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FREE ENERGY FUNCTIONS FOR GASEOUS MONOXIDES

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June 1960

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ABSTRACT

Free energy functions for gaseous monoxides have been calculated from presently available spectroscopic results. However, the electronic contributions to the free energy functions have been estimated. A simple ionic model has been assumed since the molecular electronic states for most of these oxides are not known. In some instances where experimental data are insufficient to calculate the interatomic distances and the equilibrium frequencies of vibrations, they have been estimated. The results of these calculations are tabulated for 500° intervals from room temperature up to 3000°K.

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In predicting the stability of refractory oxides at high temperatures, thermodynamic data for both the condensed and gaseous phases at these temperatures will be of great help. An ideal situation will be tabulations of accurate thermodynamic functions for all oxides. Unfortunately, presently available experimental data are insufficient to do a thorough job of calculating these thermodynamic functions. Hence, one has to estimate them in many cases. For such estimates, different investigators have used different approximations and it is not always quite clear what approximations have been made in their calculations. Also, the combination of thermodynamic functions calculated by different methods introduces unnecessary errors.

Even though the presently available experimental data are insufficient for accurate calculations of thermodynamic quantities for all oxides, tabulation of self-consistent, though approximate, thermodynamic functions for the oxides would eliminate many of these difficulties.

In recent years, such compilations of thermodynamic data for elements,¹ for condensed oxides^{2,3} etc., have been published. Brewer⁴ has calculated the dissociation energies for gaseous metal monoxides. Because of the importance of gaseous monoxides in the vaporization of metal oxides and as a continuation of similar programs in this laboratory, free energy functions of the gaseous monoxides are calculated from the available spectroscopic data. Results are tabulated for 500° intervals from room temperature up to 3000°K.

Emission spectra for many of these diatomic molecules have been analyzed and the molecular constants have been evaluated. The excellent compilation of Rosen⁵ et al, covers the literature survey up to 1951. Recently, Sutton⁶ et al, published a comprehensive report on the internuclear distances. Liberal use of these tabulations of the molecular constants have been made in these calculations. In spite of voluminous reported results in the literature for diatomic molecular spectra, estimates of r_e and ω_e values had to be made for a number of oxides. The method of estimation is fairly simple and straightforward.

A. Calculation of Electronic Contributions

Experimental results to fix the molecular electronic states of these oxides are lacking, particularly so in case of transition metal oxides. In many instances even the ground state is not firmly established. Hence the electronic contribution to the partition function has to be estimated in almost all cases. A simple ionic model approximation has been assumed in calculating the free energy functions.

To make the calculation uniform, only estimated values for the electronic contributions to the free energy functions are employed for all oxides. It is assumed that the molecular states may be approximated by the energy levels of the corresponding +2 metal ions and that the approach of an oxide ion causes no drastic perturbations. The electronic partition functions are thus approximated by the electronic partition functions of the free gaseous ions. Electronic partition functions are calculated from the energy levels of the corresponding cations (+2) taken from Moore's tabulation.⁷ Table 1 contains the results of these calculations.

B. Calculation of Rotational and Vibrational Contributions

In calculating rotational and vibrational partition functions, r_e and ω_e values are taken from References (5) and (6) whenever available. But for a number of oxides, rotational analysis of spectra are incomplete and hence r_e values have to be estimated. Where the ω_e values for the molecules are available, interatomic distances are approximated by Badger's rule⁸ from the force constant data. In a few cases, both r_e and ω_e values are estimated by interpolating between the neighboring molecules in the periodic table of elements. The r_e and ω_e values employed in this calculation are given in Table 2. The ground state values of r_e and ω_e were also used for the excited electronic states.

So far, there have been no experimental results for any of the alkali oxides. All molecular constants are estimated. In evaluating electronic contributions to free energy functions, a modification in the method of estimating is made. Instead of approximating the molecular levels with those of the +2 cations, it is approximated with the energy levels of O^- ion or its isoelectronic fluorine atom. Thus both the alkali metal and oxygen are considered to be in oxidation states of +1 and -1, respectively.

Tables 3 and 4 contain the rotational and vibrational contribution to the free energy function of oxides respectively. The calculation of translation contribution is simple and straightforward. Table 5 contains these results. The total free energy functions for the gaseous monoxides are given in Table 6.

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Table 1

$$- \left(\frac{F_T^{\circ} - H_o^{\circ}}{T} \right)_{\text{ele}} \quad \text{for oxides in e.u.}$$

Temp °K	298°	1000°	1500°	2000°	2500°	3000°
LiO [†]	3.3	3.3	3.3	3.3	3.3	3.3
BeO	0	0	0	0	0	0
BO	1.38	1.38	1.38	1.38	1.38	1.38
CO	0	0	0	0	0	0
NaO [†]	3.3	3.3	3.3	3.3	3.3	3.3
MgO	0	0	0	0	0	0
AlO	1.38	1.38	1.38	1.38	1.38	1.38
SiO	0	0	0	0	0	0
KO [†]	3.3	3.3	3.3	3.3	3.3	3.3
CaO	0	0	0	0	0	0
ScO	3.7	4.3	4.3	4.4	4.4	4.5
TiO	4.3	5.3	5.6	5.7	5.8	5.8
VO	4.4	5.8	6.0	6.2	6.3	6.3
CrO	3.9	5.5	5.8	5.9	6.0	6.1
MnO	3.6	3.6	3.6	3.6	3.6	3.6
FeO	4.6	5.4	5.7	5.8	6.0	6.0
CoO	3.2	5.2	5.5	5.7	5.8	6.0
NiO	4.4	4.6	4.9	5.0	5.2	5.3
CuO	3.6	3.7	3.7	3.8	4.0	4.0
ZnO	0	0	0	0	0	0
GaO	1.38	1.38	1.38	1.38	1.38	1.38
GeO	0	0	0	0	0	0
RbO [†]	3.3	3.3	3.3	3.3	3.3	3.3
SrO	0	0	0	0	0	0
YO	2.8	3.6	3.9	4.0	4.1	4.2
ZrO	3.3	4.3	4.7	5.0	5.2	5.3
NbO	2.9	4.4	4.9	5.3	5.5	5.7
MoO*	(3.2)	(3.2)	(3.2)	(3.2)	(3.2)	(3.2)
RuO	4.4	4.7	5.0	5.3	5.4	5.6
RhO	4.6	4.7	4.8	5.0	5.2	5.3
PdO	4.4	4.4	4.5	4.6	4.7	4.8
AgO	3.6	3.6	3.6	3.6	3.6	3.7
CdO	0	0	0	0	0	0
InO	1.38	1.38	1.38	1.38	1.38	1.38

(continued)

Table 1:
(continued)

$$- \left(\frac{F_T^O - H_O^O}{T} \right)_{\text{ele}} \quad \text{for oxides in e.u.}$$

Temp °K	298°	1000°	1500°	2000°	2500°	3000°
SnO	0	0	0	0	0	0
CsO [†]	3.3	3.3	3.3	3.3	3.3	3.3
BaO	0	0	0	0	0	0
LaO	2.8	3.0	3.3	3.5	3.7	3.8
HfO	3.1	3.1	3.1	3.1	3.1	3.1
TaO*	(4.1)	(4.1)	(4.1)	(4.1)	(4.1)	(4.1)
WO*	(3.2)	(3.2)	(3.2)	(3.2)	(3.2)	(3.2)
ReO*	(3.6)	(3.6)	(3.6)	(3.6)	(3.6)	(3.6)
OsO	4.4	4.4	4.4	4.4	4.4	4.4
IrO	4.4	4.4	4.4	4.4	4.4	4.4
PtO	4.4	4.4	4.4	4.4	4.4	4.4
AuO	3.6	3.6	3.6	3.6	3.6	3.6
HgO	0	0	0	0	0	0
TlO	1.38	1.38	1.38	1.38	1.38	1.38
PbO	0	0	0	0	0	0
BiO	1.38	1.38	1.38	1.38	1.38	1.38

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* Estimated by comparing the other elements of the same group. No analysis of electronic levels for M⁺² ions are given.

† Estimated assuming M⁺O⁻ and using F levels for O⁻ as described in text.

Table 2

The interatomic distances and ω_e values for oxides

Molecules	r_e	ω_e	Reference No.†
	$\text{\AA}^\circ$	cm^{-1}	
LiO*	1.41	1320	
BeO	1.3308	1487.3	
BO	1.2049	1885.4	
CO	1.12819	2170.2	
NO	1.1503	1903.68	
O ₂	1.2074	1580.36	
NaO*	1.76	758	
MgO	1.749	785.1	
AlO	1.6176	978.2	
SiO	1.509	1242	
PO	1.4488	1230.6	
SO	1.4933	1123.7	
KO*	2.1	670	
CaO	1.822	732.1	
ScO†	1.62	971.55	
TiO	1.620	1008.1	
VO	1.590	1012.3	(9)
CrO	1.627	897.5	(10)
MnO†	1.67	840.7	
FeO†	1.65	880	
CoO*	1.65	875	
NiO*	1.64	875	
CuO†	1.79	628	
ZnO*	1.74	680	
GaO†	1.65	767.7	
GeO	1.651	985.7	
AsO†	1.60	966.6	
SeO†	1.616	907.1	
RbO*	2.2	561	
SrO	1.940	653.5	
YO†	1.77	852.5	
ZrO	1.728	936.5	(6)
NbO†	1.691	838	(11)
MoO*	1.73	840	
TcO*	1.77		
RuO*	1.77	820	
RhO*	1.775	819	
PdO*	1.78	815	
AgO†	1.98	493	
CdO*	1.85	550	
InO†	1.83	703.1	
SnO	1.838	822.4	
SbO†	1.81	817.2	
TeO†	1.823	785.2	
CsO*	2.26	488	
BaO	1.940	669.8	

(continued)

Table 2

(continued)

The interatomic distances and ω_e values for oxides			
<u>Molecules</u>	r_e <u>Å</u>	ω_e <u>cm⁻¹</u>	<u>Reference No.[‡]</u>
LaO†	1.88	811.6	
HfO*	1.74	895	(12)
TaO†	1.827	926	(13)
WO*	1.78	803	(14)
ReO*	1.82	760	
OsO*	1.85	785	
IrO*	1.85	785	
PtO*	1.855	785	
AuO*	2.08	416	
HgO*	1.95	478	
TlO*	1.93	664	
PbO	1.922	721.8	
BiO†	1.93	693.2	
PoO*	1.94		

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*both r_e and ω_e are estimated by extrapolation

†the values of r_e or ω_e are estimated using Badger's rule

‡Except for the references noted here, the rest of the data are taken from Rosen and Sutton, References (5) and (6).

Table 3

$$- \left(\frac{F_T^O - H_O^O}{T} \right)_{\text{rot}} \text{ for oxides}$$

Temp °K	298°	1000°	1500°	2000°	2500°	3000°
LiO*	9.49	11.89	12.70	13.27	13.71	14.07
BeO	9.61	12.01	12.82	13.39	13.83	14.19
BO	9.44	11.84	12.65	13.22	13.66	14.02
CO	9.30	11.70	12.51	13.08	13.52	13.88
NaO*	11.70	14.10	14.91	15.48	15.92	16.28
MgO	11.72	14.12	14.93	15.50	15.94	16.30
AlO	11.49	13.89	14.70	15.27	15.71	16.07
SiO	11.24	13.64	14.45	15.02	15.46	15.82
PO	11.14	13.54	14.35	14.92	15.36	15.72
SO	11.25	13.65	14.46	15.03	15.47	15.83
KO*	12.77	15.17	15.98	16.55	16.99	17.35
CaO	12.22	14.62	15.43	16.00	16.44	16.80
ScO [†]	11.81	14.21	15.02	15.59	16.03	16.39
ThO	11.84	14.24	15.05	15.62	16.06	16.42
VO	11.80	14.20	15.01	15.58	16.02	16.38
CrO	11.90	14.30	15.11	15.68	16.12	16.48
MnO [†]	12.03	14.43	15.24	15.81	16.25	16.61
FeO [†]	11.99	14.39	15.20	15.77	16.21	16.57
CoO*	12.01	14.41	15.22	15.79	16.23	16.59
NiO*	11.94	14.34	15.15	15.72	16.16	16.52
CuO [†]	12.36	14.76	15.57	16.14	16.58	16.94
ZnO*	12.29	14.69	15.50	16.07	16.51	16.87
GaO [†]	12.08	14.48	15.29	15.86	16.30	16.66
GeO [†]	12.09	14.50	15.31	15.88	16.32	16.68
AsO [†]	11.78	14.38	15.19	15.76	16.20	16.56
SeO [†]	12.04	14.44	15.25	15.82	16.26	16.62
RbO*	13.37	15.77	16.58	17.15	17.59	17.95
SrO	12.76	15.16	15.97	16.54	16.98	17.34
YO [†]	12.44	14.84	15.65	16.22	16.66	17.02
ZrO	12.35	14.75	15.56	16.13	16.57	16.93
NbO	12.27	14.67	15.48	16.05	16.49	16.85
MoO*	12.38	14.78	15.59	16.16	16.60	16.96
RuO*	12.48	14.88	15.69	16.26	16.70	17.06
RhO*	12.50	14.90	15.71	16.28	16.72	17.08
PdO*	12.50	14.91	15.72	16.29	16.73	17.09
AgO [†]	12.94	15.34	16.15	16.72	17.16	17.52
CdO*	12.48	15.08	15.89	16.46	16.90	17.26
InO [†]	12.64	15.04	15.85	16.42	16.86	17.22
SnO	12.67	15.07	15.88	16.45	16.89	17.25
SbO [†]	12.61	15.01	15.82	16.39	16.83	17.19

(continued)

Table 3
(continued)

$$- \left(\frac{F_T^{\circ} - H_o^{\circ}}{T} \right)_{\text{rot}} \quad \text{for oxides}$$

Temp °K	298°	1000°	1500°	2000°	2500°	3000°
TeO†	12.65	15.05	15.86	16.43	16.87	17.24
CsO*	13.52	15.92	16.73	17.30	17.74	18.10
BaO	12.91	15.32	16.12	16.69	17.14	17.50
LaO†	12.79	15.19	16.00	16.57	17.01	17.37
HfO*	12.53	14.93	15.74	16.31	16.75	17.12
TaO*	12.73	15.13	15.94	16.51	16.95	17.31
WO*	12.62	15.03	15.83	16.41	16.85	17.21
ReO*	12.71	15.12	15.92	16.50	16.94	17.30
OsO*	12.78	15.18	16.00	16.56	17.00	17.37
IrO*	12.78	15.19	16.00	16.57	17.00	17.37
PtO*	12.80	15.20	16.01	16.58	17.02	17.38
AuO*	13.27	15.67	16.48	17.05	17.49	17.85
HgO*	13.06	15.46	16.27	16.84	17.28	17.64
TlO*	12.96	15.36	16.17	16.74	17.18	17.55
PbO	12.94	15.35	16.15	16.73	17.17	17.53
BiO†	12.96	15.37	16.17	16.74	17.19	17.55
PoO*	12.99	15.39	16.20	16.77	17.21	17.57
RaO*	13.08	15.48	16.29	16.86	17.30	17.67
AcO*	12.96	15.36	16.17	16.74	17.18	17.54
ThO	12.96	15.36	16.17	16.74	17.18	17.54
UO*	12.96	15.36	16.16	16.73	17.17	17.53

* r_e are estimated by comparing with the neighbors.

† r_e obtained from Badger rule approximation of force constant.

Table 4

$- \left(\frac{F_T^O - H_O^O}{T} \right)_{\text{vib}} \text{ for oxides}$						
Temp °K	298	1000	1500	2000	2500	3000
LiO*	0	.32	.66	.97	1.25	1.51
BeO	0	.25	.55	.83	1.10	1.34
BO	0	.14	.36	.59	.82	1.03
CO	0	.09	.26	.47	.67	.87
NO	0	.13	.35	.59	.81	1.02
NaO*	.05	.81	1.31	1.72	2.01	2.30
MgO	.05	.78	1.26	1.67	2.01	2.30
AlO	.02	.56	.99	1.36	1.68	1.95
SiO	.00	.36	.72	1.05	1.34	1.59
PO	.01	.37	.73	1.06	1.35	1.61
SO	.01	.42	.81	1.14	1.44	1.71
KO*	.08	.95	1.49	1.92	2.27	2.57
CaO	.06	.85	1.36	1.77	2.12	2.42
ScO	.02	.56	.99	1.37	1.69	1.97
TiO	.02	.53	.95	1.32	1.63	1.91
VO	.02	.53	.95	1.31	1.62	1.90
CrO	.03	.64	1.09	1.48	1.81	2.09
MnO	.04	.70	1.18	1.57	1.90	2.19
FeO	.03	.66	1.12	1.50	1.84	2.12
CoO*	.03	.66	1.13	1.51	1.84	2.14
NiO*	.03	.66	1.13	1.51	1.84	2.14
CuO	.10	1.03	1.58	2.01	2.37	2.68
ZnO*	.08	.94	1.45	1.89	2.25	2.51
GaO	.05	.80	1.30	1.70	2.05	2.34
GeO	.02	.55	.98	1.35	1.66	1.94
AsO	.02	.57	1.00	1.37	1.69	1.97
SeO	.03	.63	1.08	1.46	1.79	2.07
RbO*	.14	1.17	1.74	2.20	2.57	2.86
SrO	.09	.98	1.52	1.95	2.31	2.61
YO	.03	.69	1.16	1.55	1.88	2.17
ZrO	.02	.60	1.04	1.42	1.74	2.02
NbO	.04	.71	1.18	1.57	1.91	2.20
MoO*	.04	.71	1.18	1.57	1.91	2.19
RuO*	}	.04	.73	1.21	1.61	1.93
RhO*						
PdO*						
AgO	.19	1.35	1.93	2.40	2.78	3.10
CdO*	.15	1.20	1.76	2.22	2.59	2.93
InO	.07	.90	1.42	1.84	2.19	2.49
SnO	.04	.73	1.20	1.60	1.94	2.23
SbO	.04	.73	1.21	1.61	1.95	2.24
TeO	.05	.78	1.27	1.67	2.01	2.30

(continued)

Table 4
(continued)

$- \left(\frac{F_T^{\circ} - H_o^{\circ}}{T} \right)_{\text{vib}} \text{ for oxides}$						
Temp °K	298	1000	1500	2000	2500	3000
CsO*	.20	1.36	1.95	2.58	2.80	3.11
BaO	.08	.95	1.48	1.91	2.27	2.57
LaO	.04	.74	1.22	1.62	1.96	2.25
HfO*	.03	.64	1.11	1.47	1.80	2.10
TaO*	.03	.64	1.09	1.47	1.80	2.08
WO*	.04	.75	1.23	1.64	1.98	2.28
ReO*	.05	.81	1.31	1.72	2.06	2.37
OsO*	.05	.78	1.26	1.68	2.01	2.34
IrO*						
PtO*						
AuO*	.3	1.58	2.20	2.67	3.08	3.38
HgO*	.21	1.38	1.98	2.46	2.84	3.14
TlO*	.08	0.97	1.51	1.93	2.28	2.59
PbO	.06	.87	1.38	1.80	2.15	2.44
BiO	.07	.92	1.44	1.86	2.21	2.51

* Estimated ω_e values by comparing with neighbors.

Table 5

$$\left(\frac{F_T^{\circ} - H_O^{\circ}}{T} \right)_{\text{translation}} \quad \text{for oxides}$$

Temp °K	298	1000	1500	2000	2500	3000
LiO	30.36	36.38	38.39	39.82	40.93	41.83
BeO	30.62	36.63	38.65	40.08	41.19	42.09
BO	30.83	36.84	38.86	40.29	41.39	42.30
CO	30.96	36.97	38.99	40.41	41.52	42.43
NO	31.07	37.08	39.09	40.51	41.63	42.54
NaO	31.95	37.96	39.97	41.40	42.51	43.42
MgO	32.05	38.06	40.07	41.50	42.61	43.52
AlO	32.24	38.25	40.26	41.69	42.80	43.71
SiO	32.31	38.32	40.34	41.77	42.88	43.78
PO	32.50	38.51	40.53	41.96	43.07	43.97
SO	32.57	38.58	40.60	42.03	43.13	44.04
KO	32.97	38.99	41.00	42.43	43.53	44.44
CaO	33.03	39.04	41.06	42.48	43.59	44.50
ScO	33.28	39.30	41.31	42.73	43.84	44.75
TiO	33.41	39.43	41.44	42.87	43.98	44.89
VO	33.55	39.57	41.58	43.01	44.12	45.03
CrO	33.60	39.62	41.63	43.06	44.17	45.07
MnO	33.73	39.74	41.76	43.18	44.29	45.20
FeO	33.76	39.78	41.79	43.22	44.33	45.24
CoO	33.89	39.91	41.92	43.35	44.45	45.35
NiO	33.88	39.90	41.91	43.34	44.45	45.35
CuO	34.07	40.08	42.10	43.53	44.64	45.54
ZnO	34.14	40.15	42.17	43.59	44.70	45.61
GaO	34.29	40.31	42.32	43.75	44.86	45.76
GeO	34.39	40.40	42.42	43.85	44.96	45.86
AsO	34.47	40.48	42.50	43.92	45.03	45.94
SeO	34.60	40.61	42.63	44.05	45.16	46.07
RbO	34.79	40.81	42.82	44.25	45.36	46.26
SrO	34.86	40.87	42.89	44.31	45.42	46.33
YO	34.89	40.91	42.92	44.35	45.46	46.36
ZrO	34.95	40.97	42.98	44.41	45.52	46.42
NbO	35.00	41.02	43.03	44.46	45.57	46.47
MoO	35.08	41.10	43.11	44.54	45.65	46.55
RuO	35.23	41.25	43.26	44.69	45.79	46.70
RhO	35.27	41.28	43.30	44.72	45.83	46.74
PdO	35.36	41.38	43.39	44.82	45.93	46.83
AgO	35.38	41.41	43.42	44.85	45.96	46.86
CdO	35.49	41.51	43.52	44.95	46.06	46.96
InO	35.54	41.56	43.57	45.00	46.11	47.01
SnO	35.64	41.65	43.67	45.10	46.21	47.11
SbO	35.71	41.72	43.74	45.16	46.27	47.18

(continued)

Table 5
(continued)

$$- \left(\frac{F_T^{\circ} - H_O^{\circ}}{T} \right)_{\text{translation}} \quad \text{for oxides}$$

Temp ^o K	298	1000	1500	2000	2500	3000
TeO	35.83	41.84	43.86	45.29	46.40	47.30
CsO	35.93	41.95	43.96	45.39	46.50	47.40
BaO	36.03	42.04	44.06	45.48	46.59	47.50
LaO	36.05	42.07	44.08	45.51	46.62	47.52
CeO	36.08	42.10	44.11	45.54	46.65	47.55
SmO	36.27	42.29	44.30	45.73	46.84	47.74
EuO	36.29	42.31	44.32	45.75	46.86	47.76
GdO	36.38	42.40	44.41	45.84	46.95	47.85
LuO	36.66	42.68	44.69	46.13	47.24	48.14
HfO	36.73	42.75	44.76	46.19	47.30	48.20
TaO	36.77	42.79	44.80	46.23	47.34	48.24
WO	36.81	42.83	44.84	46.27	47.38	48.28
ReO	36.85	42.87	44.88	46.31	47.42	48.32
OsO	36.90	42.92	44.93	46.36	47.47	48.37
IrO	36.95	42.97	44.98	46.41	47.52	48.42
PtO	36.98	42.99	45.01	46.44	47.55	48.45
AuO	37.00	43.02	45.03	46.46	47.57	48.47
HgO	37.05	43.07	45.08	46.51	47.62	48.52
TlO	37.11	43.12	45.14	46.56	47.67	48.58
PbO	37.15	43.16	45.17	46.60	47.71	48.62
BiO	37.17	43.18	45.20	46.63	47.74	48.64
PoO	37.18	43.20	45.21	46.64	47.75	48.65
RaO	37.38	43.40	45.41	46.84	47.95	48.86
AcO	37.39	43.41	45.42	46.85	47.96	48.87
ThO	37.46	43.48	45.49	46.92	48.03	48.94
UO	37.52	43.54	45.55	46.98	48.09	49.00

Table 6

Estimated - $\left(\frac{F_T^O - H_O^O}{T} \right)$ in cal/deg mole for gaseous metallic diatomic oxides

Temp °K	298	1000	1500	2000	2500	3000
LiO*	43.2	51.9	55.1	57.4	59.2	60.7
NaO*	47.0	56.2	59.5	61.9	63.8	65.3
MgO	43.8	53.0	56.3	58.7	60.6	62.1
KO*	49.1	58.4	61.8	64.2	66.1	67.7
CaO	45.3	54.5	57.9	60.3	62.2	63.7
ScO†	48.8	58.4	61.6	64.1	66.0	67.7
TiO	49.6	59.5	63.0	65.5	67.5	69.0
VO	49.8	60.1	63.5	66.1	68.1	69.7
CrO	49.4	60.1	63.6	66.0	68.1	69.8
MnO†	49.4	58.5	61.8	64.2	66.2	67.6
FeO	50.4	60.2	63.9	66.3	68.4	69.9
CoO	49.1	60.2	63.8	66.4	68.3	70.1
NiO	50.3	59.5	63.1	65.6	67.7	69.4
CuO†	50.1	59.5	62.9	65.5	66.6	69.1
ZnO*	46.5	55.8	59.1	61.5	63.4	65.0
GaO†	47.8	57.0	60.3	62.7	64.6	66.1
RbO*	51.6	61.1	64.4	67.0	68.8	70.4
SrO	47.7	57.0	60.4	62.8	64.7	66.3
YO	50.2	60.1	63.6	66.2	68.1	69.8
ZrO	50.6	60.6	62.7	67.0	69.0	70.6
NbO	50.1	60.8	64.6	67.4	69.6	71.2
MoO*	52.1	61.2	64.4	66.8	68.7	70.3
RuO*	52.2	61.6	65.2	67.9	69.7	71.6
RhO*	52.3	61.6	65.0	67.6	69.8	71.4
PdO*	52.3	61.4	64.8	67.3	69.3	71.0
AgO†	52.1	61.7	65.2	67.6	69.6	71.2
CdO*	48.3	57.8	61.2	63.6	65.6	67.2
InO†	49.6	58.9	62.2	64.6	66.5	68.1
CsO*	53.0	62.5	65.9	68.6	70.3	71.9
LaO†	51.7	61.6	64.5	67.2	69.3	71.0
HfO*	52.4	61.4	64.7	67.1	69.0	70.5
TaO*	53.6	62.7	65.9	68.3	70.2	71.7
WO*	52.7	61.8	65.1	67.5	69.4	71.0
ReO*	53.2	62.4	65.7	68.1	70.0	71.6
OsO*	54.1	63.3	66.6	69.0	70.9	72.5
IrO*	54.2	63.3	66.6	69.1	70.9	72.5
PtO*	54.2	63.3	66.7	69.09	71.0	72.5
AuO*	54.2	63.9	67.3	69.8	71.7	73.3
HgO*	50.3	69.9	63.3	65.8	67.7	69.3
TlO*	51.5	60.8	64.2	66.61	68.5	70.1
BiO†	51.6	60.9	64.2	66.6	68.5	70.1

* r_e are estimated by comparing with the neighbors.

† r_e are obtained from Badger rule approximation of force constant.

Table 6a

Gaseous MO free energy functions known to better than 0.1 cal/deg mole

$$- \left(\frac{F_T^O - H_O^O}{T} \right) \text{ for MO(g)}$$

Temp °K	<u>298</u>	<u>1000</u>	<u>1500</u>	<u>2000</u>	<u>2500</u>	<u>3000</u>
AlO	45.13	54.11	57.38	59.77	61.66	63.23
BO	41.66	50.21	53.26	55.51	57.30	58.79
BaO	49.02	58.31	61.66	64.08	66.00	67.57
BeO	40.24	48.92	52.06	54.37	56.20	57.72
CO	40.25	48.77	51.78	53.99	55.75	57.23
ClO	47.04	56.14	59.46	61.88	63.79	65.38
GeO	46.50	55.45	58.71	61.10	62.97	64.52
HO	36.82	45.39	48.30	50.41	52.11	53.52
NO	42.98	51.86	54.96	57.24	59.04	60.55
OO	42.06	50.70	53.81	56.10	57.94	59.48
PbO	50.16	59.38	62.71	65.13	67.03	68.59
SO	46.03	54.87	58.09	60.43	62.30	63.85
SiO	43.55	52.32	55.51	57.84	59.70	61.25
SnO	48.35	57.47	60.77	63.19	65.09	66.65

The values for AlO, BO, BeO, CO, ClO, HO, NO, O₂, and SO are taken from Appendix 7 of Pitzer and Brewer, "Thermodynamics," McGraw-Hill, N. Y. (1961).

Most of the values in Table 6a are slightly larger at high temperatures than the values obtained from Tables 1 - 5 due to inclusion of anharmonic and stretching terms.

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