

AT THE THEORY OF GEOCHEMICAL GEOTHERMOMETERS. 3. NEW INTERPRETATION OF PARAMETERS OF THE GEOTHERMOMETER EQUATION

Makarov V.P. (Geol. Dep. RSGPU, Moscow)

The problem of definition T-P - conditions of formation of minerals is one of the major in the analysis of a nature of rocks formation. With the purpose of its decision were created numerous geochemical geobarothermometers (further geothermometers and GGT). According to these data empirical expression for GGT is described by the hyperbolic equation (Thermond - Straser's equation [9])

$$\ln K_p = -A/T + B. \quad (1)$$

The physical sense of parameters A and B is not established. With this purpose in works [1, 2] the analysis (1) is carried out and their interpretation is offered. The basic properties of this equation are established and is shown, that the equation (1) should look like

$$\ln(K_p/K_{po}) = -A/T + B. \quad (2)$$

If for a basis to take mole shares of pure components $K_{po} \approx 1$, and, the more difficultly the mineral, the K_{po} is closer to 1.

Let's present function (1) as the piece-linear continuous function having the following properties:

- The diagram of function consists of slices of lines;
- These lines are portions, each of which is described by the equation (1);
- The end of each portion is the beginning of the following segment (condition of continuity). The point of connection of both segments is referring to as a note point of function;
- A node point of function - a point of phase transition;
- Within the limits of each segment function reflects uniformity of a phase composition. This segment we shall name an interval of uniformity.

On an interval of uniformity we shall transform (1), having considered it as the equation of the straight line which is taking place through a note point with coordinates $[1/T_o, (\ln K)_o]$. Then we have $\ln K = -A/T + [(\ln K)_o + A/T_o]$. Believing $(\ln K)_o = \ln K_o$, we come to representation of the equation (1) as

$$\ln(K/K_o) = -A(1/T - 1/T_o), \quad (3)$$

whence $B = A/T_o$ or $T_o = A/B$. These equalities connect parameters A and B. Probable interpretation of parameter A is described as follows: in fraction A/T (or A/T_o) we shall increase numerator and a denominator on size R (a gas constant). Then product RT has dimension of energy, because dimension of energy has also expression RA.

Let's take advantage of the equation of an isobar [3, pg. 193], having copied it as

$$\int_{K_o}^K \frac{dK}{K} = \int_{T_o}^T \frac{\Delta H}{R} \frac{dT}{T^2}$$

Let's put, that $\Delta H = \text{const}$, and, integrating, we receive the equation:

$$\ln K - \ln K_o = -\frac{\Delta H}{R} \left(\frac{1}{T} - \frac{1}{T_o} \right) = -\frac{\Delta H}{RT} + \frac{\Delta H}{RT_o} \quad (4)$$

Whence $RT \ln(K/K_o) = -\Delta H + \Delta H T/T_o = -\Delta H + \Delta H (T/T_o)$. As $RT \ln(K/K_o) = -\Delta G$ we receive the equation $\Delta G = \Delta H - \Delta S T$, whence $\Delta S = \Delta H/RT_o$. In result we receive the required equation which is looking like (2), where $A = \Delta H/R$, $B = \Delta H/RT_o$.

Expression (4) is similar to the equation of distribution of an impurity between two phases at solubility of an impurity in the fused and crystal matrix, this equation looks like $\ln(N_l/N_c) = (-\Delta H_m/R)(1/T - 1/T_m)$, where N_l and N_c - a mole share of solvent in the melt and crystal phases, ΔH_m and T_m - accordingly heat and melt temperature of solvent [8]. This equation refers to in one cases as the Van- Laar's equation [6, pg. 69; 9], in others- Vant-Goff's isochore [7, pg. 180].

On an interval of uniformity one of points - a point with coordinates $(1/T_{pt}, \ln K_{pt})$. By analogy to the equation of solubility of an impurity the size ΔH is a heat of phase transition (pt), i.e. $\Delta H = \Delta H_{pt}$. More often $T_{pt} = T_m$, and $\Delta H_{pt} = \Delta H_m$.

In tab.1 are given T_m some minerals, included in geothermometers, and their average values are de-

signed. On these data in tab. 2 the estimation of B parameter, well conterminous with its actual value is given.

Table 1. Temperatures of fusion of the minerals making GGT

Mineral	Ann	Phl	Fa	Fo	Pyr	Alm	Wol	Ens	Dio	Fs
T _m °K	1000 * (?)	1000 * (?)	1490	2163	2025	1600 (?)	1400 **	1830	1665	1413
ΔH _m (Kcal / m)	-	-	21, 2	14,00				14,8	3,06	
ΔH _h (Kcal / m)							1,29			

*-Decomposition **-solid phase transition.

Table 2. Estimation of B parameter on data T_m.

ГТТ	Temperatures ΣT _m	T _m average	A average	B average	Estima-tion B
Opx/Grn	(1400 + 1798 + 2000 + 2000)/4	1800	2645	1,33	1,47
Cpx/Opх	(1400+1830)/2	1615	3481	2,25	2,16
Bio/Grn	(1000 + 1000+2000+2000)/4	1500	3018	2,033	2,012

As well as for Тпл, for the majority of minerals of the data on heats of fusion DH_{ф.л} is not present. On the data [4] and [5] best convergence is observed at use ΔH_{ф.л} (for example, for wollastonite).

Thus, the geothermometer is described by the equation:

$$R \ln(K/K_{pt.}) = -\Delta H_{pt.}(1/T - 1/T_{pt.})$$

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