Bond dissociation energies for alkaline fluorides.

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Abstract. The whole array of experimental data on the bond dissociation energy (*BDE*) and bond length values for alkaline fluorides was analysed. To this end the fundamental correlation of bond energy with its length was applied. According to experimental data the bond M-F (M = Li, Na, K, Rb, Cs) is formed via overlapping of the occupied *p*-orbital of fluorine and unoccupied *p*-orbital of alkaline metal, which can be considered as "π-bond". These bonds can be either in degenerate or non-degenerate states. The influence of measuring process on the result, as well as application of the resonance theory to alkaline fluorides, is discussed.

Introduction. The chemical bond in alkaline fluorides is formed by two atoms "situated" at the opposite poles of electronegativity. Therefore, one should expect the complete electron transfer from lithium to fluorine and consequently the ionic bond formation according to Kossel [1]. However, Coulomb correlation of bond length and dissociation energy of the bond metal-fluorine does not correspond to experimental data.

Swepston et al. in their work [2] dealt with geometry of LiF molecule. The authors suggested that, besides electrostatic interaction, there is a stabilising interaction between HOMO of fluorine atom and LUMO of lithium atom to form an acetylene-like structure i.e. so called "π-bonds". In the case of other metals, *d*- and *f*-orbitals can act as LUMO. The possibility of the reverse donorship and HOMO-LUMO interaction in lanthanides fluorides was also discussed in the work [3]. Initially the reverse donorship to form the "π-bonding" was suggested in the Dewar-Chatt-Duncanson model [4, 5] regarding transition metals carbonyls.

Thus far the hypothesis of the "π-bonding", present in alkaline fluorides, was not confirmed by any experimental data. All carried out theoretical researches (both quantum calculations and phenomenological approach) dealing with bond dissociation energy values *BDE* (M-F), where M = Li, Na, K, Rb, Cs, suffer from one common drawback: the researchers pick one experimental value *BDE* (M-F) and attempt to reproduce it with varying degrees of success (See, for example, the review [6]). However, there are a lot of experimentally obtained *BDE* (M-F) values corresponding to the same chemical bond but at the same time differing from each other (See, for instance, [7-13]). The observed values differences are too high to be considered as a simple error of the experiment or a width of the spectral line.

At the same time, taking into account the hypothesis of "π-bonding" in alkaline fluorides, one can give an explanation of the obtained data *BDE* (M-F). First of all, "π-bond" can be in

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either degenerate or two non-degenerate states. Moreover, in HOMO-LUMO interaction the participation of *p*-orbitals, as well as *d*- and *f*-orbitals as LUMO, in combination with its possible degenerate and non-degenerate states, can give close but different values *BDE* (M-F). Since this splitting is quite low, it does not have a significant effect on the bond energy, but it can dramatically influence on the geometry of ligands surrounding the central atom. It can also be, however, a result of such quantum phenomenon as effect of measuring device on the experiment outcome (See, for example, a recent review [14]). For instance, the bond length values in cesium halides, determined by spectroscopic methods and electron diffraction method, have a systematic difference approximately 1.5% [15].

In previous work [16, 17] we successfully applied the law of correlation of bond energy with its length for calculations. Herein, we provide the calculations for all experimentally observed values *BDE* depending on reasonable parameters such as quantum numbers. We are going to test a hypothesis of "π-bonding" in alkaline fluorides by using some aspects of the resonance theory, as well as to consider the previously not-discussed influence of measuring process on the experimental outcome.

Calculation method. The correlation between the energy of chemical bond and its length is described by equations (1-4). Equation (1) is derived from Yukawa's ideas applied to the problems of the chemical bond [18]. It serves as an answer to a simple question: "Is there any particle corresponding to the strength holding two protons in the molecule of hydrogen? If yes, what is mass of such particle?" Equation (2) determines the wave length of the first valence electron in any atom. In equation (3), instead of gauge electromagnetic field (Coulomb interaction), we use curvature of space *via* replacement of bond length r with effective bond length R. Due to the fact that parameter R is of discrete nature, it greatly facilitated the mathematic calculations. Quantisation is due to the experimental fact that kinetic energy of the first valence electron is always higher than bond energy.

$$BDE = \frac{n \cdot z_1 \cdot z_2}{R} \cdot e^{-\frac{n \cdot R}{k \cdot \lambda}} \qquad (1)$$

$$\lambda = \frac{\alpha \cdot \hbar \cdot c}{2 \cdot \left(m \cdot \alpha^2 \cdot c^2 - I_D\right)} \qquad (2)$$

$$R = r + \lambda \cdot \sum_{i=0}^{2} t_i \cdot \left(\frac{\beta}{\alpha}\right)^{2 \cdot i} \qquad (3)$$

$$\beta = \frac{g^2}{\hbar \cdot c} \qquad (4)$$

where $\hbar$ – Planck constant; m – rest mass of an electron; c – speed of light, α – fine structure constant; r – bond length; R – effective bond length; z_i – coupling constant (charge), has following values: $e = \sqrt{\alpha \cdot \hbar \cdot c} = 1.518885 \times 10^{-14} J^{\frac{1}{2}} \cdot m^{\frac{1}{2}}$, $q = \frac{1}{3}e$,

$g = 1.03682 \times 10^{-14} J^{1/2} \cdot m^{1/2}$, it should be noted that $g \approx \frac{2}{3}e$; n – bond order; k – integer parameter[2]; I_D – donor ionisation potential, as a rule, donor is an atom which forms cation after heterolytic bond dissociation[3]. All values of first ionisation potential were used from the work [4], t_i – integer parameters having properties of quantum numbers and taking values: $t_0 = 0, \pm 1, \pm 2, \ldots$; $t_1 = 0, \pm 1, \pm 2, \ldots$; $t_2 = 0, \pm \frac{1}{4}, \pm \frac{1}{2}, \pm \frac{3}{4}, \pm 1, \ldots$; etc.

Results and discussion. Equations (1-4) contain parameters, characterising the chemical bond in question (BDE – bond energy, r – bond length, z_i – coupling constant (charge), n – bond order; k – acceptor integer parameter; I_D – donor ionisation potential), and parameters describing the state of this bond (quantum numbers t_i). In present work we aim to find the values of bond parameters (first of all, n, I_D) which give a good agreement of calculation results of several values BDE (for one exact chemical bond) with experimental data when varying one quantum number. Ideally, the varied quantum number should form a continuous sequence.

In all calculations we used following values $z_1 \cdot z_2 = e \cdot e$; $k_F = 7$, $t_0 = 0$; the values of other parameters are given for each case separately.

Li-F. Using molecule Li-F as an example, we share in detail how the known experimental data on bond energy and length were analysed. For other alkaline fluorides the procedure is analogous and only the results are given.

Equation (2) contains one parameter, which directly indicates the donor in the pair of atoms forming chemical bond, namely first ionisation potential of donor. To determine the state of the chemical bond (σ or π) in the molecule one should compare the calculations results by equations (1-4) for I_{Li} (σ-bond) and I_F (π-bond).

At first, we calculate the step change of effective bond length for various values $\Delta t_i = 1$.

Table 1. Step change of effective bond length (A°) when varying $\Delta t_i = 1$

Quantum numbers	Donor	
	Metal (σ-bond) A°	Fluorine (π-bond) A°
t_0	0.33	0.7355
t_1	0.0716	**0.1597**
t_2	0.0039	0.0087

We calculate effective bond length R, and its difference ΔR with experimental bond length $r_{Li-F} = 1.564$ A° [19, 20] for both cases – I_D of lithium (σ-bond) and I_D of fluorine (π-bond), taking into account the recommended experimental value BDE (Li-F)= 5,98 eV [7, 8].

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[2] Parameter k in all cases (except for $k_N=5$, $k_O=6$, and $k_F=7$) equals doubled number of valence electrons of acceptor, i.e. atom having higher electronegativity and forming anion after heterolytic bond dissociation.

[3] However, in the case when the bond is formed *via* electron pair of ligand, first ionization potential of anion is used in calculations.

Table 2. Effective bond length R_{Li-F} and its deviation ΔR from experimental value r_{Li-F}=1.564 Aº

	Donor	
	Li (σ-bond) Aº	F (π-bond) Aº
R	1.3452	1.7237
ΔR	-0.2188	**0.1597**

Comparing results from Tables 1 and 2 one can observe the agreement of calculated and experimental values *BDE* (Li-F) with the use of the following parameters in equations 1-4.

Table 3. Calculations of *BDE* (Li-F) for cases «σ-bond» I_{Li} and «π-bond» I_F

parameter				*BDE*(Li-F) eV	
r Aº	I_D eV[a]	t_1	t_2	calk.	exp.
1.564	5.3918(Li)	1	0	4.337	5.98[a]
1.564	17.4231(F)	1	0	**5.978**	5.98±0.2[b]

[a] reference [7], [b] reference [8]

There are also other experimental values *BDE* (Li-F) [10-13]. The calculations results for all of them are given in Table 4.

Table 4. The calculations of all experimental values *BDE* (Li-F) for which the following data were used: r_{Li-F}=1.564 Aº, I_F=17.4231 eV, t_1=1, $n = 1$ (an ethylene-like structure). The only varying parameter was t_2.

parameter	*BDE*(Li-F) eV	
t_2	calk.	exp.
0	5.978	5.98[a], 5.98±0.2[b], 5.975[c]
¼	5.938	5.963[d]
¼	5.938	5.938 average[e]
½	5.898	5.909[f]
½	5.898	5.898±0.35[g]

[a] reference [7]; [b] reference [8]; [c] reference [13]; [d] reference [11]; [e] average between extreme values; [f] reference [10], [g] reference [12].

In Table 3 it was shown that calculated values *BDE* (Li-F) are in good agreement with experimental data when I_D of fluorine was used. Table 4 shows that experimental values *BDE* (Li-F) in range 5.98 eV, 5.98±0.2 eV, 5.975 eV and those in range 5.909 eV, 5.898±0.35 eV both correspond to two non-degenerate states of π-bond. At the same time, the average values *BDE* (Li-F) 5.963 eV and 5.938 eV correspond to non-degenerate state of π-bond. Therefore, according to all above, we have a conclusion that in alkali fluorides π-bonding takes place.

In all following calculations we use by default fluorine ionisation potential as donor ionisation potential and bond order equals 1.

NaF. Sodium fluoride has following experimental data: r_{Na-F}=1.926 Aº [19] and *BDE* (Na-F) equaling 5.3296 eV[10] and 4,95±0,2 eV [7, 8, 11]. We assume that values *BDE* (Na-F) correspond to two non-degenerate states. In this case, their average, corresponding to degenerate

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state, should reproduce by calculations for r_{Na-F}=1.926 Aº. The validation results of this assumption are given in Table 5.

Table 5. The calculations of all experimental values *BDE* (Na-F) for which the following data were used: r_{Na-F}=1.926Aº [19], I_F=17.4231 eV, t_1= 0, n = 1. The only varying parameter was t_2.

parameter	*BDE*(Na-F) эв	
t_2	calk.	exp.
1½	4.958	4,95±0,2[a]
0	5.143	5.14 average
-1½	5.34	5.33[b]

[a] reference [7, 8, 11]; [b] reference [10]

KF, RbF, CsF. The work [9] contains the upper dissociation limits measured spectroscopically for these molecules. The results of our calculations for all experimentally observed data *BDE* (K-F), *BDE* (Rb-F), and *BDE* (Cs-F) are given in Tables 6, 7, and 8 correspondingly.

Table 6. The calculations of all experimental values *BDE* (K-F) for which the following data were used: r_{K-F}=2.1714Aº [19], I_F=17.4231 eV, t_1= -1, n = 1. The only varying parameter was t_2.

parameter	*BDE*(K-F) eV	
t_2	calk.	exp.
-2	5.084	5.0695[a]; 5.0699[b]
-2 ¼	5.115	5.0998[c]; 5.117±0,087[d] 5.113 average[e]
-2 ½	5,147	5.156[f]
-3 ¾	5.31	<5.317[g]

[a] reference [8]; [b] reference [10]; [c] reference [11]; [d] reference [7]; [e] average between extreme values; [f]thermodynamic data used from [9]; [g] upper limits for the dissociation energies, data from [9].

Table 7. The calculations of all experimental values *BDE* (Rb-F) for which the following data were used: r_{Rb-F}=2.2704Aº [19], I_F=17.4231 eV, t_1= -2, n = 1. The only varying parameter was t_2.

parameter	*BDE*(Rb-F) eV	
t_2	calk.	exp.
½	4.993	5.000[a];
0	5.053	5.035[b]
- ½	5.115	5.117±0,216[c]; 5.102 average[d]
-1 ¼	5.211	5.182[e]; 5.204±0,3[f]
-3	5.446	<5.451[g]

[a] reference [10]; [b] reference [11]; [c] reference [8]; [d] average between extreme values; [e] thermodynamic data used from [9]; [f] data used from [12]; [g] upper limits for the dissociation energies, data from [9].

Table 8. The calculations of all experimental values *BDE* (Cs-F) for which the following data were used: r_{Cs-F}=2.345A° [19], I_F=17.4231 eV, t_1= -3, n = 1. The only varying parameter was t_2.

parameter	*BDE*(Cs-F) eV	
t_2	calk.	exp.
1 ¾	5.141	5.15[a]
1 ½	5.173	5.187[b]
1	5.238	5.255 average[c]
¾	5.271	5,269 ±0.06[d]
½	5.304	5.29±0.087[e] 5.291[f]
0	5.371	5,360±0,078[d]
-1 ¾	5.617	<5.633[g]

[a] reference [10]; [b] reference [11]; [c] average between extreme values; [d] reference [8]; [e] reference [7]; [f] thermodynamic data used from [9]; [g] upper limits for the dissociation energies, data from [9].

The influence of measuring process on the result. As it was mentioned above, in work [15] the bond length values in cesium halides, determined by spectroscopic methods and electron diffraction method, have a systematic difference approximately 1.5%. The measurement result was defendant on the measurement method. In work [21] there was an assumption that these differences are the result of incorrect interpretation of experimental data since it was likely that the mixture of monomer and dimer of alkali halide could be used. In work [15] the values r_{Cs-F}=2.33±0,02 A° are given for electron diffraction and r_{Cs-F}=2.375 A° are given for spectroscopy, whereas recommended value r_{Cs-F} equals 2.345 A° [19].

Our calculations results of *BDE* (Cs-F) are given in Table 9 with two varying parameters – t_2 and r_{Cs-F}. The varying of two parameters gives approximately the same effective bond length and gives a good agreement with experimental data. It should be noted that one of two parameters is an experimentally observed value whereas the second one is an element of a series formed by sequence with a step ¼.

Table 9. The calculation of experimental values *BDE* (Cs-F) for which the following data were used: I_F=17.4231 eV, t_1= -3, n = 1. The only varying parameters were t_2 and r_{Cs-F}.

parameter			*BDE*(Cs-F) eV	
r_{Cs-F} A°	t_2	R_{Cs-F} A°	calk.	exp.
2.33	1	1.8856	5.295	5.29±0.087[a]
2.345	½	1.8833	5.304	5.29±0.087[a]
2.375	-¼	1.8786	5.288	5.29±0.087[a]

[a] reference [7].

The calculations of *BDE* (Cs-F) were also carried out with the constant value t_2=½ and the only varying parameter was r_{Cs-F}. The results are summarised in Table 10.

Table 10. The calculation of experimental values *BDE* (Cs-F) for which the following data were used: I_F=17.4231 eV, t_1= -3, t_2= ½, n = 1. The only varying parameters was r_{Cs-F}.

parameter		*BDE*(Cs-F) эв	
r_{Cs-F} Aº	t_2	calk.	exp.
2.33	½	5.362	5.360±0,078[a]
2.345	½	5.304	5.29±0.087[b]
2.375	½	5.19	5.187[c]

[a] reference [8]; [b] reference [7]; [c] reference [11].

From Tables 9 and 10 it appears that all three experimental values of bond length Cs-F are correct. We assume that the differences in bond length values (while bond energy is constant) are due to the fact that different devices lead to excitation of different energy levels having different values t_2. Moreover, the different wave lengths having identical values t_2 give experimentally observed bond energies. When bond energy is constant the change of bond length with simultaneous change of quantum number value proceeds without energy barrier. The simultaneous change of both these parameters does not influence on the bond energy but it does influence on dipole moment of the bond. And vice versa, the change of dipole moment of the bond under the action of external factors, such as solvent, substrate, catalyst, etc., can lead to adiabatic change of bond length and quantum level, which in turn can affect the reaction direction.

As for assumption referring to the mixture of monomer and dimer, some of the observed bond lengths can be attributed to it, for instance r_{Li-F}=1.68 Aº [22]. It is close to average (r_{Li-F}=1.655 Aº) between recommended values 1.564 Aº [19] and 1.74 Aº [23] for monomer and dimer correspondingly. However, the measured values r_{Li-F}=1.547 Aº [11] and r_{Li-F}=1.5397 Aº [24] correspond to observation of different quantum levels by different devices. The calculations are given in Tables 11 and 12.

Table 11. The calculation of experimental values *BDE* (Li-F) for which the following data were used: I_F=17.4231 eV, t_1= 1, n = 1. The only varying parameters were t_2 and r_{Li-F}.

| parameter			*BDE*(Li-F) eV	
r_{Li-F} Aº	t_2	R_{Li-F} Aº	calk.	exp.
1.5397	¾	1.72538	5.970	
1.547	½	1.724	5.976	5.98[a], 5.98±0.2[b], 5.975[c]
1.564	0	1.72368	5.978	

[a] reference [7]; [b] reference [8]; [c] reference [13].

Table 12. The calculation of experimental values *BDE* (Li-F) for which the following data were used: I_F=17.4231 eV, t_1= -3, t_2= ½, n = 1. The only varying parameter was r_{Li-F}.

parameter		*BDE*(Li-F) eV	
r_{Li-F} Aº	t_2	calk.	exper.
1.5397	½	6.01	-
1.547	½	5.976	5.98[a], 5.98±0.2[b], 5.975[c]
1.564	½	5.898	5.898±0.35[d]

[a] reference [8]; [b] reference [7]; [c] reference [13]; [d] reference [12].

Resonance theory. Swepston et al. in their work [2] suggested a hypothesis that there is a stabilising interaction between HOMO of fluorine atom and LUMO of lithium atom to form an acetylene-like structure i.e. so called "π-bonds". But, as we showed above with our calculations, an ethylene-like structure (with only one stabilising HOMO-LUMO interaction) is more suitable since the calculations are in good agreement with experiment. Nonetheless, the validation of the presence of an acetylene-like structure should be done as well and it is possible with the use of resonance theory concept (See, for example, the Pauling's review [24]). According to that, the multiple bonds are in the equilibrium between several structures, for instance (5):

$$C=C \leftrightarrow C^+ \text{---} C^- \quad (5)$$
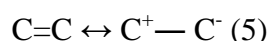
The calculations of *BDE* for C-C bond in ethylene with parameters $z_1 \cdot z_2 = g \cdot g$, $n=2$ for double bond and $z_1 \cdot z_2 = g \cdot e$, $n=1$ for polarised σ-bond give results 7.297 eV and 7.121 eV correspondingly.

We think that the transfer from ionic to so called π-bond can be considered proven. In table 13 the validation of the presence of an acetylene-like structure is given with the application of resonance theory towards alkaline fluorides.

Table 13. The calculations of *BDE* (M-F) for ethylene-like structure ($n =1$) and acetylene-like structure ($n =2$). For comparison, we give the calculations of *BDE* (C=C) and the energy difference Δ*BDE* for the structures in equation (5).

spacies	n	$z_1 \cdot z_2$	r A°	t_1	t_2	calk	Δ *BDE*	exp.
		parameter				*BDE* eV		
C=C	1	$e \cdot g$	1.33[a]	-3	0	7.121	0.176	7.298±0.13[b]
	2	$g \cdot g$				7.297		
Li-F	1	$e \cdot e$	1.564	1	0	5.987	0.148	5.98
	2	$e \cdot g$				5.839		
Na-F	1	$e \cdot e$	1.926	0	1½	4.958	0.349	4.95±0.2
	2	$e \cdot g$				4.609		
K-F	1	$e \cdot e$	2.1714	-1	¼	5.061	0.329	5.0695
	2	$e \cdot g$				4.732		
Rb-F	1	$e \cdot e$	2.2704	-2	-½	5.115	0.383	5.117±0,21
	2	$e \cdot g$				4.797		
Cs-F	1	$e \cdot e$	2.345	-3	½	5.304	0.282	5.29±0.087
	2	$e \cdot g$				5.022		

[a] reference [26]; [b] reference [7]. There are other experimental data *BDE*(C=C) and $r_{C=C}$, but this is not the aim of the present work.

We were looking for the difference Δ*BDE* (C=C) for both structures from equation (5) and its comparison with the difference Δ*BDE* (M-F) for acetylene-like and ethylene-like structures. Since we think that resonance theory is a good theory and if Δ*BDE* (M-F) ≤ Δ*BDE* (C=C), the formation of an acetylene-like structure is as equally possible as the formation of

structures from equation (5). However, an ethylene-like structure is more preferable energetically. From Table 5 one can see that only Li-F meets this criterion.

It should be noted that quantum number t_1 and period number of alkaline change symbatically.

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