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Review

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Cybernetic Prediction of Inorganic Compounds and its Correlation with Experiment

The reserves of most chemical elements of our planet are limited, therefore the use of many of them in a pure state is becoming economically injustified. In this connection chemical compounds may be considered as a natural and practically unlimited reserve of new materials. They often exhibit the properties which are not the characteristics of pure elements. So, for example, maximum critical temperature of superconductivity transition (T_C) known for chemical elements, equals 10 K (for niobium films) and maximum upper critical magnetic field $H_{c2} = 4$ KOe (for niobium) (SAVITSKIY, EFIMOV et al. 1976 a), while compounds with the structure A15 posses a $T_C = 23{,}4$ K (thin Nb_3Ge films) and Chevrel phase $PbMo_{5.1}S_8$ has the value of H_{c2} above 500 kOe (SAVITSKIY, EFIMOV et al. 1976 b). The best refractory substances with the melting temperature of 4215 °C is a solid solution of hafnium and titanium carbides. Compounds of nickel with titanium (53—57% Ni), gold with cadmium, copper with aluminium etc. exhibit the phenomenon of "mechanical memory" (SAVITSKIY 1972). A number of analogous examples may be cited, known to the specialists, deeling with the magnetic, semiconductor, luminescence and other branches of materials science.

Thus the use of chemical compounds to produce new materials is a trend of a modern materials science. The search for new inorganic compounds with a predetermined set of properties is one of the most important tasks of chemistry. Most commonly the problem is solved empirically. Modern theoretical physics and chemistry can only explain the reason of the phase formation. However, theoretical explanation of the phase formation usually proves to be restricted by the experimental data already known, while prediction of new phases of a predetermined type, based upon physical theories, remains rather problematic one.

On the other hand, a huge amount of experimental data available and a number of well established regularities should contain information about causality of phenomena of the phases' formation and their stability under given conditions. Therefore in 1967 we proposed a principcally new way of using the information available to establish the regularities and predict the character of interaction of components of physico-chemical systems (SAVITSKIY et al. 1968 a). Its basis consists in computer learning using the known experimental examples and data on chemical elements available.

Computer learning may be considered as a method of retrieving multidimensional interconnections between separate values of the properties of the components of various physico-chemical systems and the property to be predicted. As is known, almost all the properties of physico-chemical systems are determined by the nature of components. Certain quantitative conditions of the physico-chemical system often correlate with the determined intervals of changing component properties. This circumstance is widely used in various empirical rules. For example, the graphs of Darken-Gurry are widely known for estimation of solubility in a solid state. Shown

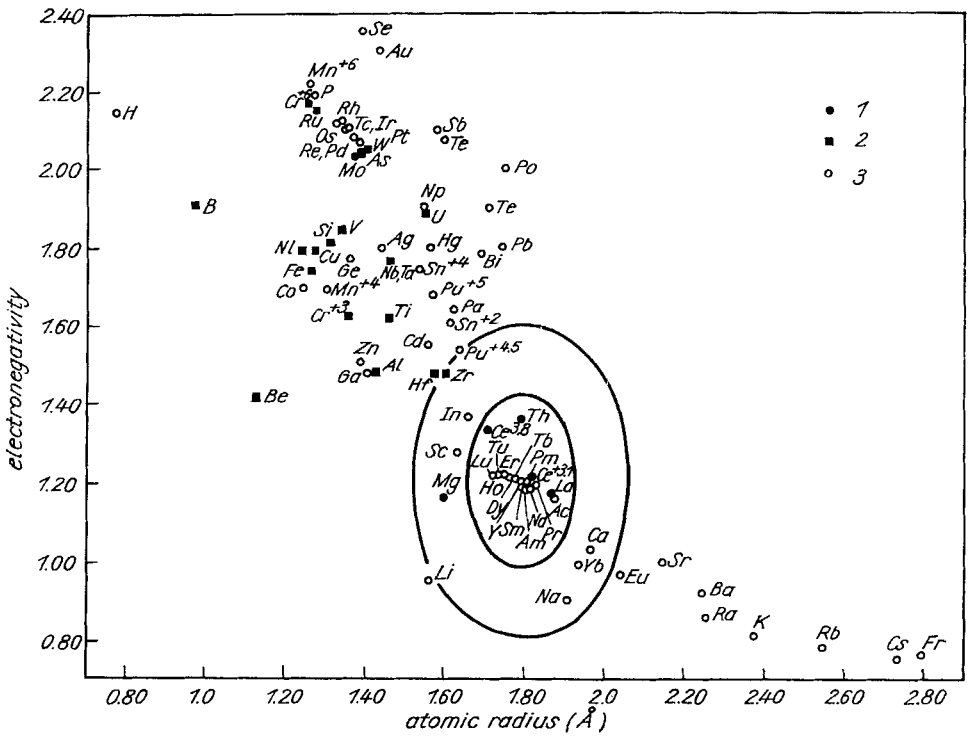

Fig. 1. Estimation of the mutual stability of yttrium with the other elements of Periodic system after DARKEN and GURRY (cf. TEREKHOVA, SAVITSKIY)

Figure 1 is such a graph of the solubility for yttrium (TEREKHOVA, SAVITSKIY). Within the limits of a small ellipse with the axes ($r = \pm 8\%$; $E = \pm 0.2$ units) the points are placed, corresponding to the elements forming a wide region of solid solutions with yttrium. Between the small and big ellipses with the axes ($r = \pm 15\%$; $E = \pm 0.4$ units) lie the points of the elements, forming the terminal solid solutions with yttrium, while beyond the big ellipse are those elements the dimensional and electrochemical factors of which are unfavourable for formation of solid solutions.

In crystal chemistry the two-dimensional graphs $r_A - r_B$ (r_A, r_B are atomic and cation radii of the components A and B, respectively) are widely used to reveal the regions of stability of various crystallographic structures. Numerous geometrical criteria are developed for the tolerance factors of existing of various types of crystalline structures (perovskites, pyrochlores, LAVES phases, A15 phases etc.). To classify the components according to their structural types the two-dimensional graphs $f_1(X_{1A}, X_{1B}) - f_2(X_{2A}, X_{2B})$ are widely used where f_1 and f_2 are some functions of the properties measured of the components X_{1A}, X_{1B}, X_{2A}, and X_{2B}. For example, in Figure 2 to separate the regions of stability of the crystalline structural types of the ternary chalcogenide compounds with the composition of AB_2X_4 the graph is used of the dependence of the force factor K_{AB} on the ratio between the cation radii r_A/r_B. Here

$$K_{AB} = \chi_A \chi_B / r_e^2$$

where χ_A and χ_B are the electronegativity factors of the cations A and B, respectively; r_e is some specifically determined equilibrium distance (IGLESIAS, STEINFINK). Even from this figure one may see, that the two dimensional graphs not only of the simple properties of the components, but also of their specially constructed functions do not

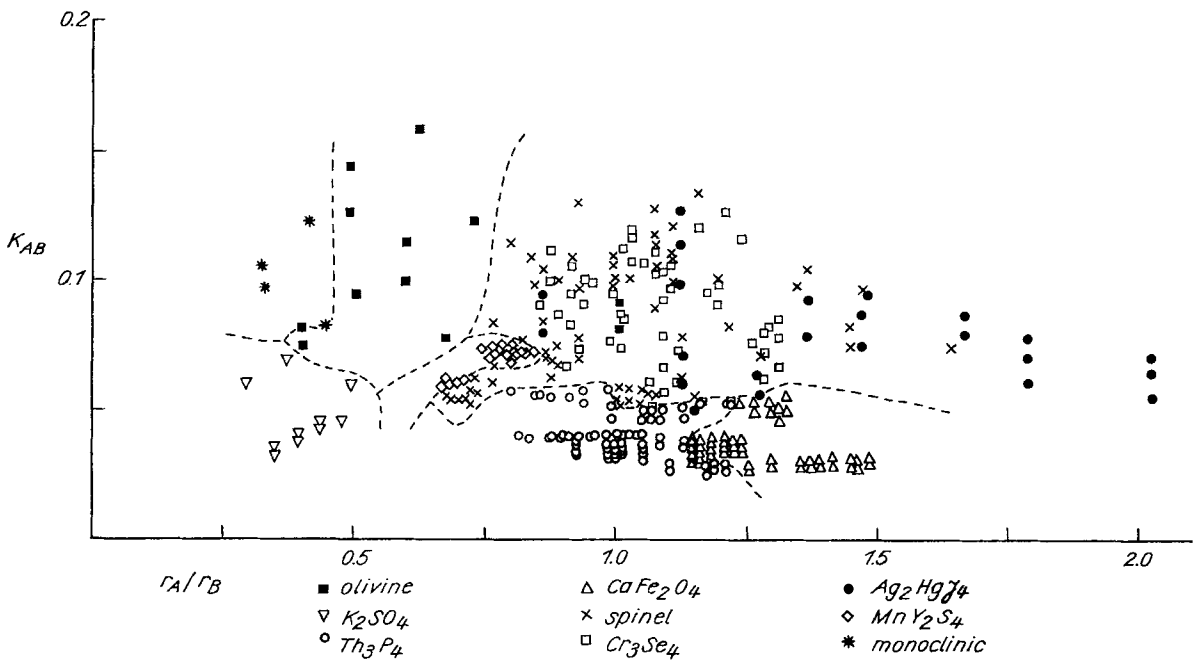

Fig. 2. Separation of the stability areas of the crystalline structures of ternary chalcogenides in the coordinates: $K_{AB} - r_A/r_B$, where K_{AB} is the force constant, r_A and r_B are the cation radii of the components A and B of the compounds AB_2X_4 (X is a chalcogen) (cf. IGLESIAS, STEINFINK)

allow to separate in a satisfactory manner the areas of stability of various structures. In these cases the investigators usually hope, that the use of additional properties of components will enable them to distinguish more exactly between the structural types. However, the transition to the four-dimensional space is technically unrealistic. The approach, which we proposed, can solve the problem. It can be considered as a method of retrieving complex, partially linear hyperplanes, separating various classes of physico-chemical systems in multidimensional spaces of the components' properties.

From the algorithmic point of view the problem comes to trying the subintervals of changing properties and separation of those combinations, within which some certain classes of systems are realized. On the one hand it is necessary to take the interval of changing properties as small as possible, to decrease the probability of getting into one subinterval of physico-chemical systems of various classes. On the other hand, when increasing the number of subintervals, the number of trials sharply increases.[1])

The problem of quantizing the properties is not completely formalized and is mainly solved using the experience and intuition of investigator. Reduction of the number of trials is achieved due to the use of various algorithms (cf. DEVINGTAL; GLADUN).

The approach proposed proved to be useful for the prediction of existence of the phases of a certain type in physico-chemical systems as well as their structure and properties. In the binary systems the existence of compounds was predicted with the

[1]) The number of trials equals 2^{NK}, where N is the number of properties, K is the number of subintervals.

compositions AB, A_2B and A_3B. Of particular interest for crystallographers may be our prediction of the known types of crystalline structure of binary compounds, which can potentially exist in respective physico-chemical systems. Earlier E. M. SAVITSKIY (1977) already considered some achievements of the development of this new scientific direction.

The problem of computer learning relates to the field of constructing the models of artificial intellect and, in a general case, is characterized by a large variety of the algorithms.

From this variety we choosed those solutions, which proved to be the most effective for the classes of problems studied. For details compare DEVINGTAL; GLADUN. The principle of learning consists in the search of regularities generalizing the similarity of experimental examples within the limits of one class on the basis of the alternative of various classes. For example, in the system Li-Pb the compound is formed with the structure of CsCl type, while this is not formed in the system Al-Si. This alternative, presented by the set of a number of systems serves as a standard set for learning. The teaching examples are given by the set of the components' properties. As a result, all the multitude of conceivable systems of the dimension considered (binary systems, ternary, etc.) are arranged into predetermined classes, i.e. each object, not included into teaching refers to one of the groups of the standard examples.

The results of prediction are collected in the Tables, published in the run of their obtaining. In the present stage of investigation it seems to be possible to give an objective estimation of the results obtained before. Table 1 gives the data of the first publication of prediction of the binary phases and estimation of their correlation with experiment.

The reliability of prediction is evaluated using the examination sample, i.e. those data which were not used in the computer learning.

$$p = \frac{a}{a_1} 100 ,$$

where p is the reliability (correlation) of the prediction, %, a is the number of examples which are tested for coincidence (the volume of the examination sample); a_1 is the number of examples, coinciding with the prediction.

The examination sample is formed in a random manner (using the Table of Random Numbers). When the results of the prediction contradict to the experimental results, or in the case of a failure due to incompleteness of original data the system may additionally learn itself. In this connection the choice of experimental results is rather a substantial part of the work. Their correctness affects the result of learning.

When one considers the existence of a compound, then, as a rule the probability of the class of existence-examples is higher than that of the alternative class (of nonexisting compounds). This nonequality is due to the nature of the chemical objects themselves. It is known, that if the compound is not synthesized, this does not mean, that it cannot exist. Therefore the results of prediction of each of the classes are also not of the equal value.

In 1968 the first prediction was published of the binary inorganic compounds with the composition A_3B (SAVITSKIY, DEVINGTAL, GRIBULYA 1968 b). Figure 3 shows the example of this prediction with the indications about the correlation with experiment for the data, obtained since the date of publication up to now. The figure deals with only 30 compounds of the type to be predicted in the corresponding systems. Nowadays 73 compounds are known and 17 compounds are not yet synthesized. The prediction of the stoichiometric phases, as it follows from the Table, is in a good agreement with the experimental results. Nevertheless, the crystalline structure of the solid phases is of the greatest interest. Various properties of solids are theoretically connect-

Table 1
Characteristics of the results of prediction of the binary phases

Composition	the characteristic to be predicted	number of the objects		number of tested predictions on 8.80	reliability of prediction		references
		of learning	of prediction		exam.	liter. data	
AB	possibility of formation of the compound	362	2404	945	91	92	SAVITSKIY, GRIBULYA 1973;
A_2B	CsCl type of the structure	215	3174	101	99	98	SAVITSKIY, GRIBULYA 1977;
A_2B	NiAs type of the structure	78	557	40	95	—	
A_2B	estimation of the melting point	14	14	—	90	—	SAVITSKIY, SHELEST, GRIBULYA
A_2B	possibility of formation of the compound	1077	3533	793	91	92	SAVITSKIY, GRIBULYA 1973;
A_2B	Laves phase type of the structure	200	1548	222	98	98	SAVITSKIY, GRIBULYA 1972, 1978 b;
A_3B	possibility of formation of the compound	1457	2534	483	91	93	SAVITSKIY, GRIBULYA 1971;
A_3B	A 15 type of the structure	85	766	20	99	99	SAVITSKIY, GRIBULYA 1975 a;
A_3B	estimation of the T_k of the phases A 15	47	766	86	T_k less than 30 K is predicted		SAVITSKIY, GRIBULYA 1978 a;
A_5B	Cu_5Ca type of the structure	87	1060	68	99	99	SAVITSKIY, GRIBULYA 1974;
the phases of variable composition	γ-b-rass type of the structure	93	551	—	—	—	SAVITSKIY, GRIBULYA 1977;
	σ-phases (β-uranium type)	106	174	1	99	99	SAVITSKIY, GRIBULYA 1975 b;

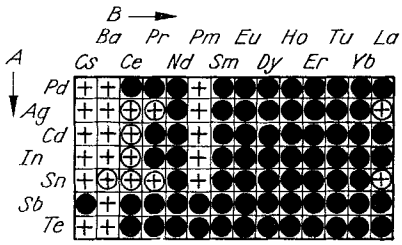

Fig. 3. The fragment of predicition of the composition A_3B, obtained in 1968 SAVITSKIY, DEVINGTAL, GRIBULYA 1968b. The conventional designations: "+" -not yet synthesized; "⊕"-known before prediction and used to learn the computer

ed with the crystalline structure. The first experiment of prediction of the crystalline phases was carried out with the binary Laves phases (SAVITSKIY, GRIBULYA 1972). That time 297 compounds of this type were known with the composition A_2B. The error of prediction was estimated 1.6%. The learning of computer was effected with 100 examples of existence was effected with 100 examples of existence and 100 examples of the absence of the phase in the system. Now we know 325 Laves phases, including the known modifications of these compounds ($MgCu_2$, $MgZn_2$, $MgNi_2$) formed at the ratio of atomic radii from 1.04 ($NbZn_2$) to 1.65 ($BaRh_2$). Since the range of variation of the size factor in this case is determined only by the experimental data with the use of atomic radii by Goldschmidt, then one may assume that the limits of variation given are not limited ones. The prediction was performed without using the data on atomic radii of chemical elements. The chemical elements were described by the data on the electron structure of isolated atom. After learning with the known experimental examples the prediction was obtained for the binary phases considered, which gave their possible number about 2000. Here one means the existence under any conceivable conditions. In this case no question is considered about the stability of these phases.

Table 1 shows that the error did not change with the increasing volume of data. The coincidence of prediction with the experiment is nowadays about 98% in round figures. Figure 4 shows the fragment of the prediction of binary Laves phases in the systems with rare-earth metals. Earlier SAVITSKIY, GRIBULYA 1972 stated according to the results of prediction, that the rare-earth elements do not form Laves phases on their basis, i.e. for the stoichiometry. A_2B they participate only as the component B. Up to now this hypothesis has no exceptions. The figure shows, that a number of refractory and some alkali and alkali-earth metals should form Laves phases with the rare-earth metals. In most of these systems so far no miscibility of compounds was obtained.

In this connection of greatest interest are the experiments on synthesizing new alloys with the use of new trends in technology: melting under zero gravity, powder technology, high pressures, super-rapid quenching, etc. The new data, which do not coincide with the prediction, are also of great interest since the systems to be learned are adaptive ones. Their relearning makes it possible to modify the prediction.

The other phases of analogous type identical to $CaCu_5$ were predicted in 1973 (SAVITSKIY, GRIBULYA 1974). The fragment of the prediction of these phases is given in Figure 5. Until now there are practically no controversies with the experiment. However, when taking into account a relatively small volume of the data accumulated, one may assume the average percent of the error for the prediction of various phases to be 4%. Thus, with some overinsurance the reliability of the prediction may be accepted as equal to 96%.

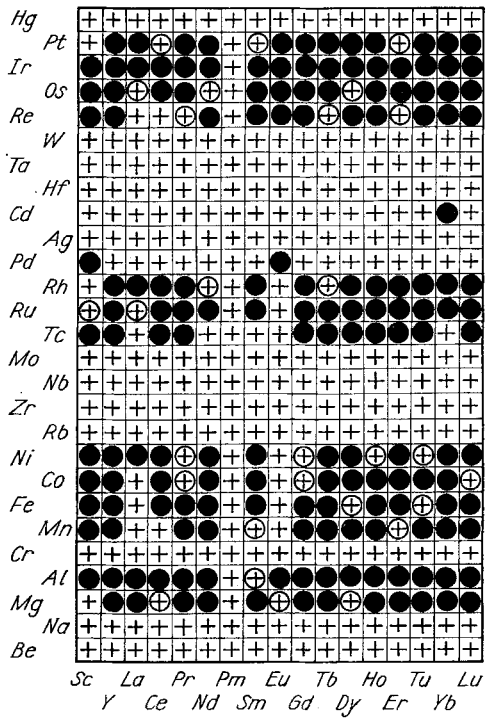

Fig. 4. The fragment of prediction of the Laves phases A_2B in the system with rare-earth elements. The conventional designations are given in Figure 3

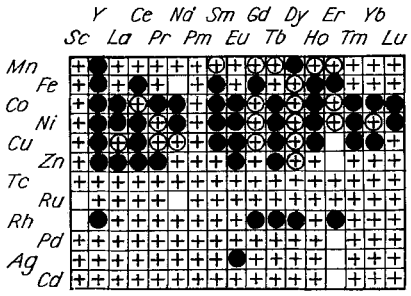

Fig. 5. The fragment of prediction of the $CaCu_5$-type phases (composition A_5B). Conventional designations are the same as in Figure 3 (SAVITSKIY, GRIBULYA 1974).

The main criterion of the choice of the crystalline structures, to be considered as an object of prediction, is their abundance in the metal systems, which are of interest from the viewpoint of theory and practice of producing inorganic materials with the properties required. Therefore, it is the most important practical task to estimate and predict the quantitative characteristics of materials.

The phases of the type A15 proved to be an interesting object for estimating the properties. These phases, together with the Laves-phases, sigma-phases (of the type β-U), α-Mn, are abundoned in metallic systems and sometimes are met with them in one and the same system. Prediction of the A15 phases is given in Figure 6. Prediction of the sigma-phases and phases of the α-Mn type is given in the Figures 7 and 8, respectively. The experimental data on the A15 phases are rather comprehensive

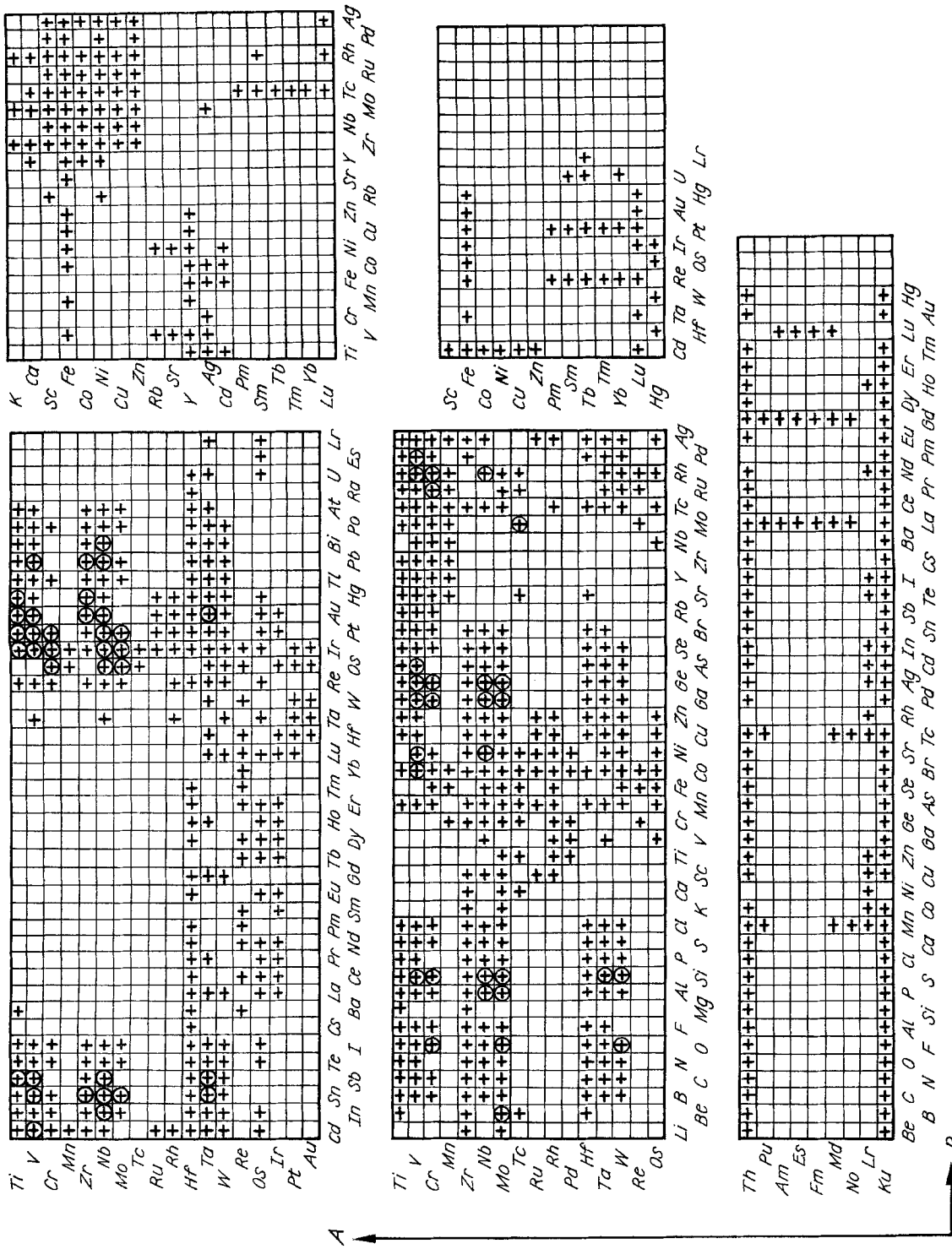

Fig. 6. Prediction of the phases A15

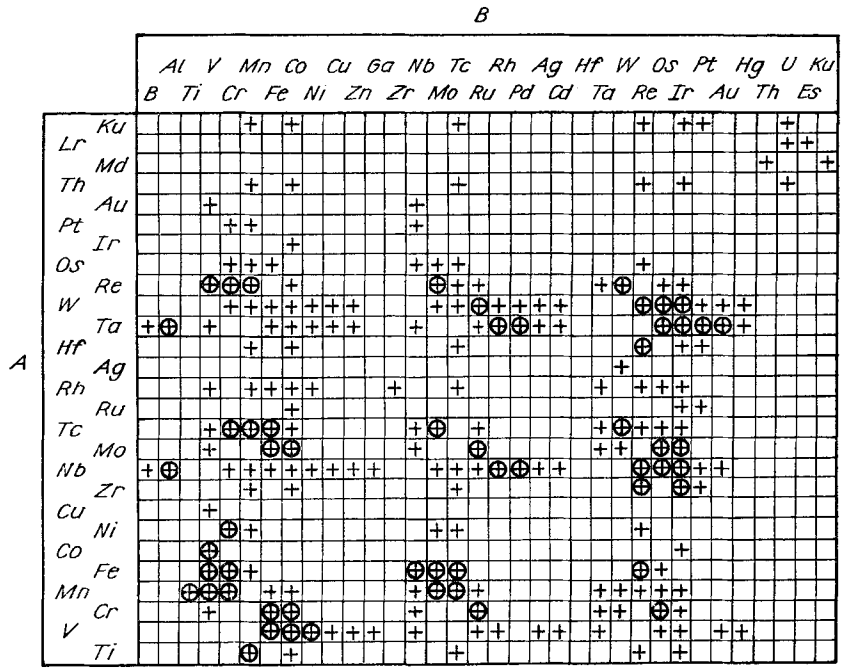

Fig. 7. Prediction of the σ-phases

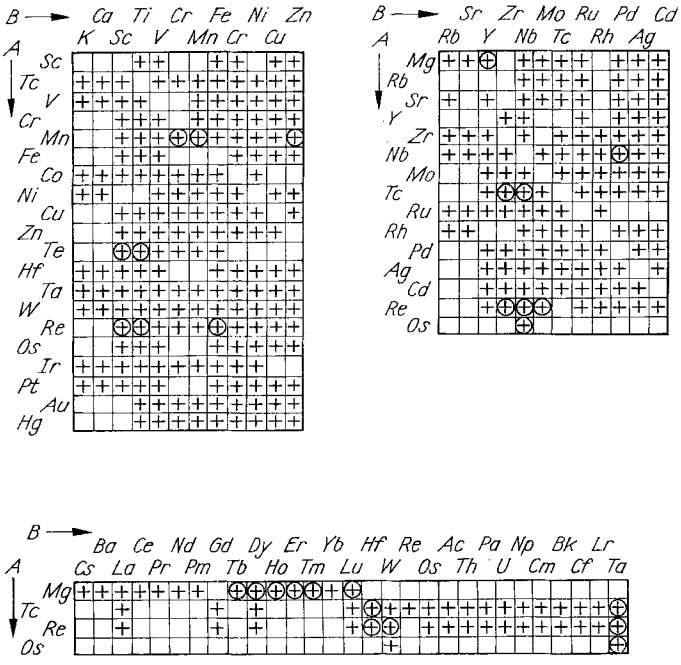

Fig. 8. Prediction of the binary phases of α-Mn type

and they are tested by a large number of investigations in connection with the superconductivity problem, though the volume of information on $CuCa_5$ compound is more.

The data of NOVOTNY concerning the alloys $Cr_{0.8}Fe_{0.2}$; $Cr_{0.75}Ru_{0.25}$; $Cr_{0.6}Co_{0.4}$ should be used in addition to the confirmation of predicting A15 phases, which are considered by SAVITSKIY, GRIBULYA 1975 a to have the same structure.

The A15 phases are known to be the most extensively studied superconductors (SAVITSKIY et al. 1976 a). Therefore, it is of interest to estimate their potential capabilities in achieving high critical transition temperatures (T_c) using the distinctive features, indicated by computer in the process of predicting A15 phase (SAVITSKIY, GRIBULYA 1978 a). Figure 9 shows the graphical interpretation of the regularities obtained. The distribution of the phases over the temperature interval enables to assume that T_c temperatures are limited by 30 K. Thus, estimating the ultimate level of properties, one may design the experiment, giving maximum attention to the most promising composition of the substances under consideration.

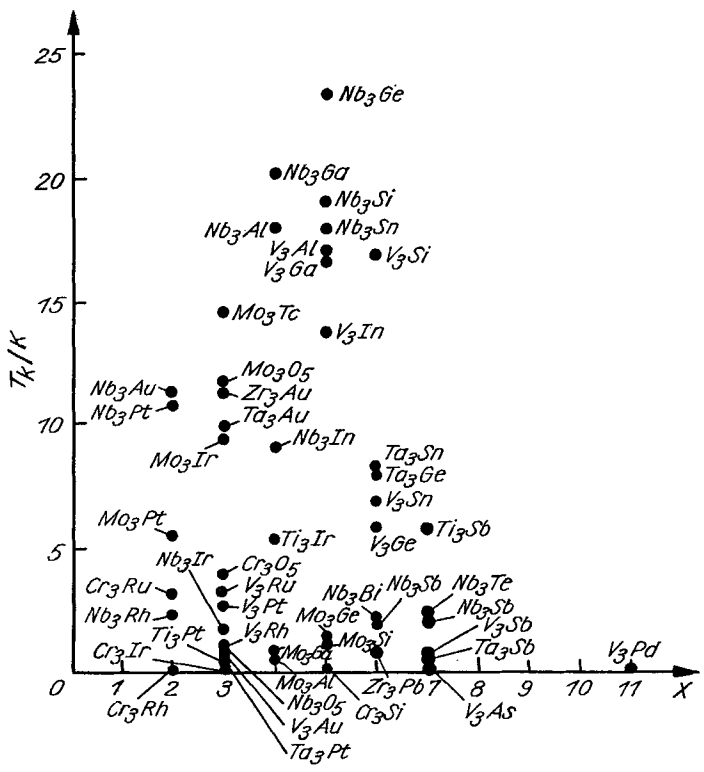

Fig. 9. Evaluation of the physical property using the example of superconducting transition temperature for the binary phase of A15 type (O_s read Os)

The modifying of the approach proposed, which opens new possibilities for the researches in both practice and theory, makes it possible to consider in a new way the well known ideas. This is especially true with respect to the clarity of existing definitions and classifications being fundamental for the theory of solids.

Naturally, the investigations were extended by using the approach for predicting the ternary inorganic compounds. Most widely met compositions ABX_2 and AB_2X_4 were predicted (A and B are the elements of periodic Table, X may be O, S, Se, Te),

Table 2
Characteristics of the prediction results for the ternary phases

Composition	the characteristics to be predicted	number of the objects		number of the predictions tested for 8.80	reliability of the prediction		references
		learning	prediction		exam.	liter. data	
ABO_2	possibility of formation of the compound	165	360	54	92	93	KISELYOVA, SAVITSKIY 1977
ABS_2	possibility of formation of the compound	175	610	19	89	74	SAVITSKIY, KISELYOVA 1979
$ABSe_2$	possibility of formation of the compound	111	674	17	85	94	
$ABTe_2$	possibility of formation of the compound	73	712	9	75	89	
ABO_3	possibility of formation of the compound	382	1967	53	88	79	KISELYOVA, POKROVSKIY
ABO_3	the perovskite type structure	247	2102	26	95	70	
ABO_4	possibility of formation of the compound	223	1872	38	97	99	
AB_2O_4	possibility of formation of the compound	313	2194	48	95	96	
AB_2O_4	the spinel type structure	190	2317	27	88	85	
AB_2S_4	possibility of formation of the compound	375	1479	32	89	97	KISELYOVA, SAVITSKIY 1979
AB_2S_4	the spinel type structure	218	1636	8	81	99	
AB_2Se_4	possibility of formation of the compound	220	950	30	80	99	
AB_2Se_4	the spinel type of the structure	167	1003	18	75	99	
AB_2Te_4	possibility of formation of the compound	40	627	19	—	94	SANTSKIY, KISELYOVA, VASHCHENKO
$A_2B_2O_7$	possibility of formation of the compound	274	674	34	80	79	SAVITSKIY, GLADUN
$A_2B_2O_7$	the pyrochlore types structure	174	714	24	78	92	
$A_XB_6S_8$	the Chevrel-phase type of structure	55	325	3	—	—	SAVITSKIY, KISELYOVA 1978

ABO_3, ABO_4 and $A_2B_2O_7$ and most typical types of the crystalline structures: spinels, pyrochlores, perovskites, Chevrel phases (KISELYOVA, SAVITSKIY 1977, 1979; SAVITSKIY, KISELYOVA 1978, 1979; KISELYOVA, POKROVSKIJ; SAVITSKIY, KISELYOVA, VASHCHENKO). More complex composition made it necessary to use the more powerful computers (of the БЭСМ-6-type) and new algorithms (GLADUN). The use of parameters of electronic structure of isolated atoms proved to be insufficient for the prediction of ternary phases. Therefore, together with the distribution of electrons over the energy shells, some other physical, thermodynamical, structural and other parameters of chemical elements and ordinary chalcogenides in the solid and gaseous states were used to describe the physico-chemical systems. The use of these parameters made it possible to improve considerably the reliability of predictions. In five years passed the data were published about the existence of 353 compounds of the compositions predicted and the crystalline structures of 105 compounds were determined.

Table 2 contains the statistical data about the results of prediction as known for the August, 1980. The total error of prediction of compounds is about 10%, this being somewhat less, than the average error of examination prediction —13%. The total error of prediction of the type of the crystalline structure equals 11%, and that is also less, than the average examination error —17%.

The most precise predictions are obtained for the compositions ABO_2, $ABSe_2$, $ABTe_2$, ABO_4, AB_2X_4 as well as for the spinel and pyrochlor types of the structure.

Figure 10 shows the fragments of the Table of prediction of the compounds ABO_2 (KISELYOVA, SAVITSKIY 1977), published in 1977. The marks "+" stand for the predictions of compounds' formation, the circles show the objects used when learning

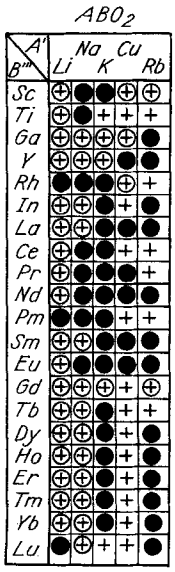

Fig. 10

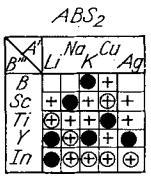

Fig. 11

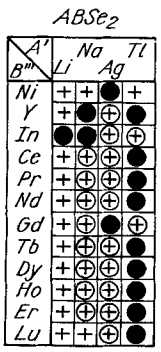

Fig. 12

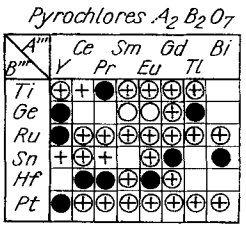

Fig. 13

Fig. 10. The fragment of prediction of the ternary compounds ABO_2 (KISELYOVA, SAVITSKIY 1977)

Fig. 11. The fragment of prediction of the compounds ABS_2 (SAVITSKIY, KISELYOVA 1979)

Fig. 12. The fragment of prediction of the compounds $ABSe_2$ (SAVITSKIY, KISELYOVA 1979)

Fig. 13. The fragment of prediction of the pyrochlores $A_2B_2O_7$ (SAVITSKIY, GLADUN), published in 1977 (B^{III} read B^{IV})

the computers. The black circles correspond to the experimentally confirmed compounds which were predicted and synthesized within 3 years passed (LAZAREV, SHAPLYGIN; BEVAN, SUMMERVILLE; LAZAREV, KRASOV).

Figures 11 and 12 show the fragments of the Prediction Tables for the semiconducting phases ABS_2 and $ABSe_2$, published in the last year (SAVITSKIY; KISELYOVA 1979). These Tables use the same marks as before. The mark "—" means the absence of the compound with the composition under prediction in the physico-chemical system A—B-chalcogen. During the last year numerous data were published (FLAHAUT; SEMRAD; LE NAGARD; ALIEV), confirming our predictions.

Figure 13 shows the fragment of the Prediction Table for the pyrochlores $A_2B_2O_7$, published in 1977 (SAVITSKIY, GLADUN). The empty circles stand for the experimentally confirmed (BEVAN, SUMMERVILLE; LAZAREV, KRASOV) predictions of the absence under normal conditions of the pyrochlore structure for the germanium compounds.

In all examples, given above, dealing with the verification of the predictions, the experimental data are taken from the literary sources, published after the Prediction Tables. However, some of the results were tested in the Institute of Metallurgy of the Academy of Sciences of the USSR. In particular, it was shown, that under ordinary conditions with the compositions $SnRe_6S_8$ no CHEVREL phase is formed and this is in accordance with our prediction (SAVITSKIY, KISELYOVA 1978). The Chevrel phase $Ag_{0.8-0.9}Mo_6S_8$ is obtained, for which we predicted $T_c > 4.2$ K, and its T_c was proved to be 7.8 K.

Discrepancy between the experimental data and those predicted is the impetus for relearning, i.e. learning the computer with the use of noncoinciding examples. Such correction of the classification scheme is possible due to the use of the high-speed computers, capable of carrying out such calculations in several hours or even minutes. Thereby, only some fragments of the Prediction Table are changed, namely those, which correspond to the physico-chemical systems close to the noncoinciding ones.

One of the greatest advantages of the cybernetic predicting systems used by us is their adaptivity, the methodological and technical basis of which is the use of the programs of the artificial intellect (GLADUN; DEVINGTAL) and high-speed computers.

Despite a short term (only 12 years (SAVITSKIY, DEVINGTAL, GRIBULYA)) passed since the first works on cybernetic prediction of inorganic phases had been published, this method made it possible to solve a number of the problems, which could not be solved before.

The criterion of the correctness of any theoretical method is a correctness of practical results, obtained on its basis. Now one may definitely say, that the method has passed its practical examination. Moreover, the method proved to be versatile: without changing general principles it was extended for predicting inorganic compounds in the ternary physico-chemical systems and in future it may be used for the prediction in multicomponent systems. The use of computers and formal cybernetic and mathematical methods has urgently put the question about clarification of the main notions of chemistry: what is a compound? what is a solid solution? what is a component? etc. The search of the answers for these questions will considerably deepen the ideas about the interactions in the physico-chemical systems. The further development of cybernetic prediction in chemistry is connected with the development and deepening the methods of prediction, extending the methodology for evaluation of the quantitative parameters of the phases, whith the merge of the prediction systems and automized information retrieval systems, as well as with the development of the physical ideas about the nature of the substances.

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