New candidates for the Pt₈Ti structures in intermetallics

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— The only known intermetallic structure with an 8:1 stoichiometry is that of Pt₈Ti. Because of its uniqueness, this structure has been studied in Pt, Pd, and Ni rich systems. However, these metals have only been paired with a handful of other elements. Are there more elements that when alloyed with Pt, Pd, or Ni order with the Pt₈Ti structure? We explored ≈40 different Pd- and Pt-based binary systems. We calculated their formation enthalpies for the Pt₈Ti structure, compared the value to the tie line between pure Pd/Pt and experimentally-observed ground states. We find that there are other (beyond those experimentally observed) possible alloys with this structure. These new Pt/Pd-rich alloys could find application in the jewelry and catalysis industries.