The development of the student's of Physics notions of enthalpy and entropy in the course of General Chemistry

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Abstract. The article contains methodology of the development of notions about enthalpy and entropy factors, characterizing the physical system orderliness. The stages of actualization of thermodynamics notions, motivation of putting the problem and methodology of forming of knowledge and ideas of entropy, enthalpy and Gibbs's energy have been described. We have shown how one should organize general conclusion and review of mastered skills. Examples of physical and chemical experiments, calculations of standard free energy of substance interaction reaction have been given.

Keywords: enthalpy, entropy, free energy, interdiscipline connections.

Topicality. The formation of professional competences of a future teacher of Physics must also be realized in the courses of other disciplines, indicated by the educational and professional curriculum in the section of the both the state component of higher education standard and the component of an institution of higher education. It particularly concerns the disciplines of Science and Mathematics type, especially General Chemistry. More attention has lately been paid to the problem of Chemistry's interdiscipline connections with other sciences in training specialists of different fields [1, 2, 3]. From the history of the chemical science development, we know that General Chemistry had for a long time being the umbilical cord which connected Chemistry with Physics. And now there are a lot of common issues, discussed both in the courses of Physics and Chemistry. It enables to form intersubject competences of the teacher of Physics through mastering subject competences by the students of Physics. As an example, we will examine some methodical resources of the development of the notions about enthalpy and entropy in the course of General Chemistry in studying the theme "Energetics of chemical reactions".

Methodology. To understand their essence, one should actualize basic knowledge of Hess's law and improve skills of thermochemical calculations. These notions enlarge the students' ideas of the phenomena of thermodynamics productions, animate and inanimate nature.

The teacher explains that the heating effect of a reaction can be determined not only by means of a calorimetre but through thermochemical calculations as well. And he calls attention to a simple example of the thermochemical equation of the complete coal combustion reaction:

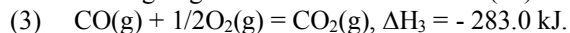(1) $C(c) + O_2(g) = CO_2(g)$, $\Delta H = - 393.5$ kJ.

The students' attention is sure to be paid to the fact that in thermochemical equations, the substance physical state is lettered in brackets: c – crystalline, g – gased, l – liquid.

Basing on Hess's law, the reaction is conventionally divided into two stages. At first, carbon (II) oxide forms:

(2) $C(c) + 1/2O_2(g) = CO(g)$, $\Delta H_2 = - 110.5$ kJ.
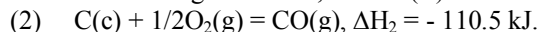
The following stage is the formation of carbon (IV) oxide:

(3) $CO(g) + 1/2O_2(g) = CO_2(g)$, $\Delta H_3 = - 283.0$ kJ.

The sum of the equations (2) and (3) will be equal to (1).

Proceeding from the absolute significance of enthalpy of the carbon oxides formation, a conclusion is drawn that the substance, in which the formation enthalpy is greater, is thermically more stable. From the reference book, we can also see that enthalpy of the formation, for example, of aluminium chloride $\Delta H^o_{298} = - 704.0$ kJ/ mol, and enthalpy of the formation of aluminium iodide $\Delta H^o_{298} = - 308.0$ kJ/ mol, which shows considerably greater stability of aluminium chloride, and energy consumption is almost twice higher for its dissolution. Using magnesium and silicium oxides, the students are shown that it is necessary to compare the formation enthalpies of these substances by taking into consideration a number of atoms in a molecule or in a minimum compound unit of nonmolecular structure. In the conversation, the students recollect that Δ (delta) is the enthalpy change $\Delta H = H_2 - H_1$, where H_2 and H_1 correspond to enthalpy of products and reagents. For exotermal reactions $\Delta H < O$, but for endothermic ones $\Delta H > O$.

It is reasonable to analyze an example of enthalpy of 1 mol of liquid water with 25^0 C and twice increased enthalpy of doubled quantity of water under the same conditions. In this case, we may say about enthalpy as well as about the mass the mass falling to some quantity of substance or about the mass corresponding to the same quantity of substance, for example, 1 mol. It is mentioned that enthalpy depends on substance aggregate state. If this statement is considered in reference to water, enthalpy of ice, liquid water or steam, even under similar conditions, all the more under different conditions, will be dissimilar. The students come to a conclusion that although it is impossible to determine the absolute significance of substance enthalpy, but its change can be calculated for chemical reactions.

The next didactic task is the students' mastering the enthalpy notions of the substance formation, which characterizes the enthalpy change during the formation of 1 mol compound out of simple substances. As an example, we should study enthalpy of the formation of water, oxides, salts and other substances, known for students.

The logical continuation of the development of the notions about the energetics of chemical processes is examining the combustion enthalpy, which is determined by the heat quantity, emanating as a result of the combustion of 1 mol of fuel. The students can be reminded of the fact that they got the information about fuel and its kinds from the school subjects in Physical geography, Physics and Chemistry.

The students should also comprehend that both enthalpy and entropy factor, as a performance of system regulation, influence a direction of a chemical reaction course. These factors determine opposite tendencies. A reaction direction will depend on the fact which of the factors is more influential at a certain moment.

In order to motivate the students' mental activity for understanding the notion of entropy, the lecturer demonstrates examples of some physical and chemical processes. Thus, if you open a bottle of aerated water, gas will begin to escape, and the level of water will even rise a little, i.e. it will expand. If you open a gas cylinder, gas will fill an apartment size. Iodine dissolves in alcohol; sugar, hydrogen chloride or ammoniac – in water, etc. These processes occur spontaneously, without a change of reaction conditions, without additional initiating, without a change of activation energy, etc. The common thing for these processes is the fact that molecules of substances before the beginning of a process had some size and they were in some order, but after breaking the state of immobility, the system transition from a more ordered state to a less ordered state took place, i.e. a degree of the system chaos increased.

The problem question "Why did it happen?" is put.

Another problem arises owing to the fact that chemists know over 20 mln organic and 0.5 mln inorganic substances, and using them one can make lots of chemical equations. But the issue lies in the fact whether these reactions will occur, and if so, under which conditions?

An answer to this question requires learning the notion of entropy (in Greek it means "transformation"). Entropy is marked by the symbol S. If the change of entropy is $\Delta S > 0$, it increases, i.e. the system changes from a more ordered state to a less ordered state. If $\Delta S < 0$, entropy decreases in connection with changing the system from a less ordered to a more ordered state.

Comparing the changes of entropy in the system transition from a certain state, the students, using concrete examples, make sure that according to $\Delta S < 0$ a spontaneous process run is impossible. Can one fancy that carbonic acid gas will again dissolve, in the same quantity, in a bottle of water without assistance?

In order to express the change of enthalpy (ΔH^0) and entropy (ΔS^0) in equal units, the numerical value of the entropy change of a reaction must be multiplied by T. The product ($T\Delta S$) is called the entropy factor; T is a temperature value according to Kelvin.

The instructor informs that the entropy factor characterizes a tendency to increasing a disorder in the system. The issue "Why not only gased, but also solid and liquid substances exist" is examined. The students recall that molecules are formed from atoms thanks to giving off energy ($\Delta H < 0$). Thus, a tendency of the system transition to a minimum energy state manifests itself in nature. This tendency is the enthalpy (or energy) factor.

After finding out the fact that there are two opposite factors influencing the system orderliness, the students are put another problem question: what occurs if the enthalpy factor action balances the entropy factor action?

An account of the following experiment (according to N. S. Akhmetov) is suitable. If an ampoule of water is broken in a closed vessel, water will evaporate. And it will occur until the vessel capacity is filled with steam,

and then the evaporation process ceases. Why? Answering this question, the students remember that there are two factors – the entropy and the enthalpy ones. Everybody knows that water vaporization is an endothermic process. So, the enthalpy factor limits an action of the entropy factor.

The students realize that a dynamic balance of the process begins. It means that the movement of molecules does not stop, but, on the contrary, steam molecules collide with molecules of water surface and change into liquid. At the same time, an opposite process of taking molecules off water surface and their changing into stem occurs. The number of molecules, evaporating for a certain time, is equal to the number of molecule condensing:

$$H_2O_{(l)} \rightleftarrows H_2O_{(s)}$$
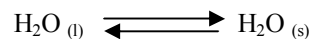
A conclusion, that the dynamic balance is a reversible process, is drawn. Moreover, the dynamic balance concerns both physical and chemical processes. Then a hypothesis is suggested: if one resists enthalpy or entropy from outside, one can manage a process and turn it in a necessary direction. This hypothesis is proved in the following themes of the course "General Chemistry". For proving the hypothesis the students have to systematize and generalize the knowledge of entropy (according to N.V. Romanova): (a) the standard entropy is a substance entropy under such condition as T=298K, P=101325Pa; (b) enlarging a number of atoms in a molecule causes growth of entropy; (c) entropy lessens with increasing substance is larger than that of crystalline substance; (d) entropy of simple and complex substances is a periodic feature. Entropy of simple substances within a certain subgroup of elements in the Periodic Law increases.

The formation of the nations of free energy, or Gibbs's energy (G), is carried into practice on the basis of the students' knowledge of the principle that the system disorder state is expressed by the product $T\Delta S$. The presence of a temperature value in this formula affirms that increasing a disorder degree in the system can be achieved by heating. The entropy factor $T\Delta S$ contrarily affects the enthalpy factors (ΔH) which influences a change of free energy:

$$\Delta G = \Delta H - T\Delta S.$$

The following conclusions result from this:

● If $\Delta G < 0$, but $\Delta H < 0$ and $\Delta S > 0$, a spontaneous run of a chemical reaction is essentially possible.

● If $\Delta G > 0$, a hypothetic reaction under the conditions cannot spontaneously take place, on the contrary, only a reverse reaction is possible.

● If $\Delta G = 0$, the system is in the chemical balance state, it means that in the system under the conditions there are both reagent and products of a reaction at the same time.

For chemical reaction, Gibb's energy is determined in two ways:

1. If a temperature of a reaction differs from the standard temperature, the equation $\Delta G = \Delta H - T\Delta S$ is used, besides that, the thermodynamic functions ΔH and ΔS are computed according to the same principle which is formulated as a result of Hess's law:

$\Delta H_{\text{of a chemical reaction}} = \sum \Delta H^0_{\text{of formed products}} - \sum \Delta H^0_{\text{of formed outgoing substances}}$,

$\Delta S_{\text{of a chemical reaction}} = \sum \Delta S^0_{\text{of formed products}} - \sum \Delta S^0_{\text{of formed outgoing substances}}$.

2. If a reaction occurs under the standard conditions, ΔG is computed in this way:

ΔG of a chemical reaction $= \sum \Delta G^0$ of formed products $- \sum \Delta G^0$ of formed outgoing substances.

The report of the fact that Gibbs's energy is the part of energy which escapes or absorbs during a chemical reaction under the conditions of a stable temperature and pressure and which can be changed into useful work ($\Delta G = A_{max}$) will be to the point. Maximum work (A_{max}) determines a so-called motive power of a reaction: the greater this power is, the more completely the process of changing outgoing reagents into products of a reaction is accomplished under the conditions.

For consolidating the theoretical material and perfecting the notions of enthalpy and entropy, it may not be out of place to solve problems of quantitative character, for instance, a problem for calculating the free energy of the reaction of the formation of calcium hydroxide by interacting calcium hydride with water:

CaH_2 (c) $+ 2H_2O$ (l) $= Ca(OH)_2$ (c) $+ 2H_2$ (g).
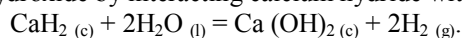
ΔH^0_{298} kJ/$_{mol}$ -189 2(-286) -986 0

ΔS^0_{298} kJ/$_{mol}$ 42 2(69.9) 83 2(130.6)

In accord with reference data, standard values of ΔH^0 and ΔS^0 for every compound are found, and then a change of reaction enthalpy and entropy is calculated:

ΔH^0 of a reaction $= -986 + 0 - [-189 + 2(-286)] = -225$ (kJ);

ΔS^0 of a reaction $= (83 + 2*130.6) - (42 + 2*69.9) = 162.4$ (J/K), or 0.1624 (kJ/K).

Entropy increasing, as a result of the reaction, is caused by the formation of 2 mols of hydrogen which testifies strengthening a disorder of the reaction system.

The entropy factor is computed in this way:

$T\Delta S^0 = 298K*0.1624$ kJ/K $= 48.4$ kJ.

Gibbs's energy of this reaction is equal to:

$\Delta G = \Delta H - T\Delta S^0 = -225$ kJ $- 48.4$ kJ $= -273.4$ kJ.

The value of Gibbs's energy shows that the reaction of calcium hydride with water is in principle possible. It is really so, the reaction occurs under usual conditions without heating.

The students perceive that both the enthalpy ($\Delta H^0 < 0$) and the entropy ($T\Delta S^0 > 0$) factors influence a displacement of the process in the same direction – increasing the reaction products. Such reactions occur to the end, i.e. to a complete change of reagents into the reaction products, therefore they are called irreversible. If there is an opposite influence of enthalpy and entropy, a reaction will be reversible.

Prospects. The study of this material is a base for solving calculation problems, connected with the standard free energy, that can be realize in the courses of Physics and General Chemistry.

Conclusions. The notions of enthalpy and entropy, formed in the course of General Chemistry on the examples of physical and chemical phenomena as well as mastered ways of solving problems for calculating enthalpy and entropy, will promote understanding the energetics of chemical reactions, the reasons of a direction displacement of their run, etc. by future specialists in the field of Physics. Such an example of an interdiscipline connection, when a learning material in Chemistry "works" for the formation of the students' of Physics competences, is also a basis for working out structural and logical schemes of curriculum of a certain specialized field.

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Формирование понятий «энтропия» и «энтальпия» у будущих учителей физики в курсе общей химии
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Аннотация. В статье рассмотрена методика формирования понятий «энтальпия» и «энтропия» на междисциплинарной основе. Значительное внимание уделяется расширению представлений студентов о законе Гесса и энергии Гиббса, усвоение которых углубляет и расширяет понимание процессов и закономерностей термодинамики. Развивается идея о том, что подобный подход к изучению материала является базой для решения расчетных задач, способствует пониманию вопросов, касающихся энергетики химических реакций.

Ключевые слова: энтальпия, энтропия, свободная энергия, межпредметные связи.