Analysis and Calculation of Thermodynamic Functions of Atoms and Organic Compounds of I-VII Groups of Mendeleev's Periodic Table in Gaseous and Condensed Phases

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The values of free energies, the heats and entropies of formation of atoms of I-VI groups of Mendeleev's periodic table in gaseous and condensed phases were analyzed. Seventy nine equations of such type as $\Delta_{c,f,s}Y^o = i \pm f\ N$, in which $\Delta_{c,f,s}Y^o$ is thermodynamic function, i and f are stoichiometric coefficients. The obtained equations can be used for the calculations of the same functions for other atoms, for wich they are not known. The same equations can also be used for the next calculation of bond strength. 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 [1]. The heat of vaporization ($\Delta_{vap}H^o$), all thermodynamic functions $\Delta_{c,f}G^o$, $\Delta_{c,f}H^o$, S^o, $\Delta_c S^o_{cond}$ and heat capacity (C_p) of organic compounds of I-VII groups of Mendeleev's Periodic table can be well characterized with the number of valence electrons N without taking into account the number (h) of lone electrons pairs (g) of them in equation $\Delta_{vap,c,f,s}\Psi^o = i \pm f\ *(N - hg)$. The stoichiometric coefficients i and f reflect partially a various spatial structure of all investigated compounds. The free energy and entropy of combustion and formation are calculated only for oxygen, sulfur and partly fluorine compounds [2, 3].

References

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[3] Ovchinnikov V.V. (2013) American Journal of Physical Chemistry 2, 4, 60-71.