THERMODYNAMIC PROPERTIES OF TWO– AND THREE–LANTHANIDES HYDRIDES

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In present work the results of value calculations of thermodynamic properties ($\Delta_f H^o_{298}$, S^o_{298} and Cp^o_{298}) two- and ($\Delta_f H^o_{298}$) three- lanthanides hydrides (Ln) are presented. Calculation is carried out by the help of semi-empirical method [1,2], considering the number of f-electrons (N_f), and also the influence of spin (S) and orbital (L) moments of linear momentum of ground state of lanthanide ion.

Available bank of thermodynamic quantities for binar lanthanides hydrides [3, 4] and interconsistent data for dihydrides Ln, received experimentally [5] and by semi-empirical structural-thermodynamic model [6] allow to carry out calculation of thermodynamic properties of these compounds. Calculated standard thermodynamic properties of lanthanides dihydrides (table 1).

At calculation of S^o and Cp^o values the method of regression analysis for results comparison and assessment of missed base value was also applied.

Available in literature unit values of enthalpy formation for some theoretically crystalline compounds of LnH_3 (table 2) [8] of berthollide type are not sufficient for reliable assessment of their thermodynamic properties. That's why we carried out comparative analysis of enthalpy values of bromides, iodides and three-hydride formation [7] for assessment of unknown values of base compounds (LaH_3, GdH_3, LuH_3) with the help of comparative calculation method. On their basis and experimentally definite quantity [7] the values of enthalpy formation of theoretically lanthanide three-hydrides are calculated, which are presented on the table 2.

References

1. Poluektov N.S., Meshkova S.B., Korovin Y.V., Oksinenko I.I. // Dokl.ANSSR 1982.v.266.№5.p.1157.
2. Meshkova S.B., Poluektov N.S., Topilova Z.M., Danilkovich M.M. // Coord. Khimiya. 1986.v.12.№4.p.481.
3. Termicheskiye konstanti veshestv. Spravochnik.M.: ANSSSR, VINTI, IVT.1978, edition.8.4.1.572p.
4. Antonova M.M. Svoistva gidridov metallov. Spravochnik. Kiev: Nauk.dumka, 1975.127p.
5. Ward I.W. Hascke I.M. // Handbook on the Physics and chemistry of Rare Earths.v.18. Lanthanides (3/) Actinides: Chemistry/Eds Gshneidner K.A,Eyring Ir.L., Choppin G.K. Lander G.N. Oxford N.Y.: Elsevier Science,1994.p.294.
6. Ionov S.P., Kuznetsov N.T. // Coord.khimiya. 2000.v.26, №12.p.943.
7. Mackay K.M. //Comprehensive inorganic/ Oxford: Pergamon Press, 1975, v 1. p.40.

Table 1

Thermodynamic properties of $LnH_{2(kp)}$

Ln	$-\Delta fH^0_{298}, \frac{kJoule}{mole}$		$S^0_{298,} \frac{Joule}{mole \cdot K}$		
	Liter.	equation	Liter	Our calculation	
La	201.3 207.9 207.5	207.5*	51.62 51.67	-	56.3
Ge	202.1 205.9 229.7 225.9	212.8	55.72 55.77	55.5	57.0
Pr	208.8 209.2 200.8	216.2	56.72 56.78	57.8	57.7
Nd	210.9 187.4 211.3	217.7	58.85 58.9	59.6	58.4
Pm	-	217.3	-	61.0	59.1
Sm	179.9 196.9 223.0	215.0	-	61.9	59.9
Eu	-	196.0	-	58.1	60.1
Gd	189.1 196.2 204.4	204.4*	-	-	61.3
Tb	209.0 216.7	211.9	74.2	65.4	62.0
Dy	209.0 231.8	216.8	64.58 64.64	67.7	62.7
Ho	220.3 220.5	219.4	55.34 55.22	69.1	63.4
Er	226.8 219.9	219.5	-	69.9	64.1
Tm	225.1	217.2	-	69.8	64.8
Yb	181.0 181.2	203.0	-	66.7	65.5
Lu	205.4 201.5	205.4*	-	-	66.2

Table 2

Values of enthalpy formation of $LnH_{3(kp)}$

Ln	$-\Delta fH^0_{298,} \kappa Joule \cdot mole^{-1}$				
	Literary		Our calculation according to equation		
La	231.8	261.8	235*	235*	235*
Ge	237.7	252.3			238.2
Pr	234.7	253.3			241.1
Nd		238.9			237.9
Pm		256.8			228.8
Sm		229.5			213.6
Eu	-	-	-	-	166.3
Gd		179.8	153	168	168.0*
Tb		110.9			181.0
Dy		36.6			190.7
Ho		17.1			194.6
Er		-44.9			192.3
Tm		-70.8			183.9
Yb		102.2			149.6
Lu		-64.7	147	152	152*

*- base value