

# Thermodynamic Functions for Molecular Oxygen in the Ideal Gas State

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The thermodynamic functions for molecular oxygen in the ideal gas state have been calculated using recent values of physical and spectroscopic constants. Values of  $C_p^\circ$ ,  $H^\circ - E_0^\circ$ ,  $-(F^\circ - E_0^\circ)/T$ , and  $S^\circ$  are given, directly calculated or interpolated, for every twenty degrees up to 700°K and for every hundred degrees up to 5,000°K.

## I. Introduction

A table of thermodynamic functions for molecular oxygen based on the latest spectroscopic data and values of physical constants was desired. Simple adjustment of the values published by Johnston and Walker [1, 2]<sup>1</sup> seemed inadequate because of the complexity of the changes to be made in the spectroscopic constants. The new table is based entirely on newly computed values.

## II. Spectroscopic Constants

The spectroscopic data used by Johnston and Walker have been revised to conform to the results of Curry and Herzberg [3] and Schlapp [4] for the ground state. For the  $^1\Delta_g$  state, the constants used are based on the recent values of Herzberg and Herzberg [5]. Constants for the  $^1\Sigma_v^+$  state and the  $^3\Sigma_u^-$  state have been taken from the tables of Sponer [6]. For the  $^3\Sigma_u^+$  state, approximate values of spectroscopic constants were selected, using a tentative identification of the Herzberg bands [7] proposed by Swings [8]. Several minor spectroscopic constants have been obtained with Dunham's formulas [9]. The improved theory of the ground state given by Schlapp introduces a slight shift in the calculated value of the unobserved lowest level. As this is the level to which all other levels are referred for purposes of thermochemical calculations, numerical values are altered slightly for all electronic states.

<sup>1</sup> Figures in brackets indicate the literature references at the end of this paper.

For states of diatomic molecules for which no splitting occurs due to spin or orbital interaction, the sum of electronic, vibrational, rotational, and vibrational-rotational interaction energies may be represented in wave numbers by the power series

$$W = \sum_{j,k} Y_{jk} \left(v + \frac{1}{2}\right)^j K^k (K+1)^k, \quad (1)$$

using the notation of Dunham. Each electronic state has its own set of  $Y_{jk}$ 's. The electronic energy can be considered as represented by  $Y_{00}$ , the vibrational by

$$\sum_{j=1} Y_{j0} \left(v + \frac{1}{2}\right)^j,$$

and the sum of rotational and rotational-vibrational interaction energy by

$$\sum_{j=0, k=1} Y_{jk} \left(v + \frac{1}{2}\right)^j K^k (K+1)^k.$$

The vibrational quantum number,  $v$ , can assume any integral value, and the rotational quantum number,  $K$ , can assume various integral values. For a homonuclear molecule, such as  $O_2^{16}$ , there are half as many rotational states as for a comparable heteronuclear molecule. The ground state of  $O_2^{16}$  is a  $^3\Sigma_u^-$  state with odd values of  $K$ . For the ground state, spin interactions are important, and triplet splitting occurs with the  $F_1$  and  $F_3$  components, averaging about  $2 \text{ cm}^{-1}$  lower than the  $F_2$  component. The results of an adequate theoretical treatment of the splitting have been given by Schlapp, including inter-

actions neglected in the original treatment of Kramers [10]. The term values of the  $F_1$ ,  $F_2$ , and  $F_3$  components with  $J=K+1$ ,  $K$ , and  $K-1$ , respectively, are given by the formulas

$$W_{K+1} = W_0 + (2K+3)B - \lambda - \frac{[(2K+3)^2 B^2 + \lambda^2 - 2\lambda B]^{\frac{1}{2}} + \mu(K+1)}{2},$$

$$W_K = W_0, \quad (2)$$

$$W_{K-1} = W_0 - (2K-1)B - \lambda + \frac{[(2K-1)^2 B^2 + \lambda^2 - 2\lambda B]^{\frac{1}{2}} - \mu K}{2},$$

with  $B = 1.438 \text{ cm}^{-1}$ ,  $\lambda = 1.985 \text{ cm}^{-1}$ , and  $\mu = -0.008 \text{ cm}^{-1}$ .  $W_0$  is given by eq 1 with constants listed below for the  $^3\Sigma_g^-$  state. In accord with these equations, the lowest state is the  $F_3$  level for  $K=1$  and is  $3.96 \text{ cm}^{-1}$  below the corresponding  $F_2$  level, or  $1.09 \text{ cm}^{-1}$  below the non-existent  $K=0$  level.

For the  $^1\Delta_g$  state, a double weighting due to  $\Lambda$  doubling provides single levels for both odd and even values of  $K$ , with levels beginning at  $K=1$ , the value of  $\Lambda$ . For the  $^1\Sigma_g^+$  state,  $K$  has even values.

The states and spectroscopic constants used for  $O_2^{16}$  are

$^3\Sigma_g^-$  (ground state)

$$\begin{array}{ll} Y_{00} = -786.08 \text{ cm}^{-1} & Y_{01} = 1.4456 \text{ cm}^{-1} \\ Y_{10} = 1580.36 \text{ cm}^{-1} & Y_{11} = -0.0158 \text{ cm}^{-1} \\ Y_{20} = -12.073 \text{ cm}^{-1} & Y_{02} = -4.838 \times 10^{-6} \text{ cm}^{-1} \\ Y_{30} = 0.0546 \text{ cm}^{-1} & Y_{12} = -4.96 \times 10^{-9} \text{ cm}^{-1} \\ Y_{40} = -0.00143 \text{ cm}^{-1} & Y_{03} = 0.1387 \times 10^{-12} \text{ cm}^{-1} \\ & Y_{04} = -32.2 \times 10^{-18} \text{ cm}^{-1} \end{array}$$

$^1\Delta_g$

$$\begin{array}{ll} Y_{00} = 7132.1 \text{ cm}^{-1} & Y_{01} = 1.4264 \text{ cm}^{-1} \\ Y_{10} = 1509.3 \text{ cm}^{-1} & Y_{11} = -0.0171 \text{ cm}^{-1} \\ Y_{20} = -12.9 \text{ cm}^{-1} & Y_{02} = -4.86 \times 10^{-6} \text{ cm}^{-1} \end{array}$$

$^1\Sigma_g^+$

$$\begin{array}{ll} Y_{00} = 12409.2 \text{ cm}^{-1} & Y_{01} = 1.4014 \text{ cm}^{-1} \\ Y_{10} = 1432.615 \text{ cm}^{-1} & Y_{11} = -0.0188 \text{ cm}^{-1} \\ Y_{20} = -13.925 \text{ cm}^{-1} & Y_{02} = -5.36 \times 10^{-6} \text{ cm}^{-1} \end{array}$$

$^3\Sigma_u^+$

$$\begin{array}{ll} Y_{00} = 35,385 & Y_{40} = -0.099 \\ Y_{10} = 791.5 & Y_{01} = 1.13 \\ Y_{20} = -20.83 & Y_{11} = -0.06 \\ Y_{30} = 0.83 & Y_{02} = -9 \times 10^{-6} \end{array}$$

$^3\Sigma_u^-$

$$\begin{array}{ll} Y_{00} = 49,007 & Y_{01} = 0.820 \\ Y_{10} = 709.57 & Y_{11} = -0.014 \\ Y_{20} = -10.708 & \end{array}$$

Corresponding spectroscopic constants were obtained for lower states of the heteronuclear  $O^{16}-O^{17}$  and  $O^{16}-O^{18}$  molecules, for which both odd and even rotational levels are present in each state.

### III. Method of Calculation

The thermodynamic functions for the ideal gas state at atmospheric pressure are obtained from the partition function  $Q$  by evaluating the formulas

$$\frac{H^\circ - E_0^\circ}{RT} = \frac{T}{Q} \frac{dQ}{dT} + \frac{5}{2} \quad (3)$$

$$-\frac{(F^\circ - E_0^\circ)}{RT} = \ln Q + \frac{3}{2} \ln M + \frac{5}{2} \ln T - 3.6644 \quad (4)$$

$$\frac{S^\circ}{R} = \frac{H^\circ - E_0^\circ}{RT} - \frac{F^\circ - E_0^\circ}{RT} \quad (5)$$

$$\frac{C_p^\circ}{R} = \frac{T^2}{Q} \frac{d^2Q}{dT^2} - \left[ \frac{T}{Q} \frac{dQ}{dT} - 1 \right]^2 + \frac{7}{2} \quad (6)$$

where  $T$  is temperature in degrees K;  $M$  is the molecular weight on the chemical scale, 31.9913 for  $O_2$ , 32.9955 for  $O^{16}-O^{17}$ , and 33.9956 for  $O^{16}-O^{18}$ ; and  $Q$ , the partition function, or state sum, is given by  $pe^{-\epsilon/kT}$ , where  $p=2J+1$  and  $\epsilon=hcW$ . The contributions of the different electronic states are included by evaluating  $Q = Q_1 + Q_2 + Q_3 + \dots$  and its derivatives, where  $Q_1$  is for the  $^3\Sigma_g^-$  state,  $Q_2$  for the  $^1\Delta_g$  state,  $Q_3$  for the  $^1\Sigma_g^+$  state, etc.

In evaluating the  $Q$ 's, or values of  $\sum(2J+1)e^{-hcW/kT}$ , the [rotational energy is separated from the rest of the energy  $W$ , and the sum over rotation levels is expressed in terms of an integral. In this way it is found that the functions  $Q_i$  and their derivatives are given by the formulas

$$Q_i = g \sum f e^{-x} \quad (7)$$

$$T \frac{dQ_i}{dT} = g [\sum T f' e^{-x} + \sum f x e^{-x}] \quad (7a)$$

$$\begin{aligned} T^2 \frac{d^2Q_i}{dT^2} = & g [\sum T^2 f'' e^{-x} + 2 \sum T f' x e^{-x} \\ & - 2 \sum f x e^{-x} + \sum f x^2 e^{-x}], \end{aligned} \quad (7b)$$

where  $x$  is  $G_v hc/kT$ , with  $G_v$  representing the sum of electronic and purely vibrational energy in  $\text{cm}^{-1}$ , and where the summation extends over all vibrational levels up to dissociation.  $G_v$  is thus that part of the total energy that is completely

independent of the rotational quantum number, and is given by

$$\sum_{j=0}^{\infty} Y_{j0} \left( v + \frac{1}{2} \right)^j$$

or its equivalent expressed as a polynomial in  $v$ .

$$f = \frac{4}{315} \frac{c_2^2 B_v^2}{T^2} + \frac{1}{15} \frac{c_2 B_v}{T} + \frac{1}{3} + \frac{T}{c_2 B_v} + \frac{T^2}{c_2^2} \left( -\frac{2D_v}{B_v^3} \right) + \frac{T^3}{c_2^3} \frac{12D_v^2 - 6B_v F_v}{B_v^5} + \frac{T^4}{c_2^4} \frac{120B_v D_v F_v - 24B_v^2 H_v - 120D_v^3}{B_v^7} \dots, \quad (8)$$

with  $c_2 = hc/k$ , as in the derivation given in reference [11]. Convergence difficulties discussed in that paper for the hydrogens do not occur for such molecules as  $O_2$ . The spectroscopic constants  $B_v$ ,  $D_v$ ,  $F_v$ , and  $H_v$ , are given by  $\sum_{j=0}^{\infty} Y_{jk} (v + 1/2)^j$ , with  $k$  taking the values 1, 2, 3, and 4, respectively.

$g$  is an average weight factor in addition to the factor  $2J+1$  typical for the rotational levels of a simple rotating vibrator. For each electronic state, the quantity  $f$ , and its temperature derivatives,  $f'$  and  $f''$ , are functions of  $T$  and  $v$  obtained from

In using the above expressions, the vibrational energy,  $G_v$ , is ordinarily to be evaluated with respect to the lowest level of the ground state. The partition function for the ground state, including the effect of triplet splitting, as detailed in eq. 2, may be represented as

$$\begin{aligned} Q_1 &= \sum_v \left\{ f_e + [e^{-hc(2\lambda + \mu - 2B)/kT} + 2e^{-hc(\lambda + 5\mu/2 - 2B)/kT}] \sum_{K=1,3,\dots} (2K+1) e^{-\frac{hcW}{KT}} \right\} \\ &= \sum_v \left\{ f_e + \left[ \frac{1}{3} e^{-hc(2\lambda + \mu - 2B)/kT} + \frac{2}{3} e^{-hc(\lambda + 5\mu/2 - 2B)/kT} \right] \frac{3}{2} f_0 \right\} \\ &= \sum_v \left\{ f_e + e^{-hc(4\lambda/3 + 2\mu - 2B)/kT} \cdot \frac{3}{2} f_0 \left[ 1 + \frac{1}{9} \left( \frac{hc}{kT} \right)^2 (\lambda - 3\mu/2)^2 - \frac{1}{81} \left( \frac{hc}{kT} \right)^3 (\lambda - 3\mu/2)^3 + \dots \right] \right\} \\ &= e^{-hc(4\lambda/3 + 2\mu - 2B)/kT} \frac{3}{2} \sum_v \left\{ \frac{2}{3} f_e \left[ 1 + \frac{hc}{kT} (4\lambda/3 + 2\mu - 2B) + \dots \right] \right. \\ &\quad \left. + f_0 \left[ 1 + \frac{1}{9} \left( \frac{hc}{kT} \right)^2 (\lambda - 3\mu/2)^2 - \frac{1}{81} \left( \frac{hc}{kT} \right)^3 (\lambda - 3\mu/2)^3 \dots \right] \right\} \quad (9) \end{aligned}$$

$f_0$  represents the partition function that would be obtained for the ground state if the triplet splitting were negligibly small, and energies were reckoned from  $K=0$ .  $f_e$  is a small correction term to which the only significant contribution above very low temperatures comes from the  $K=1$  levels:

$$f_e = 5e^{-\frac{hc}{kT} [5B - (25B^2 + \lambda^2 - 2\lambda B)^{1/2} + \lambda + 3\mu - 2B]} + 1 - 6e^{-\frac{hc}{kT} [\lambda + 5\mu/2 - 2B]} = \frac{1.963}{T} - \frac{1.48}{T^2} + \dots \quad (10)$$

Equation 9 shows that the effect of the triplet splitting is most readily included for ordinary and elevated temperatures by introducing a small additive correction  $4\lambda/3 + 2\mu - 2B$ , or  $-0.244 \text{ cm}^{-1}$ , in the vibrational energy formula for the ground state and introducing small correction terms in the formula for  $f$  to take account of its trends toward lower temperatures.

Evaluation of the expressions as far as appears justified with the present data gives the following for the various states for  $O_2^6$ .

$${}^3\Sigma_v^- \text{ state, } g = \frac{3}{2}$$

$$\begin{aligned} G_v &= -0.244 + 1568.33v - 11.993v^2 + 0.0517v^3 - 0.00143v^4 \\ f &= -\frac{1.232}{T^2} + \frac{1.8902}{T} + \frac{1}{3} + (0.483562 + 0.005311v)T + (1.5746 \cdot 10^{-6} + 0.0535 \cdot 10^{-6}v)T^2 + 14.89 \cdot 10^{-12}T^3 + 267 \cdot 10^{-18}T^4. \end{aligned}$$

$${}^1\Delta_g \text{ state, } g = 1$$

$$\begin{aligned} G_v &= 7883.5 + 1496.4v - 12.9v^2 \\ f &= \frac{1}{3} + (0.49033 + 0.00599v)T + 1.709 \cdot 10^{-6}T^2 \quad (11) \end{aligned}$$

$${}^1\Sigma_v^+ \text{ state, } g = \frac{1}{2}$$

$$G_v = 13122 + 1418.69v - 13.925v^2$$

$$f = \frac{1}{3} + (0.49944 + 0.006837v)T + 1.921 \cdot 10^{-6}T^2$$

$${}^3\Sigma_u^+ \text{ state, } g = \frac{3}{2}$$

$$G_v = 35776 + 771.2v - 19.74v^2 + 0.63v^3 - 0.099v^4$$

$$f = \frac{1}{3} + 0.632T/(1 - 0.0545v) + 6 \times 10^{-6}T^2$$

$${}^3\Sigma_u^- \text{ state, } g = \frac{3}{2}$$

$$G_v = 49359 + 698.86v - 10.708v^2$$

$$f = \frac{1}{3} + (0.855 + 0.0145v)T$$

The values used for  $R$  and  $hc/k$  were 1.98714 (defined) cal deg<sup>-1</sup>mole<sup>-1</sup> and 1.4384 deg cm, respectively.

For all electronic states treated, each summation over rotational levels for a given vibrational level was broken off at the top of the predissociation region applying to the vibrational level, by using a suitable upper limit in the integration given in reference [11]. This complicating restriction, which requires special treatment, is significant only at the highest temperatures.

The contributions of the several electronic states to the partition function and its derivatives for O<sub>2</sub><sup>16</sup> are listed in tables 1, 2, and 3. These values may facilitate any future revision of thermodynamic functions for oxygen if new spectroscopic data make it desirable. It is thought that in general these sums and their derivatives have been carried to more digits than correspond to the accuracy of the spectroscopic data. This is particularly the case for the <sup>1</sup>Δ<sub>g</sub> state for which the anharmonicity constant has not been determined experimentally. The values given in brackets are the additional contributions that would be obtained if the rotational sums were extended to infinite energy as has been customary instead of limiting them to the region of quantized levels. These additional contributions are given to more decimal places than were used for the entire sums because of possible theoretical interest in their magnitudes. The information necessary for a satisfactory calculation of the state sums for the vibrational states near the dissociation limit is not available. An analysis of the problem has been started in connection with this paper and previous work [11] and may be completed in a future publication.

TABLE 1. Values of  $Q$  for O<sub>2</sub><sup>16</sup>

Temperature	<sup>3</sup> Σ <sub>g</sub> <sup>-</sup> (Q <sub>1</sub> )	<sup>1</sup> Δ <sub>g</sub> (Q <sub>2</sub> )	<sup>1</sup> Σ <sub>g</sub> <sup>+</sup> (Q <sub>3</sub> )	<sup>3</sup> Σ <sub>u</sub> <sup>+</sup> (Q <sub>4</sub> )	<sup>3</sup> Σ <sub>u</sub> <sup>-</sup> (Q <sub>5</sub> )	Total (Q)
°K						
100	73.344					73.344
200	145.931					145.931
300	218.705					218.705
400	292.374					292.374
600	447.681					447.681
800	620.90	0.00				620.90
1,000	816.90	.01				816.91
1,250	1097.27	.09				1097.36
1,500	1418.91	.51	0.00			1419.42
1,750	1783.03	1.90	.01			1784.94
2,000	2190.46	5.26	.06			2195.78
2,500	3138.02	23.52	.61			3162.15
3,000	4266.61	68.37	2.96	0.00		4337.94
4,000	7086.4	293.7	23.97	.04	0.00	7404.1
	[.02]	[.01]	[.004]	[.024]		
5,000	10690.4	784.8	93.8	.76	.02	11569.8
	[.47]	[.24]	[.12]	[.66]		

TABLE 2. Values of  $TdQ/dT$  for O<sub>2</sub><sup>16</sup>

Temperature	<sup>3</sup> Σ <sub>g</sub> <sup>-</sup> (TQ <sub>1</sub> )	<sup>1</sup> Δ <sub>g</sub> (TQ <sub>2</sub> )	<sup>1</sup> Σ <sub>g</sub> <sup>+</sup> (TQ <sub>3</sub> )	<sup>3</sup> Σ <sub>u</sub> <sup>+</sup> (TQ <sub>4</sub> )	<sup>3</sup> Σ <sub>u</sub> <sup>-</sup> (TQ <sub>5</sub> )	Total (TQ)
°K						
100	72.551					72.551
200	145.272					145.272
300	219.098					219.098
400	298.152					298.152
600	489.366	0.000				489.366
800	736.328	.005				736.333
1,000	1041.33	.08				1041.41
1,250	1503.77	.91	0.00			1504.68
1,500	2056.30	4.62	.02			2060.94
1,750	2699.56	15.22	.17			2714.95
2,000	3434.68	38.16	.71			3473.55
2,500	5186.33	146.06	5.66			5338.05
3,000	7324.29	377.28	23.81	0.0		7725.38
	[.002]	[.001]				
4,000	12819.6	1370.2	157.6	.6	0.0	14348.0
	[.3]	[.14]	[.07]	[.4]		
5,000	20050.9	3267.1	534.2	8.8	.4	23861.4
	[6.3]	[3.2]	[1.6]	[8.9]		

The calculations which have been described were for O<sub>2</sub><sup>16</sup>. Thermodynamic functions for ordinary oxygen may be obtained from those for O<sub>2</sub><sup>16</sup> by making small adjustments in the values. In the naturally occurring mixture of isotopic oxygen, 99.526 percent of the molecules are O<sub>2</sub><sup>16</sup>, 0.394 percent are O<sup>16</sup>-O<sup>18</sup>, and 0.080 percent are O<sup>16</sup>-O<sup>17</sup>, according to the isotope data given by Birge [12]. The tables of Gordon and Barnes [13] were used in calculating the minute changes in the thermodynamic functions due to the

presence of isotopic molecules and for some other calculations for which the tables were advantageous. The contribution to  $S^\circ$  and to  $-(F^\circ - E_0^\circ)/T$  due to the presence of both odd and even rotational levels in  $O^{16}-O^{17}$  and  $O^{16}-O^{18}$  amounts to  $0.0065 \text{ cal deg}^{-1} \text{ mole}^{-1}$  in the final table. The entropy of mixing of isotopes, amounting to  $0.0677 \text{ cal deg}^{-1} \text{ mole}^{-1}$ , was not included. Similarly, no entropy of nuclear spin has been included. The quantities that were added to the thermodynamic functions for  $O_2^{16}$  to obtain values for the isotope mixture are given in table 4.

TABLE 3. Values of  $T^2 d^2 Q/dT^2$  for  $O_2^{16}$

Temperature ° K	${}^3\Sigma_g^-$ ( $T^2 Q_1''$ )	$\Delta_g$ ( $T^2 Q_2''$ )	${}^1\Sigma_g^+$ ( $T^2 Q_3''$ )	${}^3\Sigma_u^-$ ( $T^2 Q_4''$ )	${}^1\Sigma_u^-$ ( $T^2 Q_5''$ )	Total ( $T^2 Q'$ )
100	0.108					0.108
200	.466					.466
300	7.523					7.523
400	35.539	0.000				35.539
600	164.969	.001				164.970
800	367.677	.061				367.738
1,000	628.33	.91	0.00			629.24
1,250	1033.40	7.85	.03			1041.28
1,500	1530.12	33.43	.30			1563.85
1,750	2123.25	95.23	1.75			2220.23
2,000	2817.34	211.16	6.54			3035.04
2,500	4525.96	662.84	42.32	0.0		5231.12
3,000	6691.38	1469.47	150.44	.1	0.0	8311.39
	[.03]	[.02]	[.01]	[.1]		
4,000	12544.2	4278.8	772.6	7.6	.2	17603.4
	[4.0]	[2.1]	[1.1]	[5.6]		
5,000	20662.3	8769.0	2174.1	83.3	5.2	31693.9
	[72.5]	[37.4]	[18.9]	[104.5]		

TABLE 4. Increments to functions for  $O_2^{16}$  to obtain functions for the naturally occurring isotope mixture

T	$C_p^\circ$	$(H^\circ - E_0^\circ)$	$-(F^\circ - E_0^\circ)/T$	
° K	cal deg <sup>-1</sup> mole <sup>-1</sup>	cal mole <sup>-1</sup>	cal deg <sup>-1</sup> mole <sup>-1</sup>	cal deg <sup>-1</sup> mole <sup>-1</sup>
100	0	0.013	0.00770	0.00783
200	0	.013	.00776	.00782
300	0.00005	.015	.00779	.00784
400	.00011	.023	.00780	.00786
600	.00017	.053	.00783	.00792
800	.00016	.09	.00785	.00796
1,000	.00013	.12	.00788	.00800
1,250	.00010	.14	.00790	.00801
1,500	.00007	.16	.00792	.00802
1,750	.00006	.18	.00794	.00804
2,000	.00005	.20	.00795	.00805
2,500	.00003	.22	.00797	.00806
3,000	.00002	.23	.00799	.00807
4,000	.00002	.25	.00801	.00807
5,000	.00001	.26	.00802	.00807

TABLE 5. Thermodynamic functions for the natural isotopic mixture of molecular oxygen in the standard ideal gas state at 20-degree intervals up to 700° K

T	$C_p^\circ$	$H^\circ - E_0^\circ$	$-(F^\circ - E_0^\circ)/T$	$S^\circ$
° K	cal deg <sup>-1</sup> mole <sup>-1</sup>	cal mole <sup>-1</sup>	cal aeg <sup>-1</sup> mole <sup>-1</sup>	cal deg <sup>-1</sup> mole <sup>-1</sup>
20	6.984	136.39	23.373	30.193
40	6.964	275.81	28.130	35.025
60	6.960	415.03	30.930	37.848
80	6.958	554.20	32.922	39.850
100	6.958	693.36	34.469	41.402
120	6.958	832.52	35.733	42.671
140	6.958	971.67	36.803	43.743
160	6.958	1110.85	37.730	44.672
180	6.959	1250.0	38.547	45.492
200	6.961	1389.2	39.279	46.225
220	6.966	1528.5	39.941	46.889
240	6.974	1667.9	40.546	47.495
260	6.986	1807.4	41.102	48.054
280	7.002	1947.3	41.618	48.572
300	7.023	2087.6	42.097	49.056
320	7.050	2228.3	42.547	49.510
340	7.080	2369.6	42.969	49.938
360	7.115	2511.5	43.368	50.344
380	7.154	2654.2	43.745	50.730
400	7.196	2797.7	44.104	51.098
420	7.240	2942.1	44.445	51.450
440	7.286	3087.3	44.771	51.788
460	7.334	3233.5	45.083	52.113
480	7.382	3380.7	45.383	52.426
500	7.431	3528.8	45.671	52.728
520	7.480	3678.0	45.948	53.021
540	7.529	3828.0	46.215	53.304
560	7.577	3979.1	46.473	53.579
580	7.624	4131.1	46.723	53.845
600	7.670	4284.1	46.964	54.105
620	7.715	4437.9	47.199	54.357
640	7.759	4592.7	47.426	54.602
660	7.802	4748.3	47.648	54.842
680	7.843	4904.7	47.863	55.075
700	7.883	5062.0	48.072	55.303

Calculated with  $R=1.98714 \text{ cal deg}^{-1} \text{ mole}^{-1}$

Values of the thermodynamic functions were computed in the manner described for every 20 degrees up to 200° and for temperatures 300°, 400°, 600°, 800°, 1,000°, 1,250°, 1,500°, 1,750°, 2,000°, 2,500°, 3,000°, 4,000°, and 5,000° K. Intermediate values were interpolated for  $C_p^\circ$  at every 20 degrees up to 700° K and at every 100 degrees throughout the remainder of the temperature range covered. Using tabular integration, tables of  $H^\circ - E_0^\circ$ ,  $S^\circ$  and  $-(F^\circ - E_0^\circ)/T$  were built up from the  $C_p^\circ$  table. Good agreement was obtained with the directly computed values at all the above reference temperatures. The results are given at 20-degree intervals up to 700° K in table 5 and at 100-degree

intervals up to 5,000° K in table 6 for the naturally occurring mixture of oxygen isotones.

TABLE 6. *Thermodynamic functions for the natural isotopic mixture of molecular oxygen in the standard ideal gas state at 100-degree intervals up to 5,000° K*

<i>T</i>	<i>C<sub>p</sub></i> <sup>o</sup>	<i>H</i> <sup>o</sup> - <i>E</i> <sub>0</sub> <sup>o</sup>	-( <i>F</i> <sup>o</sup> - <i>E</i> <sub>0</sub> <sup>o</sup> )/ <i>T</i>	<i>S</i> <sup>o</sup>
° K	<i>cal deg</i> <sup>-1</sup> <i>mole</i> <sup>-1</sup>	<i>cal mole</i> <sup>-1</sup>	<i>cal deg</i> <sup>-1</sup> <i>mole</i> <sup>-1</sup>	<i>cal deg</i> <sup>-1</sup> <i>mole</i> <sup>-1</sup>
100	6.958	693.36	34.469	41.402
200	6.961	1389.2	39.279	46.225
300	7.023	2087.6	42.097	49.056
400	7.196	2797.7	44.104	51.098
500	7.431	3528.8	45.671	52.728
600	7.670	4284.1	46.964	54.105
700	7.883	5062.0	48.072	55.303
800	8.063	5859.6	49.044	56.368
900	8.212	6673.7	49.912	57.327
1,000	8.336	7501.2	50.697	58.199
1,100	8.439	8340.1	51.416	58.998
1,200	8.527	9188.6	52.079	59.736
1,300	8.604	10045.2	52.695	60.422
1,400	8.674	10909.2	53.270	61.062
1,500	8.738	11779.8	53.810	61.663
1,600	8.800	12656.8	54.318	62.229
1,700	8.858	13539.7	54.799	62.764
1,800	8.916	14428.4	55.256	63.272
1,900	8.973	15322.8	55.691	63.756
2,000	9.029	16223	56.106	64.217
2,100	9.084	17129	56.503	64.659
2,200	9.139	18040	56.883	65.083
2,300	9.194	18956	57.248	65.490
2,400	9.248	19879	57.600	65.883
2,500	9.301	20806	57.939	66.261
2,600	9.354	21739	58.266	66.627
2,700	9.405	22677	58.582	66.981
2,800	9.455	23620	58.889	67.324
2,900	9.503	24568	59.185	67.657
3,000	9.551	25520	59.473	67.980
3,100	9.596	26478	59.753	68.294
3,200	9.640	27440	60.024	68.599
3,300	9.682	28406	60.289	68.896
3,400	9.723	29376	60.546	69.186
3,500	9.762	30350	60.797	69.468
3,600	9.799	31328	61.042	69.744
3,700	9.835	32310	61.280	70.013
3,800	9.869	33295	61.514	70.276
3,900	9.901	34284	61.742	70.532
4,000	9.932	35275	61.965	70.783

TABLE 6. *Thermodynamic functions for the natural isotopic mixture of molecular oxygen in the standard ideal gas state at 100-degree intervals up to 5,000° K—Continued*

<i>T</i>	<i>C<sub>p</sub></i> <sup>o</sup>	<i>H</i> <sup>o</sup> - <i>E</i> <sub>0</sub> <sup>o</sup>	-( <i>F</i> <sup>o</sup> - <i>E</i> <sub>0</sub> <sup>o</sup> )/ <i>T</i>	<i>S</i> <sup>o</sup>
° K	<i>cal deg</i> <sup>-1</sup> <i>mole</i> <sup>-1</sup>	<i>cal mole</i> <sup>-1</sup>	<i>cal deg</i> <sup>-1</sup> <i>mole</i> <sup>-1</sup>	<i>cal deg</i> <sup>-1</sup> <i>mole</i> <sup>-1</sup>
4,100	9.961	36270	62.183	71.029
4,200	9.988	37267	62.396	71.269
4,300	10.015	38267	62.605	71.505
4,400	10.039	39270	62.810	71.735
4,500	10.062	40275	63.011	71.961
4,600	10.084	41282	63.208	72.182
4,700	10.104	42292	63.401	72.399
4,800	10.123	43303	63.591	72.613
4,900	10.140	44316	63.777	72.821
5,000	10.156	45331	63.960	73.026

(Calculated with  $R=1.98714$  cal deg<sup>-1</sup> mole<sup>-1</sup>)

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