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Enthalpy increment measurements of $SrMoO_4$(s) and $BaMoO_4$(s)

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Abstract

Enthalpy increment measurements on $SrMoO_4$(s) and $BaMoO_4$(s) were carried out using a Calvet micro-calorimeter. The enthalpy increment values were least squares analyzed with the constraints that $H^o(T)-H^o(298.15\ K)$ at 298.15 K is equal to zero and $C_p^o(298.15\ K)$ is equal to the known value. The dependence of enthalpy increments with temperature can be given as:

$$H^o(T) - H^o(298.15\ K)(J\ mol^{-1}) = 126.810\ T(K) + 24.571 \times 10^{-3} T^2(K) + 21.782 \times 10^5 / T(K) - 47299.\ (SrMoO_4(s),\ 299.0 \leq T(K) \leq 1020.3)$$

$$H^o(T) - H^o(298.15\ K)(J\ mol^{-1}) = 136.280 T(K) + 15.122 \times 10^{-3} T^2(K) + 20.502 \times 10^5 / T(K) - 48852.\ (BaMoO_4(s),\ 299.0 \leq T(K) \leq 1020.3)$$

Thermodynamic functions of $SrMoO_4$(s) and $BaMoO_4$(s) have been generated using the experimental $\Delta_f H_m^o(298.15\ K)$, $\Delta_f G_m^o(T)$ and estimated $S_m^o(298.15\ K)$ values for $SrMoO_4$(s) and $BaMoO_4$(s) from the literature.

Keywords: Strontium molybdates; Barium molybdates; Heat capacity; Enthalpy increments; Thermodynamic functions; Calorimetry

1. Introduction

The injection of fission products in fuel has a significant effect on the stoichiometry of the fuel as the burnup progresses. Post irradiation examination of UO_2(s) or (U,Pu)O_2(s) oxide fuel reveals two families of fission products [1]. The first group precipitates as a hexagonal multicomponent metallic phase [2] and the second group exists as a multicomponent oxide phase which crystallizes in the cubic perovskite type ABO_3 and contains Ba, Sr and Cs in the lattice site A as well as Zr, Mo and RE, and the fuel components U and Pu in the lattice site B [2]. The composition of these two phases varies continuously and depends on the fission yield and initial O/M ratio of the fuel. Paschoal et al. [3] have found that $BaMoO_4$(s) will be formed if the solubility limit of $BaMoO_3$ is exceeded in the Ba(U,Zr,Mo,U.Pu,RE)O_3 oxide phase. They predicted $BaMoO_4$ to be formed in very high burnt oxide fuels at temperatures greater than 1650 K. Similarly, the formation of $SrMoO_4$ could be possible. To predict these compounds in an operating reactor fuel pin, the thermodynamic properties of these compounds are needed. We have already determined the Gibbs energy of formation of $SrMoO_4$(s) and $BaMoO_4$(s) using e.m.f. method [4,5]. In this study we have measured $H^o(T)-H^o(298.15\ K)$ of $SrMoO_4$(s) and $BaMoO_4$(s) using a high temperature Calvet calorimeter in the temperature range 299 to 1020.3 K. In this paper we have made an attempt to put together all the thermodynamic functions of these two compounds which have been computed from the experimental measurements.

2. Experimental

$SrMoO_4$(s) and $BaMoO_4$(s) were synthesized by precipitating $SrMoO_4$(s) and $BaMoO_4$(s) separately by the respective addition of an excess solution of $Sr(NO_3)_2$(aq) or $BaCl_2$(aq) to a solution containing Na_2MoO_4(aq). The detailed procedure of preparation is given elsewhere [4,6]. The X-ray diffraction patterns of the white coloured dried precipitates were identical to that reported [7] for tetragonal $SrMoO_4$(s) and tetragonal $BaMoO_4$(s) reported by Swanson et al. [8]. Impurity analysis of $SrMoO_4$(s) and $BaMoO_4$(s) are given in Table 1. Dried samples of $SrMoO_4$(s) and $BaMoO_4$(s) were made into pellets of 4

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Table 1
Analysis of impurities present in $SrMoO_4$(s) and $BaMoO_4$(s) by emission spectrometry

$SrMoO_4$(s)				$BaMoO_4$(s)			
Elements	ppm	Elements	ppm	Elements	ppm	Elements	ppm
Al	<35	Mn	<7	Al	<35	Mn	<7
B	<0.35	Mo	–	B	<0.35	Mo	–
Be	<0.35	Ni	<18	Be	<0.35	Ni	<18
Ca	<18	Pb	<18	Ca	<18	Pb	<18
Cd	<0.35	Si	<420	Cd	<0.35	Si	<420
Co	<10	Sn	<4	Co	<10	Sn	<4
Cr	<18	Ta	<35	Cr	<18	Ta	<35
Cu	<7	Ti	<35	Cu	<7	Ti	<35
Fe	<35	V	<18	Fe	<35	V	<18
Li	<7	W	340	Li	<7	W	<494
Mg	<18	Zn	<35	Mg	<18	Zn	<35

mm diameter and 1 mm thickness under a pressure of 100 MPa. These pellets were annealed in air at 800 K for 50 h and stored in a desiccator for $H^o(T)-H^o(298.15\ \mathrm{K})$ measurements.

The Calvet calorimeter model HT-1000, supplied by SETARAM, France, has been used for enthalpy increment measurements of $SrMoO_4$(s) and $BaMoO_4$(s). The technique used was a drop calorimetry. The calorimeter has an isothermal alumina block which contains two identical one end closed alumina cells surrounded by a series of thermopiles. The sample, in the form of a pellet, maintained at 298.15 K in the sample holder, was dropped into the sample cell maintained at the experimental temperature. The temperature of the isothermal block was measured using a platinum–platinum + 10 mass % rhodium thermocouple (+0.1 K). The heat flow between the isothermal block and either of the cells was recorded in the form of a millivolt signal. The details of the experimental measurements have been described elsewhere [9]. The heat calibration was carried out using a synthetic sapphire [NIST SRM-720].

3. Results

The $H^o(T)-H^o(298.15\ \mathrm{K})$ values for $SrMoO_4$(s) and $BaMoO_4$(s) obtained at different temperatures are given in Tables 3 and 4, respectively. Experimental $C^o_p(298.15\ \mathrm{K})$ values for $SrMoO_4$(s) and $BaMoO_4$(s) are not available in the literature. $C^o_p(298.15\ \mathrm{K})$ at different temperatures has been calculated from our low temperature enthalpy increment data using the equation:

$$C^o_{p,m}(T_1+T_2)/2=\{H^o(T_2)-H^o(298.15\ \mathrm{K})\}-\{H^o(T_1)-H^o(298.15\ \mathrm{K})\}/(T_2-T_1) \quad (1)$$

where T_2 and T_1 are two different temperatures. The low temperature $C^o_{p,m}(T)$ values for $SrMoO_4$(s) and $BaMoO_4$(s) were calculated from Eq. (1) and are given in Table 2. These heat capacity values were plotted against temperature. The best least-squares line passing through the maximum number of points was extrapolated to 298.15 K. The corresponding $C^o_{p,m}(298.15\ \mathrm{K})$ values from these plots were found to be 116.96 and 122.23 $\mathrm{J\,K^{-1}\,mol^{-1}}$ for $SrMoO_4$(s) and $BaMoO_4$(s), respectively. Observed enthalpy increment data given in Tables 2 and 3 were fitted using Shomate's method [10] with the boundary conditions: $H^o(T)-H^o(298.15\ \mathrm{K})=0$ at 298.15 K and known $C^o_{p,m}(298.15\ \mathrm{K})$ value. The $H^o(T)-H^o(298.15\ \mathrm{K})$ expression for $SrMoO_4$(s) and $BaMoO_4$(s) were obtained using $C^o_{p,m}(298.15\ \mathrm{K})$ values: 116.95 and 122.33 $\mathrm{J\,K^{-1}\,mol^{-1}}$, respectively, and are represented by the equations:

$$H^o(T)-H^o(298.15\ \mathrm{K})(\mathrm{J\,mol^{-1}})=126.810T(\mathrm{K})+24.571\times10^{-3}T^2(\mathrm{K})+21.782\times10^5/T(\mathrm{K})-47299.\ (SrMoO_4(s),299.0\le T(\mathrm{K})\le1020.3) \quad (2)$$

and

$$H^o(T)-H^o(298.15\ \mathrm{K})(\mathrm{J\,mol^{-1}})=136.280T(\mathrm{K})+15.122\times10^{-3}T^2(\mathrm{K})+20.502\times10^5/T(\mathrm{K})-48852.\ (BaMoO_4(s),299.0\le T(\mathrm{K})\le1020.3). \quad (3)$$

Other thermodynamic functions for $SrMoO_4$(s) were calculated using $S^o_m(298.15\ \mathrm{K})=140.0\ \mathrm{J\,K^{-1}\,mol^{-1}}$ [11], $\Delta_f H^o_m(298.15\ \mathrm{K})=-1543.8\ \mathrm{kJ\,mol^{-1}}$ [12] and $\Delta_f G^o_m(T)$ for $T\ge1300$ K from Zharkova et al. [13] and for $T\le1200$ K from Singh et al. [4]. Similarly, for $BaMoO_4$(s) they were calculated using $S^o_m(298.15\ \mathrm{K})=145\ \mathrm{J\,K^{-1}\,mol^{-1}}$

Table 2
Low temperature heat capacity values for $SrMoO_4$(s) and $BaMoO_4$(s)

$SrMoO_4$(s)		$BaMoO_4$(s)	
T(K)	$C^o_{p,m}(T)$ $\mathrm{J\,K^{-1}\,mol^{-1}}$	T(K)	$C^o_{p,m}(T)$ $\mathrm{J\,K^{-1}\,mol^{-1}}$
303.65	117.74	303.65	123.58
306.75	118.39	314.0	126.92
309.35	119.05	317.6	127.85
350.40	125.78	316.55	127.45
		322.25	128.62

Table 3
Experimental enthalpy increment values of $SrMoO_4$(s)

T(K)	$H^\circ(T)-H^\circ$(298.15 K) (J mol^{-1})			T(K)	$H^\circ(T)-H^\circ$(298.15 K)(J mol^{-1})		
	Exp.	Cal.	*Δ% Error		Exp.	Cal.	*Δ% Error
299.0	99.5+2.1	99.5	−0.01	662.9	51612+1548	50847	−1.48
301.0	334+9	334	0.06	675.2	53541+1874	52752	−1.47
302.1	463+26	464	0.14	685.5	55352+2269	54354	−1.80
305.2	828+37	830	0.21	700.8	57695+1274	56746	−1.64
308.3	1195+33	1197	0.24	711.1	59258+1879	58364	−1.51
310.4	1445+102	1448	0.23	754.1	65611+701	65182	−0.65
319.7	2555+95	2568	0.49	766.3	67413+690	67147	−0.39
324.8	3165+365	3188	0.73	798.0	72078+1679	72273	0.27
376.0	9605+390	9649	0.46	825.4	76187+1932	76750	0.74
448.2	19352+387	19333	−0.09	871.0	83006+2051	84295	1.55
453.6	20519+739	20080	−2.14	877.2	84061+1630	85330	1.50
474.0	23915+1195	22925	−4.14	901.0	87775+2037	89322	1.76
484.3	25420+1321	24376	−4.10	921.8	90928+2179	92837	2.10
500.6	27735+1109	26691	−3.76	937.6	93359+3012	95523	2.32
516.0	29659+593	28899	−2.56	946.5	94745+3256	97041	2.42
580.7	39811+1194	38377	−3.60	1000.1	103931+3560	106279	2.26
591.0	41292+479	39914	−3.33	1020.3	105523+2078	109800	4.05
650.6	49717+1201	48953	−1.53				

* Δ% Error=(fit value−Measured value)×100/fit value.

[14], $\Delta_f H^\circ_m(298.15\ K) = -1546.7$ kJ mol^{-1} (an average solution calorimetry value of Sukhla et al. [12] and O'Hare [15]) and $\Delta_f G^\circ_m(T)$ for $T \geq 1400$ K from Rezukhina and Levitskii [16] and $T \leq 1300$ K from Singh et al. [5]. The calculated thermodynamic functions for $SrMoO_4$(s) and $BaMoO_4$(s) are given in Tables 5 and 6, respectively.

4. Discussion

A summary of the reported enthalpy increments and heat capacity data for $SrMoO_4$(s) and $BaMoO_4$(s), available in the literature, is given in Tables 7 and 8, respectively. Enthalpy increments for $SrMoO_4$(s) and $BaMoO_4$(s) from the present study are compared with the literature in Figs. 1 and 2, respectively. Similarly, the variation of heat capacities, the first differential of $H^\circ(T)-H^\circ$(298.15 K), with temperature for $SrMoO_4$(s) and $BaMoO_4$(s) is compared with the experimental data of Saha et al. [17,18] along with the other literature values [19] in Figs. 3 and 4, respectively.

Saha et al. [17,18] have measured the enthalpy increments of $SrMoO_4$(s) and $BaMoO_4$(s) in the respective temperature ranges 1042 to 1636 K and 986 to 1732 K

Table 4
Experimental enthalpy increment values of $BaMoO_4$(s)

T(K)	$H^\circ(T)-H^\circ$(298.15 K) (J mol^{-1})			T(K)	$H^\circ(T)-H^\circ$(298.15 K) (J mol^{-1})		
	Exp.	Cal.	*Δ% Error		Exp.	Cal.	*Δ% Error
299.0	104.6+3	104	−0.61	650.6	49960+1599	49362	−1.20
301.0	339+16	349	2.98	662.9	52980+795	51224	−3.31
302.1	485+5	484	−0.16	675.2	53919+1456	53092	−1.53
305.2	868+20	866	−0.21	685.5	56366+1691	54662	−3.02
308.3	1250+37	1250	−0.01	700.8	57091+1656	57003	−0.15
310.4	1508+61	1511	0.18	711.1	58576+1757	58584	0.01
319.7	2697+95	2674	−0.84	754.1	65258+2610	65232	−0.04
324.8	3353+135	3318	−1.03	766.3	66430+3322	67132	1.06
376.0	10235+819	9974	−2.54	798.0	70028+2521	72096	2.95
448.2	19981+1650	19814	−0.83	871.0	82479+3217	83671	1.44
453.6	20570+820	20567	−0.01	901.0	87670+2068	88485	0.93
474.0	24126+1013	23429	−2.89	921.8	91082+1188	91841	0.83
484.3	25662+1104	24885	−3.03	937.6	91814+2112	94401	2.82
500.6	28066+982	27201	−3.08	946.5	93567+3368	95847	2.43
516.0	30369+760	29404	−3.17	1000.1	103275+4131	104613	1.30
580.7	39317+1376	38798	−1.32	1020.3	104890+2510	107942	2.91
591.0	41804+1588	40312	−3.57				

* Δ% Error=(Fit value−Measured value)×100/Fit value.

Table 5
Thermodynamic functions for $SrMoO_4$(s)

T(K)	$C^{\circ}_{p,m}(T)$ (J K^{-1} mol^{-1})	$S^{\circ}_{m}(T)$ (J K^{-1} mol^{-1})	$-(G^{\circ}(T)-H^{\circ}(298.15\ \text{K}))/T$ J K^{-1} mol^{-1}	$H^{\circ}(T)-H^{\circ}(298.15\ \text{K})$ (J mol^{-1})	$\Delta_f H^{\circ}_{m}(T)$ (kJ mol^{-1})	$\Delta_f G^{\circ}_{m}(T)$ (kJ mol^{-1})
298.15	116.96	140.00	140.00	0	−1543.7	−1472.6
300	117.40	140.72	140.00	218	−1543.7	−1471.9
400	133.35	176.98	144.83	12859	−1542.3	−1435.0
500	141.48	207.70	154.42	26638	−1540.0	−1398.0
600	146.55	233.97	165.54	41056	−1537.4	−1361.0
700	150.17	256.84	176.99	55901	−1534.8	−1324.1
800	153.01	277.09	188.26	71064	−1532.2	−1287.1
900	155.40	295.25	199.15	86487	−1530.2	−1250.2
1000	157.51	311.74	209.60	102135	−1527.3	−1213.2
1100	159.45	326.84	219.58	117984	−1532.3	−1176.2
1200	161.25	340.79	229.11	134020	−1530.2	−1139.3
1300	162.97	353.77	238.21	150232	−1528.1	−1098.7
1400	164.63	365.91	246.90	166612	−1525.9	−1065.5
1500	166.24	377.32	255.22	183156	−1523.8	−1032.3
1600	167.81	388.10	263.19	199858	−1521.5	−999.1
1700	169.36	398.32	270.84	216717	−1519.3	−965.9
1800	170.88	408.04	278.19	233729	−1517.0	−932.6

using a drop method in a high temperature differential calorimeter. In the present study a drop method is also used but the temperature range is 299 to 1020.3 K. To cover the entire temperature range, the experimental data of the present study is combined with that of Saha et al. [17,18] and refitted using Shomate's method and can be represented by the following equations for $SrMoO_4$(s) and $BaMoO_4$(s), respectively:

$$H^{\circ}(T) - H^{\circ}(298.15\ \text{K})(\text{J mol}^{-1}) = 146.380T(\text{K}) + 7.062 \times 10^{-3}T^2(\text{K}) + 29.893 \times 10^{5}/T(\text{K}) - 54296.\ (\text{SrMoO}_4\text{(s)},\ 299.0 \le T(K) \le 1636) \quad (4)$$

and

$$H^{\circ}(T) - H^{\circ}(298.15\ \text{K})(\text{J mol}^{-1}) = 138.510T(\text{K}) + 12.509 \times 10^{-3}T^2(\text{K}) + 21.101 \times 10^{5}/T(\text{K}) - 49486.\ (\text{BaMoO}_4\text{(s)},\ 299.0 \le T(K) \le 1732). \quad (5)$$

It is clear from Fig. 1 that all the enthalpy values for $SrMoO_4$(s) match excellently well up to 1100 K, beyond this temperature our values are slightly higher than those of Saha et al. [17] and also those obtained from the combined Eq. (4). Cordfunke and Konnings [14] have refitted the experimental data of Saha et al. [18] for $BaMoO_4$(s) and the same polynomials have been plotted in Fig. 2 along with the other data. In Fig. 2 it is shown that all the lines are almost superimposed over one another. To

Table 6
Thermodynamic functions for $BaMoO_4$(s)

T(K)	$C^{\circ}_{p,m}(T)$ (J K^{-1} mol^{-1})	$S^{\circ}_{m}(T)$ (J K^{-1} mol^{-1})	$-(G^{\circ}(T)-H^{\circ}(298.15\ \text{K}))/T$ (J K^{-1} mol^{-1})	$H^{\circ}(T)-H^{\circ}(298.15\ \text{K})$ (J mol^{-1})	$\Delta_f H^{\circ}_{m}(T)$ (kJ mol^{-1})	$\Delta_f G^{\circ}_{m}(T)$ (kJ mol^{-1})
298.15	122.23	145.00	145.00	0	−1546.7	−1436.1
300	122.57	145.76	145.00	227	−1546.7	−1435.4
400	135.33	182.98	149.99	13195	−1545.1	−1399.9
500	142.58	214.01	159.78	27117	−1543.7	−1364.4
600	147.66	240.48	171.08	41641	−1542.7	−1328.9
700	151.72	263.55	182.67	56616	−1540.7	−1293.4
800	155.23	284.05	194.09	71966	−1539.1	−1257.8
900	158.42	302.52	205.13	87650	−1536.9	−1222.3
1000	161.42	319.36	215.72	103644	−1534.5	−1186.8
1100	164.29	334.88	225.86	119930	−1540.4	−1151.3
1200	167.07	349.30	235.55	136498	−1538.0	−1115.8
1300	169.78	362.78	244.82	153341	−1535.4	−1080.2
1400	172.46	375.46	253.71	170454	−1532.5	−1056.7
1500	175.10	387.45	262.23	187832	−1529.4	−1021.1
1600	177.71	398.83	270.41	205473	−1526.2	−985.5
1700	180.31	409.68	278.29	223374	−1522.8	−949.9
1800	182.89	420.06	285.88	241534	−1519.4	−914.4

Table 7
Reported enthalpy increments and heat capacity expressions for $SrMoO_4$(s)

Authors	Methods	Temperature range (K)	Thermodynamic data
Saha et al. [17]	SC	1042–1636	$H^o(T)-H^o(298.15\ K)=98.934\ T(K)+29.411\times10^{-3}\ T^2(K)-\{4.930\times10^4/T(K)\}-31946.3$
	c		$C_{p,m}o(T)=98.934+58.822\times10^{-3}T(K)+4.930\times10^4/T^2(K)$
Kubaschewski et al. [19]	C		$C^o_{p,m}(T)=134.140+29.370\times10^{-3}T(K)-23.010\times10^5/T^2(K)$
JANAF tables [20]	AD	–	$C^o_{p,m}(T)=119.575+46.824\times10^{-3}\ T(K)-11.688\times10^5/T^2(K)$
Present study	CV	299–1020.3	$H^o(T)-H^o(298.15\ K)=126.820\ T(K)+24.571\times10^{-3}\ T^2(K)+\{21.782\times10^5/T(K)\}-47299$
			$C^o_{p,m}(T)=126.820+49.142\times10^{-3}T(K)-21.782\times10^5/T^2(K)$
	COM	299–1636	$H^o(T)-H^o(298.15\ K)=146.380\ T(K)+7.062\times10^{-3}\ T^2(K)+\{29.893\times10^5/T(K)\}-54296$
			$C^o_{p,m}(T)=146.380+14.124\times10^{-3}T(K)-29.893\times10^5/T^2(K)$

DC = Drop calorimetry, c = calculated in the present study, C = calculated by Cordfunke and Konings [14], CM = compilation, AD = calculated using additive oxide method by present study, CV = Calvet calorimeter, COM = experimental data of present study is combined with that of Saha et al. [17,18].

resolve this ambiguity of the best $H^o(T)-H^o(298.15\ K)$ polynomials for $SrMoO_4$(s) and $BaMoO_4$(s), the variation of heat capacities with the temperature are compared in Figs. 3 and 4, respectively.

The first differential of the combined Eq. (4) and Eq. (5) gives the molar heat capacity for $SrMoO_4$(s) and $BaMoO_4$(s), respectively. The resulting equations are:

$$C^o_{p,m}(T)(J\ K^{-1}\ mol^{-1}) = 146.380 + 14.124\times10^{-3}T(K) - 29.893\times10^5/T^2(K).\ (SrMoO_4(s),\ 299.0 \le T(K) \le 1636) \quad (6)$$

and

$$C^o_{p,m}(T)(J\ K^{-1}\ mol^{-1}) = 138.510 + 25.018\times10^{-3}T(K) - 21.101\times10^5/T^2(K).\ (BaMoO_4(s),\ 299.0 \le T(K) \le 1732). \quad (7)$$

The heat capacity values for $SrMoO_4$(s) and $BaMoO_4$(s) have also been calculated by applying the molar additivity rule by using heat capacities of SrO(s) or BaO(s) and

Table 8
Reported enthalpy increments and heat capacity expressions for $BaMoO_4$(s)

Authors	Methods	Temperature range (K)	Thermodynamic data
Saha et al. [18]	DC	986–1732	$H^o(T)-H^o(298.15\ K)=129.393T(K)+16.814\times10^{-3}\ T^2(K)+\{14.662\times10^5/T(K)\}-44991$
	c		$C^o_{p,m}(T)=129.393+33.628\times10^{-3}T(K)-14.662\times10^5/T^2(K)$
Kubaschewski et al. [19]	CM	–	$C^o_{p,m}(T)=135.270+28.450\times10^{-3}\ T(K)-25.100\times10^5/T^2(K)$
Cordfunke and Konings [14]	C	986–1732	$H^o(T)-H^o(298.15\ K)=91.977\ T(K)+35.533\times10^{-3}\ T^2(K)-\{7.854\times10^5/T(K)\}-27947.5$
	c		$C^o_{p,m}(T)=91.977+71.066\times10^{-3}T(K)+7.854\times10^5/T^2(K)$
JANAF tables [20]	Ad	–	$C^o_{p,m}(T)=125.480+39.840\times10^{-3}T(K)-13.390\times10^5/T^2(K)$
Present study	CV	299–1020.3	$H^o(T)-H^o(298.15\ K)=136.280\ T(K)+15.122\times10^{-3}\ T^2(K)+\{20.502\times10^5/T(K)\}-48852$
			$C^o_{p,m}(T)=136.280+30.244\times10^{-3}T(K)-20.502\times10^5/T^2(K)$
	COM	299–1732	$H^o(T)-H^o(298.15\ K)=138.510\ T(K)+12.509\times10^{-3}\ T^2(K)+\{21.101\times10^5/T(K)\}-49486$
			$C^o_{p,m}(T)=138.510+25.018\times10^{-3}T(K)-21.101\times10^5/T^2(K)$

Abbreviations as per Table 7.

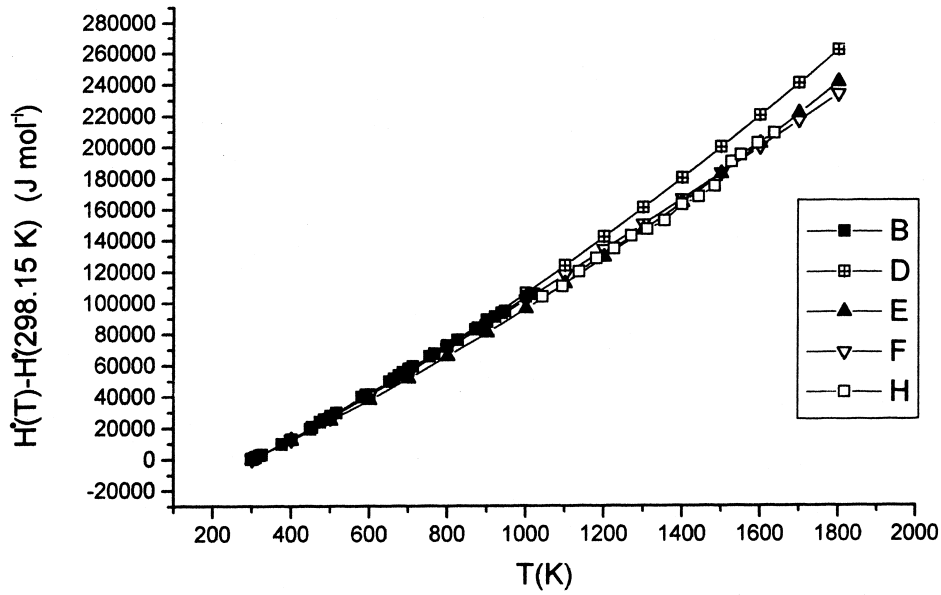

Fig. 1. Change in enthalpy increments with the temperature for $SrMoO_4$(s). B, experimental data (present study); D, least-squares values (present study); E, least-squares values (Saha et al. [17]); F, combined experimental data of present study and Saha et al. [17]; H, experimental data of Saha et al. [17].

MoO_3(s) from JANAF tables [20]. The heat capacity values derived from Eq. (6) and Eq. (7), from the additivity method and heat capacity values reported in the literature [19] for $SrMoO_4$(s) and $BaMoO_4$(s), have been taken for the comparison in Figs. 3 and 4, respectively.

It is clear from Fig. 3 that the low temperature heat capacity up to 500 K match reasonably well with all the data except those of Saha et al. [17]. However, our combined Eq. (6) is more close to the equation given by Kubaschewski et al. [19] up to 900 K and between 900 to 1800 K the combined Eq. (6) is the lowest among all the reported data. The combined heat capacity curve in Fig. 3

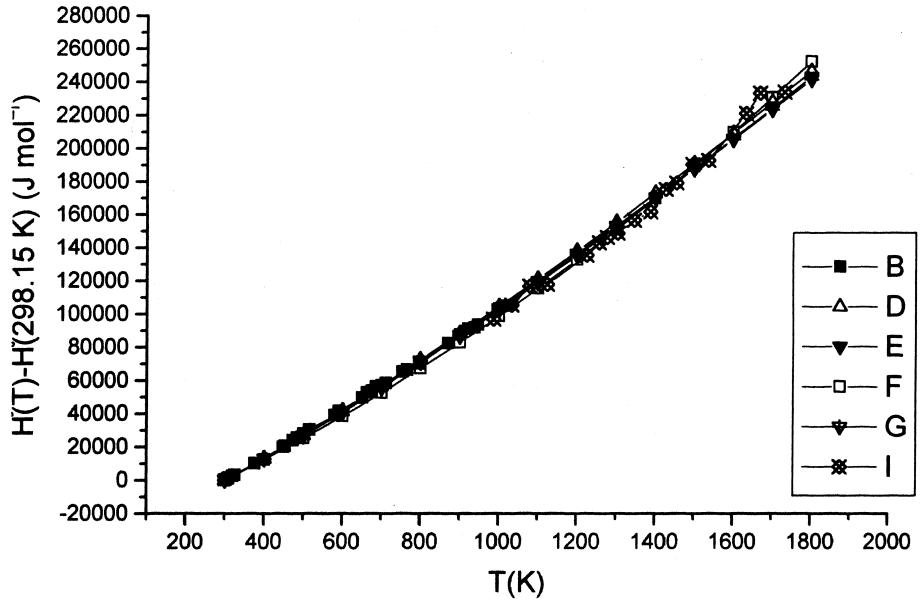

Fig. 2. Change in enthalpy increments with the temperature for $BaMoO_4$(s). B, experimental data (present study); D, least-squares values (present study); E, least-squares values (Saha et al. [18]); F, least-squares values of Cordfunke and Konings [14]; G, combined experimental data of present study and Saha et al. [18]; I, experimental data of Saha et al. [18].

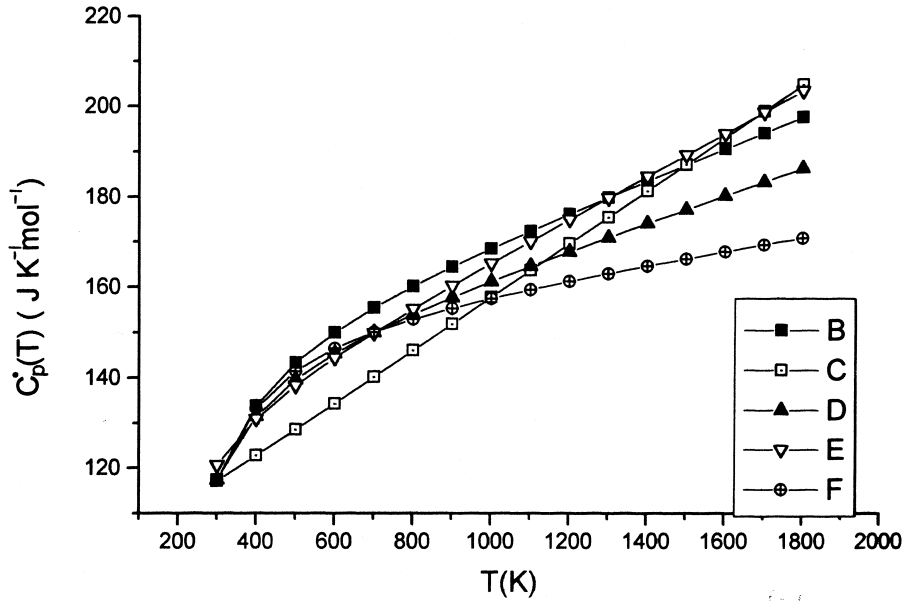

Fig. 3. Change in heat capacity values with the temperature for $SrMoO_4$(s). B, present study; C, Saha et al. [17]; D, Kubaschewski et al. [19]; E, calculated using additivity method; F, combined data of present study and Saha et al. [17].

seems to be more reasonable as it is based on the experimental data in the entire temperature range. Thus, Eq. (6) is selected as the heat capacity expression for $SrMoO_4$(s).

In the case of $BaMoO_4$(s), as seen in Fig. 4, heat capacity values of Cordfunke and Konnings [14] are quite different from the other data. Our heat capacity values match with all other values within a small error band except that of Cordfunke and Konnings [14]. Our combined heat capacity expression (Eq. (7)) matches excellent-

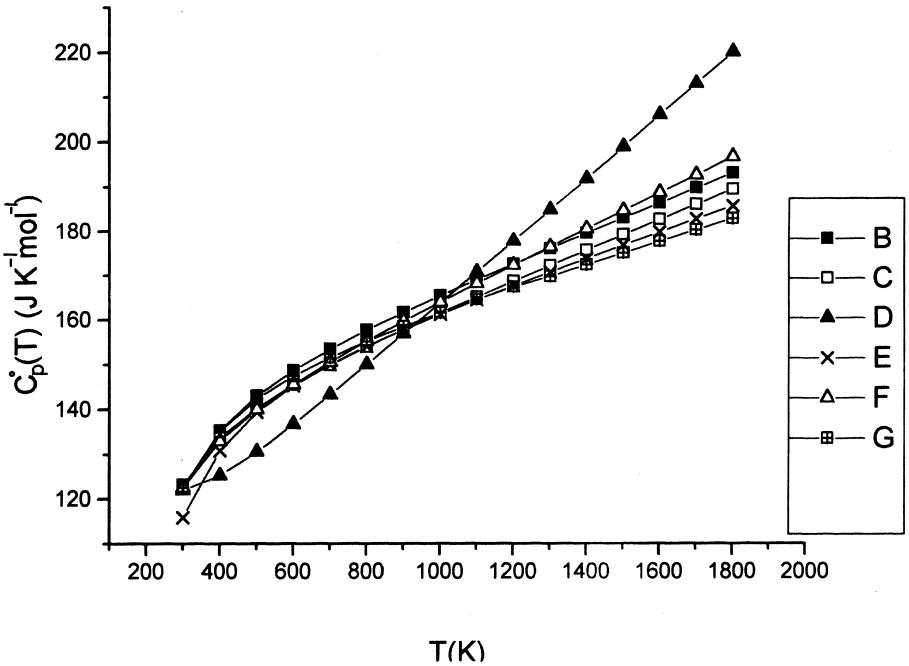

Fig. 4. Change in heat capacity values with the temperature for $BaMoO_4$(s). B, present study; C, Saha et al. [18]; D, Cordfunke and Konings [14]; E, Kubaschewski et al. [19]; F, calculated using additivity method; G, combined data of present study and Saha et al. [18].

ly well with that reported by Kubaschewski et al. [19] and hence Eq. (7) is selected as the heat capacity expression for $BaMoO_4$(s).

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