metal group (including La) reveals an unexpected wealth of new predictions—36 in total. Furthermore, several predictions occur in common alloy systems (e.g., Cu-Zn, Cu-Ni) which are believed to be well characterized. The results of a finite temperature simulation involving the cluster expansion method are presented for one system predicted to form the A_8B phase, Rh-W. Computed order-disorder transitions suggests the phase may be experimentally realizable in Rh-W.

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