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COMPUTER PROCESSING OF THERMODYNAMIC DATA FOR CALCULATION OF EQUILIBRIUM CONSTANT

Assoc. Prof. Temenuzhka Haralanova, PhD
Department of Chemistry and Chemical Technologies, Razgrad Branch,
"Angel Kanchev" Univesity of Ruse
E-mail: tharalanova@uni-ruse.bg

Ch. Assistant Mariyka Petrova, PhD
Department of Chemistry and Chemical Technologies, Razgrad Branch,
"Angel Kanchev" Univesity of Ruse
E-mail: mgpetrova@uni-ruse.bg

Senior Lecturer Ilina Ivanova
Department of Biotechnology and Food Technology, Razgrad Branch,
"Angel Kanchev" Univesity of Ruse
E-mail: iivanova@uni-ruse.bg

Abstract: *There is a number of ways for calculating the equilibrium constant of a chemical reaction. One of them is through the variation of Gibbs' standard energy.*

The present work presents a way of calculating the thermodynamic characteristic of chemical equilibrium by computer processing of reference data. The development is an example of students' independent extracurricular work. The method of calculation is in line with current trends in the development of science, with the establishment of interdisciplinary links of information technology with chemistry. Modern chemistry training is demonstrated through the use of modern computer methods.

Keywords: *chemical equilibrium, equilibrium constant, Gibbs energy, relational data, electronic application.*

INTRODUCTION

It is known from the literature (Atkins, P., & J.Paula, 2006) that most of the chemical reactions are reversible processes. What characterizes them is that they do not fully run and at one point chemical equilibrium is established (1). As the process progresses, the speeds of the forward and backward reactions are equalized and a state of chemical equilibrium occurs in the system, leaving the composition in the system constant over time. The main thermodynamic characteristic of the chemical equilibrium is the equilibrium constant. It can determine the yield of the chemical reaction products (2). That is why different methods have been developed - experimental and computational to determine its value. Depending on the particular reaction and the conditions under which it takes place, various equations known in the literature are used. The criterion for a reliable value of a constant is its constant when the concentration of the reagents changes over a wide range.

EXPOSITION

Method for calculating the equilibrium constant of a chemical reaction using the Gibbs standard energy

An arbitrary equilibrium chemical reaction can be expressed in general by the equation:

$$\nu_1 A_1 + \nu_2 A_2 \leftrightarrow \nu_1^{\mathrm{I}} A_1^{\mathrm{I}} + \nu_2^{\mathrm{I}} A_2^{\mathrm{I}}$$

where A_1 and A_2 are starting substance, and A_1^{I} and A_2^{I} are reaction products.

Since the Gibbs standard energy () is a function of the state, its change () in the course of a chemical reaction depends only on the initial reagents and the end products of the same (Berry, R., S. D. Rice, J. Ross, 2000). In thermodynamics, an equation is derived giving the relation between the change in the Gibbs standard energy () and the equilibrium constant () of any chemical reaction:

$$\ln K_p = -\frac{\Delta G_T^0}{RT}, \quad (1)$$

where ΔG_T^0 can be calculated according to the equations:

$$\Delta G_T^0 = \Delta H_T^0 - T\Delta S_T^0 \quad (2)$$

$$\Delta H_T^0 = \Delta H_{298}^0 + \int_{298}^{T} \Delta c_p dT \quad (3)$$

$$\Delta S_T^0 = \Delta S_{298}^0 + \int_{298}^{T} \Delta c_p \frac{dT}{T} \quad (4)$$

$$\Delta c_p = \Delta a + \Delta bT + \Delta aT^2 + \Delta c^{\mathrm{I}} T^{-2} \quad (5)$$

The values of the quantity ΔH_{298}^0, ΔS_{298}^0, a, b and c^{I} „„ and for the tested reaction components are reported from an electronic reference (table database) Table 1. MS Excel is used to organize the electronic directory and to create an electronic application for calculation the equilibrium constant of a chemical reaction using Gibbs standard energy. The vast program capabilities (Kancheva, A., S. Parusheva, M. Todorova, D. Koleva, J. Aleksandrova, 2005) for managing database tables, the wide range of built-in functions and the user-friendly interface make the process easy and enjoyable.

Table. 1. Thermochemical table

№	substance	ΔH^0_f,298kj/mol	S^0_{298},J/(mol,K)	α	$10^3\beta$	$10^{-5}c'$
1	Ag	0	42,69	23,97	5,28	-0,25
2	Al	0	28,31	20,67	12,39	-
3	Au	0	47,45	23,68	5,19	-
…	…	…	…	…	…	…
38	O_2	0,0	205,03	31,46	3,39	-3,77
39	O_3	142,3	238,80	47,03	8,03	-9,01
…	…	…	…	…	…	…
147	SO2	-296,9	248,1	42,55	12,55	-5,65
148	SO3	-395,2	256,23	57,32	23,86	-13,05
…	…	…	…	…	…	…

In our work, we demonstrate how students use their knowledge of physicochemistry (Haralanova, T., & M. Petrova, 2011). and using information technology, using the above method, can calculate the equilibrium constant of a chemical reaction: $2SO_2 + O_2 \leftrightarrow 2SO_3$

For creation the electronic application, one starts from analyzing the input data involved in the computational process, extracting from the electronic directory (Table 1) the information related to the input data, performing the calculations and outputting the outputs. Students should consider the equilibrium chemical reaction, which are the starting materials, the products of the reaction, the coefficients in front of the corresponding elements, and set them (Table 2).

The outputs in the electronic application are displayed as soon as the input data is set and the values associated with it are displayed in the electronic directory.

Table. 2. Setting reaction data

starting materials		set a factor in front of the element	$\Delta H^0_{f,298}$kj/mol	S^0_{298},J/(mol,K)	α	$10^3\beta$	$10^{-5}c'$
set item1	SO_2	2					
set item2		1					
set item3							
set item4							
Reaction products		set a factor in front of the element	$\Delta H^0_{f,298}$kj/mol	S^0_{298},J/(mol,K)	α	$10^3\beta$	$10^{-5}c'$
set item1	SO_3	3					
set item2							
set item3							
set item4							

Table. 3. Setting and results of the processing of reaction data

starting materials		set a factor in front of the element	$\Delta H^0_{f,298}$kj/mol	S^0_{298},J/(mol,K)	α	$10^3\beta$	$10^{-5}c'$
set item1	SO_2	2	-296,9	248,10	42,55	12,55	-5,65
set item2	O_2	1	0,0	205,03	31,46	3,39	-3,77
set item3							
set item4							
Reaction products		set a factor in front of the element	$\Delta H^0_{f,298}$kj/mol	S^0_{298},J/(mol,K)	α	$10^3\beta$	$10^{-5}c'$
set item1	SO_3	3	-395,2	256,23	57,32	23,86	-13,05
set item 2							
set item 3							
set item 4							
ΔS^o_{298}= -188,77			Results		$\Delta\alpha$= -1,92		
ΔS^o_{400}= -190,14			ΔH^o_{298}= -196600		$\Delta\beta$= 0,019		
ΔG^o_{400}= 272000			ΔH^o_{400}= 196000		$\Delta c'$= -1,103E+06		
				K_p= 3,01E-36			

The results field in Table 3 shows the values obtained in MS Excel. The type of numerical results depends on the formatting specified in the electronic application. From IT classes, students know that when the initial numerical results of the calculations are very small or large, they are output in Scientific format, which means that: $\Delta b = 19,23x10^{-3}$, $\Delta c^{I} = -11,03x10^{5},\ldots, K_p = 3,01x10^{-36}$.

CONCLUSIONS

1. The equilibrium constant of a specific chemical reaction was calculated on the basis of thermochemical data tables using the Gibbs standard energy using the applied method. This is an important practical application of thermodynamics.

2. The method described in current work makes it possible to determine the equilibrium constant of any chemical reaction for which data are available in thermochemical tables.

3. The created electronic application of MS Excel gives ease in mathematical calculations and shows the application of Information Technology for automation of annoying and calculating activities in chemistry.

4. The use of such electronic applications motivates students to upgrade their knowledge of Higher Mathematics and Information Technology so that they can successfully apply them in the workplace where they will be pursued after completing their higher education.

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