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SECTION VI. CHEMISTRY

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EQUATIONS OF TEMPERATURE DEPENDENCE OF AN ENTHALPY AND AVERAGE HEAT CAPACITY FOR EuCl₃•6H₂O

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In this work for europium chloride hexahydrate EuCl₃•6H₂O the equations of dependence of a molar enthalpy $H_T - H_{_{298,15}}$ and average isobaric molar heat capacity $\overline{C_n}$ from absolute temperature *T* are offered.

Now in literature [1] there are only of EuCl₃•6H₂O 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:

$$C_{p} = \overline{C_{p}} + \left(T - 298.15\right) \frac{d\overline{C_{p}}}{dT}$$
(1)

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

$$\overline{C_p} = (H_T - H_{298.15}) / (T - 298.15)$$
⁽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 EuCl₃•6H₂O are offered:

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

$$H_{T} - H_{298,15} = 362T + 7 \cdot 10^{-3} T^{2} + 37 \cdot 10^{4} T^{-1} - 109794$$
(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 1.

Table 1

Comparison of enthalpies of EuCl₃•6H₂O in the range 298.15–600.00 K, received at different approaches

Т, К	$H_{T} - H_{298.15}$,			${H}_{T}-{H}_{298.15}$,	
	kJ/mol		$\Delta(H_T - H_{298.15})$,	kJ/mol	$\Delta(H_T - H_{298.15}),$
	data [1]	by the	%	by the	%
	uala[1]	equation (3)		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 EuCl₃•6H₂O formulas (5) and (6) describing the temperature course $\overline{C_{a}}$ is offered:

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

$$\overline{C_{p}} = 364.087 + 0.007T - 1240.986T^{-1}$$
(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 $LnCl_3•6H_2O$, where Ln - rare-earth metals.

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