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Dissolution Properties of $M(NTO)_n \cdot mH_2O$ in Water

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Abstract: With the help of the amount of the complex (a), the concentration of the solution (b), the heat effect of dissolution process (Q) and the molar enthalpy of dissolution in water ($\Delta_{diss}H$) of $M(NTO)_n \cdot mH_2O$ (M = Ba, n = 1, m = 3; M = Li, n = 1, m = 2; M = Ca, n = 2, m = 4; M = Na, $n = m$ = 1; M = Co, Mg, n = 2, m = 8; M = Ce, Pr, Gd, n = 3, m = 7; M = Tb, Dy, n = 3, m = 5; M = Y, Yb, n = 3, m = 6; NTO = 3-nitro-1, 2, 4-triazol-5-one) obtained by a Calvet microcalorimeter, five empirical formulae describing the differential enthalpy of dissolution($\Delta_{dif}H_m^\theta$), standard molar enthalpy of dissolution [$\Delta_{diss}H_m^\theta(b=0)$], relative apparent molar enthalpy ($\Delta_{diss}H_{apparent}$), relative partial molar enthalpy ($\Delta_{diss}H_{partial}$) and enthalpies of dilution ($\Delta_{dil}H_{1,2}$) in water of these metal complexes of NTO were obtained.

Key words: physical chemistry; enthalpy; dissolution property; NTO; metal complex
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In three previous papers[1-3], the molar enthalpies of dissolution in water ($\Delta_{diss}H$) of metal complexes of 3-nitro-1, 2, 4-triazol-5-one (NTO) were reported. In order to obtain more information about the dissolution properties of $M(NTO)_n \cdot mH_2O$ (M = Ba, n = 1, m = 3; M = Li, n = 1, m = 2; M = Ca, n = 2, m = 4; M = Na, $n = m$ = 1; M = Co, Mg, n = 2, m = 8; M = Ce, Pr, Gd, n = 3, m = 7; M = Tb, Dy, n = 3, m = 5; M = Y, Yb, n = 3, m = 6; NTO = 3-nitro-1, 2, 4-triazol-5-one) in water, by substituting the amount of the complex (a), the concentration of the solution (b), the heat effect of dissolution process (Q) and the molar enthalpy of dissolution in water ($\Delta_{diss}H$) from Refs. [1-3] in Table 1 into Eqs. (1)-(5):

$$Q = \Delta_{dif}H \cdot a + Q^\theta \quad (1)$$

$$\Delta_{diss}H = A + Bb + Cb^{\frac{1}{2}} \quad (2)$$

$$\Delta_{diss}H_{apparent} = \Delta_{diss}H(b=b) - \Delta_{diss}H(b=0) = Bb + Cb^{\frac{1}{2}} \quad (3)$$

$$\Delta_{diss}H_{partial} = b\left(\frac{\partial \Delta_{diss}H}{\partial b}\right) + \Delta_{diss}H_{apparent} \quad (4)$$

$$\Delta_{dil}H_{1,2} = \sum_{2}^{1} A_i \Delta_{dil}[(b_2^{1/2})^i - (b_1^{1/2})^i] \quad (5)$$

The enthalpies of dissolution ($\Delta_{diss}H$), relative apparent molar enthalpies ($\Delta_{diss}H_{apparent}$) and relative partial molar enthalpies ($\Delta_{diss}H_{partial}$) for the complexes at different concentrations listed in Table 1 and the following differential enthalpies of dissolution process ($\Delta_{dif}H_m^\theta$), heat effect of dissolution process of the complexes corresponding to $a \rightarrow 0$ (Q^θ), standard molar enthalpy of dissolution [$\Delta_{diss}H_m^\theta(b=0)$] and five empirical formulae used for the calculation of $\Delta_{dif}H_m^\theta$, $\Delta_{diss}H$, $\Delta_{diss}H_{apparent}$, $\Delta_{diss}H_{partial}$ and enthalpies of dilution ($\Delta_{dil}H_{1,2}$) were obtained:

for $BaNTO \cdot 3H_2O$

$Q = 43259.75354 \cdot a + 1.06191$, $r^2 = 0.99913$
$\Delta_{dif}H_m^\theta = 43.26\ kJ \cdot mol^{-1}$
$Q^\theta = 1.06\ J$
$\Delta_{diss}H = 45.2975 + 1193.44b - 99.1601b^{\frac{1}{2}}$
$\Delta_{diss}H_m^\theta = 45.30\ kJ \cdot mol^{-1}$
$\Delta_{diss}H_{apparent} = 1193.44b - 99.1601b^{\frac{1}{2}}$
$\Delta_{diss}H_{partial} = 2386.87b - 148.71b^{\frac{1}{2}}$
$\Delta_{dil}H_{1,2} = 1193.44(b_2 - b_1) - 99.1601(b_2^{\frac{1}{2}} - b_1^{\frac{1}{2}})$

for $LiNTO \cdot 2H_2O$

$Q = 22318.89063 \cdot a - 5.55887$, $r^2 = 0.99945$
$\Delta_{dif}H_m^\theta = 22.32\ kJ \cdot mol^{-1}$
$Q^\theta = 5.56\ J$
$\Delta_{diss}H = 21.7993 - 2.37159b + 4.86691b^{\frac{1}{2}}$
$\Delta_{diss}H_m^\theta = 21.80\ kJ \cdot mol^{-1}$
$\Delta_{diss}H_{apparent} = -2.37159b + 4.86691b^{\frac{1}{2}}$
$\Delta_{diss}H_{partial} = -4.74319b + 7.3003b^{\frac{1}{2}}$
$\Delta_{dif}H_{1,2} = -2.37159(b_2 - b_1) + 4.86691(b_2^{\frac{1}{2}} - b_1^{\frac{1}{2}})$

for $Ca(NTO)_2 \cdot 4H_2O$

$Q = 30482.86367 \cdot a + 15.08359$, $r^2 = 0.99975$
$\Delta_{dif}H_m^\theta = 30.48\ kJ \cdot mol^{-1}$
$Q^\theta = 15.08\ J$
$\Delta_{diss}H = 31.528 + 44.9345b - 13.0422b^{\frac{1}{2}}$
$\Delta_{diss}H_m^\theta = 31.53\ kJ \cdot mol^{-1}$
$\Delta_{diss}H_{apparent} = 44.9345b - 13.0422b^{\frac{1}{2}}$
$\Delta_{diss}H_{partial} = 89.869b - 19.5632b^{\frac{1}{2}}$
$\Delta_{dil}H_{1,2} = 44.9345(b_2 - b_1) - 13.0422(b_2^{\frac{1}{2}} - b_1^{\frac{1}{2}})$

for $Gd(NTO)_3 \cdot 7H_2O$

$Q = 50058.05794 \cdot a + 1.12507$, $r^2 = 0.99996$
$\Delta_{dif}H_m^\theta = 50.06\ kJ \cdot mol^{-1}$

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$Q^{\theta}=1.12$ J

$\Delta_{diss}H=49.9453-305.849b+17.3055b^{\frac{1}{2}}$

$\Delta_{diss}H_m^{\theta}=49.94$ kJ·mol^{-1}

$\Delta_{diss}H_{apparent}=-305.849b+17.3055b^{\frac{1}{2}}$

$\Delta_{diss}H_{partial}=-611.698b+25.9583b^{\frac{1}{2}}$

$\Delta_{dil}H_{1,2}=-305.849(b_2-b_1)+17.3055(b_2^{\frac{1}{2}}-b_1^{\frac{1}{2}})$

for $NaNTO\cdot H_2O$

$Q=30441.41957\cdot a-3.6596$, $r^2=0.99953$

$\Delta_{dif}H_m^{\theta}=30.44$ kJ·mol^{-1}

$Q^{\theta}=3.66$ J

$\Delta_{diss}H=29.8866-47.0189b+9.89477b^{\frac{1}{2}}$

$\Delta_{diss}H_m^{\theta}=29.89$ kJ·mol^{-1}

$\Delta_{diss}H_{apparent}=-47.0189b+9.89477b^{\frac{1}{2}}$

$\Delta_{diss}H_{partial}=-94.0377b+14.8422b^{\frac{1}{2}}$

$\Delta_{dil}H_{1,2}=-47.0189(b_2-b_1)+9.89477(b_2^{\frac{1}{2}}-b_1^{\frac{1}{2}})$

for $Ce(NTO)_3\cdot 7H_2O$

$Q=41143.44229\cdot a-2.99413$, $r^2=0.99976$

$\Delta_{dif}H_m^{\theta}=41.14$ kJ·mol^{-1}

$Q^{\theta}=2.99$ J

$\Delta_{diss}H=40.9574+259.205b-11.6066b^{\frac{1}{2}}$

$\Delta_{diss}H_m^{\theta}=40.96$ kJ·mol^{-1}

$\Delta_{diss}H_{apparent}=259.205b-11.6066b^{\frac{1}{2}}$

$\Delta_{diss}H_{partial}=518.409b-17.4098b^{\frac{1}{2}}$

$\Delta_{dil}H_{1,2}=259.205(b_2-b_1)-11.6066(b_2^{\frac{1}{2}}-b_1^{\frac{1}{2}})$

for $Pr(NTO)_3\cdot 7H_2O$

$Q=37694.50379\cdot a-13.14711$, $r^2=0.99934$

$\Delta_{dif}H_m^{\theta}=37.70$ kJ·mol^{-1}

$Q^{\theta}=13.15$ J

$\Delta_{diss}H=40.4107+1027.99b-116.208b^{\frac{1}{2}}$

$\Delta_{diss}H_m^{\theta}=40.41$ kJ·mol^{-1}

$\Delta_{diss}H_{apparent}=1027.99b-116.208b^{\frac{1}{2}}$

$\Delta_{diss}H_{partial}=2055.98b-174.312b^{\frac{1}{2}}$

$\Delta_{dil}H_{1,2}=1027.99(b_2-b_1)-116.208(b_2^{\frac{1}{2}}-b_1^{\frac{1}{2}})$

for $Y(NTO)_3\cdot 6H_2O$

$Q=33631.59307\cdot a-11.31506$, $r^2=0.99936$

$\Delta_{dif}H_m^{\theta}=33.63$ kJ·mol^{-1}

$Q^{\theta}=11.32$ J

$\Delta_{diss}H=30.4255-828.515b+109.402b^{\frac{1}{2}}$

$\Delta_{diss}H_m^{\theta}=30.42$ kJ·mol^{-1}

$\Delta_{diss}H_{apparent}=-828.515b+109.402b^{\frac{1}{2}}$

$\Delta_{diss}H_{partial}=-1657.03b+164.103b^{\frac{1}{2}}$

$\Delta_{dil}H_{1,2}=-828.515(b_2-b_1)+109.402(b_2^{\frac{1}{2}}-b_1^{\frac{1}{2}})$

for $Yb(NTO)_3\cdot 6H_2O$

$Q=36050.5514\cdot a+5.67728$, $r^2=0.99975$

$\Delta_{dif}H_m^{\theta}=36.05$ kJ·mol^{-1}

$Q^{\theta}=5.68$ J

$\Delta_{diss}H=34.1789-1066.35b+98.06397b^{\frac{1}{2}}$

$\Delta_{diss}H_m^{\theta}=34.18$kJ·mol^{-1}

$\Delta_{diss}H_{apparent}=-1066.35b+98.0697b^{\frac{1}{2}}$

$\Delta_{diss}H_{partial}=-2132.17b+147.105b^{\frac{1}{2}}$

$\Delta_{dil}H_{1,2}=-1066.35(b_2-b_1)+98.0697(b_2^{\frac{1}{2}}-b_1^{\frac{1}{2}})$

for $Dy(NTO)_3\cdot 5H_2O$

$Q=41596.5547\cdot a-3.08558$, $r^2=0.9998$

$\Delta_{dif}H_m^{\theta}=41.60$ kJ·mol^{-1}

$Q^{\theta}=3.09$ J

$\Delta_{diss}H=42.7641+523.734b-52.8761b^{\frac{1}{2}}$

$\Delta_{diss}H_m^{\theta}=42.76$ kJ·mol^{-1}

$\Delta_{diss}H_{apparent}=523.734b-52.8761b^{\frac{1}{2}}$

$\Delta_{diss}H_{partial}=1047.47b-79.3141b^{\frac{1}{2}}$

$\Delta_{dil}H_{1,2}=523.734(b_2-b_1)-52.8761(b_2^{\frac{1}{2}}-b_1^{\frac{1}{2}})$

for $Tb(NTO)_3\cdot 5H_2O$

$Q=42296.44154\cdot a-3.35507$, $r^2=0.9999$

$\Delta_{dif}H_m^{\theta}=42.30$ kJ·mol^{-1}

$Q^{\theta}=3.36$ J

$\Delta_{diss}H=41.6989-62.5126b+11.9891b^{\frac{1}{2}}$

$\Delta_{diss}H_m^{\theta}=41.70$ kJ·mol^{-1}

$\Delta_{diss}H_{apparent}=-62.5126b+11.9891b^{\frac{1}{2}}$

$\Delta_{diss}H_{partial}=-125.025b+17.9837b^{\frac{1}{2}}$

$\Delta_{dil}H_{1,2}=-62.5126(b_2-b_1)+11.9891(b_2^{\frac{1}{2}}-b_1^{\frac{1}{2}})$

for $Co(NTO)_2\cdot 8H_2O$

$Q=61400.88503\cdot a-0.9908$, $r^2=0.99969$

$\Delta_{dif}H_m^{\theta}=61.40$ kJ·mol^{-1}

$Q^{\theta}=0.99$ J

$\Delta_{diss}H=61.5109+134.305b-9.93207b^{\frac{1}{2}}$

$\Delta_{diss}H_m^{\theta}=61.51$ kJ·mol^{-1}

$\Delta_{diss}H_{apparent}=134.305b-9.93207b^{\frac{1}{2}}$

$\Delta_{diss}H_{partial}=268.61b-14.8954b^{\frac{1}{2}}$

$\Delta_{dil}H_{1,2}=134.305(b_2-b_1)-9.93027(b_2^{\frac{1}{2}}-b_1^{\frac{1}{2}})$

for $Mg(NTO)_3\cdot 8H_2O$

$Q=60593.40768\cdot a-0.67305$, $r^2=0.9999$

$\Delta_{dif}H_m^{\theta}=60.68$ kJ·mol^{-1}

$Q^{\theta}=0.67$ J

$\Delta_{diss}H=57.9951-2390.71b+157.767b^{\frac{1}{2}}$

$\Delta_{diss}H_m^{\theta}=58.00$ kJ·mol^{-1}

$\Delta_{diss}H_{apparent}=-2390.71b+157.767b^{\frac{1}{2}}$

$\Delta_{diss}H_{partial}=-4781.42b+236.6651b^{\frac{1}{2}}$

$\Delta_{dil}H_{1,2}=-2390.71(b_2-b_1)+157.767(b_2^{\frac{1}{2}}-b_1^{\frac{1}{2}})$

Table 1 Dissolution properties in water for 13 complexes

No.	b/mol · kg^{-1}	a/mol	Q/J	$\Delta_{diss}H$/kJ · mol^{-1}		$\Delta_{diss}H_{partial}$ /kJ · mol^{-1}	$\Delta_{diss}H_{apparent}$ /kJ · mol^{-1}
				found	calculated		
1	$BaNTO \cdot 3H_2O$						
	0.00069760	0.011791	514.68	43.65	43.51	−1.79	−2.26
	0.00082991	0.014670	638.58	43.53	43.43	−1.87	−2.30
	0.00085290	0.014312	618.41	43.21	43.42	−1.88	−2.31
	0.0011710	0.020717	894.97	43.20	43.30	−2.00	−2.29
	0.0012910	0.022786	980.02	43.01	43.28	−2.02	−2.26
	0.0015290	0.027088	1175.37	43.39	43.24	−2.05	−2.17
	0.0019140	0.033709	1446.47	42.91	43.24	−2.05	−1.94
	0.0019370	0.034234	1472.42	43.01	43.25	−2.05	−1.92
	0.0017490	0.034372	1512.38	44.00	43.24	−2.06	−2.05
			mean 43.32 ±0.39				
2	$LiNTO \cdot 2H_2O$						
	0.0020510	0.014729	324.04	22.00	22.01	0.22	0.32
	0.0021420	0.015345	337.60	22.00	22.02	0.22	0.33
	0.0033861	0.027848	615.17	22.09	22.07	0.28	0.41
	0.0052609	0.038340	850.00	22.17	22.14	0.34	0.50
	0.0056643	0.040060	893.75	22.31	22.15	0.35	0.52
	0.0060223	0.042519	942.23	22.16	22.16	0.36	0.54
	0.0072850	0.050802	1118.66	22.02	22.20	0.40	0.59
	0.0082968	0.058126	1285.75	22.12	22.22	0.42	0.63
	0.0082317	0.058364	1295.69	22.20	22.22	0.42	0.62
	0.0083117	0.058300	1300.10	22.30	22.22	0.42	0.63
	0.0089505	0.064066	1426.12	22.26	22.24	0.44	0.65
	0.0090555	0.075761	1677.36	22.14	22.24	0.44	0.65
	0.0090452	0.063764	1415.57	22.20	22.24	0.44	0.65
	0.0097706	0.069548	1547.44	22.25	22.26	0.46	0.68
	0.0097912	0.069484	1575.89	22.68	22.26	0.46	0.68
	0.0097517	0.069472	1529.78	22.02	22.26	0.46	0.67
			mean 22.16 ±0.08				
3	$Ca(NTO)_2 \cdot 4H_2O$						
	0.0019460	0.016423	513.05	31.24	31.04	−0.49	−0.69
	0.0028680	0.025500	787.94	30.90	30.96	−0.57	−0.79
	0.0033960	0.028643	883.36	30.84	30.92	−0.61	−0.83
	0.0045269	0.045736	1412.77	30.89	30.85	−0.67	−0.91
	0.0061218	0.051615	1565.48	30.33	30.78	−0.75	−0.98
	0.0068953	0.058161	1777.41	30.56	30.75	−0.77	−1.00
	0.0075473	0.063568	1975.06	31.07	30.73	−0.79	−1.02
	0.0086630	0.073080	2266.94	31.02	30.70	−0.82	−1.04
	0.0097244	0.081989	2494.93	30.43	30.68	−0.85	−1.06
	0.01132	0.095495	2929.80	30.68	30.65	−0.88	−1.06
	0.01261	0.10633	3267.45	30.73	30.63	−0.90	−1.06
	0.014520	0.12248	3734.42	30.49	30.61	−0.92	−1.05
	0.016369	0.13802	4237.29	30.70	30.59	−0.93	−1.03
	0.017721	0.14931	4613.80	30.90	30.59	−0.94	−1.01
	0.021237	0.17903	5424.51	30.30	30.58	−0.95	−0.94
			mean 30.74 ±0.21				
4	$Gd(NTO)_3 \cdot 7H_2O$						
	0.00040900	0.0038174	191.63	50.20	50.17	0.22	0.27
	0.00093360	0.0087099	437.32	50.21	50.19	0.24	0.22
	0.0010420	0.0097253	487.34	50.11	50.19	0.24	0.20
	0.0010760	0.010047	501.77	49.94	50.18	0.24	0.19
	0.0013140	0.012315	619.84	50.33	50.17	0.23	0.14
	0.0013890	0.012973	651.12	50.19	50.17	0.22	0.12
	0.0011860	0.014068	707.46	50.29	50.18	0.23	0.17
	0.0020160	0.019727	988.69	50.12	50.11	0.16	−0.07
	0.0023030	0.021532	1077.26	50.03	50.07	0.13	−0.16
			mean 50.19 ±0.13				

(Table 1 continued)

No.	b/mol·kg^{-1}	a/mol	Q/J	$\Delta_{diss}H$/kJ·mol^{-1}		$\Delta_{diss}H_{partial}$ /kJ·mol^{-1}	$\Delta_{diss}H_{apparent}$ /kJ·mol^{-1}
				found	calculated		
5	$NaNTO \cdot H_2O$						
	0.0046950	0.042218	1278.78	30.29	30.34	0.46	0.58
	0.0053160	0.047804	1453.71	30.41	30.36	0.47	0.58
	0.0078890	0.070941	2174.35	30.65	30.39	0.51	0.58
	0.0088560	0.079579	2409.65	30.28	30.40	0.51	0.56
	0.0089840	0.080779	2429.82	30.08	30.40	0.52	0.56
	0.010480	0.094226	2885.20	30.62	30.41	0.52	0.53
	0.013100	0.11895	3613.73	30.38	30.40	0.52	0.47
			mean 30.39 ±0.28				
6	$Ce(NTO)_3 \cdot 7H_2O$						
	0.00081400	0.0073154	297.00	40.60	40.84	−0.12	−0.07
	0.0010880	0.0097793	402.22	41.13	40.86	−0.10	−0.01
	0.0012400	0.011149	457.56	41.04	40.87	−0.09	0.03
	0.0014640	0.013162	536.99	40.80	40.89	−0.06	0.09
	0.0016120	0.014493	595.95	41.12	40.91	−0.05	0.14
	0.0017110	0.015390	625.29	40.63	40.92	−0.04	0.17
	0.0018640	0.016758	688.25	41.07	40.94	−0.02	0.21
	0.0021880	0.023293	948.48	40.72	40.98	0.02	0.32
	0.0031500	0.028328	1167.68	41.22	41.12	0.17	0.66
			mean 40.93 ±0.24				
7	$Pr(NTO)_3 \cdot 7H_2O$						
	0.0019120	0.017191	632.82	36.81	37.29	−3.12	−3.69
	0.0021040	0.018916	715.96	37.85	37.24	−3.17	−3.67
	0.0024310	0.021858	810.06	37.06	37.18	−3.23	−3.60
	0.0031060	0.027926	1036.91	37.13	37.13	−3.28	−3.33
	0.0033590	0.030204	1127.21	37.32	37.13	−3.28	−3.20
	0.0039180	0.035218	1303.05	37.00	37.16	−3.25	−2.86
	0.0042090	0.037847	1413.19	37.34	37.20	−3.21	−2.66
	0.0049080	0.044137	1627.76	36.88	37.31	−3.10	−2.12
	0.0051730	0.046513	1745.18	37.52	37.37	−3.04	−1.90
	0.0062490	0.056189	2121.70	37.76	37.65	−2.76	−0.93
			mean 37.27 ±0.36				
8	$Y(NTO)_3 \cdot 6H_2O$						
	0.0023720	0.021328	717.69	33.65	33.79	3.36	4.06
	0.0030360	0.027297	931.64	34.13	33.94	3.51	4.01
	0.0043460	0.039078	1321.24	33.81	34.04	3.61	3.62
	0.0046140	0.041489	1426.37	34.38	34.03	3.61	3.50
	0.0056200	0.050530	1719.53	34.03	33.97	3.55	2.99
	0.0060920	0.054758	1861.76	34.00	33.92	3.49	2.71
	0.0061560	0.055357	1852.24	33.46	33.91	3.48	2.67
	0.0078940	0.070985	2395.03	33.74	33.61	3.18	1.50
			mean 33.89 ±0.38				
9	$Yb(NTO)_3 \cdot 6H_2O$						
	0.0012240	0.011006	398.51	36.21	36.30	2.13	2.54
	0.0014810	0.013317	487.15	36.58	36.37	2.19	2.50
	0.0021850	0.019647	711.22	36.20	36.43	2.25	2.22
	0.0028800	0.025902	937.38	36.19	36.37	2.19	1.75
	0.0028940	0.026021	952.12	36.59	36.37	2.19	1.74
	0.0029700	0.026710	974.36	36.48	36.36	2.18	1.68
	0.0039240	0.035284	1273.03	36.08	36.14	1.96	0.85
	0.0039340	0.035373	1278.75	36.15	36.13	1.96	0.84
			mean 36.31 ±0.25				
10	$Dy(NTO)_3 \cdot 5H_2O$						
	0.0016250	0.014349	597.34	41.63	41.48	−1.28	−1.50
	0.0020130	0.018100	746.44	41.24	41.45	−1.32	−1.45
	0.0022940	0.020632	850.25	41.21	41.43	−1.33	−1.40
	0.0023720	0.021328	881.04	41.31	41.43	−1.33	−1.38
	0.0025300	0.022773	949.88	41.71	41.43	−1.33	−1.34
	0.0025780	0.023180	963.35	41.56	41.43	−1.33	−1.33
	0.0034070	0.030636	1274.13	41.59	41.46	−1.30	−1.06
	0.0039440	0.035468	1465.20	41.31	41.51	−1.26	−0.85
	0.0043580	0.039185	1630.89	41.62	41.56	−1.21	−0.67
			mean 41.46 ±0.22				

(Table 1 continued)

No.	b/mol·kg^{-1}	a/mol	Q/J	$\Delta_{diss}H$/kJ·mol^{-1} found	$\Delta_{diss}H$/kJ·mol^{-1} calculated	$\Delta_{diss}H_{partial}$ /kJ·mol^{-1}	$\Delta_{diss}H_{apparent}$ /kJ·mol^{-1}
11	$Tb(NTO)_3 \cdot 5H_2O$						
	0.0015990	0.014383	606.52	42.17	42.08	0.38	0.52
	0.0018130	0.016300	683.64	41.94	42.10	0.40	0.54
	0.0021410	0.019256	815.47	42.35	42.12	0.42	0.56
	0.0022310	0.020062	845.01	42.12	42.13	0.43	0.57
	0.0022410	0.020152	845.16	41.94	42.13	0.43	0.57
	0.0023320	0.020969	882.79	42.10	42.13	0.43	0.58
	0.0026570	0.023893	1005.64	42.09	42.15	0.45	0.59
	0.0027750	0.024955	1055.36	42.29	42.16	0.46	0.60
	0.0042240	0.037985	1602.95	42.20	42.21	0.52	0.64
			mean 42.14 ±0.17				
12	$Co(NTO)_2 \cdot 8H_2O$						
	0.0011660	0.010484	643.91	61.42	61.33	−0.18	−0.20
	0.0013430	0.012077	737.81	61.09	61.33	−0.18	−0.19
	0.0013940	0.012533	769.39	61.39	61.33	−0.18	−0.18
	0.0016860	0.015156	929.85	61.35	61.33	−0.18	−0.16
	0.0019730	0.017737	1090.45	61.48	61.33	−0.18	−0.13
	0.0022620	0.020339	1242.90	61.11	61.34	−0.17	−0.10
	0.0022730	0.020443	1259.27	61.60	61.34	−0.17	−0.10
	0.0028940	0.026020	1584.86	60.91	61.37	−0.15	−0.02
	0.0030540	0.027451	1694.26	61.72	61.37	−0.14	0.00
			mean 61.34 ±0.26				
13	$Mg(NTO)_2 \cdot 8H_2O$						
	0.00043800	0.0039384	238.00	60.43	60.25	2.25	2.86
	0.00050300	0.0045245	272.87	60.31	60.33	2.34	2.90
	0.00062600	0.0056263	337.63	60.01	60.45	2.45	2.93
	0.00083000	0.0075720	459.32	60.66	60.56	2.56	2.85
	0.00090000	0.0080878	492.63	60.91	60.58	2.58	2.80
	0.0010010	0.0089317	541.35	60.61	60.59	2.60	2.70
	0.0011410	0.010256	618.96	60.35	60.60	2.60	2.54
	0.0014360	0.012917	784.19	60.71	60.54	2.55	2.10
	0.0016010	0.014394	869.10	60.38	60.48	2.49	1.81
			mean 60.49 ±0.30				

The results reveal that the values of r^2 of Eq. (1) for 13 complexes are more than 0.99 and the values of $\Delta_{diss}H_m^\theta$ ($b = 0$) approach the values of $\Delta_{diss}H_m^\theta$ at infinite dilution in Ref. [1−3], indicating that 65 empirical formulae describing the dissolution properties in water of 13 complexes and derived values of $\Delta_{diss}H_m^\theta$, $\Delta_{diss}H_m^\theta$ ($b = 0$), $\Delta_{diss}H_{apparent}$, $\Delta_{diss}H_{partial}$ and are believable to a great extent.

References:

[1] HU Rong-zu, MENG Zi-hui. Thermochemical and thermodynamic properties of $M(NTO)_n$ and $M(NTO)_n \cdot mH_2O$[J]. *Chinese Journal of Energetic Materials*, 1995, 3(3): 9−27.

[2] HU Rong-zu, MENG Zi-hui, KANG Bing. Thermochemical and thermodynamic properties of $M(NTO)_n$ and $M(NTO)_n \cdot mH_2O$ [J]. *Thermochim Acta*, 1996, 275(2): 159−172.

[3] MENG Zi-hui, HU Rong-zu. Standard enthalpy of formation of metal (K, Ba, Li, Ca, Gd, Pb, Cu and Zn) salts of NTO[J]. *J Therm Anal*, 1995, 45(1−2): 79−86.

$M(NTO)_n \cdot mH_2O$ 在水中的溶解行为

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摘　要: 借助 $M(NTO)_n \cdot mH_2O$ (M = Ba, n = 1, m = 3; M = Li, n = 1, m = 2; M = Ca, n = 2, m = 4; M = Na, n = m = 1; M = Co, Mg, n = 2, m = 8; M = Ce, Pr, Gd, n = 3, m = 7; M = Tb, Dy, n = 3, m = 5; M = Y, Yb, n = 3, m = 6; NTO = 3-nitro-1, 2, 4-triazol-5-one)的摩尔用量(a)、水溶液浓度(b)及由 Calvet 微热量计所得的溶解过程热效应(Q)和摩尔溶解焓($\Delta_{diss}H$),得到了描述这些 NTO 金属配合物的微分溶解焓($\Delta_{dil}H_m^\theta$)、标准摩尔溶解焓[$\Delta_{diss}H_m^\theta$($b = 0$)]、相对表观摩尔焓($\Delta_{diss}H_{apparent}$)、相对偏摩尔焓($\Delta_{diss}H_{partial}$)和稀释焓($\Delta_{dil}H_{1,2}$)的 5 个经验式。

关键词: 物理化学; 焓; 溶解性质; NTO; 金属配合物

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