**NIST-JANAF THERMOCHEMICAL TABLE** 

IP(O, g) =  $109837.02 \pm 0.06 \text{ cm}^{-1}$  $S^{\circ}(298.15 \text{ K}) = 161.058 \pm 0.020 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$   $\Delta_t H^{\circ}(0 \text{ K}) = 246.79 \pm 0.10 \text{ kJ} \cdot \text{mol}^{-1}$  $\Delta_t H^{\circ}(298.15 \text{ K}) = 249.17 \pm 0.10 \text{ kJ} \cdot \text{mol}^{-1}$ 

Electronic Levels and Quantum Weights						
State	$\epsilon_i$ , cm <sup>-1</sup>	$g_i$				
<sup>3</sup> P <sub>2</sub>	0	5				
${}^{3}P_{1}$	158.265	3				
$^{3}P_{0}$	226,977	1				
${}^{3}P_{0}$ ${}^{1}D_{2}$	15867.862	5				
¹So	33792.583					

## **Enthalpy of Formation**

The enthalpy of formation is based on the dissociation energy of  $O_2(g)$ ,  $41260 \pm 15$  cm<sup>-1</sup> (493.579  $\pm 0.18$  kJ·mol<sup>-1</sup>), as recommended by CODATA. This value is derived from the spectroscopic study of Brix and Herzberg. The products of dissociation are assumed to be oxygen atoms in their ground states. The justification for this is discussed by Gaydon<sup>3</sup> and Krupenie.

### **Heat Capacity and Entropy**

The electronic levles for O(g) are given in the compilation by Moore.<sup>5</sup> Our calcualtions indicate that, except for the five states lying below 34000 cm<sup>-1</sup>, the inclusion of levels up to n=12 has no effect on the thermodynamic functions to 6000 K. This is a result of the high energy of these levels; the fifth excited state lies at 73768.20 cm<sup>-1</sup> above the ground state. Since the inclusion of these upper levels has no effect on the thermodynamic functions (to 6000 K) we list only the lowest lying status ( $\epsilon_i$ < 34000 cm<sup>-1</sup>). The reported uncertainty in S°(298.15 K) is due to uncertainties in the relative atomic mass, the fundamental constants, and the position of the low lying electronic levles. The calculated value of S(298.15 K) is 0.0094 J·K<sup>-1</sup>·mol<sup>-1</sup> greater than that recommended by CODATA<sup>1</sup> due to the use of a 1 bar standard state pressure (CODATA used 1 atm). The difference is due to our use of the current CODATA fundamental constants.<sup>6</sup> Extension of these calculations above 6000 K may require consideration of the higher excited states and utilization of proper fill and cut off procedures.<sup>7</sup>

#### References

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TAR         C*         S* −[G°−H*(T)]/T         H°−H*(T)         ΔH*         ΔG°         log K₁           0         0.         0.         INFINITE         −6.725         246.790         246.790         INFINITE           100         23.703         135.947         131.131         −4.518         247.544         242.615         −16.786           250         22.734         152.153         163.085         −2.186         248.421         237.339         −61.986           298.15         21.911         161.088         16.058         0.         249.187         231.176         −40.599           300         21.901         161.194         161.099         0.041         249.187         231.628         −40.330           350         21.657         164.551         161.324         11.29         249.537         228.670         −29.48           450         21.354         169.953         162.668         3.278         250.188         225.670         −29.49           450         21.254         170.060         165.291         6.462         251.013         213.312         121.57         172.549         −22.936           500         21.244         176.060         157.377         10.6	Enthalpy Reference Temperature = $T_r$ = 298.15 K J·K <sup>-1</sup> mol <sup>-1</sup>				к 5	Standard State Pressure = $p^{\circ}$ = 0.1 MPa			
0 0. 0. INFINITE	<i>T/</i> K	C;		$-H^{\circ}(T_{r})]/T$	$H^{\circ}-H^{\circ}(T_{r})$		$\Delta_{r}G^{\circ}$	log Kr	
100		•						INFINITE	
200         22,734         152,153         163,085         -2,186         248,421         227,339         -61,986           298,15         21,911         161,058         161,058         0.         29,173         231,736         -40,599           300         21,901         161,194         161,058         0.         29,173         231,736         -40,599           300         21,677         164,551         161,324         1,129         249,537         22,8673         -40,330           400         21,482         167,450         161,918         2,207         24,968         22,2676         -22,989           500         21,237         172,197         103,518         4,443         220,474         219,549         -22,936           600         21,124         176,060         165,291         6,462         251,1934         20,094         18,458         171,930         14,860         225,266         15,482           900         20,944         182,116         186,797         10,771         25,230         194,163         -11,299           1100         20,893         188,782         171,393         14,860         252,682         187,681         -9,803           1100	-				-4.518	247.544	242.615	126,729	
298.15 21.211 161.058 161.058 0. 249.173 231.736 -40.599 300 21.901 161.194 161.059 0.041 249.187 231.628 -40.330 330 21.657 164.551 161.324 1.129 249.537 231.638 -40.330 330 21.657 164.551 161.324 1.129 249.537 231.638 -40.330 400 21.482 167.430 161.912 2.220 249.868 223.650 -2.469 450 21.354 169.953 162.668 3.278 250.180 223.650 -2.5492 450 21.257 172.197 163.511 4.343 250.474 219.549 -22.396 600 21.124 176.060 165.291 6.462 251.013 213.312 11.8570 700 21.040 179.310 167.067 8.570 251.494 200.599 -15.466 800 20.984 182.116 168.777 10.671 251.926 200.692 -13.099 900 20.944 184.855 170.3599 12.767 252.320 194.163 -11.209 1100 20.987 190.599 174.734 19.039 252.682 187.681 -9.803 1200 20.887 190.599 174.734 19.039 253.332 174.619 -7.601 1200 20.887 190.599 174.734 19.039 253.332 174.619 -7.601 1200 20.884 192.270 176.019 21.126 233.667 168.047 -6.752 1400 20.838 193.816 177.236 23.212 233.906 161.435 -6.024 1400 20.838 196.599 179.486 27.381 254.211 154.840 -5.392 1600 20.838 196.599 179.486 27.381 254.211 148.210 -4.839 1700 20.833 197.862 180.530 29.464 254.659 141.564 -4.350 1800 20.833 197.862 180.530 29.464 254.659 141.564 -4.350 1800 20.837 20.079 182.479 33.630 255.96 254.171 154.840 -3.992 2000 20.826 201.247 183.391 35.713 255.299 121.552 -3.175 2000 20.827 20.079 182.479 33.630 255.697 128.234 -3.552 2000 20.830 20.3232 185.106 39.878 255.667 108.159 -2.568 2000 20.841 20.5045 188.591 4 41.962 255.845 114.860 -2.857 2000 20.841 20.5045 188.591 4 41.962 255.845 101.450 -2.304 2400 20.841 20.5045 188.591 4 41.962 255.845 101.450 -2.304 2400 20.841 20.5045 188.6693 44.045 255.992 49.734 -2.062 200.20.850 20.1247 183.391 255.675 108.159 -2.568 200 20.862 20.1247 183.391 255.675 108.159 -2.568 200 20.862 20.6714 188.170 48.216 255.277 49.484 1.633 2000 20.894 208.261 188.170 30.303 256.405 74.551 -1.442 2500 20.881 20.5045 186.6693 44.045 255.992 40.826 -2.304 2600 21.397 20.910 19.086 56.774 27.345 60.077 4.345 60.079 40.205 3300 20.991 21.057 20.268 80.275 20.275 20.206 20.877 20.206 20.206 20.206 20.207 2	200	22.734	152.153	163.085	-2.186	248,421	237.339	-61.986	
298.15	250	22.246	157.170	161.421	-1.063	248.816	234.522	-49.001	
1800   21,901   161,194   161,059   0,041   249,187   231,628   -40,330   21,657   64,551   161,324   1,199   249,537   228,673   -34,128   400   21,482   167,430   161,912   2,2077   249,868   222,5670   -29,469   450   21,354   169,953   162,668   3,278   250,180   222,562   -25,842   500   21,257   172,197   163,511   4,343   250,474   219,549   -22,936   600   21,124   716,060   165,291   6,462   251,013   213,312   -18,570   21,040   179,310   167,067   8,570   251,494   206,999   -15,446   800   20,984   82,116   168,777   10,671   251,926   200,602   -13,008   800   20,984   82,116   168,777   10,671   251,926   200,602   -13,008   800   20,984   82,116   168,777   10,671   251,926   200,602   -13,008   1100   20,991   186,789   173,373   19,059   12,767   253,300   194,163   -11,269   20,877   190,599   173,373   16,950   233,018   181,165   -8,603   1200   20,877   190,599   176,019   21,126   233,627   168,047   -6,752   1400   20,833   193,816   177,236   23,221   233,906   161,453   -6,024   1400   20,833   195,854   178,390   25,256   254,171   154,840   -5,392   1600   20,833   199,352   180,530   29,464   254,689   141,564   -4,350   1800   20,833   199,352   180,530   29,464   254,689   141,564   -4,350   1800   20,837   190,599   31,530   255,290   126,233   20,323   180,000   20,826   201,247   183,391   35,713   255,299   122,234   -3,515   2000   20,826   201,247   183,391   35,713   255,299   122,234   -3,515   2000   20,835   203,232   185,106   39,878   255,665   144,660   -2,857   2000   20,835   203,232   185,106   39,878   255,665   144,660   -2,857   200,000   20,835   203,232   185,106   39,878   255,665   144,660   -2,857   200,000   20,835   203,232   185,106   39,878   255,665   144,660   -2,857   200,000   20,835   203,232   185,106   39,878   255,665   144,600   -2,255   200,000   20,835   203,232   185,106   39,878   255,665   144,600   -2,255   200,000   20,835   203,232   185,106   39,878   255,665   144,600   20,835   203,232   203,232   203,233   203,232   203,233   203,2	298.15	21.911	161,058	161.058	0.				
1.63	300	21.901	161.194	161.059	0.041	249.187	231.628		
400 21.482 167.430 161.912 2.207 249.868 225.670 -25.842 500 21.257 172.197 163.511 4.343 250.474 219.549 -22.936 600 21.1257 172.197 163.511 4.343 250.474 219.549 -22.936 600 21.1247 160.600 165.291 6.462 251.013 21.3312 -18.570 700 21.040 179.310 167.057 8.570 251.494 206.990 -15.446 800 20.984 182.116 168.777 10.671 251.926 200.602 -13.098 900 20.944 184.585 170.399 12.767 252.320 194.163 -11.269 1000 20.915 186.790 171.930 14.860 252.682 187.681 9.803 1100 20.833 188.782 173.373 16.950 253.018 181.165 -8.603 1200 20.837 190.559 174.734 19.039 253.332 174.619 -7.601 1200 20.831 193.816 177.236 23.212 233.906 161.453 -6.024 140.20.833 195.254 178.390 25.296 254.171 154.840 -5.392 1600 20.838 196.599 179.486 27.381 254.421 148.210 -4.839 1700 20.833 197.862 180.530 29.464 254.659 141.564 -4.350 1800 20.830 199.053 181.527 31.547 254.884 134.905 -3.915 1900 20.827 20.0179 182.479 33.630 255.097 124.234 -3.525 200 20.826 201.247 183.391 35.713 255.299 121.552 -3.175 2000 20.827 20.0179 182.479 33.630 255.097 124.234 -3.525 200 20.830 203.232 185.106 39.878 255.667 108.159 -2.568 200.20.835 204.188 185.91 4 1.962 255.835 101.450 -2.304 2400 20.841 205.045 186.693 44.045 255.992 94.734 -2.062 200.20.831 20.02.856 186.693 44.045 255.992 94.734 -2.062 200.20.851 20.5896 184.466 37.796 255.488 114.866 2.2857 20.00 20.852 20.04.188 185.91 4 1.962 255.835 101.450 -2.304 2400 20.881 205.045 188.693 44.045 255.992 94.734 -2.062 20.00 20.882 20.02.188 185.06 39.878 255.667 108.159 -2.568 20.00 20.884 20.00 20.886 185.906 87.444 46.130 256.139 88.012 -1.839 2600 20.8870 20.00 20.886 187.444 46.130 256.139 88.012 -1.839 2600 20.8870 20.00 20.886 187.488 187.07 30.305 256.405 74.551 -1.442 2800 20.884 208.261 188.150 30.205 30.20	350	21.657	164,551	161.324	1.129	249.537	228.673	-34.128	
500         21,257         172,197         163,511         4,343         250,474         219,549         -22,936           600         21,124         176,060         165,291         6,462         251,013         21,3312         -18,570           700         21,040         179,310         167,067         8,570         251,494         206,990         -18,466           800         20,944         184,585         170,399         12,769         194,163         -11,269           1000         20,951         186,790         171,337         16,950         253,018         181,165         -8,603           1200         20,887         190,599         174,734         19,059         253,332         174,619         -7,601           1300         20,864         192,270         176,019         21,126         253,627         186,047         -6,752           1400         20,833         193,816         177,236         23,212         253,906         161,433         -6,024           1500         20,845         195,254         178,390         25,266         254,171         154,840         -5,392           1600         20,833         197,862         180,330         29,464         254,659		21.482	167.430						
Corner   C									
700         21,040         179,310         167,067         8,570         251,494         206,990         -15,446           800         20,984         182,116         168,777         10,671         251,926         200,602         -13,098           900         20,944         184,585         170,399         12,767         252,320         194,163         -11,309           1100         20,893         188,782         173,373         16,950         253,018         181,165         -8,603           1200         20,887         190,599         174,734         19,039         253,332         174,619         -7,601           1300         20,864         192,270         176,019         21,126         253,627         168,047         -6,752           1400         20,833         195,599         179,486         27,381         254,421         148,240         -4,839           1700         20,833         195,599         179,486         27,381         254,421         148,210         -4,839           1800         20,830         199,053         181,527         31,547         254,884         134,905         -3,915           200         20,827         20,0179         182,479         33,630									
800         20.944         182.116         168.777         10.671         251.926         200.602         -13.098           900         20.944         184.885         170.399         12.767         252.320         194.163         -11.269           1000         20.891         186.790         171.930         14.860         252.682         187.681         -9.803           1100         20.807         190.599         174.734         190.99         253.332         174.619         -7.601           1300         20.864         192.270         176.019         21.126         253.627         168.047         -6.752           1400         20.853         193.816         177.236         23.212         253.906         161.453         -6.024           1500         20.834         195.5254         178.390         25.296         254.171         154.840         -5.392           1600         20.833         197.862         180.530         29.464         254.659         141.564         -4.350           1700         20.833         197.862         180.530         29.464         254.659         141.564         -4.350           1800         20.821         200.179         182.479         33.630 <td></td> <td></td> <td></td> <td></td> <td>8,570</td> <td>251.494</td> <td>206.990</td> <td>-15.446</td>					8,570	251.494	206.990	-15.446	
900 20.944 184.585 170.399 12.767 252.320 194.163 -11.269 1000 20.915 186.790 171.930 14.860 252.682 187.681 -9.803 1100 20.893 188.782 173.373 16.950 253.032 174.619 -7.601 1200 20.877 190.599 174.734 19.039 253.332 174.619 -7.601 1300 20.864 192.270 176.019 21.126 253.627 168.047 -6.752 1400 20.853 193.816 177.236 23.212 253.906 161.453 -6.024 1500 20.845 195.254 178.399 253.332 174.619 -7.801 1500 20.845 195.254 178.399 253.332 174.619 -7.631 1500 20.845 195.254 178.399 253.332 174.619 -7.631 154.800 20.833 197.862 180.530 29.464 254.629 141.564 -4.839 1700 20.833 197.862 180.530 29.464 254.659 141.564 -4.350 1800 20.830 199.053 181.527 31.547 254.884 134.905 -3.915 1900 20.820 179 182.479 33.630 255.097 128.234 -3.525 2000 20.826 201.247 183.391 35.713 255.299 121.552 -3.175 2100 20.827 200.179 182.479 33.630 255.097 128.234 -3.525 200 20.826 201.247 183.391 35.713 255.299 121.552 -3.175 2100 20.831 205.000 18.81 185.914 41.962 255.835 101.450 -2.304 2400 20.831 205.045 186.693 44.045 255.935 101.450 -2.304 2400 20.841 205.045 186.693 44.045 255.939 94.734 -2.062 2500 20.861 205.046 186.693 44.045 255.037 88.012 -1.839 250.0 20.812 205.896 187.444 46.130 256.139 88.012 -1.839 250.0 20.894 208.626 185.550 185.500 185.500 74.551 -1.442 2800 20.894 208.261 185.550 52.391 256.625 67.814 -1.633 2700 20.894 208.261 185.550 52.391 256.625 67.814 -1.633 2700 20.991 211.057 192.068 60.767 256.637 61.072 -1.100 3000 20.993 20.9910 211.057 192.068 60.767 256.639 40.826 -78.14 -1.265 2900 20.914 208.995 190.208 54.481 256.637 61.072 -1.100 3000 20.993 20.991 211.057 192.068 60.767 256.639 40.826 -33.583 40.593 25.000 21.032 21.792 12.833 193.777 67.079 257.169 20.555 -0.307 3600 21.032 21.572 196.835 77.675 257.496 -1.3270 0.073 3600 21.032 21.572 196.835 77.675 257.496 -1.3270 0.073 3600 21.032 21.572 196.535 77.675 257.496 -1.3270 0.073 3600 21.032 21.572 196.535 77.675 257.496 -1.3270 0.073 3600 21.032 21.572 196.535 77.675 257.496 -1.3270 0.073 3600 21.032 21.572 196.535 77.675 257.496 -1.3270 0.073 3600 21.039 21.	800	20.984	182.116	168,777	10,671	251.926	200,602	-13.098	
1000   20.891   188.782   173.373   16.950   253.018   181.165   -8.603   1200   20.877   190.599   174.734   19.039   253.332   174.619   -7.601   1300   20.844   192.270   176.019   21.126   253.627   168.047   -6.752   1400   20.853   193.816   177.236   23.212   253.906   161.453   -6.024   1500   20.845   195.254   178.390   25.296   254.171   154.840   -5.392   1700   20.838   196.599   179.486   27.381   254.421   148.210   -4.839   1700   20.833   197.862   180.530   29.464   254.659   141.564   -4.350   1800   20.830   199.053   181.527   31.547   254.884   134.905   -3.915   1900   20.827   200.179   182.479   33.630   255.097   128.234   -3.525   1900   20.827   200.2263   184.266   37.796   255.488   114.860   -2.857   2200   20.826   201.247   183.391   35.713   255.299   121.552   -3.175   2100   20.827   202.263   184.266   37.796   255.488   114.860   -2.857   2200   20.830   203.232   185.106   39.878   255.667   108.159   -2.2568   200.2084   200.5386   187.444   44.962   255.835   101.450   -2.304   2400   20.841   205.896   187.444   46.130   256.139   88.012   1.839   2600   20.862   206.714   188.170   48.216   256.277   81.284   -1.633   2600   20.877   207.502   188.871   50.303   256.405   74.551   -1.442   2800   20.894   208.261   189.550   52.391   256.525   67.814   -1.265   2900   20.914   208.995   190.208   4.481   526.637   61.072   -1.100   3000   20.937   207.502   188.871   50.303   256.405   74.551   -1.442   2800   20.991   211.057   192.068   60.767   256.838   47.578   -0.802   3000   20.937   207.502   188.701   30.303   256.405   74.551   -0.403   3000   20.937   207.502   207.503   30.503   207.503   207.503   207.503   207.503   207.503   207.503   207.504   207.505   207.504   207.505   207	900	20.944	184.585	170.399	12.767	252.320			
1200   20.817   190.599   174.734   19.039   253.332   174.619   -7.601   1300   20.864   192.270   176.019   21.126   253.627   168.047   -6.752   1400   20.853   193.816   177.236   23.212   253.906   161.453   -6.024   1500   20.884   195.254   178.390   25.296   254.171   154.840   -5.392   1600   20.838   196.599   179.486   27.381   254.421   148.210   -4.839   1700   20.833   197.862   180.530   29.464   254.659   141.564   -4.350   1800   20.830   199.053   181.527   31.547   254.884   314.955   -3.915   1900   20.827   200.179   182.479   33.630   255.097   128.234   -3.525   2000   20.826   201.247   183.391   35.713   255.299   121.552   -3.175   2100   20.827   202.263   184.266   37.796   255.488   114.860   -2.857   2200   20.835   204.158   185.914   41.962   255.835   101.450   -2.304   2400   20.841   205.045   186.693   44.045   255.992   94.734   -2.062   2500   20.851   205.896   187.444   46.130   256.139   88.012   -1.839   2600   20.862   206.714   188.170   48.216   256.277   81.284   -1.633   2700   20.894   208.261   185.550   32.391   256.525   67.814   -1.265   2900   20.991   20.997   20.991   20.895   190.208   34.481   256.537   61.072   -1.100   3000   20.993   20.997   20.9084   63.676   256.939   40.826   -2.304   20.909   211.057   192.068   60.767   256.939   40.826   -0.666   3300   21.022   211.704   192.668   60.767   257.496   -13.270   0.107   3000   21.022   211.704   192.668   60.767   257.496   -13.270   0.173   3400   21.032   213.537   194.318   69.190   257.241   34.071   -0.539   3400   21.032   213.537   194.318   69.190   257.241   34.071   -0.539   3400   21.032   213.537   194.318   69.190   257.241   34.071   -0.539   3400   21.032   213.537   194.318   69.190   257.241   34.071   -0.539   3400   21.032   213.537   194.318   69.190   257.241   34.071   -0.539   3400   21.224   21.1318   197.63   84.867   257.566   -33.583   0.408   4000   21.130   213.537   194.318   69.190   257.241   34.071   -0.009   3800   21.232   214.682   195.360   34.481   257.554	1000	20.915							
1300   20.864   192.270   176.019   21.126   253.627   168.047   -6.752   1400   20.831   193.816   177.236   23.212   253.906   161.453   -6.024   1500   20.845   195.254   178.390   25.296   254.171   154.840   -5.392   1600   20.838   195.599   179.486   27.381   254.421   148.210   -4.839   1700   20.833   197.862   180.530   29.464   254.659   141.564   -4.350   1800   20.830   199.053   181.527   31.547   254.884   134.905   -3.915   1900   20.827   200.179   182.479   33.630   255.097   128.234   -3.525   2000   20.826   201.247   183.391   35.713   255.299   121.552   -3.175   2100   20.827   202.263   184.266   37.796   255.488   114.860   -2.857   2200   20.830   203.232   185.106   39.878   255.667   108.159   -2.568   2300   20.835   204.158   185.914   41.962   255.835   101.450   -2.304   2400   20.841   205.045   186.693   44.045   255.992   24.734   -2.062   2500   20.851   205.896   187.444   46.130   256.139   88.012   -1.839   2600   20.862   206.714   188.170   48.216   256.277   81.284   -1.633   2700   20.877   207.502   188.871   50.303   256.405   74.551   -1.442   2800   20.944   208.995   190.208   54.481   256.637   61.072   -1.100   3000   20.937   209.704   190.846   56.574   256.741   54.327   -1.100   3000   20.937   209.704   190.846   56.574   256.741   54.327   -0.802   300   21.025   211.704   192.653   62.867   257.044   34.071   -0.539   3400   21.025   211.704   192.653   62.867   257.441   34.071   -0.539   3400   21.025   212.332   193.233   64.971   257.094   27.315   -0.420   3700   21.170   214.117   194.845   71.305   257.241   37.94   -0.200   3700   21.170   214.117   194.845   71.305   257.544   34.071   -0.539   3400   21.056   212.332   193.233   64.971   257.094   27.315   -0.400   3700   21.170   214.117   194.845   71.305   257.309   70.000   21.277   215.234   195.862   75.547   257.496   -13.270   0.173   3600   21.275   215.234   195.862   75.547   257.496   -13.270   0.173   3600   21.279   215.234   195.862   36.834   79.808   257.554   -20.040   0.255									
1400   20.833   193.816   177.236   23.212   253.906   161.453   -6.024   1500   20.845   195.254   178.390   25.296   254.171   154.840   -5.392   1600   20.838   196.599   179.486   27.381   254.421   148.210   -4.839   1700   20.833   197.862   180.530   29.464   254.659   141.564   -4.350   1800   20.827   200.179   182.479   33.630   255.097   128.234   -3.525   2000   20.826   201.247   183.391   35.713   255.299   121.557   -3.175   2100   20.827   202.263   184.266   37.796   255.488   114.860   -2.857   2200   20.830   203.232   185.106   39.878   255.667   108.159   -2.568   2300   20.835   204.158   185.914   41.962   255.835   101.450   -2.304   2400   20.841   205.045   186.693   44.045   255.992   94.734   -2.062   2500   20.851   205.896   187.444   46.130   256.139   88.012   -1.839   2600   20.862   206.714   188.170   48.216   256.277   81.284   -1.633   2700   20.894   208.261   188.951   32.391   236.525   67.814   -1.265   2900   20.914   208.995   190.208   34.481   236.637   61.072   -1.100   3000   20.937   209.704   90.846   56.574   236.741   34.327   -0.946   3100   20.937   209.704   90.846   56.574   256.741   34.327   -0.946   3300   21.022   211.704   192.688   60.767   257.044   27.304   27.305   27.307   20.991   21.1057   192.088   60.767   257.049   42.332   393.223   64.971   257.049   42.332   30.000   21.032   211.374   192.068   60.766   3500   21.302   212.332   193.223   64.971   257.094   42.315   -0.420   3000   21.302   21.577   196.353   77.675   257.496   -13.270   0.173   4000   21.302   215.772   196.353   77.675   257.496   -13.270   0.173   4000   21.302   21.577   196.353   77.675   257.496   -13.270   0.173   4000   21.302   215.772   196.353   77.675   257.496   -13.270   0.173   4000   21.302   215.772   196.353   77.675   257.496   -13.270   0.173   4000   21.302   215.772   196.353   77.675   257.496   -13.270   0.173   4000   21.397   21.684   197.763   84.087   257.596   -3.5880   0.499   21.445   21.318   197.763   84.087   257.596   -3.5880   0.499								-6,752	
1500   20.845   195.254   178.390   25.296   254.171   154.840   -5.392   1600   20.838   196.599   179.486   27.381   254.421   148.210   -4.839   1700   20.833   197.862   180.530   29.464   254.659   141.564   -4.350   1800   20.830   199.053   181.527   31.547   254.884   134.905   -3.915   1900   20.827   200.179   182.479   33.630   255.097   128.234   -3.525   2000   20.826   201.247   183.391   35.713   255.299   121.552   -3.175   2100   20.827   202.263   184.266   37.796   255.488   114.860   -2.857   2200   20.830   203.232   185.106   39.878   255.667   108.159   -2.568   2300   20.835   204.158   185.914   41.962   255.835   101.450   -2.304   2400   20.841   205.045   186.693   44.045   255.995   94.734   -2.062   2500   20.851   205.896   187.444   46.130   256.139   88.012   -1.839   2600   20.862   206.714   188.170   48.216   256.277   81.284   -1.633   2700   20.877   207.502   188.871   50.303   256.405   74.551   -1.442   2800   20.994   208.261   189.550   52.391   236.525   67.814   -1.633   200.20.937   209.704   190.846   56.574   256.777   81.284   -1.633   300   20.937   209.704   190.846   56.574   256.774   34.327   -0.946   3300   20.991   211.057   192.068   60.767   256.929   40.826   -0.656   3300   21.022   211.704   192.653   62.867   237.014   34.071   -0.394   34.00   21.130   21.2332   193.223   64.971   237.094   27.135   -0.420   3500   21.192   212.943   193.777   67.079   257.169   20.555   -0.307   3600   21.130   21.3537   394.318   69.190   257.241   13.794   -0.200   3000   21.397   214.117   194.845   71.305   257.399   7.030   -0.094   40.000   21.397   21.4682   195.360   73.424   257.373   0.265   -0.504   4000   21.397   21.4845   217.318   197.633   84.087   257.576   -0.507   -0.004   40.000   21.397   216.814   197.303   81.945   257.576   -0.507   -0.004   40.000   21.397   216.814   197.303   81.945   257.576   -0.507   -0.004   40.000   21.397   216.814   197.303   81.945   257.576   -0.508   -0.666   -0.563   -0.666   -0.563   -0.666   -0.563   -0.666							161.453	-6.024	
1600         20.838         196.599         179.486         27.381         254.421         148.210         -4.839           1700         20.833         197.862         180.530         29.464         254.659         141.564         -4.359           1800         20.830         199.053         181.527         31.547         254.884         134.905         -3.915           1900         20.827         200.179         182.479         33.630         255.097         128.234         -3.525           2000         20.830         203.232         185.106         39.878         255.667         108.159         -2.568           2200         20.830         203.232         185.106         39.878         255.667         108.159         -2.568           2300         20.841         205.045         186.693         44.045         255.992         94.734         -2.062           2500         20.851         205.896         187.444         46.130         256.277         81.284         -1.633           2700         20.877         207.502         188.871         50.303         236.405         74.551         -1.442           2800         20.9874         207.510         188.871         50.303								-5.392	
1700   20.833   197.862   180.530   29.464   254.659   141.564   -4.350   1800   20.830   199.053   181.527   31.547   254.884   314.905   -3.915   1900   20.827   200.179   182.479   33.630   255.097   128.234   -3.525   2000   20.826   201.247   183.391   35.713   255.299   121.552   -3.175   2100   20.827   202.653   184.266   37.796   255.488   114.860   -2.857   2200   20.830   203.232   185.106   39.878   255.667   108.159   -2.568   2300   20.835   204.158   185.914   41.962   255.835   101.459   -2.304   2400   20.841   205.045   186.693   44.045   255.992   94.734   -2.062   2500   20.851   205.896   187.444   46.130   2256.139   88.012   -1.839   2700   20.877   207.502   188.871   50.303   256.405   74.551   -1.442   2800   20.894   208.261   189.550   52.391   256.525   67.814   -1.265   2900   20.914   208.995   190.208   54.481   256.637   61.072   -1.100   3000   20.937   209.704   190.846   56.574   256.734   54.327   -0.946   3300   21.932   211.057   192.068   60.767   256.929   40.826   -0.666   3300   21.022   211.704   192.653   62.867   257.094   27.315   -0.420   3500   21.302   212.943   193.777   67.079   257.094   27.315   -0.420   3700   21.357   213.537   94.318   69.190   257.241   13.794   -0.200   3700   21.130   213.537   94.318   69.190   257.241   13.794   -0.200   3700   21.130   214.682   195.360   73.424   257.794   27.315   -0.420   3700   21.397   214.117   94.845   71.305   257.994   27.315   -0.420   3700   21.397   214.117   94.845   71.305   257.994   27.315   -0.420   3700   21.130   21.3537   94.318   69.190   257.241   13.794   -0.200   3700   21.130   21.3537   94.318   69.190   257.241   13.794   -0.200   3700   21.130   21.5772   196.353   77.675   257.496   -13.270   -0.173   3000   21.237   215.234   195.862   75.547   257.436   -6.501   0.087   4000   21.349   21.485   21.318   197.63   84.887   257.554   -20.040   0.255   4200   21.397   216.814   97.303   81.945   257.554   -20.040   0.255   4200   21.397   21.485   21.318   197.63   84.887   257.956   -33			196,599	179.486	27.381	254.421	148,210		
1800         20,830         199,053         181,527         31,547         254,884         134,905         -3.915           2000         20,827         200,179         182,479         33,630         255,097         128,234         -3.525           2000         20,826         201,247         183,391         35,713         255,299         121,552         -3.175           2100         20,827         202,263         184,266         37,796         255,488         114,860         -2.568           2300         20,831         203,321         185,914         41,962         255,835         101,450         -2.568           2400         20,841         205,045         186,693         44,045         255,992         94,734         -2.062           2500         20,811         205,045         187,444         46,130         256,139         88.012         -1.839           2600         20,862         206,114         188,170         48,216         256,277         81,284         -1.633           2700         20,877         207,502         188,871         50,303         256,635         61,072         -1.104           2800         20,894         208,295         190,208         54,481	1700	20.833	197.862	180,530	29.464	254,659	141.564	-4.350	
2000   20.826   201.247   183.391   35.713   255.299   121.552   -3.175	1800	20.830	199.053	181.527					
2100         20.827         202.263         184.266         37.796         255.488         114.860         -2.857           2200         20.830         203.232         185.106         39.878         255.667         108.159         -2.568           2300         20.831         204.158         185.914         41.962         255.835         101.450         -2.304           2400         20.841         205.045         186.693         44.045         255.992         94.734         -2.062           2500         20.851         205.896         187.444         46.130         256.139         88.012         -1.839           2600         20.862         206.714         188.170         48.216         256.277         81.284         -1.633           2700         20.877         207.502         188.871         50.303         256.405         74.551         -1.442           2800         20.844         208.261         189.550         52.391         256.525         67.814         -1.265           2900         20.914         208.995         190.208         54.481         256.637         61.072         -1.100           3100         20.993         211.057         192.068         60.767									
2200   20.830   203.232   185.106   39.878   255.667   108.159   -2.508   2300   20.835   204.158   185.914   41.962   255.835   101.450   -2.304   2400   20.841   205.045   186.693   44.045   255.992   94.734   -2.062   2500   20.851   205.896   187.444   46.130   255.139   88.012   -1.839   2600   20.852   206.714   188.170   48.216   256.277   81.284   -1.633   2700   20.877   207.502   188.871   50.303   256.405   74.551   -1.442   2800   20.894   208.261   189.550   52.391   256.525   67.814   -1.265   2900   20.914   208.995   190.208   54.481   256.637   61.072   -1.100   3000   20.937   209.704   190.846   56.574   256.741   54.327   -0.946   3100   20.963   210.391   191.466   58.669   256.838   47.578   -0.802   3200   20.991   211.057   192.068   60.767   256.929   40.826   -0.666   3300   21.022   211.704   192.663   62.867   257.014   34.071   -0.539   3400   21.036   212.332   193.277   67.079   257.169   20.555   -0.307   3600   21.130   213.537   194.318   69.190   257.241   13.794   -0.200   3800   21.130   213.537   194.318   69.190   257.241   13.794   -0.200   3800   21.213   214.682   195.360   73.424   257.330   7.030   -0.099   3800   21.213   214.682   195.360   73.424   257.373   0.265   -0.004   3900   21.257   216.814   197.303   81.945   257.566   -33.583   0.408   4400   21.349   216.299   196.834   79.808   257.541   -20.040   0.255   -0.004   4400   21.349   216.299   196.834   79.808   257.566   -33.583   0.408   4400   21.495   217.812   198.213   86.234   257.566   -33.583   0.408   4400   21.495   217.812   198.213   86.234   257.720   -40.355   0.479   4500   21.545   218.759   199.086   90.543   257.566   -33.583   0.408   4400   21.495   217.812   198.213   86.234   257.756   -60.687   0.674   4900   21.748   221.338   200.333   70.045   257.926   -67.465   0.734   4900   21.445   217.318   197.63   84.087   257.566   -33.583   0.408   4400   21.949   21.485   217.812   198.213   86.234   257.756   -33.698   0.486   4400   21.949   21.2224   21.924   21.935   21.335   20.									
2300								-2.568	
2400         20,841         205,045         186,693         44,045         255,992         94,734         -2,062           2500         20,851         205,896         187,444         46,130         256,139         88,012         -1,839           2600         20,862         206,714         188,170         48,216         256,277         81,284         -1,633           2700         20,877         207,502         188,871         50,303         256,405         74,551         -1,442           2800         20,994         208,261         189,550         52,391         256,525         67,814         -1,265           2900         20,914         208,995         190,208         54,481         256,637         61,072         -1,100           3000         20,937         209,704         190,846         56,574         256,741         54,327         -0,946           3100         20,963         210,391         211,668         58,669         256,838         47,578         -0,802           3200         21,921         211,074         192,663         62,867         257,014         34,071         -0,802           3300         21,022         211,704         192,663         62,867					41.962	255.835	101.450	-2.304	
2500         20.851         205.896         187,444         46.130         256.139         88.012         -1.839           2600         20.862         206.714         188.170         48.216         256.277         81.284         -1.633           2700         20.877         207.502         188.871         50.303         256.405         74.551         -1.442           2800         20.894         208.261         189.550         52.391         256.525         67.814         -1.265           2900         20.914         208.995         90.208         54.812         256.637         61.072         -1.100           3000         20.937         209.704         190.846         56.574         256.741         54.327         -0.946           3100         20.963         210.391         191.466         58.669         256.838         47.578         -0.802           3200         20.291         211.1074         192.653         62.867         257.014         34.071         -0.802           3300         21.056         21.332         193.233         64.971         257.044         34.071         -0.539           3400         21.150         21.332         193.237         67.079         <	2400	20.841	205.045	186,693	44.045	255.992	94.734	-2.062	
2700         20,877         207,502         188,871         50,303         256,405         74,551         -1,442           2800         20,894         208,261         189,550         52,391         256,525         67,814         -1,265           2900         20,914         208,995         190,208         54,481         256,637         61,072         -1,100           3000         20,937         209,704         190,846         56,574         256,741         54,327         -0,946           3100         20,963         210,391         191,466         58,669         256,838         47,578         -0,802           3200         20,991         211,074         192,653         62,867         257,014         34,071         -0,539           3400         21,052         212,332         193,223         64,971         257,094         27,315         -0,420           3500         21,092         212,943         193,777         67,079         257,169         20,555         -0,307           3600         21,130         213,573         194,318         69,190         257,241         13,794         -0,200           3700         21,170         214,117         194,845         71,305	2500	20.851	205,896	187.444					
2800         20.894         208 261         189.550         52.391         256.525         67.814         -1.265           2900         20.914         208.995         190.208         54.481         256.637         61.072         -1.100           3000         20.937         209.704         190.846         56.574         256.741         54.327         -0.946           3100         20.963         210.391         191.466         58.669         256.838         47.578         -0.802           3200         20.991         211.057         192.068         60.767         256.929         40.826         -0.666           3300         21.022         211.704         192.653         62.867         257.014         34.071         -0.539           3400         21.036         212.332         193.273         64.971         257.169         20.555         -0.307           3600         21.130         213.537         194.318         69.190         257.241         13.794         -0.200           3700         21.170         214.117         194.845         71.305         257.309         7.030         -0.099           3800         21.213         214.682         195.360         73.424			206.714						
2900   20.914   208.995   190.208   54.481   256.637   61.072   -1.100   3000   20.937   209.704   190.846   56.574   256.741   54.327   -0.946   3100   20.953   210.391   191.466   58.669   256.838   47.578   -0.802   3200   20.991   211.057   192.068   60.767   256.929   40.826   -0.666   3300   21.022   211.704   192.653   62.867   257.014   34.071   -0.539   3400   21.056   212.332   193.273   64.971   257.094   27.315   -0.420   3500   21.092   212.943   193.777   67.079   257.169   20.555   -0.307   3600   21.130   213.537   194.318   69.190   257.241   13.794   -0.200   3700   21.170   214.117   194.845   71.305   257.309   7.030   -0.099   3800   21.213   214.682   195.360   73.424   257.373   0.265   -0.004   3900   21.257   215.234   195.862   75.547   257.436   -6.501   0.087   4000   21.302   215.772   196.353   77.675   257.496   -13.270   0.173   4100   21.349   216.299   196.834   79.808   257.554   -20.040   0.255   4200   21.397   216.814   197.303   81.945   257.661   -26.811   0.333   4300   21.445   217.318   197.763   84.087   257.666   -33.583   0.408   4400   21.595   218.795   198.654   88.386   257.773   -47.133   0.547   4600   21.596   218.769   199.086   90.543   257.825   -53.909   0.612   4700   21.647   219.234   199.510   92.705   257.876   -60.687   0.674   4800   21.697   219.690   199.925   94.872   257.926   -67.465   0.734   4900   21.748   220.138   200.333   97.045   257.976   -74.244   0.791   5000   21.899   221.435   201.514   103.592   258.105   -101.371   0.999   5000   21.899   221.435   201.514   103.592   258.105   -101.371   0.999   5400   21.997   222.668   202.667   107.982   258.105   -101.371   0.999   5400   21.997   222.668   202.667   107.982   258.821   -14.208   1.258   5500   22.093   223.457   203.351   114.602   258.282   -118.506   1.178   5500   22.184   223.842   203.701   116.818   258.304   -13.296   1.218   5900   22.229   224.222   204.046   119.039   258.321   -142.083   1.258   6000   22.273   224.596   204.385   121.264   258.332   -148.869			207,502						
3000   20,937   209,704   190,846   56,574   256,741   54,327   -0.946						256.637	61.072	-1.100	
3100   20.963   210.391   191.466   58.669   256.838   47.578   -0.802   20.991   211.057   192.068   60.767   256.929   40.826   -0.666   3300   21.022   211.704   192.653   62.867   257.014   34.071   -0.539   3400   21.056   212.332   193.223   64.971   257.094   27.315   -0.420   3500   21.092   212.943   193.777   67.079   257.169   20.555   -0.307   3600   21.130   213.537   194.318   69.190   257.241   13.794   -0.200   3700   21.170   214.117   194.845   71.305   257.309   7.030   -0.099   3800   21.213   214.682   195.360   73.424   257.373   0.265   -0.004   3900   21.257   215.234   195.862   75.547   257.436   -6.501   0.087   4000   21.302   215.772   196.353   77.675   257.496   -13.270   0.173   4100   21.349   216.814   197.303   81.945   257.514   -20.040   0.255   4200   21.397   216.814   197.303   84.987   257.611   -26.811   0.333   4300   21.445   217.318   197.633   84.987   257.666   -33.583   0.408   4400   21.495   217.812   198.213   86.234   257.720   -40.358   0.479   4500   21.545   218.295   198.654   88.386   257.773   -47.133   0.547   4600   21.596   218.796   199.925   94.872   257.875   -60.687   0.674   4800   21.697   219.234   199.510   92.705   257.876   -60.687   0.674   4800   21.697   219.639   199.925   94.872   257.926   -67.465   0.734   4900   21.748   220.138   200.333   97.045   257.974   -74.244   0.791   4800   21.799   220.578   200.734   99.222   258.021   -81.025   0.846   5100   21.849   221.835   201.833   97.045   257.974   -74.244   0.791   5000   21.799   220.578   200.734   99.222   258.021   -81.025   0.846   5500   21.899   221.835   201.891   105.842   258.284   -111.940   1.092   1.092   1.092   1.394   221.835   201.891   105.842   258.284   -114.940   1.092   1.092   1.092   1.245   22.668   202.664   110.184   258.284   -114.940   1.092   1.092   1.092   1.093   22.445   22.668   202.664   110.184   258.284   -114.940   1.092   1.090   22.2445   22.2668   202.664   110.184   258.234   -114.940   1.092   1.092   1.092   1.092   1.093   1.05.84			209.704					-0.946	
10.00	3100	20.963	210.391	191.466	58.669	256.838	47.578		
3300 21.022 211.704 192.653 62.867 257.014 34.071 -0.539 3400 21.056 212.332 193.223 64.971 257.094 27.315 -0.420 3500 21.092 212.943 193.777 67.079 257.169 20.555 -0.307 3600 21.130 213.537 194.318 69.190 257.241 13.794 -0.200 3700 21.170 21.41.17 194.845 71.305 257.309 7.030 -0.099 3800 21.213 214.682 195.360 73.424 257.373 0.265 -0.004 3900 21.257 215.234 195.862 75.547 257.436 -6.501 0.087 4000 21.302 215.772 196.353 77.675 257.496 -13.270 0.173 4100 21.349 216.299 196.834 79.808 257.554 -20.040 0.255 4000 21.397 216.814 197.303 81.945 257.611 -26.811 0.333 4300 21.445 217.318 197.763 84.087 257.666 -33.583 0.408 4400 21.495 217.812 198.213 86.234 257.720 -40.358 0.479 4500 21.545 218.295 198.654 88.386 257.773 -47.133 0.547 4600 21.596 218.796 199.086 90.543 257.825 -53.909 0.612 4700 21.647 219.234 199.510 92.705 257.876 -60.687 0.674 4800 21.495 217.812 29.20578 20.333 97.045 257.926 -67.465 0.734 4900 21.748 220.138 200.333 97.045 257.926 -67.465 0.734 4900 21.748 220.138 200.333 97.045 257.926 -67.465 0.734 4900 21.748 220.138 200.333 97.045 257.926 -67.465 0.734 4900 21.799 220.578 200.734 99.222 258.021 81.025 0.846 5100 21.899 221.435 201.514 103.592 258.100 -94.589 0.950 5200 21.899 221.435 201.514 103.592 258.100 -94.589 0.950 5500 22.045 222.264 202.267 107.982 258.180 -94.589 0.950 5500 22.045 222.668 202.6674 110.184 258.224 -114.940 1.092 5500 22.199 223.845 203.351 114.602 258.282 -128.510 1.178 5900 22.184 223.842 203.701 116.818 258.302 -118.869 1.296 6000 22.299 224.222 204.046 119.039 258.321 -142.083 1.258 6000 22.299 224.222 204.046 119.039 258.321 -142.083 1.258 6000 22.273 224.596 204.385 121.264 258.332 -148.869 1.296	3200	20.991	211.057	192.068	60.767	256.929	40.826	-0.666	
3500   21.092   212.943   193.777   67.079   257.169   20.555   -0.307		21.022							
3600 21.130 213.537 194.318 69.190 257.241 13.794 -0.200 3700 21.170 214.117 194.845 71.305 257.309 7.030 -0.099 3800 21.213 214.682 195.360 73.424 257.373 0.265 -0.004 3900 21.257 215.234 195.862 75.547 257.436 -6.501 0.087 4000 21.302 215.772 196.353 77.675 257.496 -13.270 0.173 4100 21.349 216.299 196.834 79.808 257.554 -20.040 0.255 4200 21.397 216.814 197.303 81.945 257.611 -26.811 0.333 4300 21.445 217.318 197.763 84.087 257.666 -33.583 0.408 4400 21.495 217.812 198.213 86.234 257.720 -40.358 0.479 4500 21.545 218.295 198.654 88.386 257.773 -47.133 0.547 4500 21.545 218.295 198.654 88.386 257.773 -47.133 0.547 4600 21.697 219.234 199.510 92.705 257.876 -60.687 0.674 4800 21.697 219.690 199.925 94.872 257.926 -67.465 0.734 4900 21.748 220.138 200.333 97.045 257.974 -74.244 0.791 4900 21.748 220.138 200.333 97.045 257.974 -74.244 0.791 21.849 221.318 200.333 97.045 257.974 -74.244 0.791 21.899 221.435 201.514 103.592 258.021 -81.025 0.846 5500 21.899 221.435 201.891 105.784 258.150 -101.371 0.999 5400 21.997 222.264 202.267 107.982 258.100 -94.589 0.950 22.093 223.065 202.995 112.391 258.255 -121.775 1.056 5500 22.045 22.2668 202.654 110.184 258.224 -114.940 1.092 5500 22.1939 223.457 203.351 114.602 258.282 -128.510 1.178 5500 22.184 223.842 203.701 116.818 258.304 -135.296 1.218 5500 22.2184 223.842 203.701 116.818 258.304 -135.296 1.218 5500 22.2184 223.842 203.701 116.818 258.304 -135.296 1.218 5500 22.2184 223.842 203.701 116.818 258.304 -135.296 1.218 5500 22.2184 223.842 203.701 116.818 258.304 -135.296 1.218 5500 22.229 224.222 204.046 119.039 258.332 -148.869 1.296									
3700         21.170         214.117         194.845         71.305         257.309         7.030         -0.099           3800         21.213         214.682         195.360         73.424         257.373         0.265         -0.004           3900         21.237         215.234         195.862         75.547         257.436         -6.501         0.087           4000         21.302         215.772         196.353         77.675         257.496         -13.270         0.173           4100         21.349         216.299         196.834         79.808         257.554         -20.040         0.255           4200         21.397         216.814         197.303         81.945         257.611         -26.811         0.333           4300         21.495         217.812         198.213         86.234         257.720         -40.358         0.408           4400         21.956         217.812         198.213         86.234         257.720         -40.358         0.479           4500         21.595         198.654         88.386         257.773         -47.133         0.547           4600         21.697         219.234         199.510         92.705         257.876 <t< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></t<>									
3800   21,213   214,682   195,366   73,424   257,373   0,265   -0,004								-0.099	
3900 21.257 215.234 195.862 75.547 257.436 -6.501 0.087 4000 21.302 215.772 196.353 77.675 257.496 -13.270 0.173 4100 21.349 216.299 196.834 79.808 257.554 -20.040 0.255 4200 21.397 216.814 197.303 81.945 257.611 -26.811 0.333 4300 21.445 217.318 197.763 84.087 257.666 -33.583 0.408 4400 21.495 217.812 198.213 86.234 257.720 -40.358 0.479 4500 21.545 218.295 198.654 88.386 257.773 -47.133 0.547 4600 21.596 21.8769 199.086 90.543 257.825 -53.909 0.612 4700 21.647 219.234 199.510 92.705 257.876 -60.687 0.674 4800 21.697 219.690 199.925 94.872 257.926 -67.465 0.734 4900 21.748 220.138 200.333 97.045 257.974 -74.244 0.791 5000 21.799 220.578 200.734 99.222 258.021 -81.025 0.846 5100 21.899 221.435 201.514 103.592 258.066 -87.806 0.899 5200 21.899 221.435 201.514 103.592 258.110 -94.589 0.950 5300 21.949 221.853 201.893 105.784 258.150 -101.371 0.999 5400 21.997 222.664 202.267 107.982 258.189 -108.155 1.046 5500 22.193 223.457 203.351 114.602 258.282 -114.940 1.092 5600 22.193 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.	3800	21,213	214.682	195.360	73.424	257.373	0,265	-0.004	
4000         21,302         215,772         196,353         77.675         257,496         -13,270         0.173           4100         21,349         216,299         196,834         79,808         257,554         -20,040         0.255           4200         21,397         216,814         197,303         81,945         257,561         -26,811         0.333           4300         21,445         217,318         197,763         84,087         257,666         -33,583         0.408           4400         21,495         217,812         198,213         86,234         257,720         -40,358         0.479           4500         21,545         218,769         199,086         90,543         257,825         -53,909         0.612           4700         21,647         219,234         199,510         92,705         257,876         -60,687         0.674           4800         21,697         219,690         199,925         94,872         257,926         -67,465         0.734           4900         21,748         220,158         200,333         97,045         257,974         -74,244         0.791           5000         21,899         221,435         201,514         103,592	3900	21.257	215.234	195.862	75.547	257,436	-6.501	0.087	
4200         21.397         216.814         197.303         81.945         257.611         -26.811         0.333           4300         21.445         217.318         197.763         84.087         257.666         -33.583         0.408           4400         21.495         217.812         198.213         86.234         257.720         -40.358         0.479           4500         21.545         218.295         198.654         88.386         257.773         -47.133         0.547           4600         21.596         218.769         199.086         90.543         257.825         -53.909         0.612           4700         21.647         219.234         199.510         92.705         257.876         -60.687         0.674           4800         21.697         219.690         199.925         94.872         257.926         -67.465         0.734           4900         21.748         220.138         200.333         97.045         257.974         -74.244         0.791           5000         21.899         221.435         201.514         10.359         228.026         87.806         0.899           5200         21.899         221.435         201.514         10.359		21.302							
4300 21.445 217.318 197.763 84.087 257.666 -33.583 0.408 4400 21.495 217.812 198.213 86.234 257.720 -40.358 0.479 4500 21.545 218.295 198.654 88.386 257.773 -47.133 0.347 4600 21.596 218.769 199.086 90.543 257.825 -53.909 0.612 4700 21.647 219.234 199.510 92.705 257.876 -60.687 0.674 4800 21.748 220.138 200.333 97.045 257.976 -67.465 0.734 4900 21.748 220.138 200.333 97.045 257.974 -74.244 0.791 5000 21.799 220.578 200.734 99.222 258.021 -81.025 0.846 5100 21.849 221.010 201.127 101.405 258.066 -87.806 0.899 5200 21.899 221.435 201.514 103.592 258.100 -94.589 0.950 5300 21.949 221.853 201.893 105.784 258.150 -101.371 0.999 5400 21.949 222.264 202.267 107.982 258.180 -101.371 0.999 5500 22.045 222.668 202.634 110.184 258.224 -114.940 1.992 5500 22.093 223.065 202.995 112.391 258.255 -121.725 1.135 5700 22.184 223.842 203.701 116.818 258.232 -128.510 1.178 5800 22.184 223.842 203.701 116.818 258.332 -148.869 1.296									
4400 21.495 217.812 198.213 86.234 257.720 -40.358 0.479 4500 21.545 218.295 198.654 88.386 257.773 -47.133 0.547 4600 21.596 218.769 199.086 90.543 257.825 -53.909 0.612 4700 21.647 219.234 199.510 92.705 257.876 -60.687 0.674 4800 21.697 219.690 199.92.2 94.872 257.926 -67.465 0.734 4800 21.748 220.138 200.333 97.045 257.974 -74.244 0.791 5000 21.799 220.578 200.734 99.222 258.021 -81.025 0.846 100 21.899 221.435 201.514 103.592 258.10 -94.589 0.950 5300 21.949 221.853 201.514 103.592 258.110 -94.589 0.950 5300 21.949 222.658 201.593 105.784 258.150 -101.371 0.999 5400 21.997 222.644 202.267 107.982 258.189 -108.155 1.046 15500 22.045 222.668 202.634 110.184 258.224 -114.940 1.092 5600 22.093 223.065 202.995 112.391 258.255 -121.725 1.135 5700 22.189 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.184 223.842 203.701 116.818 258.304 -135.296 1.218 5900 22.229 224.222 204.046 119.039 258.332 -148.869 1.296									
4500 21.545 218.295 198.654 88.386 257.773 -47.133 0.547 4600 21.596 218.769 199.086 90.543 257.825 -53.909 0.612 4700 21.697 219.639 199.925 94.872 257.826 -60.687 0.674 4800 21.697 219.690 199.925 94.872 257.926 -67.465 0.734 4900 21.748 220.138 200.333 97.045 257.974 -74.244 0.791 5000 21.789 220.578 200.734 99.222 258.021 81.025 0.846 5100 21.849 221.010 201.127 101.405 258.066 -87.806 0.899 5200 21.899 221.435 201.514 103.592 258.110 -94.589 0.950 5300 21.899 221.435 201.514 103.592 258.110 -94.589 0.950 5300 21.949 221.853 201.893 105.784 258.150 -101.371 0.999 5400 21.997 222.264 202.267 107.982 258.189 -108.155 1.046 5500 22.045 222.668 202.634 110.184 258.224 -114.940 1.092 5600 22.093 223.065 202.995 112.391 258.255 -121.725 1.135 5700 22.139 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.184 223.842 203.701 116.818 258.304 -135.296 1.218 5900 22.229 224.222 204.046 119.039 258.321 -142.083 1.258 6000 22.273 224.596 204.385 121.264 258.332 -148.869 1.296							-40.358	0.479	
4600         21.596         218.769         199.086         90.543         257.825         -53,909         0.612           4700         21.647         219.234         199.510         92.705         257.876         -60.687         0.674           4800         21.697         219.690         199.925         94.872         257.926         -67.465         0.734           4900         21.748         220.138         200.333         97.045         257.974         -74.244         0.791           5000         21.899         220.578         200.734         99.222         258.021         -81.025         0.846           5100         21.849         221.010         201.127         101.405         258.066         -87.806         0.899           5200         21.899         221.435         201.514         103.592         258.110         -94.589         0.950           5300         21.997         222.264         202.267         107.982         258.150         -10.371         0.999           5400         22.095         223.065         202.995         112.391         258.224         -114.940         1.092           5500         22.095         223.365         202.995         112.391		21.545					-47.133	0.547	
4700 21.647 219.234 199.510 92.705 257.876 -60.687 0.674 4800 21.697 219.690 199.925 94.872 257.926 -67.465 0.734 4800 21.748 220.138 200.333 97.045 257.974 -74.244 0.791 5000 21.749 220.578 200.734 99.222 258.021 -81.025 0.846 100 21.849 221.010 201.127 101.405 258.066 -87.806 0.899 5200 21.899 221.435 201.514 103.592 258.110 -94.589 0.950 5300 21.949 221.853 201.893 105.784 258.150 -101.371 0.999 5400 21.997 222.264 202.267 107.982 258.189 -108.155 1.046 5500 22.045 222.668 202.6534 110.184 258.224 -114.940 1.092 5600 22.093 223.065 202.995 112.391 258.255 -121.725 1.135 5700 22.139 223.457 203.351 114.602 258.282 -128.510 1.178 5800 22.184 223.842 203.701 116.818 258.304 -135.296 1.218 5900 22.229 224.222 204.046 119.039 258.321 -142.083 1.258 6000 22.273 224.596 204.385 121.264 258.332 -148.869 1.296	4600	21.596	218.769	199.086	90,543				
4800         21,697         219,690         199,925         94,872         257,926         -67,465         0,734           4900         21,748         220,138         200,333         97,045         257,974         -74,244         0,791           5000         21,799         220,578         200,734         99,222         258,021         -81,025         0,846           5100         21,849         221,010         201,127         101,405         258,066         -87,806         0,899           5200         21,899         221,435         201,514         103,592         258,110         -94,589         0,950           5300         21,949         221,853         201,893         105,784         258,150         -101,371         0,999           5400         21,997         222,264         202,267         107,982         258,189         -108,155         1.046           5500         22,043         222,668         202,695         112,391         258,224         -11,494         1.092           5600         22,093         223,457         203,351         114,602         258,285         -121,725         1.135           5700         22,139         223,847         203,301         114,602 <td>4700</td> <td>21.647</td> <td>219.234</td> <td>199.510</td> <td>92,705</td> <td>257.876</td> <td>-60.687</td> <td>0.674</td>	4700	21.647	219.234	199.510	92,705	257.876	-60.687	0.674	
5000         21.799         220.578         200.734         99.222         258.021         -81.025         0.846           5100         21.849         221.010         201.127         101.405         258.066         -87.806         0.899           5200         21.899         221.435         201.514         103.592         258.110         -94.589         0.950           5300         21.949         221.853         201.893         105.784         258.150         -101.371         0.999           5400         21.997         222.664         202.667         107.982         258.189         -108.155         1.046           5500         22.045         222.668         202.634         110.184         258.224         -114.940         1.092           5600         22.093         223.065         202.995         112.391         258.255         -121.725         1.135           5700         22.184         223.842         203.701         116.818         258.304         -135.296         1.218           5900         22.2199         224.222         204.046         119.039         258.321         -142.083         1.258           6000         22.273         224.596         204.385         121.	4800	21.697	219.690	199.925	94,872				
5100         21.849         221.010         201.127         101.405         258.066         -87.806         0.899           5200         21.899         221.435         201.514         103.592         258.110         -94.589         0.950           5300         21.949         221.853         201.893         105.784         258.150         -101.371         0.999           5400         21.997         222.264         202.267         107.982         258.189         -108.155         1.046           5500         22.045         222.668         202.634         110.184         258.224         -114.940         1.092           5600         22.093         233.065         202.995         112.391         258.255         -121.725         1.135           5700         22.139         223.457         203.351         114.602         258.282         -128.510         1.178           5800         22.184         223.842         203.701         116.818         258.304         -135.296         1.218           5900         22.229         224.222         204.046         119.039         258.321         -142.083         1.258           6000         22.273         224.596         204.385         121		21.748							
5200         21.899         221.435         201.514         103.592         258.110         -94.589         0.950           5300         21.949         221.853         201.893         105.784         258.150         -101.371         0.999           5400         21.997         222.264         202.267         107.982         258.189         -108.155         1.046           5500         22.045         222.668         202.634         110.184         258.224         -114.940         1.092           5600         22.093         223.457         203.351         114.602         258.252         -121.725         1.135           5700         22.184         223.842         203.701         116.818         258.304         -135.296         1.218           5900         22.229         224.222         204.046         119.039         258.321         -142.083         1.258           6000         22.273         224.596         204.385         121.264         258.332         -148.869         1.296									
3300         21,949         221,853         201,893         105,784         258,150         -101,371         0.999           5400         21,997         222,264         202,267         107,982         258,189         -108,155         1.046           5500         22,045         222,668         202,634         110,184         258,224         -114,940         1.092           5600         22,093         223,065         202,995         112,391         258,282         -121,725         1.135           5700         22,139         223,457         203,351         114,602         258,282         -128,510         1.178           5800         22,184         223,842         203,701         116,818         258,304         -135,296         1.218           5900         22,299         224,222         204,046         119,039         258,321         -142,083         1.258           6000         22,273         224,596         204,385         121,264         258,332         -148,869         1.296							-94.589	0.950	
5400         21.997         222.264         202.267         107.082         258.189         -108.155         1.046           5500         22.045         222.668         202.634         110.184         258.224         -114.940         1.092           5600         22.093         223.065         202.995         112.391         258.255         -121.725         1.135           5700         22.139         223.457         203.351         114.602         258.282         -128.510         1.178           5800         22.184         223.842         203.701         116.818         258.304         -135.296         1.218           5900         22.229         224.222         204.046         119.039         258.321         -142.083         1.258           6000         22.273         224.596         204.385         121.264         258.332         -148.869         1.296	5300	21.949	221.853	201.893	105.784	258.150	-101.371	0.999	
5500         22,045         222,668         202,634         110,184         258,224         -114,940         1.092           5600         22,093         223,065         202,995         112,391         258,255         -121,725         1.135           5700         22,139         223,457         203,351         114,602         258,282         -128,510         1.178           5800         22,184         223,842         203,701         116,818         258,304         -135,296         1.218           5900         22,229         224,222         204,046         119,039         258,321         -142,083         1.258           6000         22,273         224,596         204,385         121,264         258,332         -148,869         1,296	5400	21.997	222.264	202,267	107.982	258.189	-108.155	1.046	
5700         22.139         223.457         203.351         114.602         258.282         -128.510         1.178           5800         22.184         223.842         203.701         116.818         258.304         -135.296         1.218           5900         22.229         224.222         204.046         119.039         258.321         -142.083         1.258           6000         22.273         224.596         204.385         121.264         258.332         -148.869         1.296	5500	22.045	222.668	202.634	110.184	258.224			
5700         22,139         223,457         203,351         114,602         258,282         -128,510         1.178           5800         22,184         223,842         203,701         116,818         258,304         -135,296         1.218           5900         22,229         224,222         204,046         119,039         258,321         -142,083         1,258           6000         22,273         224,596         204,385         121,264         258,332         -148,869         1,296									
5900         22.229         224.222         204.046         119.039         258.321         -142.083         1.258           6000         22.273         224.596         204.385         121.264         258.332         -148.869         1.296	5700	22.139	223.457						
6000 22.273 224.596 204.385 121.264 258.332 -148.869 1.296									
REVIOUS: March 1977 (1 atm) CURRENT; September 1982 (1 bar)				_ ,					
	REVIOUS:	March 197	77 (1 atm)			CURR	ENT: Septemb	er 1982 (1 bar)	

**NIST-JANAF THERMOCHEMICAL TABLES** 

 $S^{\circ}(298.15 \text{ K}) = 186.251 \pm 0.04 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ 

 $\Delta_{\rm f} H^{\circ}(0 \text{ K}) = -66.911 \pm 0.34 \text{ kJ} \cdot \text{mol}^{-1}$  E  $\Delta_{\rm f}H^{\circ}(298.15~{\rm K}) = -74.873 \pm 0.34~{\rm kJ \cdot mol^{-1}}$ 

Vibrational Frequencies and Degeneracies ν, cm<sup>-1</sup> 2916.5 (1) 1534.0 (2) 3018.7 (3) 1306 (3)

Ground State Quantum Weight: [1]  $\sigma = 12$ Point Group: T<sub>d</sub> Bond Distance:  $C-H = 1.091 \pm 0.002 \text{ Å}$ Bond Angle: H-C-H = 109.4712° Product of the Moments of Inertia:  $I_A I_B I_C = 1.499 \times 10^{-118} \text{ g}^3 \cdot \text{cm}^6$ .

# **Enthalpy of Formation**

Rossini1 measured the enthalpy of combustion of methane gas. His value at 298.15 K was corrected to the presently accepted molecular weight of water. The enthalpy of formation was calculated using -68.3174 and -94.0540 kcal·mol<sup>-1</sup> for the enthalpy of formation of H<sub>2</sub>O(1) and CO<sub>2</sub>(g), respectively.

## **Heat Capacity and Entropy**

Stevenson and Ibers,<sup>2</sup> calculated the bond distance from an analysis of available spectroscopic data. Vibrational frequencies listed by Jones and McDowell,3 are consistent with their results of a force constant calculation. The principal moments of inertia are:  $I_A = I_B = I_C = 0.5313 \times 10^{-39} \text{ g} \cdot \text{cm}^2$ .

## References

<sup>1</sup>F. D. Rossini, J. Res. Nat. Bur. Stand. 6, 37 (1931).

<sup>2</sup>D. P. Stevenson and J. A. Ibers, J. Chem. Phys. 33, 100 (1960).

<sup>3</sup>L. H. Jones and R. S. McDowell, J. Mol. Spectrosc. 3, 632 (1959).

Enthalpy R	eference To	emperature _J·K <sup>-1</sup> mol <sup>-</sup>	= T <sub>r</sub> = 298.15 I	<u> </u>	Standard Stat kJ·mol <sup>-1</sup>	e Pressure =	$p^{\circ} = 0.1 \text{ MPa}$
T/K	$C_p^o$		$G^{\circ}-H^{\circ}(T_{r})]/T$	$H^{\circ}-H^{\circ}(T_r)$	$\Delta_l H^\circ$	$\Delta_{\rm r}G^{\circ}$	log Kr
0	0.	0.	INFINITE	-10.024	-66.911	-66.911	INFINITE
100	33.258	149,500	216.485	-6.698	-69.644	-64.353	33.615
200 250	33,473 34,216	172.577	189.418	-3.368	-72.027	-58.161	15.190
		180.113	186.829	-1.679	-73,426	-54.536	11.395
298,15 300	35.639	186.251	186.251	0.	-74.873	-50.768	8.894
350 350	35.708 37.874	186.472 192.131	186.252 186.694	0.066 1.903	-74.929 -76.461	-50.618 -46.445	8.813 6.932
400	40,500	197.356	187.704	3.861	-76.461 -77.969	-40.443 -42.054	5,492
450	43,374	202.291	189.053	5.957	-79,422	-37.476	4.350
500	46.342	207,014	190.614	8,200	-80.802	-32.741	3.420
600	52.227	215.987	194.103	13.130	-83.308	-22.887	1.993
700	57.794	224.461	197.840	18.635	-85,452	-12.643	0.943
800	62.932	232.518	201.675	24.675	-87.238	-2.115	0.138
900	67.601	240.205	205,532	31.205	-88.692	8.616	-0.500
1000	71.795	247.549	209,370	38.179	-89.849	19.492	-1.018
1100	75.529	254.570	213,162	45,549	-90,750	30.472	-1.447
1200	78.833	261.287	216,895	53.270	-91.437	41,524	-1.807
1300	81.744	267.714	220.558	61.302	-91.945	52,626	-2.115
1400 1500	84.305	273.868	224,148	69.608	-92.308	63,761	-2.379
	86,556	279.763	227,660	78.153	-92.553	74.918	-2.609
1600	88.537	285.413	231.095	86.910	-92,703	86.088	-2.810
1700 1800	90.283 91.824	290.834 296.039	234.450	95.853	-92.780	97.265	-2.989
1900	91.824	301.041	237.728 240.930	104.960 114.212	-92.797 -92.770	108.445 119.624	-3.147 -3.289
2000	94,399	305.853	244.057	123.592	-92.770 -92.709	130.802	-3.416
		310.485					
2100 2200	95,477 96,439	314.949	247.110 250.093	133.087 142.684	-92.624 -92.521	141,975 153,144	-3.531 -3.636
2300	97.301	319.255	253.007	152.371	-92.409	164.308	-3,732
2400	98.075	323.413	255,854	162,141	-92.291	175,467	-3,819
2500	98,772	327,431	258,638	171.984	-92.174	186,622	-3.899
2600	99,401	331.317	261.359	181.893	-92,060	197,771	-3.973
2700	99,971	335.080	264.020	191.862	-91.954	208,916	-4.042
2800	100.489	338.725	266.623	201.885	-91.857	220.058	-4.105
2900	100.960	342.260	269.171	211.958	-91.773	231.196	-4.164
3000	101,389	345,690	271.664	222.076	-91.705	242.332	-4.219
3100	101.782	349.021	274,106	232,235	-91.653	253.465	-4.271
3200	102.143	352.258	276.498	242.431	-91.621	264.598	-4.319
3300	102.474	355.406	278.842	252,662	-91.609	275.730	-4.364
3400	102.778	358.470	281.139	262.925	-91.619	286.861	-4.407
3500	103.060	361.453	283.391	273,217	-91.654	297.993	-4.447
3600	103.319	364.360	285.600	283.536	-91.713	309.127	-4,485
3700 3800	103.560 103.783	367.194	287,767	293.881	-91.798	320.262	-4.521
3900	103,783	369.959 372.658	289.894 291.982	304.248 314.637	-91.911 -92.051	331.401 342.542	-4.555 -4.588
4000	104,183	375.293	294.032	325.045	-92.031 -92.222	353.687	-4.619
4100	104,363	377.868	296.045	335.473	-92.422	364.838	-4.648
4200	104,533	380,385	298.023	345.918	-92.422 -92.652	375.993	-4.676
4300	104,688	382.846	299.967	356.379	-92.914	387.155	-4.703
4400	104.834	385.255	301.879	366,855	-93.208	398.322	-4.729
4500	104.972	387.612	303.758	377.345	~93.533	409.497	-4.753
4600	105,101	389.921	305.606	387.849	-93.891	420,679	-4.777
4700	105.223	392.182	307,424	398,365	-94.281	431,869	-4.800
4800	105.337	394.399	309.213	408,893	-94.702	443.069	-4.822
4900	105.445	396.572	310.973	419.432	-95.156	454.277	-4.843
5000	105.546	398.703	312.707	429.982	95.641	465.495	-4.863
5100	105.642	400.794	314.414	440.541	-96.157	476.722	-4.883
5200	105,733	402.847	316.095	451.110	-96.703	487.961	-4.902
5300	105.818	404,861	317.750	461.688	-97.278	499.210	-4.920
5400 5500	105,899 105,976	406,840 408,784	319,382	472.274	-97.882	510,470	-4.938
			320.990	482.867	-98,513	521.741	-4,955
5600	106.049	410.694	322.575	493.469	-99.170	533.025	-4.972
5700 5800	106.118	412.572	324.137	504.077	-99.852	544.320	-4.988
5900 5900	106.184 106.247	414.418 416.234	325,678 327,197	514,692 525,314	-100.557 -101.284	555.628 566.946	-5.004 -5.019
6000	106.247	418.020	327.197 328.696	535.942	-101.284 -102.032	506.946 578.279	-5.019 -5.034
0000	150,500	410,040	540.070	JJJ.744	102.032	310.219	3.034

MALCOLM W. CHASE

 $S^{\circ}(298.15 \text{ K}) = 194.171 \pm 1.3 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ 

 $\Delta_1 H^{\circ}(0 \text{ K}) = 149.031 \pm 0.8 \text{ kJ} \cdot \text{mol}^{-1}$  $\Delta_0 H^{\circ}(298.15 \text{ K}) = 145.687 \pm 0.8 \text{ kJ·mol}^{-}$ 

Electronic Levels and	d Quantum Weights
$\epsilon_i$ , cm <sup>-1</sup>	g <sub>i</sub>
0	2
46205	2
Vibrational Frequencie ν, cm	
[3002] (	1)
580 (	(1)
[3184] (	(2)
1383 (	2)

Point Group: D3h

Bond Distance: C-H = 1.079 Å

Bond Angle:  $H-C-H = 120^{\circ}$ 

Product of the Moments of Inertia:  $I_A I_B I_C = 4.99 \times 10^{-119} \text{ g}^3 \cdot \text{cm}^6$ 

## **Enthalpy of Formation**

Chupka' measured the photoionization spectrum of methane and from the onset of  $CH_1^*$  production has reported  $\Delta_a H^o$  $(CH_3-H) = 103.244 \pm 0.12$  kcal mol<sup>-1</sup>. The value was corrected for the thermal rotation energy of the fragment ions and is the value adopted

 $\sigma = 6$ 

Dibeler et al. had earlier reported  $\Delta_{al}H^{o}(CH_{3}-H) = 101.7 \pm 0.5 \text{ kcal} \cdot \text{mol}^{-1}$  but they did not apply the rotational energy correction, which bring them closer to Chupka.

The photoionization values are in good agreement with earlier electron impact determinations as summarized by Stevenson<sup>3</sup> who gives  $\Delta_{ai}H^{\circ}(CH_3-H) = 101.9 \pm 1 \text{ kcal·mol}^{-1}$ . Kinetic determinations have been recently reviewed by Kerr<sup>4</sup> and yield  $\Delta_{ai}H^{\circ}(CH_3-H) = 102.5 \pm 1$ kcal·mol<sup>-1</sup> again in excellent agreement.

## **Heat Capacity and Entropy**

The structure, bond length, angles and electronic levels are those reported by Herzberg.<sup>5</sup> A set of vibrational frequencies have been reported by Andrews and Pimentel<sup>6</sup> in an argon matrix, of which only two were observed. Milligan and Jacox<sup>7</sup> observed  $\nu_2 = 611 \text{ cm}^{-1}$  in an argon matrix and disagreed with Andrews and Pimentel who reported 730 cm<sup>-1</sup>. Later, Tan and Pimentel<sup>8</sup> agreed that the earlier values were for a methyl radical interacting with an alkali halide molecule. This would affect the v<sub>2</sub> mode strongest, thus, we adopt the remaining in plane frequencies which appear to be of the correct magnitudes. The  $\nu_2$  mode is taken from the analysis of Herzberg<sup>5</sup> since this represents the gas phase molcule and is in resonable agreement with the matrix value of Milligan and Jacox. The uncertainty in the entropy reflects the uncertainties in the vibrational frequencies.

The principal moments of inertia are:  $I_A = I_B = 0.2923 \times 10^{-39}$ , and  $I_C = 0.5846 \times 10^{-39}$  g·cm<sup>2</sup>.

### References

<sup>1</sup>W. A. Chupka, J. Chem. Phys. 48, 2337 (1968).

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Inthalpy Reference Temperature = $T_r$ = 298.15 K 				K S	Standard State Pressure = p° = 0.1 MPa			
<i>T/</i> K	C° C	-	°-H°(T,)]/T	$H^{\circ}-H^{\circ}(T_{r})$	$\Delta_t H^\circ$	Δ <sub>r</sub> G°	log K <sub>f</sub>	
0	0.	0.	INFINITE	-10.407	149.031	149,031	INFINITE	
100	33.395	155.665	226.465	-7.080	147.800	147,438	-77.014	
200	35.638	179.380	197.609	-3.646	146.868	147.432	-38.505	
250	37.162	187,495	194.799	-1.826	146.297	147.637	-30.847	
298.15	38.693	194.170	194.170	0.	145.687	147.950	-25.920	
300	38.753	194.410	194.171	0.072	145.663	147.964	-25.763	
350	40.392	200.506	194.649	2.050	144.997	148.400	-22.147	
400	42.041	206.008	195.730	4.111	144.320	148.932	-19.449	
450 500	43.668 45.252	211.054 215.737	197.156 198.783	6.254 8.477	143.644 142.976	149,549 150,241	-17.359 -15.696	
600	48.288	224.258	202,333	13.155	141.682	151.817	- 13,217	
700	51.174	231.921	206.021	18.130	140,477	153,602	-11.462	
800	53,926	238.935	209.703	23,386	139.383	155.554	-10.157	
900	56.527	245.438	213.316	28.910	138.411	157.635	-9.149	
1000	58.954	251.521	216.836	34.686	137.557	159.817	-8.348	
1100	61.187	257.247	220.252	40.694	136.814	162.080	-7.697	
1200	63.217	262.659	223.562	46.916	136.167	164.406	-7.156	
1300 1400	65.048 66.690	267,793 272,675	226.769 229.875	53,331 59,919	135.602	166.783 169.201	-6.701 -6.313	
1500	68.156	277,327	232.885	66,663	135.105 134.662	171,652	-5.97 <b>7</b>	
1600	69.463	281.768	235,802	73.545	134,262	174,131	-5.685	
1700	70.628	286.015	238,632	80.551	133,896	176.634	-5.427	
1800	71,667	290.082	241,378	87.667	133,554	179.158	-5.199	
1900	72.594	293,982	244.045	94.881	133.230	181.701	-4.995	
2000	73.422	297,727	246.636	102.182	132.917	184,260	-4.812	
2100	74.165	301,327	249.155	109.562	132.610	186.835	-4.647	
2200	74.831	304.793	251,606	117.013	132,305	189.424	-4.497	
2300 2400	75.430	308.133	253,991	124.526	131.999	192.027	-4.361 -4.236	
2500	75.971 76.459	311.355 314.466	256.315 258.579	132.097 139.719	131.688 131.369	194.644 197.273	-4.236 -4.122	
2600	76.902	317.474	260.787	147,387		199.916	-4.016	
2700	77.304	320.384	262.940	155.098	131.041 130.701	202.571	-3.919	
2800	77.670	323.202	265.042	162.847	130.348	205.239	-3.829	
2900	78.003	325.933	267.095	170.630	129,980	207.921	-3.745	
3000	78.309	328,583	269.101	178.446	129.595	210,615	-3,667	
3100	78.588	331.155	271.061	186.291	129.193	213.322	-3.594	
3200	78.845	333.655	272.979	194.163	128.772	216.042	-3.527	
3300 3400	79.082	336.084 338.449	274,854	202.060	128.331	218.777	-3.463 -3.403	
3500	79,300 79,501	340.750	276,690 278,488	209.979 217.919	127.869 127.385	221.524 224.286	-3.347	
3600	79.687	342.992	280.248	225,879	126.879	227.061	-3.295	
3700	79.860	345,178	281.974	233,856	126.349	229,852	-3.245	
3800	80.020	347.310	283.665	241,850	125.796	232,656	-3.198	
3900	80.169	349.391	285.324	249,860	125.217	235.476	-3.154	
4000	80.308	351.422	286.951	257.884	124.613	238.311	-3.112	
4100	80.438	353.407	288.548	265.921	123.984	241.161	-3.072	
4200	80,559	355.346	290.115	273.971	123,328	244.027	-3.035	
4300 4400	80.672 80.778	357.243 359.099	291.654 293.166	282.033 290.105	122.645 121.936	246,909 249,807	-2.999 -2.966	
4500	80.778	360.916	294.652	298.188	121.930	252.721	-2.934	
4600	80.972	362.694	296.112	306.281	120,436	255.652	-2.903	
4700	81.060	364.437	297.547	314.382	119.645	258.600	-2.874	
4800	81.143	366.144	298.958	322.492	118.827	261.565	-2.846	
4900	81.221	367.818	300.347	330.611	117.982	264.547	-2.820	
5000	81.295	369.460	301.712	338,737	117.111	267.548	-2.795	
5100	81,365	371.070	303,057	346.870	116,214	270.565	-2.771	
5200	81,432	372.651	304,380	355.009	115.292	273,601	-2.748	
5300 5400	81.495 81.554	374.203	305.683	363.156	114.345	276,654	-2.727	
5500	81.554	375,726 377,223	306,966 308,230	371,308 379,467	113.373 112.379	279,726 282,815	-2.706 -2.686	
5600	81.666	378.694	309,475			285.923	-2.667	
5700	81.718	380.140	309.473	387.630 395.800	111.362 110.324	285.923 289.050	-2.667 2.649	
5800	81.767	381.562	311.911	403,974	109.266	292.195	-2.631	
5900	81.815	382.960	313,104	412.153	108.188	295.357	-2.615	
6000	81.860	384.336	314,280	420.337	107.094	298,539	-2.599	
EVIOUS-	June 1969	(1 atm)				CURRENT: Jun	ic 1969 (1 har)	
		·						

Methyl (CH<sub>3</sub>) C1H3(g)

MALCOLM W. CHAS

## **Enthalpy of Formation**

 $\Delta_t H^o(OH, g, 0 \text{ K})$  is calculated from the relation  $\Delta$   $H^o(OH, g, 0 \text{ K}) = 1/2$   $D_0^o(O_2) + 1/2$   $D_0^o(H_2) = D_0^o(OH)$ . are as follows:  $D_0^o(O_2) = 117.967 \pm 0.042$  kcal·mol<sup>-1</sup> and  $D_0^o(H_2) = 103.267 \pm 0.003$  kcal·mol<sup>-1</sup> were taken from the CODATA¹ selection. Barrow² in a refinement of the work of Barrow and Downie³ obtains a value of  $D_0^o$  for  $OH(X^2\Pi_{3/2}) \to O(^3P_2) + H(^2S_{1/2})$  of 35427 cm<sup>-1</sup> from an extrapolation of  $\Delta_{vap}G$  versus v; it was increased to 35450  $\pm$  100 cm<sup>-1</sup> to account for the fact that  $\Delta_{vap}G$  yields slightly low values at high v. Fehlenbok⁴ obtains a value of  $D_0^o$  for  $OH(B^2\Sigma^+)$  of 1315 cm<sup>-1</sup> and O(D) for this state of 441 cm<sup>-1</sup>. Using  $T_e(B^2\Sigma^+)$  given by Rosen⁵ and the zero point energy of HO (including the Dunham correction, see Herzberg)⁶ of 847.0 cm<sup>-1</sup>, this yields  $D_0^o(OH) = 35451$  cm<sup>-1</sup> with an estimated uncertainty of 100 cm<sup>-1</sup>. A value of  $D_0^o(OH) = 35450 \pm 100$  cm<sup>-1</sup> = 101.356  $\pm$  0.29 kcal·mol<sup>-1</sup> was adopted. Combining the above values, one obtains  $\Delta_t H^o(OH, g, 0 \text{ K}) = 9.261 \pm 0.29$  kcal·mol<sup>-1</sup> which is in good agreement with the last JANAF<sup>7</sup> selection.

### Heat Capacity and Entropy

The vibrational and rotational constants of the respective electronic levels were taken from Rosen.<sup>5</sup> Comparison of the results of these calculations with those of the more exact treatment given by Haar et al.<sup>10</sup> suggests that errors in the tables due to approximations in our calculations may be neglected above 400 K. Below this, they may be appreciable. It is recommended that  $H^o(0 \text{ K})-H^o(298.15 \text{ K})$ ,  $S^o(298.15 \text{ K})$  and  $C_p^o(298.15 \text{ K})$  be taken as  $-2.107 \text{ kcal·mol}^{-1}$ ,  $43.890 \text{ kJ·mol}^{-1}$ , and  $7.144 \text{ kJ·mol}^{-1}$ , respectively. These errors result from dealing with the ground state ( $X^2\Pi_0$ ) as two separate electronic states separated by 139.7 cm<sup>-1</sup>

The thermodynamic functions are calculated using first-order anharmonic corrections to  $Q_i^t$  and  $Q_v^t$  in the partition function  $Q = Q_v \Sigma Q_v^t Q_v^t Q_v = x_0 - x_0 - x_0 = x_0$ . The National Bureau of Standards prepared this table 11 by critical analysis of data existing in 1972. Using molecular constants and  $\Delta_t H^0$  selected by NBS, 11 we recalculate the table in terms of 1973 fundamental constants, 12 1975 atomic weights 13 and current JANAF reference states for the elements.

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Enthalpy Reference Temperature = $T_r$ = 298.15 K Standard State Pressure = $p^{\circ}$ = 0.1 MPa $J$ -K- $J$ -mol <sup>-1</sup> $J$ -							
<i>T/</i> K	C,°		$G^{\circ}-H^{\circ}(T_{r})]/T$	$H^{\circ}-H^{\circ}(T_{r})$	_kJ·mol¯¹_ ∆ <sub>r</sub> H°	Δ <sub>r</sub> G°	log Kr
0	0.	0.	INFINITE	-9.172	38.390	38.390	INFINITE
100	32.627	149,590	210,980	-6,139	38.471	37.214	-19.438
200	30,777	171,592	186,471	-2.976	38.832	35.803	-9.351
250	30.283	178.402	184.204	-1.450	38.930	35.033	-7.320
298,15	29.986	183.708	183.708	0.	38.987	34,277	6.005
300	29.977	183.894	183,709	0.055	38,988	34,248	-5.963
350	29.780	188.499	184.073	1.549	39.019	33.455	-4.993
400	29.650	192.466	184.880	3.035	39.029	32.660	-4.265
450	29.567	195.954	185.921	4.515	39.020	31.864	-3.699
500	29.521	199.066	187.082	5.992	38,995	31.070	-3.246
600	29,527	204,447	189,542	8.943	38.902	29.493	-2.568
700	29,663	209.007	192,005	11.902	38.764	27.935	-2.085
800	29.917	212.983	194.384	14.880	38,598	26.399	-1.724
900	30.264	216.526	196.651	17.888	38.416	24.884	1.444
1000	30.676	219.736	198.801	20.935	38.230	23.391	-1.222
1100	31.124	222.680	200.840	24.024	38.046	21,916	1.041
1200	31.586	225.408	202.775	27.160	37.867	20,458	-0.891
1300	32.046	227.955	204.615	30.342	37.697	19,014	-0.764
1400	32.492	230.346	206.368	33.569	37.535	17,583	-0.656
1500	32.917	232.602	208.043	36,839	37.381	16.163	-0.563
1600	33.319	234.740	209,645	40,151	37.234	14.753	-0.482
1700	33.694	236.771	211.182	43.502	37.093	13.352	-0.410
1800 1900	34.044 34.369	238.707 240.557	212.657	46.889 50,310	36.955 36,819	11.960 10.575	-0.347 -0.291
2000	34,670	240.337	214.078 215.446	53,762	36.685	9.197	-0.240
2100 2200	34.950 35,209	244.026 245,658	216.767 218.043	57.243 60.752	36,551 36,416	7.826 6.462	-0.195 -0.153
2300	35,449	247,228	219.278	64.285	36.278	5.103	-0.116
2400	35,673	248.741	220.474	67.841	36.137	3.750	-0.082
2500	35.881	250.202	221,635	71.419	35.992	2,404	-0.050
2600	36.075	251.613	222.761	75.017	35.843	1,063	-0.021
2700	36.256	252.978	223.855	78.633	35.689	-0.271	0.005
2800	36.426	254,300	224.918	82.267	35.530	-1.600	0.030
2900	36,586	255,581	225.954	85.918	35.365	-2.924	0.053
3000	36.736	256.824	226.962	89.584	35.194	-4.241	0.074
3100	36.878	258.031	227.945	93.265	35.017	-5.552	0.094
3200	37.013	259.203	228,904	96.960	34.834	-6.858	0.112
3300	37.140	260,344	229.839	100.667	34.644	-8.158	0.129
3400	37.261	261.455	230.753	104.387	34.448	-9.452	0,145
3500	37.376	262.537	231.645	108.119	34.246	-10.741	0.160
3600	37.486	263.591	232.518	111.863	34.037	-12.023	0.174
3700	37.592	264.620	233.372	115.617	33.821	-13.300	0.188
3800	37.693	265.624	234.208	119.381	33.599	-14.570 -15.834	0.200 0.212
3900 4000	37.791 37.885	266.604 267.562	235.026 235.827	123.155 126.939	33,371 33,136	-17,093	0.212
							0.234
4100 4200	37.976 38.064	268.499 269.415	236.613 237.383	130.732 134.534	32,894 32,646	-18.346 -19.593	0.234
4300	38.150	270.311	238.138	138,345	32,340	-20.833	0.253
4400	38.233	271.189	238.879	142.164	32.130	-22.068	0.262
4500	38.315	272.050	239.607	145.991	31.862	-23.297	0.270
4600	38.394	272.893	240.322	149.827	31.587	-24.520	0.278
4700	38,472	273,719	241,023	153.670	31.305	-25.737	0.286
4800	38,549	274,530	241,713	157,521	31.017	-26.947	0.293
4900	38,625	275,326	242,391	161,380	30.722	-28.152	0.300
5000	38.699	276.107	243.057	165,246	30.420	-29.350	0.307
5100	38.773	276.874	243.713	169.120	30.111	-30.542	0.313
5200	38.846	277.627	244.358	173.001	29.796	-31.729	0.319
5300	38,919	278,368	244.993	176.889	29.473	-32.909	0.324
5400	38.991	279,096	245,617	180,784	29.144	-34.083	0.330
5500	39.062	279.812	246.233	184.687	28.807	-35.251	0.335
5600	39.134	280.517	246.839	188.597	28.464	-36.412	0.340
5700	39.206	281.210	247.436	192.514	28,113	-37.568	0.344
5800	39.278	281.892	248.024	196,438	27.756	-38.716	0.349
5900	39.350	282.564	248.604	200.369	27,391	-39,860	0.353
6000	39.423	283.226	249.175	204.308	27,019	-40.997	0.357
PREVIOUS: .	June 1977	(1 atm)				CURRENT: Ju	ine 1977 (1 bar)