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# Computer-Aided Design of $AD_2X_2$ Intermetallics with a $ThCr_2Si_2$-Type of Crystal Structure

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**Abstract**—Several hundred new $AD_2X_2$ ($A$ and $D$ are various elements; $X$ = B, Al, Si, P, Ga, Ge, As, Sn, Sb) compounds are computer designed, and the types of their crystal structures under normal conditions are predicted. A special software package is used for the calculations; it includes a set of databases on the properties of inorganic substances and materials and a system for an analysis of these data, which is based on precedent pattern recognition methods. Only data on the properties of the elements entering into the compound compositions are used to predict unknown compounds. The parameters of elements in positions $A$ and $D$ (i.e., the Mendeleev–Pettifor numbers, the pseudopotential radii, and their algebraic functions) are found to mainly determine the possibility of formation of $AD_2X_2$ compounds and the type of their crystal structures. New compounds of $AD_2B_2$, $AD_2Ga_2$, and $AD_2Sn_2$ compositions are predicted for the first time.

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## INTRODUCTION

Intermetallics $AD_2X_2$ ($A$ and $D$ are elements given in the tables below; $X$ = B, Al, Si, P, Ga, Ge, As, Sn, Sb) with a $ThCr_2Si_2$-type of crystal structure are being extensively studied due to searching for new ferro- and antiferromagnetic materials [1–6]. Compounds of this composition exhibit superconducting ($T_c \leq 40$ K) [2, 7–14] and thermoelectric properties [15, 16].

## THEORETICAL ANALYSIS

At present, database "Phases" on the properties of inorganic compounds [17] contains information on 1327 $AD_2X_2$ ($X$ = B, Al, Si, P, Ga, Ge, As, Sn, Sb) compounds. Most of them crystallize into a $ThCr_2Si_2$-type of crystal structure (space group I4/*mmm*) at room temperature and atmospheric pressure (Fig. 1). The representativeness of the families with crystal structures of the types $FeMo_2B_2$ ($U_3Si_2$) (space group P4/*mbm*), $CaAl_2Si_2$ (space group $P\bar{3}m1$), $CaBe_2Ge_2$ (space group P4/*nmm*), and $CoSc_2Si_2$ (space group C2/*m*) is significantly smaller.

Criteria for the formation of $AD_2X_2$ intermetallics with many types of crystal structures were searched for in many works [18–23], and almost all found criteria include size factors: most often, these are the lattice parameters of well-known phases [19–23], which makes it impossible to predict unknown compounds. Only Pearson [18] tried to predict a $ThCr_2Si_2$-type crystal structure for intermetallics. His criterion included a sum of the metallic radii of elements $D$ and $X$ [18, 24].

To test the correctness of the criterion proposed in [18], we plotted the stability diagrams of structure types for $AD_2X_2$ ($X$ = B, Al, Si, P, S, Fe, Co, Ni, Cu, Ga, Ge, As, Se, Rh, Pd, Sn, Sb, Te, Ir, Pt, Au, Bi) phases in the coordinates $(R_{metD} + R_{metX}) - (R_{metA} + R_{metD})$, $(R_{metD} + R_{metX}) - R_{metA}$, where $R_{met}$ is the metallic radius of the corresponding element in an $AD_2X_2$ compound [23], and in the coordinates $(R_{ppD} + R_{ppX}) - (R_{ppA} + R_{ppD})$ and $(R_{ppD} + R_{ppX}) - R_{ppA}$, where $R_{pp}$ is the pseudopotential radius of the corresponding element according to Zunger [25]. We failed to separate the structure types of $AD_2X_2$ compounds in the space of element $A$, $D$, and $X$ radii in none of the plotted diagrams. Similar conclusions were made by us earlier, when we studied the diagrams of silicide and germanide phases with a $ThCr_2Si_2$-type of structure, whose coordinates were the Bokii–Belov metallic radius of component $A$ and Bokii–Belov metallic radius of component $D$ [26, 27].

The application of widely used electron concentrations as diagram coordinates in the case of $AD_2Ge_2$ germanides [28] shows that this parameter also does not determine the stability boundaries of the $ThCr_2Si_2$ structure type. It was concluded that a wide range of the properties of components, including the electron, thermodynamic, size, and energy parameters of the chemical elements constituting intermetallics should be analyzed to obtain stability criteria for $ThCr_2Si_2$-type of phases. In [26–29], we proposed this approach

to predict new $AD_2X_2$ ($X$ = Al, Si, Ge, P, As, Sb) compounds with a $ThCr_2Si_2$-type of crystal structure.

In [26–29], we analyzed the data on synthesized intermetallics of the given compositions using the precedent-based pattern recognition methods [30] and formed multidimensional criteria that included a wide range of the properties of chemical elements, namely, the ionization potential, the metallic radii, the entropies of individual substances, the melting points, the electron distribution over the energy levels of isolated atoms, and so on. As a result, we found rules to separate $AD_2Si_2$ and $AD_2Ge_2$ compounds with a $ThCr_2Si_2$-type structure [26, 27] from compounds with other crystal structures and systems without forming compounds of given compositions under normal conditions. A similar problem was solved for $AD_2Al_2$, $AD_2P_2$, $AD_2As_2$, and $AD_2Sb_2$ compounds [28, 29] when we searched for the stability regions (i.e., compact groups of points each of which corresponds to a compound with a certain type of crystal structure in a plot whose coordinates are the properties of the components and algebraic functions of these properties) of $ThCr_2Si_2$ and $CaAl_2Si_2$.

In more than two decades, we tested 41 $AD_2Al_2$ compositions (six predictions were wrong), 134 $AD_2Si_2$ compositions (17 predictions were wrong), 40 $AD_2P_2$ compositions (one prediction was wrong), 91 $AD_2Ge_2$ compositions (eight predictions were wrong), 13 $AD_2As_2$ compositions (one predictions was wrong), and 18 $AD_2Sb_2$ compositions (three predictions were wrong). Thus, the average prediction error was 12%.

Since several hundred new $AD_2X_2$ compounds have been recently synthesized, we decided to train a computer using new data, a wider range of the properties of elements, and a more powerful set of pattern recognition programs. Thus, the purpose of this work is to revise the criteria of forming $AD_2X_2$ intermetallics with different types of crystal structure and to predict new compounds of this composition in ternary $A$–$D$–$X$ ($A$ and $D$ are various elements; $X$ = B, Al, Si, P, Ga, Ge, As, Sn, Sb) systems and the types of their structures under normal conditions.

## COMPUTER EXPERIMENTAL TECHNIQUE

For computer analysis (computer training), we used a specially designed information-analytical system (IAS), which included databases on the properties of inorganic substances and materials and a set of pattern recognition programs [31].

After estimating the experimental data extracted from database "Phases" on the properties of inorganic compounds (http://phases.imet-db.ru) [17], for computer analysis we selected information on 670 well-known $AD_2X_2$ compounds with a $ThCr_2Si_2$-type of structure under normal conditions (293 K, 0.1 MPa), 125 compounds with a $CaAl_2Si_2$-type of structure, 76 compounds with a $CaBe_2Ge_2$-type of structure, 49 compounds with a $CoSc_2Si_2$-type of structure, 59 compounds with a $FeMo_2B_2$-type of structure, and 252 compounds with structures other than those given above and information on 921 examples of the absence of compounds of the $AD_2X_2$ composition.

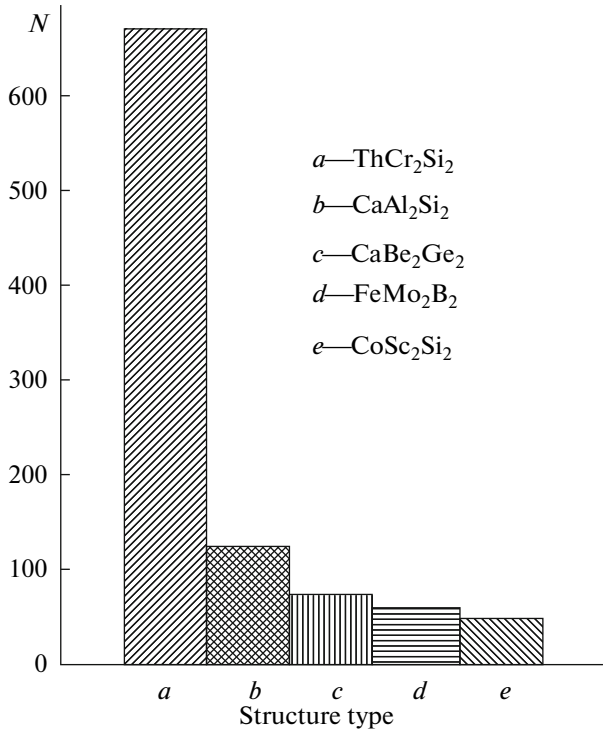


**Fig. 1.** ($a$)–($e$) Distribution diagram for the structure types of intermetallics $AD_2X_2$ ($X$ = B, Al, Si, P, Ga, Ge, As, Sn, Sb) at room temperature and atmospheric pressure ($N$ is the number of compounds).

Based on standpoint of physical chemistry, we used the following properties of elements $A$, $D$, and $X$ to describe intermetallics at the initial stage: the pseudopotential radius [25]; the melting and boiling points, the first three ionization potentials, the distances from core and valence electrons (after Schubert), the element number (after Mendeleev–Pettifor) [32, 33], the electronegativity (after Pauling), the Miedema chemical potential, the quantum number, the thermal conductivity, the group number in the periodic system, the molar heat capacity, the enthalpies of evaporation and atomization, the entropy for a solid state, the metallic [24] and covalent (after Bokii and Belov) radii, and the number of valence electrons (in total, 93 parameters for each chemical system). The data on the properties of elements were borrowed from our database "Elements" (http://phases.imet-db.ru/elements), which was included into IAS [31].

The prediction of new $AD_2X_2$ intermetallics consisted of the following four stages:

(i) selection of the properties of elements most important to classify $AD_2X_2$ intermetallics into structure types;

(ii) searching for the stability regions of $AD_2X_2$ intermetallics in the space of the properties of elements $A$, $D$, and $X$ and predicting of $A–D–X$ chemical systems with the formation or absence of intermetallics of the given composition;

(iii) searching for the stability regions of $AD_2X_2$ intermetallics with the structure types given above under normal conditions and multiclass prediction of the type of crystal structure (seven classes);

(iv) searching for the stability regions of $AD_2X_2$ intermetallics with a certain type of crystal structure and sequential division of systems into three classes (e.g., class 1, compounds with a $ThCr_2Si_2$-type of structure; class 2, compounds with structures other than $ThCr_2Si_2$; and class 3, no $AD_2X_2$ intermetallics in an $A–D–X$ system) followed by prediction.

With the designed IAS [31], we can select the parameters of chemical elements and algebraic functions using these parameters, in the space of which the stability regions of different classes of inorganic compounds are divided best of all.

When training a computer, we present information on chemical systems on a computer memory in the form of a set of the properties of elements $A$, $D$, and $X$ and indicated the class (type of crystal structure or the formation/absence of $AD_2X_2$ compound) to which a certain system belongs. Thus, the initial information for computer analysis consisted of a matrix (training sample) the number of lines in which was equal to the number of the $A–D–X$ chemical systems used to train a computer. As the parameters of elements, we decided to use the initial properties of elements and the most informative algebraic functions found by IAS.

To train a computer, we used the following pattern recognition programs included into IAS [30, 31, 34]: an estimate calculation algorithm, two-dimensional linear separators, a linear machine, a linear Fisher discriminant, logical regularities, multiplicative neural network learning, neural network training, a multilevel perceptron, a $k$ nearest neighbors method, the supporting vector machine, the method of binary decision trees, statistically weighed syndromes, deadlock test selection, the method of inductive concept formation ConFor (which is based on growing pyramidal networks), and L1-regularized multinomial regression [35].

At each prediction stage 2–4 (prediction of the formation of $AD_2X_2$ compound, multiclass prediction of the type of crystal structure, prediction of compounds with a certain type of crystal structure), we used cross-validation to choose the best computer training algorithm.[1] The chosen algorithms (in most cases, they were the following programs: linear machine, training of neural networks and $k$ nearest neighbors) were used in the procedure of collective decision making using a number of algorithms from IAS [31]. As a rule, the collective decision strategy can improve the prediction accuracy due to the mutual compensation of the disadvantages of one algorithm by the advantages of other ones. The best "collective" algorithm (as a rule, they were the clustering and selection algorithm, the Bayes method, or the complex committee method of "majority voting") was found from the results of examination recognition of 100 examples randomly chosen from a training sample and not used in computer training (at the final stage of prediction, control examples were returned to a training sample). With the best algorithms, we predicted new $AD_2X_2$ compounds and estimated the types of their crystal structure under normal conditions.

The final prediction was formed by comparing the results of stages 2–4. If the results were conflicting, the prediction was taken to be indefinite and a blank cell was retained in the corresponding prediction table. It should be noted that, using a "collective" of algorithms, we were able to increase the prediction accuracy from 95.7 to 99.7% for the prediction of the possibility of compound formation and from 90.3 to 97.0% for the multiclass prediction of the type of crystal structure and to increase the prediction accuracy during the sequential division of systems into three classes, e.g., from 94.5 to 95.2% for the prediction of the type of $CaAl_2Si_2$ crystal structure.

## RESULTS OF COMPUTER-AIDED DESIGN AND THEIR DISCUSSION

Using the subsystems of selecting informative attributes introduced into IAS [31], we found that, to classify $A–D–X$ systems into systems with and without $AD_2X_2$ compounds, the most important parameters are $M5(A) \cdot M5(D)$ and $S1(A) + S1(D)$, where $M5(A)$ and $M5(D)$ are the Mendeleev–Pettifor numbers [33, 34] and $S1(A)$ and $S1(D)$ are the pseudopotential radii of elements $A$ and $D$, respectively [25]. For solving the problems of the multiclass prediction of the type of crystal structure, the most important parameters are $S1(A)$, $M5(A)$, and $M5(A)/M3(X)$, where $M3(X)$ is the Mendeleev–Pettifor number of element $X$ (H d-t start left) [32, 33]. For dividing objects into three classes (stage 4), the most important parameters are $M5(A)$, $S1(A)$, $S1(A)–S1(X)$, $M5(A)/M5(X)$, and $M5(A) \cdot M5(D)$, where $M5(X)$ is the Mendeleev–Pettifor number and $S1(X)$ is the pseudopotential radius of element $X$ (class of compounds with a $ThCr_2Si_2$-type of structure), and $M5(A) \cdot M5(D)$ and $S1(A)+S1(D)$ (class of $CaAl_2Si_2$).

It should be noted that the use of only informative parameters for describing $A–D–X$ systems not always increases the accuracy of prediction by pattern recognition algorithms having different ideologies. This conclusion is supported by the results of both visualization with the detected most important attributes and examination recognition with cross-validation. From the standpoint of chemistry, this is related to the

[1] The procedure of cross-validation was described in detail in [34, 36].

**Table 1.** Prediction of the type of crystal structure of $AD_2B_2$ compounds

| Element *D* | Element *A* | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Y | La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu | Ac | Th | Pa | U | Np | Pu | Am |
| Fe | #1 | 1 | #4 | 4 | #5 | 1 | 1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | 1 | 4 | | 4 | | 4 | 1 |
| Co | #1 | #1 | #1 | #1 | #1 | 1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | 1 | 1 | 1 | 1 | 4 | 1 | 1 | 1 | 1 | 1 |

**Table 2.** Prediction of the type of crystal structure of $AD_2Al_2$ compounds

| Element *D* | Element *A* | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Ca | Sr | Y | Ba | La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu | Ac | Th | Pa | U | Np | Pu | Am |
| Zn | #1 | 1 | | 1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | #1 | | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Au | 3 | #3 | 3 | 3 | #3 | #3 | #3 | #3 | 3 | #3 | #3 | #3 | #3 | #3 | 3 | 3 | 3 | 3 | 3 | 3 | #3 | 3 | #3 | 3 | 3 | 3 |

fact that the possibility of formation and the type of crystal structure of a compound are determined by a set of the properties of all compound components rather than by the parameters of only two of them. Therefore, when training a computer and predicting new compounds, we decided to use a set of the initial properties of elements *A*, *D*, and *X* in combination with the most informative parameters found using IAS.

Tables 1–9 present some results for predicting the type of crystal structure of $AD_2X_2$ ($X$ = B, Al, Si, P, Ga, Ge, As, Sn, Sb) compounds under normal conditions. We used the following designations: 1, $AD_2X_2$ compound with a $ThCr_2Si_2$-type crystal structure; 2 and 3, the same with $CaAl_2Si_2$- and $CaBe_2Ge_2$-type structures, respectively; 4, compound with a structure that differs from those given in 1–3; 5, no $AD_2X_2$ compounds. Symbol # indicates the systems studied earlier and used for computer training. Blank cells indicate conflicting predictions obtained at stages 2–4.

An analysis of Tables 1–9 demonstrates that a $ThCr_2Si_2$-type of crystal structure is characteristic of $AD_2X_2$ compounds in which $X$ = Si, P, Ga, Ge, or As, under normal conditions (Fig. 2). A $CaAl_2Si_2$-type of structure is much rare (Fig. 2): it is most often detected in $AD_2X_2$ ($X$ = As, Sb) pnictides under normal conditions. This structure is not predicted for compounds with boron, aluminum, and tin, although a $CaAl_2Si_2$-type of structure was experimentally detected in

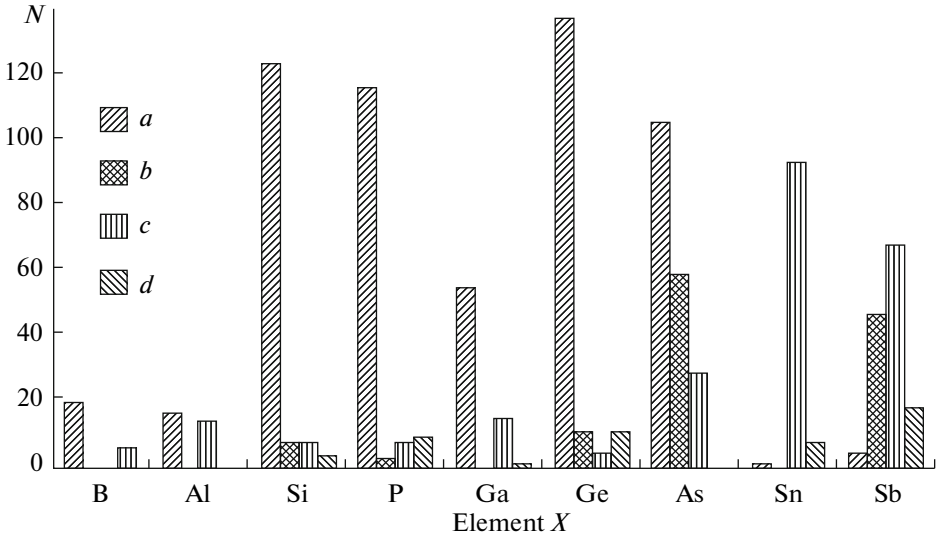


**Fig. 2.** Distribution diagram for the structure types of (*a*)–(*c*) intermetallics $ThCr_2Si_2$, $CaAl_2Si_2$, and $CaBe_2Ge_2$, respectively, and (*d*) another structure for the predicted intermetallics of composition $AD_2X_2$ ($X$ = B, Al, Si, P, Ga, Ge, As, Sn, Sb).

**Table 3.** Prediction of the type of crystal structure of $AD_2Si_2$ compounds

| Element *D* | Element *A* | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Ca | Sc | Sr | Y | Zr | Ba | La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu | Hf | Ac | Th | Pa | U | Np | Pu | Am |
| Al | #2 | | #2 | #2 | 5 | #4 | #2 | #2 | #2 | #2 | 2 | #2 | #2 | #2 | #2 | #2 | #2 | #2 | 2 | #2 | 2 | 5 | 2 | 2 | | #4 | | | |
| Cr | | 1 | 1 | #1 | 5 | 1 | | #5 | | #1 | 1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #5 | 1 | #1 | 1 | #1 | #1 | #1 | 1 |
| Mn | #1 | 1 | #1 | #1 | | #1 | #1 | #1 | #1 | #1 | 1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 5 | 1 | #1 | 1 | #1 | #1 | #1 | 1 |
| Fe | #5 | #4 | 1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #4 | 1 | #1 | 1 | #1 | #1 | #1 | 1 |
| Co | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | 1 | #1 | #1 | #1 | 1 |
| Ni | #1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | 1 | #1 | #1 | #1 | 1 |
| Cu | #1 | #1 | #1 | #1 | | #1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | | 1 | #1 | 1 | #1 | #1 | #1 | 1 |
| Zn | #1 | | #1 | 1 | | #1 | 1 | 1 | 1 | #1 | 1 | 1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Ru | 1 | 1 | | #1 | | | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | | 1 | #1 | 1 | #1 | #1 | #1 | 1 |
| Rh | 1 | 1 | | 1 | 1 | #4 | 1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | 1 | 1 | #1 | 1 | #1 | #1 | #1 | 1 |
| Pd | #1 | 1 | #1 | #1 | 1 | 1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | 1 | #1 | 1 | #1 | #1 | #1 | 1 |
| Ag | #1 | 1 | #1 | 1 | | #1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | 1 | 1 | 1 | 1 | 1 | #1 | 1 | | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Os | | 1 | | #1 | 5 | 4 | #1 | #1 | #1 | #1 | 1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | | 1 | #1 | 1 | #1 | #1 | #1 | 1 |
| Ir | | 1 | 4 | #1 | | #4 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | 1 | 1 | #1 | 1 | 1 | 1 | | 1 | 1 | | 3 | #3 | #3 | |
| Pt | #3 | | 4 | #3 | | #4 | 1 | 3 | #3 | 3 | | #3 | #1 | 3 | #3 | #1 | #3 | 3 | | 1 | | 1 | | | * | #1 | #3 | #3 | 3 |
| Au | #1 | 1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | 1 | 1 | 1 | #1 | 1 | #1 | #3 | #1 | 1 |

**Table 4.** Prediction of the type of crystal structure of $AD_2P_2$ compounds

| Element *D* | Element *A* | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Li | K | Ca | Rb | Sr | Y | Zr | Cs | Ba | La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu | Hf | Ac | Th | Pa | U | Np | Pu | Am |
| Mn | 1 | 1 | #2 | 1 | 1 | | 5 | 1 | #1 | | | | | | 1 | #2 | | | | | | | | | | 1 | | | | | | 1 |
| Fe | 1 | #1 | #1 | #1 | #1 | 1 | | 1 | #1 | #1 | #1 | #1 | 1 | 1 | 1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | | 1 | | 1 | #1 | 1 | 1 | 1 |
| Co | 1 | #1 | #1 | #1 | #1 | 1 | | 1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | #3 | 3 | #3 | 3 | | 1 |
| Ni | #1 | 1 | #1 | 1 | #4 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | 1 | 1 | | 1 | #1 | 1 | 1 | 1 |
| Cu | #1 | 1 | #1 | | #1 | | #2 | | #1 | | | | | | | #1 | | | | 1 | 1 | | | | #2 | | #2 | | #2 | | | |
| Ru | 1 | #1 | #1 | #1 | #1 | #1 | | 1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | 1 | 1 | 1 | #4 | 4 | | 1 | 1 | 1 |
| Rh | 1 | #1 | #1 | #1 | #1 | 1 | 1 | #1 | #1 | #3 | #3 | #3 | #3 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 3 | 4 | 4 | 3 | 3 | 3 | 3 |
| Pd | 1 | 1 | #1 | 1 | #1 | #1 | 1 | 1 | 1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Os | 1 | 1 | 4 | 1 | #1 | 1 | 1 | 1 | #1 | | | | | 1 | | #1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 4 | | 4 | 4 | | | | |
| Ir | 1 | #1 | #4 | #1 | #4 | | | #1 | #1 | | | | | 4 | | #4 | | | | | | | | 1 | 1 | 1 | 4 | | | | | |

**Table 5.** Prediction of the type of crystal structure of $AD_2Ga_2$ compounds

| Element *D* | Element *A* | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Sr | Y | La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu | Ac | Th | Pa | U | Np | Pu | Am |
| Al | 1 | #1 | #1 | #1 | #1 | #1 | 1 | 1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | #1 | 5 | 1 | 1 | 1 | | 1 | 1 | 1 |
| Zn | 1 | 1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | 1 | #1 | #1 | 1 | 1 | 1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Pd | 4 | 3 | #3 | #3 | 3 | 3 | 3 | #1 | 1 | 3 | 3 | 3 | 3 | | | 1 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | |
| Cd | #1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |

**Table 6.** Prediction of the type of crystal structure of $AD_2Ge_2$ compounds

| Element *D* | Element *A* | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Ca | Sr | Y | Ba | La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu | Ac | Th | Pa | U | Np | Pu | Am |
| Al | #2 | #2 | #2 | 2 | #2 | #2 | #2 | #2 | 2 | #2 | #2 | #2 | #2 | #2 | #2 | #2 | #2 | #2 | #2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |
| Mn | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | 1 | #1 | #1 | 1 | 1 |
| Fe | 1 | 1 | #1 | 1 | #1 | #1 | #1 | #1 | 1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | 1 | #1 | 1 | #1 | #1 | 1 | 1 |
| Co | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | 1 | #1 | 1 | 1 | 1 |
| Ni | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | 1 | #1 | 1 | 1 | 1 |
| Cu | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | 1 | #1 | 1 | #1 | 1 | 1 | 1 |
| Zn | #1 | #1 | 1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Ru | #1 | 1 | #1 | | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | 1 | 1 | 1 | 1 | 1 |
| Rh | 1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | #1 | 1 | 1 | #1 | 1 | #1 | #1 | 1 | 1 |
| Pd | 1 | #1 | 1 | #1 | #1 | #1 | 1 | #1 | 1 | #1 | #1 | #1 | 1 | #1 | #1 | 1 | 1 | 1 | 1 | 1 | #1 | 1 | #1 | #1 | 1 | 1 |
| Ag | #1 | #1 | 1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Os | | 1 | | 4 | | | | | | | 1 | | | | | | 1 | 1 | 1 | | #1 | 1 | 1 | 1 | 1 | |
| Ir | 1 | #1 | 1 | #4 | #3 | #3 | #3 | #3 | 4 | #3 | #1 | #4 | #3 | 3 | 3 | 3 | | 1 | | | #1 | 1 | #1 | | | 3 |
| Pt | #4 | #1 | #4 | #1 | #4 | 4 | #4 | #4 | 4 | #4 | #4 | #4 | #4 | #4 | #4 | 4 | 4 | 4 | 4 | 4 | #1 | 1 | #1 | 1 | 1 | 4 |
| Au | #1 | #1 | 1 | #4 | 1 | 1 | 1 | #1 | 1 | 1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | #1 | 1 | 1 | | 1 | 1 |

17 compounds with aluminum and information on this fact was used to train a computer. A $CaBe_2Ge_2$-type of structure is most often predicted for intermetallics with arsenic, tin, and antimony. New compounds with $CoSc_2Si_2$- and $FeMo_2B_2$-type of structures are not predicted for the combinations of elements given in Tables 1–9.

## CONCLUSIONS

(1) Using precedent-based pattern recognition methods, we predicted several hundred new $AD_2X_2$ intermetallics in $A$–$D$–$X$ systems, where $A$ and $D$ are various chemical elements and $X$ = B, Al, Si, P, Ga, Ge, As, Sn, or Sb, and found the types of their crystal structures under normal conditions. The predicted compounds are promising for searching for new magnetic materials.

(2) It is shown that a $ThCr_2Si_2$-type of structure is characteristic of $AD_2X_2$ compounds in which $X$ = Si, P, Ga, Ge, or As. A $CaAl_2Si_2$-type of structure is most often in $AD_2X_2$ ($X$ = As, Sb) pnictides under normal conditions. A $CaBe_2Ge_2$-type of structure is most often predicted for $AD_2X_2$ ($X$ = As, Sn, Sb) compounds.

**Table 7.** Prediction of the type of crystal structure of $AD_2As_2$ compounds

| Element *D* | Element *A* | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | K | Ca | Rb | Sr | Y | Cs | Ba | La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu | Ac | Th | Pa | U | Np | Pu | Am |
| Cr | 1 | #1 | 1 | #1 | 1 | 1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | | | | | | | | |
| Mn | 1 | #2 | 1 | #2 | 1 | 1 | #1 | | | | | 2 | | #2 | 2 | 2 | 2 | 2 | 2 | 2 | #2 | 2 | 2 | | | | | | |
| Fe | #1 | #1 | #1 | #1 | 1 | #1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | 2 | 1 | 1 | | | | | 1 | 1 |
| Co | #1 | #1 | #1 | #1 | 1 | 1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | #3 | 3 | 3 | 3 | 1 | 1 |
| Ni | 1 | #1 | 1 | #1 | 1 | 1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | | #3 | 3 | | 1 |
| Cu | 1 | #1 | 1 | #1 | | 1 | #1 | 1 | | | | 1 | 1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 2 | 2 | #2 | 2 | 2 | 2 |
| Zn | | #2 | #1 | #2 | 2 | 1 | #4 | 2 | 2 | 2 | 2 | 2 | 2 | #2 | 2 | 2 | 2 | 2 | 2 | 2 | #2 | 2 | 2 | | 2 | 2 | 2 | 2 | 2 |
| Ru | #1 | #1 | #1 | #1 | 1 | #1 | #1 | #1 | 3 | 3 | 3 | 1 | | #1 | | 3 | 1 | 1 | 1 | 1 | 1 | | 1 | 3 | 3 | 3 | 3 | 3 | |
| Rh | #1 | 1 | #1 | #4 | 3 | #1 | #1 | #3 | #3 | #3 | #3 | 3 | 3 | #3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 1 | 3 | 3 | 3 | #3 | 3 | 3 | 3 |
| Pd | 1 | #1 | 1 | #1 | 1 | 1 | #1 | #1 | #1 | #1 | #1 | 1 | #1 | #1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | 1 | | | | | 1 | 1 |
| Cd | 2 | #2 | #2 | #2 | 2 | | #2 | 2 | 2 | 2 | 2 | 2 | 2 | #2 | 2 | 2 | 2 | 2 | 2 | 2 | #2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |

**Table 8.** Prediction of the type of crystal structure of $AD_2Sn_2$ compounds

| Element *D* | Element *A* | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Sr | Y | Ba | La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu | Ac | Th | Pa | U | Np | Pu | Am |
| Cu | #4 | 3 | 4 | #3 | #3 | #3 | #3 | | #3 | #4 | 3 | 3 | | | | | | | | | 3 | 3 | 3 | 3 | 3 |
| Rh | 4 | 3 | | 3 | #3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | | 3 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| Pd | 4 | | 1 | 3 | #3 | 3 | 3 | | 3 | 4 | 4 | | | | | | | | | 3 | 3 | 3 | 3 | 3 | 3 |
| Ag | #1 | 3 | #1 | 3 | 3 | 3 | 3 | | 3 | 4 | 3 | 3 | | | | | | | | 3 | 3 | 3 | 3 | 3 | 3 |
| Ir | | 3 | | 3 | #3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| Pt | 3 | 3 | | 3 | #3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | | | 3 | 4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |

**Table 9.** Prediction of the type of crystal structure of $AD_2Sb_2$ compounds

| Element *D* | Element *A* | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Ca | Sr | Y | Ba | La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu | Ac | Th | Pa | U | Np | Pu | Am |
| Mg | #2 | #2 | 2 | #2 | | | | | | 2 | #2 | | | 2 | 2 | 2 | 2 | #2 | 2 | 2 | | | | | | 2 |
| Mn | #2 | #2 | 4 | #1 | | | | | 2 | 2 | #2 | 5 | 5 | | 5 | 5 | | #2 | 5 | 4 | 4 | 4 | 4 | | | |
| Fe | | | 4 | 1 | #4 | | #4 | #4 | | 4 | | | | 5 | 5 | #5 | 5 | | | 4 | | | | | | |
| Ni | | #1 | | 1 | #1 | | | #1 | 3 | 3 | #1 | 3 | #3 | #3 | #3 | #3 | 3 | | 3 | 1 | | 3 | | | | |
| Cu | 3 | #3 | 3 | 3 | 3 | #3 | #3 | 3 | 3 | 3 | #3 | #3 | 3 | 3 | 3 | 3 | 3 | 3 | | | 3 | 3 | 3 | 3 | 3 | 3 |
| Zn | #2 | #2 | 2 | #4 | 2 | 2 | 2 | 2 | 2 | 2 | #2 | 2 | 2 | 2 | 2 | 2 | 2 | #2 | 2 | | | | | | 2 | 2 |
| Rh | 1 | | | 1 | #1 | #1 | #1 | #1 | | | | | | | | | | | | | | | | | | |
| Pd | 3 | #3 | 3 | 3 | #3 | #3 | #3 | #3 | 3 | #3 | #3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | | 3 | 3 | 3 | 3 | 3 | 3 |
| Cd | #2 | #2 | 2 | #2 | 2 | 2 | 2 | 2 | 2 | 2 | #2 | 2 | 2 | 2 | 2 | 2 | 2 | #2 | 2 | 2 | 2 | | | 2 | 2 | 2 |
| Pt | 3 | #3 | | 3 | #4 | #4 | #4 | 4 | 4 | 3 | #4 | 4 | 4 | 4 | 4 | | | | 3 | 4 | 4 | 4 | 4 | | | 4 |
| Au | | | 3 | #4 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | | 3 | 3 | 3 | 3 | 3 | 3 |

(3) The parameters of elements in positions *A* and *D* (i.e., the Mendeleev–Pettifor numbers, the pseudopotential radii, and their algebraic functions) were found to mainly determine the possibility of formation of $AD_2X_2$ compounds and the type of their crystal structure.

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