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THEORETICAL
INORGANIC CHEMISTRY

Prediction of New $A^{3+}B^{3+}C^{2+}O_4$ Compounds

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Abstract—Hitherto unprepared $ABCO_4$ compounds (where A and B stand for tervalent metals ($r_A \geq r_B$) and C stands for a divalent metal) are predicted. Criteria are found to predict the possibility for these compounds to crystallize in some type of structure (K_2NiF_4, $CaFe_2O_4$, $YbFe_2O_4$, or spinel) at room temperature and atmospheric pressure. The prediction is based only on the properties of elements and simple oxides. A special software system for computer-aided analysis of information is used for calculations involving pattern recognition based on use case.

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Oxide compounds of composition $A^{3+}B^{3+}C^{2+}O_4$ ($r_A \geq r_B$) are promising for search for new magnetic [1–3], dielectric [4], superconducting [5], and other functional materials [6, 7]. These compounds are well studied [8–13]. A number of reviews over the methods for their preparation and properties have been published [14–20]. The "Phases" database [21] compiles information on about 800 compounds of this composition, most of them (281 compounds) having K_2NiF_4 type crystal structures (space group $I4/mmm$, $Z = 2$) (Fig. 1); 102 compounds have spinel structure (space group $Fd\bar{3}m$, $Z = 8$), 89 compounds have $YbFe_2O_4$ structure (space group $R\bar{3}m$, $Z = 3$), and 57 compounds have $CaFe_2O_4$ structure (space group $Pnam$, $Z = 4$). There are far less $A^{3+}B^{3+}C^{2+}O_4$ compounds that have other (e.g., olivine or hausmannite) crystal structures. However, the number of possible compounds of the above composition is several orders of magnitude larger than the number of already studied compounds. Therefore, the aim of this study is to predict the $ABCO_4$ compounds not yet prepared in A_2O_3–B_2O_3–CO system.

THEORETICAL ANALYSIS

Numerous attempts to find a criterion for predicting the possible formation of $A^{3+}B^{3+}C^{2+}O_4$ compounds with certain types of crystal structures that would include only data on the parameters of the constituent elements, involved information on the ionic radii of divalent and tervalent cations in these compounds, or ratios of these radii. Attempts were also made to find a correlation between the crystal-structure types of compounds where A = Sc, In, Y, or Ln and B = Fe, Ga, Cr, or Al and the divalent cation radius [16, 22]. Ganguly [15] and Pajaczkowska and Gloubokov [20] used cation radius ratios to predict compounds with K_2NiF_4 and β-K_2SO_4 type structures. Beznosikov [23–25] proposed to use cationic and anionic radii and their ratios for predicting crystal structure type for $ABCX_4$ compounds. Patel et al. [11] used the well-known Goldschmidt's tolerance factor for predicting compounds having K_2NiF_4 type structures. Zvereva et al. [18] pointed to the insufficiency of this criterion for predicting the structure types of oxides, and proposed to take into account the thermochemical parameters of an $A^{3+}B^{3+}C^{2+}O_4$ compound, such as the enthalpy of formation. Gerardin et al. [26] proposed the criterion $1/2(r_{A(3+)} + r_{C(2+)}) + r_{O(2-)}$ for predicting rhombohedral structure; the limitations of this criterion were noticed by Kimizuka et al. [16]. Our calculations were performed using all of the aforemen-

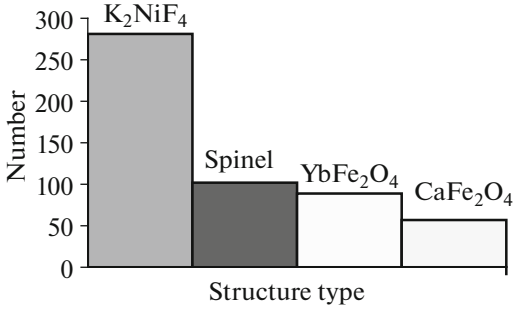

Fig. 1. Bar diagram showing the abundances of crystal structure types for $A^{3+}B^{3+}C^{2+}O_4$ compounds.

tioned criteria (except for the criterion that includes data on the enthalpy of formation of the $ABCO_4$ compound [18]) and visual analysis of the location of points in the spaces of ionic radii (according to Shannon) and their ratios, as well as information on crystal structure types for about 800 $A^{3+}B^{3+}C^{2+}O_4$ compounds from the "Phases" database [21]. These calculations showed that none of the proposed criteria based solely on taking into account ion sizes could provide a sufficiently good separation of the existing compounds by the structure type. It became clear that, in order to improve the prediction accuracy, the criteria should comprise not only dimensional parameters but also other properties of chemical elements and simple oxides. However, the search for such multidimensional criteria is extremely complex; therefore, methods for detecting complex patterns involving pattern recognition based on use case were used earlier [27] for predicting new $Ln^{3+}Cu^{3+}C^{2+}O_4$ compounds and the possibility of their crystallization in K_2NiF_4 type structure.

METHODS OF CALCULATION

We used our developed information analysis system (IAS) [28]. The IAS comprises databases for the properties of inorganic compounds and materials and an information analysis subsystem based on pattern recognition by use case. The IAS operation procedure is described in detail in [29].

The initial information for computer-aided analysis was found in the "Phases" database [21], which is part of the IAS. Before being included in the sample for computer training, the information was subjected to a thorough expert evaluation. The goal of the evaluation was to exclude erroneous data that could in future reduce the reliability of prediction. This stage is the most time-consuming and long-lasting. In carrying out this work, we attempted to partially automate the procedure for searching for erroneous data. In the context, the error means an erroneous classification of a chemical system (for example, the researchers pointed out that there is a compound of a certain composition under given conditions, but actually a solid solution is formed at this ratio of the components).

The sample for computer analysis (training sample) is a matrix, where each line contains a set of values of component properties, selected by the expert, of the compound of a particular composition, with an indication of one of the previously known classes (for example, a class of chemical systems with the formation of a compound of a certain composition, or a class of compounds with a certain type of crystal structure, etc.) to which the compound belongs. In this case, conditionally erroneous can be considered a compound belonging to some class, the values of component properties of which differ substantially from the values of component properties of compounds of the same class. The software system developed by us identifies compounds that fall into the "alien" class and provides the chemist with data for the expert evaluation of information on this compound and for deciding on its status. The principal possibility of finding such an experimental errors is connected with the periodicity in properties of inorganic compounds depending on the atomic number of the component elements of chemical systems. Although these dependences are extremely complex and cannot yet be described analytically, the consequence of this periodicity in variation of properties is the "compact" sets of compounds of a certain class where the values of component properties differ only insignificantly.

The software error detection system was based on the use of three known statistical criteria, which allow finding outlying values, namely, the rule of three sigmas [30], Grubbs's criterion [31], and Dixon's criterion [32]. The search for "erroneous" compounds was carried out separately for each class. The assignment of the compound to a given class was considered erroneous when at least two statistical criteria for a certain property of a component classified it as such. We also took into account the number of properties of the components for which the material was classified as erroneous (the larger this number, the greater the probability of error). The result of the work of the software system was a list of compounds whose component properties differed most strongly from the properties of the components of most compounds of this class. As a rule, the number of such compounds was an order of magnitude smaller than the initial set obtained from the database, which significantly shortened the time for subsequent review by the expert.

Next, the expert carefully analyzed the list of compounds obtained using information from the full texts of articles, monographs, and reference books included in the Database "Phases", as well as the opinions of other persons skilled in the art. The task of this analysis was to determine whether the identified "erroneous" compound (1) is unique (for example, a representative of a new class of compounds that have just begun to be studied, or a class of compounds that are poorly studied for some reasons (complex production technology, expensive and rare components)); (2) the error is related to the incorrect value of component properties (for example, incorrect interpolation or calculation of the properties of the element or simple compound); or (3) a real mistake in classifying the compound as belonging to a certain class. The result of the above analysis was the exclusion of information about 10% of the experimentally studied compounds from the sample for computer training.

An important step in the preparation of data for computer analysis is the selection of the properties of components (chemical elements and simple oxides). The initial property sets were formed on the basis of physicochemical concepts of the nature of the classes of compounds under consideration. Information about the properties of the elements was obtained from

the "Elements" database developed by us (http://phases.imet-db.ru/elements), and information on oxides was obtained from the database on the properties of simple oxides included in the IAS. The properties of components most important for the classification were selected using a special software, which is part of the IAS [33]. Not only the component properties, but also automatically generated algebraic functions of these properties were evaluated, which greatly simplified the subsequent formation of the required criteria. The result of these programs was finding of the most informative component parameters for classification.

To find the formation criteria for $ABCO_4$ compounds in A_2O_3–B_2O_3–CO systems and the criteria for predicting the type of their crystal structure under normal conditions, we used a suite of 15 image recognition programs by use case, incorporated into the IAS [28]. For assessing the prediction accuracy of the criteria, we employed a popular sliding control procedure, which is widely used for these purposes; for its details, see [34, 35]. As a result, the most accurate pattern recognition algorithms were selected.

Due to the specifics of the algorithms, the selected pattern recognition programs mutually complement each other, giving exact results for different sets of compounds. Therefore, the procedure for making a collective decision based on special programs of the IAS [28, 34] is used to form a generalized criterion that would use the advantages of various algorithms. For assessing the accuracy of the criteria obtained using these programs, we used the examination recognition of information on 100 compounds, the data about which were randomly selected from training samples and were not used in computer training (at the final prediction stage, these test cases were returned to the sample for analysis). As a result, generalized criteria were found for the formation of $ABCO_4$ compounds belonging to different classes. The thus-found criteria comprise only the component properties and can have various forms (Boolean expression, a set of equations or inequalities, a neural or growing pyramidal network, etc.). A special subsystem of the IAS was used to automate the forecasting procedure. This subsystem substitutes the values of the properties of components in the found criteria, predicts the belonging of the compound to a given class, and outputs the results in a tabular form, which is customary for chemists.

The task of predicting new $ABCO_4$ compounds in A_2O_3–B_2O_3–CO systems included solving three intermediate problems. In the first of them (problem 1), the formation of $ABCO_4$ compounds was predicted. The next problem involved the search for criteria and the prediction of formation of compounds of this composition with the most common types of crystal structures (K_2NiF_4, $YbFe_2O_4$, spinel, or $CaFe_2O_4$). The last problem was divided into two. In solving the first of them, we conducted a multi-class prediction of belonging to one of the following six classes: compounds having (1) K_2NiF_4, (2) $YbFe_2O_4$, (3) spinel, or (4) $CaFe_2O_4$ structure; (5) compounds having structures other than above; and (6) systems having no $A^{3+}B^{3+}C^{2+}O_4$ compounds (problem 2). Then, four problems were solved (for targeted K_2NiF_4, $YbFe_2O_4$, spinel, and $CaFe_2O_4$ classes) for consecutively separating the oxide systems into three classes: e.g., targeted class 1: K_2NiF_4; class 2: compounds having structures other than K_2NiF_4; and class 3: no $A^{3+}B^{3+}C^{2+}O_4$ compounds in the A_2O_3–B_2O_3–CO system (four problems 3). All forecasts were for atmospheric pressure and room temperature. The final decision on the class to which the predicted compound belongs was made on the basis of a comparison of the predictions obtained in solving all problems. When the results contradicted each other, the prediction was considered uncertain, and an empty position was left in the corresponding prediction table.

CALCULATIONS

After the expert evaluation, the sample for computer analysis included information on 255 $A^{3+}B^{3+}C^{2+}O_4$ compounds having K_2NiF_4 structure, 102 compounds having spinel structure, 82 compounds having $YbFe_2O_4$ structure, 56 compounds having $CaFe_2O_4$ structure, 124 compounds whose crystal structure under ambient temperature and pressure differed from the above structures, and 63 A_2O_3–B_2O_3–CO systems in which $ABCO_4$ compounds are not formed.

The initial set of component parameters included the following properties of chemical elements A, B, and C (for the values of properties, see the "Elements" database: http://phases.imet-db.ru/elements): pseudopotential radius (according to Zangger); ionic radius (according to Shannon); distances to internal and to valence electrons (according to Schubert); ionization energies of the first, second, and third electrons (E5–E7); Mendeleev–Pettyfor numbers (M1–M11); the group number in the Periodic Table; quantum number (A5); the number of valence electrons; electronegativity (by Pauling) (E2); Midema chemical potential; melting and boiling temperatures; standard entropy; standard enthalpy of atomization; thermal conductivity; molar heat capacity, etc., as well as thermal parameters of simple oxides of divalent and tervalent elements (melting (decay) point, standard entropy (S), standard heat of formation, isobaric heat capacity, and isobaric potential of formation), altogether 134 values for each A–B–C–O system.

RESULTS AND DISCUSSION

First, the hypothesis was tested that the set comprising a limited number of even most "informative" parameters found with the help of the program [33],

the components, and algebraic functions of these parameters fails to provide a sufficiently good separation between A_2O_3–B_2O_3–CO systems where $ABCO_4$ compounds are formed and where they are not formed, and the separation of the latter with respect to the crystal structure type. Conclusions were made on the basis of a comparison of the results of examination recognition and analysis of the projection points in the spaces of most "informative" component parameters.

Calculations showed that S(B)/S(C) and M9(O)/M6(B) are the most important algebraic functions for the classification of A_2O_3–B_2O_3–CO systems with and without $ABCO_4$ compounds. The highest accuracy of examination forecasting in the sliding control mode (94.5%) was achieved in the case of a criterion obtained using the linear machine algorithm. On the projection the coordinates of which were these parameters, more than half the points corresponding to A_2O_3–B_2O_3–CO systems without $ABCO_4$ compounds were in the regions of high values of S(B)/S(C) and M9(O)/M6(B). Nevertheless, it was not possible to achieve a sufficiently complete separation of the classes of systems with and without compounds of the indicated composition. Therefore, computer experiments were conducted to find more classified sets of components. The criteria that include only the properties of chemical elements and were formulated as a result of the work of pattern recognition programs (algorithms for learning the neural network, the *k*-nearest neighbors and support vectors methods), provided the highest prediction accuracy in the sliding control mode (95.4, 96.7 and 96.9%, respectively). The further application of the collective decision-making program for the three above-mentioned algorithms based on the Bayesian method gave the best estimate of the prediction accuracy, namely, 98%.

An attempt to separate $ABCO_4$ compounds having different crystal structure types using only the most classified functions (E2(A)/E2(B), M10(A)/M5(B), S(A)-S(B), and E7(A)/E7(B)), which were found as a result of calculations, did not lead to a satisfactory separation between compounds with different types of structures. The highest accuracy (64.5%) of estimation in the sliding control mode was obtained for the *k*-nearest neighbors algorithm. Visual analysis of all constructed projections also indicated a significant overlap of the compounds with different types of crystal structures. When only the properties of elements were included in the sought-for criterion and when the algorithms based on the methods of constructing logical regularities, *k*-nearest neighbors, support vectors, and training of the neural network were used to form the criterion, it became possible to obtain much more accurate results (reliability of the results of sliding control was 83.7, 85.8, 84.7 and 87.1%, respectively). The application of the set of the above algorithms and the generalized polynomial corrector for collective decision making increased the prediction accuracy to 91%.

Similar results were obtained in solving problems 3. Using only the found "informative" properties did not allow us to achieve high prediction accuracy. When searching for a criterion that would allow us to separate $ABCO_4$ compounds with K_2NiF_4 type structure from compounds with other structures and from A_2O_3–B_2O_3–CO systems with no $ABCO_4$ compounds, we obtained the highest prediction accuracy (95%) when using the collective algorithms that combined the training of a neural network, *k*-nearest neighbors and support vectors methods, and the committee method (averaging) to make a collective decision. The criterion comprised only the properties of the elements. For the target class of compounds having $CaFe_2O_4$ type structure, the most classified criterion (99% accuracy) also included only the properties of elements and was obtained as a result of using collective algorithms (training a neural network, a linear machine, *k*-nearest neighbors, and support vectors methods) and the template method for making a collective decision. For separating $ABCO_4$ spinels from compounds having other structures and from systems where compounds of this composition are not formed, it was necessary to additionally include the properties of simple oxides into the criterion. The accuracy of the criterion obtained by the use of the collective pattern recognition algorithms (training a neural network, *k*-nearest neighbors, and support vectors methods) using the Bayes method to make a collective decision, reached 95%. It was only in solving the problem of separating the compounds having $YbFe_2O_4$ structure and the compounds having other crystal structures that the most classified criterion included, in addition to the properties of elements and simple oxides, the most "informative" parameters M5(3)/M6(1) and A5(2)/A5(3). In this case, where we used the collective algorithms based on training a neural network, a linear machine, *k*-nearest neighbors, and support vectors methods, and the majority voting committee method for making a collective decision, we attained 95% prediction accuracy.

The formulated criteria were used to predict the possibility of formation and crystal-structure type under the ambient conditions for yet-to-prepare compounds. Tables 1–4 show selected results of comparison of the forecasts obtained in solving all three of the classification problems. The following notations are used in the tables: K—forecasts of compounds having K_2NiF_4 crystal structure; C—forecasts of compounds having $CaFe_2O_4$-type crystal structure; S—forecasts of compounds having spinel structure; Y—forecasts of compounds having $YbFe_2O_4$ crystal structure; A—forecasts of compounds having crystal structures other than listed above; and N—forecasts of the absence of an $ABCO_4$ compound in the A_2O_3–B_2O_3–CO system. The # symbol denotes previously studied systems, information about which is used for computer training.

Table 1. Predicted crystal-structure types for $ABCO_4$ (C = Mg, Mn, or Ca) compounds

$ABMgO_4$

A / B	Sc	V	Mn	Fe	Ga	Y	Rh	In	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Am
Al	#Y		S		S	Y		#Y					Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Sc	#C							S									N	N			N			
V		#S	S	#S			S	S							Y	Y	Y	Y	Y	Y	Y	Y	Y	
Cr		S	S		S		S	#S					Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	
Mn	Y		#A	S			S			A		A	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Fe			S	#S			S	#S	#A				Y	Y	Y	Y	Y	Y	Y	#Y	#Y	#Y	#Y	
Ga	#Y	S	#S	S		#Y		#Y	#N				Y	Y	Y	Y	Y	Y	#Y	#Y	#Y	#Y	#Y	Y
Y									N	N	N	N		N	N		N	N	N					
Rh							#S	S							Y		Y	Y	Y	Y	Y	Y	Y	
In								#S				N				Y	Y	Y	Y	Y	Y	Y	Y	

$ABMnO_4$

A / B	Sc	V	Cr	Mn	Fe	Y	Rh	In	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Am
Al	Y	S	S	S	#S	#Y	S	#Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	#Y	#Y	#Y	#Y	#Y	Y
Sc	A			A				A						A										
V	Y	#S		S	S	Y	S		Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Cr	Y	S	#S	A	S	Y	S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Fe				A	#S	#Y	S	#Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	#Y	#Y	#Y	#Y	Y
Ga	Y	S		S	#S	#Y	S	#Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	#Y	#Y	#Y	#Y	#Y	Y
Y									K	K	K	K												
Rh	Y					Y	#S			Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
In						Y		#S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y						Y

$ABCaO_4$

A / B	Sc	V	Mn	Fe	Y	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Am
Al	K				#K	#K	#K	#K	#K	K	#K	#K	#K	#K	#K	#K	#K	#K	#K	#K	K
Sc	#C				C	A					A										A
V	C	#C			A	K			K	K	K	K	K	K	K	K	K	K	K	K	K
Cr		C	C	C	#A	#A	#A	#A	#A	A	#A	#A	#A	#A	#A	#A	A	A	A	A	K
Mn	C		#C	C	K	#K	#K	#K	#K	K	#K	#K	#K	#K	#K	#K	K	K	K	K	K
Fe	#C		C	#C		#K	#K	#K	#K	K	#K	#K	#K	#K	#K	#K	K	K	K	K	K
Ga	A	A	A		#A	#A	#A	#A	#A	A	#A	#A	#A	#A	#A	#A	#A	#A	#A	A	A
Y						N				N			N	N	N	N					
Rh	C					K	K	K	K	K	K	K	K	K	K	K	K	K	K	K	K
In						A	A	A	A	A	A	A							C	A	

Table 2. Predicted crystal-structure types for $ABCO_4$ (C = Fe, Co, or Ni) compounds

$ABFeO_4$

A / B	Sc	V	Cr	Mn	Fe	Ga	Y	Rh	In	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Am
Al	#Y	S	S	S	S		Y	S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Sc												A	A												
V	Y	#S		S	S		Y	S		Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Cr	Y	S	#S	S	S	S	Y	S	S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Mn				#A	S		Y	S	#Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Ga	Y	S		#S	S	#S	Y	S	#Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	#Y	#Y	#Y	Y
Y							Y				K	K					N	N	N	N					
Rh	Y						Y	S	S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
In							Y		S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y

$ABCoO_4$

A / B	Sc	V	Cr	Mn	Fe	Ga	Y	Rh	In	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Am
Al	#Y	S	S	S	S		Y	S	#Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Sc										A	A	A													
V	Y	#S		S	S		Y	S	S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Cr	Y	S	#S	#S	#S	S	Y	S		Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Mn	Y			#A	S		Y	S	Y		Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Fe	Y			S	#S		#Y	#S	#S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	#Y	#Y	#Y	#Y	Y
Ga	Y	S		#S	S	#S	#Y	S	#Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	#Y	#Y	#Y	#Y	#Y	Y
Y										K	K	K					N	N	N	N					
Rh	Y						Y	#S	S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
In							Y		#S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y

$ABNiO_4$

A / B	Sc	V	Cr	Mn	Fe	Ga	Y	Rh	In	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Am
Al		S	S	S	S	S		S	#S																Y
Sc																						N	N		
V	Y	S		#S	#S		Y	S	S		Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y			
Cr	Y		#A	#S	#S	S	Y	S	#S		Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Mn	Y			#S	#S		Y		S		Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Fe				#S	#S		Y		#S		Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Ga	Y	S		S	S	#S	Y	S	#S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Y										K								N	N	N				
Rh	Y						Y	#A	S					Y		Y	Y	Y	Y	Y	Y	Y	Y	Y	
In							Y		#N																Y

Table 3. Predicted crystal-structure types for $ABCO_4$ (C = Cu, Zn, or Sr) compounds

$ABCuO_4$

A / B	Sc	V	Cr	Mn	Fe	Y	Rh	In	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Am
Al	#Y	S	S	S	S	Y	S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Sc	#N																							K
V	Y				S	Y	S		Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Cr	Y	A	#A	#S	S	Y			Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Mn	Y					Y	#S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Fe					#A	Y		#Y			Y	Y	Y	Y	Y		Y	Y	Y	Y	#Y	#Y	#Y	Y
Ga	#Y	S		#S	S	#Y	S	#Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	#Y	#Y	#Y	#Y	#Y	Y
Y						#N				K	K	K		K										K
Rh						Y	#A	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
In						Y		#N		Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y

$ABZnO_4$

A / B	Sc	V	Cr	Mn	Fe	Ga	Y	Rh	In	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Am
Al	#Y	S	S	S		S	Y	S	#Y	Y							Y	Y	Y	Y		Y		Y	Y
Sc	#A						A		A	A	A	A	A	A		S	A	A	A	A	A	A		A	S
V	Y	#S			#S		Y	S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Cr	Y	S	#S	#A	S	S	Y	S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Mn	Y			#A	#A		Y	S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Fe	Y			#A	#S		#Y	S	#Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	#Y	Y	#Y	#Y	#Y	Y
Ga	#Y	S		S	S	#S	#Y	S	#Y	Y				Y		Y	Y	Y	Y	#Y	#Y	#Y	#Y	#Y	Y
Y											A	A	S		S	S									S
Rh							Y	#S	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
In							Y		#A													Y	Y	Y	

$ABSrO_4$

A / B	Sc	V	Mn	Fe	Ga	Y	Rh	In	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Am
Al	K				A	#K			#K	#K	#K	#K	K	#K	#K	#K	#K	#K	#K	#K	#K	#K	K	K
Sc	#C					C		A	#A	#A	#A	#A	A	#A	#A								C	A
V	A	A	A	A		K	A		#K	#K	#K	#K	K	#K	#K	#K	#K	#K	#K	#K	#K	#K	#K	K
Cr		A	A	A	A	A	A		#K	#K	#K	#K	K	#K	#K	#K	#K	#K	#K	#K	K	K	K	K
Mn			#C	A		K	A		#N	#K	#K	#K	K	#K	#K	#K	#K	#K	#K	#K	K	K	K	K
Fe			A	#A		K	A		#K	#K	#K	#K	K	#K	#K	#K	#K	#K	#K	#K	K	K	K	K
Ga	K				#A	#K		A	#K	#K	#K	#K	K	#K	#K	#K	#K	#K	#K	#K	#K	#K	K	K
Y						#C										C	C	C	C					
Rh	A					K	#A	A	#K	K	K	K	K	K	K	K	K	K	K	K	K	K	K	K
In						A		#C	#A	A	#A	A	A	A	A	A	A	A	A	A		A		A

Table 4. Predicted crystal-structure types for $ABCO_4$ (C = Cd or Ba) compounds

$ABCdO_4$

A / B	Sc	V	Fe	Ga	Y	Rh	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Am
Al	Y		S	S	Y	S	Y				Y		Y	Y	Y	Y	Y	Y	Y		Y	
Sc	#S													S	S	S	S	S			S	S
V	Y	#S	S		Y	S					Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	
Cr	Y	S	S	S	Y	S		Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Mn	Y				Y	S		Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Fe	Y		#S		Y	S		Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Ga	Y	S	S	#S	Y	S	Y			Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Y							A	A	A	A				A	A	A						
Rh	Y				Y	#S					Y			Y	Y	Y	Y	Y	Y	Y	Y	Y
In					Y						Y	Y		Y	Y	Y	Y	Y	Y	Y		

$ABBaO_4$

A / B	Sc	V	Mn	Fe	Ga	Y	Rh	In	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Am
Al	K			#N	#A	K			#K	#K	#K	#K	K	#K	#K	#K	#K	#K	#K	#K	K	K	K	K
Sc	A					C			A	A	A	A		A							A			A
V		A	A	A		K	A	A	K	K	K	K	K	K	K	K	K	K	K	K	K	K	K	K
Cr	K	A	A	A	A	K	A	A	#K	#K	#K	#K	K	#K	#K	#K	#K	#K	#K	#K	K	K	K	K
Mn	K		#A	A		K	A	A	#K	#K	#K	#K	K	#K	#K	#K	#K	#K	#K	#K	K	K	K	K
Fe			A	#A		#K	A	A	#K	#K	#K	#K	K	#K	#K	#K	#K	#K	#K	#K	K	K	K	K
Ga				#A	#A	K		A	#A			#A							K	K	K	K		
Y						#C			C				C			C	C	C	C					
Rh						K	#A	A	K	K	K	K	K	K	K	K	K	K	K	K	K	K	K	K
In						A		#A	#A	A	A	#A	A	A		A	A	A	A	A			A	A

Analysis of the obtained tables of forecasts shows that the greatest number of new $ABCO_4$ compounds having K_2NiF_4 and $CaFe_2O_4$ type structures is predicted in systems with alkaline-earth metals (except for systems with magnesium). These systems do not typically form spinels and $ABCO_4$ compounds having $YbFe_2O_4$ type structure. These compounds are most often predicted in the systems where C = Mg, Mn, Fe, Co, Ni, Cu, Zn, or Cd.

An analysis of the results of calculations to evaluate the importance of component parameters for classifying the oxide compounds with respect to the crystal structure type or the possibility of formation under certain settings, shows that the inclusion, in the classification criteria, of only two or three parameters of elements or simple oxides (or algebraic functions of these properties) fails to ensure an acceptable accuracy of separating different classes of compounds compared to the use of a wide set of properties of the components. A possible explanation for this effect is due to the fact that, in the latter case, it is possible to take into account the features of compounds having different compositions, including those having a unique set of components. The use of pattern recognition methods involving use case automates the searching for such multidimensional criteria, predicting the yet-to-prepare compounds, and evaluating their properties.

The experimental errors in assigning compounds to the predicted classes are significant contributors to the reduced prediction accuracy. This study is the first attempt to partially automate the finding of such errors based on the use of pattern recognition ideas. However, the final decision on whether the experimental information detected by the artificial intelligence program is erroneous is to be taken by the chemist who trains the computer system.

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