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Thermochemical Study of Gaseous Salts of Oxygen-containing Acids: XXII.[1] Tin Molybdates

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Abstract—Gas-phase reactions involving tin molybdates were studied. Standard enthalpies of formation and atomization of gaseous salts $SnMoO_4$ and Sn_2MoO_5 were determined.

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At present five gaseous salts of tin(II): $SnPO_2$, $SnPO_3$ [2], $SnWO_4$, Sn_2WO_5, and SnW_2O_7 are known to exist [3]. All these salts were obtained by reactions of the corresponding gaseous oxides with SnO(gas) foperating as a cation-forming oxide in the synthesis reactions.

It was shown in [4] that the thermal stability of gaseous salts depends on a difference in acid-base properties of the oxides forming a salt. Quantitatively acid-base properties of an oxide can be estimated using the value of average orbital electronegativity [5]. The electronegativity of oxides of the IVA subgroup increases on going from PbO to SiO, therefore in reactions of the synthesis of gaseous salts of oxygen-containing acids SiO functions as an anion-forming oxide [6, 7], GeO possesses amphoteric properties forming salts of two types [8–10], and SnO and PbO are known only as cation-forming oxides [2, 3, 11–14]. To carry out the synthesis of gaseous tin molybdates it is necessary to select such heating conditions which are suitable for the simultaneous existence of SnO and molybdenum oxides in vapor.

Crystalline oxides SnO and SnO_2 were found to exist in the system tin-oxygen [15]. The most stable is the dioxide SnO_2. The vaporization of tin dioxide in the temperature range 1250–1540 K to a greater degree follows Eq. (1) and to a lesser degree, Eqs. (2) and (3) [15]. The molecules SnO and O_2 comprise more than 95% of the gas phase over tin dioxide. A part of tin monooxide (~3%) is polymerized to form the Sn_2O_2 dimer. A fraction of SnO_2 is about ~0.01 %. When a mixture of tin and tin dioxide is evaporated the temperature of the vapor formation decreases to 1050–1200 K. The vapor phase consists of Sn_nO_n molecules. The value of n varies from 1 up to 6. The main components of the vapor are SnO and Sn_2O_2. With growing temperature the part of polymeric compounds, first of all of a dimer, increases.

$$SnO_2(cr) = SnO(gas) + 0.5\ O_2(gas), \quad (1)$$

$$SnO_2(cr) = 0.5\ Sn_2O_2(gas) + 0.5\ O_2(gas), \quad (2)$$

$$SnO_2(cr) = SnO_2(gas), \quad (3)$$

$$Sn(l) + SnO_2(cr) \rightarrow Sn_nO_n(gas). \quad (4)$$

The results of studying vapor formation of MoO_3 were generalized in [15]. It was found that molybdenum trioxide is polymerized in vapor in the temperature range 800–1000 K. The main forms are Mo_3O_9 and Mo_4O_{12}, their partial pressures are similar.

The study of the vaporization of a mixture of tin and tin dioxide from a tungsten cell by high-temperature mass-spectrometry in the temperature range 1200–1348 K [16] has shown that Sn^+, SnO^+, $SnWO_3^+$, $SnWO_4^+$, and $Sn_2WO_5^+$ ions are present in the vapor mass spectrum. Alongside monatomic tin and monoxide, tin(II) tungstates originating from the reaction of tin oxide with the cell material were present in the vapor. Calculated enthalpies of reactions (5) and (6) at 0 K are 310 ± 13 and 275 ± 4 kJ mol^{-1}, respectively.

$$SnWO_4(gas) + 3\ Sn(gas) = 2\ Sn_2O_2(gas) + W(cr), \quad (5)$$

[1] For communication XXI, see [1].

$$Sn_2WO_5(gas) = SnWO_4(gas) + SnO(gas). \quad (6)$$

These values allowed us to calculate atomization enthalpies of gaseous tin tungstates $SnWO_4$ and Sn_2WO_5 equal to 2953 ± 96 and 3754 ± 145 kJ mol^{-1}, respectively.

Ionic currents of Sn^+, SnO^+, $SnWO_3^+$, $SnWO_4^+$, $SnW_2O_7^+$, and $(SnWO_4)_2^+$ were recorded in the mass spectrum of vapor over the system SnO_2–$2WO_3$ in the temperature range 1220–1400 K [11]. Appearance energies of the ions are 15.4, 12.4, 13.2, 10.8, 10.6, and 10.6 eV, respectively. On the basis of these data it was concluded that the vapor over the system SnO_2–$2WO_3$ is enriched with heavy molecular forms.

When studying vaporization of a mixture of 50 mol % SnO_2–50 mol % WO_3 in the temperature range 1250–1400 K [3] it was found that the vapor phase over the mixture consisted of SnO, W_3O_9, W_4O_{12}, $SnWO_4$, Sn_2WO_5, and SnW_2O_7. Partial pressures of the vapor molecular forms and also the enthalpy of formation of gaseous salts $SnWO_4$, Sn_2WO_5, and SnW_2O_7 of –777.9 ± 71.1, –1083.9 ± 125.5, and –1570.7 ± 104.6 kJ mol^{-1}, respectively, were determined.

To synthesize gaseous tin molybdates, we originally evaporated a mixture consisting of tin dioxide and molybdenum trioxide. The coexistence of tin and molybdenum oxides in vapor was not observed, as more volatile molybdenum oxide was preferentially removed from the system. To increase SnO partial pressure and to reduce temperature of tin dioxide vaporization, metal tin was added to the mixture. As a result we managed to create conditions for the coexistence of SnO, molybdenum oxides, and also tin molybdates in vapor.

We recorded peaks of Sn^+, SnO^+, $SnMoO_2^+$, $SnMoO_3^+$, $SnMoO_4^+$, $Sn_2MoO_5^+$, and $Mo_4O_{12}^+$ ions in the mass spectrum of vapor over the studied mixture in the temperature range of 900–1075 K. As temperature was increased up to 1175 K the intensity of $Mo_4O_{12}^+$ decreased to a background level.

To determine the nature of ions in the mass spectrum, we have measured their appearance energies by recording curves of ionization effectiveness. The effectiveness turned to be (±0.3) 15.2, 10.6, 11.1, and 11.1 eV, respectively, for the Sn^+, SnO^+, $SnMoO_4^+$, and $Sn_2MoO_5^+$ ions. The ions SnO^+, $SnMoO_4^+$, and $Sn_2MoO_5^+$ are molecular. The measured appearance energy of SnO^+ coincides with the ionization energy of tin monoxide [17]. The appearance energies of $SnMoO_4^+$ and $Sn_2MoO_5^+$ are close in values to the appearance energies of molecular ions $BaMoO_4^+$, $SnWO_4^+$, and $Ba_2MoO_5^+$ [11, 18]. The appearance energy of Sn^+ exceeds the ionization energy of monatomic tin by 7.9 eV [17]. No breaks were observed in the curve of Sn^+ ionization effectiveness, and ratios of the intensities of ionic currents Sn^+/SnO^+ in the mass spectra of vapor over the studied mixture and over individual tin oxide were equal, which points to the fact that the ion Sn^+ is a product of the dissociative ionization of the molecule SnO. Appearance energies of $SnMoO_2^+$ and $SnMoO_3^+$ estimated with an accuracy of ±1 eV are higher than the appearance energy of $SnMoO_4^+$ by 3–4 eV. In this connection we related $SnMoO_2^+$ and $SnMoO_3^+$ ions to the products of the dissociative ionization of the molecule $SnMoO_4$.

The determination of SnO, $SnMoO_4$, Sn_2MoO_5, and Mo_4O_{12} partial pressures by comparison of ionic currents using silver as an internal reference of pressure [19] has allowed us to calculate equilibrium constants and enthalpies of gas-phase reactions (7)–(9) by Eq. (10).

$$SnO + 0.25Mo_4O_{12} = SnMoO_4, \quad (7)$$

$$2SnO + 0.25Mo_4O_{12} = Sn_2MoO_5, \quad (8)$$

$$SnO + SnMoO_4 = Sn_2MoO_5, \quad (9)$$

$$\Delta_r H^0(0) = T[\Delta_r \Phi^0(T) - R\ln K_p(T)]. \quad (10)$$

Necessary thermodynamic functions of tin and molybdenum oxides were taken from the handbook [20]. Thermodynamic functions for gaseous tin molybdates were calculated by the statistical thermodynamics method in the approximation "rigid rotator–harmonic oscillator." Molecular parameters of salts were found by the density functional (DFT) quantum chemical method in the B3LYP approximation [22–23] using the GAMESS program complex [21]. For oxygen the 6-31G* basis was taken, and for molybdenum and tin, the effective Basch–Stevens–Krauss potential [24].

The structure of C_{2v} symmetry of the $SnMoO_4$ molecule analogous to that of the $GeMoO_4$ molecule [8] (Fig. 1a) has the minimal energy. It represents a MoO_4 tetrahedron with a tin atom connected with two oxygen atoms in the bidentate mode. Interatomic distances are as follows, Å: r(Mo–O_{cycl}) 1.91, r(Mo–O_{term}) 1.71, and r(Sn–O) 2.04; the angles are as follows, deg: $O_{cycl}MoO_{cycl}$ 88.3, $O_{term}MoO_{term}$ 109.7, and OSnO 81.4. Normal vibration frequencies for $SnMoO_4$ are 996, 987, 728, 638, 564, 372, 350, 306, 246, 230, 219, and 98 cm^{-1}.

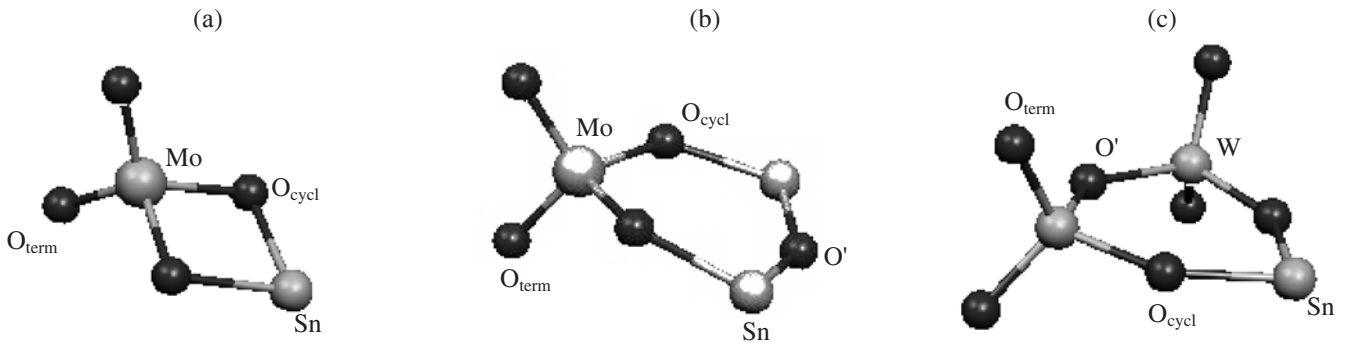

Fig. 1. Molecular structure of (a) $SnMoO_4$, (b) Sn_2MoO_5, and (c) SnW_2O_7.

For the Sn_2MoO_5 molecule the structure with C_{2v} symmetry presented in Fig. 1b has a minimal energy. Interatomic distances are as follows, Å: r(Mo–O_{cycl}) 1.88, r(Mo–O_{term}) 1.72, r(Sn–O_{cycl}) 2.01, and r(Sn–O') 1.96, the angles are as follows, deg: $O_{cycl}MoO_{cycl}$ 105.8, $O_{term}MoO_{term}$ 109.7, OSnO' 96.4, and SnO'Sn 145.7. Normal vibration frequencies for Sn_2MoO_5 are 991, 978, 812, 785, 613, 434, 423, 351, 331, 284, 274, 226, 209, 144, 136, 114, 53, and 16 cm^{-1}.

Partial vapor pressures and enthalpies of the studied gas-phase reactions at 0 K calculated by Eq. (10) are given in Table 1.

Combining the enthalpy of reaction (7) and standard enthalpies of formation of SnO(gas) and Mo_4O_{12}(gas) [20] we found the standard enthalpy of formation of $SnMoO_4$(gas) equal to –670 ± 40 kJ mol^{-1}.

The enthalpy of formation of the molecule Sn_2MoO_5 equal to –929 ± 42 kJ mol^{-1} was obtained from evaluation of the enthalpies of independent reactions (8) and (9).

The ion $SnMo_2O_7^+$ corresponding to the direct ionizations of the $SnMo_2O_7$ molecule was not found in the mass spectra of vapor over the studied mixture in

Table 1. Partial pressures of vapor of molecular forms and enthalpies of reactions (7)–(9) involving gaseous tin molybdates

T, K	p, atm				$-\Delta_r H^0$, kJ		
	$SnO\times10^7$	$Mo_4O_{12}\times10^5$	$SnMoO_4\times10^7$	$Sn_2MoO_5\times10^5$	(7)	(8)	(9)
935	1.69	0.41	2.85	0.36	34.3	315.3	262.4
943	2.18	0.77	4.56	0.61	33.0	316.8	262.9
967	4.30	1.71	8.93	1.15	31.5	317.3	263.6
991	4.65	1.38	7.92	1.02	33.0	323.3	269.4
1007	5.81	1.78	11.67	1.40	34.2	326.8	271.1
961	2.15	0.86	3.96	0.62	31.6	322.9	269.2
920	0.49	0.29	1.30	0.24	32.9	326.6	270.5
954	1.82	0.69	3.08	0.54	31.4	322.5	269.5
990	4.76	1.61	8.92	1.15	32.6	323.2	268.9
1010	7.41	2.15	10.10	1.64	31.0	324.6	272.4
1029	10.76	2.59	21.53	2.18	35.7	326.2	270.1
1050	15.53	3.15	28.41	2.60	36.4	327.5	271.3
1073	22.83	3.53	42.85	3.47	39.1	329.9	272.5
1094	31.56	3.17	50.72	3.48	41.7	330.6	273.2
1004	4.83	1.14	8.20	0.96	35.3	326.7	271.6
1031	8.18	1.58	12.85	1.41	36.1	328.8	273.6
1071	20.47	1.49	27.59	1.47	43.0	325.5	269.3
1253	4.36	–	11.53	0.09	–	–	310.3

Table 1. (Contd.)

T, K	*p*, atm				$-\Delta_r H^0$, kJ		
	$SnO\times10^7$	$Mo_4O_{12}\times10^5$	$SnMoO_4\times10^7$	$Sn_2MoO_5\times10^5$	(7)	(8)	(9)
1295	14.91	–	34.30	0.18	–	–	301.6
1317	23.74	–	44.99	0.20	–	–	299.8
1337	41.08	–	70.83	0.28	–	–	296.8
1294	13.63	–	24.36	0.10	–	–	300.0
1254	4.87	–	8.39	0.03	–	–	300.9
1275	9.30	–	16.00	0.06	–	–	299.4
1300	14.13	–	36.70	0.11	–	–	297.5
1318	23.81	–	57.06	0.18	–	–	296.3
1328	27.53	–	62.49	0.19	–	–	296.5
1353	47.14	–	103.18	0.30	–	–	295.3
1373	70.46	–	131.79	0.36	–	–	294.0
1390	115.54	–	859.47	0.35	–	–	296.5
900	0.73	0.44	1.19	0.08	27.6	305.1	254.6
927	2.12	1.22	4.02	0.69	27.9	312.1	260.8
947	3.81	2.07	7.23	1.06	27.8	311.8	260.3
968	7.06	3.40	14.00	1.70	28.6	311.4	259.4
955	2.39	2.36	4.61	0.85	24.4	319.7	268.0
903	0.59	0.28	0.87	0.38	29.0	321.6	270.8
928	0.97	0.50	1.96	0.35	30.7	320.9	267.4
971	2.85	1.36	5.67	0.88	30.6	323.6	269.6
993	4.75	1.42	9.01	0.97	33.8	323.1	268.2
994	4.97	1.33	8.31	0.88	33.6	321.9	268.0
1040	12.90	2.57	24.29	1.90	36.9	325.3	269.0
930	3.04	0.32	1.75	0.22	31.2	301.3	256.4
973	3.18	0.92	5.22	0.59	33.0	320.0	266.6
1023	8.90	1.94	13.79	1.46	34.5	324.7	270.5
1032	10.10	2.16	16.92	1.57	35.5	325.8	270.6
1052	14.42	2.50	24.34	1.92	37.3	327.2	271.1
1267	53.05	–	129.26	0.47	–	–	278.3
1284	82.55	–	176.63	0.66	–	–	277.4
1292	101.26	–	223.59	0.80	–	–	276.5
1302	130.51	–	236.88	0.96	–	–	277.1
1324	195.26	–	376.01	1.15	–	–	274.1
Average value :					33±4	322±7	277±14

the temperature range 900–1175 K. The presence of similar molecules was recorded in the vapor over the systems SnO_2–WO_3 [3], GeO_2–WO_3 [8], GeO_2–MoO_3 [9], PbO–MoO_3, and PbO–WO_3 [11–13]. It is quite probable that the absence of $SnMo_2O_7$ molecules from the vapor is due to the unsuitable ratio of components in the condensed phase and to the temperature range of measurements. Though germanium molybdate $GeMo_2O_7$ was present in the vapor over the system GeO_2–MoO_3 [9] it was not possible to determine the enthalpy of the reaction with its participation because of low intensity of the ionic current of $GeMo_2O_7^+$.

The value of the atomization enthalpy of $SnMoO_4$(gas) found in the present work in combination with known atomization enthalpies of gaseous tin(II) salts [2, 3] allows us to obtain the dependence of the atomization enthalpies of the salts on the atomization enthalpies of

the anion-forming oxides [4] for an isocation series of tin gaseous salts, which is described by Eq. (11).

$$\Delta_{at}H^0(M_mXO_n, \text{gas}, 298) = k\Delta_{at}H^0(XO_{n-1}, \text{gas}, 298) + b, \quad (11)$$

$$\Delta_rH^0(T) = -R\,\frac{\partial \ln K_p(T)}{\partial(1/T)}\,. \quad (12)$$

To construct linear dependence (11) for tin salts, it was necessary to correct values of the enthalpies of formation of tin tungstates determined in [3], as when the enthalpies of the studied reactions calculated by Eqs. (10) and (12) were reduced to standard temperature certain approximations were used and thermodynamic functions of the $SnWO_4$, SnW_2O_7, and Sn_2WO_5 molecules were only estimated. For these molecules we have carried out quantum-chemical calculations analogous to those fulfilled for $SnMoO_4$ and Sn_2MoO_5. Structures analogous to those of the appropriate molybdates correspond to the minima on the potential energy surfaces of $SnWO_4$ and Sn_2WO_5. Interatomic distances are as follows, Å: r(W–O_{cycl}) 1.90, r(W–O_{term}) 1.73, and r(Sn–O) 2.05, the angles are as follows, deg: $O_{cycl}WO_{cycl}$ 88.7, $O_{term}MoO_{term}$ 110.6, and OSnO 80.8. Normal vibration frequencies for $SnWO_4$ are 1009, 978, 737, 642, 557, 374, 331, 304, 256, 220, 198, and 91 cm^{-1}.

The structure of C_{2v} symmetry of the molecule Sn_2WO_5 presented in Fig. 1b has a minimal energy. Interatomic distances are as follows, Å: r(W–O_{cycl}) 1.87, r(Wo–O_{term}) 1.73, r(Sn–O) 2.02, and r(Sn–O') 1.96; the angles are as follows, deg: $O_{cycl}WO_{cycl}$ 106.6, $O_{term}WO_{term}$ 110.2, OSnO' 95.5, and SnO'Sn 147.2. Normal vibration frequencies for Sn_2WO_5 are 1005, 966, 816, 786, 626, 445, 416, 342, 326, 286, 279, 217, 203, 135, 134, 113, 56, and 24 cm^{-1}.

For the molecule SnW_2O_7 the structure presented on Fig. 1c has a minimal energy. Interatomic distances are as follows, Å: r(W–O_{cycl}) 1.87, r(W–O_{term}) 1.72, r(W–O') 1.91, and r(Sn–O) 2.01; the angles are as follows, deg: $O_{cycl}WO'$ 103.9, $O_{term}WO_{term}$ 109.0, WO'W 133.2, and OSnO 92.8. Normal vibration frequencies for SnW_2O_7 are 1024, 1021, 986, 983, 853, 841, 663, 487, 399, 376, 332, 330, 293, 278, 269, 211, 196, 187, 170, 123, 118, 61, 18, and 7 cm^{-1}.

Using the values of partial pressures of the vapor of molecular forms measured in [3] at 1318 K and the calculated thermodynamic functions of the molecules $SnWO_4$, SnW_2O_7, and Sn_2WO_5, we have calculated enthalpies of gas-phase reactions (13)–(18) involving gaseous tin tungstates by Eq. (10). The results obtained are presented in Table 2.

$$SnO + 1/3W_3O_9 = SnWO_4, \quad (13)$$

$$SnO + 2/3W_3O_9 = SnW_2O, \quad (14)$$

$$2SnO + 1/3W_3O_9 = Sn_2WO_5, \quad (15)$$

$$SnO + 0.25W_4O_{12} = SnWO_4, \quad (16)$$

$$SnO + 0.5W_4O_{12} = SnW_2O_7, \quad (17)$$

$$2SnO + 0.25W_4O_{12} = Sn_2WO_5, \quad (18)$$

$$WO_3 + 2/3W_3O_9 = W_3O_9, \quad (19)$$

$$WO_3 + 1/3W_3O_9 = W_2O_6. \quad (20)$$

In addition we have reduced the enthalpies of reactions (13)–(15) found in [3] by Eq. (12) to the standard temperature 298 K.

Table 2. Values of enthalpies of reactions (11, 12) involving gaseous tin tungstates

Reaction	T, K	$-\Delta_rH^0(T)$, kJ [3]	$-\Delta_rH^0(298)$, kJ [3]	$-\Delta_rH^0(298)$, kJ (our data)
(13)	1300	130.5 (12)	136.8 (12)	131.5 (12)
	1348	114.6 (11)	120.9 (11)	
	1318			107.3 (11)
(14)	1300	246.0 (12)	257.7 (12)	252.4 (12)
	1348	231.4 (11)	243.1 (11)	
	1318			188.3 (11)
(15)	1318			404.1 (11)
(16)	1318			74.4 (11)
(17)	1318			122.7 (11)
(18)	1318			369.3 (11)

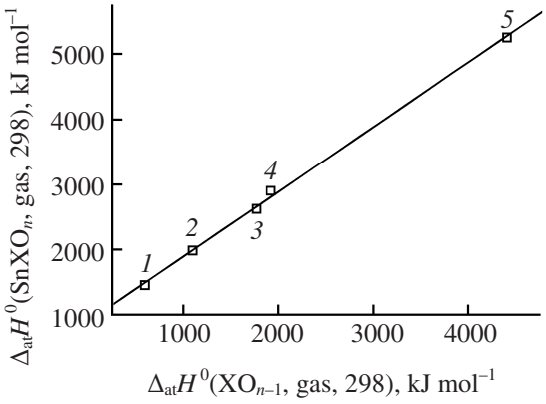

Fig. 2. Dependence of atomization enthalpies of gaseous tin(II) salts on atomization enthalpies of anion-forming oxides: (*1*) $SnPO_2$; (*2*) $SnPO_3$; (*3*) $SnMoO_4$; (*4*) $SnWO_4$; (*5*) SnW_2O_7.

The calculated values of enthalpies of gas-phase reactions (13), (14) considerably differ from the data in [3]. To reveal the reason of the discrepancies of these values, we have calculated entropies of reactions (13), (14) and have compared these data with the entropy changes for gas-phase reactions (19), (20), since it was accepted in the calculations of the enthalpies of reactions involving gaseous tin tungstates in [3] by Eq. (10) that entropy changes in reactions (13) and (18) are equal to those in reactions (14) and (20), respectively. Our calculations have shown that the entropy changes in reactions (13) and (18) at 1318 K differ by 12.9, and those in reactions (14) and (20), by 44.1 J K^{-1}. The entropy contributions $T\Delta_rS(T)$ to the Gibbs energies differ, respectively, by 16.8 and 57.3 kJ.

To construct dependence (11) for isocation series of gaseous tin(II) salts it is necessary to select the most reliable values of standard enthalpies of formation of gaseous $SnWO_4$ and SnW_2O_7. For this purpose it is necessary either to carry out a number of additional experimental determinations of enthalpies of reactions (13), (14) or to try to optimize the available data. In the second case it is possible to substitute in Eq. (11) the values of atomization enthalpies of tin gaseous salts which we have determined in the present work and in [2] in combination with the data obtained in [3] and the data which we calculated by Eq. (10) with the purpose of minimizing standard deviations. As a result the data found with the use of partial pressures of vapor of molecular forms measured in [3] at 1318 K and reduced to the standard temperature with the thermodynamic functions which we have calculated, appeared the most reliable.

The corrected values of the enthalpies of formation of gaseous $SnWO_4$, SnW_2O_7, and Sn_2WO_5 are –757, –1509, and –1031 kJ mol^{-1}, respectively.

The dependence of the atomization enthalpies of gaseous tin(II) salts on the atomization enthalpies of anion-forming oxides is presented in Fig. 2. Coefficients k and b in Eq. (11) are 0.994 ± 0.022 and 900 ± 53.

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