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Thermochemistry of Heteroatomic Compounds: The Minimization of the Bonds Strength (Enthalpy) of C-H, C-C, C-O C=O for Some Sugars in Condensed State.

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ABSTRACT

The calculations of strength of bonds (enthalpy) magnitudes of C-C, C-H, C-O, C=O and O-H bonds with the use of Widows-Excel-function «Search of the decision by a method gradient descent» of condensed carbohydrates of a various spatial structure (15 compounds) were made first time. The reduced magnitudes of the force of all bonds in condensed phase, comparing to gas state, designated as a strength of bond (S_b) carbohydrates, necessary to explain by the presence significant hydrogen bonds, dipole-dipole- and dispersive interactions in biochemical molecules.

Keywords: sugars, carbohydrates, strength of bonds, enthalpy of atomization.

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INTRODUCTION

The energy of bonds of the organic molecule, which are being in a gas or condensed state, it is possible to define not only an experimental physical method, but also to calculate on the equation (1) with the application of one of the theoretical approaches, based on use atomization enthalpy ($\Delta_a H^o$), formations of a molecule ($\Delta_f H^o_{gas/cond}$) and atoms making it ($\Delta_{atom} H^o_{gas/cond}$) in a gas/condensed phase. It is necessary to note, that size $\Delta_a H^o$ it is possible to consider to the equal sum energies (enthalpies) all compounds (ΣE_b) between atoms in a molecule

$$\Delta_a H^o = \Sigma\ \Delta_{atom} H^o_{gas/cond} - \Delta_f H^o_{gas/cond} = \Sigma E_b \qquad (1).$$

RESULTS AND DISCUSSION

Previously we presented the results of the determination of strengths of chemical bonds (bond enthalpies) of saturated alkanes, chlor- and nitro alkanes with the use of they the heat of atomization ($\Delta_a H^o_{gas/cond}$) in the gaseous and condensed phases [1-3]. In the present communication we present the results of calculations of strength of C-H, C-C, C-O, C=O, O-H bonds (the heat or enthalpy) for some sugars (carbohydrates), which exist in the condensed phase only.

The calculation of the heats of the given above bonds was conducted with the use of the program Microsoft-Excel-function «Search of the decision by a method of the interfaced gradients». It is the equation (2), in which R_i^2 is the sum of quadrates of the differences between the experimental and calculated values of atomization function ($\Delta_a H^o$) of carbohydrates in the condensed phase and g_i is their weight contributions was accepted as equal 1. The minimization of the heats of bonds has been conducted until the smallest value of R_i^2.

$$R_i^{\ 2} = \Sigma\{|\ \Delta_a H^o_{exp} - \Delta_a H^o_{calc}\ |\ g_i\}^2 \qquad (2).$$

The heat of atomization was calculated by the equation (3) with the use of the known the heats of formation of carbohydrates molecules ($\Delta_f H^o_{mol}$) [4] and the heats of formation of simple atoms ($\Delta_f H^o_{atom}$), composite of they in the condensed state [1]. It is known that the heat of atomization is equal to the sum of all strengths of bonds (S_b) in molecule. Necessary to note that the strength of bond in the literature was called as the bond energy (E_b) or bond dissociation energy (BDE), taking into account that the organic bond can dissociate for different manner: on two radical or two charged particles [5]

$$\Delta_a H^o = \Sigma\ \Delta_{atom} H^o_{cond} - \Delta_f H^o_{cond} = \Sigma S_b(E_b, \text{BDE}) \qquad (3).$$

Table 1: The heats of atomization (kJ mol^{-1}) of carbohydrates, some alcohols and parameter $R_i^{\ 2}$ from Eq. (2).

No	Compound, formula,	$\Delta_a H^o_{exp}$	$\Delta_a H^o_{calc}$	$R_i^{\ 2}$
1	*α-D*-Glucose $C_6H_{12}O_6$,	1398.2	1401.9	13.9
2	*D*-Fructofuranose, $C_6H_{12}O_6$,	1387.6	1383.9	13.9
3	*α-D*-Lactose $C_{12}H_{22}O_{11}$	2460.6	2460.6	0.0
4	*α-D*-Saccharose, $C_{12}H_{22}O_{11}$	2467.6	2467.6	0.0
5	*α-D*-methylglucose, $C_7H_{14}O_6$	1374.9	1371.2	13.9
6	α-Methylglucofuranoside, $C_7H_{14}O_6$	1349.4	1353.1	13.9
7	*α-D*-galactose, $C_6H_{12}O_6$	1396.9	1388.9	64.0
8	*D*-ribose, $C_5H_{10}O_5$	1153.6	1157.3	13.7
9	*D*-arabinose, $C_5H_{10}O_5$	1162.4	1157.3	26.0
10	*α-D*-xylofuranose, $C_5H_{10}O_5$	1162.3	1162.3	0.0
11	*D*-Xylose, $C_5H_{10}O_5$	1155.9	1157.3	1.9
12	*D*-Sorbose, $C_6H_{12}O_6$	1402.3	1396.6	31.9
13	*D*-Mannose, $C_6H_{12}O_6$	1388.8	1388.9	0.0
14	*D*-Gulose, $C_6H_{12}O_6$	1381.1	1388.9	61.4
15	*α-D*-Fructose, $C_6H_{12}O_6$	1391.0	1396.6	31.9
16	Eritrol, $C_4H_{10}O_4$	998.8	998.8	0.0
17	2- Tetrahydrofuran-methanol, $C_5H_{10}O_2$	541.3	541.3	0.0
				Σ 285.8

The atomization values of the simple hydrogen, carbon and oxygen atoms in condensed phase ($\Delta_a H^o_{cond}$) are taken from the work [1]; all results are given in Table 1.

We compared the calculated enthalpy magnitudes of C-C and C-H bonds (Table 2) with the same values of bonds, which known in the literature for condensed phase [1]. The magnitudes of C-C bonds are essentially much higher than values for a condensed phase received previously (1.1 ± 0.01kJ mol^{-1}), but the C-H bonds are practically in the same ranges as calculated earlier (23.8 ± 0.3 kJ mol^{-1}) for the saturated alkanes [1]. As far as is concerned of other C-O, C=O and OH bonds is it appear that they are essentially lesser than known in the literature [6]. We can explained the last circumstance only by the presence of hydrogen bonds, a dipole-dipole- and Van der Vaals-interactions, which are absent for this type of biochemical molecules, if they will in a gas conditions.

Table 2: The enhalpies (kJ mol^{-1}) of different bonds of carbohydrates.

C–C Bonds					
C–C in pyrane cycles	**C–C** in furane cycles	**C**–CH$_2$OH in exocyclic groups	**C–C**H(=O) alongside to aldehyde groups	**C–C**(=O)-C alongside to ketone groups	**C–C** in the middle of chain
33.6	37.0	23.2	34.2	83.4	52.8
C–H Bonds					
	H–CH$_2$(OH)	**H–C**(OH)	(O)-H$_2$**C–H**		
	16.3	25.0	36.1		
	C-O Bonds				
	C–O(H)	**C=O**	**C–O–C** glycoside bond		
	115.5	60.9	32.6		
H–O Bonds					
88.7					

CONCLUSIONS

The calculations of strength of bonds (enthalpy) magnitudes of C-C, C-H, C-O, C=O and O-H bonds with the use of Widows-Excel-function «Search of the decision by a method gradient descent» of condensed carbohydrates of a various spatial structure (15 compounds) were made first time. The reduced magnitudes of the force of all bonds in condensed phase, comparing to gas state, designated as a strength of bond (S_b) carbohydrates, necessary to explain by the presence significant hydrogen bonds, dipole-dipole- and dispersive interactions in biochemical molecules.

REFERENCES

[1] Ovchinnikov VV. American J Physical Chem 2014;3:54-60.

[2] Vitaly Ovchinnikov and Alexey Kulakov. Res J Pharm Biol Chem Sci 2014;5: 1436-1439.

[3] Ovchinnikov VV and Kulakov AA. Bull Kazan Technol Univ 2014;17:68-70.

[4] Ovchinnikov VV. Chemistry J 2013;2: 59-65.

[5] Mortimer CT. Reaction heats and bond strength. Pergamon Press Ltd.; 1962;pp238 .

[6] Luo, Yu-Ran. Handbook of bond dissociation energies in organic compounds, CRC PRESS. Boca Raton-London-New York-Washington, D.C.; 2003;pp362 .