Self-consistent database for atoms and molecules

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Abstract. The scheme of construction of modern databases ideologically no different from specialized directories of the last century. The main drawback of such repositories is the accumulation of all the measured values of a particular atom or molecule with a subjective assessment by a distinguished group of authors reliability of the obtained values. Nevertheless, there are various methods of comparative analysis allows using those or other approximations to evaluate the compliance of measured value data of other authors. Much more advanced ways to approach the evaluation of data is based on the notions of unitary symmetry, developed in several papers. The presentation of such an approach present article is devoted.

Keywords: Periodic table, Combinatorics, Homologous series, Unitary Symmetry, Ionization energy of the atoms, Databases for molecules.

1. Introduction

It was shown earlier [1,2,3,4,5], that for objects, starting with elementary particles and to complex molecules and their mixtures, combinatorial operations lead to the formation of a homologous series (series of combinatorial objects). These homologous series have a universal property - in the space of physical and chemical parameters is saved some of the parameter in relation to certain pairs of combinatorial objects. This versatile property has been called unitary symmetry SU (n).
Mathematical interpretation of the SU (5) as an example of the halogenated methane was given in [2]. In [3] were able to show the physical meaning of unitary symmetry for many physical and chemical properties that have a combinatorial nature. In contrast to the geometric symmetry which preserves the shape of the object, in the case of unitary symmetry is saved ratio parameters (features, functions) for homologous pairs of combinatorial objects.

Recall that for baryons [1] can be written, for example, equation (1):

$$RM(dss) - RM(dus) = RM(uss) - RM(uus)$$

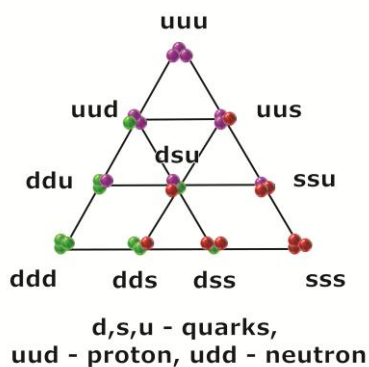where RM is a Rest mass of baryons (MeV/c^2), u,d,s - кварки. (see Fig.1)

d,s,u - quarks,
uud - proton, udd - neutron

Fig.1. Combinations of three **u, d**, **s** quarks forming baryons with a spin $-3/2$ form the **uds** baryon decuplet [5]

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Similar laws are known, for example, for the mirror nuclei (Equation 2):

$$E_b[(K)P + (K-1)N] - E_b[(K-1)P + (K)N] = E_b[(K-1)P + (K-2)N] - E_b(K-2)P + (K-1)N]$$

where E_b is binding energy of protons (P) and neutrons (N) in mirror nuclei, K is a number of nucleons. (see Fig.2).
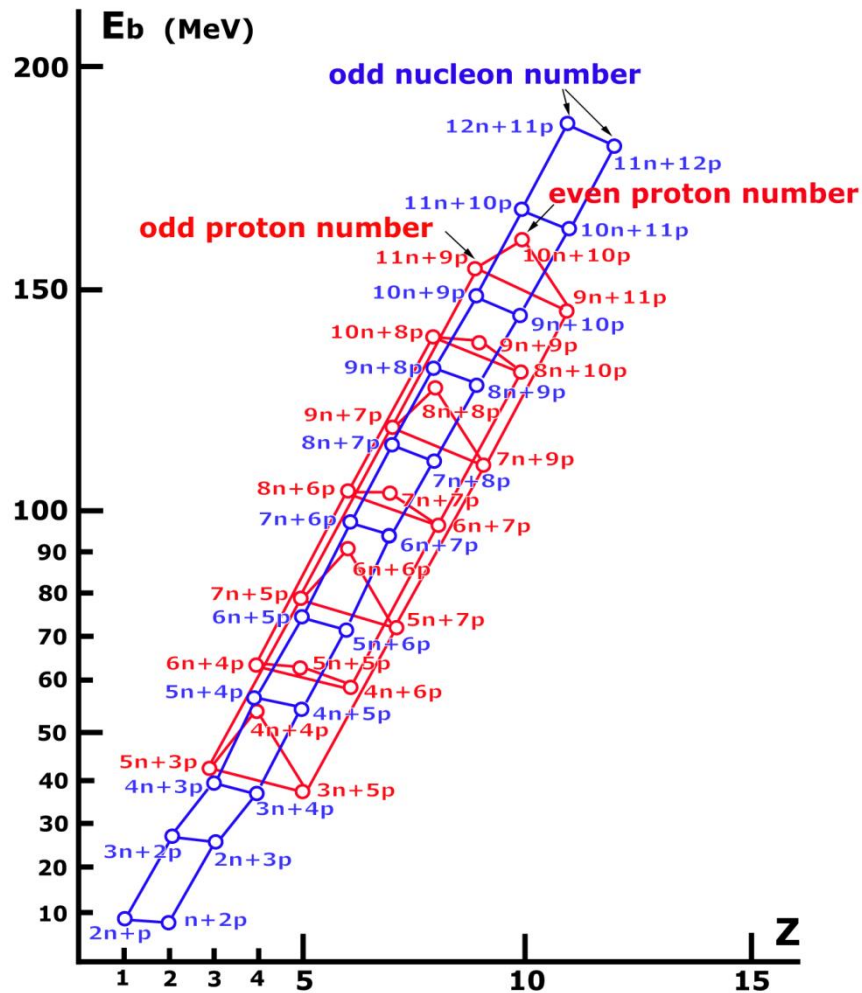

Fig.2. The binding energy of the nucleons in the mirror nuclei. (Z - charge of the nucleus).

For homologous series of halogenated methanes were obtained [6] 90 equations corresponding to the replacement of one atom in one molecule to another atom to form another molecule. An example of such equations is shown Table 1:

Table 1. The system of equations for the replacement F-H. Before each chemical compound in order to save space omitted designations of some physical or chemical parameter of the molecule (A). For some parameters, for which the geometric symmetry does not play a big role, the equation with (*) and without ( ) can be combined.

	Replacement: F ⟷ H
1	CF3Cl - CF3Br = CH3Cl - CH3Br
1*	CHF2Cl - CHF2Br = CH2FCl - CH2FBr
2	CF3Br - CF3I = CH3Br - CH3I
2*	CHF2Br - CHF2I = CH2FBr - CH2FI
3	CF3Cl - CF3I = CH3Cl - CH3I
3*	CHF2Cl - CHF2I = CH2FCl - CH2FI
4	CF2Cl2 - CF2Br2 = CHFCl2 - CHFBr2 = CH2Cl2 - CH2Br2
5	CF2Cl2 - CF2I2 = CHFCl2 - CHFI2 = CH2Cl2 - CH2I2
6	CF2Br2 - CF2I2 = CHFBr2 - CHFI2 = CH2Br2 - CH2I2
7	CFCl3 - CFBr3 = CHCl3 - CHBr3
8	CFBr3 - CFI3 = CHBr3 - CHI3
9	CFI3 - CFCl3 = CHI3 - CHCl3

Not all of these and similar equations are completely accurate, but the reasons for the low invariance are the subject of additional studies of violations of a particular symmetry.

It is important that these equations not only have great predictive power, but also the identification of false values previously measured parameters

Ideologically, the proposed method consists in the fact that each parameter of the molecule is at the intersection of values for the homologous series of isostructural isovalent substituted molecules (see Fig 3).
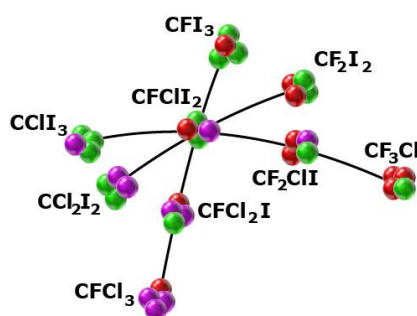

Fig. 3. One of the knots of system of homologous series of halogenated methane. Thus, there is a mutual self correlation position of the molecule in the space of its physical and chemical parameters.

Virtually the proposed method consists in finding pairs of objects for which the difference between the values of the parameter under consideration are almost equal. This follows from the symmetry of the considered class of objects and is a conservation law. Consider some examples.

2. Ionization potentials of atoms

We analyze the ionization potentials of the first 20 atoms [7]. Input data is presented in Table. 2 and in Fig. 4 - 20.

Table 2. Regularities in the ionization potentials and their differences for chemical elements with $Z = 1 - 20$. To save space, the designation of the ionization potential (I_i) to the atoms in the 4 and 5 columns are omitted.

The number of protons, the nuclear charge Z	atom	Ionization potentials (I) of the 1s^1 electron. (eV)	The difference between the ionization potentials of the 1s^1 electron of two neighboring elements. (eV)		The difference between the differences of ionization potentials for the 1s^1 electrons for two neighboring groups of atoms – – [I$_i$ (A$_Z$) – I$_i$(A$_{Z+1}$)] – [I$_i$ (A$_{Z+1}$) – I$_i$(A$_{Z+2}$)], (eV)	
1	H	13,598				
			(H-He)	40,818		
2	He	54,416			(H-He) - (He-Li)	27,217
			(He-Li)	68,035		
3	Li	122,451			(He-Li) - (Li - Be)	27,227
			(Li-Be)	95,262		
4	Be	217,713			(Li-Be) - (Be - B)	27,242
			(Be-B)	122,504		
5	B	340,217			(Be-B) - (B-C)	26,360
			(B-C)	148,864		
6	C	489,081			(B-C) - (C-N)	29,084
			(C-N)	177,948		
7	N	667,029			(C-N) - (N-O)	26,410
			(N-O)	204,358		
8	O	871,387			(N-O) - (O-F)	27,344
			(O-F)	231,702		
9	F	1103,089			(O-F) - (F-Ne)	27,373
			(F-Ne)	259,075		
10	Ne	1362,164			(F-Ne) - (Ne-Na)	27,420
			(Ne-Na)	286,495		
11	Na	1648,659			(Ne-Na) - (Na-Mg)	27,459
			(Na-Mg)	313,954		
12	Mg	1962,613			(Na-Mg) - (Mg-Al)	27,513
			(Mg-Al)	341,467		
13	Al	2304,080			(Mg-Al) - (Al-Si)	27,561
			(Al-Si)	369,028		
14	Si	2673,108			(Al-Si) - (Si-P)	27,626
			(Si-P)	396,654		
15	P	3069,762			(Si-P) - (P-S)	27,683
			(P-S)	424,337		
16	S	3494,099			(P-S) - (S-Cl)	27,757
			(S-Cl)	452,094		
17	Cl	3946,193			(S-Cl) - (Cl-Ar)	27,827
			(Cl-Ar)	479,921		
18	Ar	4426,114			(Cl-Ar) - (Ar-K)	27,896
			(Ar-K)	507,817		
19	K	4933,931			(Ar-K) - (K-Ca)	27,990
			(K-Ca)	535,807		
20	Ca	5469,738				

Table 1

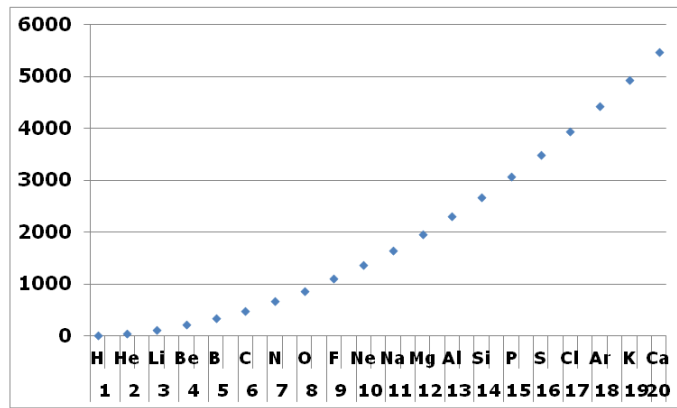Ionisation Energies (eV) of 1s^1 electrons vs Z for atoms Z = 1 - 20 presented in Fig.4

Fig 4. Ionisation Energies (eV) of $1s^1$ electrons vs Z for atoms $Z = 1 - 20$

This regularity very attractive because of its smooth non-linear pattern. Now consider the difference between the ionization energies of neighboring atoms (see. Fig.5).
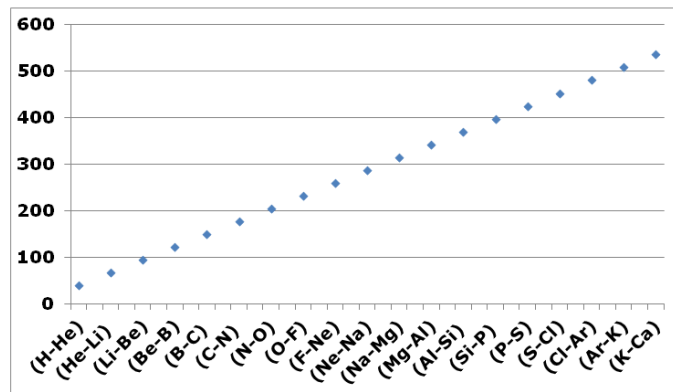

Fig.5. The Ionisation Energies difference between the values of the $1s^1$ electron of two neiboring elements - $[I_i (A_Z) - I_i(A_{Z+1})]$, (eV) vs Z for atoms $Z = 1 - 20$

This regularity even more attractive because of its smooth linear pattern. But that's what happens when considering the differences of adjacent differences (see. Fig.6-20).
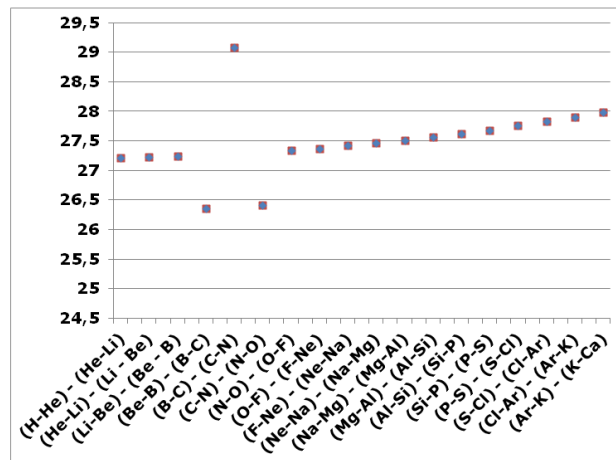

Fig.6. The Ionisation Energies difference between the values of the $1s^1$ electron of two groups of the neiboring elements - $[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})]$, (eV)

As can be seen from the Fig.6 the almost linear dependence

$$[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})] \quad vs \quad [Z_i (A_Z) - Z_i(A_{Z+1})] - [Z_i (A_{Z+1}) - Z_i (A_{Z+2})]$$

drop out the point which corresponds to the difference of the ionization energies for the elements Be, B, C, N and O

$$\{[I(Be) - I(B)] - [I(B) - I(C)]\},$$

$$\{[I(B) - I(C)] - [I(C) - I(N)]\},$$

$$\{[I(C) - I(N)] - [I(N) - I(O)]\}$$

Doing similar calculations for the following on nucleus electrons, it is easy to verify that

$$[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})] = const,$$

where I_i - ionization energy of (i) electron of the atom A_Z with atomic number Z.

Below is a graph of

$$[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})] \quad vs \quad [Z_i (A_Z) - Z_i(A_{Z+1})] - [Z_i (A_{Z+1}) - Z_i (A_{Z+2})]$$
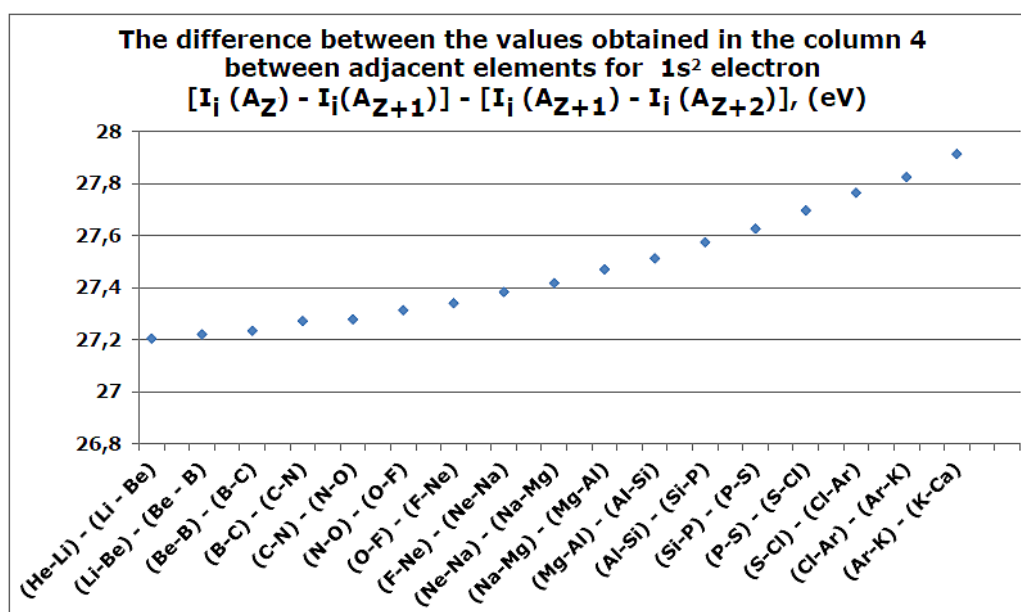
for the subsequent electrons.

Fig.7. The Ionisation Energies difference between the values of the $1s^2$ electron of two groups of the neiboring elements - $[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})]$, (eV). In this case, we do not observe the values that fall outside of the smooth running of the graph.

In the transition from the electron shell $1s^2$ to $1s^2 2s^1$ there is a change of values of the Ionisation Energies differences - from ~ 27 eV to ~ 7 eV.
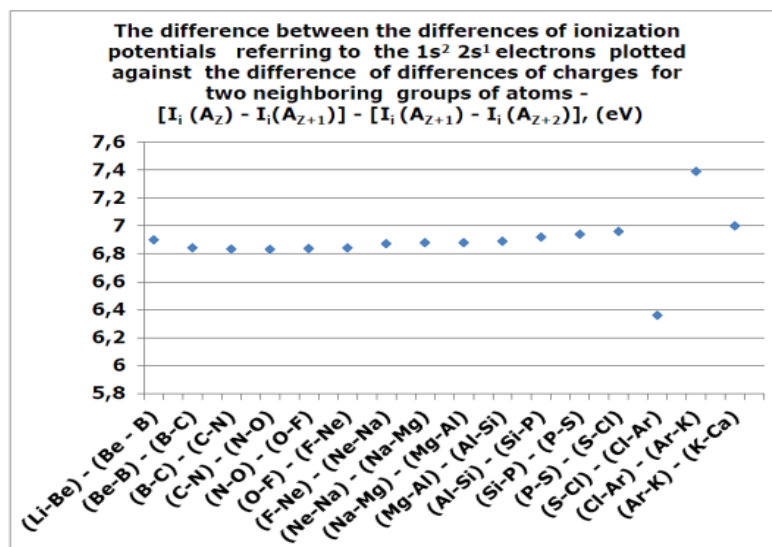
Fig.8. The Ionisation Energies difference between the values of the $1s^2 2s^1$ electron of two groups of the neiboring elements - $[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})]$ (eV). The irregularities were identified for the following values :
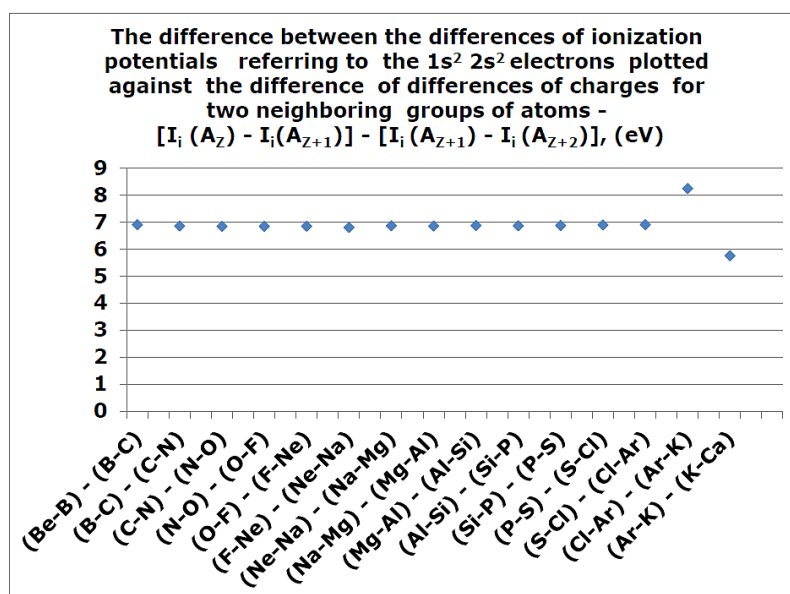$\{[I(S) - I(Cl)] - [I(Cl) - I(Ar)]\}$ and $\{[I(Cl) - I(Ar)] - [I(Ar) - I(K)]\}$

Fig.9. The Ionisation Energies difference between the values of the $1s^2 2s^2$ electron of two groups of the neiboring elements - $[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})]$, (eV). The irregularities were identified for the following values :
$\{[I(Cl) - I(Ar)] - [I(Ar) - I(K)]\}$ and $\{[I(Ar) - I(K)] - [I(K) - I(Ca)]\}$
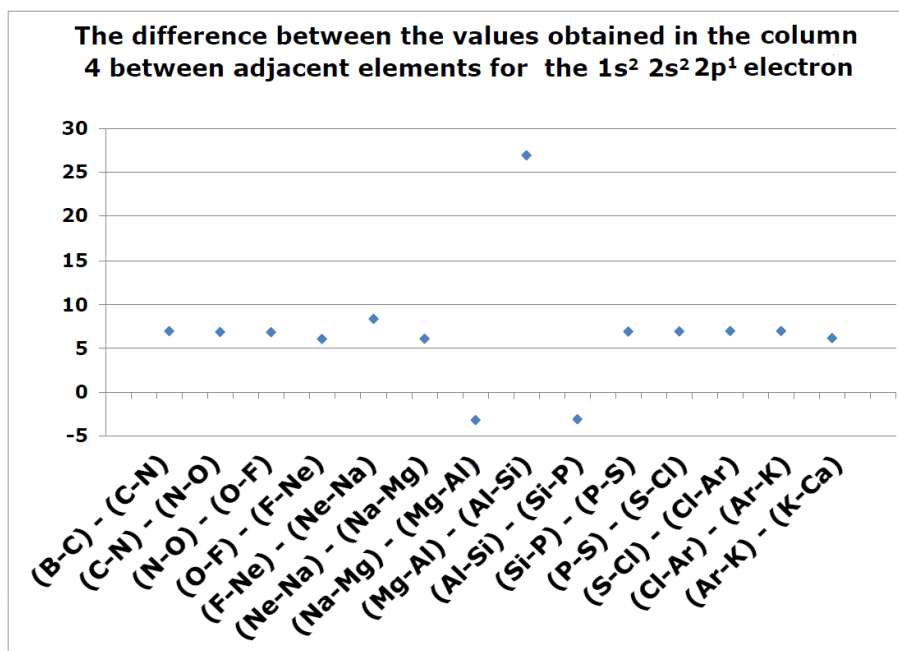
Fig.10. The Ionisation Energies difference between the values of the $1s^2 2s^2 2p^1$ electron of two groups of the neiboring elements - $[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})]$, (eV). The irregularities were identified for the following values :

$$\{[I(Na) - I(Mg)] - [I(Mg) - I(Al)]\}$$

$$\{[I(Mg) - I(Al)] - [I(Al) - I(Si)]\}$$

$$\{[I(Al) - I(Si)] - [I(Si) - I(P)]\}$$

Fig.11. The Ionisation Energies difference between the values of the $1s^2 2s^2 2p^2$ electron of two groups of the neiboring elements - $[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})]$, (eV). The irregularities were identified for the following values :

$$\{[I(Ne) - I(Na)] - [I(Na) - I(Mg)]\}$$
$$\{[I(Na) - I(Mg)] - [I(Mg) - I(Al)]\}$$
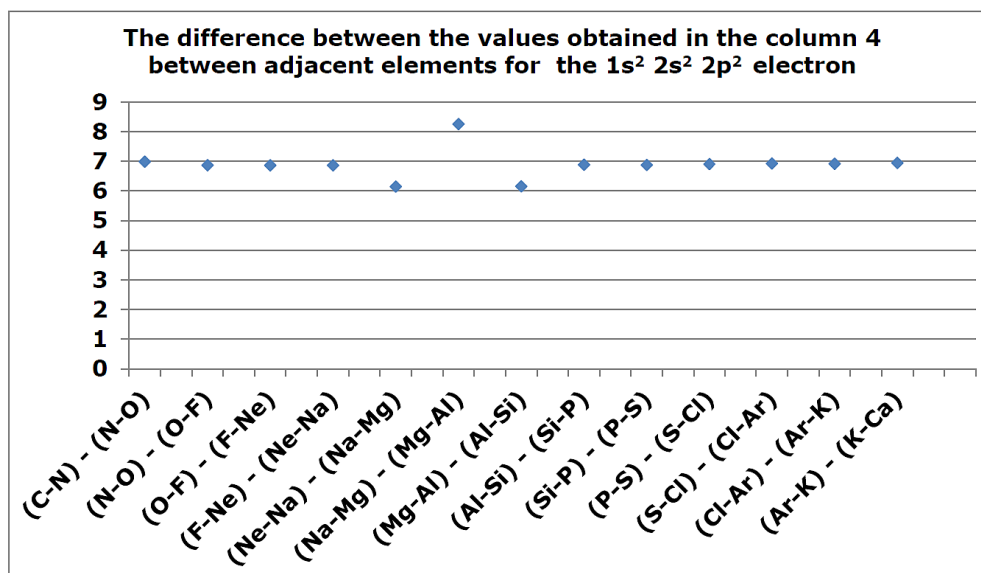$$\{[I(Mg) - I(Al)] - [I(Al) - I(Si)]\}$$

Fig.12. The Ionisation Energies difference between the values of the $1s^2 2s^2 2p^3$ electron of two groups of the neiboring elements - $[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})]$, (eV). The irregularities were identified for the following values :
$$\{[I(N) - I(O)] - [I(O) - I(F)]\}$$
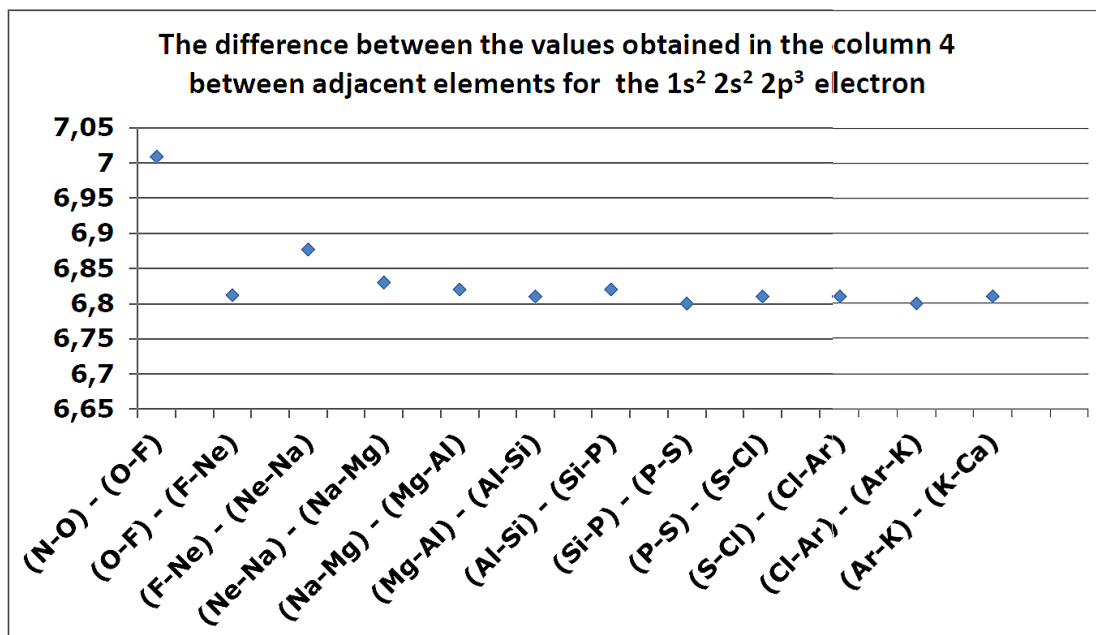$$\{[I(F) - I(Ne)] - [I(Ne) - I(Na)]\}$$

Fig.13. The Ionisation Energies difference between the values of the $1s^2 2s^2 2p^4$ electron of two groups of the neiboring elements - $[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})]$, (eV). The irregularities were identified for the following values :
$$\{[I(O) - I(F] - [I(F) - I(Ne)]\}$$
$$\{[I(F) - I(Ne)] - [I(Ne) - I(Na)]\}$$

But this case requires further investigation. It is possible that since the $1s^2 2s^2 2p^2$ electron changed the power characteristics of the interaction of charged particles in atoms.

Fig.14. The Ionisation Energies difference between the values of the $1s^2 2s^2 2p^5$ electron of two groups of the neiboring elements - $[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})]$, (eV).
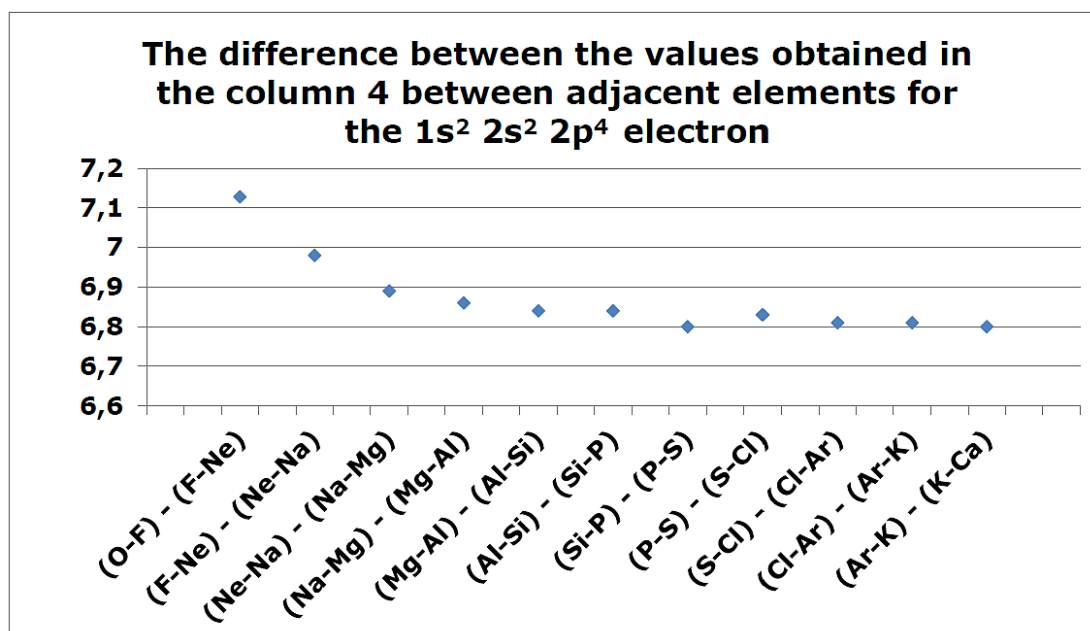

Fig.15. The Ionisation Energies difference between the values of the $1s^2 2s^2 2p^6$ electron of two groups of the neiboring elements - $[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})]$, (eV).

In the transition from the electron shell $1s^2 2s^2 2p^5$ to $1s^2 2s^2 2p^6$ there is a change of values of the Ionisation Energies differences - with ~ 7 eV to ~ 3 eV.
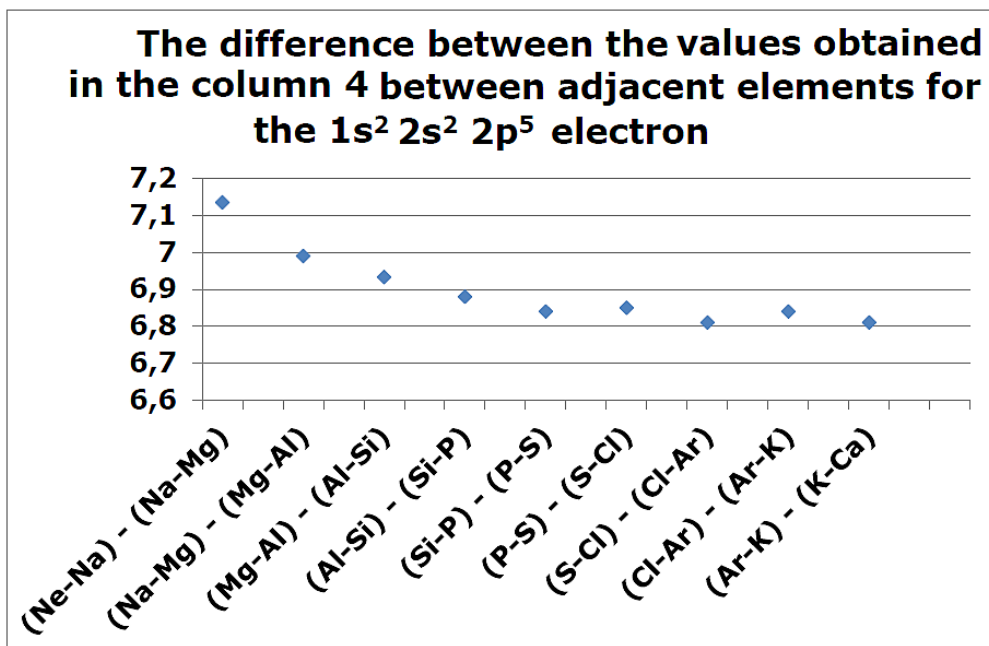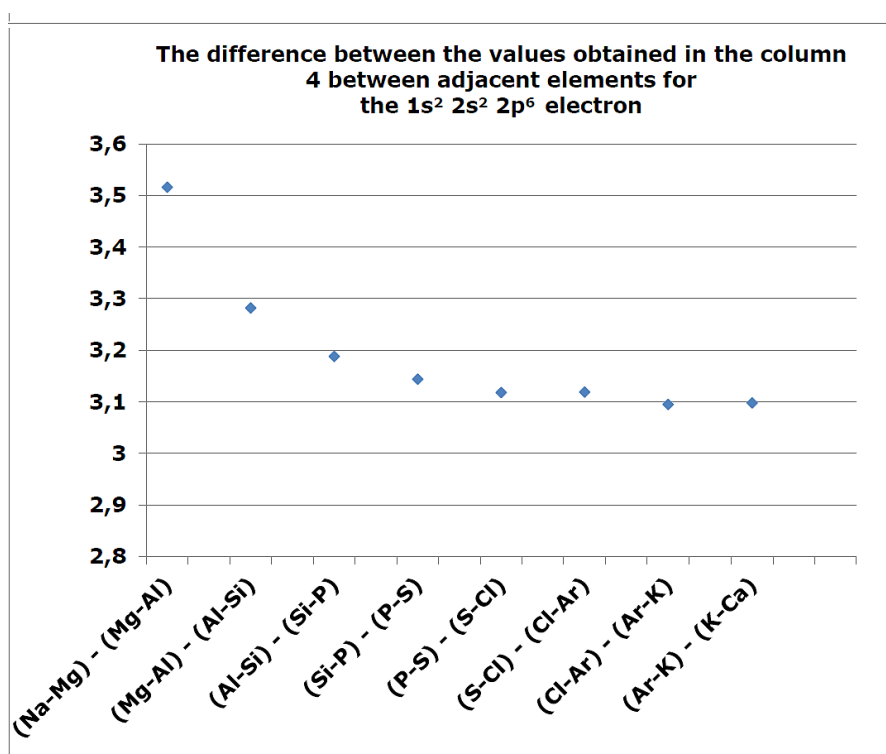
Fig.17. The Ionisation Energies difference between the values of the $1s^2 2s^2 2p^6 3s^1$ electron of two groups of the neiboring elements -
$$[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})], (eV).$$

Here, the observed spread of the values for Ionisation Energies difference between the values of the $1s^2 2s^2 2p^6 3s^1$ electron of two groups of the neiboring elements is too large to to make any conclusions.

Fig.18. The Ionisation Energies difference between the values of the $1s^2 2s^2 2p^6 3s^2$ electron of two groups of the neiboring elements -
$$[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})], (eV).$$

Here, the observed spread of the values for Ionisation Energies difference between the values of the $1s^2 2s^2 2p^6 3s^2$ electron of two groups of the neiboring elements is too large to to make any conclusions as well.
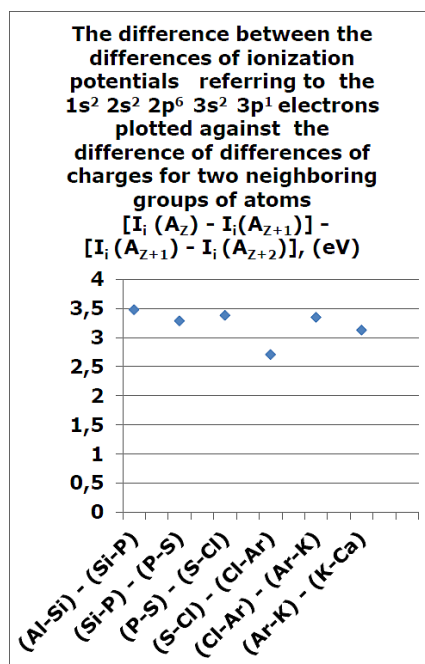
Fig.19. The Ionisation Energies difference between the values of the $1s^2 2s^2 2p^6 3s^2 3p^1$ electron of two groups of the neiboring elements -

$$[I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})], (eV).$$

For the case of the $1s^2 2s^2 2p^6 3s^2 3p^1$ electron "falling out point" is the value for [(S-Cl) - (Cl-Ar)].
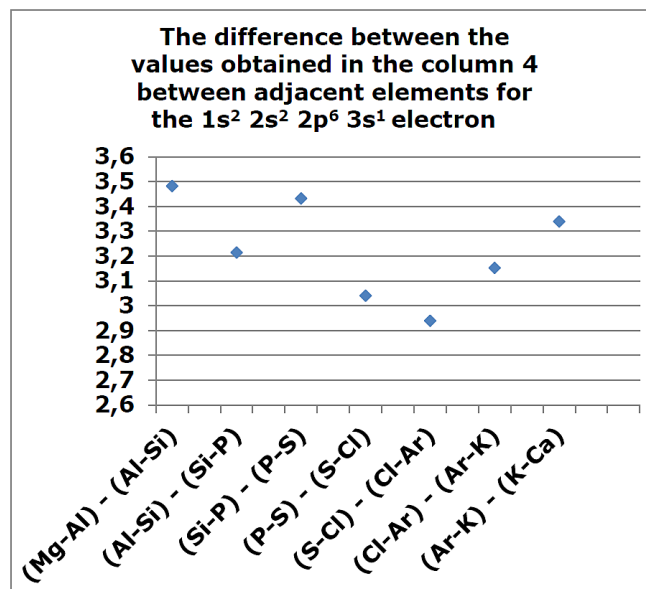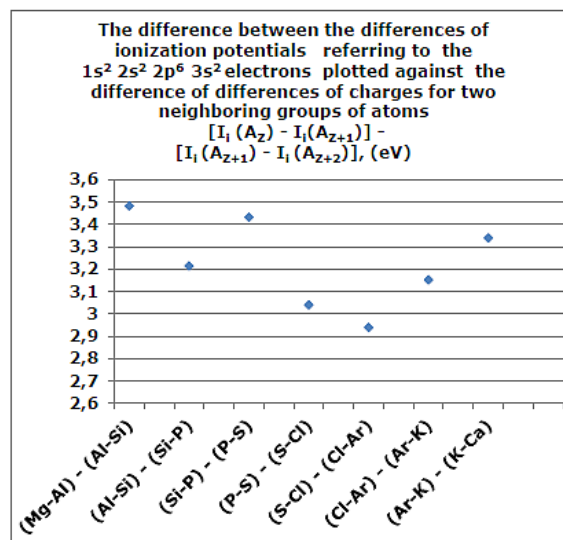

Fig.20. The Ionisation Energies difference between the values of the $1s^2 2s^2 2p^6 3s^2 3p^2$ electron of two groups of the neiboring elements -

$$I_i (A_Z) - I_i(A_{Z+1})] - [I_i (A_{Z+1}) - I_i (A_{Z+2})], (eV).$$

Here, the observed spread of the values for Ionisation Energies difference between the values of the $1s^2 2s^2 2p^6 3s^2 3p^2$ electron of two groups of the neiboring elements is too large to to make any conclusions again.
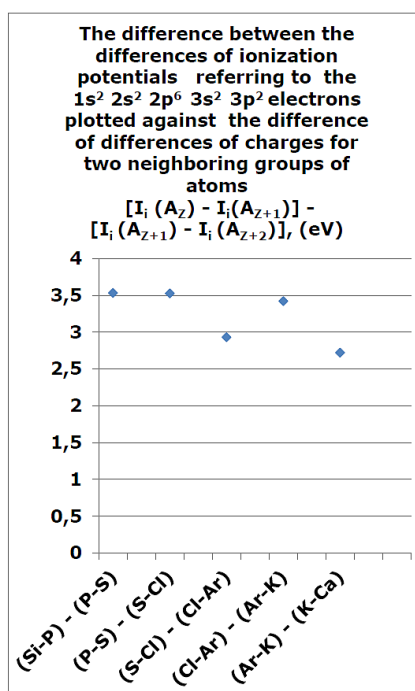
To conclude this section we would like to note that it is not difficult to find such regularities of the other physical and chemical properties of atoms and ions and create a significant Self consistent database (SCD).

2. Self-consistent values of the molecules

One of the most conservative notions in chemistry is a concept of Homology. So, the concept of homology refers to the comparative analysis. But in order to compare (as a process) the objects need to decompose them into elementary components (parts). Then two objects that differ only in one (essential) part can be called Homology. Sequence of objects that appears when replacing one part of the qualitative characteristics of the other part of the same characteristics can be called **Homologous series.**
Therefore such series as CH4 - CH3F - CH2F2 - CHF3 - CF4 and the like will also be called homologous series. Combination of H, F, Cl, Br, I around tetravalent carbon atom (n = 5, k = 4 - "n choose k") according to the formula $^{n-1}C_{n+k-1} = (n+k-1)! / k!(n - 1)!$ gives the total amount of the halogen-substituted methanes (70). All homologous series multiply intersect and form a structure which formally presented at Fig.21.
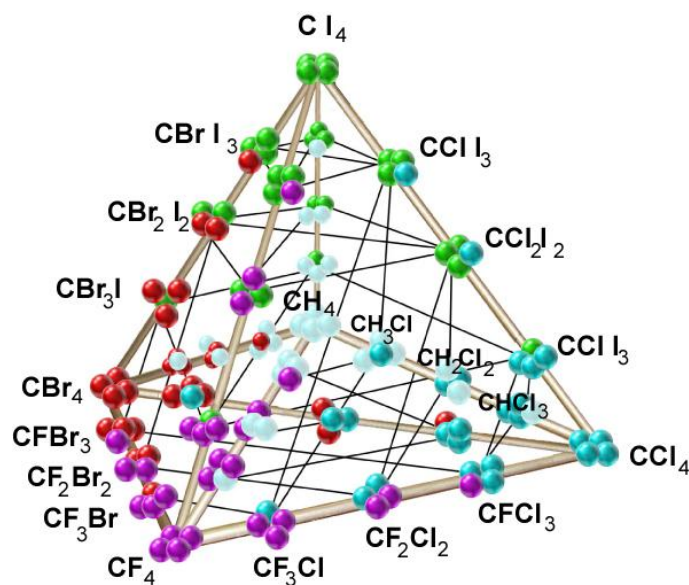
Fig. 21. This is an illustration of all possible combinations of 5 different objects (H,F,Cl,Br,I) with 4 repetitions. Building such a structure allows for more intuitive form to submit a combinatorial nature, such as the family of halogenated methanes.

In our studies [2], [3], [4] it was shown that making certain symmetry operations in the space of physical parameters of the elements of the set of halogenated methane traced constancy of the parameter in the difference in specific transitions from one compound to another. That is, there is almost the same pattern as in the systematics of baryons, which Gell-Mann pointed out in [1].
Placing the system of the homologous series of halogenated methanes in the space of physical and chemical parameters, we can obtain a distribution with great predictive power.
The results are discussed in terms of first-principles of the symmetry influence to the core-ionization energies and to thermochemical parameters.

2.1. The system of equations for halogenated methane

So much for the value of Vertical Ionization Energies [6] division is illustrated in Fig.22

Fig. 22a. Vertical Ionization Energies (VIE - I_{VIE}) and Enthalpy ΔH_f^o. of halogenated methanes v.s. on their molecular weight. Black letters and b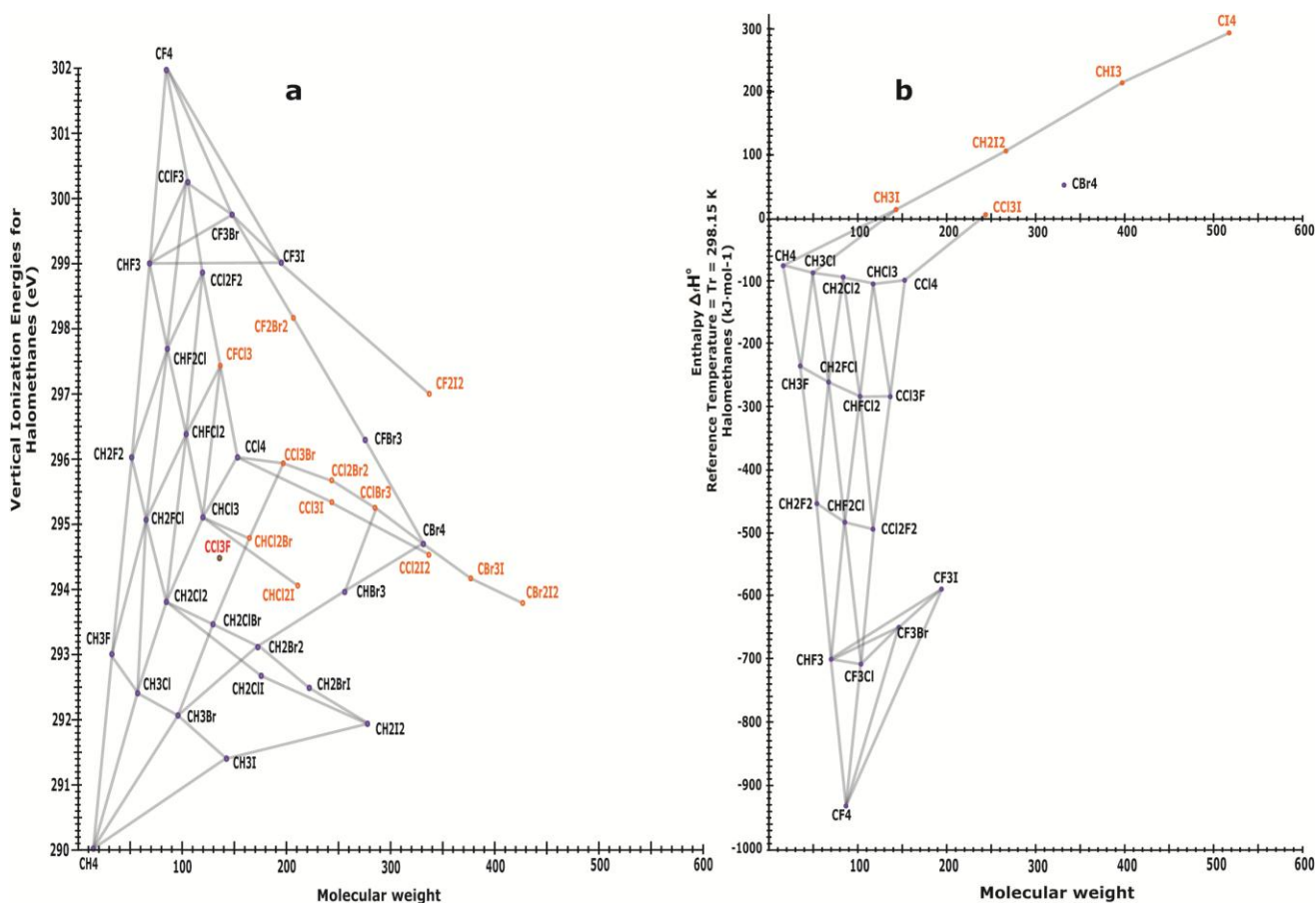lue dots indicate the compounds listed in [6] (for $I_{VIE)}$. Orange color compounds and their values (VIE), the resulting calculations similar to those of Table 3. Red marked compound CFCl3, which in [6] is erroneous.

Fig. 22b. Black letters and blue dots indicate ΔH_f^o for compounds listed in [7]. Orange color compounds and their values (VIE) is the resulting calculations of ΔH_f^o [8]. The value ΔH_f^o (ClCl3) is the result of calculations similar to those of Table 3.

Such representations are useful as a zero approximation in the evaluation of data. If the authors of the work [6] have not missed this simple step, the errors could have been avoided. The same can be said about a large number of theoretical and experimental data, which are listed in various reference books, including the Database (NIST) As seen in Fig.22, each parameter value is at the intersection of several homologous series. This fact determines the correlated (depending on other values) location for each connection.

For the entire class of halogenated methanes $CH_{4-n-m} X_n Y_m$ (X,Y = F,Cl,Br,I) in accordance with the combinatorial substituting one atom to another for combinations ($^{n-1}C_{n+k-1}$ = (n+k-1)! / k!(n - 1)! , where n = 5, k = 2 - "n choose k") can be obtained the total amount of substituting (10): F - H, F - Cl, F - Br, F - I, Cl - H, Cl - Br, Cl - I, Br - H, Br - I, I - H. For each substitution is made 9 basic equations of conservation of the difference (I_{VIE}) for molecules with the same geometric symmetry operations groups . The total number of basic equations is 90. Below is a table of equations to replace the F - H.

Table 3. The system of equations for the replacement F-H. Before each chemical compound formula omitted designation (I_{VIE}) in order to save space. Blue marked data have been cited in [6] (see Table. 1, [6]). Red marked values (I_{VIE}) calculated based on the data (see Table 1, [6]). In Equation 7 clearly shows the consequences of an erroneous value for CFCl3. New value (I_{VIE}) for CFCl3, as reported to me one of the authors [6] is 297.48 eV.

	.Replacement: F ⟷ H				
	The law of conservation within the same point group symmetry - C_{3v} or C_s **The highest degree of accuracy**				
1	**CF3Cl - CF3Br**	=	**(C_{3v})**	=	**CH3Cl - CH3Br**
	300,25 - 299,77	0,48	~	0,374	292,43 - 292,056
1a		**CHF2Cl - CHF2Br =**	**(C_s)**	**= CH2FCl - CH2FBr**	
		297.700 - ( )	~	295.036 - ( )	
2	**CF3Br - CF3I**	=	**(C_{3v})**	=	**CH3Br - CH3I**
	299,77 - 299,00	0,77	~	0,626	292,056 - 291,43
2a		**CHF2Br - CHF2I =**	**(C_s)**	**= CH2FBr - CH2FI**	
		( ) - ( )	~	( ) - ( )	
3	**CF3Cl - CF3I**	=	**(C_{3v})**	=	**CH3Cl - CH3I**
	300,25 - 299,00	1,25	~	1,00	292,43 - 291,43
3a		**CHF2Cl - CHF2I =**	**(C_s)**	**CH2FCl - CH2FI**	
		297.700 - ( )	~	295.036 - ( )	
	The law of conservation within the same point group symmetry - C_{2v} **The highest degree of accuracy**				
4	**CF2Cl2 - CF2Br2**	=	**(C_{2v})**	=	**CH2Cl2 - CH2Br2**
	298,87 - 298,161	**0,709**	=	0,709	293,81 - 293,101
		CHFCl2 - CHFBr2			
		296,372 - ( )			
		(C_s)			
5	**CF2Cl2 - CF2I2**	=	**(C_{2v})**	=	**CH2Cl2 - CH2I2**
	298,87 - 297,043	**1.827**	=	1.827	293,81 - 291,983
		CHFCl2 - CHFI2			
		296,372 - ( )			
		(C_s)			
6	**CF2Br2 - CF2I2**	=	**(C_{2v})**	=	**CH2Br2 - CH2I2**
	298,161 - 297,043	**1,118**	=	1,118	293,101 - 291,983
		CHFBr2 - CHFI2			
		( ) - ( )			
		(C_s)			
	The law of conservation within the same point group symmetry - C_{3v} **The highest degree of accuracy**				
7	**CFCl3 - CFBr3**	=	**(C_{3v})**	=	**CHCl3 - CHBr3**
	297,445 (294.48) - **296,276**	**1,169 (- 1,796)**	=	**1,169**	295,16 - 293,991
8	**CFBr3 - CFI3**	=	**(C_{3v})**	=	**CHBr3 - CHI3**
	296,276 - ( )				293,991- ( )
9	**CFI3 - CFCl3**	=	**(C_{3v})**	=	**CHI3 - CHCl3**
	( ) - **297,445** **(294,48)**				( ) - 295,16

2.2. Results and discussion

It is interesting that, if you follow the exact sequence conservation geometric symmetry group within differences (I_{VIE}), then each of the first three equations splits into two equations - the first saved group C_{3v}, while in the second group C_S. Three subsequent equations also break - every two preserving the geometrical symmetry groups C_{2v} or C_S , respectively.
While differences between (I_{VIE}) for compounds belonging to different groups - C_{3v} and C_S are not observed exact equality (replacement of H - Cl):

$$I_{VIE} \text{ (CH3F) - } I_{VIE} \text{ (CH3Br)} \sim I_{VIE} \text{ (CH2FCl) - } I_{VIE} \text{ (CH2ClBr)}$$
$$1{,}501 = 293.557 \text{- } 292.056 \quad \sim \quad 295.036 \text{ - } 293{,}456 = 1{,}58$$
$$I_{VIE} \text{ (CH3Br) - } I_{VIE} \text{ (CH3I)} \sim I_{VIE} \text{ (CH2ClBr) - } I_{VIE} \text{ (CH2ClI)}$$
$$0{,}626 = 292.056 \text{ - } 291.43 \quad \sim \quad 293.456 \text{ - } 292.696 = 0{,}76$$

Although it should be noted that (I_{VIE}) of the core-ionization energies within the real error of the difference between " different symmetric" equations probably be neglected.
To an even greater extent this applies to thermochemical parameters, which by their nature should have experimental at times (if not the order) large error and significantly less dependent on the geometric symmetry of the compound.
Moreover, if the trust values (I_{VIE}) [6], the difference $\Delta(I_{VIE})$ with fluorine molecules to exceed the difference $\Delta(I_{VIE})$ with hydrogen molecules. In addition, the replacement of one " secondary " ligand with Br on I leads to a marked increase in both the differences $\Delta(I_{VIE})$, and their inequality (see Tab.4). In the language of the theory of symmetry - a " broken symmetry SU " and its causes should be considered in further calculations.

Table 4. Dependence differences Δ (I_{VIE}) from the secondary ligand

$(F - H)_{Cl,Br}$	$(I_{VIE})CF3Cl - (I_{VIE})CF3Br$	$(I_{VIE})CH3Cl - (I_{VIE})CH3Br$	
	$300.25 - 299.77 = 0{,}48$	$292.43 - 292.056 = 0{,}374$	$0{,}106$
$(F - H)_{Cl,I}$	$(I_{VIE})CF3Cl - (I_{VIE})CF3I$	$(I_{VIE})CH3Cl - (I_{VIE})CH3I$	
	$300{,}25 - 299{,}00 - = 1{,}25$	$292{,}43 - 291{,}43 = 1{,}00$	$0{,}25$

According to [6] with the whole set of equations to obtain new values (I_{VIE}) for the following molecules : CF2I2 (297,043), CCl2I2 (294,507), CF2Br2 (298,161), CFCl3 (297,445), CCl3Br (295,944), CCl3I (295,318) , CCl2Br2 (295,625), CClBr3, 295,241, CBr3I (294,149), CBr2I2 (293,798), CHCl2I (294,032), CHCl2Br (294,792).

Missing values (I_{VIE}) related to compounds containing in the structure I$_3$ (any of the molecules CHI3, CFI3, CClI3, CBrI3) and the lack of data for several molecules of symmetry C_s do not allow the calculation and analysis of the entire set of 70 compounds of halogenated methanes.
Similar calculations were carried out for the thermochemical parameters of halogenated methanes. However, the data presented in [8] are so irrational in terms of following dependence of the enthalpy of the geometric symmetry of the molecules (see Fig.22b) that either should increase measurement error, or use simple additive schemes.
Everything in this case, sufficient reliability can be done using this equation ΔH_f^{o} (**CIF3**) - ΔH_f^{o} (**CICl3**) = ΔH_f^{o} (**CHF3**) - ΔH_f^{o} (**CHCl3**) is to determine ΔH_f^{o} (**CICl3**) = 4, 77 kJ mol $^{-1}$
 But the scope of this work does not allow them to consider in detail.

2.3. Conclusions

The proposed approach provides the basis for a new simple method of analyzing and calculating purposeful experimental and calculated data for the physical and chemical properties of chemical compounds. And considering that the database and the authors of the vast number of works do not result in proper calculation errors , the system of equations , in which the parameter in question for the same molecule contains several times produces correlating the intersection of several homologous series parameter.

In addition, the presentation of data in the database is not in the form of individual values (see base NIST), as well as a distribution similar to that shown in Fig.22 , make it easy to make a preliminary assessment of the parameter for the desired compound and concentrate on measuring or calculating precisely the connections that are required to complete the correlated analysis on the set of homologous molecules

The proposed system of equations can be easily transformed by organic compounds (replacing C - CH3, C2H5 ...) or inorganic nature (replacing C - Si, Ge, Sn, Pb).

3. Unitary Symmetry and   database

Using the concepts of unitary symmetry enables fundamentally change construction of databases values of physical and chemical parameters of atoms and molecules. Concepts such as self-consistency and reliability of the parameter values within the closed class of objects composed of a single set of elements is the main feature of the new databases.

Currently, physical and chemical data in NIST represented as a set of experimental data or estimated for each object individually. Also presents the works of other authors.

In fact, all atomic and molecular objects are elements of a set of homologous series.

The essence of the future database is as follows:

1. Each molecule is known to consist of at least two atoms.
2. Each atom is part of a group of atoms with an equally filled electron shell (shells), involved in the formation of chemical bonds. (Homologous atoms).
3. Consistently replacing one atom at its homologous one, we get either a homologous series of molecules:

    CO - CS - CSe -CTe - CPo

    or a set of homologous series, as in the case of halogen methanes (см. Fig. 21).

4. All of the experimental and calculated data scattered molecules must be located in a folder under the code name "homology with elements (for example) 5 period. This folder, in turn, will have subsections related to the permanent element (e.g., carbon) or a group of elements (e.g., benzene ring).
5. Advance may be made of the system of equations similar to the equation shown in Table 3.
6. Substitution into the these equations the experimental data and their variation within the experimental error will provide a self-consistent set of parameters and produce estimates have not yet measured values.
7. An exemplary embodiment of the database should look like as shown in Fig. 23
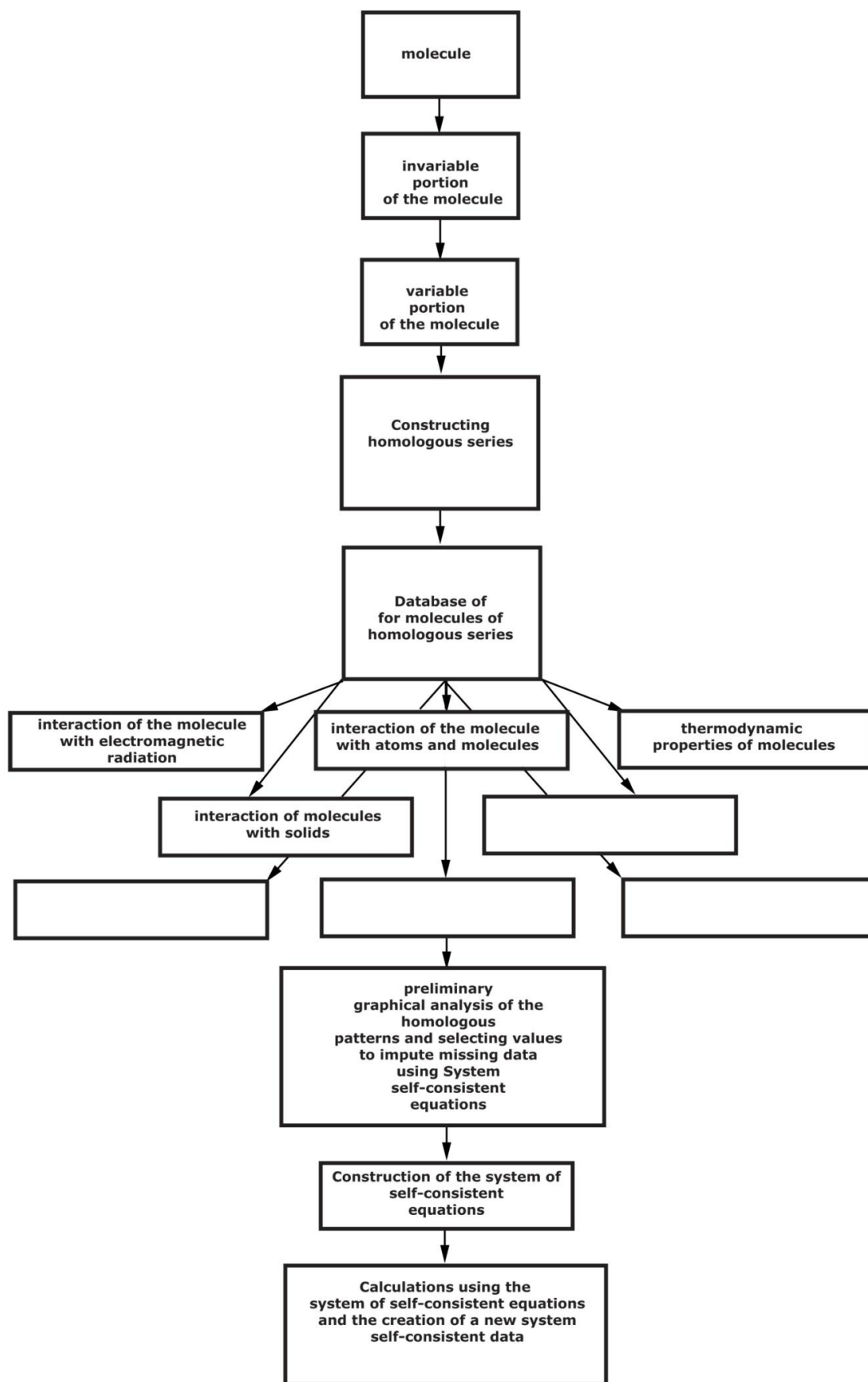
Fig.23. Block diagram of the construction of a database of physical and chemical properties of molecules. Empty cells are reserved for a variety of physical and chemical parameters of stable nuclei and their isotopes, atoms, atomic ions, molecules and radicals.

Building a database for atoms and molecules based on the basic properties of nature is more

reasonable from a scientific point of view and easier for users of any level.

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