

## BASIC AND SUBSIDIARY ATOM PARAMETERS. 2. ELECTRONEGATIVITY, BINDING ENERGY, AND FERSMANS OF ATOMS

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UDC 539.183 + 539.218

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№ 2001

We show that the electronegativity of an atom is connected with its Fersman by the equations of the first and second degrees, and the energy of the cation-anion interaction is connected with the difference of the Fersmans of atoms. Fersman is a complex parameter connected with the serial number of an element, an ion radius, and a summary potential of ionization at a maximum valency.

In [1], we introduced the new complex atom parameters, namely,  $R_F = (r \Sigma I)/N$ ,  $R_p = R_F/r^2$ , and  $R_G = R_F/v$  named by us Fersman and Goldshmidt with  $\Sigma I$  as a total ionization potential of valent electrons,  $N$  - an element serial number,  $r$  - an ion radius. The availability of those atom parameters enabled us with high exactness to determine the density of metals, which was obtained with the help of linear equations.

While introducing new atom parameters, its very important to find out their relationship with the previously known ones to be able to describe the properties of compounds and, first of all, the relationship of a given atom to others. We calculated Fersmans of anions which are given in Tab. 1 in the second line under the symbol of the corresponding element. The values of electronegativity  $X$  of those elements are given above. As is generally known, the notion of electronegativity was introduced for the first time in 1932 by L. Pauling. The problem was thoroughly studied in the voluminous literature, but we would like to attract readers' attention only to two papers [2, 3]. To calculate electronegativity  $X$ , Pauling used the binding energy of  $A^-A$ ,  $B^-B$ , and  $A^-B$  atoms for 14 elements specially underlined in Tab. 1.

Let us take into consideration the fact that 13 elements among them belong to 25  $B$ -elements whose  $p$ -shells are filled partly. It is  $\Delta X$  difference that matters, and Pauling assigned a special part to hydrogen and postulated the value of  $X$  equal to 2.1 for it. He noted that the limit of exactness in calculations was the first decimal number.

The H - At diagonal separates metals from non-metals [4]. If we place  $Tl^{1+}$  having the lowest value of  $R_F$  against H in the left low corner of Tab. 1, the

Tl - F diagonal connects, in this case, an ion of the lowest values of  $X$  and  $R_F$  (Tl) with an ion of the highest values of  $X$  and  $R_F$  (F). Let us note that fluorine has  $X$  equal to 4.0 and called by Pauling superhalogen. It has the maximum of  $R_F$  which is approximately three times higher than oxygen and chlorine, fluorine's nearest neighbours, have. There is no any more leap of  $R_F$  changes in the Periodic system during the transition from one element to another. And this is not casual. We investigated the change of  $X$  depending on the change  $R_F$  during the transition from one element to another, and we did it both along the periods and along the subgroups. Their interdependence is well approximated by linear equations

$$X = \alpha R_F + \beta \quad (1)$$

for  $A^-$  elements and by square equations

$$X = \gamma (R_F)^3 + \delta R_F + \varepsilon, \quad (2)$$

Table 1

H 2.1				
	B 2.0 23.03	C 2.5 39.80	N 3.0 46.13	O 3.5 43.03
	Al 1.5 12.51	Si 1.8 23.17	P 2.1 33.28	S 2.5 33.46
	Ga 1.7 8.68	Ge 1.9 12.24	As 2.0 14.70	Se 2.4 21.15
	In 1.8 7.65	Sn 1.9 2.55	Sb 1.9 13.53	Te 2.1 19.32
	Tl 2.0 5.62	Pb 2.2 7.61	Bi 1.9 10.50	Po 2.0 17.66
$Tl^{1+}$ 1.6 0.83				F 4.0 129.91
				Cl 3.0 42.66
				Br 2.8 33.18
				J 2.6 29.96
				At 2.2 23.05

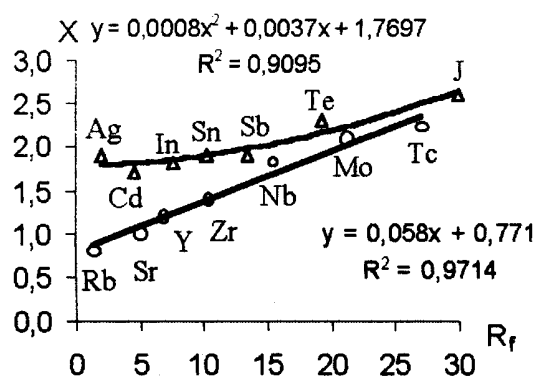


Fig. 1

for B-elements. Fig. 1 shows the graphs and the equations for one of the periods. For other periods, the tendencies are analogous. The coefficients of the equations for corresponding subgroups are given in Tab. 2. The genuine truth of values for elements of

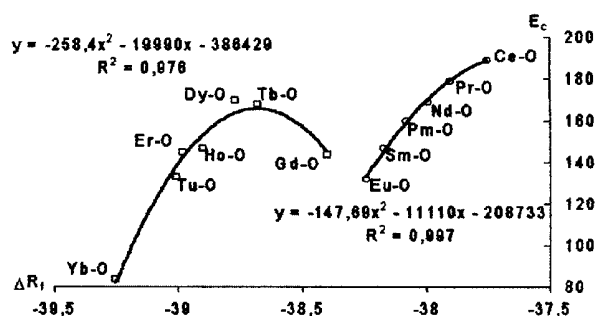


Fig. 2

1-B, 2-B subgroups is conditioned by the fact that there are only 3 elements in each subgroup. We used X values calculated for molecules. The picture of X values calculated for crystals shows the same tendencies with some differences of minor importance.

As electronegativity was calculated on the basis of the binding energy  $E_c$  of atoms (ions), we investigated the dependence of  $E_c$  on the difference of the Fermans

Table 2

Cations	Functions	Arguments		Anions	Coefficients					$R^2$
		$R_F$	$\Delta R_F$		$\alpha$	$\beta$	$\gamma$	$\delta$	$\epsilon$	
1A	X	+	~	~	0.0262	0.7543	-	-	-	0.9037
2A	X	+	~	~	0.0403	0.7661	-	-	-	0.9499
3A	X	+	~	~	0.0302	0.9844	-	-	-	0.9998
4A	X	+	~	~	0.0257	1.1151	-	-	-	0.9830
5A	X	+	~	~	0.0257	1.5205	-	-	-	0.9934
6A	X	+	~	~	0.0070	1.9859	-	-	-	0.7080
1B	X	+	~	~	-	-	0.7061	~2.9939	5.0634	1
2B	X	+	~	~	-	-	~0.0029	~0.1381	2.3940	1
3B	X	+	~	~	-	-	0.0028	~0.0673	2.0762	0.9147
4B	X	+	~	~	-	-	0.0016	~0.0627	2.4598	0.9743
5B	X	+	~	~	-	-	0.0012	~0.0310	1.9095	0.9550
7B	X	+	~	~	-	-	~0.0002	0.0407	1.4331	0.9978
1A	$E_c$	~	+	F	-	-	0.7152	~179.78	11412	0.9968
1A	$E_c$	~	+	Cl	-	-	0.0321	~0.4073	65.028	0.9831
1A	$E_c$	~	+	Br	-	-	0.0073	~0.2131	91055	0.7632
1A	$E_c$	~	+	J	-	-	0.0836	~0.7950	33.691	0.9762
4B	$E_c$	~	+	F	-	-	~0.0881	~17.653	~747.31	0.8307
4B	$E_c$	~	+	Cl	-	-	~0.0997	~3.3657	84.354	0.7450
4B	$E_c$	~	+	Br	-	-	~0.0763	~0.7901	94.723	0.7901
4B	$E_c$	~	+	J	-	-	~0.1241	~1.4150	75.966	0.9994
4B	$E_c$	~	+	O	-	-	~0.0944	1.0341	258.29	0.9570
4B	$E_c$	~	+	S	-	-	~0.1028	0.3430	169.95	0.9012
4B	$E_c$	~	+	Se	-	-	~0.0987	2.2167	129.42	0.8712
4B	$E_c$	~	+	Te	-	-	~0.3535	1.3092	120.34	0.9883
Ln	$E_c$	~	+	O	-	-	~147.69	~11110	~208733	0.997
b	$E_c$	~	+	O	-	-	~258.40	~19940	~386429	0.976
a	$E_c$	~	+	S	-	-	~87.442	~4851.8	~671480	0.9926
b	$E_c$	~	+	S	-	-	~127.16	~7345.5	105951	0.9264
a	$E_c$	~	+	Se	-	-	0.7955	125.17	1899.3	0.9930
b	$E_c$	~	+	Se	-	-	~48.554	~1578.1	~12717	0.7874
a	$E_c$	~	+	Te	-	-	89.369	2628	19373	0.9796
b	$E_c$	~	+	Te	-	-	~58.451	~1696.1	12220	0.7790

$\Delta R_F$  of a cation and an anion<sup>1</sup>. The values of  $E_c$  were taken from [5]. As the determination errors of different bound pairs usually change from parts of percentage to 30 per cent, we chose those atom groups for our investigation which determination errors are minimal:  $A^1 - B^7$ ,  $B^4 - B^6$ ,  $B^4 - B^7$ ,  $Ln - B^6$ . Fig. 2 and Tab. 2 show that the function  $E_c = F(\Delta R_F)$  is described by the equation of type 2. For lanthanides, it's necessary to have two equations. The tendency of the binding energy change of six elements (*a*) (Ce, Pr, Nd, Pm, Sm, Eu) is observed rather clearly both for oxygen and chalcogens. For other elements (*b*), this tendency is expressed less clearly and lutecium has such a high value of  $E_c$  that it is described neither by Eq. (1) nor by Eq. (2).

The analysis of 112 bound pairs enables us to come to the conclusion that the atom binding energy  $E_c$  as well as electronegativity  $X$  are conditioned by basic atom parameters: a serial number, a total ionization potential of valent electrons and an ion radius. This opens wide perspectives for the more exact determination of  $X$  and the investigation of properties of compounds in those cases where the conception of electronegativity has not realized itself.

Nowadays a great number of different atom parameters are used for the classification of compounds and the description of their properties. The main quantum number and charge as well as their effective values are introduced into practice. The mentioned effective values are calculated according to definite rules. A few variants of radii are brought forward. They are ionic, covalent, metallic, tetrahedral, octahedral, and so on. Besides that, the value of a radius depends on the multiplicity of a bond. An atom valence in compounds is not a constant value, and atom ionization

potentials depend on the environment of a given atom. One can speak with certainty only about the invariability of an element serial number. This is why, the attempts to use one parameter or two-three parameters like the energy of atomization [6], the difference and the sum of radii of *s*-shells and *p*-shells [7], and the sum of serial numbers [8] give only a limited result. It is natural that, by passing from one compound to another, a Fersman also undergoes certain changes. Maybe, it is the tendencies of the change of complex parameters analogous to those of a Fersman that will enable one to move essentially forward to the solution of the most important problem in materials science, the prognosis of compounds' properties depending on their structure and their composition, as the use of multiciphered coefficients in the epoch of computers does not complicate this solution.

It is a pleasure for the author to thank V.G. Bar'yakhtar for stimulating discussions. The author is grateful to A.S. Menilenko and O. Biratshna for their help.

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Received 31.08.99

<sup>1</sup>The sum of Fersmans leads to analogous equations with less truth.