

# EQUATIONS OF TEMPERATURE DEPENDENCE OF AN ENTHALPY AND AVERAGE HEAT CAPACITY FOR $\text{EuCl}_3 \cdot 6\text{H}_2\text{O}$

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In this work for europium chloride hexahydrate  $\text{EuCl}_3 \cdot 6\text{H}_2\text{O}$  the equations of dependence of a molar enthalpy  $H_T - H_{298.15}$  and average isobaric molar heat capacity  $\overline{C_p}$  from absolute temperature  $T$  are offered.

Now in literature [1] there are only of  $\text{EuCl}_3 \cdot 6\text{H}_2\text{O}$  in temperature range 298.15–600.00 K given for true isobaric molar heat capacity  $C_p$ , but there are no equations for the description it  $H_T - H_{298.15}$  and  $\overline{C_p}$ . In article [2] it is shown that  $C_p$  and  $\overline{C_p}$  are connected by a ratio:

$$C_p = \overline{C_p} + (T - 298.15) \frac{d\overline{C_p}}{dT} \quad (1)$$

It is also  $\overline{C_p}$  possible to define from molar values of enthalpies [2]:

$$\overline{C_p} = (H_T - H_{298.15}) / (T - 298.15) \quad (2)$$

From the publication [3] it is known, that the dependence  $H_T - H_{298.15}$  on absolute temperature  $T$  can be presented in the form  $H_T - H_{298.15} = aT + bT^2 + cT^{-1} + d$ , where  $a, b, c, d$  – coefficients. In this work, in view of results [2-4], the corresponding equations for  $\text{EuCl}_3 \cdot 6\text{H}_2\text{O}$  are offered:

$$H_T - H_{298.15} = 366.909T + 0.007T^2 + 0.037 \cdot 10^7 T^{-1} - 111.257 \cdot 10^3 \quad (3)$$

$$H_T - H_{298.15} = 362T + 7 \cdot 10^{-3} T^2 + 37 \cdot 10^4 T^{-1} - 109794 \quad (4)$$

The equation (3) well describes data from the book I. Barin [1] (the maximum deviation does not exceed 0.13 %). To expression (4) we come on the basis of results [4]. Its maximum deviation is slightly higher (-1.36 %), if to compare with [1]. Additional examples are given in the table.

**Table.** Comparison of enthalpies of  $\text{EuCl}_3 \cdot 6\text{H}_2\text{O}$  in the range 298.15–600.00 K, received at different approaches

T, K	$H_T - H_{298.15}$ , kJ/mol	$H_T - H_{298.15}$ , kJ/mol	$\Delta(H_T - H_{298.15})$ , %	$H_T - H_{298.15}$ , kJ/mol	$\Delta(H_T - H_{298.15})$ , %
	data [1]	by the equation (3)		by the equation (4)	
300.00	0.679	0.679	0.00	0.670	-1.36
400.00	37.505	37.551	0.12	37.051	-1.21
500.00	74.593	74.687	0.13	73.696	-1.20
600.00	111.943	112.025	0.07	110.543	-1.25

Note. In all considered cases at a temperature of 298.15 K an enthalpy  $H_T - H_{298.15} = 0.000$  kJ/mol.

On the basis of the equations (3) and (4), having applied recommendations from [2, 3] and some results from [4], for  $\text{EuCl}_3 \cdot 6\text{H}_2\text{O}$  formulas (5) and (6) describing the temperature course  $\overline{C_p}$  is offered:

$$\overline{C_p} = 368.996 + 0.007T - 1240.986T^{-1} \quad (5)$$

$$\overline{C_p} = 364.087 + 0.007T - 1240.986T^{-1} \quad (6)$$

The maximum difference between the values, received when calculating behind the equations (5) and (6), does not exceed 1.34 %.

In conclusion we will note, that equation (4) and (6), received by means of a method [4], are perhaps less exact. However approach from [4] can be more universal. Likely with its help it is possible to predict heat capacity for many compounds  $\text{LnCl}_3 \cdot 6\text{H}_2\text{O}$ , where Ln – rare-earth metals.

[1] I. Barin (in collab. with G. Platzki). Thermochemical Data of Pure Substances. Weinheim: VCH (Germany), 3 ed., 1885 (1995).

[2] D. Sh. Tsagareishvili, G. G. Gvelesiani, V. P. Orlovsky, T. V. Belyavskaya, Enthalpy and thermal capacity of scandium and europium orthophosphates at high temperatures, Inorg. Mater. **11**, 491-493 (1975).

[3] D. Sh. Tsagareishvili, G. G. Gvelisiani, V. P. Orlovsky, T. V. Belyaevskaya, V. P. Repko, Enthalpy and thermal capacity of lanthanum, neodymium and yttrium orthophosphates under high temperatures, Inorg. Mater. **8**, 1790-1793 (1972).

[4] A.A. Козьма, Оцінка ізобарної теплоємності  $\text{EuCl}_3 \cdot 6\text{H}_2\text{O}$  при температурах 298–600 К та її порівняння з відомими даними, IXth International scientific conference «Relaxed, nonlinear and acoustic optical processes and materials» – RNAOPM'2018, The first Volyn-Pomerania Interdisciplinary Summer School on «Art-Science Technology» – VPISSAST'2018, ISBN 978-966-940-159-5, Lutsk–Lake «Svityaz'», Ukraine, 64 (2018).