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Thermochemical Study of Gaseous Salts of Oxygen-containing Acids: XIX.[1] Nickel(II) Salts

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Abstract—Existence of gaseous salts formed by nickel oxide NiO was established, and their standard enthalpies of formation and atomization were determined.
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Nickel-containing composite materials are often exploited at high temperatures under oxidative conditions, when transfer of volatile components into vapor becomes essential and affects the composition and properties of the materials. The presently available information on possible forms of existence of gaseous oxygen-containing nickel compounds is restricted by the research into of NiO vaporization [2–4]. According to the data in these works, nickel oxide practically completely dissociates on heating with transfer of oxygen and atomic nickel into vapor. Therewith, the condense phase is impoverished with oxygen and comes to the composition NiO_{1-x}. Nickel oxide is present in the vapor only in the beginning of vaporization at a maximum partial pressure of oxygen. As for more complex oxygen-containing nickel compounds, it was shown in [5] that the vapor above lithium nickelate contains molecules of $LiNiO_2$ which can be considered as a salt formed by Li_2O and Ni_2O_3. The enthalpy of sublimation of lithium nickelate at 1491 K is 293 ± 5 kJ.

According to the reactivity criterion for gaseous oxides in the gas-phase synthesis of oxygencontaining salts, proposed in [6], nickel(II) oxide, by analogy with CrO, FeO, and CoO [1, 7–9], should have amphoteric properties and form two types of salts, acting as both an anion- and a cation-forming oxide. The purpose of this work was to obtain gaseous salts formed by nickel(II) oxide and to determine their thermodynamic properties.

Our preliminary experiments showed that, when nickel oxide(II) is heated up to 1850–1900 K in molybdenum or tungsten chambers, NiO is present in the vapor within first 2–3 min only. As the sample vaporizes further, the vapor contains nothing more than oxygen and atomic nickel. To increase the relative content of nickel in the vapor, we added into chambers silicon dioxide that dissociated according to Eq. (1) in the above-mentioned temperature range [10].

$$SiO_2(cr., l.) \rightleftarrows SiO_2(gas) + 0.5\ O_2(gas). \quad (1)$$

The liberated oxygen shifted the equilibrium of gas-phase reaction (2) to the left, thus much increasing the partial pressure of NiO.

$$NiO \rightleftarrows Ni + 0.5O_2. \quad (2)$$

The addition of silicon dioxide into the chamber favored not only increased NiO content in the vapor, but also formation of gaseous molybdenum(VI) or tungsten(VI) oxides, respectively, as well as synthesis of gaseous nickel(II) molybdates and tungstates. Gaseous barium nickelate $BaNiO_2$ was synthesized by heating mixtures of BaO, NiO, and SiO_2 in molybdenum chambers, and nickel phosphates, by vaporization of NiO and $MgHPO_4$ from a double two-temperature chamber that made it possible to synthesize salts from oxides much differing in volatility [11]. In the latter case, NiO placed in a ceramic beaker and a pressure standard (gold) were loaded in the upper compartment of the chamber, and magnesium hydrophosphate that dissociates on heating into PO and PO_2 [12], in the lower compartment.

The mass spectra of the vapor over the samples contained the following ions: system NiO–SiO_2–Mo(W): NiO^+, SiO^+, XO^+, XO_2^+, XO_3^+, and $NiXO_4^+$; (hereinafter, X = Mo, W); system NiO–$MgHPO_4$: Ni^+, NiO^+, PO^+, PO_2, $NiPO_2^+$, and $NiPO_3^+$; and system

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

$NiO–SiO_2–BaO$: Ni^+, NiO^+, SiO^+, Ba^+, BaO^+, XO_2^+, XO_3^+, $BaXO_3^+$, $BaXO_4$, and $BaNiO_2$. The ratio of ion currents depended on temperature and vaporization time.

To determine the nature of ions in the mass spectrum, we measured their appearance energies by recording ionization efficiency curves. The appearance energies were (+0.5 eV): 7.6 (Ni^+), 9.2 (NiO^+), 10.0 (WO_2^+), 11.7 (WO_3^+), 9.5 (MoO_2^+), 12.1 (MoO_3^+), 10.6 (SiO^+), 8.3 (PO^+), 11.2 (PO_2^+), 13+2 ($NiMoO_4^+$), 9.1 ($NiPO_2^+$), 10.0 ($NiPO_3^+$), 6.5 (BaO^+), 5.6 (Ba^+), and 12 ± 2 ($BaNiO_2^+$). The appearance energies of Ni^+, NiO^+, XOd^+, XO_3^+, PO^+, BA^+, and BaO^+ coincided with the ionization energies of the corresponding molecules and atoms within the measurement accuracy [13]. The appearance energies of $NiMoO_4^+$, $NiPO_2^+$, $NiPO_3^+$, and $NiBaO_2^+$ were measured for the first time. The resulting values are in a good agreement with the earlier determined appearance energies of chromium [7], manganese [14, 15], iron [8, 9], and cobalt [1] molybdates and phosphates and also of barium ferrate and cobaltate [1, 8, 9], which points to the molecular origin of the ions. We did not measure appearance energies for the $NiWO_4^+$ ion because of its low intensity. Nevertheless, by analogy with chromium [7], manganese [14], and iron [9] tungstates, we suggest that the $NiWO_4^+$ ions to originate from direct ionization of the $NiWO_4$ molecules.

Analysis of the vapor mass spectra, dependences of ion currents on vaporization time and temperature, and measured appearances energies of ions allow us to state that the vapor formed on the vaporization of mixtures of nickel and silicon oxides from molybdenum or tungsten chambers comprises the molecules NiO, XO_2, XO_3, SiO, and $NiXO_4$ and atomic nickel. The vapor over the $NiO–MgHPO_4$ system contains nickel phosphates $NiPO_2$ and $NiPO_3$ along with gaseous NiO, PO, and PO_2, as well as atomic nickel, whereas the vapor over the $NiO–SiO_2–BaO$ mixture in the temperature range under study contains atomic nickel and barium, their oxides BaO and NiO, and barium nickelate $BaNiO_2$.

To find the standard enthalpies of formation of the gaseous salts formed by nickel(II) oxide, we determined the equilibrium constants of gas-phase reactions (3)–(6).

$$NiO + XO_3 \rightleftarrows NiXO_4, \quad (3)$$

$$NiO + PO_2 \rightleftarrows NiPO_3, \quad (4)$$

$$NiO + PO \rightleftarrows NiPO_2, \quad (5)$$

$$BaO + NiO \rightleftarrows BaNiO_2. \quad (6)$$

Table 1. Partial pressures and enthalpies of reaction (3) for molecular species in the vapor over the $NiO–SiO_2$ system evaporated from molybdenum and tungsten chambers

T, K	p, atm			$-\Delta_r H^0(0)$, kJ
	NiO, $\times 10^7$	MoO_3, $\times 10^5$	$NiMoO_4$, $\times 10^8$	
1881	4.06	0.21	0.08	373.2
1878	11.46	6.89	4.14	364.1
1876	11.45	5.69	2.67	359.0
1871	7.14	3.73	1.70	363.0
1914	9.25	4.89	2.23	365.8
1918	7.32	3.21	1.74	371.9
1836	4.90	2.93	2.49	374.5
1834	5.34	2.46	1.59	368.6
1826	4.43	3.06	1.58	366.5
1825	4.43	2.92	1.80	369.0
1813	4.54	2.90	1.57	364.3
1849	6.28	3.52	2.74	371.9
1849	5.83	3.33	2.51	372.6
1850	5.09	2.77	1.83	372.8
1858	1.95	2.64	0.46	368.6
1898	7.83	4.19	2.81	375.6
			Average	373 ± 5
	NiO, $\times 10^7$	WO_3, $\times 10^6$	$NiWO_4$, $\times 10^8$	
1854	7.00	2.93	7.74	457.2
1864	5.18	3.64	6.22	457.6
1866	2.69	4.34	4.05	458.8
1862	2.59	5.03	3.42	453.5
1862	1.53	12.30	4.66	452.6
1854	1.24	13.17	5.57	455.7
1862	1.02	7.19	3.11	460.9
1892	4.42	1.88	2.29	461.4
1878	1.29	3.97	2.85	469.1
1875	0.58	3.11	0.57	459.4
1890	8.61	0.81	2.54	465.4
1887	2.34	1.80	1.27	461.6
1890	1.50	2.68	0.63	452.2
			Average	458.9 ± 4.9

The enthalpies of these reactions were calculated by Eq. (7).

$$\Delta_r H^0(0) = T[\Delta_r \Phi^0(T) - R\ln K_e(T)]. \quad (7)$$

Here $\Delta_r H^0(0)$ and $\Delta_r \Phi^0(T)$ are the enthalpy and reduced Gibbs energy of the reaction at the temperatures 0°C and T, respectively; R, gas constant; and K_e, equilibrium constant of the reaction. The partial pressures of molecular species in the vapor over the systems and the enthalpies of reactions (3)–(6) are given in Tables 1–3.

Table 2. Partial pressures over the NiO–$MgHPO_4$ system and enthalpies of reactions (4) and (5)

T, K	*p*, atm					$-\Delta_r H^0(0)$, kJ	
	NiO, $\times 10^5$	PO, $\times 10^5$	PO_2, $\times 10^5$	$NiPO_2$, $\times 10^6$	$NiPO_3$, $\times 10^6$	Eq. (4)	Eq. (5)
1757	3.23	17.74	1.83	0.66	0.30	340.8	388.6
1771	2.82	21.42	2.4	0.72	0.46	344.1	395.7
1787	2.16	19.44	2.22	0.42	0.38	344.5	401.8
1689	3.56	8.78	5.12	2.46	1.74	354.6	382.4
1694	3.84	7.88	4.85	1.99	2.01	353.1	385.2
1695	3.76	6.20	3.71	1.58	2.75	353.8	394.0
1703	3.50	5.81	4.01	1.34	1.76	355.0	389.4
1703	3.59	4.84	2.87	0.96	1.41	352.4	390.6
1687	3.10	4.93	2.98	0.95	1.48	350.8	389.2
1687	2.64	3.88	2.20	0.88	1.13	355.4	391.9
1700	2.94	3.37	2.29	0.83	1.23	357.7	394.0
1677	4.57	4.84	5.33	2.03	3.74	354.2	386.3
1681	4.25	3.85	4.71	1.81	3.12	357.6	387.5
1687	3.94	3.50	4.47	1.70	3.29	360.5	391.4
1687	4.26	2.99	4.86	1.59	3.29	360.6	389.1
1693	3.29	2.96	4.10	1.37	2.99	363.5	395.1
1692	3.78	2.81	3.84	1.48	3.14	363.2	394.6
1692	3.62	2.76	3.59	1.37	2.98	362.9	395.4
1691	3.78	2.74	3.67	1.37	2.51	362.2	391.8
1703	3.48	2.30	3.40	1.15	2.37	366.0	396.1
1700	3.31	2.39	3.43	1.14	2.37	365.5	395.9
1692	3.24	2.40	3.33	1.10	2.04	363.4	392.7
1693	3.13	2.29	3.38	1.14	2.36	365.3	395.3
					Average	356 ± 7.1	391.9 ± 4.3

Table 3. Partial pressures of molecular species in the vapor over the NiO–BaO–SiO_2 system and enthalpies of reaction (6)

T, K	*p*, atm			$-\Delta_r H^0(0)$, kJ
	NiO, $\times 10^8$	BaO, $\times 10^6$	$BaNiO_2$, $\times 10^8$	
1915	3.45	0.90	0.47	421.5
1918	2.66	0.71	0.31	423.6
1990	3.86	2.18	0.98	433.4
1822	7.87	0.55	3.36	426.1
1848	10.41	1.62	5.45	418.6
1854	4.52	2.35	3.76	421.3
1856	4.88	1.79	3.76	424.8
1819	3.37	0.88	2.17	420.8
1868	8.33	2.05	6.14	420.9
1872	9.05	2.61	5.47	415.0
1879	13.97	4.43	5.14	400.5
1889	12.64	3.26	4.48	406.8
1884	8.75	3.50	4.47	410.4
1930	14.71	5.00	3.40	401.9
			Average	418 ± 10

The thermodynamic functions of gaseous oxides, required for calculation of reaction enthalpies and their reduction to the standard temperature of 298 K were taken from the reference books [16, 17]. The thermodynamic functions of gaseous nickel salts were calculated by statistical thermodynamics methods in the rigid rotor–harmonic oscillator approximation. Therewith, the structure, interatomic distances, and normal mode frequencies of the anionic groups XO_4, PO_3, and PO_2 were transferred from the corresponding molecules of alkaline-earth metals [18].

For gaseous salts $NiXO_4$, $NiPO_3$, and $NiPO_2$ we carried out quantum-chemical calculations of structures and vibration spectra. The calculations were carried out using the GAMESS program package [19] by the *ab initio* SCF method. The computational technique has been described in detail in [1, 7, 9, 14, 20]. The calculated molecular parameters of $NiXO_4$ salts are given in Tables 4 and 5. The Ni–O interatomic distance was accepted to be 1.89 Å on the basis of the calculations. The normal mode frequencies of the Ni–O group (510, 259, and 109 cm^{-1}) were taken from data for nickel molybdate.

Table 4. Geometric parameters of gaseous nickel salts[a]

Molecule	r(Ni–O), Å	r(X–O_{cycl}), Å	r(X–O_{term}), Å	∠OXO_{cycl}, deg	∠OXO_{term}, deg
$NiMoO_4$	1.872	1.878	1.676	88.6	110.7
$NiWO_4$	1.880	1.870	1.695	88.8	11.7
$NiPO_3$	2.113	1.490	1.432	106.6	126.7
$NiPO_2$	2.090	1.509	–	103.6	–
$CaNiO_2$	1.669	2.187	–	108.7	–

[a] O_{cycl} is an oxygen atom in a cycle, and O_{term} is a terminal oxygen atom.

To determine molecular parameters of $BaNiO_2$, we carried out a quantum-chemical study of its structural analog $CaNiO_2$. For this molecule a planar structure of C_{2v} symmetry has a minimum energy. It represents a planar tetragon with bidentate nickel and calcium atoms. As the multiplicity of the ground state of $CaNiO_2$ is one, we used the Møller–Plesset second-order perturbation theory for calculations [21]. The calculated interatomic distances are as follows, Å: r(Ni–O) 1.669 and r(Ca–O) 2.187. The ONiO angle is 108°. The calculated Ca–O interatomic distance coincides with the respective interatomic distances in calcium molybdate and tungstate [18]. The corresponding normal mode frequencies are 772, 747, 596, 460, 283, and 116 cm^{-1}.

According to data in Table 4, the nickel–oxygen bond length in calcium nickelate is shorter than in nickel molybdate, tungstate, and phosphates, which points to different valence states of nickel in gaseous salts where nickel acts as a cation- or an anion-forming element. This conclusion is also supported by the fact that the effective charge of the nickel atom in $CaNiO_2$ is, on average, higher by 0.2 e than in $NiPO_2$, $NiPO_3$, $NiMoO_4$, and $NiWO_4$.

The resulting standard enthalpies of formation and atomization of gaseous salts formed by NiO are given in Table 6.

As shown earlier [22], the atomization enthalpy of a gaseous salt in an isocationic series of gaseous salts of oxygen-containing acids linearly depends on the atomization enthalpy of a gaseous anion-forming oxide [Eq. (8)].

$$\Delta_{at}H^0(M_nXO_n,\ \text{gas},\ 298) = k\Delta_{at}H^0(XO_{n-1},\ \text{gas},\ 298) + b. \quad (8)$$

On the basis of our present data we constructed the corresponding dependence for the isocationic series of gaseous nickel salts (see figure) and determined the coefficients k and b in Eq. (8), $1.03l \pm 0.25$ and 727 ± 36, respectively. The high regression coefficient (0.9994) and small standard deviation (26.65) point to reliability of the data obtained. The resulting atomization enthalpy of gaseous barium nikelate also nicely fits the dependence for the isocationic series of barium salts in [22].

Table 6 lists the standard enthalpies of atomization and formation, calculated by Eq. (8) for certain gaseous nickel salts that should be stable according to the criterion in [6].

Our present data together with those reported in [1, 7–9, 14, 15, 20] make it possible to compare the reactivities of gaseous nickel oxide and other 3*d* element oxides in the synthesis of gaseous salts of oxygen-containing acids. In the series MnO–CrO–FeO–CoO–NiO, nickel(II) oxide has the highest average orbital electronegativity [6]. As a result, all gaseous salts in which nickel oxide acts as a cation-forming oxide have the lowest thermal stability and enthalpy of formation compared with analogous salts of manganese, chromium, iron, and cobalt. The existence of gaseous salts $MnXO_4$, $MnXO_3$, $CrXO_4$, and $CrXO_3$ formed by reactions of manganese and chromium oxides with molybdenum and tungsten oxides XO_2 and XO_3 was proved experimentally in [7, 20]. Iron, cobalt, and nickel oxides react with the same

Table 5. Normal mode frequencies (cm^{-1}) of gaseous nickel salts $NiXO_4$, and their assignment

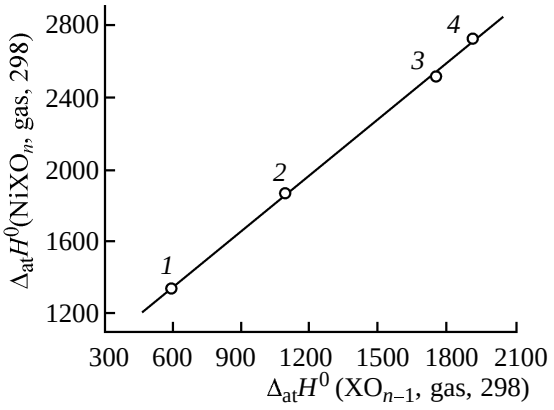
$NiMoO_4$	$NiWO_4$	Assignment
109.4	99.2	Torsion Ni–O_{cycl}–X–O_{term}
258.5	230.3	Torsion O_{cycl}–X–O_{term}–O_{term}
277.2	279.8	Bending O_{cycl}–X–O_{cycl}, asym.
287.4	281.7	Bending O_{term}–X–O_{cycl}, sym.
354.6	349.0	Bending O_{term}–X–O_{term}
390.5	368.2	Bending O_{term}–X–O_{term}
510.0	503.0	Bending O_{cycl}–Ni–O_{cycl}
665.7	657.9	Bending O_{cycl}–Ni–O_{cycl}
706.9	696.9	Bending O_{cycl}–Ni–O_{cycl}
787.8	783.6	Bending O_{cycl}–Ni–O_{cycl}
1075.2	1301.2	Stretching X–O_{term}, asym.
1110.0	1336.2	Stretching X–O_{term}, sym.

Table 6. Standard entropies and enthalpies of formation and atomization of gaseous salts formed by nickel(II) oxide[a]

Salt	$-\Delta_f H^0(298)$, kJ mol^{-1}	$-\Delta_{at} H^0(298)$, kJ mol^{-1}	$S^0(298)$, J kmol^{-1}
$NiWO_4$	479 ± 17	2754 ± 18	346.4
$NiMoO_4$	432 ± 19	2513 ± 20	356.9
$NiPO_3$	375 ± 13	1868 ± 13	309.1
$NiPO_2$	86 ± 10	1330 ± 7	296.5
$BaNiO_2$	243 ± 15	1348 ± 15	340.9
$NiMoO_3$	102	1935	–[b]
$NiWO_3$	61	2088	–
$NiVO_3$	321	2014	–
$NiTiO_3$	413	2062	–
$NiNbO_3$	295	2194	–
$NiTaO_3$	269	2227	–
$NiBO_2$	65	1556	–
NiB_2O_4	969	3524	–
$CaNiO_2$	159	1263	–
$SrNiO_2$	201	1288	–

[a] Values calculated by Eq. (8) are printed italic. [b] Standard entropies were not calculated for gaseous salts whose existence is not proved experimentally.

anion-forming oxides to yield nothing more than $FeXO_4$ [8, 9], $CoXO_4$ [1], and $NiXO_4$. To estimate the relative content of NiWO in the reaction mixture of NiO, WO_2, and $NiWO_3$, we estimated the partial pressure of $NiWO_3$. The resulting value is $\sim 1 \times 10^{-9}$ atm, which is lower by an order of magnitude than the partial pressures of $MnWO_3$ and $CrWO_3$ at the same pressures of MnO, CrO and WO_2. Gaseous salts $NiMoO_3$ and $NiWO_3$ were not found in the vapor over the $NiO–SiO_2$ mixture evaporated from molybdenum and tungsten chambers, as the estimated partial pressures of these salts are beyond the lower sensitivity limit of the mass spectrometer.



Atomization enthalpies of gaseous nickel salts vs. atomization enthalpies of gaseous anion-forming oxides. (*1*) $NiPO_2$, (*2*) $NiPO_3$, (*3*) $NiMoO_4$, and (*4*) $NiWO_4$.

With gaseous salts in which CrO, FeO, CoO, and NiO act as anion-forming oxides, the dependences of the thermal stability and relative content of their salts in vapor on the position of the metal in the 3*d* element series is not so unambiguous. The standard enthalpies of formation of barium nickelate, cobaltate [1], and ferrate [8, 9] coincide with each other within measurement accuracy, but they are lower in absolute values than the enthalpy of formation of barium chromate [7]. Barium salts are thermally more stable than calcium and strontium salts, as the enthalpies of formation of barium cobaltates, ferrates, and chromates are higher in absolute values than the enthalpies of the corresponding calcium and strontium salts. We failed to synthesize gaseous calcium and strontium nickelates because of the low NiO content in the vapor, even at increased partial pressure of oxygen.

EXPERIMENTAL

The work was carried out on an MS-1301 mass spectrometer at the electron ionizing energy 25 eV. Samples were evaporated from single and double molybdenum and tungsten effusion chambers and also from a double two-temperature molybdenum chamber [11]. The chambers were heated by electron bombardment, the temperature was measured with an EOP-66 optical pyrometer. The partial pressures of vapor components were determined by comparison of ion currents, using gold as a pressure standard [23]. The ionization cross sections were calculated by the additivity method [24], and those of gaseous salts were multiplied by 0.7 [25]. To determine the molecular composition of the vapor, the appearance energies of ions in the mass spectrum were determined by the method of vanishing ion current, using the ionization energies of gold and nickel as standards [13]. The instrument was preliminarily calibrated by CaF_2 vapor pressure [16].

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