APPLICATION OF PYRAMIDAL NETWORKS TO THE SEARCH FOR NEW ELECTRO-OPTICAL INORGANIC MATERIALS

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Abstract: The problem of predicting new inorganic material systems with predefined properties on the basis of elemental properties remains largely unsolved. Within the context of this problem, a computer learning method (concept formation), based on semantic networks of a special kind - growing pyramidal networks (GPNs), was used in the process of searching for novel compounds with electro-optical (EO) properties. The basic chemical hypothesis of this investigation was that only compounds with acentric crystal space groups possess EO properties. It is expected that new EO compounds will be similar in composition and crystal structure to already known compounds. The crystal chemical types used to build the GPN were selected on the basis of known acousto-optical, electro-optical, and nonlinear-optical materials. Hundreds of new ternary and quaternary EO compounds are predicted using the resultant GPN.

Keywords: electro-optical materials, artificial intelligence, growing pyramidal networks, prediction, database.

1. INTRODUCTION

The electro-optical (EO) effect, discovered by Kerr in 1875, where the index of refraction of a material varies under the action of an electric field, has widespread application to modern opto-electronics. EO materials are used as an actuating medium for light modulators, deflectors, shutters, filters and other transducers of parameters involving a light beam (in particular, laser radiation) (Rez and Poplavko, 1989; Narasimhamurty, 1981; Yariv and Yeh, 1984). There are two kinds of EO effect: 1) linear (referred to as the Pockels effect) where the index of refraction variation linearly depends on a force field ($D(1/n^2)_{ij} = r_{ijk}E_k$); and 2) quadratic (effect by Kerr) where the index of refraction varies with the square of the force field ($D(1/n^2)_{ij} = r_{ijkl}E_kE_l$). The first effect is exhibited by acentric crystal structures only, while the second one is observed in any dielectric. As a consequence of it's low operating voltage the Pockels effect is of more practical use (Rez and Poplavko, 1989). The present research is focused on the "*a priori*" prediction of new acentric material systems having linear EO properties. The term "*a priori*" means that only constituent elemental information is used for predicting acentric EO material systems.

2. EXISTING APPROACHES TO SEARCHING FOR NEW EO MATERIAL SYSTEMS

The analysis of known approaches has shown that at present the basic method of searching for EO substances is by the synthesis of crystal chemical analogs of known materials, e.g., an investigator uses an isovalent substitution for one cation or anion by the element of the same group of the Periodic Table. However, in this case, it is not always possible to produce crystals with a similar structure type to the prototype. The problem becomes complicated when searching for new EO materials on the basis of heterovalent substitution of the elements of other neighborhood groups. In this case it is necessary to take into account a set of the factors which influence the formation of compounds with the desired predefined crystal structure type.

Theoretical methods of searching for EO materials are limited by various empirical rules and regularities. Abrahams (1986,1990,1996) was among the first to develop such theoretical methods of searching for compound-analogs with special ferro-electrical properties. The basic idea of his research coincides with the below discussion wherein the point group determines ferro-electrical properties, and therefore, it is logical that the search for new substances of this class involve analogs using information from crystallographic DBs. However, Abrahams could not predict new compounds with desired ferro-electrical properties from already known compounds.

Previous unsuccessful attempts by the authors (Rabe, et al., 1992) at predicting new high-temperature ferro-electrics with composition ABO_3 (A and B are hereafter chemical elements, O - oxygen) have involved two- dimensional projections of the elemental properties of known compounds. The approach employs quantum structural diagrams (where the coordinates are functions of electronegativities, obtained by spectroscopic methods, the numbers of valence electrons and pseudo-potential radii of cations A and B) all of which are properties associated with classes of known compounds was observed. But due to nonlinearities in the relationships of theses properties relative to predicting ferro-electrics, the projection approach did not yield the desired consistent prediction results.

To accommodate these nonlinear relationship artificial intelligence (AI) methods (Gladun and Vashchenko, 1995) were employed. Using these AI methods promising new EO materials in systems A-B-X were predicted (Kiselyova, et al., 1998; Kiseleva, 1997). It should be noted that the termination criteria of the algorithm used in this work (Gladun and Vashchenko, 1995) was 100% separation of known compounds belonging to various classes. In addition, prediction of more complicated compounds was also carried-out.

3. Used methods

Our approach to the problem of predicting new EO inorganic substances via computer design is based on the process of development of new materials used by the chemists. As a rule the research begins with the analysis of a materials dataset similar to the materials sought. The result of such a review is a list of the most promising classes of materials. In addition, a selection of the most promising elements for substitution of already known compounds is carried-out. The basis of such selection is the Mendeleev periodic law and various empirical rules (for example, Goldschmidt rule for estimation of possibility of formation of compounds with perovskite crystal structure), and also data on proximity of properties of the substituting elements to substituted. In addition, non-formalizable techniques and rules, which are imparted from one generation of the chemists to other, can be used.

The proposed approach is to automate the process of inorganic (including EO) materials design, described above via the development of computer system which could provide the investigator with qualitative information about properties of known materials. Such a computer system would allow the analysis of experimental data with the aim of identifying regularities between properties of compounds and their constituent components (chemical elements or more simple compounds), which could further be used for predicting the new compounds, similar to those already known. The developed system will never be completely automatic, since it is impossible to take into account all factors which cause a choice of one or other class of compounds, and all empirical experience of the investigators. However, such a system, referred to as an 'information-predicting' system (Kiselyova, 1993), allows to reduce the time required in searching for new inorganic materials.

Initially, the problem of computer memory for storing multi-dimensional empirical relationships among inorganic compounds and their component properties arises. Considering the fact that the developed system simulates the intelligence of chemist, it would be expedient to use human memory methods in the storage of such knowledge. One possibility is the use of a neural network structure accelerating a search for correlations and optimizing the computer memory for their storage.

The most appropriate algorithm was found using the "trial-and-error" method. It is the best from the viewpoint of reliability of new compound prediction. This algorithm, developed in Institute of Cybernetics of National Academy of Sciences of Ukraine, is a special system for semantic network formation. These networks are called semantic growing pyramidal networks (GPN) (Gladun and Vashchenko, 1995) and have dendritic (pyramidal) form. A pyramidal network is an acyclic graph having no vertices with only one entering arc. The terminating ends of the network (receptors) correspond to the range of appropriate values of components properties (the chemical elements or more simple compounds) of the considered physical-chemical systems. The nodes within the interior of the network correspond to combinations of values of component properties occurring in the analyzed physical-chemical systems. If the process of concept formation is active then the pyramidal network is designated as a growing one. GPN is built while classifying process of objects. Concept formation involves the analysis of network vertices and the choice of vertices is based upon associativity with the most similar class (checking vertices).

Table 1. Promising Crystal Families to Search for New Electro-Optical Materials

Composition	Crystal Structure Type	Space Group	Examples	Application
ABO_3	$LiNbO_3$	acentric groups	$LiNbO_3$, $LiTaO_3$	EO, AO, NO materials
ABO_3	distorted perovskite	acentric groups	$PbTiO_3$, $PbZrO_3$, $BaTiO_3$	EO materials
ABX_2, AB_2Chal_4	chalcopyrite	I4(-)2d	$ZnGeP_2$, $AgTlSe_2$, $AgGaS_2$, $HgGa_2S_4$	EO, AO, NO materials
A_2BF_6	-	acentric groups	Ba_2ZnF_6, Sr_2CuF_6	EO, AO materials
A_3BCl_5	-	acentric groups	Tl_3PbCl_5	IR-EO and IR-AO materials
ABF_5	-	acentric groups	$SrAlF_5$, $SrGaF_5$	EO materials, laser matrix
$ABCF_6$	colquirite	P31c	$LiCaAlF_6$	EO materials, vacuum UV-optics
$ABCF_6$	Na_2SiF_6	P321	$LiMgAlF_6$	EO materials, vacuum UV-optics
$A_2B_2C_3O_{12}$	langbeinite	$P2_13$	$K_2Mg_2(SO_4)_3$, $Tl_2Cd_2(SO_4)_3$	EO materials
$A_2BC_2O_7$	melililte	P4(-)2_1m	$Ba_2ZnGe_2O_7$, $Ba_2MgGe_2O_7$, $Ca_2MgSi_2O_7$, $Ca_2Al_2SiO_7$	EO materials, laser matrix
$AB_3C_4O_{12}$	hantite	R32	$YAl_3B_4O_{12}$	EO materials, "d"- and "f"-lasers
ABC_2F_7	weberite	Imm2 or $P3_12'1$	Na_2MgAlF_7, Na_2MnFeF_7	EO materials, "d"-lasers

A, B, C - chemical elements; Chal - S, Se, or Te.

Each material system to be analyzed was entered into the computer as a set of values of component properties. The resultant networks are a primary intermediate product for the next stage - searching for connections between properties of components and properties of physical-chemical systems of fixed classes which occur frequently across the set of analyzed material systems. It is possible to receive the sought regularity only after intelligent system learning. During process of identifying regularities, the computer is informed of the various classes of physical-chemical system which have evolved. The regularities can be used for predicting new inorganic compounds and/or forecasting their properties. It is necessary to note that the prediction procedure input need only consist of information on property values of the chemical elements comprising a hypothesized new system. Thus, it can be said that the prediction is from 'first principles'.

4. ANALYSIS OF INFORMATION

The next stage of the analysis involved the prediction of new EO materials based upon known compounds. Databases, developed by A.A.Baikov Institute of Metallurgy and Materials Science of Russian Academy of Sciences: DB on properties of acousto-optical (AO), electro-optical and nonlinear optical (NO) substances (Yudina, et al., 1996; Degtyaryov et al., 1999) and properties of inorganic compounds (Kiseleva, et al., 1996), including results of statistical studies, published in (Rez and Poplavko, 1989; Narasimhamurty, 1981; Yariv and Yeh, 1984), were used. The analysis of the information has enabled the selection of classes (crystal chemical families) of new EO materials (Table 1).

Crystal chemical families whose members can exhibit significant EO properties is not limited to those listed in Table 1. It is known (Rez and Poplavko, 1989; Narasimhamurty, 1981; Yariv and Yeh, 1984) that crystals of the KDP-family (KH_2PO_4, KD_2PO_4, CsD_2AsPO_4, etc.), $Bi_{12}XO_{20}$ (X = Ge, Si, Ti), $K_3Li_2Nb_5O_{15}$, $Ba_2NaNb_5O_{15}$, $(Ba,Sr)Nb_2O_6$, $KTiOPO_4$, $(NH_4)_2C_2H_4{*}H_2O$, etc., have the most significant linear EO effect. However, analysis of the information on properties of inorganic compounds (Kiseleva, et al., 1996) has shown that the number of known compounds in these families is not a sufficient data set to establish regularities for use in prediction of new compounds.

5. PREDICTION OF COMPOUNDS

The final stage in the process is the prediction of new inorganic compounds, belonging to families, listed in

Table 1. At this point, the basic information for computer learning was extracted from a database on properties of inorganic compounds (Kiseleva, et al., 1996) containing information on more than 38,000 inorganic compounds. The properties of the chemical elements (the distribution of electrons in the energy levels of isolated atoms, the ionization potentials, the ionic or covalent radii, the electronegativities, Debay temperatures, the standard isobaric thermal capacity, melting points and heat of melting, etc.), and also property of the appropriate simple compounds (halogenides, chalcogenides, oxides) (the standard heat and the standard entropy of formation, melting points, etc.) were used for representation of information on each of the compounds.

By applying this approach the formation of compounds with composition A_3BCl_5 and the formation and crystal structure type of the following compounds with composition were predicted

$A^{I}_2B^{IV}F_6$ (more specifically, the formation of crystal modifications with K_2GeF_6-II, β_1-K_2UF_6, Na_2SiF_6, trirutile, K_2PtCl_6, K_2MnF_6-II, or K_2ZrF_6 types under normal conditions were predicted),

$A^{II}_2B^{II}F_6$ (crystal modifications with Ba_2MnF_6, rutile, Pb_2ZnF_6, or Ba_2CuF_6 types were predicted),

$A^{II}B^{III}_2Se_4$ (spinel, chalcopyrite, olivine, $PbGa_2Se_4$, Yb_3Se_4, Yb_3S_4, $CaFe_2O_4$, Th_3P_4, or $NiCr_2Se_4$ crystal structure types were predicted),

ABX_2 (where X is O, S, Se, Te, N, P, As, Sb, or Bi) (the formation of structures resembling chalcopyrite, α-$NaFeO_2$, β-$NaFeO_2$, α-$LiFeO_2$, or TlSe at normal conditions were predicted),

$A^{II}B^{III}F_5$ (structure types $BaFeF_5$, $BaGaF_5$, $CaCrF_5$, $CaFeF_5$, or $SrFeF_5$ were predicted), and

$A^{I}B^{V}O_3$ and $A^{II}B^{IV}O_3$ (types considered included cubic perovskite, calcite, aragonite, ilmenite, $NaClO_3$, $KBrO_3$, $LiNbO_3$, and also types of distortion (rhombic, hexagonal, monoclinic, or tetragonal) of ideal perovskites under normal conditions were predicted).

Illustrated in Table 2-4 is a subset of the above predictions which hold promise for new EO materials. In all of these tables the symbol * designates those compositions which do not form compounds in the appropriate system at 298 K and 1 atm. The symbol ? denotes those compounds which the computer could not predict crystal structure type at standard conditions. The empty square is an indetermine result. The parentheses designate experimentally investigated systems which are used for computer learning.

The predictions of crystal structure types for compounds with composition $A^{I}_2B^{IV}F_6$ (Table 2) are the acentric phases resembling the structure types Na_2SiF_6 (space group P321), β_1-K_2UF_6 (space group P62m) and K_2MnF_6-II (space group $P6_3mc$).

Table 2. Part of Predictions of the Crystal Structure Type for Compounds with Composition $A^{I}_2B^{IV}F_6$

A^{I} / B^{IV}	Li	Na	K	Rb	Cs
Si	(N)	(N)	(K)	(K)	(K)
Ti	(R)	(N)	(K)	(G)	(G)
V	(R)	N	(M)	(M)	↔
Cr	(R)	(N)	(K)	(K)	(K)
Mn	(N)	(N)	(M)	(M)	(K)
Fe		R	K	M	M
Co		R	K	M	K
Ge	(R)	(N)	(G)	(K)	(K)
Mo	(R)	(R)	G		M
Ru		(N)	(G)	(K)	(G)
Rh	R	N	G	G	M
Pd	(R)	(N)	(G)	(K)	(K)
Ce		(U)	(U)	(U)	(U)
Pr		↔	U	G	G
Os		(N)	(G)		(G)
Ir		(N)	(G)	(G)	(G)
Pt	(R)	(N)	(G)	(G)	(G)
Th	(*)	(N)	(U)	(U)	?
Pa		N		G	
U	(*)	(N)	(U)	(Z)	(Z)
Np		(N)	(U)	(Z)	Z
Pu		(N)	U	(Z)	(Z)
Cm		?	U	Z	Z
Bk		?	U	Z	Z
Cf		?	U	Z	Z

Designations: **G** - formation of compound with the crystal structure type K_2GeF_6-II is predicted; **U** - formation of compound with the crystal structure type β_1-K_2UF_6 is predicted; **N** - formation of compound with the crystal structure type Na_2SiF_6 is predicted; **R** - formation of compound with the trirutile crystal structure type is predicted; **K** - formation of compound with the crystal structure type K_2PtCl_6 is predicted; **M** - formation of compound with the crystal structure type K_2MnF_6-II is predicted; **Z** - formation of compound with the crystal structure type K_2ZrF_6 is predicted; - - the crystal structure differing from those listed above is predicted; **(G), (U), (N), (R), (K), (M), (Z)** - compound with corresponding type of crystal structure was synthesized and this information was used in the computer learning process; ↔ - compound with the crystal structure differing from those listed above does not exist under normal conditions and this information was used in the computer learning process; (*) - compound A_2BF_6 is not formed and this fact was used in the computer learning process.

Table 3. Part of Predictions of the Crystal Structure Type for Compounds with Composition ABX_2

	B = Si								B = Ge								B = Sn				
X / A	N	P	As	Sb	Bi	S	Se	Te	N	P	As	Sb	Bi	S	Se	Te	N	P	As	Sb	Bi
Mg	(B)	(C)	*	(*)	*	*	*	*	(B)	↔	C	C	*	*	*	*			*	(*)	(*)
Ca	B	-	*	*		*	*	*	(C)	-	C	C	*	*	*	*					C
Sr			*	*		*	*	*	B	-	C	C	*	*	*	*			*	*	
Ba			*	*		*	*	*	B	-	C	C	*	*	*	*			*	*	*
Zn		(C)	(C)	*				*	(B)	(C)	(C)	B				(*)	C	(C)	(C)	(C)	
Cd		(C)	(C)	*	*	*	*	(*)		(C)	(C)	*	*	*	(*)	(C)		(C)	(C)	(*)	(*)
Hg			*	*		*	*	*	B	-	C	C	*	(*)	(*)	(*)		*	*	*	(*)

Designations: **C** - formation of compound with the chalcopyrite crystal structure type is predicted; **B** - formation of compound with the crystal structure type β-$NaFeO_2$ is predicted; - - the crystal structure differing from those listed above is predicted; **(C), (B)** - compound with corresponding type of crystal structure was synthesized and this information was used in the computer learning process; ↔ - compound with the crystal structure differing from those listed above does not exist under normal conditions and this information was used in the computer learning process; (*) - compound ABX_2 is not formed and this fact was used in the computer learning process.

Table 4. Part of Predictions of the Crystal Structure Type for Compounds with Composition $A_2B_2(XO_4)_3$

	X = S						X = Cr					X = Mo					X = W				
A / B	Na	K	Rb	Cs	Tl		Na	K	Rb	Cs	Tl	Na	K	Rb	Cs	Tl	Na	K	Rb	Cs	Tl
Mg	L	(L)	(L)	(*)	L		L	L		L	L	K	(K)	(L)	(L)	(L)		↔	(L)	L	L
Ca	(*)	(L)	L	(L)	(*)				L	L	L	(*)	?	?	?	?	(*)	*	?	?	?
Mn	(*)	(L)	(L)	L	(L)		L		(L)	L	L	K	↔	(L)	(L)	(L)					
Fe	*	L	L		(L)		L	K	L	L	L	K	K	?	?	?		K			
Co	(*)	(L)	L		(L)		L	K	L	L	L		(K)	(L)	(L)	↔		K			
Ni	(*)	(L)	L	L	L		L		L	L	L	K	(K)	(L)	(L)	(L)					
Cu	(*)		L	*	L		L	K	L	L	L	K	(K)	?	?	?		K			
Zn	*	(L)	L	*	L		L	K	L	L	L	↔	(K)	(K)	-	(K)		K			
Sr	(*)	?	?		(*)		*	*	?	?	?	(*)	?	?	?	?	(*)	*	*	*	*
Cd	(*)	(L)	(L)		(L)								K	↔	(L)	K	(*)		L	L	L
Ba	(*)		(*)	(*)	(*)		*	*				(*)		*	*	*	*	*			
Pb					*		(*)	*	*	*	*	(*)	*	(*)	*	*	(*)	*	(*)	(*)	*

Designations: **L** - formation of compound with the langbeinite crystal structure type is predicted; **K** - formation of compound with the crystal structure type $K_2Zn_2(MoO_4)_3$ is predicted; - - the crystal structure differing from those listed above is predicted; **(L), (K)** - compound with corresponding type of crystal structure was synthesized and appropriate information was used in the computer learning process; ↔ - compound with the crystal structure differing from those listed above does not exist under normal conditions and this information was used in the computer learning process; (*) - compound $A_2B_2(XO_4)_3$ is not formed and this fact was used in the computer learning process.

In Table 3 is a subset of the results regarding the prediction of the crystal structure type for compounds with composition ABX_2 (B = Si, Ge or Sn). Chalcopyrites are best suited to searching for new EO materials.

The next step in searching for new EO materials is the prediction of more complicated compounds, e.g., quaternaries which are often the result of substitutions of cations in ternary acentric compounds. Using the growing pyramidal networks (Gladun and Vashchenko, 1995), the formation and crystal structure type (at normal conditions) of compounds with compositions were predicted

$A_2B_2(XO_4)_3$ (X = S, Cr, Mo, or W) (types considered included langbeinite and $K_2Zn_2(MoO_4)_3$),

$A^{II}{}_2B^{II}X^{IV}{}_2O_7$ (X = Si, Ge, Sn, Ti, Zr, or Hf) and $A^{I}{}_2X^{IV}B^{III}{}_2O_7$ (X = Si, Ge, or Ti) (the possibility of forming a crystal modification of melilite was also predicted).

In addition, compounds with compositions

$AD_3(BO_3)_4$ (A and D - chemical elements, B - boron) (types considered included hantite, calcite, and aragonite).

$ABCF_4$ (crystal structure types resembling trirutile, colquirite, Na_2SiF_6, $RbNiCrF_6$, or $CsAgFeF_4$ at normal conditions) were predicted, together with

A_2BCF_6 (A = Na or Ag) (types considered included weberite (orthorhombic or trigonal) and fluorite).

Illustrated in Table 4 are the prediction results involving crystal structure types of compounds with composition $A_2B_2(XO_4)_3$. These results are important because some of the predictions are of interest relative to EO applications, e.g., compounds with langbeinite structure type (space group P213) has already been checked by experiment (shaded squares). Of the 7 predictions checked, all were validated by new experimental data.

6. CONCLUSIONS

The approach discussed in this paper for predicting new materials is based on a process which is analogous to the search for new materials by an inorganic chemist. It has allowed predicting hundreds of new compounds in ternary and quaternary chemical systems, not yet investigated. These compounds are crystal chemical analogs to known EO substances and are predicted to exhibit EO properties. The predictions have been based on the interaction of growing pyramidal networks, computer learning and databases on properties of inorganic compounds.

It is important to note that the predictions were severely limited by available data on known compounds. However, good results were obtained in spite of these conditions for the algorithms used. Given the costs associated with generating experimental data, it is clear this approach affords many opportunities for designers of new materials. Although databases represent a growing source of organized quantitative and qualitative information for the consequent analysis and classification of materials, and the chemist possesses powerful tools to evaluate experimental data, these databases and tools are typically limited to a few factors and depend on correlations to identify multi-dimensional regularities. In addition, human limitations in conducting simultaneous perception and analysis of rather large data sets of numeric and symbolic information are bounded. Thus, the proposed approach not only simulates the process of design of new inorganic materials but also extends the capabilities of the chemist in discovering new materials with powerful multi-dimensional data analysis tools.

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