

Thermochemistry of heteroatomic compounds: Analysis of thermodynamic functions of Mendeleev's Periodic table atoms in various phases; possibility for the bond strengths calculations in condensed state

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Abstract: The values of free energies, the heats and entropies of formation and heat capacities of gaseous and condensed atoms of I-VII main and lateral groups and three groups of transitive elements of Mendeleev's Periodic table were analyzed. Seventy nine equations of such type as $\Delta_{g,f,s} \Psi^0 = i \pm f N$, in which $\Delta_{g,f,s} \Psi^0$ is thermodynamic function, i and f are stoichiometric coefficients, have been calculated. The obtained equations can be used for the calculations of the same functions for other atoms, for with they are not known. The same equations can be used for the next calculation of bond strength in they also. Instead of bond energy (E_b) or bond dissociation energy (BDE) the bond strength (S_b) new symbol of the bond powers for organic and organometallic substances has been suggested. It has been done because there are all thermodynamic functions for practically all atoms of Periodic table and hard to define the bond power with the use the heat function (enthalpy) only; probably is necessary to present the all thermodynamic parameters for the calculating bonds between atoms.

Keywords: Atom, Free Energy, Heat of Formation, Entropy, Heat of Capacity, Bond Energy, Strength of Bond

1. Introduction

The bond energies of organic and bioorganic compounds define not only a direction and energy of organic reactions, but the possibility and activity of the live organisms also. Their values and the importance draw attention of the researchers in chemistry and biochemistry during very big period of time [1, 2].

It is known, that the new formation and destruction of the old bonds in organic and biochemical molecules play a very important significance for the understanding of synthetic ways of the mentioned substances not only for an industry, but for the vital objects. The important attention to this process is shown not only synthetic, but the theoretical biochemists also.

2. Results and Discussion

The quantitative definition of bond energy is connected

both with labour-consuming physical experiment and with the different theoretical calculations. One of such calculations is based on the data about the heat of atomization ($\Delta_a H^0$) an organic molecule in a gas phase. In turn, the heat of atomization depends on the sum of the heats of its atoms ($\Delta_{at} H^0_{gas}$) and the heat (enthalpy) of molecule formation in a gas phase ($\Delta_f H^0_{gas}$) [1, 2]. Necessary to note, that the heat of atomization is equal to the sum of all bond energies of (E_b) in such molecule also (Eq. 1).

$$\Delta_a H^0 = \sum \Delta_{at} H^0_{gas} - \Delta_f H^0_{gas} = \sum E_b \quad (1)$$

Earlier we conducted the analysis of thermodynamic functions ($\Delta_{c,f,s} \Psi^0$) of free energies ($\Delta_{c,f} G^0$), the heats of combustion and formation ($\Delta_{c,f} H^0$) and formation entropy (S^0) in condensed and gaseous phases of organic compounds I-VII of groups of Mendeleev's Periodic system of elements. Also it has been found that all functions depend from the number of valence electrons N without of the number (h) of lone electron pairs (g) of all investigated molecules (Eq. 2)

[3-7]

$$\Delta_{g,f,s}\Psi^{\circ} = i \pm f*(N - hg) \quad (2)$$

here i and f are stoichiometric coefficients

Also we have become interested not only the heat of formation of simple atoms in gaseous and condensed states, but and their other thermodynamic functions, which are known in the literature and summed in Table 1 [8, 9].

After the painstaking analysis of all thermodynamic functions and the heat of capacities of gaseous and condensed atoms was found that all they depend on the general number of electrons N in atoms I-VIII of groups in the different periods only (Table 1 and equations in it). Therefore the equation (2) necessary was changed into equation (3) before the use

$$\Delta_{g,f,s}\Psi^{\circ} = i \pm f*N \quad (3)$$

The correlations like (3) established and presented in Table 1 allow to calculate the unknown values of thermodynamic functions in the condensed condition for such necessary for the formation of organic molecules atoms as hydrogen, calcium, oxygen and others.

However there are some positions in Table 1 in the last column, in which there are not real correlations; they are marked as "no correlations".

The above mentioned correlations are necessary for the subsequent calculations of thermodynamic parameters of such important heteroatomic compounds as sugars, amino acids and others useful in the industry, biochemistry and medicine of substances. These data are collected in Table 2 and presented in square cells.

Nevertheless at the consideration of the data in Table 1 there are some questions and offers for their discussion. One of them is connected with the use of the thermodynamic characteristic for the name of the bond energy. Till now for the designation of bond energy (E_b) or bond dissociation energy (BDE) was used the heat function (enthalpy) only [2].

It is known, that there are practically all thermodynamic functions ($\Delta_f G^{\circ}$, $\Delta_f H^{\circ}$, fS° and C_p , see Table 1 also) for simple atoms in the literature, which can be used for the calculations and description of any bonds in gaseous and condensed

phases. That's why we suggest to use for all heteroatomic bonds by the term "strength of bond (S_b)" but not "bond energy or bond dissociation energy" in organic molecule and to show all thermodynamic functions of examined bond in molecules.

For the revision of this offer we have chosen a some linear and cyclic alkanes and have defined for them the basic thermodynamic functions and their sizes of atomizations in gas and condensed phases: ($\Delta_{g,f,s}\Psi^{\circ}$, Table 3).

The analysis of the results of Table 3 shows that all atomizations of all chosen thermodynamic functions (values of heat capacities were not considered) of different alkanes are depended from the number of valence electrons (Eqs. 4-8; there is bad correlation between $\Delta_a G^{\circ}_{\text{cond}}$ and N , r 0.763), as it was shown earlier for the organic molecules [3-7].

The C-H and C-C bond strengths ($\pm 1.5\%$) of alkanes can calculated with the use of Eq. 1, but instead the enthalpy could be used the other functions - free energy and entropy (Table 4).

$$\Delta_a G^{\circ}_{\text{gas}} = (-20.6 \pm 48.0) + (145.1 \pm 1.6)N, r \ 0.999, S_o \ 55.6, n \ 7, \text{ compounds (I-VII)} \quad (4)$$

$$\Delta_a H^{\circ}_{\text{gas}} = (90.5 \pm 46.6) + (194.2 \pm 1.5)N, r \ 0.999, S_o \ 54.0, n \ 7, \text{ compounds (I-VII)} \quad (5)$$

$$\Delta_a H^{\circ}_{\text{cond}} = (31.0 \pm 20.9) + (7.5 \pm 0.7)N, r \ 0.979, S_o \ 24.2, n \ 7, \text{ compounds (I-VII)} \quad (6)$$

$${}_a S^{\circ}_{\text{gas}} = (-1.7 \pm 37.0) + (67.1 \pm 1.2)N, r \ 0.999, S_o \ 49.9, n \ 7, \text{ compounds (I-VII)} \quad (7)$$

$${}_a S^{\circ}_{\text{cond}} = (9.9 \pm 49.8) + (7.8 \pm 1.6)N, r \ 0.903, S_o \ 57.6, n \ 7, \text{ compounds (I-VII)} \quad (8)$$

The data of Table 4 shows that the bond strength of all chosen gaseous functions are on about two order more than for condensed phase. Probably it can explain that alkanes in the condensed phase have a sensitive dispersion interaction between C-H bonds each other. At the same time to hard explain the some negative values of C-C bond strength for linear and cyclic alkanes (!).

Table 1. Thermodynamic functions (kJ mol^{-1} , $\text{J mol}^{-1} \text{K}^{-1}$) of atoms in the gaseous and condensed states of different groups of Periodic Table

First Main Group		Li, 3	Na, 11	K, 19	Rb, 37	Cs, 55	Equations
Functions, Ψ°	Atoms, N /Phases						
$\Delta_f G^{\circ}$	gaseous	128.0	77.8	61.2	54.0	50.9	$\Delta_f G^{\circ} = (104.2 \pm 16.8) - (1.2 \pm 0.5) N \ r \ 0.787, S_o \ 22.5, n \ 5^a$
	condense	0.9	0.5	0.3			$\Delta_f G^{\circ} = (1.0 \pm 0.1) - (0.04 \pm 0.01) N \ r \ 0.981, S_o \ 0.1, n \ 3^a$
$\Delta_f H^{\circ}$	gaseous	105.5	107.3	89.0	80.9	76.5	$\Delta_f H^{\circ} = (107.3 \pm 7.7) - (0.6 \pm 0.2) N \ r \ 0.963, S_o \ 0.04, n \ 5^b$
	condensed	2.4	2.4	2.3	2.2	2.1	$\Delta_f H^{\circ} = (2.4 \pm 0.03) - (0.02 \pm 0.01) N \ r \ 0.987, S_o \ 0.02, n \ 5^b$
fS°	gaseous	138.7	153.6	160.3	170.1	175.6	$fS^{\circ} = (143.4 \pm 4.0) + (0.7 \pm 0.1) N \ r \ 0.942, S_o \ 5.6, n \ 5^b$
	condensed	29.1	51.5	64.6	76.8	85.1	$fS^{\circ} = (36.9 \pm 6.9) + (1.0 \pm 0.2) N \ r \ 0.932, S_o \ 9.3, n \ 5^b$
C_p	condensed	31.3	32.7	32.7	31.4	31.4	No correlation
First Lateral Group							

Functions, Ψ^o	Atoms, N /Phases		Cu, 29 299.7	Ag, 47 247.4	Au, 79 325.6		Equations
$\Delta_f G^o$	gaseous						No correlation
$\Delta_f H^o$	gaseous		337.6	284.9	83.7		$\Delta_f H^o = (505.0 \pm 48.5) - (5.2 \pm 0.9) N r 0.986,$ $S_o 31.2, n 3^b$
	condensed		11.9				
ρS^o	gaseous		166.4	172.0	180.4		$\rho S^o = (158.6 \pm 0.8) + (0.3 \pm 0.01) N r 0.998,$ $S_o 0.5, n 3^b$
Cp	condensed		24.5	25.5			
Second Main Group							
Functions, Ψ^o	Atoms, N /Phases	Be, 4	Mg, 12	Ca, 20	Sr, 38	Ba, 56	Equations
	gaseous	288.1	114.4	142.8	130.1	143.2	$\Delta_f G^o = (106.2 \pm 1.3) + (0.6 \pm 0.02) N r 0.999, S_o 1.1, n 3(\text{no Mg,Sr})^a$
$\Delta_f G^o$	condensed	10.0	6.1			136.1	$\Delta_f G^o = (-11.7 \pm 14.8) + (2.6 \pm 0.4) N r 0.986,$ $S_o 17.7, n 3(\text{no Sr,Ca})^a$
$\Delta_f H^o$	gaseous	327.4	149.0	176.6	163.5	174.6	$\Delta_f H^o = (320.4 \pm 62.2) - (4.7 \pm 2.5) N r 0.884,$ $S_o 60.1, n 3(\text{no Mg,Ba})^a$
	condensed	12.0	9.0	7.79	0.91	4.99	No correlation
ρS^o	gaseous	136.1	148.5	154.8	164.5	170.1	$\rho S^o = (138.9 \pm 3.4) + (0.6 \pm 0.1) N r 0.956, S_o 4.5, n 5^a$
	condensed	9.4	32.7	45.5	50.9	62.5	$\rho S^o = (17.3 \pm 7.4) + (0.9 \pm 0.2) N r 0.910, S_o 9.7, n 5^b$
Cp	condensed	15.9	24.9	26.3	27.3	28.3	$Cp = (24.4 \pm 0.4) + (0.07 \pm 0.01) N r 0.970,$ $S_o 0.4, n 4 (\text{no Be})^a$
Second Lateral Group							
Functions, Ψ^o	Atoms, N /Phases		Zn, 30	Cd, 48	Hg, 80		Equations
$\Delta_f G^o$	gaseous		94.9	77.4	31.8		$\Delta_f G^o = (135.5 \pm 6.6) - (1.3 \pm 0.1) N r 0.995,$ $S_o 4.2, n 3^a$
$\Delta_f H^o$	gaseous		128.6	111.9	61.3		$\Delta_f H^o = (172.9 \pm 9.5) - (1.4 \pm 0.1) N r 0.992,$ $S_o 6.9, n 3^a$
	condensed		6.52				
ρS^o	gaseous			167.6	174.8		
	condensed		41.6	51.7	76.0		$\rho S^o = (19.8 \pm 2.9) + (0.7 \pm 0.05) N r 0.997, S_o 1.8, n 3^a$
Cp	condensed		25.3	26.0	28.0		$Cp = (23.5 \pm 0.3) + (0.05 \pm 0.01) N r 0.993,$ $S_o 0.2, n 3^a$
Third Main Group							
Functions, Ψ^o	Atoms, N /Phases	B, 5	Al, 13	Ga, 31	In, 39	Tl, 81	Equations
$\Delta_f G^o$	gaseous	545.2	285.8	233.8	208.1	145.1	$\Delta_f G^o = (299.8 \pm 13.6) - (2.0 \pm 0.3) N r 0.970,$ $S_o 18.4, n 4 (\text{no B})^a$
	condensed	19.3	7.2				
$\Delta_f H^o$	gaseous	556.5	326.3	272.0	238.5	179.9	$\Delta_f H^o = (338.8 \pm 17.7) - (2.1 \pm 0.4) N r 0.975,$ $S_o 16.7, n 4 (\text{no B})^a$
	condensed	22.0	10.0	246.8			$\Delta_f H^o = (-60.7 \pm 67.4) + (9.4 \pm 3.9) N r 0.939,$ $S_o 64.7, n 3^a$
ρS^o	gaseous	153.3	164.4				
	condensed	14.8	37.8	40.9	57.8	64.2	$\rho S^o = (23.9 \pm 7.9) + (0.6 \pm 0.2) N r 0.873, S_o 10.8, n 5^a$
	gaseous		21.4	25.3			
Cp	condensed		29.3	26.9	26.7	26.3	$Cp = (28.8 \pm 1.0) + (0.04 \pm 0.02) N r 0.775,$ $S_o 1.0, n 4^a$
Third Lateral Group							
Functions, Ψ^o	Atoms, N /Phases		Sc, 21	Y, 39	La, 57		Equations
$\Delta_f G^o$	gaseous		302.2	387.0	381.8		$\Delta_f G^o = (270.8 \pm 60.1) + (2.2 \pm 1.4) N r 0.837, S_o 36.7, n 3^a$
	condensed				430.8		
$\Delta_f H^o$	gaseous		381.6	426.8	430.9		$\Delta_f H^o = (359.2 \pm 30.1) + (1.2 \pm 0.7) N r 0.901, S_o 16.8, n 3^a$
	condense				431.8		
ρS^o	gaseous		174.7		182.3		
	condensed		37.6	46.0	57.1		$\rho S^o = (25.8 \pm 1.8) + (0.5 \pm 0.04) N r 0.997, S_o 1.1, n 3^a$
	gaseous		22.1		22.8		
Cp	condensed		25.1	25.1	27.2		$Cp = (23.5 \pm 1.4) + (0.06 \pm 0.03) N r 0.866,$ $S_o 0.8, n 3^a$
Fourth Main Group							
Functions, Ψ^o	Atoms, N /Phases	C, 6	Si, 14	Ge, 32	Sn, 50	Pb, 82	Equations
$\Delta_f G^o$	gaseous	669.5	399.1	335.8	267.3	162.9	$\Delta_f G^o = (569.7 \pm 78.1) - (5.5 \pm 1.7) N r 0.881,$

	condensed	2.9				2.2	S_o 104.0, n 5 ^a
$\Delta_f H^\circ$	gaseous	715.0	468.7	376.6	302.1	195.8	$\Delta_f H^\circ = (626.7 \pm 73.1) - (5.8 \pm 1.6) N r$ 0.904, S_o 97.3, n 5 ^a
	condensed	16.5	50.6		2.1	4.3	No correlation
ρS°	gaseous	157.9	167.9	167.8		175.3	$\rho S^\circ = (158.3 \pm 2.9) + (0.2 \pm 0.01) N r$ 0.966, S_o 3.2, n 3 (no Si, Sn) ^a
	condensed	5.8	47.2	31.1	51.4	71.7	$\rho S^\circ = (16.5 \pm 11.6) + (0.7 \pm 0.2) N r$ 0.839, S_o 15.5, n 5 ^a
C_p	gaseous	20.4	22.2	30.7			$C_p = (17.3 \pm 1.2) + (0.4 \pm 0.06) N r$ 0.990, S_o 1.1, n 3 ^a
	condensed	6.1	25.6	23.3	27.0	26.8	No correlation
Fourth Lateral Group							
Functions, Ψ°	Atoms, N /Phases		Ti, 22	Zr, 40	Hf, 72		Equations
$\Delta_f G^\circ$	gaseous		429.9	568.4	660.8		$\Delta_f G^\circ = (355.8 \pm 61.3) + (4.4 \pm 1.2) N r$ 0.962, S_o 44.6, n 3 ^a
	condensed		14.8	18.7			
$\Delta_f H^\circ$	gaseous		474.5	610.9	702.9		$\Delta_f H^\circ = (400.9 \pm 60.0) + (4.3 \pm 1.2) N r$ 0.963, S_o 43.7, n 3 ^a
	condensed		16.2	22.0			
ρS°	gaseous		180.3	183.0	186.9		$\rho S^\circ = (177.6 \pm 0.4) + (0.1 \pm 0.02) N r$ 0.998, S_o 0.3, n 3 ^b
	condensed		39.18	47.60	71.94		$\rho S^\circ = (23.1 \pm 3.7) + (0.7 \pm 0.1) N r$ 0.993, S_o 2.7, n 3 ^b
C_p	gaseous		24.4	26.6			
	condensed		33.5	25.7	25.5		$C_p = (34.6 \pm 5.4) - (0.1 \pm 0.1) N r$ 0.789, S_o 4.0, n 3 ^a
Fifth Main Group							
Functions, Ψ°	Atoms, N /Phases	N, 7	P, 15	As, 33	Sb, 51	Bi, 83	Equations
$\Delta_f G^\circ$	gaseous	455.6	292.1	247.3	222.2	168.2	$\Delta_f G^\circ = (313.1 \pm 6.9) - (1.8 \pm 0.1) N r$ 0.994, S_o 6.7, n 4 (no N) ^a
	condensed		12.1				
$\Delta_f H^\circ$	gaseous	472.8	333.9	288.7	262.3	207.1	$\Delta_f H^\circ = (355.7 \pm 6.7) - (1.8 \pm 0.1) N r$ 0.994, S_o 6.5, n 4 (no N) ^a
	condensed	316.4	18.1	13.5	10.6		$\Delta_f H^\circ = (20.9 \pm 10.0) - (0.2 \pm 0.02) N r$ 0.991, S_o 0.7, n 3 (P, As, Sb) ^a
ρS°	gaseous	153.2	163.1	174.1		186.9	$\rho S^\circ = (155.4 \pm 4.2) + (0.4 \pm 0.1) N r$ 0.950, S_o 5.5, n 4 (no Sb) ^a
	condensed		41.1	35.1	45.7	56.8	$\rho S^\circ = (38.4 \pm 4.4) + (0.2 \pm 0.07) N r$ 0.933, S_o 3.7, n 3 (no As) ^a
C_p	gaseous	32.9	20.8	20.8		20.8	No correlation
	condensed		26.3	24.7	25.2	25.6	No correlation
Fifth Lateral Group							
Functions, Ψ°	Atoms, N /Phases		V, 23	Nb, 41	Ta, 73		Equations
$\Delta_f G^\circ$	gaseous		468.0	698.0	738.7		$\Delta_f G^\circ = (409.7 \pm 149.7) + (4.9 \pm 3.0) N r$ 0.855, S_o 106.8, n 3 ^a
$\Delta_f H^\circ$	gaseous		515.3	721.9	781.6		$\Delta_f H^\circ = (448.4 \pm 124.9) + (4.9 \pm 2.0) N r$ 0.892, S_o 89.2, n 3 ^a
	condensed		17.3	29.6			
ρS°	gaseous		180.3	183.0	186.9		$\rho S^\circ = (177.4 \pm 0.4) + (0.1 \pm 0.02) N r$ 0.998, S_o 0.3, n 3 ^b
	condensed		28.7	36.5	41.5		$\rho S^\circ = (24.4 \pm 3.6) + (0.2 \pm 0.07) N r$ 0.959, S_o 2.6, n 3 ^a
C_p	gaseous		24.5		20.9		
	condensed		24.2	24.9	25.3		$C_p = (23.8 \pm 0.3) + (0.02 \pm 0.01) N r$ 0.950, S_o 0.2, n 3 ^a
Sixth Main Group							
Functions, Ψ°	Atoms, N /Phases	O, 8	S, 16	Se, 34	Te, 52	Po, 84	Equations
$\Delta_f G^\circ$	gaseous	231.8	197.6	166.7	154.9	106.5	$\Delta_f G^\circ = (229.9 \pm 9.3) - (1.5 \pm 0.2) N r$ 0.976, S_o 11.9, n 5 ^a
	condensed		0.4	2.6			
$\Delta_f H^\circ$	gaseous	249.2	278.8	206.7	194.5	144.1	$\Delta_f H^\circ = (276.8 \pm 15.8) - (1.6 \pm 0.3) N r$ 0.941, S_o 20.3, n 5 ^a
	condensed		1.4	6.7	11.2		$\Delta_f H^\circ = (-2.8 \pm 0.5) + (0.3 \pm 0.01) N r$ 0.998, S_o 0.3, n 3 ^a
ρS°	gaseous	161.1	167.7	176.6	182.6	188.8	$\rho S^\circ = (161.6 \pm 2.6) + (0.3 \pm 0.05) N r$ 0.966, S_o 3.3, n 5 ^a
	condensed		35.3	48.9	49.7	64.8	$\rho S^\circ = (30.9 \pm 3.9) + (0.4 \pm 0.1) N r$ 0.968, S_o

C_p	gaseous	21.9	23.7	21.0	24.3		3.7, n 4 ^a $C_p = (22.2 \pm 2.6) + (0.04 \pm 0.03)N$ r 0.806, S_o 1.0, n 3 (no Se) ^a
	condensed		31.7	35.6	25.7	26.4	$C_p = (35.7 \pm 4.4) - (0.1 \pm 0.08)N$ r 0.768, S_o 4.2, n 3 (no Te) ^a
Sixth Lateral Group							
Functions, Ψ^o	Atoms, N /Phases		Cr, 24	Mo, 42	W, 74		Equations
$\Delta_f G^o$	gaseous		352.6	604.9	802.3		$\Delta_f G^o = (182.2 \pm 103.8) + (8.7 \pm 2.0)N$ r 0.973, S_o 72.9, n 3 ^a
	condensed				27.8		
$\Delta_f H^o$	gaseous		397.5	660.2	844.3		$\Delta_f H^o = (234.3 \pm 117.0) + (8.6 \pm 2.3) N$ r 0.966, S_o 82.1, n 3 ^a
	condensed				30.1		
ρS^o	gaseous		174.2	181.8	173.8		No correlation
	condensed		23.8	28.6	32.8		$\rho S^o = (20.3 \pm 1.8) + (0.2 \pm 0.03)N$ r 0.980, S_o 1.2, n 3 ^a
C_p	gaseous		46.9		21.3		
	condensed		23.3	23.5	24.2		$C_p = (22.8 \pm 0.1) + (0.02 \pm 0.01)N$ r 0.989, S_o 0.1, n 3 ^a
Seventh Main Group							
Functions, Ψ^o	Atoms, N /Phases	F, 9	Cl, 17	Br, 35	I, 53	At, 85	Equations
$\Delta_f G^o$	gaseous	62.4	105.3	82.4	70.2	54.4	$\Delta_f G^o = (112.2 \pm 6.6) - (0.7 \pm 0.1) N$ r 0.972, S_o 6.2, n 4 (no F) ^a
$\Delta_f H^o$	gaseous	78.9	121.1	111.8	106.8	92.0	$\Delta_f H^o = (127.8 \pm 1.4) - (0.4 \pm 0.03) N$ r 0.996, S_o 1.3, n 4 (no F) ^a
ρS^o	gaseous	158.7	165.1	174.9	180.7	186.9	$\rho S^o = (158.4 \pm 2.8) + (0.4 \pm 0.1)N$ r 0.963, S_o 3.5, n 5 ^a
C_p	gaseous	22.8	21.8				
Seventh Lateral Group							
Functions, Ψ^o	Atoms, N /Phases		Mn, 25	Tc, 43	Re, 75		Equations
$\Delta_f G^o$	gaseous		238.7	604.5	733.4		$\Delta_f G^o = (86.5 \pm 219.5) + (9.2 \pm 4.2) N$ r 0.909, S_o 151.3, n 3 ^a
$\Delta_f H^o$	gaseous		290.0	648.5	778.6		$\Delta_f H^o = (138.2 \pm 213.5) + (9.1 \pm 4.1)N$ r 0.911, S_o 147.2, n 3 ^a
ρS^o	gaseous		32.0	180.9			
	condensed		32.0	49.7	36.5		No correlation
C_p	gaseous		27.6				
	condensed		25.5	25.8	25.7		No correlation
First Group of Transitive Elements							
Functions, Ψ^o	Atoms, N /Phases		Fe, 26	Co, 27	Ni, 28		Equations
$\Delta_f G^o$	gaseous		372.0	380.5	378.3		$\Delta_f G^o = (291.9 \pm 83.3) + (3.1 \pm 3.1) N$ r 0.714, S_o 4.4, n 3 ^a
$\Delta_f H^o$	gaseous		417.7	425.1	429.6		$\Delta_f H^o = (263.5 \pm 23.0) + (5.9 \pm 0.8) N$ r 0.990, S_o 1.2, n 3 ^a
ρS^o	gaseous		180.4	179.4	182.1		
	condensed		34.3	30.0	29.9		$\rho S^o = (90.8 \pm 32.7) - (2.2 \pm 1.2)N$ r 0.876, S_o 1.7, n 3 ^a
C_p	gaseous		25.7	23.0	23.3		$C_p = (55.0 \pm 22.6) - (1.1 \pm 0.8)N$ r 0.808, S_o 1.2, n 3 ^a
	condensed		25.0	24.8	26.1		$C_p = (10.4 \pm 12.0) + (0.5 \pm 0.4)N$ r 0.786, S_o 0.6, n 3 ^a
Second Group of Transitive Elements							
Functions, Ψ^o	Atoms, N /Phases		Ru, 44	Rh, 45	Pd, 46		Equations
$\Delta_f G^o$	gaseous		601.4	510.9	354.8		$\Delta_f G^o = (6038 \pm 851) - (123.3 \pm 3.5) N$ r 0.988, S_o 26.7, n 3 ^a
$\Delta_f H^o$	gaseous		648.1	556.5	393.3		$\Delta_f H^o = (6265 \pm 930) - (127.4 \pm 20.7)N$ r 0.987, S_o 29.2, n 3 ^a
ρS^o	gaseous		186.4		166.9		
	condensed		28.5	31.5	37.9		$\rho S^o = (-178.9 \pm 44.2) + (4.7 \pm 1.0)N$ r 0.979, S_o 1.4, n 3 ^a
C_p	gaseous		21.5	21.0			
	condensed		23.8	25.0	26.0		$C_p = (-24.6 \pm 2.6) + (1.0 \pm 0.4)N$ r 0.998, S_o 0.1, n 3 ^a
Third Group of Transitive Elements							
Functions, Ψ^o	Atoms, N /Phases		Os, 76	Ir, 77	Pt, 78		Equations
$\Delta_f G^o$	gaseous		621.8	622.3	519.1		$\Delta_f G^o = (4541 \pm 2305) - (51.3 \pm 29.9) N$ r 0.864, S_o 42.3, n 3 ^a
$\Delta_f H^o$	gaseous		790.7	673.2	564.0		$\Delta_f H^o = (9404 \pm 172) - (113.3 \pm 2.2)N$ r

ρS°	gaseous	192.5	178.4	0.995, S_0 3.2, n 3 ^a	
	condensed		35.5	41.6	
C_p	gaseous			25.5	
	condensed		25.5	25.9	

^a Data have been used from Ref. [8]; ^b Data have been used from Ref. [9].

Table 2. The calculated thermodynamic functions (kJ mol^{-1} and $\text{J mol}^{-1}\text{K}^{-1}$) in the condensed state, which are given as bold type

Func-tions	Atoms, N /Phases	H, 1	Ca, 20	C, 6	N, 7	O, 8	P, 15	Sb, 51	Bi, 83	Sn, 50	Pb, 82	Po, 84
$\Delta_f G^\circ$	gaseous	103.0	142.8	669.5	455.6	231.8	292.1	222.2	168.2	267.3	162.9	106.5
	condensed	1.0	40.3	2.9			12.1				2.2	
$\Delta_f H^\circ$	gaseous	218.0	176.6	715.0	472.8	249.2	333.9	262.3	207.1	302.1	195.8	144.1
	condensed	2.4	7.79	16.5	316.4	-0.4	18.1	10.6	74.3	2.1	4.3	22.4
ρS°	gaseous	144.1	154.8	157.9	153.2	161.1	163.1	175.8	186.9	168.3	175.3	188.8
	condensed	37.9	45.5	5.8			41.1	45.7	56.8	51.4	71.7	64.8
C_p	gaseous	114.7		20.4	32.9	21.9	20.8		20.8	37.3	50.1	
	condensed		26.3	6.1		31.7	26.3	25.2	25.6	27.0	26.8	26.4

Table 3. Thermodynamic functions and calculated through Eq. 1 ($\pm 1.5\%$) the atomizations in the gaseous and condensed phases (kJ mol^{-1} and $\text{J mol}^{-1}\text{K}^{-1}$) of some linear and cyclic alkane

No, Compound, formula, N	Free energy				Heat contribution (enthalpy)	
	$\Delta_f G^\circ$, gas	$\Delta_f G^\circ$, cond	$\Delta_a G^{\circ b}$, gas	$\Delta_a G^{\circ b}$, cond	$\Delta_f H^\circ$, gas	$\Delta_f H^\circ$, cond
Linear alkanes						
I, Methane, CH_4 , 8	-50.6 ^[10]	-31.0 ^a ± 1.5	1132.1 ± 17.0	37.9 ± 0.6	-74.9 ^[9]	-70.8 ^c ± 0.3
II, Ethane, C_2H_6 , 14	-33.0 ^[10]	-25.6 ^a ± 1.3	1990.0 ± 29.8	37.4 ± 0.6	-84.7 ^[11]	-96.6 ^c ± 0.5
III, Propane, C_3H_8 , 20	-23.0 ^[10]	-20.2 ^a ± 1.0	2855.5 ± 43.0	39.7 ± 0.6	-104.7 ^[10]	-122.4 ^c ± 0.6
IV, <i>n</i> -Pentane, C_5H_{12} , 32	-8.4 ^[10]	-9.5 ^[10]	4591.9 ± 68.9	36.0 ± 0.5	-146.8 ^[4] ± 0.6	-173.5 ^[5] ± 0.6
V, <i>n</i> -Oktane, C_8H_{18} , 50	16.7 ^[4] ± 0.9	6.4 ^[4]	7193.3 ± 107.9	34.8 ± 0.5	-208.4 ^[13] ± 0.7	-250.0 ^[13] ± 0.8
Cyclic alkanes						
VI, Cyclohexane, C_6H_{12} , 36	31.8 ^[10]	26.7 ^[10]	5221.2 ± 78.3	2.7 ± 0.04	-123.0 ^[10]	-156.2 ^[10]
VII, Cyclopentane, C_5H_{10} , 30	38.6 ^[10]	36.5 ^[3]	4438.9 ± 65.1	-12.0 ± 0.2	-76.9 ^[14]	-105.6 ^[14] ± 1.8

Table 3. Continued

No, Compound, xxxformula, N	Heat contribution (enthalpy)		Entropy			
	$\Delta_a H^{\circ b}$, gas	$\Delta_a H^{\circ b}$, cond	ρS° , gas	ρS° , cond	ρS° , gas	ρS° , cond
Linear alkanes						
I, Methane, CH_4 , 8	1661.9 ± 25.0	96.9 ± 1.4	188.7 ^[9]	106.2 ^[9] ± 6.1	545.6 ± 8.2	51.2 ± 0.8
II, Ethane, C_2H_6 , 14	2822.5 ± 42.3	144.0 ± 2.1	230.0 ^[10]	126.7 ^[13]	950.4 ± 14.2	112.3 ± 1.7
III, Propane, C_3H_8 , 20	3993.7 ± 60.0	188.5 ± 2.8	270.0 ^[10]	171.0 ^[12]	1356.5 ± 20.3	149.6 ± 2.2
IV, <i>n</i> -Pentane, C_5H_{12} , 32	6337.8 ± 95.1	284.8 ± 4.3	347.8 ^[4] ± 0.8	263.5 ^[4]	2170.9 ± 32.6	220.3 ± 3.3
V, <i>n</i> -Oktane, C_8H_{18} , 50	9852.4 ± 147.8	425.2 ± 6.4	467.1 ^[4] ± 0.9	361.2 ^[4]	3389.9 ± 50.8	367.4 ± 5.5
Cyclic alkanes						
VI, Cyclohexane, C_6H_{12} , 36	7029.0 ± 105.4	284.0 ± 4.3	298.0 ^[10]	204.0 ^[10]	2378.6 ± 35.7	285.6 ± 4.3
VII, Cyclopentane, C_5H_{10} , 30	5831.9 ± 87.5	212.1 ± 3.2	293.0 ^[10]	49.0 ^[10]	1937.5 ± 29.1	359.0 ± 5.4

^a Calc. via Eq. (3) in Ref. [4]; ^b Calc. via Eq. (1) with the use of $\Delta_f G^\circ$, $\Delta_f H^\circ$, ρS° functions; ^c Calc. via Eq. (7) in Ref. [4].

Table 4. The calculated of the gaseous and condensed inner (i) and cyclic (c) bond strength ($S_b \pm 1.5\%$, kJ mol^{-1} and $\text{J mol}^{-1}\text{K}^{-1}$) on the basis of their thermodynamic functions

No, Compound	S_b through free energy, G°		S_b through enthalpy, H°		S_b through entropy, S°	
	C-H	C-C	C-H	C-C	C-H	C-C
Linear alkanes						
I, Methane	gas 283.0 ± 0.4 cond 9.5 ± 0.1		gas 415.5 ± 6.2 Lit 439.3 ± 0.4 ^[2] cond 24.2 ± 0.4		gas 136.4 ± 2.0 cond 12.8 ± 0.2	
II, Ethane		gas 292.0 ± 4.4 cond -19.6 ± 0.3		gas 329.5 ± 4.9 Lit 377.4 ± 0.8 ^[2] cond -1.2 ± 0.01		gas 132.0 ± 2.0 cond 35.5 ± 0.5
III, Propane	gas (i) 286.7 ± 4.3 cond (i) 10.9 ± 0.2		gas (i) 420.8 ± 6.3 Lit (i) 410.5 ± 2.9 ^[2] cond (i) 22.8 ± 0.3		gas (i) 137.0 ± 2.0 cond (i) 0.9 ± 0.01	
IV, <i>n</i> -Pentane	gas (i) 287.6 ± 4.3 cond (i) 9.5 ± 0.08	gas (i) 294.8 ± 4.4 cond (i) -23.6 ± 0.3	gas (i) 421.1 ± 6.3 Lit (i) 415.1 ^[2]	gas (i) 330.5 ± 5.0 Lit (i) 365.3 ± 2.9 ^[2]	gas (i) 137.4 ± 2.1 cond (i) 0.3 ± 0.005	gas (i) 133.2 ± 2.0 cond (i) 33.5 ± 0.5

No, Compound	S_b through free energy, G°		S_b through enthalpy, H°		S_b through entropy, S°	
	C-H	C-C	C-H	C-C	C-H	C-C
V, <i>n</i> -Oktane	gas (i) 287.6 ± 4.3 cond (i) 9.6 ± 0.1	gas (i) 294.2 ± 4.4 cond (i) -22.8 ± 0.3	cond (i) 24.1 ± 0.4 gas (i) 421.1 ± 6.3 Lit (i) $415.1^{[2]}$ cond (i) 24.0 ± 0.4	cond (i) 2.6 ± 0.03 gas (i) 330.2 ± 4.9 Lit (i) $364.0 \pm 3.8^{[2]}$ cond (i) 1.8 ± 0.02	gas (i) 137.3 ± 2.0 cond (i) 3.5 ± 0.05	gas (i) 132.7 ± 2.0 cond (i) 41.8 ± 0.6
The middle values of S_b of C-H and C-C bonds Cycloalkanes	gas 286.2 ± 4.3 cond 9.9 ± 0.1	gas 293.7 ± 4.4 cond -22.0 ± 0.3	gas 419.6 ± 6.3 cond 23.8 ± 0.3	gas 330.1 ± 4.9 cond 1.1 ± 0.01	gas 137.0 ± 2.0 cond: hard define	gas 132.6 ± 2.0 cond 36.9 ± 0.5
VI, Cyclohexane		gas (c) 296.8 ± 4.3 cond (c) -21.3 ± 0.3	Lit (e) $403.3 \pm 2.5^{[2]}$	gas (c) 329.9 ± 4.9 Lit (c) $371.5 \pm 2.9^{[2]}$ cond (c) 1.7 ± 0.02		gas (c) 123.6 ± 1.8 cond (c) 22.0 ± 0.3
VII, Cyclopentane		gas (c) 314.4 ± 4.7 cond (c) -24.2 ± 0.4	Lit (e) $400.0 \pm 4.2^{[2]}$	gas (c) 324.8 ± 4.9 Lit (c) $371.5 \pm 2.9^{[2]}$ cond (c) -3.2 ± 0.04		gas (c) 113.5 ± 1.7 cond (c) 71.6 ± 1.1

3. Conclusions

On the base of the consideration of all presented data is possible to make some conclusions.

First of all it was established that practically all thermodynamic functions and heat capacities of simple atoms of Mendeleev's table are depended from the number of electrons in they.

The second of them is connected with the necessity to present all thermodynamic functions of the calculated bonds in organic or organometallic compounds, that to have a really understanding about the bond strength of they.

The third is connected with the necessity of calculations of all bonds in the condensed phase especially because the large number of heteroatomic compounds have a reactivity in the condensed conditions than in gaseous phase.

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