ANALYSIS OF THERMOCHEMICAL DATA OF FATTY ORGANIC ACIDS

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It is known that fatty acids can be included in the structure of lipides. Many fatty acids have one or several double C=C bonds. Such type of acids plays an important role in steel industry, in particular. On this reason is important to unite their thermochemical data on vaporization $\Delta_{vap}H^o$, combustion $\Delta_c H^o$, formation $\Delta_f H^o$ and make on their base the equations, which can serve for the prediction of properties of new similar fatty acids. Analysis of the mentioned above thermodynamic functions of fatty acids: dodecanoic ($C_{12}H_{24}O_2$), meristic ($C_{14)H_{28}O_2}$), palmitic ($C_{16}H_{32}O_2$), margarinic ($C_{17}H_{34}O_2$), stearic ($C_{18}H_{36}O_2$) and arachidic ($C_{20}H_{40}O_2$), represented in the works [1, 2] allows to calculate the equations (1-3), in which the functions $\Delta_{vap}H^o$, $\Delta_c H^o$ and $\Delta_f H^o$ depended from the number of valence electrons N without of the number of lone electron pairs g of oxygen atoms (2 pairs) in the consistence of acids.

$\Delta_{vap}H^o = (27.1 \pm 7.9) + (1.4 \pm 0.2)$ (N-g); r 0.974, So 7.3, n 6 (1)
$\Delta_c H^o = (5.7 \pm 80.5)$ - (108.7 ± 0.8) (N-g); r 0.999, So 32.0, n 6 (2)
$\Delta_f H^o = (-433.5 \pm 50.1)$ - (4.9 ± 0.5) (N-g); r 0.977, So 20.4, n 6 (3)

The correlation parameters of calculated equations for fatty acids, having from 12 to 20 carbon atoms in their structures are practically equal to the same for simple carbon acids [3], but have a different errors at correlation coefficients.

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1. Adriaanse N., Dekker H, Heats of combustion of normal saturated fatty acids and their methyl esters. J. Coops, Rec. Trav. Chim. Pays/Bas, 1965, 84, 393.

2. Stephenson R.M., Malanowski S., Handbook of the Thermodynamics of Organic Compounds 1987.

3. Ovchinnikov V.V. Thermochemistry of heteroatomic compounds. The analysis and calculation of thermodynamic functions of organic acids. Harold of Kazan technological university. 2014, 17, 144.