

CNN : CNN Radical

Enthalpy of Formation at 0 K:

JANAF [1]:	$\Delta H(0K)=584.00 \pm 126.00$ kJ/mol
Gurvich et al[2]:	$\Delta H(0K)=632.83 \pm 100.00$ kJ/mol
A. Burcat and B. Ruscic[3]:	$\Delta H(0K)=591.22 \pm 3.19$ kJ/mol
ORCA[2, 4] DFT:	$\Delta H(0K)=535.79 \pm 10.00$ kJ/mol

Molar Mass : 40.024399 g/mol

σ 1

Vibrational Frequencies and Degeneracies (cm^{-1}) [4]:

1285.74(1) 407.9(1) 1513.07(1) 407.84(1)

Inertia Moment I :

6.34947e-46 ($\text{kg}\cdot\text{m}^2$)

Electronic Levels Energy and Degeneracies (cm^{-1}) [4]:

0.00(3)

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References:

- [1] NIST-JANAF Thermochemical Tables NIST Standard Reference Database 13 Last Update to Data Content: 1998 DOI: 10.18434/T42S31
- [2] L.V. Gurvich, I.V. Veyts, C.B. Alcock, Thermodynamic Properties of Individual Substances, Hemisphere Publishing Corporation, 1991
- [3] A. Burcat and B. Ruscic, Third Millennium Ideal Gas and Condensed Phase Thermochemical Database for Combustion with Updates from Active Thermochemical Tables, 2005
- [4] Neese, F. Software update: the ORCA program system, version 5.0 WIREs Comput. Molec. Sci., 2022 12(1)e1606 doi.org/10.1002/wcms.1606

CALCULATION AT THERMAL EQUILIBRIUM Tex=Tvib=Trot=Th
(P=1 bar=0.1 MPa)

T	Cp	h	s	g	zint	ztr
K	J/K/mol	kJ/mol	J/K/mol	kJ/mol	-	-
100.00	30.729	2.938	192.011	-16.263	4.756e+02	6.570e+05
150.00	34.406	4.564	205.150	-26.208	7.387e+02	1.811e+06
200.00	37.680	6.370	215.517	-36.733	1.055e+03	3.717e+06
250.00	40.196	8.319	224.206	-47.732	1.447e+03	6.493e+06
298.15	42.209	10.304	231.462	-58.706	1.910e+03	1.008e+07
300.00	42.282	10.383	231.724	-59.135	1.930e+03	1.024e+07
350.00	44.157	12.544	238.384	-70.890	2.522e+03	1.506e+07
400.00	45.897	14.796	244.396	-82.962	3.241e+03	2.103e+07
450.00	47.509	17.132	249.896	-95.321	4.109e+03	2.822e+07
500.00	48.984	19.545	254.979	-107.945	5.148e+03	3.673e+07
550.00	50.318	22.028	259.711	-120.813	6.384e+03	4.661e+07
600.00	51.511	24.574	264.142	-133.911	7.847e+03	5.794e+07
650.00	52.571	27.177	268.307	-147.223	9.568e+03	7.077e+07
700.00	53.509	29.829	272.238	-160.738	1.158e+04	8.518e+07
750.00	54.337	32.526	275.959	-174.444	1.392e+04	1.012e+08
800.00	55.069	35.261	279.490	-188.331	1.664e+04	1.189e+08
850.00	55.715	38.031	282.848	-202.390	1.977e+04	1.384e+08
900.00	56.287	40.831	286.049	-216.613	2.335e+04	1.597e+08
950.00	56.794	43.659	289.106	-230.992	2.745e+04	1.828e+08
1000.00	57.244	46.510	292.031	-245.521	3.212e+04	2.078e+08
1050.00	57.646	49.382	294.834	-260.193	3.741e+04	2.347e+08
1100.00	58.004	52.274	297.524	-275.003	4.339e+04	2.637e+08
1150.00	58.326	55.182	300.110	-289.944	5.012e+04	2.947e+08
1200.00	58.614	58.106	302.598	-305.012	5.767e+04	3.277e+08
1250.00	58.875	61.043	304.996	-320.202	6.612e+04	3.630e+08
1300.00	59.110	63.993	307.310	-335.510	7.554e+04	4.004e+08
1350.00	59.322	66.954	309.545	-350.932	8.602e+04	4.400e+08
1400.00	59.516	69.925	311.706	-366.463	9.765e+04	4.818e+08
1450.00	59.692	72.905	313.797	-382.101	1.105e+05	5.260e+08
1500.00	59.852	75.894	315.824	-397.842	1.247e+05	5.726e+08
1550.00	59.999	78.890	317.789	-413.683	1.404e+05	6.215e+08
1600.00	60.134	81.893	319.696	-429.620	1.575e+05	6.728e+08
1650.00	60.258	84.903	321.548	-445.651	1.764e+05	7.266e+08
1700.00	60.372	87.919	323.349	-461.774	1.970e+05	7.829e+08
1750.00	60.477	90.940	325.100	-477.985	2.196e+05	8.417e+08
1800.00	60.574	93.967	326.805	-494.283	2.441e+05	9.032e+08
1850.00	60.664	96.998	328.466	-510.665	2.708e+05	9.672e+08
1900.00	60.748	100.033	330.085	-527.129	2.999e+05	1.034e+09
1950.00	60.825	103.072	331.664	-543.673	3.314e+05	1.103e+09
2000.00	60.897	106.115	333.205	-560.295	3.655e+05	1.175e+09
2050.00	60.965	109.162	334.710	-576.993	4.024e+05	1.250e+09
2100.00	61.027	112.212	336.180	-593.765	4.422e+05	1.328e+09
2150.00	61.086	115.265	337.616	-610.610	4.851e+05	1.408e+09
2200.00	61.141	118.320	339.021	-627.526	5.313e+05	1.492e+09
2250.00	61.193	121.379	340.396	-644.512	5.810e+05	1.578e+09
2300.00	61.241	124.439	341.741	-661.566	6.344e+05	1.667e+09
2350.00	61.286	127.503	343.059	-678.686	6.916e+05	1.759e+09
2400.00	61.329	130.568	344.350	-695.871	7.529e+05	1.854e+09
2450.00	61.369	133.636	345.615	-713.120	8.185e+05	1.952e+09
2500.00	61.407	136.705	346.855	-730.432	8.886e+05	2.053e+09
2550.00	61.443	139.776	348.071	-747.805	9.635e+05	2.157e+09
2600.00	61.477	142.849	349.265	-765.239	1.043e+06	2.265e+09
2650.00	61.509	145.924	350.436	-782.731	1.128e+06	2.375e+09
2700.00	61.540	149.000	351.586	-800.282	1.219e+06	2.489e+09

2750.00	61.568	152.078	352.715	-817.890	1.315e+06	2.606e+09
2800.00	61.596	155.157	353.825	-835.553	1.418e+06	2.726e+09
2850.00	61.622	158.237	354.916	-853.272	1.526e+06	2.849e+09
2900.00	61.646	161.319	355.987	-871.044	1.641e+06	2.976e+09
2950.00	61.670	164.402	357.041	-888.870	1.764e+06	3.106e+09
3000.00	61.692	167.486	358.078	-906.748	1.893e+06	3.239e+09
3050.00	61.713	170.571	359.098	-924.678	2.030e+06	3.375e+09
3100.00	61.733	173.657	360.102	-942.658	2.174e+06	3.516e+09
3150.00	61.753	176.745	361.090	-960.688	2.327e+06	3.659e+09
3200.00	61.771	179.833	362.062	-978.767	2.488e+06	3.806e+09
3250.00	61.789	182.922	363.020	-996.894	2.658e+06	3.956e+09
3300.00	61.806	186.012	363.964	-1015.068	2.837e+06	4.110e+09
3350.00	61.822	189.102	364.893	-1033.290	3.026e+06	4.268e+09
3400.00	61.837	192.194	365.809	-1051.557	3.225e+06	4.429e+09
3450.00	61.852	195.286	366.712	-1069.871	3.434e+06	4.593e+09
3500.00	61.866	198.379	367.602	-1088.229	3.654e+06	4.762e+09
3550.00	61.880	201.473	368.480	-1106.630	3.885e+06	4.934e+09
3600.00	61.893	204.567	369.345	-1125.076	4.127e+06	5.109e+09
3650.00	61.905	207.662	370.199	-1143.565	4.382e+06	5.288e+09
3700.00	61.917	210.757	371.041	-1162.096	4.649e+06	5.471e+09
3750.00	61.929	213.853	371.873	-1180.669	4.929e+06	5.658e+09
3800.00	61.940	216.950	372.693	-1199.283	5.222e+06	5.849e+09
3850.00	61.951	220.047	373.503	-1217.938	5.529e+06	6.043e+09
3900.00	61.961	223.145	374.302	-1236.633	5.850e+06	6.241e+09
3950.00	61.971	226.244	375.092	-1255.368	6.186e+06	6.443e+09
4000.00	61.980	229.342	375.871	-1274.142	6.538e+06	6.649e+09
4050.00	61.989	232.442	376.641	-1292.955	6.905e+06	6.858e+09
4100.00	61.998	235.541	377.402	-1311.806	7.289e+06	7.072e+09
4150.00	62.007	238.641	378.153	-1330.695	7.689e+06	7.290e+09
4200.00	62.015	241.742	378.896	-1349.621	8.107e+06	7.511e+09
4250.00	62.023	244.843	379.630	-1368.584	8.543e+06	7.737e+09
4300.00	62.031	247.944	380.355	-1387.584	8.997e+06	7.966e+09
4350.00	62.038	251.046	381.073	-1406.620	9.471e+06	8.200e+09
4400.00	62.045	254.148	381.782	-1425.691	9.965e+06	8.438e+09
4450.00	62.052	257.250	382.483	-1444.798	1.048e+07	8.679e+09
4500.00	62.059	260.353	383.176	-1463.939	1.101e+07	8.925e+09
4550.00	62.065	263.456	383.862	-1483.115	1.157e+07	9.175e+09
4600.00	62.072	266.560	384.540	-1502.325	1.215e+07	9.429e+09
4650.00	62.078	269.663	385.211	-1521.569	1.275e+07	9.688e+09
4700.00	62.084	272.768	385.875	-1540.846	1.338e+07	9.950e+09
4750.00	62.089	275.872	386.532	-1560.157	1.403e+07	1.022e+10
4800.00	62.095	278.976	387.182	-1579.500	1.470e+07	1.049e+10
4850.00	62.100	282.081	387.826	-1598.875	1.540e+07	1.076e+10
4900.00	62.105	285.186	388.463	-1618.282	1.613e+07	1.104e+10
4950.00	62.111	288.292	389.094	-1637.721	1.688e+07	1.133e+10
5000.00	62.115	291.398	389.718	-1657.191	1.766e+07	1.161e+10
5050.00	62.120	294.503	390.336	-1676.693	1.848e+07	1.191e+10
5100.00	62.125	297.610	390.948	-1696.225	1.932e+07	1.220e+10
5150.00	62.129	300.716	391.554	-1715.787	2.019e+07	1.251e+10
5200.00	62.134	303.822	392.154	-1735.380	2.109e+07	1.281e+10
5250.00	62.138	306.929	392.749	-1755.003	2.202e+07	1.312e+10
5300.00	62.142	310.036	393.338	-1774.655	2.299e+07	1.344e+10
5350.00	62.146	313.143	393.921	-1794.336	2.399e+07	1.376e+10
5400.00	62.150	316.251	394.500	-1814.047	2.503e+07	1.408e+10
5450.00	62.154	319.358	395.072	-1833.786	2.610e+07	1.441e+10
5500.00	62.157	322.466	395.640	-1853.554	2.721e+07	1.474e+10
5550.00	62.161	325.574	396.203	-1873.350	2.835e+07	1.508e+10
5600.00	62.164	328.682	396.760	-1893.174	2.953e+07	1.542e+10

5650.00	62.168	331.791	397.313	-1913.026	3.075e+07	1.577e+10
5700.00	62.171	334.899	397.860	-1932.906	3.202e+07	1.612e+10
5750.00	62.174	338.008	398.403	-1952.812	3.332e+07	1.647e+10
5800.00	62.178	341.117	398.942	-1972.746	3.466e+07	1.683e+10
5850.00	62.181	344.226	399.476	-1992.706	3.605e+07	1.720e+10
5900.00	62.184	347.335	400.005	-2012.693	3.749e+07	1.757e+10
5950.00	62.187	350.444	400.530	-2032.707	3.896e+07	1.794e+10
6000.00	62.189	353.553	401.050	-2052.746	4.049e+07	1.832e+10
6050.00	62.192	356.663	401.566	-2072.812	4.206e+07	1.871e+10
6100.00	62.195	359.773	402.078	-2092.903	4.368e+07	1.909e+10
6150.00	62.198	362.882	402.586	-2113.019	4.535e+07	1.949e+10
6200.00	62.200	365.992	403.089	-2133.161	4.707e+07	1.989e+10
6250.00	62.203	369.102	403.589	-2153.328	4.884e+07	2.029e+10
6300.00	62.205	372.213	404.085	-2173.520	5.067e+07	2.070e+10
6350.00	62.207	375.323	404.576	-2193.737	5.255e+07	2.111e+10
6400.00	62.210	378.433	405.064	-2213.978	5.448e+07	2.153e+10
6450.00	62.212	381.544	405.548	-2234.243	5.647e+07	2.195e+10
6500.00	62.214	384.654	406.029	-2254.532	5.852e+07	2.238e+10
6550.00	62.217	387.765	406.505	-2274.846	6.063e+07	2.281e+10
6600.00	62.219	390.876	406.979	-2295.183	6.280e+07	2.325e+10
6650.00	62.221	393.987	407.448	-2315.543	6.503e+07	2.369e+10
6700.00	62.223	397.098	407.914	-2335.927	6.732e+07	2.414e+10
6750.00	62.225	400.209	408.377	-2356.335	6.968e+07	2.459e+10
6800.00	62.227	403.321	408.836	-2376.765	7.210e+07	2.505e+10
6850.00	62.229	406.432	409.292	-2397.219	7.459e+07	2.552e+10
6900.00	62.231	409.544	409.745	-2417.694	7.715e+07	2.598e+10
6950.00	62.232	412.655	410.194	-2438.193	7.978e+07	2.646e+10
7000.00	62.234	415.767	410.640	-2458.714	8.248e+07	2.694e+10
7050.00	62.236	418.879	411.083	-2479.257	8.525e+07	2.742e+10
7100.00	62.238	421.990	411.523	-2499.822	8.810e+07	2.791e+10
7150.00	62.239	425.102	411.960	-2520.409	9.102e+07	2.840e+10
7200.00	62.241	428.214	412.393	-2541.018	9.402e+07	2.890e+10
7250.00	62.243	431.326	412.824	-2561.648	9.710e+07	2.941e+10
7300.00	62.244	434.439	413.252	-2582.300	1.003e+08	2.992e+10
7350.00	62.246	437.551	413.677	-2602.973	1.035e+08	3.043e+10
7400.00	62.247	440.663	414.099	-2623.668	1.068e+08	3.095e+10
7450.00	62.249	443.776	414.518	-2644.383	1.102e+08	3.148e+10
7500.00	62.250	446.888	414.934	-2665.120	1.137e+08	3.201e+10
7550.00	62.252	450.001	415.348	-2685.877	1.173e+08	3.254e+10
7600.00	62.253	453.113	415.759	-2706.654	1.210e+08	3.308e+10
7650.00	62.254	456.226	416.167	-2727.452	1.247e+08	3.363e+10
7700.00	62.256	459.339	416.573	-2748.271	1.286e+08	3.418e+10
7750.00	62.257	462.451	416.976	-2769.110	1.325e+08	3.474e+10
7800.00	62.258	465.564	417.376	-2789.969	1.366e+08	3.530e+10
7850.00	62.260	468.677	417.774	-2810.847	1.407e+08	3.587e+10
7900.00	62.261	471.790	418.169	-2831.746	1.450e+08	3.645e+10
7950.00	62.262	474.903	418.562	-2852.664	1.493e+08	3.703e+10
8000.00	62.263	478.017	418.952	-2873.602	1.538e+08	3.761e+10
8050.00	62.264	481.130	419.340	-2894.559	1.583e+08	3.820e+10
8100.00	62.266	484.243	419.726	-2915.536	1.630e+08	3.880e+10
8150.00	62.267	487.356	420.109	-2936.532	1.678e+08	3.940e+10
8200.00	62.268	490.470	420.490	-2957.547	1.727e+08	4.001e+10
8250.00	62.269	493.583	420.868	-2978.581	1.777e+08	4.062e+10
8300.00	62.270	496.697	421.245	-2999.634	1.828e+08	4.124e+10
8350.00	62.271	499.810	421.619	-3020.705	1.880e+08	4.186e+10
8400.00	62.272	502.924	421.990	-3041.795	1.934e+08	4.249e+10
8450.00	62.273	506.037	422.360	-3062.904	1.988e+08	4.312e+10
8500.00	62.274	509.151	422.727	-3084.031	2.044e+08	4.377e+10

8550.00	62.275	512.265	423.093	-3105.177	2.101e+08	4.441e+10
8600.00	62.276	515.378	423.456	-3126.341	2.160e+08	4.506e+10
8650.00	62.277	518.492	423.817	-3147.522	2.220e+08	4.572e+10
8700.00	62.278	521.606	424.176	-3168.722	2.281e+08	4.639e+10
8750.00	62.279	524.720	424.533	-3189.940	2.343e+08	4.706e+10
8800.00	62.280	527.834	424.887	-3211.176	2.407e+08	4.773e+10
8850.00	62.281	530.948	425.240	-3232.429	2.472e+08	4.841e+10
8900.00	62.282	534.062	425.591	-3253.699	2.539e+08	4.910e+10
8950.00	62.282	537.176	425.940	-3274.988	2.607e+08	4.979e+10
9000.00	62.283	540.290	426.287	-3296.293	2.676e+08	5.049e+10
9050.00	62.284	543.405	426.632	-3317.616	2.747e+08	5.119e+10
9100.00	62.285	546.519	426.975	-3338.957	2.819e+08	5.190e+10
9150.00	62.286	549.633	427.317	-3360.314	2.893e+08	5.262e+10
9200.00	62.287	552.747	427.656	-3381.688	2.969e+08	5.334e+10
9250.00	62.287	555.862	427.994	-3403.080	3.046e+08	5.407e+10
9300.00	62.288	558.976	428.329	-3424.488	3.125e+08	5.480e+10
9350.00	62.289	562.091	428.663	-3445.912	3.205e+08	5.554e+10
9400.00	62.290	565.205	428.996	-3467.354	3.287e+08	5.629e+10
9450.00	62.290	568.320	429.326	-3488.812	3.370e+08	5.704e+10
9500.00	62.291	571.434	429.655	-3510.287	3.456e+08	5.780e+10
9550.00	62.292	574.549	429.982	-3531.777	3.543e+08	5.856e+10
9600.00	62.292	577.663	430.307	-3553.285	3.631e+08	5.933e+10
9650.00	62.293	580.778	430.631	-3574.808	3.722e+08	6.010e+10
9700.00	62.294	583.893	430.953	-3596.348	3.814e+08	6.089e+10
9750.00	62.294	587.007	431.273	-3617.903	3.908e+08	6.167e+10
9800.00	62.295	590.122	431.592	-3639.475	4.004e+08	6.247e+10
9850.00	62.296	593.237	431.909	-3661.062	4.102e+08	6.327e+10
9900.00	62.296	596.352	432.224	-3682.666	4.202e+08	6.407e+10
9950.00	62.297	599.466	432.538	-3704.285	4.303e+08	6.489e+10
10000.00	62.298	602.581	432.850	-3725.920	4.407e+08	6.570e+10

CALCULATION OUT THERMAL EQUILIBRIUM: Tex=1.5*Th Tvib=√ 1.5 Trot=Th
(P=1 bar=0.1 MPa)

Th	Cp	h	s	g	zint	ztr
K	J/K/mol	kJ/mol	J/K/mol	kJ/mol	-	-
100.00	32.323	2.992	192.492	-16.732	4.809e+02	6.570e+05
150.00	36.708	4.783	206.458	-26.971	7.714e+02	1.811e+06
200.00	39.967	6.809	217.489	-37.855	1.146e+03	3.717e+06
250.00	42.523	9.010	226.689	-49.273	1.631e+03	6.493e+06
298.15	44.698	11.268	234.368	-60.701	2.226e+03	1.008e+07
300.00	44.778	11.357	234.645	-61.148	2.251e+03	1.024e+07
350.00	46.837	13.836	241.704	-73.426	3.037e+03	1.506e+07
400.00	48.697	16.435	248.082	-86.068	4.019e+03	2.103e+07
450.00	50.346	19.142	253.915	-99.042	5.238e+03	2.822e+07
500.00	51.785	21.943	259.296	-112.323	6.734e+03	3.673e+07
550.00	53.028	24.826	264.292	-125.889	8.557e+03	4.661e+07
600.00	54.097	27.780	268.953	-139.720	1.076e+04	5.794e+07
650.00	55.015	30.795	273.320	-153.800	1.340e+04	7.077e+07
700.00	55.803	33.861	277.427	-168.114	1.654e+04	8.518e+07
750.00	56.482	36.973	281.300	-182.650	2.026e+04	1.012e+08
800.00	57.069	40.123	284.965	-197.394	2.463e+04	1.189e+08
850.00	57.577	43.307	288.440	-212.336	2.973e+04	1.384e+08
900.00	58.020	46.519	291.744	-227.466	3.566e+04	1.597e+08
950.00	58.407	49.757	294.892	-242.776	4.252e+04	1.828e+08
1000.00	58.747	53.018	297.896	-258.256	5.041e+04	2.078e+08
1050.00	59.046	56.297	300.770	-273.901	5.944e+04	2.347e+08
1100.00	59.311	59.595	303.523	-289.702	6.974e+04	2.637e+08
1150.00	59.547	62.907	306.165	-305.653	8.143e+04	2.947e+08
1200.00	59.757	66.233	308.704	-321.748	9.467e+04	3.277e+08
1250.00	59.945	69.571	311.147	-337.983	1.096e+05	3.630e+08
1300.00	60.114	72.920	313.501	-354.351	1.264e+05	4.004e+08
1350.00	60.266	76.279	315.773	-370.848	1.451e+05	4.400e+08
1400.00	60.404	79.647	317.967	-387.470	1.661e+05	4.818e+08
1450.00	60.528	83.023	320.089	-404.212	1.894e+05	5.260e+08
1500.00	60.642	86.406	322.143	-421.071	2.153e+05	5.726e+08
1550.00	60.745	89.796	324.133	-438.043	2.440e+05	6.215e+08
1600.00	60.839	93.191	326.063	-455.124	2.757e+05	6.728e+08
1650.00	60.926	96.593	327.937	-472.312	3.107e+05	7.266e+08
1700.00	61.005	99.999	329.757	-489.602	3.491e+05	7.829e+08
1750.00	61.078	103.410	331.526	-506.993	3.912e+05	8.417e+08
1800.00	61.146	106.825	333.248	-524.482	4.374e+05	9.032e+08
1850.00	61.208	110.245	334.924	-542.065	4.878e+05	9.672e+08
1900.00	61.266	113.668	336.557	-559.741	5.428e+05	1.034e+09
1950.00	61.319	117.094	338.149	-577.507	6.027e+05	1.103e+09
2000.00	61.369	120.524	339.702	-595.361	6.677e+05	1.175e+09
2050.00	61.415	123.956	341.218	-613.300	7.383e+05	1.250e+09
2100.00	61.458	127.391	342.699	-631.324	8.148e+05	1.328e+09
2150.00	61.499	130.829	344.145	-649.429	8.975e+05	1.408e+09
2200.00	61.536	134.269	345.559	-667.614	9.868e+05	1.492e+09
2250.00	61.572	137.712	346.943	-685.878	1.083e+06	1.578e+09
2300.00	61.605	141.156	348.296	-704.218	1.187e+06	1.667e+09
2350.00	61.636	144.603	349.622	-722.633	1.298e+06	1.759e+09
2400.00	61.665	148.051	350.920	-741.121	1.418e+06	1.854e+09
2450.00	61.692	151.501	352.191	-759.681	1.547e+06	1.952e+09
2500.00	61.718	154.953	353.438	-778.311	1.685e+06	2.053e+09
2550.00	61.742	158.406	354.660	-797.011	1.832e+06	2.157e+09
2600.00	61.766	161.860	355.859	-815.778	1.989e+06	2.265e+09
2650.00	61.787	165.316	357.036	-834.612	2.158e+06	2.375e+09
2700.00	61.808	168.774	358.191	-853.511	2.337e+06	2.489e+09

2750.00	61.827	172.232	359.326	-872.474	2.528e+06	2.606e+09
2800.00	61.846	175.692	360.440	-891.500	2.732e+06	2.726e+09
2850.00	61.863	179.153	361.535	-910.588	2.949e+06	2.849e+09
2900.00	61.880	182.615	362.611	-929.736	3.179e+06	2.976e+09
2950.00	61.896	186.078	363.669	-948.944	3.423e+06	3.106e+09
3000.00	61.911	189.541	364.709	-968.211	3.682e+06	3.239e+09
3050.00	61.925	193.006	365.733	-987.536	3.957e+06	3.375e+09
3100.00	61.939	196.472	366.740	-1006.917	4.248e+06	3.516e+09
3150.00	61.952	199.938	367.731	-1026.354	4.555e+06	3.659e+09
3200.00	61.965	203.405	368.707	-1045.847	4.881e+06	3.806e+09
3250.00	61.976	206.873	369.667	-1065.393	5.224e+06	3.956e+09
3300.00	61.988	210.342	370.614	-1084.993	5.587e+06	4.110e+09
3350.00	61.999	213.811	371.546	-1104.646	5.970e+06	4.268e+09
3400.00	62.009	217.281	372.464	-1124.350	6.373e+06	4.429e+09
3450.00	62.019	220.751	373.370	-1144.105	6.798e+06	4.593e+09
3500.00	62.029	224.223	374.262	-1163.911	7.245e+06	4.762e+09
3550.00	62.038	227.694	375.142	-1183.766	7.716e+06	4.934e+09
3600.00	62.047	231.167	376.010	-1203.670	8.211e+06	5.109e+09
3650.00	62.055	234.639	376.866	-1223.622	8.731e+06	5.288e+09
3700.00	62.063	238.113	377.710	-1243.622	9.277e+06	5.471e+09
3750.00	62.071	241.586	378.543	-1263.669	9.850e+06	5.658e+09
3800.00	62.078	245.061	379.365	-1283.762	1.045e+07	5.849e+09
3850.00	62.085	248.535	380.177	-1303.901	1.108e+07	6.043e+09
3900.00	62.092	252.011	380.978	-1324.085	1.174e+07	6.241e+09
3950.00	62.099	255.486	381.769	-1344.313	1.243e+07	6.443e+09
4000.00	62.105	258.962	382.550	-1364.586	1.316e+07	6.649e+09
4050.00	62.112	262.438	383.322	-1384.902	1.391e+07	6.858e+09
4100.00	62.118	265.915	384.084	-1405.261	1.470e+07	7.072e+09
4150.00	62.123	269.392	384.837	-1425.662	1.553e+07	7.290e+09
4200.00	62.129	272.870	385.581	-1446.105	1.640e+07	7.511e+09
4250.00	62.134	276.347	386.316	-1466.590	1.730e+07	7.737e+09
4300.00	62.139	279.825	387.043	-1487.115	1.824e+07	7.966e+09
4350.00	62.144	283.304	387.762	-1507.681	1.922e+07	8.200e+09
4400.00	62.149	286.783	388.472	-1528.287	2.024e+07	8.438e+09
4450.00	62.154	290.261	389.174	-1548.933	2.131e+07	8.679e+09
4500.00	62.158	293.741	389.869	-1569.617	2.242e+07	8.925e+09
4550.00	62.163	297.220	390.555	-1590.341	2.358e+07	9.175e+09
4600.00	62.167	300.700	391.235	-1611.102	2.478e+07	9.429e+09
4650.00	62.171	304.180	391.907	-1631.901	2.604e+07	9.688e+09
4700.00	62.175	307.660	392.572	-1652.738	2.734e+07	9.950e+09
4750.00	62.179	311.141	393.230	-1673.612	2.870e+07	1.022e+10
4800.00	62.182	314.622	393.881	-1694.522	3.011e+07	1.049e+10
4850.00	62.186	318.103	394.525	-1715.469	3.157e+07	1.076e+10
4900.00	62.189	321.584	395.163	-1736.451	3.309e+07	1.104e+10
4950.00	62.193	325.065	395.795	-1757.469	3.467e+07	1.133e+10
5000.00	62.196	328.547	396.420	-1778.523	3.631e+07	1.161e+10
5050.00	62.199	332.029	397.039	-1799.611	3.801e+07	1.191e+10
5100.00	62.202	335.511	397.651	-1820.733	3.977e+07	1.220e+10
5150.00	62.205	338.993	398.258	-1841.890	4.159e+07	1.251e+10
5200.00	62.208	342.475	398.859	-1863.080	4.349e+07	1.281e+10
5250.00	62.211	345.958	399.455	-1884.304	4.545e+07	1.312e+10
5300.00	62.214	349.440	400.044	-1905.561	4.748e+07	1.344e+10
5350.00	62.217	352.923	400.628	-1926.851	4.959e+07	1.376e+10
5400.00	62.219	356.406	401.207	-1948.174	5.177e+07	1.408e+10
5450.00	62.222	359.890	401.781	-1969.529	5.402e+07	1.441e+10
5500.00	62.224	363.373	402.349	-1990.915	5.635e+07	1.474e+10
5550.00	62.227	366.856	402.912	-2012.334	5.877e+07	1.508e+10
5600.00	62.229	370.340	403.470	-2033.784	6.126e+07	1.542e+10

5650.00	62.231	373.824	404.023	-2055.265	6.384e+07	1.577e+10
5700.00	62.234	377.308	404.572	-2076.776	6.650e+07	1.612e+10
5750.00	62.236	380.792	405.115	-2098.319	6.926e+07	1.647e+10
5800.00	62.238	384.276	405.654	-2119.891	7.210e+07	1.683e+10
5850.00	62.240	387.760	406.188	-2141.494	7.503e+07	1.720e+10
5900.00	62.242	391.245	406.718	-2163.126	7.807e+07	1.757e+10
5950.00	62.244	394.729	407.243	-2184.788	8.119e+07	1.794e+10
6000.00	62.246	398.214	407.764	-2206.479	8.442e+07	1.832e+10
6050.00	62.248	401.699	408.281	-2228.199	8.775e+07	1.871e+10
6100.00	62.249	405.184	408.793	-2249.949	9.118e+07	1.909e+10
6150.00	62.251	408.669	409.301	-2271.726	9.473e+07	1.949e+10
6200.00	62.253	412.154	409.805	-2293.532	9.838e+07	1.989e+10
6250.00	62.255	415.639	410.305	-2315.366	1.021e+08	2.029e+10
6300.00	62.256	419.124	410.801	-2337.228	1.060e+08	2.070e+10
6350.00	62.258	422.610	411.294	-2359.118	1.100e+08	2.111e+10
6400.00	62.259	426.095	411.782	-2381.035	1.141e+08	2.153e+10
6450.00	62.261	429.581	412.266	-2402.979	1.184e+08	2.195e+10
6500.00	62.262	433.067	412.747	-2424.950	1.227e+08	2.238e+10
6550.00	62.264	436.553	413.224	-2446.949	1.272e+08	2.281e+10
6600.00	62.265	440.038	413.698	-2468.973	1.318e+08	2.325e+10
6650.00	62.267	443.524	414.168	-2491.024	1.366e+08	2.369e+10
6700.00	62.268	447.010	414.634	-2513.102	1.414e+08	2.414e+10
6750.00	62.269	450.497	415.097	-2535.205	1.465e+08	2.459e+10
6800.00	62.271	453.983	415.557	-2557.334	1.516e+08	2.505e+10
6850.00	62.272	457.469	416.013	-2579.489	1.570e+08	2.552e+10
6900.00	62.273	460.956	416.466	-2601.669	1.624e+08	2.598e+10
6950.00	62.274	464.442	416.915	-2623.875	1.680e+08	2.646e+10
7000.00	62.276	467.929	417.362	-2646.106	1.738e+08	2.694e+10
7050.00	62.277	471.415	417.805	-2668.361	1.797e+08	2.742e+10
7100.00	62.278	474.902	418.245	-2690.641	1.858e+08	2.791e+10
7150.00	62.279	478.389	418.682	-2712.946	1.920e+08	2.840e+10
7200.00	62.280	481.875	419.116	-2735.275	1.984e+08	2.890e+10
7250.00	62.281	485.362	419.547	-2757.629	2.050e+08	2.941e+10
7300.00	62.282	488.849	419.975	-2780.006	2.118e+08	2.992e+10
7350.00	62.283	492.336	420.400	-2802.408	2.187e+08	3.043e+10
7400.00	62.284	495.823	420.823	-2824.833	2.258e+08	3.095e+10
7450.00	62.285	499.311	421.242	-2847.281	2.331e+08	3.148e+10
7500.00	62.286	502.798	421.659	-2869.753	2.406e+08	3.201e+10
7550.00	62.287	506.285	422.073	-2892.249	2.483e+08	3.254e+10
7600.00	62.288	509.772	422.484	-2914.767	2.562e+08	3.308e+10
7650.00	62.289	513.260	422.892	-2937.308	2.642e+08	3.363e+10
7700.00	62.290	516.747	423.298	-2959.872	2.725e+08	3.418e+10
7750.00	62.291	520.235	423.701	-2982.459	2.810e+08	3.474e+10
7800.00	62.292	523.722	424.102	-3005.068	2.897e+08	3.530e+10
7850.00	62.293	527.210	424.500	-3027.700	2.986e+08	3.587e+10
7900.00	62.293	530.697	424.895	-3050.354	3.077e+08	3.645e+10
7950.00	62.294	534.185	425.288	-3073.030	3.170e+08	3.703e+10
8000.00	62.295	537.673	425.679	-3095.728	3.266e+08	3.761e+10
8050.00	62.296	541.161	426.067	-3118.447	3.364e+08	3.820e+10
8100.00	62.297	544.648	426.453	-3141.188	3.464e+08	3.880e+10
8150.00	62.297	548.136	426.836	-3163.951	3.567e+08	3.940e+10
8200.00	62.298	551.624	427.217	-3186.736	3.672e+08	4.001e+10
8250.00	62.299	555.112	427.596	-3209.541	3.780e+08	4.062e+10
8300.00	62.300	558.600	427.972	-3232.368	3.890e+08	4.124e+10
8350.00	62.300	562.088	428.346	-3255.215	4.002e+08	4.186e+10
8400.00	62.301	565.576	428.718	-3278.084	4.118e+08	4.249e+10
8450.00	62.302	569.065	429.088	-3300.973	4.235e+08	4.312e+10
8500.00	62.302	572.553	429.456	-3323.883	4.356e+08	4.377e+10

8550.00	62.303	576.041	429.821	-3346.813	4.479e+08	4.441e+10
8600.00	62.304	579.529	430.184	-3369.764	4.605e+08	4.506e+10
8650.00	62.304	583.018	430.546	-3392.735	4.734e+08	4.572e+10
8700.00	62.305	586.506	430.905	-3415.727	4.866e+08	4.639e+10
8750.00	62.306	589.994	431.262	-3438.738	5.000e+08	4.706e+10
8800.00	62.306	593.483	431.617	-3461.769	5.138e+08	4.773e+10
8850.00	62.307	596.971	431.970	-3484.820	5.279e+08	4.841e+10
8900.00	62.307	600.460	432.321	-3507.891	5.422e+08	4.910e+10
8950.00	62.308	603.948	432.670	-3530.982	5.569e+08	4.979e+10
9000.00	62.308	607.437	433.017	-3554.092	5.719e+08	5.049e+10
9050.00	62.309	610.925	433.362	-3577.221	5.872e+08	5.119e+10
9100.00	62.310	614.414	433.706	-3600.369	6.029e+08	5.190e+10
9150.00	62.310	617.903	434.047	-3623.537	6.189e+08	5.262e+10
9200.00	62.311	621.391	434.386	-3646.724	6.352e+08	5.334e+10
9250.00	62.311	624.880	434.724	-3669.930	6.518e+08	5.407e+10
9300.00	62.312	628.369	435.060	-3693.154	6.688e+08	5.480e+10
9350.00	62.312	631.858	435.394	-3716.397	6.862e+08	5.554e+10
9400.00	62.313	635.346	435.727	-3739.660	7.039e+08	5.629e+10
9450.00	62.313	638.835	436.057	-3762.940	7.220e+08	5.704e+10
9500.00	62.314	642.324	436.386	-3786.239	7.404e+08	5.780e+10
9550.00	62.314	645.813	436.713	-3809.557	7.592e+08	5.856e+10
9600.00	62.315	649.302	437.038	-3832.892	7.784e+08	5.933e+10
9650.00	62.315	652.791	437.362	-3856.246	7.980e+08	6.010e+10
9700.00	62.315	656.280	437.684	-3879.618	8.180e+08	6.089e+10
9750.00	62.316	659.769	438.005	-3903.008	8.384e+08	6.167e+10
9800.00	62.316	663.258	438.323	-3926.416	8.592e+08	6.247e+10
9850.00	62.317	666.747	438.641	-3949.841	8.804e+08	6.327e+10
9900.00	62.317	670.236	438.956	-3973.284	9.020e+08	6.407e+10
9950.00	62.318	673.725	439.270	-3996.745	9.240e+08	6.489e+10
10000.00	62.318	677.215	439.582	-4020.224	9.465e+08	6.570e+10

CALCULATION OUT THERMAL EQUILIBRIUM: Tex=2.0*Th Tvib=√ 2.0 Trot=Th
(P=1 bar=0.1 MPa)

Th	Cp	h	s	g	zint	ztr
K	J/K/mol	kJ/mol	J/K/mol	kJ/mol	-	-
100.00	33.766	3.066	193.057	-17.209	4.882e+02	6.570e+05
150.00	38.348	5.023	207.670	-27.757	8.080e+02	1.811e+06
200.00	41.597	7.252	219.168	-39.014	1.239e+03	3.717e+06
250.00	44.285	9.688	228.745	-50.858	1.816e+03	6.493e+06
298.15	46.611	12.204	236.748	-62.745	2.544e+03	1.008e+07
300.00	46.695	12.303	237.036	-63.211	2.576e+03	1.024e+07
350.00	48.842	15.080	244.399	-76.014	3.560e+03	1.506e+07
400.00	50.707	17.999	251.046	-89.225	4.821e+03	2.103e+07
450.00	52.295	21.039	257.113	-102.809	6.415e+03	2.822e+07
500.00	53.633	24.183	262.694	-116.737	8.410e+03	3.673e+07
550.00	54.756	27.413	267.860	-130.985	1.088e+04	4.661e+07
600.00	55.697	30.717	272.666	-145.530	1.391e+04	5.794e+07
650.00	56.489	34.081	277.156	-160.354	1.758e+04	7.077e+07
700.00	57.158	37.497	281.368	-175.438	2.202e+04	8.518e+07
750.00	57.726	40.957	285.331	-190.768	2.731e+04	1.012e+08
800.00	58.210	44.454	289.072	-206.330	3.360e+04	1.189e+08
850.00	58.626	47.982	292.614	-222.112	4.101e+04	1.384e+08
900.00	58.985	51.538	295.976	-238.103	4.970e+04	1.597e+08
950.00	59.296	55.117	299.173	-254.291	5.982e+04	1.828e+08
1000.00	59.567	58.717	302.222	-270.669	7.154e+04	2.078e+08
1050.00	59.806	62.335	305.134	-287.227	8.506e+04	2.347e+08
1100.00	60.015	65.969	307.921	-303.958	1.006e+05	2.637e+08
1150.00	60.201	69.617	310.593	-320.855	1.183e+05	2.947e+08
1200.00	60.365	73.277	313.159	-337.910	1.384e+05	3.277e+08
1250.00	60.512	76.948	315.626	-355.118	1.613e+05	3.630e+08
1300.00	60.644	80.629	318.002	-372.473	1.870e+05	4.004e+08
1350.00	60.762	84.318	320.293	-389.970	2.160e+05	4.400e+08
1400.00	60.869	88.016	322.505	-407.604	2.485e+05	4.818e+08
1450.00	60.965	91.721	324.642	-425.370	2.848e+05	5.260e+08
1500.00	61.053	95.432	326.711	-443.264	3.253e+05	5.726e+08
1550.00	61.133	99.149	328.714	-461.282	3.703e+05	6.215e+08
1600.00	61.205	102.872	330.656	-479.420	4.202e+05	6.728e+08
1650.00	61.272	106.600	332.540	-497.674	4.753e+05	7.266e+08
1700.00	61.333	110.332	334.370	-516.042	5.361e+05	7.829e+08
1750.00	61.389	114.068	336.149	-534.519	6.030e+05	8.417e+08
1800.00	61.440	117.808	337.879	-553.103	6.765e+05	9.032e+08
1850.00	61.488	121.551	339.563	-571.791	7.569e+05	9.672e+08
1900.00	61.532	125.298	341.204	-590.580	8.449e+05	1.034e+09
1950.00	61.573	129.048	342.802	-609.467	9.409e+05	1.103e+09
2000.00	61.611	132.800	344.362	-628.451	1.046e+06	1.175e+09
2050.00	61.646	136.555	345.884	-647.529	1.159e+06	1.250e+09
2100.00	61.679	140.313	347.369	-666.699	1.283e+06	1.328e+09
2150.00	61.709	144.073	348.821	-685.958	1.416e+06	1.408e+09
2200.00	61.738	147.834	350.240	-705.304	1.561e+06	1.492e+09
2250.00	61.765	151.598	351.628	-724.736	1.718e+06	1.578e+09
2300.00	61.790	155.364	352.986	-744.252	1.886e+06	1.667e+09
2350.00	61.813	159.131	354.315	-763.849	2.068e+06	1.759e+09
2400.00	61.835	162.900	355.616	-783.527	2.263e+06	1.854e+09
2450.00	61.856	166.671	356.892	-803.283	2.474e+06	1.952e+09
2500.00	61.876	170.443	358.142	-823.116	2.699e+06	2.053e+09
2550.00	61.894	174.216	359.367	-843.025	2.941e+06	2.157e+09
2600.00	61.912	177.990	360.569	-863.008	3.199e+06	2.265e+09
2650.00	61.928	181.766	361.749	-883.063	3.476e+06	2.375e+09
2700.00	61.944	185.543	362.906	-903.190	3.771e+06	2.489e+09

2750.00	61.959	189.321	364.043	-923.386	4.086e+06	2.606e+09
2800.00	61.973	193.100	365.159	-943.651	4.422e+06	2.726e+09
2850.00	61.986	196.880	366.257	-963.984	4.780e+06	2.849e+09
2900.00	61.998	200.660	367.335	-984.383	5.161e+06	2.976e+09
2950.00	62.010	204.442	368.395	-1004.847	5.565e+06	3.106e+09
3000.00	62.022	208.225	369.437	-1025.375	5.995e+06	3.239e+09
3050.00	62.033	212.008	370.462	-1045.967	6.450e+06	3.375e+09
3100.00	62.043	215.792	371.471	-1066.620	6.933e+06	3.516e+09
3150.00	62.053	219.577	372.464	-1087.334	7.445e+06	3.659e+09
3200.00	62.062	223.362	373.441	-1108.109	7.986e+06	3.806e+09
3250.00	62.071	227.148	374.403	-1128.943	8.559e+06	3.956e+09
3300.00	62.080	230.935	375.351	-1149.835	9.164e+06	4.110e+09
3350.00	62.088	234.722	376.285	-1170.784	9.802e+06	4.268e+09
3400.00	62.096	238.510	377.205	-1191.790	1.048e+07	4.429e+09
3450.00	62.103	242.298	378.111	-1212.851	1.119e+07	4.593e+09
3500.00	62.111	246.087	379.005	-1233.968	1.193e+07	4.762e+09
3550.00	62.117	249.877	379.886	-1255.138	1.272e+07	4.934e+09
3600.00	62.124	253.667	380.755	-1276.362	1.355e+07	5.109e+09
3650.00	62.130	257.457	381.612	-1297.639	1.442e+07	5.288e+09
3700.00	62.136	261.248	382.457	-1318.967	1.534e+07	5.471e+09
3750.00	62.142	265.039	383.291	-1340.347	1.630e+07	5.658e+09
3800.00	62.148	268.831	384.114	-1361.777	1.731e+07	5.849e+09
3850.00	62.153	272.623	384.927	-1383.258	1.837e+07	6.043e+09
3900.00	62.159	276.415	385.729	-1404.787	1.948e+07	6.241e+09
3950.00	62.164	280.208	386.521	-1426.365	2.065e+07	6.443e+09
4000.00	62.168	284.001	387.303	-1447.991	2.187e+07	6.649e+09
4050.00	62.173	287.794	388.075	-1469.665	2.314e+07	6.858e+09
4100.00	62.177	291.588	388.838	-1491.385	2.448e+07	7.072e+09
4150.00	62.182	295.382	389.591	-1513.152	2.587e+07	7.290e+09
4200.00	62.186	299.177	390.336	-1534.964	2.733e+07	7.511e+09
4250.00	62.190	302.971	391.072	-1556.822	2.886e+07	7.737e+09
4300.00	62.194	306.766	391.800	-1578.724	3.045e+07	7.966e+09
4350.00	62.198	310.561	392.519	-1600.670	3.211e+07	8.200e+09
4400.00	62.201	314.357	393.229	-1622.660	3.384e+07	8.438e+09
4450.00	62.205	318.153	393.932	-1644.693	3.565e+07	8.679e+09
4500.00	62.208	321.949	394.627	-1666.769	3.753e+07	8.925e+09
4550.00	62.211	325.745	395.315	-1688.887	3.950e+07	9.175e+09
4600.00	62.215	329.541	395.995	-1711.046	4.154e+07	9.429e+09
4650.00	62.218	333.338	396.667	-1733.247	4.367e+07	9.688e+09
4700.00	62.221	337.135	397.333	-1755.489	4.588e+07	9.950e+09
4750.00	62.224	340.932	397.991	-1777.771	4.818e+07	1.022e+10
4800.00	62.226	344.729	398.643	-1800.093	5.058e+07	1.049e+10
4850.00	62.229	348.527	399.288	-1822.454	5.307e+07	1.076e+10
4900.00	62.232	352.324	399.926	-1844.855	5.565e+07	1.104e+10
4950.00	62.234	356.122	400.558	-1867.295	5.834e+07	1.133e+10
5000.00	62.237	359.920	401.183	-1889.773	6.112e+07	1.161e+10
5050.00	62.239	363.718	401.802	-1912.288	6.402e+07	1.191e+10
5100.00	62.241	367.517	402.416	-1934.842	6.702e+07	1.220e+10
5150.00	62.244	371.315	403.023	-1957.433	7.013e+07	1.251e+10
5200.00	62.246	375.114	403.624	-1980.060	7.336e+07	1.281e+10
5250.00	62.248	378.913	404.220	-2002.724	7.671e+07	1.312e+10
5300.00	62.250	382.712	404.810	-2025.425	8.018e+07	1.344e+10
5350.00	62.252	386.511	405.395	-2048.161	8.377e+07	1.376e+10
5400.00	62.254	390.310	405.974	-2070.932	8.749e+07	1.408e+10
5450.00	62.256	394.109	406.547	-2093.739	9.134e+07	1.441e+10
5500.00	62.258	397.909	407.116	-2116.581	9.533e+07	1.474e+10
5550.00	62.260	401.709	407.679	-2139.457	9.945e+07	1.508e+10
5600.00	62.261	405.508	408.238	-2162.367	1.037e+08	1.542e+10

5650.00	62.263	409.308	408.791	-2185.312	1.081e+08	1.577e+10
5700.00	62.265	413.108	409.340	-2208.290	1.127e+08	1.612e+10
5750.00	62.266	416.908	409.884	-2231.301	1.174e+08	1.647e+10
5800.00	62.268	420.709	410.423	-2254.346	1.223e+08	1.683e+10
5850.00	62.269	424.509	410.957	-2277.423	1.273e+08	1.720e+10
5900.00	62.271	428.309	411.487	-2300.532	1.325e+08	1.757e+10
5950.00	62.272	432.110	412.013	-2323.674	1.378e+08	1.794e+10
6000.00	62.274	435.911	412.534	-2346.848	1.434e+08	1.832e+10
6050.00	62.275	439.712	413.051	-2370.053	1.491e+08	1.871e+10
6100.00	62.277	443.512	413.563	-2393.290	1.550e+08	1.909e+10
6150.00	62.278	447.313	414.072	-2416.558	1.611e+08	1.949e+10
6200.00	62.279	451.114	414.576	-2439.857	1.673e+08	1.989e+10
6250.00	62.281	454.916	415.076	-2463.187	1.738e+08	2.029e+10
6300.00	62.282	458.717	415.572	-2486.547	1.804e+08	2.070e+10
6350.00	62.283	462.518	416.065	-2509.937	1.873e+08	2.111e+10
6400.00	62.284	466.320	416.553	-2533.357	1.943e+08	2.153e+10
6450.00	62.285	470.121	417.038	-2556.807	2.016e+08	2.195e+10
6500.00	62.286	473.923	417.519	-2580.286	2.091e+08	2.238e+10
6550.00	62.288	477.724	417.996	-2603.795	2.168e+08	2.281e+10
6600.00	62.289	481.526	418.470	-2627.332	2.248e+08	2.325e+10
6650.00	62.290	485.328	418.940	-2650.898	2.329e+08	2.369e+10
6700.00	62.291	489.130	419.407	-2674.493	2.413e+08	2.414e+10
6750.00	62.292	492.932	419.870	-2698.117	2.500e+08	2.459e+10
6800.00	62.293	496.734	420.329	-2721.768	2.589e+08	2.505e+10
6850.00	62.294	500.536	420.786	-2745.448	2.680e+08	2.552e+10
6900.00	62.295	504.338	421.239	-2769.155	2.774e+08	2.598e+10
6950.00	62.295	508.140	421.689	-2792.889	2.871e+08	2.646e+10
7000.00	62.296	511.943	422.135	-2816.651	2.970e+08	2.694e+10
7050.00	62.297	515.745	422.579	-2840.441	3.072e+08	2.742e+10
7100.00	62.298	519.547	423.019	-2864.257	3.177e+08	2.791e+10
7150.00	62.299	523.350	423.456	-2888.100	3.285e+08	2.840e+10
7200.00	62.300	527.152	423.890	-2911.969	3.395e+08	2.890e+10
7250.00	62.301	530.955	424.321	-2935.865	3.509e+08	2.941e+10
7300.00	62.301	534.758	424.750	-2959.787	3.625e+08	2.992e+10
7350.00	62.302	538.560	425.175	-2983.736	3.745e+08	3.043e+10
7400.00	62.303	542.363	425.597	-3007.710	3.868e+08	3.095e+10
7450.00	62.304	546.166	426.017	-3031.709	3.994e+08	3.148e+10
7500.00	62.304	549.969	426.434	-3055.735	4.123e+08	3.201e+10
7550.00	62.305	553.772	426.848	-3079.786	4.256e+08	3.254e+10
7600.00	62.306	557.575	427.259	-3103.861	4.391e+08	3.308e+10
7650.00	62.307	561.378	427.667	-3127.962	4.531e+08	3.363e+10
7700.00	62.307	565.181	428.073	-3152.088	4.674e+08	3.418e+10
7750.00	62.308	568.984	428.477	-3176.239	4.820e+08	3.474e+10
7800.00	62.309	572.787	428.877	-3200.413	4.970e+08	3.530e+10
7850.00	62.309	576.590	429.275	-3224.613	5.124e+08	3.587e+10
7900.00	62.310	580.393	429.671	-3248.836	5.282e+08	3.645e+10
7950.00	62.310	584.197	430.064	-3273.084	5.443e+08	3.703e+10
8000.00	62.311	588.000	430.455	-3297.355	5.609e+08	3.761e+10
8050.00	62.312	591.803	430.843	-3321.651	5.778e+08	3.820e+10
8100.00	62.312	595.607	431.229	-3345.970	5.952e+08	3.880e+10
8150.00	62.313	599.410	431.612	-3370.312	6.129e+08	3.940e+10
8200.00	62.313	603.214	431.993	-3394.678	6.311e+08	4.001e+10
8250.00	62.314	607.017	432.372	-3419.067	6.497e+08	4.062e+10
8300.00	62.314	610.821	432.749	-3443.479	6.688e+08	4.124e+10
8350.00	62.315	614.624	433.123	-3467.914	6.883e+08	4.186e+10
8400.00	62.315	618.428	433.495	-3492.372	7.082e+08	4.249e+10
8450.00	62.316	622.232	433.865	-3516.852	7.287e+08	4.312e+10
8500.00	62.316	626.036	434.233	-3541.355	7.495e+08	4.377e+10

8550.00	62.317	629.839	434.598	-3565.880	7.709e+08	4.441e+10
8600.00	62.317	633.643	434.961	-3590.427	7.927e+08	4.506e+10
8650.00	62.318	637.447	435.323	-3614.997	8.151e+08	4.572e+10
8700.00	62.318	641.251	435.682	-3639.589	8.379e+08	4.639e+10
8750.00	62.319	645.055	436.039	-3664.202	8.612e+08	4.706e+10
8800.00	62.319	648.859	436.394	-3688.837	8.851e+08	4.773e+10
8850.00	62.320	652.663	436.747	-3713.494	9.095e+08	4.841e+10
8900.00	62.320	656.466	437.098	-3738.172	9.344e+08	4.910e+10
8950.00	62.321	660.271	437.447	-3762.872	9.598e+08	4.979e+10
9000.00	62.321	664.075	437.795	-3787.593	9.858e+08	5.049e+10
9050.00	62.321	667.879	438.140	-3812.335	1.012e+09	5.119e+10
9100.00	62.322	671.683	438.483	-3837.098	1.040e+09	5.190e+10
9150.00	62.322	675.487	438.825	-3861.882	1.067e+09	5.262e+10
9200.00	62.323	679.291	439.164	-3886.687	1.096e+09	5.334e+10
9250.00	62.323	683.095	439.502	-3911.512	1.125e+09	5.407e+10
9300.00	62.323	686.899	439.838	-3936.358	1.154e+09	5.480e+10
9350.00	62.324	690.704	440.172	-3961.225	1.184e+09	5.554e+10
9400.00	62.324	694.508	440.505	-3986.111	1.215e+09	5.629e+10
9450.00	62.325	698.312	440.835	-4011.018	1.246e+09	5.704e+10
9500.00	62.325	702.117	441.164	-4035.945	1.278e+09	5.780e+10
9550.00	62.325	705.921	441.491	-4060.893	1.311e+09	5.856e+10
9600.00	62.326	709.725	441.817	-4085.860	1.344e+09	5.933e+10
9650.00	62.326	713.530	442.141	-4110.847	1.378e+09	6.010e+10
9700.00	62.326	717.334	442.463	-4135.853	1.413e+09	6.089e+10
9750.00	62.327	721.139	442.783	-4160.879	1.449e+09	6.167e+10
9800.00	62.327	724.943	443.102	-4185.925	1.485e+09	6.247e+10
9850.00	62.327	728.748	443.419	-4210.990	1.522e+09	6.327e+10
9900.00	62.328	732.552	443.735	-4236.075	1.559e+09	6.407e+10
9950.00	62.328	736.357	444.049	-4261.178	1.597e+09	6.489e+10
10000.00	62.328	740.161	444.361	-4286.301	1.636e+09	6.570e+10

CALCULATION OUT THERMAL EQUILIBRIUM: Tex=3.0*Th Tvib=√ 3.0 Trot=Th
(P=1 bar=0.1 MPa)

Th	Cp	h	s	g	zint	ztr
K	J/K/mol	kJ/mol	J/K/mol	kJ/mol	-	-
100.00	36.033	3.252	194.230	-18.184	5.066e+02	6.570e+05
150.00	40.630	5.520	209.776	-29.377	8.856e+02	1.811e+06
200.00	44.027	8.125	221.944	-41.394	1.429e+03	3.717e+06
250.00	46.976	11.003	232.093	-54.102	2.192e+03	6.493e+06
298.15	49.437	14.001	240.583	-66.909	3.193e+03	1.008e+07
300.00	49.524	14.120	240.889	-67.412	3.238e+03	1.024e+07
350.00	51.649	17.439	248.688	-81.260	4.646e+03	1.506e+07
400.00	53.381	20.924	255.702	-95.596	6.508e+03	2.103e+07
450.00	54.779	24.545	262.073	-110.377	8.934e+03	2.822e+07
500.00	55.906	28.274	267.905	-125.568	1.205e+04	3.673e+07
550.00	56.819	32.091	273.278	-141.136	1.598e+04	4.661e+07
600.00	57.563	35.980	278.255	-157.055	2.091e+04	5.794e+07
650.00	58.175	39.927	282.887	-173.301	2.700e+04	7.077e+07
700.00	58.682	43.923	287.218	-189.853	3.446e+04	8.518e+07
750.00	59.105	47.959	291.281	-206.692	4.350e+04	1.012e+08
800.00	59.462	52.028	295.107	-223.801	5.438e+04	1.189e+08
850.00	59.765	56.126	298.722	-241.166	6.735e+04	1.384e+08
900.00	60.024	60.248	302.145	-258.772	8.273e+04	1.597e+08
950.00	60.247	64.391	305.397	-276.609	1.008e+05	1.828e+08
1000.00	60.440	68.552	308.492	-294.664	1.220e+05	2.078e+08
1050.00	60.609	72.728	311.445	-312.927	1.465e+05	2.347e+08
1100.00	60.756	76.919	314.268	-331.390	1.750e+05	2.637e+08
1150.00	60.886	81.121	316.972	-350.043	2.077e+05	2.947e+08
1200.00	61.001	85.334	319.565	-368.880	2.452e+05	3.277e+08
1250.00	61.103	89.556	322.058	-387.892	2.879e+05	3.630e+08
1300.00	61.194	93.786	324.456	-407.073	3.364e+05	4.004e+08
1350.00	61.276	98.024	326.767	-426.418	3.913e+05	4.400e+08
1400.00	61.349	102.269	328.997	-445.919	4.532e+05	4.818e+08
1450.00	61.416	106.520	331.151	-465.572	5.227e+05	5.260e+08
1500.00	61.476	110.776	333.234	-485.372	6.005e+05	5.726e+08
1550.00	61.530	115.037	335.251	-505.314	6.874e+05	6.215e+08
1600.00	61.580	119.303	337.205	-525.393	7.841e+05	6.728e+08
1650.00	61.626	123.573	339.101	-545.606	8.914e+05	7.266e+08
1700.00	61.667	127.846	340.941	-565.948	1.010e+06	7.829e+08
1750.00	61.705	132.124	342.729	-586.416	1.141e+06	8.417e+08
1800.00	61.740	136.404	344.468	-607.007	1.286e+06	9.032e+08
1850.00	61.773	140.687	346.160	-627.716	1.445e+06	9.672e+08
1900.00	61.803	144.973	347.808	-648.541	1.619e+06	1.034e+09
1950.00	61.830	149.261	349.413	-669.479	1.810e+06	1.103e+09
2000.00	61.856	153.552	350.979	-690.527	2.018e+06	1.175e+09
2050.00	61.880	157.844	352.507	-711.682	2.245e+06	1.250e+09
2100.00	61.902	162.139	353.998	-732.942	2.492e+06	1.328e+09
2150.00	61.923	166.436	355.455	-754.304	2.760e+06	1.408e+09
2200.00	61.942	170.734	356.879	-775.766	3.051e+06	1.492e+09
2250.00	61.960	175.034	358.271	-797.326	3.367e+06	1.578e+09
2300.00	61.977	179.336	359.633	-818.981	3.708e+06	1.667e+09
2350.00	61.993	183.639	360.966	-840.730	4.075e+06	1.759e+09
2400.00	62.008	187.943	362.271	-862.571	4.472e+06	1.854e+09
2450.00	62.022	192.248	363.550	-884.501	4.899e+06	1.952e+09
2500.00	62.035	196.555	364.803	-906.519	5.358e+06	2.053e+09
2550.00	62.048	200.863	366.032	-928.623	5.851e+06	2.157e+09
2600.00	62.059	205.172	367.237	-950.812	6.380e+06	2.265e+09
2650.00	62.070	209.481	368.419	-973.084	6.946e+06	2.375e+09
2700.00	62.081	213.792	369.579	-995.437	7.551e+06	2.489e+09

2750.00	62.091	218.104	370.719	-1017.870	8.199e+06	2.606e+09
2800.00	62.100	222.416	371.837	-1040.381	8.890e+06	2.726e+09
2850.00	62.109	226.729	372.937	-1062.969	9.627e+06	2.849e+09
2900.00	62.118	231.044	374.017	-1085.633	1.041e+07	2.976e+09
2950.00	62.126	235.358	375.079	-1108.371	1.125e+07	3.106e+09
3000.00	62.133	239.674	376.123	-1131.183	1.214e+07	3.239e+09
3050.00	62.141	243.990	377.150	-1154.066	1.308e+07	3.375e+09
3100.00	62.148	248.306	378.161	-1177.020	1.408e+07	3.516e+09
3150.00	62.154	252.624	379.155	-1200.044	1.514e+07	3.659e+09
3200.00	62.160	256.941	380.134	-1223.136	1.627e+07	3.806e+09
3250.00	62.166	261.260	381.098	-1246.296	1.746e+07	3.956e+09
3300.00	62.172	265.579	382.047	-1269.522	1.872e+07	4.110e+09
3350.00	62.178	269.898	382.982	-1292.814	2.005e+07	4.268e+09
3400.00	62.183	274.218	383.903	-1316.170	2.146e+07	4.429e+09
3450.00	62.188	278.538	384.811	-1339.590	2.294e+07	4.593e+09
3500.00	62.193	282.859	385.706	-1363.072	2.451e+07	4.762e+09
3550.00	62.197	287.180	386.588	-1386.616	2.616e+07	4.934e+09
3600.00	62.202	291.501	387.458	-1410.221	2.790e+07	5.109e+09
3650.00	62.206	295.823	388.316	-1433.886	2.973e+07	5.288e+09
3700.00	62.210	300.145	389.162	-1457.610	3.165e+07	5.471e+09
3750.00	62.214	304.468	389.997	-1481.393	3.367e+07	5.658e+09
3800.00	62.218	308.791	390.822	-1505.233	3.580e+07	5.849e+09
3850.00	62.222	313.114	391.635	-1529.130	3.803e+07	6.043e+09
3900.00	62.225	317.438	392.438	-1553.083	4.037e+07	6.241e+09
3950.00	62.228	321.762	393.230	-1577.092	4.282e+07	6.443e+09
4000.00	62.232	326.086	394.013	-1601.155	4.539e+07	6.649e+09
4050.00	62.235	330.410	394.786	-1625.272	4.809e+07	6.858e+09
4100.00	62.238	334.735	395.550	-1649.443	5.091e+07	7.072e+09
4150.00	62.241	339.060	396.304	-1673.667	5.386e+07	7.290e+09
4200.00	62.243	343.385	397.050	-1697.942	5.695e+07	7.511e+09
4250.00	62.246	347.710	397.786	-1722.270	6.018e+07	7.737e+09
4300.00	62.249	352.036	398.514	-1746.648	6.355e+07	7.966e+09
4350.00	62.251	356.362	399.234	-1771.076	6.707e+07	8.200e+09
4400.00	62.254	360.688	399.946	-1795.554	7.075e+07	8.438e+09
4450.00	62.256	365.014	400.649	-1820.081	7.459e+07	8.679e+09
4500.00	62.258	369.340	401.345	-1844.657	7.859e+07	8.925e+09
4550.00	62.260	373.667	402.033	-1869.281	8.276e+07	9.175e+09
4600.00	62.263	377.994	402.713	-1893.953	8.711e+07	9.429e+09
4650.00	62.265	382.321	403.386	-1918.671	9.163e+07	9.688e+09
4700.00	62.267	386.648	404.052	-1943.436	9.635e+07	9.950e+09
4750.00	62.268	390.975	404.711	-1968.247	1.013e+08	1.022e+10
4800.00	62.270	395.303	405.363	-1993.104	1.064e+08	1.049e+10
4850.00	62.272	399.631	406.008	-2018.005	1.117e+08	1.076e+10
4900.00	62.274	403.958	406.647	-2042.952	1.172e+08	1.104e+10
4950.00	62.276	408.286	407.279	-2067.942	1.229e+08	1.133e+10
5000.00	62.277	412.615	407.905	-2092.976	1.289e+08	1.161e+10
5050.00	62.279	416.943	408.525	-2118.054	1.351e+08	1.191e+10
5100.00	62.280	421.271	409.139	-2143.174	1.415e+08	1.220e+10
5150.00	62.282	425.600	409.746	-2168.337	1.481e+08	1.251e+10
5200.00	62.283	429.929	410.348	-2193.542	1.550e+08	1.281e+10
5250.00	62.285	434.257	410.944	-2218.788	1.622e+08	1.312e+10
5300.00	62.286	438.586	411.534	-2244.076	1.696e+08	1.344e+10
5350.00	62.288	442.915	412.119	-2269.404	1.773e+08	1.376e+10
5400.00	62.289	447.244	412.699	-2294.773	1.853e+08	1.408e+10
5450.00	62.290	451.574	413.273	-2320.182	1.936e+08	1.441e+10
5500.00	62.291	455.903	413.842	-2345.631	2.021e+08	1.474e+10
5550.00	62.293	460.233	414.405	-2371.119	2.110e+08	1.508e+10
5600.00	62.294	464.562	414.964	-2396.646	2.201e+08	1.542e+10

5650.00	62.295	468.892	415.518	-2422.212	2.296e+08	1.577e+10
5700.00	62.296	473.222	416.067	-2447.816	2.394e+08	1.612e+10
5750.00	62.297	477.552	416.611	-2473.458	2.496e+08	1.647e+10
5800.00	62.298	481.882	417.150	-2499.138	2.600e+08	1.683e+10
5850.00	62.299	486.212	417.685	-2524.855	2.708e+08	1.720e+10
5900.00	62.300	490.542	418.215	-2550.609	2.820e+08	1.757e+10
5950.00	62.301	494.872	418.741	-2576.400	2.936e+08	1.794e+10
6000.00	62.302	499.202	419.262	-2602.227	3.055e+08	1.832e+10
6050.00	62.303	503.533	419.779	-2628.090	3.178e+08	1.871e+10
6100.00	62.304	507.863	420.292	-2653.989	3.305e+08	1.909e+10
6150.00	62.305	512.194	420.801	-2679.924	3.436e+08	1.949e+10
6200.00	62.306	516.524	421.305	-2705.894	3.571e+08	1.989e+10
6250.00	62.307	520.855	421.806	-2731.898	3.710e+08	2.029e+10
6300.00	62.307	525.186	422.302	-2757.938	3.854e+08	2.070e+10
6350.00	62.308	529.517	422.795	-2784.011	4.002e+08	2.111e+10
6400.00	62.309	533.848	423.283	-2810.119	4.154e+08	2.153e+10
6450.00	62.310	538.179	423.768	-2836.260	4.312e+08	2.195e+10
6500.00	62.311	542.510	424.249	-2862.436	4.474e+08	2.238e+10
6550.00	62.311	546.841	424.727	-2888.644	4.640e+08	2.281e+10
6600.00	62.312	551.172	425.201	-2914.886	4.812e+08	2.325e+10
6650.00	62.313	555.503	425.671	-2941.160	4.989e+08	2.369e+10
6700.00	62.313	559.835	426.138	-2967.467	5.171e+08	2.414e+10
6750.00	62.314	564.166	426.601	-2993.806	5.358e+08	2.459e+10
6800.00	62.315	568.497	427.061	-3020.178	5.550e+08	2.505e+10
6850.00	62.315	572.829	427.517	-3046.581	5.748e+08	2.552e+10
6900.00	62.316	577.160	427.971	-3073.016	5.952e+08	2.598e+10
6950.00	62.317	581.492	428.421	-3099.482	6.161e+08	2.646e+10
7000.00	62.317	585.824	428.867	-3125.979	6.377e+08	2.694e+10
7050.00	62.318	590.155	429.311	-3152.508	6.598e+08	2.742e+10
7100.00	62.318	594.487	429.751	-3179.067	6.825e+08	2.791e+10
7150.00	62.319	598.819	430.189	-3205.656	7.059e+08	2.840e+10
7200.00	62.319	603.151	430.623	-3232.276	7.298e+08	2.890e+10
7250.00	62.320	607.482	431.054	-3258.926	7.545e+08	2.941e+10
7300.00	62.321	611.814	431.482	-3285.606	7.798e+08	2.992e+10
7350.00	62.321	616.146	431.908	-3312.315	8.057e+08	3.043e+10
7400.00	62.322	620.478	432.330	-3339.054	8.324e+08	3.095e+10
7450.00	62.322	624.810	432.750	-3365.822	8.598e+08	3.148e+10
7500.00	62.323	629.143	433.167	-3392.620	8.878e+08	3.201e+10
7550.00	62.323	633.475	433.581	-3419.446	9.166e+08	3.254e+10
7600.00	62.323	637.807	433.992	-3446.301	9.462e+08	3.308e+10
7650.00	62.324	642.139	434.401	-3473.184	9.765e+08	3.363e+10
7700.00	62.324	646.471	434.807	-3500.096	1.008e+09	3.418e+10
7750.00	62.325	650.804	435.211	-3527.035	1.039e+09	3.474e+10
7800.00	62.325	655.136	435.611	-3554.003	1.072e+09	3.530e+10
7850.00	62.326	659.468	436.010	-3580.999	1.106e+09	3.587e+10
7900.00	62.326	663.801	436.405	-3608.022	1.140e+09	3.645e+10
7950.00	62.327	668.133	436.799	-3635.072	1.175e+09	3.703e+10
8000.00	62.327	672.466	437.189	-3662.150	1.211e+09	3.761e+10
8050.00	62.327	676.798	437.578	-3689.255	1.248e+09	3.820e+10
8100.00	62.328	681.131	437.964	-3716.387	1.286e+09	3.880e+10
8150.00	62.328	685.463	438.347	-3743.545	1.324e+09	3.940e+10
8200.00	62.328	689.796	438.728	-3770.730	1.364e+09	4.001e+10
8250.00	62.329	694.129	439.107	-3797.942	1.405e+09	4.062e+10
8300.00	62.329	698.461	439.484	-3825.180	1.446e+09	4.124e+10
8350.00	62.330	702.794	439.858	-3852.444	1.489e+09	4.186e+10
8400.00	62.330	707.127	440.230	-3879.733	1.532e+09	4.249e+10
8450.00	62.330	711.460	440.600	-3907.049	1.577e+09	4.312e+10
8500.00	62.331	715.792	440.968	-3934.390	1.622e+09	4.377e+10

8550.00	62.331	720.125	441.334	-3961.757	1.669e+09	4.441e+10
8600.00	62.331	724.458	441.697	-3989.149	1.716e+09	4.506e+10
8650.00	62.332	728.791	442.058	-4016.566	1.765e+09	4.572e+10
8700.00	62.332	733.124	442.418	-4044.009	1.815e+09	4.639e+10
8750.00	62.332	737.457	442.775	-4071.476	1.866e+09	4.706e+10
8800.00	62.332	741.790	443.130	-4098.968	1.918e+09	4.773e+10
8850.00	62.333	746.123	443.483	-4126.484	1.971e+09	4.841e+10
8900.00	62.333	750.456	443.834	-4154.025	2.026e+09	4.910e+10
8950.00	62.333	754.789	444.184	-4181.591	2.081e+09	4.979e+10
9000.00	62.334	759.122	444.531	-4209.181	2.138e+09	5.049e+10
9050.00	62.334	763.455	444.876	-4236.794	2.196e+09	5.119e+10
9100.00	62.334	767.788	445.220	-4264.432	2.256e+09	5.190e+10
9150.00	62.334	772.121	445.561	-4292.093	2.316e+09	5.262e+10
9200.00	62.335	776.455	445.901	-4319.778	2.378e+09	5.334e+10
9250.00	62.335	780.788	446.239	-4347.487	2.441e+09	5.407e+10
9300.00	62.335	785.121	446.575	-4375.219	2.506e+09	5.480e+10
9350.00	62.335	789.454	446.909	-4402.975	2.572e+09	5.554e+10
9400.00	62.336	793.787	447.241	-4430.753	2.639e+09	5.629e+10
9450.00	62.336	798.121	447.572	-4458.555	2.708e+09	5.704e+10
9500.00	62.336	802.454	447.901	-4486.379	2.778e+09	5.780e+10
9550.00	62.336	806.787	448.228	-4514.227	2.849e+09	5.856e+10
9600.00	62.337	811.121	448.554	-4542.097	2.922e+09	5.933e+10
9650.00	62.337	815.454	448.878	-4569.989	2.997e+09	6.010e+10
9700.00	62.337	819.787	449.200	-4597.904	3.073e+09	6.089e+10
9750.00	62.337	824.121	449.520	-4625.842	3.150e+09	6.167e+10
9800.00	62.338	828.454	449.839	-4653.801	3.230e+09	6.247e+10
9850.00	62.338	832.788	450.156	-4681.783	3.310e+09	6.327e+10
9900.00	62.338	837.121	450.472	-4709.787	3.393e+09	6.407e+10
9950.00	62.338	841.455	450.786	-4737.812	3.477e+09	6.489e+10
10000.00	62.338	845.788	451.099	-4765.860	3.562e+09	6.570e+10