

UDC 541.9:666.940

*V.V. Taranenkova, Ya.N. Pitak, G.N. Shabanova***BINDING PROPERTIES OF OXIDE COMPOUNDS OF SPECIAL CEMENTS IN INTERACTION WITH WATER****National Technical University «Kharkiv Polytechnic Institute», Kharkiv, Ukraine**

To synthesize special multimineral cements, it is necessary to have information concerning binding properties of individual phases being part of given cements. Despite numerous studies, there are not yet clear theoretical criteria to evaluate the behavior of various oxide compounds (if only qualitatively, not to mention quantitatively) with respect to their possible use in chemistry of special cements. Therefore, the development of corresponding quantitative dependences as well the ascertainment of the physical and chemical conditions determining the binding properties remain the actual task of chemistry of binding materials. Our study shows that a certain range of relative electronegativity values, where compounds under consideration reveal their binding properties, can be determined clearly by means of the concept of electronegativity. It is ascertained that some binary and ternary compounds (about 100) lie within a certain range of relative electronegativity, including those ones which binding properties have not been fully studied yet. Besides, the obtained data will allow selecting the most favorable conditions for compound hardening. Thus, in terms of our findings, the binding properties of oxide compounds and prospects of their application in special cement technology can be evaluated.

**Keywords:** acid-base properties, electronegativity, binding properties, hardening conditions, special cements.

**DOI:** 10.32434/0321-4095-2020-130-3-189-196

***Introduction***

Special cements are widely used in metallurgy and machine manufacturing (melting furnace lining, ore agglomeration, mould making, and exothermic mixtures), electrical engineering and electronics (inorganic adhesives, resistors, and electrical compounds), laser engineering (matrix for laser and luminophors), chemical and petroleum refining industry (corrosion-resistant cements, fire protection of reactors, granulation and pelletizing of powdered materials, catalysts and catalyst carriers), nuclear power engineering (biological shielding), etc.

Oxide compounds are included in all types of cements that are the most important in practice. That is why great attention is paid to studying the features determining the binding properties of mentioned compounds when they interact with water. Nowadays, a number of empirical and semi-empirical generalizations in term of accumulated experimental data are made. These generalizations allow evaluating a possible use of some oxide compounds in the production of special cements. However, the

generalizations have mainly a qualitative character.

First of all, Zhuravlev's work [1] should be mentioned among the studies devoted to the problem concerned. On the basis of the Mendeleev's periodic law, he theoretically substantiated the binding properties of a number chemical compounds, such as calcium silicates, aluminates and ferrites, and experimentally confirmed theoretical statements. Having studied binding properties in 42 binary systems, Zhuravlev formulated some postulates characterizing binding properties of various oxide compounds as follows:

1) compounds like silicates, aluminates and ferrites of second group elements of Mendeleev periodic table, which are placed in even-numbered rows, exhibit binding properties; however, compounds of elements placed in odd-numbered rows of the same group do not show binding properties. From the point of view of crystal chemistry, it means that binding properties are typical of compounds, which have ionic radius of cations more than 1.03 Å;

2) binding properties are manifested in those compounds that have basicity of 2 and more.

However, some recent experimental data show that Zhuravlev's postulates are not always true.

As for the first postulate, it quite closely agrees with the fact that solubility decreases with increasing lattice energy. Since lattice energy is increased with decreasing ionic radius, it can be assumed that low solubility of beryllium, magnesium and zinc silicates results in regularities that have been observed by Zhuravlev. However, under hydrothermal hardening conditions, magnesium silicate reveals some binding properties.

With regard to the second postulate, it should be emphasized that the closest analogues of silicates, stannates and plumbates, display binding properties at the basicity of 1. This suggests that binding properties depends not only on the basicity of a compound but also on its chemical activity. For example, when moving from calcium monoaluminate to strontium and barium monoaluminates, their activity increases, and, consequently, mechanical strength of monoaluminates increases.

Thus, despite numerous studies, there are no clear theoretical criteria to evaluate the behavior of various oxide compounds (if only qualitatively, not to mention quantitatively) concerning the possibility of their use in the production of special cements.

To synthesize special multimineral cements, it is necessary to have information about the binding properties of individual phases being part of given cements. From this point of view, the most promising way for the creation of new binding materials involves studying not only ordinary binders but also their analogues. In particular, the investigation of germanates and gallates of alkaline-earth elements should be performed, which are characterized by a combination of the following useful properties: refractoriness, high density, mechanical strength, etc. Besides, it is known that some compounds show binding properties under normal conditions, while other compounds (for instance, metasilicates and titanates of alkaline earth elements) are inert under normal conditions and exhibit binding properties at the hardening under conditions of elevated temperatures.

Thus, the development of quantitative dependences and the ascertainment of the physicochemical conditions determining the binding properties is an urgent and important problem in chemistry of binding materials.

#### **Theory**

Binders are combination of two chemical reagents: a solid powder and a liquid. The occurrence

of binding properties results from chemical interaction between reagents. To bring out the regularities in binding properties, it is necessary to evaluate the reactivity of cement compounds with respect to water, when powder and liquid are an oxide compound (like calcium silicates) and water, respectively. Since reactions of calcium silicates and their analogues with water are acid-base interactions, their rate obviously will be determined by extent of difference in acid-base properties of the starting reagents, i.e. mineral compounds and water.

Traditional chemical methods for the evaluation of acid-base properties of silicates and their analogues are not applicable because these compounds are hardly dissolved in water. This does not allow characterizing their acid-base properties by means of pH determination [2].

To estimate acid-base properties of silicates, Batsanov proposed to use the values of compounds electronegativities [3]. The concept of electronegativity (EN) is important not only for theoretical chemistry but also for mineralogy, since the use of EN data can explain the regularities of changes in properties of minerals and chemical compounds.

Atom electronegativity is a measure of atom affinity for an electron. According to Lewis's theory, EN allows characterizing acid or base properties of an atom. Sanderson showed that the EN values of oxides are inversely proportional to the pH values measured after dissolution of oxides in water [3]. Therefore, the EN conception can be used for studying the compound acid-base properties.

Fedorov [4] proposed to use the concept of electronegativity for prediction of binding properties of oxide compounds. Fedorov calculated electronegativities ( $EN_{\text{comp}}$ ) of calcium silicates and aluminates-like compounds, such as silicates, stannates, plumbates, titanates and aluminates of alkali and alkaline-earth elements, for which the binding properties were known. The values of compounds electronegativities were calculated in accordance with Sanderson's technique as a geometric mean of electronegativities of the elements forming a given compound. A comparison of the values of compound relative electronegativity ( $EN_{\text{rel}}$ ), obtained by dividing  $EN_{\text{comp}}$  by the water electronegativity ( $EN(\text{H}_2\text{O})$ ), allowed drawing the conclusion that the binding properties appeared only for compounds corresponding to a certain range of  $EN_{\text{rel}}$ .

According to the calculated values of  $EN_{\text{rel}}$ , Fedorov classified the studied compounds into three groups: 1) compounds that do not form cement stone

because of too much intensive interaction with water; 2) compounds that have binding properties; and 3) compounds that are not hardened due to low reactivity with respect to water.

However, analyzing the results of calculations performed by Fedorov, we revealed numerous inaccuracies and, consequently, the range of  $EN_{rel}$ , well where binding properties occur, must be revised. For example,  $EN(H_2O)$  value calculated according to Sanderson's technique is equal to 4.0343, while the value calculated by Fedorov is 4.04. Besides, he did not consider compounds discovered in recent years that are the analogues of calcium silicates and aluminates (for instance, germanates and gallates of alkaline-earth elements). Moreover, the data concerning EN of complex ternary oxide compounds and such important compounds of cement chemistry as ferrites of alkaline-earth elements are not available.

Therefore, we calculated in the present study the  $EN_{comp}$  values for 168 silicates, germanates, stannates, plumbates, titanates, aluminates, gallates, ferrites, aluminoferrites, and aluminosilicates of alkali and alkaline-earth elements as well as zirconium-containing compounds by using the electronegativity concept in order to determine the range of  $EN_{rel}$ , where compounds show binding properties. This allowed us to select the most favorable compound that can be applied as binding materials.

The initial data for EN calculation were taken from ref. [2]. The experimental data concerning the presence of binding properties were taken from previous publications [5–14].

### Results and discussion

Results of the calculations of EN for silicates and aluminates for the elements from the first and second groups of periodic table are given in Tables 1–9.

Our investigation shows that a certain range of relative electronegativity values, where compounds exhibit binding properties, can be clearly determined. The numerous groups of binary and ternary compounds (about 100) are present within this range, including those compounds which binding properties have not been completely studied yet.

The oxide compounds with  $EN_{rel}=0.55-0.85$  display binding properties under normal conditions, while those with  $EN_{rel}=0.74-0.90$  show their binding properties under hydrothermal conditions. Compounds that do not form strength cement stone are as follows: with low  $EN_{rel}$  (less than 0.72) due to too much intensive interaction with water and with high  $EN_{rel}$  values (more than 0.90) due to low reactivity relative to water.

As can be seen from the obtained data, the

Table 1  
Relationship between electronegativities of silicates and their binding properties

Compound	$EN_{comp}$	$EN_{rel}$	Binding properties*	
			under normal conditions	under hydrothermal conditions
$2Na_2O \cdot SiO_2$	1.98	0.49	–	–
$2Li_2O \cdot SiO_2$	2.03	0.50	–	–
$K_2O \cdot SiO_2$	2.21	0.55	+	–
$Na_2O \cdot SiO_2$	2.38	0.59	+	–
$Li_2O \cdot SiO_2$	2.42	0.60	+	–
$4BaO \cdot SiO_2$	2.70	0.67	Δ	×
$3BaO \cdot SiO_2$	2.80	0.69	+	–
$Na_2O \cdot 2SiO_2$	2.86	0.71	+	–
$3SrO \cdot SiO_2$	2.87	0.71	+	+
$Li_2O \cdot 2SiO_2$	2.89	0.72	+	–
$2BaO \cdot SiO_2$	2.96	0.73	+	–
$3CaO \cdot SiO_2$	2.97	0.74	+	+
$5BaO \cdot 3CaO \cdot 4SiO_2$	3.02	0.75	+	+
$2SrO \cdot SiO_2$	3.03	0.75	+	+
$2CaO \cdot SiO_2$	3.12	0.77	+	+
$K_2O \cdot 4SiO_2$	3.22	0.80	+	+
$3CaO \cdot 2SiO_2$	3.23	0.80	–	+
$BaO \cdot SiO_2$	3.27	0.81	–	+
$SrO \cdot SiO_2$	3.33	0.83	–	+
$2MgO \cdot SiO_2$	3.34	0.83	–	Δ
$BaO \cdot 2CaO \cdot 3SiO_2$	3.35	0.83	–	+
$CaO \cdot SiO_2$	3.39	0.84	–	+
$2BaO \cdot 3SiO_2$	3.46	0.86	×	×
$5BaO \cdot 8SiO_2$	3.48	0.86	×	×
$3BaO \cdot 5SiO_2$	3.50	0.87	×	×
$MgO \cdot SiO_2$	3.57	0.88	–	–
$BaO \cdot 2SiO_2$	3.58	0.89	–	×
$Al_2O_3 \cdot SiO_2$	3.73	0.92	–	–
$2CdO \cdot SiO_2$	3.87	0.96	–	–
$CdO \cdot SiO_2$	3.95	0.98	–	–
$2ZnO \cdot SiO_2$	3.97	0.98	–	–
$ZnO \cdot SiO_2$	4.02	0.99	–	–

Note: + – the presence of binding properties has been established; – – the absence of binding properties has been established; Δ – the binding properties are suggested; × – the absence of binding properties is suggested.

compounds having high  $EN_{rel}$  values show binding properties only at autoclave treatment. However, autoclave treatment is not effective for compounds having  $EN_{rel} < 0.80$ , moreover it is even harmful for compounds with  $EN_{rel} < 0.77$  because binding properties disappear.

Thus, Table 10 summarizes the refined ranges

Table 2

**Relationship between electronegativities of germanates and their binding properties**

Compound	EN <sub>comp</sub>	EN <sub>rel</sub>	Binding properties*	
			under hydrothermal conditions	under hydrothermal conditions
3BaO·GeO <sub>2</sub>	2.90	0.72	+	Δ
3SrO·GeO <sub>2</sub>	2.98	0.74	Δ	Δ
3CaO·GeO <sub>2</sub>	3.08	0.76	+	+
2BaO·GeO <sub>2</sub>	3.10	0.77	+	+
2SrO·GeO <sub>2</sub>	3.17	0.79	Δ	Δ
5BaO·3CaO·4GeO <sub>2</sub>	3.18	0.79	Δ	Δ
3BaO·2GeO <sub>2</sub>	3.26	0.81	+	Δ
2CaO·GeO <sub>2</sub>	3.26	0.81	+	+
3CaO·2GeO <sub>2</sub>	3.41	0.85	+	+
2MgO·GeO <sub>2</sub>	3.48	0.86	×	Δ
BaO·GeO <sub>2</sub>	3.49	0.87	–	+
SrO·BaO·2GeO <sub>2</sub>	3.52	0.87	×	Δ
SrO·GeO <sub>2</sub>	3.54	0.88	×	Δ
CaO·BaO·2GeO <sub>2</sub>	3.55	0.88	×	Δ
CaO·SrO·2GeO <sub>2</sub>	3.58	0.89	×	Δ
CaO·GeO <sub>2</sub>	3.62	0.90	–	Δ
MgO·GeO <sub>2</sub>	3.79	0.94	×	×
SrO·4GeO <sub>2</sub>	3.84	0.95	×	×
CaO·2GeO <sub>2</sub>	3.92	0.97	×	×
BaO·4GeO <sub>2</sub>	4.17	1.03	×	×
CaO·4GeO <sub>2</sub>	4.22	1.05	×	×
BaO·19GeO <sub>2</sub>	4.49	1.11	×	×

\*Note: see the footnote to Table 1.

Table 3

**Relationship between electronegativities of stannates and their binding properties**

Compound	EN <sub>comp</sub>	EN <sub>rel</sub>	Binding properties*	
			under hydrothermal conditions	under hydrothermal conditions
2BaO·SnO <sub>2</sub>	3.04	0.75	+	–
2SrO·SnO <sub>2</sub>	3.10	0.77	+	–
2CaO·SnO <sub>2</sub>	3.20	0.79	+	+
BaO·SnO <sub>2</sub>	3.39	0.84	+	+
2MgO·SnO <sub>2</sub>	3.43	0.85	–	+
SrO·SnO <sub>2</sub>	3.44	0.85	+	+
CaO·SnO <sub>2</sub>	3.51	0.87	–	+
2CdO·SnO <sub>2</sub>	3.96	0.98	–	–
CdO·SnO <sub>2</sub>	4.08	1.01	–	–

\*Note: see the footnote to Table 1.

Table 4

**Relationship between electronegativities of plumbates and their binding properties**

Compound	EN <sub>comp</sub>	EN <sub>rel</sub>	Binding properties*	
			under hydrothermal conditions	under hydrothermal conditions
2BaO·PbO <sub>2</sub>	3.11	0.77	+	–
2SrO·PbO <sub>2</sub>	3.18	0.79	+	–
2CaO·PbO <sub>2</sub>	3.27	0.81	+	+
BaO·PbO <sub>2</sub>	3.51	0.87	+	+
SrO·PbO <sub>2</sub>	3.56	0.88	+	+
CaO·PbO <sub>2</sub>	3.63	0.90	+	+
2CdO·PbO <sub>2</sub>	4.06	1.01	–	–
CdO·2PbO <sub>2</sub>	4.37	1.08	–	–

\*Note: see the footnote to Table 1.

Table 5

**Relationship between electronegativities of titanates and their binding properties**

Compound	EN <sub>comp</sub>	EN <sub>rel</sub>	Binding properties*	
			under hydrothermal conditions	under hydrothermal conditions
3BaO·TiO <sub>2</sub>	2.76	0.68	+	×
3SrO·TiO <sub>2</sub>	2.83	0.70	Δ	×
2BaO·TiO <sub>2</sub>	2.90	0.72	+	+
3CaO·TiO <sub>2</sub>	2.93	0.73	+	Δ
2SrO·TiO <sub>2</sub>	2.97	0.74	+	+
3BaO·2TiO <sub>2</sub>	3.02	0.75	+	Δ
2CaO·TiO <sub>2</sub>	3.06	0.76	+	+
3SrO·2TiO <sub>2</sub>	3.08	0.76	Δ	Δ
4SrO·3TiO <sub>2</sub>	3.12	0.77	Δ	Δ
3CaO·2TiO <sub>2</sub>	3.16	0.78	+	+
BaO·TiO <sub>2</sub>	3.18	0.79	–	+
4CaO·3TiO <sub>2</sub>	3.20	0.79	×	Δ
SrO·TiO <sub>2</sub>	3.23	0.80	–	+
2MgO·TiO <sub>2</sub>	3.28	0.81	–	Δ
CaO·TiO <sub>2</sub>	3.30	0.82	–	+
BaO·2TiO <sub>2</sub>	3.45	0.86	–	+
MgO·TiO <sub>2</sub>	3.47	0.86	–	+
MgO·2TiO <sub>2</sub>	3.64	0.90	–	–
BaO·4TiO <sub>2</sub>	3.66	0.91	–	–
2CdO·TiO <sub>2</sub>	3.79	0.94	–	–
CdO·TiO <sub>2</sub>	3.84	0.95	–	–
2ZnO·TiO <sub>2</sub>	3.89	0.96	–	–
ZnO·TiO <sub>2</sub>	3.91	0.97	–	–

\*Note: see the footnote to Table 1.

Table 6  
Relationship between electronegativities of aluminates and their binding properties

Compound	EN <sub>comp</sub>	EN <sub>rel</sub>	Binding properties*
10BaO·Al <sub>2</sub> O <sub>3</sub>	2.49	0.62	×
8BaO·Al <sub>2</sub> O <sub>3</sub>	2.55	0.63	×
7BaO·Al <sub>2</sub> O <sub>3</sub>	2.57	0.64	×
5BaO·Al <sub>2</sub> O <sub>3</sub>	2.65	0.66	×
4BaO·Al <sub>2</sub> O <sub>3</sub>	2.71	0.67	×
2BaO·2SrO·Al <sub>2</sub> O <sub>3</sub>	2.74	0.68	×
3BaO·CaO·Al <sub>2</sub> O <sub>3</sub>	2.75	0.68	–
4SrO·Al <sub>2</sub> O <sub>3</sub>	2.77	0.69	+
3BaO·Al <sub>2</sub> O <sub>3</sub>	2.79	0.69	+
3SrO·Al <sub>2</sub> O <sub>3</sub>	2.85	0.71	+
3CaO·Al <sub>2</sub> O <sub>3</sub>	2.93	0.73	+
12CaO·7Al <sub>2</sub> O <sub>3</sub>	3.07	0.76	+
BaO·Al <sub>2</sub> O <sub>3</sub>	3.11	0.77	+
SrO·Al <sub>2</sub> O <sub>3</sub>	3.15	0.78	+
2CaO·SrO·3Al <sub>2</sub> O <sub>3</sub>	3.18	0.79	+
CaO·Al <sub>2</sub> O <sub>3</sub>	3.19	0.79	+
BaO·2CaO·4Al <sub>2</sub> O <sub>3</sub>	3.23	0.80	+
SrO·2Al <sub>2</sub> O <sub>3</sub>	3.29	0.82	+
CaO·2Al <sub>2</sub> O <sub>3</sub>	3.32	0.82	+
BaO·6Al <sub>2</sub> O <sub>3</sub>	3.42	0.84	–
SrO·6Al <sub>2</sub> O <sub>3</sub>	3.43	0.85	–
CaO·6Al <sub>2</sub> O <sub>3</sub>	3.44	0.85	–

\*Note: see the footnote to Table 1.

Table 7  
Relationship between electronegativities of gallates and their binding properties

Compound	EN <sub>comp</sub>	EN <sub>rel</sub>	Binding properties*
4BaO·Ga <sub>2</sub> O <sub>3</sub>	2.93	0.73	×
4SrO·Ga <sub>2</sub> O <sub>3</sub>	3.00	0.74	+
7SrO·2Ga <sub>2</sub> O <sub>3</sub>	3.06	0.76	Δ
3BaO·Ga <sub>2</sub> O <sub>3</sub>	3.07	0.76	+
3SrO·Ga <sub>2</sub> O <sub>3</sub>	3.13	0.78	Δ
3CaO·2Ga <sub>2</sub> O <sub>3</sub>	3.20	0.79	Δ
3CaO·Ga <sub>2</sub> O <sub>3</sub>	3.21	0.80	+
3SrO·2Ga <sub>2</sub> O <sub>3</sub>	3.45	0.86	Δ
BaO·Ga <sub>2</sub> O <sub>3</sub>	3.60	0.89	+
SrO·Ga <sub>2</sub> O <sub>3</sub>	3.64	0.90	+
CaO·Ga <sub>2</sub> O <sub>3</sub>	3.69	0.92	+
SrO·2Ga <sub>2</sub> O <sub>3</sub>	3.90	0.97	+
CaO·2Ga <sub>2</sub> O <sub>3</sub>	3.94	0.98	+
BaO·6Ga <sub>2</sub> O <sub>3</sub>	4.14	1.03	×
SrO·6Ga <sub>2</sub> O <sub>3</sub>	4.15	1.03	×
CaO·6Ga <sub>2</sub> O <sub>3</sub>	4.16	1.03	×

\*Note: see the footnote to Table 1.

Table 8  
Relationship between electronegativities of ferrites and their binding properties

Compound	EN <sub>comp</sub>	EN <sub>rel</sub>	Binding properties*
5BaO·Fe <sub>2</sub> O <sub>3</sub>	2.84	0.70	×
7BaO·2Fe <sub>2</sub> O <sub>3</sub>	3.00	0.74	Δ
7SrO·2Fe <sub>2</sub> O <sub>3</sub>	3.06	0.76	Δ
3BaO·Fe <sub>2</sub> O <sub>3</sub>	3.07	0.76	+
3SrO·Fe <sub>2</sub> O <sub>3</sub>	3.13	0.78	Δ
2BaO·Fe <sub>2</sub> O <sub>3</sub>	3.27	0.81	+
2SrO·Fe <sub>2</sub> O <sub>3</sub>	3.33	0.83	+
2CaO·Fe <sub>2</sub> O <sub>3</sub>	3.40	0.84	+
3SrO·2Fe <sub>2</sub> O <sub>3</sub>	3.46	0.86	×
BaO·Fe <sub>2</sub> O <sub>3</sub>	3.61	0.89	–
SrO·BaO·2Fe <sub>2</sub> O <sub>3</sub>	3.63	0.90	–
SrO·Fe <sub>2</sub> O <sub>3</sub>	3.65	0.91	–
CaO·BaO·2Fe <sub>2</sub> O <sub>3</sub>	3.66	0.91	–
CaO·Fe <sub>2</sub> O <sub>3</sub>	3.71	0.92	–
2BaO·3Fe <sub>2</sub> O <sub>3</sub>	3.79	0.94	–
CaO·2Fe <sub>2</sub> O <sub>3</sub>	3.95	0.98	–
BaO·6Fe <sub>2</sub> O <sub>3</sub>	4.16	1.03	–
SrO·6Fe <sub>2</sub> O <sub>3</sub>	4.17	1.03	–

\*Note: see the footnote to Table 1.

of EN<sub>rel</sub> values for such compounds as silicates and aluminates. These results allow evaluating the binding properties and selecting the most favorable hardening conditions.

It should be noted that the development of new special cement compositions in terms of both ternary oxide compounds [5,8,12] and even more complicated ones [13,14] is of great interest. The approach given on the present work is very promising to this end. For instance, zirconates of alkaline-earth elements do not show any binding properties and their EN<sub>rel</sub> values are not included in the range corresponding to the presence of binding properties. However, a ternary compound, calcium aluminozirconate 7CaO·3Al<sub>2</sub>O<sub>3</sub>·ZrO<sub>2</sub> (EN<sub>rel</sub>=0.76), exhibits binding properties and is an important component of zirconium-containing refractory cements [10]. The analysis of the obtained data shows that some zirconosilicates that are hardened under hydrothermal conditions can be used for the production of special binders, including bioactive materials [15].

In our opinion, our data will contribute to the study of the binding properties of complicated oxide compounds containing both polyatomic cations and complex anions.

Table 9

## Relationship between electronegativities of some ternary and quaternary compounds and their binding properties

Compound	EN <sub>comp</sub>	EN <sub>rel</sub>	Binding properties*	
			under hydrothermal conditions	under hydrothermal conditions
20CaO·3MgO·13Al <sub>2</sub> O <sub>3</sub> ·3SiO <sub>2</sub>	2.82	0.70	+	–
7CaO·3Al <sub>2</sub> O <sub>3</sub> ·ZrO <sub>2</sub>	3.07	0.76	+	–
4CaO·Al <sub>2</sub> O <sub>3</sub> ·Fe <sub>2</sub> O <sub>3</sub>	3.21	0.80	+	+
2CaO·Al <sub>2</sub> O <sub>3</sub> ·SiO <sub>2</sub>	3.28	0.81	–	+
6SrO·ZrO <sub>2</sub> ·5SiO <sub>2</sub>	3.31	0.82	×	Δ
7SrO·ZrO <sub>2</sub> ·6SiO <sub>2</sub>	3.31	0.82	×	Δ
3BaO·3Al <sub>2</sub> O <sub>3</sub> ·2SiO <sub>2</sub>	3.32	0.82	–	+
3CaO·ZrO <sub>2</sub> ·2SiO <sub>2</sub>	3.36	0.83	–	+
2SrO·6Al <sub>2</sub> O <sub>3</sub> ·ZrO <sub>2</sub>	3.40	0.84	×	Δ
BaO·Al <sub>2</sub> O <sub>3</sub> ·SiO <sub>2</sub>	3.45	0.86	–	+
BaO·Al <sub>2</sub> O <sub>3</sub> ·2SiO <sub>2</sub>	3.55	0.88	–	+
SrO·Al <sub>2</sub> O <sub>3</sub> ·2SiO <sub>2</sub>	3.57	0.88	×	Δ
2CaO·ZrO <sub>2</sub> ·4SiO <sub>2</sub>	3.59	0.89	–	–
CaO·Al <sub>2</sub> O <sub>3</sub> ·2SiO <sub>2</sub>	3.60	0.89	–	–
2BaO·2ZrO <sub>2</sub> ·3SiO <sub>2</sub>	3.61	0.90	×	×
SrO·ZrO <sub>2</sub> ·2SiO <sub>2</sub>	3.70	0.92	×	×
CaO·ZrO <sub>2</sub> ·2SiO <sub>2</sub>	3.73	0.93	×	×
BaO·ZrO <sub>2</sub> ·3SiO <sub>2</sub>	3.77	0.94	×	×

\*Note: see the footnote to Table 1.

Table 10

## Electronegativity value ranges where oxide compounds show their binding properties

Compounds	According to our calculation				According to Fedorov's calculation			
	Normal conditions		Hydrothermal conditions		Normal conditions		Hydrothermal conditions	
	EN <sub>comp</sub>	EN <sub>rel</sub>	EN <sub>comp</sub>	EN <sub>rel</sub>	EN <sub>comp</sub>	EN <sub>rel</sub>	EN <sub>comp</sub>	EN <sub>rel</sub>
Silicates	2.80–3.22	0.69–0.80	2.97–3.39	0.74–0.84	2.73–3.00	0.68–0.74	3.31–3.38	0.82–0.83
Germanates	2.90–3.41	0.72–0.85	2.90–3.62	0.72–0.90	–	–	–	–
Stannates	3.04–3.44	0.75–0.85	3.20–3.51	0.79–0.87	2.87–3.31	0.71–0.82	3.00–3.29	0.74–0.81
Plumbates	3.11–3.63	0.77–0.90	3.27–3.63	0.81–0.90	2.87–3.27	0.70–0.81	2.97–3.27	0.73–0.81
Titanates	2.76–3.16	0.68–0.77	2.90–3.47	0.72–0.86	2.75–2.90	0.68–0.72	–	–
Aluminates	2.77–3.32	0.69–0.82	–	–	2.76–3.01	0.68–0.74	–	–
Gallates	3.00–3.94	0.74–0.98	–	–	–	–	–	–
Ferrites	3.00–3.40	0.74–0.84	–	–	–	–	–	–

It is obvious that electronegativity cannot be a single criterion determining binding properties. However, it should be taken into consideration when evaluating the behavior of various oxide compounds with regard to the potential binding properties.

### Conclusions

The values of relative electronegativity for more than 168 silicates, germanates, stannates, plumbates, titanates, aluminates, gallates, ferrites, alumoferrites and aluminosilicates of alkali and alkaline-earth elements as well as zirconium-containing compounds have been calculated by using the Batsanov's

electronegativity concept. We have revised the range of relative electronegativities, where compounds display binding properties. A great number of binary and ternary compounds (about 100) are within the specified range. In terms of our data, the binding properties of oxide compounds (including those which binding properties have not been completely studied yet) and possibility of their application in special cements technology can be evaluated. Besides, the obtained data will allow selecting the most favorable conditions for compound hardening.

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Received 02.02.2020

### В'ЯЖУЧІ ВЛАСТИВОСТІ ОКСИДНИХ СПОЛУК СПЕЦІАЛЬНИХ ЦЕМЕНТІВ ПРИ ВЗАЄМОДІЇ З ВОДОЮ

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Для цілеспрямованого синтезу спеціальних полімінеральних цементів необхідно мати інформацію про в'язучі властивості окремих фаз, що входять до їх складу. Незважаючи на численні дослідження, дотепер немає чітких теоретичних критеріїв (хоча б якісних, не кажучи вже про кількісні) для оцінювання поведінки різних оксидних сполук щодо можливості їх використання в хімії спеціальних цементів. Тому актуальною проблемою хімії в'язучих матеріалів є розробка кількісних залежностей, а також виявлення фізико-хімічних умов, що визначають наявність в'язучих властивостей. Нами показано, що за допомогою концепції електронегативності можна досить чітко визначити певний інтервал значень відносних електронегативностей, в якому розглянуті сполуки виявляють в'язучі властивості. Встановлено, що в межах визначеного інтервалу знаходиться численна група бінарних і потрійних сполук (близько 100), включно з тими, в'язучі властивості яких ще не вивчені повністю. Крім того, отримані дані дозволять вибрати найбільш сприятливі умови для тверднення цих сполук. Таким чином, на основі отриманих даних можна оцінити наявність в'язучих властивостей оксидних сполук і перспективи їх застосування в технології спеціальних цементів.

**Ключові слова:** кислотно-основні властивості, електронегативність, в'язучі властивості, умови тверднення, спеціальні цементы.

### BINDING PROPERTIES OF OXIDE COMPOUNDS OF SPECIAL CEMENTS IN INTERACTION WITH WATER

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To synthesize special multiminerall cements, it is necessary to have information concerning binding properties of individual phases being part of given cements. Despite numerous studies, there are not yet clear theoretical criteria to evaluate the behavior of various oxide compounds (if only qualitatively, not to mention quantitatively) with respect to their possible use in chemistry of special cements. Therefore, the development of corresponding quantitative dependences as well the ascertainment of the physical and chemical conditions determining the binding properties remain the actual task of chemistry of binding materials. Our study shows that a certain range of relative electronegativity values, where compounds under consideration reveal their binding properties, can be determined clearly by means of the concept of electronegativity. It is ascertained that some binary and ternary compounds (about 100) lie within a certain range of relative electronegativity, including those ones which binding properties have not been fully studied yet. Besides, the obtained data will allow selecting the most favorable conditions for compound hardening. Thus, in terms of our findings, the binding properties of oxide compounds and prospects of their application in special cement technology can be evaluated.

**Keywords:** acid-base properties; electronegativity; binding properties; hardening conditions; special cements.

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