Article ID: 1006-9941(2002)01-0016-02

Relationship between the Standard Enthalpy of Formation and the Ratio of Standard Enthalpy of Formation and Exothermic Denitration Decomposition Peak Temperature of $M(NTO)_n$

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Abstract: A relationship is established, using the least-squares method, between the standard enthalpy of formation and the standard enthalpy of formation divided by the exothermic denitration decomposition peak absolute temperature corresponding to $\beta \to 0$.

Key words: denitration reaction; DSC; exothermic decomposition peak temperature; standard enthalpy of formation; NTO salt

CLC number: O159; TQ564　　**Document code**: A

In the previous paper[1], the standard enthalpies of formation[$\Delta_f H_m^\theta[M(NTO)_n, cr]$ of twenty metal salts of 3-nitro-1,2,4-triazol-5-one(NTO) in Table 1 were reported. In references [2,3], the initial data($\beta_i, T_{pdi}, i = 1, 2, \cdots n$) of the exothermic denitration decomposition reaction of these salts under the non-isothermal DSC condition were reported. Where β is the constant heating rate and T_{pd} is the exothermic denitration decomposition peak temperature. In order to obtain information about the correlation of standard enthalpies of formation and the peak temperature (T_{pdo}) corresponding to $\beta \to 0$ of the exothermic denitration decomposition reaction in the DSC curves of these salts, the values of $\Delta_f H_m^\theta[M(NTO)_n, cr]$ tabulated in Ref. [1] and T_{pdo} obtained by Eq. (1) from the initial data(β_i, T_{pdi}, $i = 1, 2, \cdots n$) tabulated in Refs. [2, 3] (for original data see Table 1) are fitted to the equation (2).

$$T_{pdi} = T_{pdo} + b\beta_i + c\beta_i^2 + d\beta_i^3 \quad i = 1, 2, \cdots n \quad (1)$$

$$\Delta_f H_m^\theta[M(NTO)_n, cr] = -19.959\,5 + 485.9\Delta_f H_m^\theta[M(NTO)_n, cr]/T_{pdo}$$
$$r = 0.996\,1 \quad (2)$$

Fig. 1 shows a linear interdependence between the parameters $\Delta_f H_m^\theta[M(NTO)_n, cr]$ and $\Delta_f H_m^\theta[M(NTO)_n, cr]/T_{pdo}$ for twenty NTO metal salts, indicating that

$$\Delta_f H_m^\theta[M(NTO)_n, cr] = \frac{19.959\,5\,T_{pdo}}{(485.9 - T_{pdo})}$$

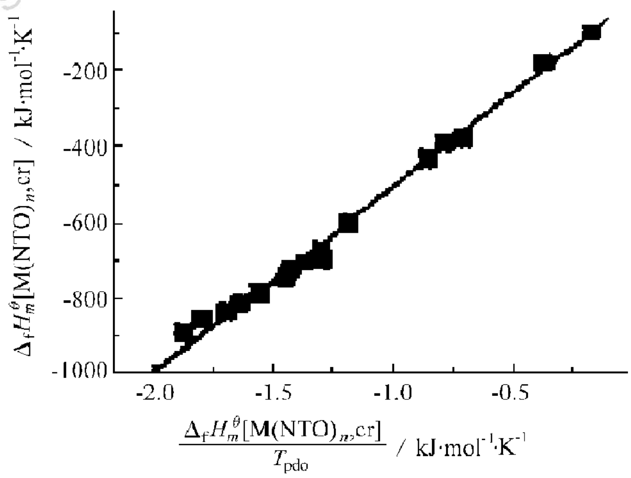

Fig. 1　$\Delta_f H_m^\theta[M(NTO)_n, cr]$ vs. $\Delta_f H_m^\theta[M(NTO)_n, cr]/T_{pdo}$ relationship for twenty NTO metal salts

Received date: 2001-10-17

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Table 1　Data for twenty NTO metal salts

Sample	β /℃·min^{-1}	T_{pd} /℃	T_{pdo} /℃	$-\Delta_f H_m^\theta[M(NTO)_n, cr]$ /kJ·mol^{-1}
$Li(NTO)\cdot 2H_2O$	2.056	280.9	274.2	388.7
	5.043	287.9		
	10.04	294.2		
	20.48	298.9		
$Na(NTO)\cdot H_2O$	2.009	246.3	237.6	397.2
	5.018	255.8		
	10.11	264.8		
	20.35	274.3		
$K(NTO)\cdot H_2O$	2.063	240.0	234.3	435.9
	5.009	246.5		
	10.50	254.8		
	20.67	263.8		
$Mg(NTO)_2\cdot 8H_2O$	2.074	264.1	248.6	446.1
	5.260	282.5		
	10.62	301.1		
	21.53	308.7		
$Ca(NTO)_2\cdot 4H_2O$	2.031	278.1	257.7	691.7
	5.123	296.5		
	10.24	304.5		
	21.39	316.7		
$[Mn(H_2O)_6](NTO)_2\cdot 2H_2O$	2.020	271.6	246.5	193.6
	5.050	293.9		
	10.43	305.3		
	20.68	336.3		
$[Co(H_2O)_6](NTO)_2\cdot 2H_2O$	2.039	296.1	279.8	97.0
	5.113	312.9		
	10.18	326.6		
	20.73	345.6		
$[Cu(NTO)_2(H_2O)_2]\cdot 2H_2O$	2.052	205.6	196.8	−298.4
	5.131	215.3		
	10.37	225.1		
	20.95	240.1		
$Zn(NTO)_2\cdot H_2O$	2.000	245.6	234.1	−38.1
	5.150	263.1		
	10.52	288.6		
	20.64	307.1		
$Y(NTO)_3\cdot 6H_2O$	2.023	243.9	239.9	698.5
	5.000	249.1		
	10.27	256.3		
	20.57	263.3		
$La(NTO)_3\cdot 7H_2O$	2.014	225.8	199.5	885.4
	5.139	248.3		
	10.14	254.6		
	20.35	268.3		
$Ce(NTO)_3\cdot 7H_2O$	2.030	224.6	199.8	851.0
	5.054	245.3		
	10.06	252.3		
	20.62	271.1		
$Pr(NTO)_3\cdot 7H_2O$	2.014	229.9	216.8	831.9
	5.015	242.9		
	10.13	252.6		
	21.40	264.9		

Table 1　(Continued)

Sample	β /℃·min^{-1}	T_{pd} /℃	T_{pdo} /℃	$-\Delta_f H_m^\theta[M(NTO)_n, cr]$ /kJ·mol^{-1}
$Nd(NTO)_3\cdot 8H_2O$	2.006	234.8	221.2	809.6
	5.034	247.6		
	10.29	255.1		
	20.69	265.3		
$Sm(NTO)_3\cdot 7H_2O$	2.081	240.8	231.4	785.6
	5.078	250.8		
	10.31	260.8		
	20.64	270.1		
$Eu(NTO)_3\cdot 7H_2O$	2.028	245.3	235.7	664.0
	4.899	256.6		
	10.31	270.8		
	20.35	274.3		
$Gd(NTO)_3\cdot 7H_2O$	1.989	242.1	237.2	740.3
	4.975	252.1		
	10.14	271.3		
	20.44	278.8		
$Tb(NTO)_3\cdot 5H_2O$	2.001	241.6	233.7	723.9
	5.122	253.1		
	10.25	268.3		
	20.68	275.8		
$Dy(NTO)_3\cdot 5H_2O$	1.998	243.8	235.0	729.3
	5.214	256.1		
	10.16	270.1		
	20.74	278.1		
$Yb(NTO)_3\cdot 6H_2O$	1.983	247.1	238.0	604.0
	5.076	255.5		
	10.16	259.3		
	20.75	269.6		

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