

Searching for Missing Binary Equiatomic Phases:

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SUPPORTING INFORMATION

Searching for Missing Binary Equiatomic Phases: Complex Crystal Chemistry in the Hf–In System

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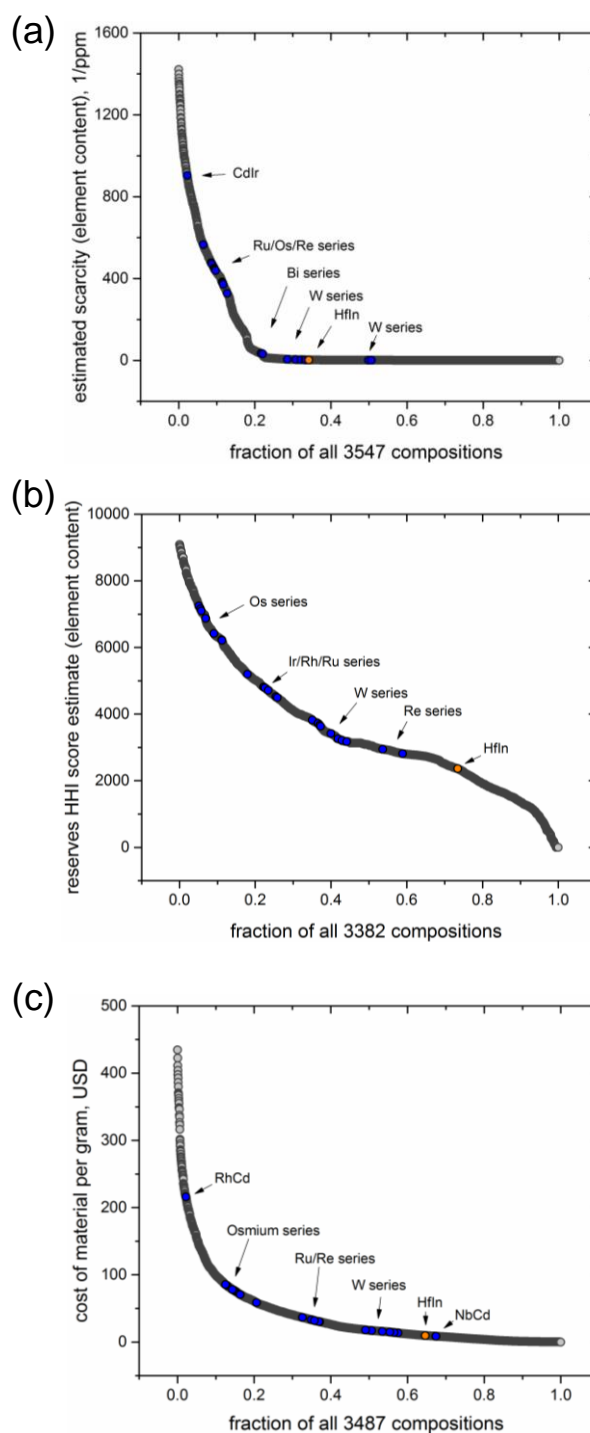


Figure S1. Estimated (a) scarcity, (b) HHI reserve score (excluding U- and Th-containing compounds), and (c) cost per gram (excluding Pm-containing compounds) for all possible *AB* combinations, with 21 uninvestigated systems highlighted. Calculations were made on the basis of a scarcity calculator and vendor internet prices.

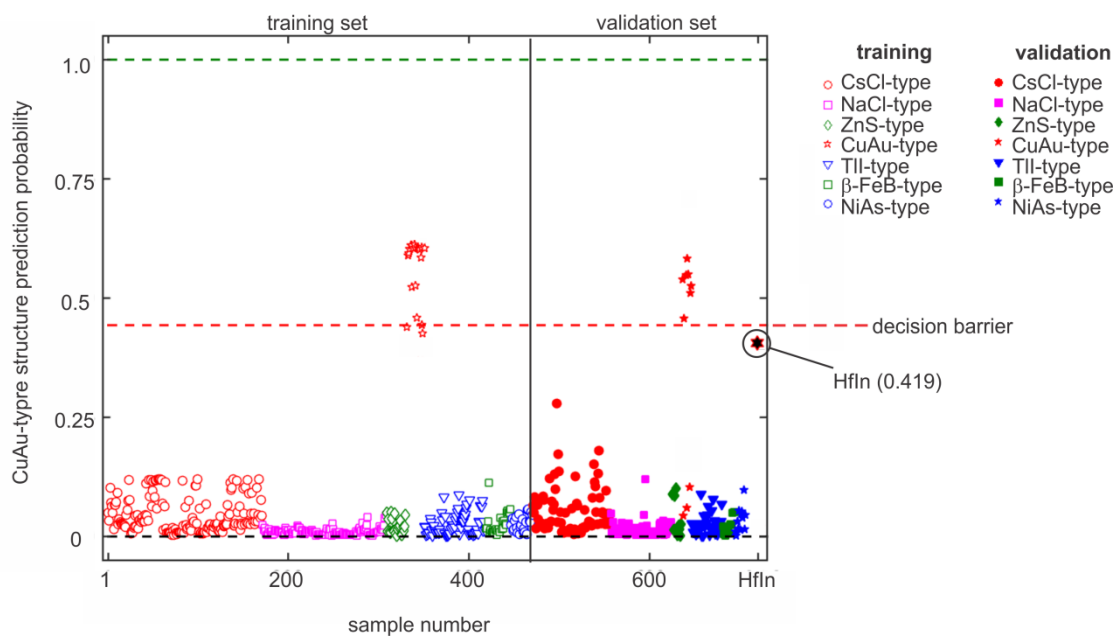
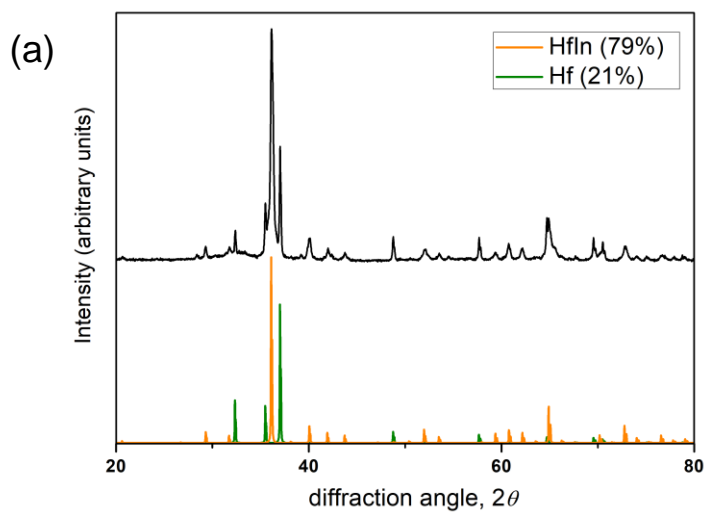


Figure S2. Probabilities predicted by machine-learning model to adopt CuAu-type structures for *AB* compounds, including HfIn.



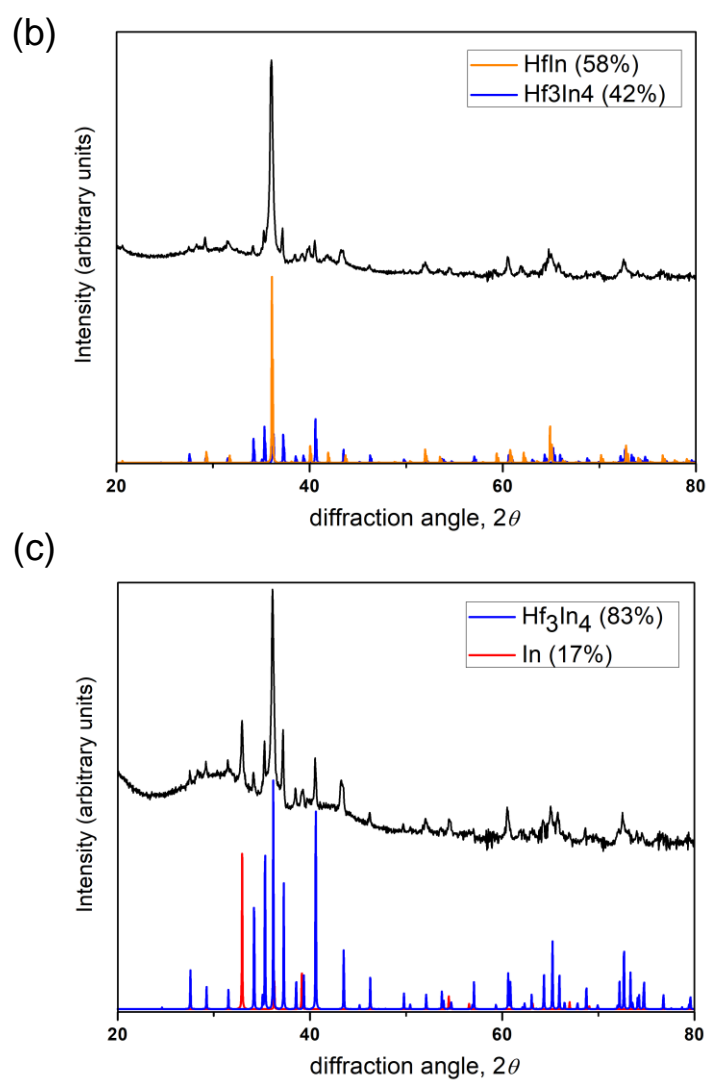


Figure S3. Powder XRD patterns for two-phase samples in Hf–In system.

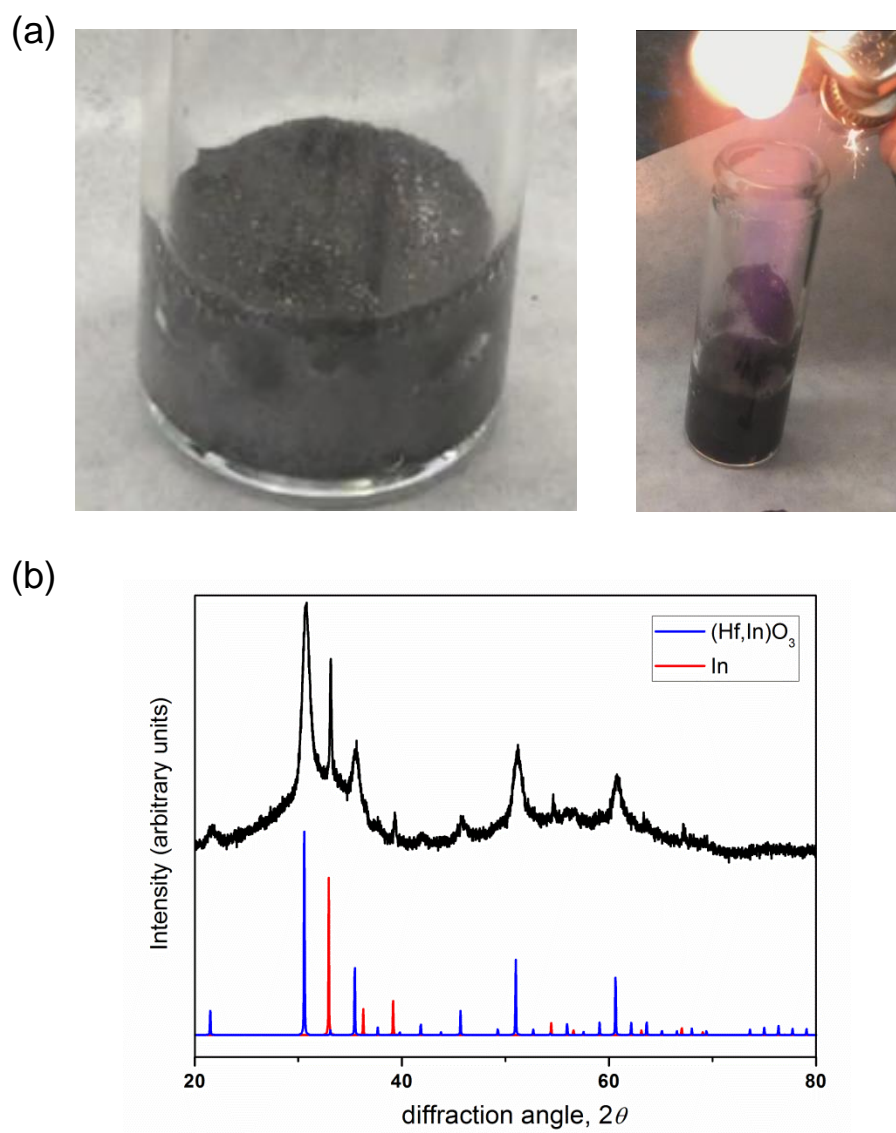


Figure S4. (a) Reaction of HfIn with water and ignition of flammable gas produced. (b) Powder XRD pattern of product after reaction with water.