Searching for Missing Binary Equiatomic Phases:

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DOI:

[10.1021/acs.inorgchem.8b01122](https://doi.org/10.1021/acs.inorgchem.8b01122)

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Document Version

Peer reviewed version

Citation for published version (Harvard):

Oliyntyk, AO, Gaultois, MW, Hermus, M, Morris, A, Mar, A & Brgoch, J 2018, 'Searching for Missing Binary Equiatomic Phases: Complex Crystal Chemistry in the Hf-In System', *Inorganic Chemistry*, vol. 57, no. 13, pp. 7966-7974. <https://doi.org/10.1021/acs.inorgchem.8b01122>, <https://doi.org/10.1021/acs.inorgchem.8b01122>

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Checked for eligibility: 28/06/2018

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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.