High-$T_c$ ternary metal hydrides, YKH$_{12}$ and LaKH$_{12}$, discovered by machine learning

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The search for hydride compounds that exhibit high $T_c$ superconductivity has been extensively studied. Within the range of binary hydride compounds, the studies have been developed well including data-driven searches as a topic of interest. Toward the search for the ternary systems, the number of possible combinations grows rapidly, and hence the power of data-driven search gets more prominent. In this study, we constructed various regression models to predict $T_c$ for ternary hydride compounds and found the extreme gradient boosting (XGBoost) regression giving the best performance. The best performed regression predicts new promising candidates realizing higher $T_c$, for which we further identified their possible crystal structures. Confirming their lattice and thermodynamical stabilities, we finally predicted new ternary hydride superconductors, YKH$_{12}$ [$C2/m$ (No.12), $T_c=143.2$ K at 240 GPa] and LaKH$_{12}$ [$R3m$ (No.166), $T_c=99.2$ K at 140 GPa] from first principles.

INTRODUCTION

The compressed polyhydrides are good candidates for high $T_c$ superconductor due to the high vibration frequencies provided by the hydrogen atoms, coupled with the introduction of other elements to get necessary pre-compression for the entire system to maintain its metallic and superconducting state even at lower pressure. The potential for high $T_c$ has been confirmed by many theoretical and experimental studies. [1–5]

The structure searching to get higher $T_c$ for these compounds has been made mainly within binary compounds, and some of the synthesis have reported the achievement of high $T_c$, e.g., LaH$_{10}$ (260 K at 200 GPa), [6] YH$_6$ (224 K at 166 GPa), [7] and TH$_{10}$ (159 K at 174 GPa) [8] etc. Recent theoretical prediction of Li$_2$MgH$_{16}$ (473 K at 250 GPa) and the experimental measurement of carbonaceous sulfur hydride (287 K at $\sim$267 GPa) indicate that multi component hydrides could have greater potential for higher $T_c$ than binary ones. [6, 10] At present, about 10-20 ternary superconducting hydrides have been proposed, but a small part of them have been experimentally verified ending up with extremely low $T_c$. [9] 29 According to 'Materials Project (MP) database', [30] the number of ternary compounds amounts around to five times larger than that of binary compounds under ambient conditions, providing us with an exciting field of materials searching. For such problems with a wide search space, data-driven approaches get to be powerful over other methods. For cuprate and iron-based superconductors, their searchings by using machine learning approaches have been reported. [31–33] For the hydrides superconductor, RbH$_{12}$, neural networks have been applied. [34] We shall then employ machine learning techniques to explore ternary polyhydrides for higher $T_c$.

The compounds to be targeted were first narrowed down according to the following policy: The target ternary system is restricted within those composed as a combination of binary hydrides having higher $T_c$ as reported. From binary hydrides that have been reported to be superconducting, [7] [21] [22] [25] [35–111] there can be about 2,800 possible combinations. Of these, except for those with very low $T_c$, we can narrow it down to about 1,800 types, and further, except for those with too high hydrogen content, to about 1,700 types. Among these, we limited our search to the Y and La systems which have tendency to achieve higher $T_c$, getting about 250 combinations of YMH$_x$ and LaMH$_x$ ($M=Ca$, K, and Na). For these target compounds, a procedure for our virtual screening via machine-learning and high-throughput ab
initio calculations is as follows: (1) machine-learning search for the chemical compositions achieving higher \( T_c \), (2) evolutionary crystal structure search for the candidate compositions, (3) stability check for the candidate structures, (4) \textit{ab initio} predictions of \( T_c \) for the stable structures.

(1) For the composition search, as described in the “Method” section, we considered various regression models to predict \( T_c \) values of the ternary hydrides, which were learned with theoretically predicted data on \( T_c \) extracted from available literature. \[7, 9, 11, 15, 18, 26, 35, 124\] Our descriptors entering the regression as input consist of 84 features such as chemical compositions, space group, and pressure-dependent electronic properties, where the composition descriptors were generated using the XenonPy software \[123\] and the pressure-dependent descriptors were computed by the VASP software \[124, 127\]. We checked their prediction performance by using the cross validation and then the best performed model, i.e., the extreme gradient boosting algorithm implemented in the XGBoost package. \[128\] was used for the high-throughput screening of the target ternary compounds. Our XGBoost model predicted ternary compositions, \( \text{YKH}_1 \) and \( \text{LaKH}_1 \), to be candidates for achieving higher \( T_c \) at 200 GPa. (2) For the predicted chemical compositions, we further predicted their crystal structures by using an evolutionary algorithm for crystal structure search implemented in the USPEX code \[129\] coupled with \textit{ab initio} geometry optimizations implemented in the VASP code. \[124, 127\] (3) For the predicted crystal structures, as shown in Fig. 1, we evaluated their thermodynamical and structural stabilities by using convex hull method and \textit{ab initio} phonon calculation. (4) Confirming the stabilities, we finally predicted that the ternary \( \text{YKH}_1 \) and \( \text{LaKH}_1 \) are promising candidates to achieve higher \( T_c \). To the best of our knowledge, this is the first example of the ternary hydride superconductors realized by alkali earth metals \((M=\text{K}, +2\) valence) while preceding studies with alkali metals \((M = \text{Ca}, \text{Mg}, +1\) valence).

\section*{METHOD}

Several ternary superconducting hydrides predicted theoretically so far, such as \( \text{CaYH}_1 \), \( \text{YSH}_6 \), and \( \text{CSH}_7 \), \[13, 25, 115\] were proposed as a composite of two different binary hydrides possibly to form a compound under high pressure. Referring 102 published papers on superconducting hydrides, \[7, 9, 11, 15, 18, 26, 35, 122\] we obtained 533 superconducting data, including 181 high-\( T_c \) hydrides \((T_c \text{ higher than liquid nitrogen})\). Additionally, we collected 150 kinds of binary compounds. Excluding those with very low \( T_c \) \((T_c < 40 \text{ K, McMillan Limit})\), 81 kinds were left. They can form 2,867 ternary combinations excluding the overlap of chemical compositions. Moreover, we excluded those with extremely higher hydrogen concentration, making \( x \leq 16 \) for \( \text{AMH}_x \), \[9\] thereby obtaining 2,366 possible compounds. To make the search space more compact, we selected the candidates only for those with \( A=\text{La and Y} \) because La- and Y-based materials have well been verified as having higher \( T_c \) by not only theoretical predictions, but also experimental observations \[6, 7\]. Resultant candidates, \( \text{YMH}_1 \) and \( \text{LaMH}_1 \), then amount to 238 compounds, which are input compounds entering the regression.

It is difficult to obtain all the structural data from the above pool of published articles. It is rather practical to use chemical compositions as the direct descriptor. In the preceding studies, \[130, 134\] it has been found that \( T_c \) correlates well with (i) space group, \( 6, 135\) (ii) density of states \((\text{DOS})\) at the Fermi level, \( D(E_F) \), as a measure of the applied pressure, \[73, 76, 101, 131, 136\] as well as (iii) the chemical composition. \[132, 137\] By the procedures explained below, we finally set up total 84 descriptors corresponding to the above three features: For (i) \( [\text{space group}] \), we took the number index for the space group \((e.g., \text{No.166 for } R3\text{m})\) as the descriptor. For (ii) \( [\text{pressure}] \), we used the scheme taken in the preceding studies, \[132, 138\] where the descriptors were composed as weighted averages over the quantities for pristine materials composed of each of elements in a compound \( (\text{averaging weight is based on the composition ratio}) \). The quantities were evaluated for the structure of each pristine material taken from the Materials Project \[59\] by using VASP \[124, 127\] to get \( \text{DOS} \) at several values of pressure \( (\text{detailed computational conditions were provided in S.I. (§)}) \). For the weighted averaging, we took the same manner as in XenonPy. \[123\] The procedure provides total 56 descriptors for (ii) at this stage. For (iii) \( [\text{chemical composition}] \), we used a XenonPy utility \[123\] that generates many possible descriptors, from which we picked up 290 descriptors at the first stage.

For total 347 descriptors \[290 \text{(ii)/Chemical composition) + 56 (ii)/pressure dependent DOS) + 1 (i/space group number)}\], we truncated them to avoid overfitting by excluding those with comparably weaker correlation with \( T_c \). The truncation can be performed during the random-forest regressions by monitoring the correlation using the scikit-learn library \[139\] \((\text{with six trees for this purpose})\), finally getting total 84 truncated descriptors \[70 \text{(iii)/Chemical composition) + 13 (ii)/pressure dependent DOS) + 1 (space group number)}\] as listed in S.I. \( (§) \).

The above constructed descriptors were thoroughly incorporated into four linear Ridge \((\text{RD})\), \[140\] Bayesian Ridge \((\text{RD})\), \[141\] LASSO \((\text{LS})\), \[140, 142–144\] and Elastic Net \((\text{EN})\) \[140, 145\] and three nonlinear Decision-Tree (DT) \[140\], Random Forest \((\text{RF})\) \[140, 146, 147\], and Extreme Gradient Boosting \((\text{XGBoost})\) \[128, 140\] regressors to predict \( T_c \) for the target compositions \( (\text{see Table I}) \); the \((\text{maximum}) \) depths of decision tree for DT, RF, and XGBoost were set to be 21, 16, and 7, respectively. To construct the regressors, 533 data \[7, 9, 11, 15, 18, 26, 35, 122\] are randomly divided into training and test data with with the ratio of 80:20. Hyperparameters in the models were chosen through the Bayesian optimization technique implemented in the Hy-
perOpt software package [148] to minimize the $R^2$ 5-fold cross-validation score. Model performance was judged from $R^2$, MAE (Mean Absolute Error), and RMSE (Root Mean Squared Error) as given in Table I. Among the above regressors, we found the XGBoost exhibiting the best performance for the test data, i.e., the lowest RMSE, $\Delta T_{\text{RMSE}} \sim 20$ K. Thus, the XGBoost was chosen as our machine learning model for $T_c$-prediction used in the successive high-throughput virtual screening of the ternary compositions.

Once a trained regression is available, it can immediately predict $T_c$ even for the chemical compositions with unknown $T_c$ by putting corresponding descriptors as the input for the regression. Since we do not know their crystal structures in advance for the predictions, we have to assume their space groups in order to complete input descriptors. Looking over the existing data, we found that a space group, $R\overline{3}m$ (No.166), often gives higher $T_c$ for binary compounds, so we adopted it as a trial. The trial setting was proved to be a fair choice by further verifications (crystal structural predictions and ab initio estimations) in a consistent manner as explained later. On the assumption of space group, we predicted $T_c$ for several choices of $XMH_x$ ($X=Y$ and La). For the candidate chemical composition giving higher $T_c$, we further predict their crystal structure by using the USPEX code [129] combined with ab initio kernel by VASP. [124–127] It randomly generates the 400 structures among from monomer upto tetramer of $AKH_{12}$ ($A=La$ or Y) as an 'initial generation' for the generic algorithm. Each generation evolves 100 structures according to 40% heredity, 40% random, 10% softmutation, and 10% transmutation. A promising candidate structure is identified when no further evolution occurs for more than 10 generations. The candidate is then subject to further ab initio geometrical optimizations by using the Perdew-Burke-Ernzerhof (GGA-PBE) functional for the exchange-correlation functional. [149] We performed the procedure at the pressure of 100 GPa, 200 GPa, and 300 GPa, to get each optimized structure.

For the predicted crystal structures, we evaluated the structural stability by phonon calculations and thermodynamic stability by the convex hull method. For the phonon evaluations, we used the PhonoPy package [150] combined with ab initio kernel by VASP. [124–127] Convex hull evaluations were made by using a utility implemented in USPEX. [129] By the ab initio phonon calculations, we finally estimated $T_c$ based on the Allen-Dynes formalism, [151] [152] to be compared with our data-driven predictions by the regression for verification. Detailed computational conditions for the phonon calculations are given in S.I. (§).

FIG. 1. Predicted structures for (a) YKH$_{12}$ with $C2/m$ (No.12), and (b) LaKH$_{12}$ with $R\overline{3}m$ (No.166), by the crystal structures search using USPEX.

TABLE I. Comparison of several regression models in terms of $R^2$, MAE (Mean Absolute Error), and RMSE (Root Mean Squared Error) for the test dataset. Each abbreviation means ‘RD’ (Ridge), ‘BR’ (Bayesian Ridge), ‘LS’ (Lasso), ‘EN’ (Elastic Net), ‘DT’ (Decision Tree), ‘RF’ (Random Forest), and ‘XGB’ (Extreme Gradient Boosting).

|                | Linear regression | Nonlinear regression |
|----------------|-------------------|----------------------|
| $R^2$          | 0.244 0.249 0.403 | 0.460 0.732 0.842 0.877 |
| MAE            | 34.66 37.57 34.06 | 32.24 18.58 16.34 13.53 |
| RMSE           | 50.34 50.17 44.75 | 42.56 29.96 23.01 20.29 |
As we mentioned in the previous section (see Table I), the XGBoost regressor is the best performed machine learning model. Fig. 2 shows the performance of our XGBoost model. Its $R^2$ values are 0.99 and 0.87 for 426 training and 107 test data, respectively, indicating our regressor is slightly overfitted. But it exhibits a better performance than the other models, especially the linear regressions. Looking at RMSE, the XGBoost value was about 20 K. This cannot matter for our purposes, judging from our XGBoost performance.

Fig. 2. Model performance. Comparison between $T_c$ in database and that interpolated by regression, proving the performance of our XGBoost regression model. Total 533 data are are randomly divided into 426 training data (80%) and 107 test data (20%).

RESULTS AND DISCUSSION

To strengthen the reality of predictions, it is indispensable to estimate the stability of the predicted structures. The thermal stability of the structure is confirmed by comparing a pressure dependence of relative formation enthalpy within the USPEX calculations as shown in Fig. 3. From the analysis, we can identify the pressure range where the structures can stably exist. Under the pressure range, we performed ab initio phonon calculations to examine the lattice stabilities. As shown in Fig. 4, any imaginary modes do not appear ensuring the lattice stability for these structures at the pressure.

For $\text{YKH}_{12}$ (at 240 GPa) and $\text{LaKH}_{12}$ (at 160 GPa), we further evaluated their electron-phonon couplings and then estimated their $T_c$ values based on the Allen-Dynes formalism. which are listed in Table II. The machine-learning predicted values overestimate ab initio ones by $\sim$ 20K and $\sim$ 60K for $\text{YKH}_{12}$ and $\text{LaKH}_{12}$, respectively. These overestimates lie within almost RMSE and three-times RMSE, respectively, which may be thought of as being allowable, judging from our XGBoost performance.

CONCLUSION

We performed a data-driven materials searching for ternary hydrides superconductors within the range of $\text{AMH}_{12}$ ($A=$La,Y) composition. The regression over 533 existing superconductors was constructed by the random forest method using 84 descriptors characterizing chemical composition, space group, and pressure. Using the regression, we estimated $T_c$ over 239 compositions to get the prediction of higher $T_c$ achieved by the choice of $M=$K, $\text{YKH}_{12}$ and $\text{LaKH}_{12}$. For the predicted compositions, we performed evolutionary structure search to get their crystal structures. For the structures, we confirmed their structural stabilities by using ab initio phonon calculations as well as getting $T_c$ estimated by Allen-Dynes formula. We finally predicted two new ternary hydrides superconductors, $\text{YKH}_{12}$ and $\text{LaKH}_{12}$.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
\textbf{Composite} & \textbf{Predicted $T_c$ [K]} & \textbf{Regression} & \textbf{Ab initio} \\
\hline
$\text{YKH}_{12}$ & 168.9 & 143.2 & \\
$\text{LaKH}_{12}$ & 162.8 & 99.2 & \\
\hline
\end{tabular}
\caption{Comparison of the $T_c$ predictions between the \textit{ab initio} DFT and the XGBoost regression.}
\end{table}
FIG. 3. Relative enthalpies for (a) YKH$_{12}$ and (b) LaKH$_{12}$, showing the pressure range where the compounds are stable.

FIG. 4. Phonon dispersions, phonon DOS, and Eliashberg functions for (a) YKH$_{12}$ at 200 GPa and (b) LaKH$_{12}$ at 160 GPa. No imaginary frequency appears ensuring the lattice stability for each compound.

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SUPPLEMENTAL INFORMATION

Ab initio calculations

The crystal structures predicted for YKH\textsubscript{12} and LaKH\textsubscript{12} at each pressure are given in Table.\textsuperscript{[III]} For electronic structure calculations (required to get pressure-dependent DOS) and phonon calculations (to evaluate dynamical stabilities), we used VASP package \textsuperscript{[124,127]} with GGA-PBE exchange-correlation functionals.\textsuperscript{[149]} Ionic cores are described by ultrasoft pseudo potentials provided in the package. To assist the convergence in the self-consistent field iterations, we used Marzari-Vanderbilt smearing scheme.\textsuperscript{[153]} Resolutions for the plane wave basis set expansions \([\text{Energy cutoff} (E_{\text{cut}})]\) and the Brillouin-zone integration \([k\text{-mesh}]\) were determined so that the resultant energy values could converge within the required accuracies, finally getting \(E_{\text{cut}}=75\) Ry with \((8 \times 8 \times 8)\) \(k\)-mesh for the electronic Brillouin-zone. Phonon calculations are performed by linear-response method\textsuperscript{[154]} with \((4 \times 4 \times 4)\) \(q\)-mesh.

To estimate \(T_c\), we used Allen-Dynes formula implemented in Quantum Espresso package\textsuperscript{[155]} with the effective Coulomb interaction \(\mu^*\) being chosen 0.1 empirically. Denser \(k\)-meshes, \(16 \times 16 \times 16\), were used for the double-delta integrations in electron-phonon calculations. The estimated results are summarized in Table\textsuperscript{[IV]}

Descriptors

Total 84 descriptors used for the regression are listed in Table\textsuperscript{[V]} corresponding to those for (i) [space group], (ii) [pressure], and (iii) [chemical composition]. A descriptor for a composition is composed from that for each atomic species, and \(f_\alpha\) as the descriptor for \(\alpha\),

\[
    f_{\text{ave}} = \sum_\alpha W_\alpha \cdot f_\alpha, \\
    f_{\text{sum}} = \sum_\alpha W_\alpha \cdot f_\alpha, \\
    f_{\text{var}} = \sum_\alpha W_\alpha \cdot (f_\alpha - f_{\text{ave}})^2, \\
    f_{\text{max}} = \max_\alpha \{f_\alpha\}, \\
    f_{\text{min}} = \min_\alpha \{f_\alpha\},
\]

are used, where \(W_\alpha\) is the number of \(\alpha\)-species included in the composition, and \(W_\alpha^*\) is the normalized fraction.

List of estimated and training data

Total 426 training data used to construct the regression are listed in Table\textsuperscript{[VII]} By using the XGBoost regression, we estimated \(T_c\) for a set of chemical compositions as shown in Table\textsuperscript{[VI]}
TABLE III. Crystal structures of YKH\textsubscript{12} and LaKH\textsubscript{12} predicted at each pressure (P). Lattice parameters (a, b and c) are given in unit of Å.

| P (GPa) | Atomic coordinates (fractional) |
|---------|--------------------------------|
|         | Atoms | x    | y    | z    |
| YKH\textsubscript{12} | C2/m  | 240  | a = 4.685 | b = 4.959 | c = 3.412 |
|         |       |      | K(2c) 0.00000 0.00000 0.50000  |
|         |       |      | Y(2b) 0.00000 0.50000 0.00000  |
|         |       |      | H(8j) 0.10546 0.13491 0.02245  |
|         |       |      | H(8j) 0.11840 0.35836 0.52932  |
|         |       |      | β = 94.640° |
| LaKH\textsubscript{12} | R\overline{3}m  | 140  | a = b = 5.457 | c = 5.844 |
|         |       |      | K(3b) 0.00000 0.00000 0.50000  |
|         |       |      | La(3a) 0.00000 0.00000 0.00000  |
|         |       |      | H(36i) 0.00522 0.29080 0.25260  |
| LaKH\textsubscript{12} | C2/m  | 250  | a = 8.126 | b = 5.479 | c = 4.379 |
|         |       |      | K(4i) 0.12534 0.00000 0.82783  |
|         |       |      | La(4i) 0.12649 0.50000 0.34168  |
|         |       |      | H(8j) 0.11445 0.17656 0.45546  |
|         |       |      | H(8j) 0.11651 0.10279 0.25125  |
|         |       |      | H(8j) 0.12613 0.30763 0.96974  |
|         |       |      | H(8j) 0.13714 0.36984 0.78838  |
|         |       |      | H(8j) 0.24797 0.21751 0.24331  |
|         |       |      | H(4g) 0.00000 0.21727 0.00000  |
|         |       |      | H(4h) 0.00000 0.26959 0.50000  |

TABLE IV. $T_c$ estimated by Allen-Dynes formula using ab initio phonon calculations for YKH\textsubscript{12} [C2/m] and KH\textsubscript{12} [R\overline{3}m] at each pressure. $\lambda$ and $\omega_{bg}$ are the parameters appearing in the formula.

| P (GPa) | $\lambda$ | $\omega_{bg}$ [K] | $T_c$ [K] |
|---------|------------|-------------------|----------|
| YKH\textsubscript{12} | 180 | 1.398 | 1289.465 | 137.7 |
| YKH\textsubscript{12} | 200 | 1.400 | 1324.987 | 141.1 |
| YKH\textsubscript{12} | 240 | 1.427 | 1318.072 | 143.2 |
| YKH\textsubscript{12} | 260 | 1.436 | 1127.344 | 123.2 |
| YKH\textsubscript{12} | 300 | 1.587 | 911.696 | 109.4 |
| LaKH\textsubscript{12} | 140 | 1.531 | 854.12 | 99.2 |
| LaKH\textsubscript{12} | 160 | 1.665 | 789.38 | 98.8 |
TABLE V. Total 84 descriptors used for the regression, corresponding to those for (i) [space group], (ii) [pressure], and (iii) [chemical composition]. Each weighting scheme (ave/sum/var/max/min) is defined in Eqs. [1].

| Weighting scheme | Property | Label | Description |
|------------------|----------|-------|-------------|
| ave (i)          | atomic_radius_rahm |          | Atomic radius by Rahm et al. |
| ave (i)          | boiling_point |          | Boiling temperature |
| ave (i)          | covalent_radius_cordero |          | Covalent radius by Cordero et al. |
| ave (i)          | covalent_radius_pyykko |          | Single bond covalent radius by Pyykko et al. |
| ave/max (i)      | covalent_radius_slater |          | Covalent radius by Slater |
| ave (i)          | en_allen |          | Allen’s scale of electronegativity |
| ave/sum (i)      | en_ghosh |          | Ghosh’s scale of electronegativity |
| ave/sum (i)      | first_ion_en |          | First ionisation energy |
| ave (i)          | fusion_enthalpy |          | Fusion heat |
| ave/sum/var (i)  | gs_bandgap |          | DFT bandgap energy of $T = 0$ K ground state |
| ave/max (i)      | gs_volume_per |          | DFT volume per atom of $T = 0$ K ground state |
| ave/sum/var/max/min (i) | hhi_p |          | Herfindahl-Hirschman Index (HHI) production values |
| ave/sum/min (i)  | hhi_r |          | Herfindahl-Hirschman Index (HHI) reserves values |
| ave/sum/var (i)  | heat_capacity_mass |          | Mass specific heat capacity |
| ave (i)          | evaporation_heat |          | Evaporation heat |
| ave/sum/max/min (i) | lattice_constant |          | Physical dimension of unit cells in a crystal lattice |
| ave/min (i)      | mendeleev_number |          | Atom number in mendeleev’s periodic table |
| ave/sum (i)      | melting_point |          | Melting point |
| ave/sum/max (i)  | molar_volume |          | Molar volume |
| ave/sum/max (i)  | num_unfilled |          | Total unfilled electron |
| ave/sum/max (i)  | num_valance |          | Total valance electron |
| ave (i)          | period |          | Period in the periodic table |
| ave (i)          | vdw_radius |          | Van der Waals radius |
| ave/max (i)      | vdw_radius_alvarez |          | Van der Waals radius according to Alvarez |
| ave/max (i)      | vdw_radius_mm3 |          | Van der Waals radius from the MM3 FF |
| sum (i)          | atomic_radius |          | Atomic radius |
| sum (i)          | atomic_volume |          | Atomic volume |
| sum (i)          | c6_gb |          | C$_6$ dispersion coefficient in a.u |
| sum/max (i)      | covalent_radius_pyykko_triple |          | Triple bond covalent radius by Pyykko et al. |
| sum/min (i)      | electron_negativity |          | Tendency of an atom to attract a shared pair of electrons |
| var/min (i)      | en_mulliken |          | Mulliken’s scale of electronegativity |
| sum/max (i)      | gs_est_bcc_latcnt |          | Estimated BCC lattice parameter based on the DFT volume |
| sum/var (i)      | num_s_unfilled |          | Unfilled electron in s shell |
| sum (i)          | specific_heat |          | Specific heat at 20oC |
| var (i)          | icsd_volume |          | Atom volume in ICSD database |
| var/max (i)      | vdw_radius_eff |          | Van der Waals radius from the UFF |
| max/min (i)      | bulk_modulus |          | Bulk modulus |
| max (i)          | num_p_unfilled |          | Unfilled electron in p shell |
| ave/var/min (ii) | s_dos |          | Density of states of s electron at Fermi surface (state/eV/atom) |
| ave/min (ii)     | Free_energy |          | Pressure-related free energy |
| var/max/sum (ii) | p_dos |          | Density of states of p electron at Fermi surface (state/eV/atom) |
| max/sum (ii)     | element_dos |          | Density of states at Fermi surface (state/eV/atom) |
| (iii) spg_number |          | space group number |
TABLE VI. 28 chemical compositions to estimate $T_c$ by using the XGBoost regression learned with the 426 training data.

| No. | $T_c$ [K]  | No. | $T_c$ [K]  |
|-----|------------|-----|------------|
| 1   | YKH$_{12}$ 168.93 | 15  | LaSH$_{12}$ 74.94 |
| 2   | LaKH$_{12}$ 162.85 | 16  | LaArH$_{12}$ 74.91 |
| 3   | YCH$_{12}$ 137.60 | 17  | YBiH$_{12}$ 72.54 |
| 4   | LaMgH$_{12}$ 135.33 | 18  | YFeH$_{12}$ 64.58 |
| 5   | LaCH$_{12}$ 132.70 | 19  | LaPH$_{12}$ 60.59 |
| 6   | LaAcH$_{12}$ 128.99 | 20  | YTaH$_{12}$ 58.93 |
| 7   | YSeH$_{12}$ 127.01 | 21  | YTiH$_{12}$ 57.21 |
| 8   | YSH$_{12}$ 123.04 | 22  | LaBiH$_{12}$ 56.59 |
| 9   | YArH$_{12}$ 99.59  | 23  | LaSbH$_{12}$ 52.38 |
| 10  | YGeH$_{12}$ 98.60  | 24  | LaSiH$_{12}$ 50.53 |
| 11  | LaSe$_{12}$ 98.25  | 25  | LaTaH$_{12}$ 42.25 |
| 12  | YInH$_{12}$ 93.81  | 26  | LaTiH$_{12}$ 39.85 |
| 13  | YPH$_{12}$ 92.78  | 27  | LaFeH$_{12}$ 24.48 |
| 14  | LaTeH$_{12}$ 77.93  | 28  | LaGeH$_{12}$ 18.47 |
### TABLE VII: Total 533 training data [7,9,11,15,18,26,35,122] used to construct our regressors (see the main text). The label 'Spg' abbreviates 'Space group' with the numbering. $\mu$ is the parameter for the effective Coulomb interactions appearing in Allen-Dynes formula.

| No. | Spg. | $P$ (GPa) | $T_c$ (K) | $\mu$ |
|-----|------|-----------|-----------|--------|
| 0   | SiH₄ | 64 $Cmca$ | 60.0      | 75.0   | 0.1   |
| 1   | SiH₄ | 64 $Cmca$ | 150.0     | 20.0   | 0.1   |
| 2   | SiH₄ | 64 $Cmca$ | 200.0     | 30.0   | 0.1   |
| 3   | SiH₄ | 64 $Cmca$ | 250.0     | 50.0   | 0.1   |
| 4   | YH₃  | 225 $Fm\bar{3}m$ | 17.7 | 40.0   | 0.1   |
| 5   | YH₃  | 225 $Fm\bar{3}m$ | 28.0 | 9.0    | 0.1   |
| 6   | YH₃  | 225 $Fm\bar{3}m$ | 35.0 | 0.0    | 0.1   |
| 7   | YH₃  | 225 $Fm\bar{3}m$ | 45.0 | 0.0    | 0.1   |
| 8   | YH₃  | 225 $Fm\bar{3}m$ | 52.0 | 6.0    | 0.1   |
| 9   | YH₃  | 225 $Fm\bar{3}m$ | 62.0 | 5.0    | 0.1   |
| 10  | YH₃  | 225 $Fm\bar{3}m$ | 67.0 | 4.0    | 0.1   |
| 11  | YH₃  | 225 $Fm\bar{3}m$ | 74.0 | 3.0    | 0.1   |
| 12  | BaH₂  | 194 $P6_3/mmc$ | 60.0 | 4.0    | 0.1   |
| 13  | Si₂H₆ | 2 $P\bar{1}$ | 175.0 | 65.0   | 0.1   |
| 14  | Si₂H₆ | 2 $P\bar{1}$ | 200.0 | 80.0   | 0.1   |
| 15  | Si₂H₆ | 221 $Pm\bar{3}m$ | 275.0 | 139.0  | 0.1   |
| 16  | Si₂H₆ | 15 $C2/c$ | 300.0 | 34.0   | 0.1   |
| 17  | SiH₆  | 68 $Ccca$ | 250.0 | 107.0  | 0.1   |
| 18  | SiH₄  | 40 $Ama2$ | 120.0 | 22.0   | 0.1   |
| 19  | SiH₄  | 194 $P6_3/mmc$ | 200.0 | 62.0   | 0.1   |
| 20  | HBr  | 11 $P2_1/m$ | 140.0 | 28.0   | 0.1   |
| 21  | HBr  | 11 $P2_1/m$ | 160.0 | 34.0   | 0.1   |
| 22  | HBr  | 11 $P2_1/m$ | 180.0 | 49.0   | 0.1   |
| 23  | HBr  | 11 $P2_1/m$ | 200.0 | 51.0   | 0.1   |
| 24  | HCl  | 11 $P2_1/m$ | 240.0 | 7.0    | 0.1   |
| 25  | HCl  | 11 $P2_1/m$ | 280.0 | 14.0   | 0.1   |
| 26  | HCl  | 11 $P2_1/m$ | 320.0 | 30.0   | 0.1   |
| 27  | HCl  | 11 $P2_1/m$ | 360.0 | 41.0   | 0.1   |
| 28  | GaH₃ | 223 $Pm\bar{3}n$ | 120.0 | 102.0  | 0.1   |
| 29  | GaH₃ | 223 $Pm\bar{3}n$ | 160.0 | 86.0   | 0.1   |
| 30  | GaH₃ | 223 $Pm\bar{3}n$ | 200.0 | 72.0   | 0.1   |
| 31  | GaH₃ | 223 $Pm\bar{3}n$ | 240.0 | 60.0   | 0.1   |
| 32  | PtH₃ | 225 $Fm\bar{3}m$ | 77.0 | 25.0   | 0.1   |
| 33  | PtH₃ | 225 $Fm\bar{3}m$ | 90.0 | 13.0   | 0.1   |
| 34  | PtH₃ | 225 $Fm\bar{3}m$ | 115.0 | 5.0    | 0.1   |
| 35  | PtH₃ | 225 $Fm\bar{3}m$ | 145.0 | 4.0    | 0.1   |
| 36  | B₃H₆  | 63 $Cmcm$ | 360.0 | 125.0  | 0.13  |
| 37  | GeH₆  | 14 $P2_1/c$ | 250.0 | 90.0   | 0.1   |
| 38  | PtH₃ | 225 $Fm\bar{3}m$ | 88.0 | 24.0   | 0.1   |
| 39  | PtH₃ | 225 $Fm\bar{3}m$ | 95.0 | 18.0   | 0.1   |
| 40  | PtH₃ | 194 $P6_3/mmc$ | 105.0 | 16.0   | 0.1   |
| 41  | PtH₃ | 194 $P6_3/mmc$ | 120.0 | 10.0   | 0.1   |
| 42  | PtH₃ | 225 $Fm\bar{3}m$ | 140.0 | 6.0    | 0.1   |
| 43  | PtH₃ | 225 $Fm\bar{3}m$ | 160.0 | 5.0    | 0.1   |
| 44  | PtH₃ | 225 $Fm\bar{3}m$ | 200.0 | 3.0    | 0.1   |
| 45  | KH₆  | 15 $C2/c$ | 166.0 | 70.0   | 0.1   |
| 46  | KH₆  | 15 $C2/c$ | 230.0 | 70.0   | 0.1   |
| 47  | KH₆  | 15 $C2/c$ | 300.0 | 46.0   | 0.1   |
| 48  | NbH₆ | 66 $Cccm$ | 0.0001 | 2.4    | 0.1   |
| 49  | NbH₂  | 225 $Fm\bar{3}m$ | 0.0001 | 2.6    | 0.1   |
| 50  | NbH₂  | 225 $Fm\bar{3}m$ | 50.0 | 1.5    | 0.1   |
| 51  | NbH₄ | 139 $I4/mmm$ | 300.0 | 47.0   | 0.1   |
| 52  | GeH₃  | 223 $Pm\bar{3}n$ | 180.0 | 160.0  | 0.1   |
| 53  | GeH₃  | 131 $P421/mmc$ | 180.0 | 110.0  | 0.1   |
| 54  | GeH₃  | 66 $Cccm$ | 180.0 | 100.0  | 0.1   |
| 55  | BaH₆ | 123 $P4/mmm$ | 100.0 | 38.0   | 0.1   |
| 56  | MgH₂ | 194 $P6_3/mmc$ | 180.0 | 24.0   | 0.1   |
| 57  | MgH₄ | 63 $Cmcm$ | 100.0 | 38.0   | 0.1   |
| Element | Molecular Formula | Space Group | a (Å) | b (Å) | c (Å) | α (°) | β (°) | γ (°) |
|---------|------------------|-------------|-------|-------|-------|-------|-------|-------|
| MgH₂    | 146 R3           | 140.0       | 60.0  | 0.1   |
| BH      | 191 P6/mmm       | 100.0       | 39.0  | 0.1   |
| BH      | 191 P6/mmm       | 125.0       | 32.0  | 0.1   |
| BH      | 191 P6/mmm       | 150.0       | 27.0  | 0.1   |
| BH      | 191 P6/mmm       | 175.0       | 21.0  | 0.1   |
| BH      | 191 P6/mmm       | 200.0       | 19.0  | 0.1   |
| LiH₆    | 127 P4/mnm       | 150.0       | 0.0   | 0.13  |
| LiH₆    | 166 R₃m          | 150.0       | 38.34 | 0.13  |
| LiH₆    | 166 R₃m          | 200.0       | 42.0  | 0.13  |
| LiH₆    | 166 R₃m          | 250.0       | 58.0  | 0.13  |
| LiH₆    | 166 R₃m          | 300.0       | 82.0  | 0.13  |
| LiH₆    | 97 I422          | 100.0       | 31.04 | 0.13  |
| LiH₆    | 97 I422          | 150.0       | 35.0  | 0.13  |
| LiH₆    | 97 I422          | 200.0       | 37.0  | 0.13  |
| BeH₂    | 63 Cmcm          | 250.0       | 44.0  | 0.1   |
| BeH₂    | 63 Cmcm          | 250.0       | 42.0  | 0.1   |
| BeH₂    | 63 Cmcm          | 270.0       | 45.0  | 0.1   |
| BeH₂    | 63 Cmcm          | 290.0       | 37.0  | 0.1   |
| BeH₂    | 63 Cmcm          | 310.0       | 33.0  | 0.1   |
| BeH₂    | 129 P4/mmm       | 350.0       | 39.0  | 0.1   |
| BeH₂    | 129 P4/mmm       | 365.0       | 50.0  | 0.1   |
| BeH₂    | 129 P4/mmm       | 390.0       | 30.0  | 0.1   |
| H₂S     | 2 P1            | 130.0       | 33.0  | 0.13  |
| H₂S     | 2 P1            | 140.0       | 40.0  | 0.13  |
| H₂S     | 2 P1            | 150.0       | 56.0  | 0.13  |
| H₂S     | 2 P1            | 158.0       | 60.0  | 0.13  |
| H₂S     | 64 Cmca         | 160.0       | 82.0  | 0.13  |
| H₂S     | 64 Cmca         | 170.0       | 75.0  | 0.13  |
| H₂S     | 64 Cmca         | 180.0       | 65.0  | 0.13  |
| BeH₂    | 63 Cmcm         | 300.0       | 45.0  | 0.1   |
| VH₂     | 225 Fm3m        | 0.0         | 0.5   | 0.1   |
| VH₂     | 62 Pnma         | 60.0        | 4.0   | 0.1   |
| NbH₃    | 225 Fm3m        | 0.0         | 1.5   | 0.1   |
| NbH₃    | 186 P6/mmc      | 60.0        | 0.5   | 0.1   |
| H₂S     | 160 R₃m        | 130.0       | 166.0 | 0.1   |
| H₂S     | 229 Im3m       | 200.0       | 191.0 | 0.1   |
| H₂S     | 229 Im3m       | 250.0       | 179.0 | 0.1   |
| XeH     | 71 I4mm        | 100.0       | 29.0  | 0.12  |
| XeH     | 71 I4mm        | 200.0       | 17.0  | 0.12  |
| XeH     | 71 I4mm        | 300.0       | 13.0  | 0.12  |
| XeH₈    | 63 Cmcm        | 400.0       | 26.0  | 0.12  |
| XeH₈    | 63 Cmcm        | 500.0       | 20.0  | 0.12  |
| XeH₈    | 63 Cmcm        | 600.0       | 16.0  | 0.12  |
| AlH₃    | 11 P2₁/m-Z     | 250.0       | 146.0 | 0.1   |
| H₂I     | 62 Pnma        | 100.0       | 5.3   | 0.1   |
| H₂I     | 62 Pnma        | 150.0       | 4.32  | 0.1   |
| H₂I     | 62 Pnma        | 200.0       | 3.67  | 0.1   |
| H₂I     | 62 Pnma        | 240.0       | 3.77  | 0.1   |
| H₂I     | 166 R₃m        | 240.0       | 33.05 | 0.1   |
| H₂I     | 166 R₃m        | 260.0       | 30.82 | 0.1   |
| H₂I     | 166 R₃m        | 300.0       | 25.09 | 0.1   |
| H₂I     | 191 P6/mmm     | 120.0       | 9.92  | 0.1   |
| H₂I     | 191 P6/mmm     | 160.0       | 8.8   | 0.1   |
| H₂I     | 191 P6/mmm     | 200.0       | 9.57  | 0.1   |
| H₂I     | 191 P6/mmm     | 250.0       | 11.26 | 0.1   |
| H₂I     | 191 P6/mmm     | 300.0       | 12.48 | 0.1   |
| GeH₄    | 40 Ama2        | 250.0       | 57.0  | 0.1   |
| GeH₄    | 15 C2/c       | 500.0       | 84.0  | 0.1   |
| OsH     | 225 Fm3m      | 100.0       | 2.1   | 0.1   |
| H₂I     | 63 Cmcm       | 100.0       | 7.8   | 0.1   |
| H₂I     | 191 P6/mmm    | 100.0       | 17.5  | 0.1   |
| H₂I     | 191 P6/mmm    | 150.0       | 20.4  | 0.1   |
| InH₃    | 148 R₃        | 200.0       | 40.5  | 0.1   |
|   | Element | Formula | Density | Melting Point | Boiling Point |
|---|---------|---------|---------|---------------|---------------|
| 121 | InH | 148 R̅ | 250.0 | 39.0 | 0.1 |
| 122 | InH | 148 R̅ | 300.0 | 38.0 | 0.1 |
| 123 | InH | 11 P2₁/m | 150.0 | 27.0 | 0.1 |
| 124 | InH | 11 P2₁/m | 200.0 | 40.5 | 0.1 |
| 125 | HCl | 12 C2/m | 250.0 | 20.0 | 0.1 |
| 126 | HBr | 12 C2/m | 120.0 | 0.01 | 0.1 |
| 127 | BiH | 194 P6₃/mmc | 250.0 | 30.0 | 0.1 |
| 128 | BiH | 194 P6₃/mmc | 300.0 | 20.0 | 0.1 |
| 129 | BiH | 11 P2₁/m | 150.0 | 59.0 | 0.1 |
| 130 | BiH | 11 P2₁/m | 200.0 | 60.0 | 0.1 |
| 131 | BiH | 11 P2₁/m | 250.0 | 63.0 | 0.1 |
| 132 | BiH | 11 P2₁/m | 300.0 | 65.0 | 0.1 |
| 133 | BiH | 59 Pmmm | 150.0 | 93.0 | 0.1 |
| 134 | BiH | 59 Pmmm | 200.0 | 88.0 | 0.1 |
| 135 | BiH | 59 Pmmm | 250.0 | 77.0 | 0.1 |
| 136 | BiH | 59 Pmmm | 300.0 | 75.0 | 0.1 |
| 137 | BiH | 12 C2/m | 200.0 | 103.0 | 0.1 |
| 138 | BiH | 12 C2/m | 250.0 | 101.0 | 0.1 |
| 139 | BiH | 12 C2/m | 300.0 | 119.0 | 0.1 |
| 140 | BiH | 2 P1̅ | 200.0 | 100.0 | 0.1 |
| 141 | BiH | 2 P1̅ | 250.0 | 107.0 | 0.1 |
| 142 | BiH | 2 P1̅ | 300.0 | 113.0 | 0.1 |
| 143 | MgH | 229 Im3m | 300.0 | 263.0 | 0.12 |
| 144 | MgH | 229 Im3m | 350.0 | 260.0 | 0.12 |
| 145 | MgH | 229 Im3m | 400.0 | 271.0 | 0.12 |
| 146 | HSe | 12 C2/m | 300.0 | 5.0 | 0.1 |
| 147 | HSe | 14 P2₁/c | 300.0 | 23.0 | 0.1 |
| 148 | HSe | 129 P4/mmm | 250.0 | 39.0 | 0.1 |
| 149 | HSe | 129 P4/mmm | 300.0 | 42.0 | 0.1 |
| 150 | HSe | 229 Im3m | 200.0 | 116.0 | 0.1 |
| 151 | HSe | 229 Im3m | 250.0 | 111.0 | 0.1 |
| 152 | HSe | 229 Im3m | 300.0 | 110.0 | 0.1 |
| 153 | H₂Se | 229 Im3m | 300.0 | 160.0 | 0.1 |
| 154 | H₂Se | 139 I4/mmm | 0.0001 | 0.192 | 0.1 |
| 155 | H₂Se | 139 I4/mmm | 10.0 | 0.081 | 0.1 |
| 156 | H₂Se | 139 I4/mmm | 30.0 | 0.021 | 0.1 |
| 157 | H₂Se | 139 I4/mmm | 50.0 | 0.008 | 0.1 |
| 158 | HH₂ | 67 Cmma | 180.0 | 8.159 | 0.1 |
| 159 | HH₂ | 67 Cmma | 240.0 | 6.207 | 0.1 |
| 160 | HH₂ | 11 P2₁/m | 260.0 | 12.804 | 0.1 |
| 161 | HH₂ | 11 P2₁/m | 280.0 | 7.962 | 0.1 |
| 162 | CrH | 194 P6₃/mmc | 0.0 | 10.6 | 0.1 |
| 163 | CrH | 194 P6₃/mmc | 60.0 | 4.3 | 0.1 |
| 164 | CrH | 194 P6₃/mmc | 120.0 | 3.3 | 0.1 |
| 165 | CrH | 194 P6₃/mmc | 200.0 | 3.1 | 0.1 |
| 166 | CrH | 194 P6₃/mmc | 81.0 | 37.1 | 0.1 |
| 167 | CrH | 194 P6₃/mmc | 120.0 | 29.5 | 0.1 |
| 168 | CrH | 194 P6₃/mmc | 160.0 | 28.2 | 0.1 |
| 169 | CrH | 194 P6₃/mmc | 200.0 | 27.2 | 0.1 |
| 170 | PbH | 12 C2/m | 158.0 | 76.0 | 0.1 |
| 171 | PbH | 12 C2/m | 180.0 | 97.0 | 0.1 |
| 172 | PbH | 12 C2/m | 230.0 | 107.0 | 0.1 |
| 173 | PbH | 12 C2/m | 250.0 | 106.0 | 0.1 |
| 174 | PbH | 12 C2/m | 300.0 | 104.0 | 0.1 |
| 175 | PbH | 12 C2/m | 350.0 | 103.0 | 0.1 |
| 176 | SiH | 15 C2/c | 300.0 | 29.65 | 0.13 |
| 177 | SiH | 14 P2₁/c | 400.0 | 31.57 | 0.13 |
| 178 | SiH | 12 C2/m | 610.0 | 106.31 | 0.13 |
| 179 | HS | 15 C2/c | 200.0 | 35.3 | 0.1 |
| 180 | HS | 12 C2/m | 250.0 | 25.1 | 0.1 |
| 181 | HS | 12 C2/m | 300.0 | 38.0 | 0.1 |
| 182 | H₂S₂ | 1 P1 | 112.0 | 70.1 | 0.1 |
| 183 | H₂S₂ | 1 P1 | 120.0 | 75.2 | 0.1 |
| 184 | H₂S₂ | 1 P1 | 130.0 | 79.1 | 0.1 |
| 185 | SnH₄ | 139 | I₄/mmm | 220.0 | 91.0 | 0.1 |
| 186 | SnH₆ | 119 | I₄/m2 | 220.0 | 81.0 | 0.1 |
| 187 | SnH₂ | 12 | C₂/m | 250.0 | 93.0 | 0.1 |
| 188 | SnH₄ | 12 | C₂/m | 300.0 | 97.0 | 0.1 |
| 189 | Fe₂S₃ | 36 | Cmcm | 173.0 | 0.3 | 0.1 |
| 190 | AsH₃ | 63 | Cmcm | 300.0 | 21.2 | 0.1 |
| 191 | AsH₅ | 63 | Cmcm | 400.0 | 20.2 | 0.1 |
| 192 | AsH₆ | 15 | C₂/c | 350.0 | 141.0 | 0.1 |
| 193 | AsH₆ | 15 | C₂/c | 400.0 | 143.9 | 0.1 |
| 194 | AsH₆ | 15 | C₂/c | 450.0 | 151.4 | 0.1 |
| 195 | SbH₃ | 62 | Pnma | 175.0 | 14.6 | 0.1 |
| 196 | SbH₅ | 62 | Pnma | 215.0 | 10.5 | 0.1 |
| 197 | SbH₆ | 62 | Pnma | 255.0 | 8.5 | 0.1 |
| 198 | SbH₆ | 62 | Pnma | 295.0 | 6.8 | 0.1 |
| 199 | SbH₇ | 47 | Pnmm | 300.0 | 25.9 | 0.1 |
| 200 | SbH₇ | 47 | Pnmm | 400.0 | 19.8 | 0.1 |
| 201 | SbH₇ | 194 | P₆₃/mmc | 150.0 | 102.2 | 0.1 |
| 202 | SbH₇ | 194 | P₆₃/mmc | 200.0 | 102.3 | 0.1 |
| 203 | SbH₇ | 194 | P₆₃/mmc | 250.0 | 99.9 | 0.1 |
| 204 | SbH₇ | 194 | P₆₃/mmc | 300.0 | 93.9 | 0.1 |
| 205 | PH₂ | 12 | C₂/m | 100.0 | 49.01 | 0.1 |
| 206 | PH₂ | 12 | C₂/m | 150.0 | 55.52 | 0.1 |
| 207 | PH₂ | 12 | C₂/m | 200.0 | 75.59 | 0.1 |
| 208 | PH₂ | 139 | I₄/mmm | 100.0 | 32.47 | 0.1 |
| 209 | PH₂ | 139 | I₄/mmm | 150.0 | 50.6 | 0.1 |
| 210 | PH₂ | 139 | I₄/mmm | 200.0 | 70.36 | 0.1 |
| 211 | RuH₂ | 225 | Pm₃m | 100.0 | 0.41 | 0.1 |
| 212 | RuH₂ | 221 | Pm₃m | 100.0 | 3.57 | 0.1 |
| 213 | RuH₂ | 223 | Pm₃m | 200.0 | 1.25 | 0.1 |
| 214 | TcH₂ | 139 | I₄/mmm | 100.0 | 5.42 | 0.1 |
| 215 | TcH₂ | 139 | I₄/mmm | 150.0 | 6.31 | 0.1 |
| 216 | TcH₂ | 139 | I₄/mmm | 200.0 | 10.65 | 0.1 |
| 217 | TcH₂ | 63 | Cmcm | 300.0 | 8.61 | 0.1 |
| 218 | TcH₂ | 131 | P₄₁/mmc | 300.0 | 9.94 | 0.1 |
| 219 | H₄Te | 191 | P₆₃/mmc | 170.0 | 104.47 | 0.1 |
| 220 | H₄Te | 191 | P₆₃/mmc | 200.0 | 99.18 | 0.1 |
| 221 | H₄Te | 191 | P₆₃/mmc | 250.0 | 91.33 | 0.1 |
| 222 | H₄Te | 166 | R₃m | 270.0 | 75.66 | 0.1 |
| 223 | H₄Te | 166 | R₃m | 300.0 | 67.7 | 0.1 |
| 224 | H₄Te | 12 | C₂/m | 200.0 | 57.98 | 0.1 |
| 225 | H₄Te | 12 | C₂/m | 300.0 | 46.0 | 0.1 |
| 226 | H₄Te | 129 | P₄₁/mmm | 150.0 | 28.28 | 0.1 |
| 227 | H₄Te | 129 | P₄₁/mmm | 200.0 | 18.71 | 0.1 |
| 228 | H₄Te | 194 | P₆₃/mmc | 300.0 | 44.26 | 0.1 |
| 229 | H₄S₃ | 62 | Pnma | 140.0 | 2.1 | 0.13 |
| 230 | KAuH₂ | 123 | P₄₁/mmm | 120.0 | 0.28 | 0.11 |
| 231 | Ba(AuH₃)₂ | 79 | I₄ | 0.0001 | 30.0 | 0.11 |
| 232 | Sr(AuH₃)₂ | 79 | I₄ | 0.0001 | 10.0 | 0.11 |
| 233 | MgGeH₆ | 200 | Pm₃ | 200.0 | 66.6 | 0.1 |
| 234 | MgGeH₆ | 200 | Pm₃ | 250.0 | 59.05 | 0.1 |
| 235 | MgGeH₆ | 200 | Pm₃ | 300.0 | 50.29 | 0.1 |
| 236 | MgSiH₆ | 12 | C₂/m | 250.0 | 63.144 | 0.1 |
| 237 | MgSiH₆ | 12 | C₂/m | 275.0 | 58.048 | 0.1 |
| 238 | MgSiH₆ | 12 | C₂/m | 300.0 | 52.651 | 0.1 |
| 239 | Li₂BH₄ | 175 | P₆₃ | 100.0 | 98.0 | 0.1 |
| 240 | Li₂BH₄ | 175 | P₆₃ | 200.0 | 81.0 | 0.1 |
| 241 | VH | 166 | R₃m | 200.0 | 2.24 | 0.1 |
| 242 | VH | 62 | Pnma | 200.0 | 6.12 | 0.1 |
| 243 | VH | 225 | Pm₃ | 200.0 | 4.59 | 0.1 |
| 244 | VH | 194 | P₆₃/mmc | 200.0 | 18.5 | 0.1 |
| 245 | VH | 63 | Cmcm | 300.0 | 25.1 | 0.1 |
| 246 | VH | 12 | C₂/m | 300.0 | 71.4 | 0.1 |
| 247 | TaH₂ | 62 | Pnma | 200.0 | 7.1 | 0.1 |
| 248 | TaH₄ | 166 | R₃m | 250.0 | 31.0 | 0.1 |
| Element | Structure | Lattice Parameter | Symmetry | Remarks |
|---------|-----------|-------------------|----------|---------|
| TaH₂   | $F d d 2$  | 300.0             | 135.8    | 0.1     |
| LaH₄   | $I 4/m m m$ | 300.0             | 10.0     | 0.1     |
| LaH₈   | $C 2/m$   | 300.0             | 131.0    | 0.1     |
| LaH₁₀  | $F n 3 m$  | 210.0             | 238.0    | 0.1     |
| LaH₁₀  | $F n 3 m$  | 250.0             | 232.0    | 0.1     |
| YH₁₀   | $I m 3 m$  | 250.0             | 215.0    | 0.1     |
| YH₁₀   | $I m 3 m$  | 250.0             | 265.0    | 0.1     |
| H₃Cl   | 166.0     | 400.0             | 44.8     | 0.1     |
| ArH₂   | 2 P $\bar{1}$ | 1400.0  | 6.0    | 0.1     |
| ArH₄   | 12 $C 2/m$ | 1500.0             | 70.0     | 0.1     |
| ArH₄   | 139 $I 4/m m m$ | 1500.0           | 72.0     | 0.1     |
| ArH₄   | 62 Pmna    | 2000.0             | 51.0     | 0.1     |
| ZrH₂   | 63 Cmcm    | 120.0             | 10.6     | 0.1     |
| ScH₆   | 194 P6₃/mmc | 300.0           | 95.03    | 0.1     |
| ScH₉   | 194 P6₃/mmc | 400.0           | 183.1    | 0.1     |
| YH₆   | 229 I m 3 m  | 120.0             | 259.6    | 0.1     |
| YH₆   | 176 P6₃/m   | 150.0             | 264.2    | 0.1     |
| YH₆   | 225 F n 3 m  | 400.0             | 308.3    | 0.1     |
| LaH₆   | 166.0     | 100.0             | 231.8    | 0.1     |
| CeH₉   | 194 P6₃/mmc | 50.0             | 60.26    | 0.1     |
| GeH₄   | 12 $C 2/m$ | 280.0             | 67.0     | 0.1     |
| GeH₄   | 12 $C 2/m$ | 300.0             | 63.0     | 0.1     |
| Ge₃H₁₁ | 119 $I 4 m 2$ | 285.0           | 43.0     | 0.1     |
| Ge₃H₁₁ | 119 $I 4 m 2$ | 300.0           | 38.0     | 0.1     |
| Ge₃H₁₁ | 119 $I 4 m 2$ | 320.0           | 35.0     | 0.1     |
| FeH₅   | 67 Cmca    | 200.0             | 48.0     | 0.1     |
| FeH₅   | 139 $I 4/m m m$ | 200.0        | 0.1     | 0.1     |
| FeH₅   | 64 Cmca    | 300.0             | 0.1     | 0.1     |
| AcH₃   | 63 Cmcm    | 150.0             | 0.0      | 0.1     |
| Ac₃H₁₀ | 65 Cmcm    | 150.0             | 3.0      | 0.1     |
| AcH₄   | 63 Cmcm    | 100.0             | 60.0     | 0.1     |
| AcH₅   | 2 P $\bar{1}$ | 150.0           | 74.9     | 0.1     |
| AcH₈   | 12 $C 2/m$ | 150.0             | 134.0    | 0.1     |
| AcH₈   | 8 Cm      | 100.0             | 152.1    | 0.1     |
| AcH₁₀  | 166 $R 3 m$ | 200.0           | 204.1    | 0.1     |
| AcH₁₀  | 166 $R 3 m$ | 250.0           | 140.1    | 0.1     |
| AcH₁₀  | 166 $R 3 m$ | 300.0           | 83.2     | 0.1     |
| AcH₁₂  | 139 $I 4/m m m$ | 150.0        | 123.3    | 0.1     |
| AcH₁₂  | 139 $I 4/m m m$ | 300.0        | 83.8     | 0.1     |
| ACH₁₆  | 175 P6₃/m 2 | 150.0           | 199.2    | 0.1     |
| ACH₁₆  | 175 P6₃/m 2 | 250.0           | 155.9    | 0.1     |
| H₃SAr  | 221 Pm3m   | 240.0             | 89.0     | 0.13    |
| H₃SAr  | 221 Pm3m   | 240.0             | 22.0     | 0.13    |
| ScH₂   | 191 P6/mmm | 300.0             | 0.0      | 0.1     |
| ScH₃   | 194 P6₃/mmc | 400.0           | 0.0      | 0.1     |
| ScH₄   | 139 $I 4/m m m$ | 120.0       | 105.0    | 0.1     |
| ScH₄   | 139 $I 4/m m m$ | 250.0       | 72.0     | 0.1     |
| ScH₆   | 229 I m 3 m  | 250.0             | 149.0    | 0.1     |
| ScH₇   | 63 Cmcm    | 300.0             | 201.0    | 0.1     |
| ScH₉   | 109 $I 4/m d$ | 300.0         | 187.0    | 0.1     |
| ScH₁₀  | 63 Cmcm    | 250.0             | 129.0    | 0.1     |
| ScH₁₂  | 71 I mm m  | 350.0             | 155.0    | 0.1     |
| ThH₃   | 166 $R 3 m$ | 100.0             | 0.0      | 0.1     |
| ThH₅   | 10.0 I m m m | 10.0         | 3.8      | 0.1     |
| ThH₆   | 139 $I 4/m m m$ | 85.0       | 2.97     | 0.1     |
| ThH₇   | 14 P2₁/c   | 100.0             | 61.4     | 0.1     |
| ThH₁₀  | 225 F n 3 m  | 100.0             | 221.1    | 0.1     |
| ThH₁₀  | 225 F n 3 m  | 200.0             | 182.6    | 0.1     |
| ThH₁₀  | 225 F n 3 m  | 300.0             | 155.4    | 0.1     |
| H₃Cl   | 229 I m 3 m  | 150.0             | 198.0    | 0.1     |
| H₃Cl   | 229 I m 3 m  | 175.0             | 122.0    | 0.1     |
| H₃Cl   | 229 I m 3 m  | 200.0             | 95.0     | 0.1     |
| \(H_{2}Cl\) | 322 | \(Im\bar{3}m\) | 250.0 | 77.0 | 0.1 |
| \(WH\) | 194 | \(P6/mmc\) | 300.0 | 4.175 | 0.1 |
| \(WH\) | 62 | \(Pnma\) | 300.0 | 1.484 | 0.1 |
| \(WH\) | 129 | \(P4/mmm\) | 140.0 | 0.065 | 0.1 |
| \(WH\) | 183 | \(P6mm\) | 230.0 | 64.16 | 0.1 |
| \(WH\) | 183 | \(P6mm\) | 250.0 | 64.87 | 0.1 |
| \(WH\) | 183 | \(P6mm\) | 270.0 | 62.41 | 0.1 |
| \(WH\) | 183 | \(P6mm\) | 300.0 | 60.792 | 0.1 |
| \(WH\) | 12 | \(C2/m\) | 240.0 | 31.586 | 0.1 |
| \(H_{2}Se\) | 221 | \(Pm3m\) | 200.0 | 196.0 | 0.1 |
| \(H_{2}Se\) | 65 | \(Cmmm\) | 200.0 | 181.0 | 0.1 |
| \(H_{2}Se\) | 227 | \(Fd\bar{3}m\) | 200.0 | 115.0 | 0.1 |
| \(ZrH_{3}\) | 161 | \(R3c\) | 260.0 | 8.0 | 0.13 |
| \(ZrH_{4}\) | 70 | \(Fdd\bar{2}\) | 140.0 | 78.0 | 0.13 |
| \(ZrH_{4}\) | 139 | \(I4/mmm\) | 230.0 | 47.0 | 0.13 |
| \(ZrH_{6}\) | 36 | \(Cmc21-HP\) | 160.0 | 55.0 | 0.13 |
| \(ZrH_{6}\) | 36 | \(Cmc21-HP\) | 215.0 | 70.0 | 0.13 |
| \(ZrH_{6}\) | 14 | \(P2_{1}/c\) | 295.0 | 153.0 | 0.13 |
| \(ZrH_{6}\) | 139 | \(I4/mmm\) | 295.0 | 114.0 | 0.13 |
| \(ZrH_{6}\) | 139 | \(I4/mmm\) | 340.0 | 107.0 | 0.13 |
| \(H_{2}SiP_{0.125}\) | 166 | \(R3m\) | 100.0 | 136.0 | 0.1 |
| \(H_{2}SiP_{0.125}\) | 166 | \(R3m\) | 150.0 | 168.0 | 0.1 |
| \(H_{2}SiP_{0.125}\) | 229 | \(Im3m\) | 200.0 | 194.0 | 0.1 |
| \(H_{2}SiP_{0.125}\) | 229 | \(Im3m\) | 250.0 | 178.0 | 0.1 |
| \(H_{2}SiP_{0.0625}\) | 166 | \(R3m\) | 100.0 | 131.3 | 0.1 |
| \(H_{2}SiP_{0.0625}\) | 166 | \(R3m\) | 150.0 | 170.5 | 0.1 |
| \(H_{2}SiP_{0.0625}\) | 229 | \(Im3m\) | 200.0 | 212.3 | 0.1 |
| \(H_{2}SiP_{0.0625}\) | 229 | \(Im3m\) | 250.0 | 190.7 | 0.1 |
| \(H_{2}SiP_{0.0625}\) | 166 | \(R3m\) | 100.0 | 126.7 | 0.1 |
| \(H_{2}SiP_{0.0625}\) | 166 | \(R3m\) | 150.0 | 145.4 | 0.1 |
| \(H_{2}SiP_{0.0625}\) | 229 | \(Im3m\) | 200.0 | 161.4 | 0.1 |
| \(H_{2}SiP_{0.0625}\) | 229 | \(Im3m\) | 250.0 | 142.3 | 0.1 |
| \(H_{2}SiP_{0.125}\) | 166 | \(R3m\) | 100.0 | 139.5 | 0.1 |
| \(H_{2}SiP_{0.125}\) | 166 | \(R3m\) | 150.0 | 147.8 | 0.1 |
| \(H_{2}SiP_{0.125}\) | 229 | \(Im3m\) | 200.0 | 136.1 | 0.1 |
| \(H_{2}SiP_{0.125}\) | 229 | \(Im3m\) | 250.0 | 119.4 | 0.1 |
| \(TiH_{2}\) | 139 | \(I4/mmm\) | 200.0 | 11.8 | 0.1 |
| \(TiH_{2}\) | 139 | \(I4/mmm\) | 30.0 | 0.0 | 0.1 |
| \(TiH_{2}\) | 129 | \(P4/mmm\) | 200.0 | 0.1 | 0.1 |
| \(TiH_{3}\) | 225 | \(Fm\bar{3}m\) | 80.0 | 13.3 | 0.1 |
| \(TiH_{3}\) | 225 | \(Fm\bar{3}m\) | 100.0 | 9.7 | 0.1 |
| \(TiH_{3}\) | 225 | \(Fm\bar{3}m\) | 150.0 | 5.0 | 0.1 |
| \(TiH_{4}\) | 225 | \(Fm\bar{3}m\) | 200.0 | 3.5 | 0.1 |
| \(TiH_{6}\) | 71 | \(Immm\) | 200.0 | 77.8 | 0.1 |
| \(VH_{3}\) | 229 | \(Fm\bar{3}m\) | 140.0 | 11.1 | 0.1 |
| \(VH_{3}\) | 229 | \(Fm\bar{3}m\) | 150.0 | 8.0 | 0.1 |
| \(VH_{3}\) | 229 | \(Fm\bar{3}m\) | 200.0 | 2.5 | 0.1 |
| \(VH_{3}\) | 229 | \(Fm\bar{3}m\) | 250.0 | 1.6 | 0.1 |
| \(PdH_{2}\) | 216 | \(F4\bar{3}m\) | 200.0 | 8.86 | 0.1 |
| \(PdH_{2}\) | 225 | \(Fm\bar{3}m\) | 200.0 | 18.78 | 0.1 |
| \(FeH_{3}\) | 139 | \(I4/mmm\) | 150.0 | 45.8 | 0.1 |
| \(FeH_{3}\) | 139 | \(I4/mmm\) | 300.0 | 35.7 | 0.1 |
| \(FeH_{6}\) | 12 | \(C2/m\) | 100.0 | 3.9 | 0.1 |
| \(FeH_{6}\) | 65 | \(Cmmm\) | 150.0 | 42.9 | 0.1 |
| \(FeH_{6}\) | 65 | \(Cmmm\) | 300.0 | 37.3 | 0.1 |
| \(H_{2}Se\) | 51 | \(Pnma\) | 150.0 | 39.0 | 0.1 |
| \(H_{2}Se\) | 51 | \(Pnma\) | 200.0 | 28.0 | 0.1 |
| \(H_{2}Se\) | 51 | \(Pnma\) | 300.0 | 26.0 | 0.1 |
| \(H_{2}Se\) | 12 | \(C2/m\) | 265.0 | 87.0 | 0.1 |
| \(H_{2}Se\) | 12 | \(C2/m\) | 270.0 | 86.0 | 0.1 |
| \(H_{2}Se\) | 12 | \(C2/m\) | 300.0 | 56.0 | 0.1 |
| \(YH_{6}\) | 229 | \(Im3m\) | 100.0 | 233.0 | 0.1 |
| \(YH_{6}\) | 229 | \(Im3m\) | 125.0 | 165.0 | 0.1 |
| Z  | Chemical Formula | Space Group | a (Å) | c (Å) | β (°) |
|----|-----------------|-------------|-------|-------|-------|
| 375 | YH₆ | Im3m | 200.0 | 285.0 | 0.1 |
| 376 | YH₆ | Im3m | 300.0 | 290.0 | 0.1 |
| 377 | CaYH₂ | Pm3m | 170.0 | 210.0 | 0.1 |
| 378 | CaYH₂ | Pm3m | 200.0 | 215.0 | 0.1 |
| 379 | CaYH₂ | Pm3m | 250.0 | 201.0 | 0.1 |
| 380 | CaYH₂ | Fd3m | 200.0 | 226.0 | 0.1 |
| 381 | MgH₆ | C2 | 300.0 | 73.0 | 0.1 |
| 382 | LiMgH₆ | P | 300.0 | 178.0 | 0.1 |
| 383 | Li₂MgH₆ | P5m1 | 300.0 | 201.0 | 0.1 |
| 384 | Li₂MgH₆ | Fd3m | 250.0 | 473.0 | 0.1 |
| 385 | Li₂MgH₆ | Fd3m | 300.0 | 357.0 | 0.1 |
| 386 | Li₂MgH₆ | Fd3m | 500.0 | 176.0 | 0.1 |
| 387 | Li₂MgH₆ | C2 | 300.0 | 212.0 | 0.1 |
| 388 | YH₆ | Im3m | 250.0 | 300.0 | 0.11 |
| 389 | YH₆ | Im3m | 350.0 | 283.0 | 0.11 |
| 390 | YH₆ | Fm3m | 250.0 | 311.0 | 0.11 |
| 391 | YH₆ | Fm3m | 300.0 | 310.0 | 0.11 |
| 392 | YH₆ | Fm3m | 350.0 | 278.0 | 0.11 |
| 393 | YSnH₄ | C2/m | 200.0 | 20.0 | 0.1 |
| 394 | FeSeH | C2/m | 150.0 | 0.2 | 0.1 |
| 395 | FeSeH | C2/m | 200.0 | 0.0 | 0.1 |
| 396 | FeSeH | C2/m | 250.0 | 0.0 | 0.1 |
| 397 | FeSeH | C2/m | 300.0 | 0.0 | 0.1 |
| 398 | Fe₂Se₇ | Immm | 150.0 | 1.1 | 0.1 |
| 399 | Fe₂Se₇ | Immm | 200.0 | 0.8 | 0.1 |
| 400 | Fe₂Se₇ | Immm | 250.0 | 3.8 | 0.1 |
| 401 | Fe₂Se₇ | Immm | 300.0 | 1.3 | 0.1 |
| 402 | Fe₄SeH₂ | Amm2 | 150.0 | 0.0 | 0.1 |
| 403 | Fe₄SeH₂ | I4/mmm | 150.0 | 8.6 | 0.1 |
| 404 | Fe₄SeH₂ | I4/mmm | 200.0 | 9.1 | 0.1 |
| 405 | Fe₄SeH₂ | Pm | 150.0 | 34.4 | 0.1 |
| 406 | Fe₄SeH₂ | Pm | 200.0 | 36.4 | 0.1 |
| 407 | Fe₄SeH₂ | Pm | 150.0 | 0.0 | 0.1 |
| 408 | CeH₉ | F43m | 90.0 | 333.111 | 0.1 |
| 409 | CeH₉ | F43m | 92.0 | 141.691 | 0.1 |
| 410 | CeH₉ | F43m | 94.0 | 142.559 | 0.1 |
| 411 | CeH₉ | F43m | 96.0 | 116.405 | 0.1 |
| 412 | CeH₉ | F43m | 98.0 | 140.482 | 0.1 |
| 413 | CeH₉ | F43m | 100.0 | 141.236 | 0.1 |
| 414 | CeH₉ | F43m | 150.0 | 130.651 | 0.1 |
| 415 | CeH₉ | F43m | 200.0 | 133.98 | 0.1 |
| 416 | CeH₉ | F43m | 250.0 | 97.608 | 0.1 |
| 417 | CeH₉ | F43m | 300.0 | 93.647 | 0.1 |
| 418 | CeH₉ | Fm3m | 92.0 | 147.143 | 0.1 |
| 419 | CeH₉ | Fm3m | 94.0 | 163.133 | 0.1 |
| 420 | CeH₉ | Fm3m | 96.0 | 117.656 | 0.1 |
| 421 | CeH₉ | Fm3m | 98.0 | 125.005 | 0.1 |
| 422 | CeH₉ | Fm3m | 100.0 | 144.022 | 0.1 |
| 423 | CeH₉ | Fm3m | 150.0 | 134.382 | 0.1 |
| 424 | CeH₉ | Fm3m | 200.0 | 105.745 | 0.1 |
| 425 | CeH₉ | Fm3m | 250.0 | 84.766 | 0.1 |
| 426 | CeH₉ | Fm3m | 300.0 | 74.129 | 0.1 |
| 427 | LiPH₃ | P2/m | 200.0 | 60.4 | 0.1 |
| 428 | LiPH₄ | P2₁/m | 150.0 | 0.05 | 0.1 |
| 429 | LiPH₄ | Pm | 200.0 | 167.3 | 0.1 |
| 430 | LiPH₄ | Pm | 250.0 | 148.3 | 0.1 |
| 431 | LiPH₄ | Pm | 300.0 | 128.6 | 0.1 |
| 432 | LiPH₄ | Pm | 300.0 | 59.2 | 0.1 |
| 433 | YCaH₂ | Pm3m | 180.0 | 229.9 | 0.1 |
| 434 | YCaH₂ | Pm3m | 200.0 | 222.0 | 0.1 |
| 435 | YCaH₂ | Pm3m | 250.0 | 210.8 | 0.1 |
| 436 | YSH₆ | P4₂/mmc | 210.0 | 91.0 | 0.1 |
| 437 | YSH₆ | P4₂/mmc | 300.0 | 61.0 | 0.1 |
| Compound | Space Group | Volume | Density | Ref. |
|----------|-------------|--------|---------|------|
| LaSH₆   | 63 Cmcm    | 200.0  | 24.0   | 0.1  |
| LaSH₆   | 63 Cmcm    | 300.0  | 35.0   | 0.1  |
| PH₃     | 63 Cmcm    | 100.0  | 13.0   | 0.13 |
| PH₃     | 12 C2/m    | 200.0  | 67.0   | 0.13 |
| UH₂₅    | 225 Fm̅3m  | 100.0  | 58.58  | 0.1  |
| UH₂₀    | 225 Fm̅3m  | 200.0  | 21.22  | 0.1  |
| UH₂₀    | 225 Fm̅3m  | 300.0  | 11.93  | 0.1  |
| UH₂₀    | 225 Fm̅3m  | 400.0  | 9.5    | 0.1  |
| UH₂₀    | 225 Fm̅3m  | 550.0  | 15.11  | 0.1  |
| S₀₂Si₅₃₈₃ | 166 R5m   | 200.0  | 110.0  | 0.1  |
| S₀₃Se₅₃₈₃ | 156 P₃m1  | 200.0  | 54.0   | 0.1  |
| S₀₅Se₅₃₈₃ | 166 R5m   | 200.0  | 99.0   | 0.1  |
| S₀₆Se₅₃₈₃ | 166 R5m   | 200.0  | 184.0  | 0.1  |
| TaH₂    | 14 P2₁/₃c | 100.0  | 23.0   | 0.1  |
| BH₅     | 15 C2/c   | 250.0  | 37.31  | 0.1  |
| BH₂₅    | 15 C2/c   | 300.0  | 34.24  | 0.1  |
| BH₂₅    | 15 C2/c   | 350.0  | 33.31  | 0.1  |
| BH₂₅    | 15 C2/c   | 400.0  | 28.03  | 0.1  |
| BH      | 191 P6/mmm | 250.0  | 4.522  | 0.1  |
| NiH₂    | 225 Fm̅3m  | 25.0   | 0.01   | 0.1  |
| Al₃H    | 156 P₃m1  | 195.0  | 3.5    | 0.13 |
| Al₃H    | 148 R3    | 195.0  | 0.6    | 0.13 |
| Al₃H    | 150 P321  | 195.0  | 0.6    | 0.13 |
| Al₃H    | 10 P2/m   | 195.0  | 1.2    | 0.13 |
| Al₃H    | 5 C2     | 195.0  | 0.4    | 0.13 |
| AlH     | 166 R5m   | 180.0  | 57.9   | 0.13 |
| AlH     | 166 R5m   | 215.0  | 45.4   | 0.13 |
| AlH     | 166 R5m   | 335.0  | 21.2   | 0.13 |
| AlH₂₅   | 223 Pm₃n  | 105.0  | 28.5   | 0.13 |
| AlH₂₅   | 223 Pm₃n  | 150.0  | 7.7    | 0.13 |
| AlH₂₅   | 223 Pm₃n  | 210.0  | 0.3    | 0.13 |
| AlH₂₅   | 223 Pm₃n  | 290.0  | 0.0    | 0.13 |
| HBS     | 40 Ama2   | 200.0  | 0.0    | 0.1  |
| HBS     | 40 Ama2   | 300.0  | 0.8    | 0.1  |
| HBS     | 40 Ama2   | 400.0  | 1.9    | 0.1  |
| Ca₅BH₃   | 38 Amm2   | 300.0  | 7.0    | 0.1  |
| CaBH₄   | 46 Ima2   | 300.0  | 0.1    | 0.1  |
| CaBH₅   | 194 P6mmc | 300.0  | 0.1    | 0.1  |
| CaBH₆   | 205 Pa₃   | 100.0  | 114.0  | 0.1  |
| CaBH₆   | 205 Pa₃   | 200.0  | 117.0  | 0.1  |
| CaBH₆   | 205 Pa₃   | 300.0  | 119.0  | 0.1  |
| Ca₅B₂H₇   | 6 Pm   | 200.0  | 63.0   | 0.1  |
| Ca₅B₂H₇   | 6 Pm   | 300.0  | 89.0   | 0.1  |
| TiPH₃   | 156 P₃m1  | 150.0  | 0.0    | 0.1  |
| TiPH₃   | 166 R5m   | 250.0  | 2.22   | 0.1  |
| TiPH₃   | 38 Amm2   | 250.0  | 30.51  | 0.1  |
| TiPH₄   | 166 R₃m   | 100.0  | 51.57  | 0.1  |
| TiPH₄   | 166 R₃m   | 200.0  | 38.09  | 0.1  |
| TiPH₄   | 166 R₃m   | 250.0  | 62.36  | 0.1  |
| TiPH₄   | 166 R₃m   | 300.0  | 57.06  | 0.1  |
| TiPH₅   | 119 I₄m2  | 250.0  | 126.06 | 0.1  |
| TiPH₆   | 8 Cm    | 250.0  | 40.89  | 0.1  |
| TiPH₇   | 8 Cm    | 250.0  | 51.32  | 0.1  |
| TiPH₈   | 12 C₂m   | 250.0  | 66.67  | 0.1  |
| TiPH₈   | 12 C₂m   | 300.0  | 54.77  | 0.1  |
| BeCH₄   | 2 P1̅    | 5.0    | 6.0   | 0.1  |
| BeCH₄   | 2 P1̅    | 60.0   | 8.5   | 0.1  |
| BeCH₄   | 2 β-P1̅ | 20.0   | 13.3  | 0.1  |
| BeCH₄   | 2 α-P1̅ | 40.0   | 18.1  | 0.1  |
| BeCH₄   | 2 α-P1̅ | 80.0   | 28.9  | 0.1  |
| Zr₂H₁₅ | 220 I43d | 40.0   | 0.8   | 0.1  |
| ZrH₃   | 223 Pm₃n | 10.0   | 16.6  | 0.1  |
| ZrH₃   | 223 Pm₃n | 20.0   | 13.8  | 0.1  |
| No. | Compounds | Space Group | Temperature (K) | Volume (Å³) | Density (g/cm³) |
|-----|------------|-------------|----------------|-------------|----------------|
| 501 | ZrH<sub>3</sub> | $Pm\bar{3}m$ | 40.0 | 12.4 | 0.1 |
| 502 | TiH<sub>2</sub> | $C2/m$ | 350.0 | 93.6 | 0.1 |
| 503 | TiH<sub>2</sub> | $C2/m$ | 250.0 | 103.1 | 0.1 |
| 504 | TiH<sub>2</sub> | $P\bar{1}$ | 200.0 | 35.0 | 0.1 |
| 505 | TiH<sub>2</sub> | $P\bar{1}$ | 150.0 | 4.8 | 0.1 |
| 506 | TiH<sub>4</sub> | $I4/mmm$ | 350.0 | 131.2 | 0.1 |
| 507 | TiH<sub>4</sub> | $Fddd$ | 350.0 | 21.2 | 0.1 |
| 508 | TiH<sub>4</sub> | $I4$ | 350.0 | 2.4 | 0.1 |
| 509 | TiH<sub>4</sub> | $I4$ | 50.0 | 5.4 | 0.1 |
| 510 | TiH<sub>4</sub> | $I4/m$ | 300.0 | 4.0 | 0.1 |
| 511 | TiH<sub>3</sub> | $Ibam$ | 150.0 | 2.1 | 0.1 |
| 512 | TiH<sub>3</sub> | $Ibam$ | 250.0 | 4.7 | 0.1 |
| 513 | TiH<sub>2</sub> | $Cmma$ | 50.0 | 7.1 | 0.1 |
| 514 | TiH<sub>2</sub> | $Cmma$ | 250.0 | 5.8 | 0.1 |
| 515 | TiH<sub>2</sub> | $I4/mmm$ | 50.0 | 0.0 | 0.1 |
| 516 | TiH<sub>2</sub> | $I4/mmm$ | 350.0 | 22.7 | 0.1 |
| 517 | TiH<sub>2</sub> | $I4/mmm$ | 50.0 | 5.4 | 0.1 |
| 518 | LiP<sub>2</sub>H<sub>4</sub> | $R3\bar{3}$ | 230.0 | 143.0 | 0.1 |
| 519 | LiP<sub>2</sub>H<sub>4</sub> | $R3\bar{3}$ | 300.0 | 112.0 | 0.1 |
| 520 | LiP<sub>2</sub>H<sub>4</sub> | $R3\bar{3}$ | 400.0 | 84.0 | 0.1 |
| 521 | LiP<sub>2</sub>H<sub>4</sub> | $R3\bar{3}$ | 400.0 | 90.0 | 0.1 |
| 522 | BeP<sub>2</sub>H<sub>4</sub> | $R3\bar{3}$ | 400.0 | 139.0 | 0.1 |
| 523 | NaP<sub>2</sub>H<sub>4</sub> | $R3\bar{3}$ | 300.0 | 0.99 | 0.1 |
| 524 | LiBH<sub>2</sub> | $Cmcm$ | 400.0 | 2.53 | 0.1 |
| 525 | LiBH<sub>2</sub> | $Cmcm$ | 500.0 | 9.12 | 0.1 |
| 526 | LiBH<sub>2</sub> | $Cmcm$ | 600.0 | 10.0 | 0.1 |
| 527 | LiBH<sub>2</sub> | $Cmcm$ | 100.0 | 98.0 | 0.1 |
| 528 | CSH<sub>7</sub> | $Cm$ | 150.0 | 152.0 | 0.1 |
| 529 | CSH<sub>7</sub> | $R3m$ | 200.0 | 137.0 | 0.1 |
| 530 | CSH<sub>7</sub> | $Pmna$ | 150.0 | 122.0 | 0.1 |
| 531 | CSH<sub>7</sub> | $Pmna$ | 200.0 | 123.0 | 0.1 |