

AlF2- : Aluminum fluoride anion

Enthalpy of Formation at 0 K:

JANAF[1] : $\Delta H(0K) = -900.00 \pm 84.00$
ORCA[2,3] DFT : $\Delta H(0K) = -815.27 \pm 10.25$

Molar Mass : 64.978897 g/mol

σ 2

Vibrational Frequencies and Degeneracies (cm^{-1}) [2]:

623.95(1) 254.95(1) 640.09(1)

Inertia Moment IA.IB.IC [2]:

4.64579e-136 ($\text{kg}\cdot\text{m}^2$)³

Electronic Levels Energy and Degeneracies (cm^{-1}) [2]:

0.00(1)
35042.93(1)
43143.03(1)
45333.53(1)
64686.57(1)
70714.69(1)
71422.98(1)
71644.33(1)
73907.39(1)

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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] 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
- [3] Paul G. Wenthold and Robert R. Squires, "Bond Dissociation Energies of F2 and HF2 . A Gas-Phase Experimental and G2 Theoretical Study", J. Phys. Chem., 99, 2002-2005, 1995 DOI: 10.1021/j100007a034

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	36.420	3.407	216.297	-18.222	2.426e+03	1.359e+06
150.00	39.857	5.314	231.708	-29.443	4.776e+03	3.745e+06
200.00	43.312	7.394	243.652	-41.337	8.127e+03	7.688e+06
250.00	46.338	9.637	253.653	-53.776	1.281e+04	1.343e+07
298.15	48.672	11.927	262.023	-66.195	1.894e+04	2.086e+07
300.00	48.751	12.017	262.324	-66.680	1.922e+04	2.119e+07
350.00	50.602	14.503	269.984	-79.991	2.782e+04	3.115e+07
400.00	52.011	17.070	276.837	-93.665	3.914e+04	4.349e+07
450.00	53.089	19.699	283.028	-107.664	5.379e+04	5.838e+07
500.00	53.924	22.375	288.667	-121.959	7.243e+04	7.598e+07
550.00	54.578	25.088	293.838	-136.523	9.580e+04	9.642e+07
600.00	55.099	27.830	298.610	-151.336	1.247e+05	1.198e+08
650.00	55.518	30.596	303.038	-166.378	1.601e+05	1.464e+08
700.00	55.860	33.381	307.165	-181.635	2.030e+05	1.762e+08
750.00	56.142	36.181	311.029	-197.090	2.543e+05	2.094e+08
800.00	56.377	38.994	314.660	-212.734	3.153e+05	2.460e+08
850.00	56.574	41.818	318.084	-228.553	3.873e+05	2.863e+08
900.00	56.742	44.651	321.323	-244.539	4.715e+05	3.303e+08
950.00	56.885	47.492	324.394	-260.683	5.694e+05	3.781e+08
1000.00	57.009	50.340	327.315	-276.976	6.825e+05	4.298e+08
1050.00	57.116	53.193	330.100	-293.412	8.125e+05	4.855e+08
1100.00	57.209	56.051	332.759	-309.984	9.611e+05	5.454e+08
1150.00	57.291	58.913	335.304	-326.686	1.130e+06	6.095e+08
1200.00	57.364	61.780	337.744	-343.512	1.322e+06	6.780e+08
1250.00	57.428	64.650	340.087	-360.458	1.538e+06	7.508e+08
1300.00	57.485	67.523	342.340	-377.520	1.780e+06	8.282e+08
1350.00	57.536	70.398	344.511	-394.691	2.051e+06	9.101e+08
1400.00	57.582	73.276	346.604	-411.969	2.354e+06	9.967e+08
1450.00	57.623	76.156	348.625	-429.350	2.690e+06	1.088e+09
1500.00	57.660	79.038	350.579	-446.831	3.063e+06	1.184e+09
1550.00	57.694	81.922	352.471	-464.407	3.475e+06	1.286e+09
1600.00	57.725	84.808	354.303	-482.077	3.929e+06	1.392e+09
1650.00	57.753	87.695	356.079	-499.837	4.427e+06	1.503e+09
1700.00	57.778	90.583	357.804	-517.684	4.974e+06	1.619e+09
1750.00	57.802	93.472	359.479	-535.616	5.572e+06	1.741e+09
1800.00	57.824	96.363	361.108	-553.631	6.225e+06	1.868e+09
1850.00	57.844	99.255	362.692	-571.726	6.935e+06	2.001e+09
1900.00	57.862	102.147	364.235	-589.900	7.708e+06	2.139e+09
1950.00	57.879	105.041	365.738	-608.149	8.545e+06	2.282e+09
2000.00	57.895	107.935	367.204	-626.473	9.452e+06	2.431e+09
2050.00	57.909	110.830	368.634	-644.869	1.043e+07	2.586e+09
2100.00	57.923	113.726	370.029	-663.336	1.149e+07	2.747e+09
2150.00	57.936	116.623	371.392	-681.871	1.263e+07	2.913e+09
2200.00	57.948	119.520	372.725	-700.474	1.386e+07	3.085e+09
2250.00	57.959	122.417	374.027	-719.143	1.517e+07	3.264e+09
2300.00	57.969	125.316	375.301	-737.876	1.658e+07	3.448e+09
2350.00	57.979	128.214	376.548	-756.673	1.810e+07	3.639e+09
2400.00	57.988	131.113	377.768	-775.531	1.971e+07	3.835e+09
2450.00	57.996	134.013	378.964	-794.449	2.144e+07	4.038e+09
2500.00	58.005	136.913	380.136	-813.427	2.329e+07	4.247e+09
2550.00	58.012	139.813	381.285	-832.462	2.525e+07	4.463e+09
2600.00	58.019	142.714	382.411	-851.555	2.734e+07	4.685e+09
2650.00	58.026	145.615	383.516	-870.703	2.957e+07	4.913e+09
2700.00	58.032	148.517	384.601	-889.906	3.193e+07	5.148e+09

2750.00	58.039	151.419	385.666	-909.163	3.443e+07	5.390e+09
2800.00	58.044	154.321	386.712	-928.472	3.709e+07	5.638e+09
2850.00	58.050	157.223	387.739	-947.834	3.991e+07	5.893e+09
2900.00	58.055	160.126	388.749	-967.246	4.288e+07	6.155e+09
2950.00	58.060	163.029	389.741	-986.708	4.603e+07	6.424e+09
3000.00	58.065	165.932	390.717	-1006.220	4.936e+07	6.700e+09
3050.00	58.069	168.835	391.677	-1025.780	5.287e+07	6.982e+09
3100.00	58.073	171.739	392.621	-1045.387	5.657e+07	7.272e+09
3150.00	58.077	174.642	393.551	-1065.042	6.046e+07	7.569e+09
3200.00	58.081	177.546	394.465	-1084.742	6.457e+07	7.873e+09
3250.00	58.085	180.450	395.366	-1104.488	6.889e+07	8.184e+09
3300.00	58.089	183.355	396.253	-1124.279	7.343e+07	8.502e+09
3350.00	58.092	186.259	397.126	-1144.113	7.820e+07	8.828e+09
3400.00	58.095	189.164	397.987	-1163.991	8.320e+07	9.161e+09
3450.00	58.099	192.069	398.835	-1183.912	8.846e+07	9.502e+09
3500.00	58.102	194.974	399.671	-1203.874	9.396e+07	9.850e+09
3550.00	58.105	197.879	400.495	-1223.878	9.973e+07	1.021e+10
3600.00	58.108	200.784	401.308	-1243.924	1.058e+08	1.057e+10
3650.00	58.111	203.690	402.109	-1264.009	1.121e+08	1.094e+10
3700.00	58.113	206.595	402.900	-1284.134	1.187e+08	1.132e+10
3750.00	58.116	209.501	403.680	-1304.299	1.256e+08	1.170e+10
3800.00	58.119	212.407	404.450	-1324.502	1.329e+08	1.210e+10
3850.00	58.121	215.313	405.210	-1344.744	1.404e+08	1.250e+10
3900.00	58.124	218.219	405.960	-1365.023	1.483e+08	1.291e+10
3950.00	58.127	221.125	406.700	-1385.339	1.565e+08	1.333e+10
4000.00	58.129	224.032	407.431	-1405.693	1.650e+08	1.375e+10
4050.00	58.132	226.938	408.153	-1426.082	1.740e+08	1.419e+10
4100.00	58.135	229.845	408.867	-1446.508	1.833e+08	1.463e+10
4150.00	58.137	232.752	409.571	-1466.969	1.929e+08	1.508e+10
4200.00	58.140	235.659	410.268	-1487.465	2.030e+08	1.554e+10
4250.00	58.143	238.566	410.956	-1507.996	2.135e+08	1.600e+10
4300.00	58.145	241.473	411.636	-1528.560	2.244e+08	1.648e+10
4350.00	58.148	244.380	412.308	-1549.159	2.357e+08	1.696e+10
4400.00	58.151	247.288	412.972	-1569.791	2.474e+08	1.745e+10
4450.00	58.154	250.195	413.630	-1590.456	2.596e+08	1.795e+10
4500.00	58.157	253.103	414.279	-1611.154	2.723e+08	1.846e+10
4550.00	58.160	256.011	414.922	-1631.884	2.854e+08	1.898e+10
4600.00	58.164	258.919	415.558	-1652.646	2.991e+08	1.951e+10
4650.00	58.167	261.828	416.186	-1673.440	3.132e+08	2.004e+10
4700.00	58.171	264.736	416.809	-1694.265	3.278e+08	2.058e+10
4750.00	58.174	267.645	417.424	-1715.120	3.430e+08	2.113e+10
4800.00	58.178	270.553	418.033	-1736.007	3.587e+08	2.170e+10
4850.00	58.182	273.462	418.636	-1756.924	3.750e+08	2.226e+10
4900.00	58.187	276.372	419.233	-1777.870	3.918e+08	2.284e+10
4950.00	58.191	279.281	419.824	-1798.847	4.093e+08	2.343e+10
5000.00	58.196	282.191	420.409	-1819.853	4.273e+08	2.403e+10
5050.00	58.201	285.101	420.988	-1840.888	4.459e+08	2.463e+10
5100.00	58.206	288.011	421.561	-1861.951	4.652e+08	2.525e+10
5150.00	58.211	290.921	422.129	-1883.044	4.851e+08	2.587e+10
5200.00	58.216	293.832	422.692	-1904.164	5.056e+08	2.650e+10
5250.00	58.222	296.743	423.249	-1925.313	5.268e+08	2.714e+10
5300.00	58.228	299.654	423.801	-1946.489	5.487e+08	2.779e+10
5350.00	58.235	302.566	424.347	-1967.693	5.714e+08	2.845e+10
5400.00	58.241	305.478	424.889	-1988.924	5.947e+08	2.912e+10
5450.00	58.248	308.390	425.426	-2010.181	6.188e+08	2.980e+10
5500.00	58.255	311.302	425.958	-2031.466	6.436e+08	3.049e+10
5550.00	58.263	314.215	426.485	-2052.777	6.692e+08	3.119e+10
5600.00	58.271	317.129	427.008	-2074.115	6.955e+08	3.190e+10

5650.00	58.279	320.042	427.526	-2095.478	7.227e+08	3.261e+10
5700.00	58.288	322.957	428.039	-2116.867	7.507e+08	3.334e+10
5750.00	58.296	325.871	428.548	-2138.282	7.795e+08	3.407e+10
5800.00	58.306	328.786	429.053	-2159.722	8.092e+08	3.482e+10
5850.00	58.315	331.702	429.554	-2181.187	8.398e+08	3.558e+10
5900.00	58.325	334.618	430.050	-2202.677	8.713e+08	3.634e+10
5950.00	58.336	337.534	430.542	-2224.192	9.036e+08	3.712e+10
6000.00	58.347	340.451	431.030	-2245.731	9.369e+08	3.790e+10
6050.00	58.358	343.369	431.515	-2267.295	9.711e+08	3.869e+10
6100.00	58.370	346.287	431.995	-2288.883	1.006e+09	3.950e+10
6150.00	58.382	349.206	432.472	-2310.494	1.043e+09	4.031e+10
6200.00	58.394	352.125	432.944	-2332.130	1.080e+09	4.114e+10
6250.00	58.407	355.045	433.413	-2353.789	1.118e+09	4.197e+10
6300.00	58.421	357.966	433.879	-2375.471	1.157e+09	4.282e+10
6350.00	58.434	360.887	434.341	-2397.177	1.198e+09	4.367e+10
6400.00	58.449	363.810	434.799	-2418.905	1.239e+09	4.454e+10
6450.00	58.464	366.732	435.254	-2440.656	1.282e+09	4.541e+10
6500.00	58.479	369.656	435.706	-2462.430	1.325e+09	4.630e+10
6550.00	58.495	372.580	436.154	-2484.227	1.370e+09	4.719e+10
6600.00	58.511	375.505	436.599	-2506.046	1.416e+09	4.810e+10
6650.00	58.527	378.431	437.040	-2527.887	1.463e+09	4.901e+10
6700.00	58.545	381.358	437.479	-2549.750	1.512e+09	4.994e+10
6750.00	58.562	384.286	437.914	-2571.635	1.561e+09	5.088e+10
6800.00	58.581	387.214	438.346	-2593.541	1.612e+09	5.182e+10
6850.00	58.599	390.144	438.776	-2615.469	1.664e+09	5.278e+10
6900.00	58.619	393.074	439.202	-2637.418	1.718e+09	5.375e+10
6950.00	58.638	396.006	439.625	-2659.389	1.773e+09	5.473e+10
7000.00	58.659	398.938	440.046	-2681.381	1.829e+09	5.572e+10
7050.00	58.680	401.872	440.463	-2703.394	1.887e+09	5.672e+10
7100.00	58.701	404.806	440.878	-2725.427	1.946e+09	5.773e+10
7150.00	58.723	407.742	441.290	-2747.481	2.006e+09	5.875e+10
7200.00	58.745	410.678	441.699	-2769.556	2.068e+09	5.978e+10
7250.00	58.768	413.616	442.106	-2791.651	2.131e+09	6.083e+10
7300.00	58.792	416.555	442.510	-2813.767	2.196e+09	6.188e+10
7350.00	58.816	419.495	442.911	-2835.902	2.262e+09	6.295e+10
7400.00	58.840	422.437	443.310	-2858.058	2.330e+09	6.402e+10
7450.00	58.866	425.380	443.706	-2880.233	2.400e+09	6.511e+10
7500.00	58.891	428.323	444.100	-2902.428	2.471e+09	6.621e+10
7550.00	58.918	431.269	444.492	-2924.643	2.544e+09	6.732e+10
7600.00	58.944	434.215	444.881	-2946.878	2.618e+09	6.844e+10
7650.00	58.972	437.163	445.267	-2969.131	2.694e+09	6.957e+10
7700.00	59.000	440.112	445.652	-2991.404	2.772e+09	7.071e+10
7750.00	59.028	443.063	446.033	-3013.696	2.852e+09	7.186e+10
7800.00	59.057	446.015	446.413	-3036.008	2.933e+09	7.303e+10
7850.00	59.087	448.969	446.791	-3058.338	3.017e+09	7.420e+10
7900.00	59.117	451.924	447.166	-3080.687	3.102e+09	7.539e+10
7950.00	59.147	454.880	447.539	-3103.054	3.189e+09	7.659e+10
8000.00	59.179	457.839	447.910	-3125.440	3.277e+09	7.780e+10
8050.00	59.210	460.798	448.279	-3147.845	3.368e+09	7.902e+10
8100.00	59.243	463.760	448.645	-3170.268	3.461e+09	8.025e+10
8150.00	59.275	466.723	449.010	-3192.710	3.556e+09	8.150e+10
8200.00	59.309	469.687	449.373	-3215.169	3.652e+09	8.275e+10
8250.00	59.343	472.653	449.733	-3237.647	3.751e+09	8.402e+10
8300.00	59.377	475.621	450.092	-3260.143	3.852e+09	8.530e+10
8350.00	59.412	478.591	450.449	-3282.656	3.955e+09	8.659e+10
8400.00	59.448	481.563	450.804	-3305.188	4.060e+09	8.789e+10
8450.00	59.484	484.536	451.156	-3327.736	4.167e+09	8.921e+10
8500.00	59.520	487.511	451.508	-3350.303	4.277e+09	9.053e+10

8550.00	59.558	490.488	451.857	-3372.887	4.389e+09	9.187e+10
8600.00	59.595	493.467	452.204	-3395.489	4.503e+09	9.322e+10
8650.00	59.633	496.448	452.550	-3418.108	4.619e+09	9.458e+10
8700.00	59.672	499.430	452.894	-3440.744	4.738e+09	9.595e+10
8750.00	59.711	502.415	453.236	-3463.397	4.859e+09	9.734e+10
8800.00	59.751	505.401	453.576	-3486.067	4.983e+09	9.873e+10
8850.00	59.791	508.390	453.915	-3508.754	5.109e+09	1.001e+11
8900.00	59.832	511.380	454.252	-3531.458	5.237e+09	1.016e+11
8950.00	59.873	514.373	454.587	-3554.180	5.368e+09	1.030e+11
9000.00	59.915	517.368	454.921	-3576.917	5.502e+09	1.044e+11
9050.00	59.957	520.365	455.253	-3599.672	5.638e+09	1.059e+11
9100.00	60.000	523.364	455.583	-3622.442	5.777e+09	1.074e+11
9150.00	60.043	526.365	455.912	-3645.230	5.918e+09	1.088e+11
9200.00	60.087	529.368	456.239	-3668.034	6.063e+09	1.103e+11
9250.00	60.131	532.373	456.565	-3690.854	6.210e+09	1.118e+11
9300.00	60.176	535.381	456.889	-3713.690	6.360e+09	1.134e+11
9350.00	60.221	538.391	457.212	-3736.543	6.512e+09	1.149e+11
9400.00	60.266	541.403	457.533	-3759.411	6.668e+09	1.164e+11
9450.00	60.312	544.418	457.853	-3782.296	6.826e+09	1.180e+11
9500.00	60.359	547.434	458.172	-3805.197	6.988e+09	1.196e+11
9550.00	60.406	550.453	458.489	-3828.113	7.152e+09	1.211e+11
9600.00	60.453	553.475	458.804	-3851.045	7.320e+09	1.227e+11
9650.00	60.501	556.499	459.118	-3873.994	7.490e+09	1.243e+11
9700.00	60.549	559.525	459.431	-3896.957	7.664e+09	1.259e+11
9750.00	60.598	562.554	459.743	-3919.937	7.841e+09	1.276e+11
9800.00	60.647	565.585	460.053	-3942.932	8.021e+09	1.292e+11
9850.00	60.696	568.618	460.361	-3965.942	8.204e+09	1.309e+11
9900.00	60.746	571.654	460.669	-3988.968	8.391e+09	1.325e+11
9950.00	60.797	574.693	460.975	-4012.009	8.581e+09	1.342e+11
10000.00	60.847	577.734	461.280	-4035.065	8.775e+09	1.359e+11

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	37.942	3.495	217.086	-18.254	2.491e+03	1.359e+06
150.00	42.214	5.576	233.277	-29.568	5.096e+03	3.745e+06
200.00	46.060	7.909	245.967	-41.628	9.047e+03	7.688e+06
250.00	49.008	10.451	256.579	-54.303	1.487e+04	1.343e+07
298.15	51.070	13.045	265.397	-67.008	2.283e+04	2.086e+07
300.00	51.137	13.147	265.713	-67.505	2.319e+04	2.119e+07
350.00	52.663	15.954	273.717	-81.167	3.475e+04	3.115e+07
400.00	53.771	18.841	280.825	-95.238	5.040e+04	4.349e+07
450.00	54.592	21.786	287.208	-109.674	7.112e+04	5.838e+07
500.00	55.211	24.776	292.994	-124.441	9.802e+04	7.598e+07
550.00	55.688	27.798	298.279	-139.509	1.323e+05	9.642e+07
600.00	56.062	30.846	303.141	-154.853	1.754e+05	1.198e+08
650.00	56.360	33.915	307.641	-170.452	2.288e+05	1.464e+08
700.00	56.601	37.000	311.827	-186.288	2.942e+05	1.762e+08
750.00	56.798	40.099	315.739	-202.346	3.734e+05	2.094e+08
800.00	56.961	43.209	319.410	-218.610	4.684e+05	2.460e+08
850.00	57.098	46.327	322.867	-235.069	5.813e+05	2.863e+08
900.00	57.213	49.454	326.134	-251.712	7.144e+05	3.303e+08
950.00	57.312	52.587	329.230	-268.529	8.703e+05	3.781e+08
1000.00	57.396	55.725	332.172	-285.511	1.052e+06	4.298e+08
1050.00	57.469	58.869	334.974	-302.650	1.261e+06	4.855e+08
1100.00	57.533	62.016	337.649	-319.939	1.502e+06	5.454e+08
1150.00	57.589	65.167	340.208	-337.371	1.777e+06	6.095e+08
1200.00	57.638	68.322	342.660	-354.940	2.090e+06	6.780e+08
1250.00	57.681	71.479	345.014	-372.641	2.444e+06	7.508e+08
1300.00	57.720	74.639	347.277	-390.468	2.844e+06	8.282e+08
1350.00	57.755	77.801	349.456	-408.417	3.293e+06	9.101e+08
1400.00	57.786	80.965	351.557	-426.483	3.795e+06	9.967e+08
1450.00	57.813	84.130	353.585	-444.662	4.355e+06	1.088e+09
1500.00	57.839	87.298	355.546	-462.950	4.977e+06	1.184e+09
1550.00	57.861	90.467	357.443	-481.344	5.667e+06	1.286e+09
1600.00	57.882	93.637	359.280	-499.840	6.429e+06	1.392e+09
1650.00	57.901	96.808	361.061	-518.435	7.268e+06	1.503e+09
1700.00	57.918	99.981	362.790	-537.126	8.191e+06	1.619e+09
1750.00	57.934	103.154	364.469	-555.911	9.202e+06	1.741e+09
1800.00	57.949	106.329	366.102	-574.786	1.031e+07	1.868e+09
1850.00	57.962	109.504	367.689	-593.750	1.152e+07	2.001e+09
1900.00	57.974	112.680	369.235	-612.799	1.283e+07	2.139e+09
1950.00	57.986	115.857	370.741	-631.932	1.426e+07	2.282e+09
2000.00	57.996	119.034	372.210	-651.147	1.581e+07	2.431e+09
2050.00	58.006	122.212	373.642	-670.441	1.748e+07	2.586e+09
2100.00	58.016	125.391	375.040	-689.812	1.930e+07	2.747e+09
2150.00	58.024	128.570	376.405	-709.259	2.125e+07	2.913e+09
2200.00	58.032	131.750	377.739	-728.780	2.336e+07	3.085e+09
2250.00	58.040	134.930	379.043	-748.374	2.562e+07	3.264e+09
2300.00	58.047	138.111	380.319	-768.038	2.805e+07	3.448e+09
2350.00	58.054	141.292	381.567	-787.771	3.066e+07	3.639e+09
2400.00	58.060	144.474	382.790	-807.572	3.346e+07	3.835e+09
2450.00	58.066	147.656	383.987	-827.439	3.645e+07	4.038e+09
2500.00	58.072	150.838	385.160	-847.371	3.964e+07	4.247e+09
2550.00	58.078	154.021	386.310	-867.367	4.304e+07	4.463e+09
2600.00	58.084	157.204	387.438	-887.425	4.667e+07	4.685e+09
2650.00	58.089	160.387	388.544	-907.545	5.054e+07	4.913e+09
2700.00	58.094	163.571	389.630	-927.724	5.464e+07	5.148e+09

2750.00	58.100	166.755	390.696	-947.963	5.901e+07	5.390e+09
2800.00	58.105	169.939	391.743	-968.259	6.363e+07	5.638e+09
2850.00	58.110	173.124	392.772	-988.612	6.854e+07	5.893e+09
2900.00	58.116	176.309	393.782	-1009.021	7.374e+07	6.155e+09
2950.00	58.121	179.495	394.776	-1029.485	7.923e+07	6.424e+09
3000.00	58.127	182.680	395.753	-1050.004	8.505e+07	6.700e+09
3050.00	58.133	185.867	396.714	-1070.575	9.118e+07	6.982e+09
3100.00	58.139	189.053	397.659	-1091.198	9.766e+07	7.272e+09
3150.00	58.145	192.240	398.589	-1111.873	1.045e+08	7.569e+09
3200.00	58.152	195.428	399.505	-1132.598	1.117e+08	7.873e+09
3250.00	58.159	198.616	400.407	-1153.373	1.193e+08	8.184e+09
3300.00	58.166	201.804	401.295	-1174.198	1.272e+08	8.502e+09
3350.00	58.174	204.993	402.169	-1195.070	1.356e+08	8.828e+09
3400.00	58.182	208.183	403.031	-1215.990	1.444e+08	9.161e+09
3450.00	58.191	211.373	403.881	-1236.957	1.537e+08	9.502e+09
3500.00	58.200	214.564	404.718	-1257.971	1.634e+08	9.850e+09
3550.00	58.210	217.755	405.544	-1279.030	1.735e+08	1.021e+10
3600.00	58.220	220.948	406.358	-1300.133	1.842e+08	1.057e+10
3650.00	58.231	224.141	407.161	-1321.282	1.953e+08	1.094e+10
3700.00	58.243	227.335	407.953	-1342.474	2.070e+08	1.132e+10
3750.00	58.255	230.529	408.735	-1363.709	2.192e+08	1.170e+10
3800.00	58.269	233.725	409.507	-1384.986	2.320e+08	1.210e+10
3850.00	58.283	236.922	410.269	-1406.306	2.453e+08	1.250e+10
3900.00	58.297	240.119	411.021	-1427.667	2.592e+08	1.291e+10
3950.00	58.313	243.318	411.764	-1449.070	2.737e+08	1.333e+10
4000.00	58.329	246.518	412.497	-1470.512	2.889e+08	1.375e+10
4050.00	58.347	249.720	413.222	-1491.995	3.047e+08	1.419e+10
4100.00	58.365	252.922	413.938	-1513.518	3.212e+08	1.463e+10
4150.00	58.385	256.126	414.646	-1535.079	3.383e+08	1.508e+10
4200.00	58.405	259.332	415.345	-1556.679	3.562e+08	1.554e+10
4250.00	58.426	262.539	416.036	-1578.317	3.748e+08	1.600e+10
4300.00	58.449	265.748	416.720	-1599.993	3.941e+08	1.648e+10
4350.00	58.472	268.958	417.396	-1621.706	4.142e+08	1.696e+10
4400.00	58.497	272.170	418.064	-1643.457	4.351e+08	1.745e+10
4450.00	58.522	275.384	418.725	-1665.243	4.568e+08	1.795e+10
4500.00	58.549	278.600	419.379	-1687.066	4.794e+08	1.846e+10
4550.00	58.577	281.818	420.026	-1708.925	5.028e+08	1.898e+10
4600.00	58.606	285.038	420.667	-1730.819	5.270e+08	1.951e+10
4650.00	58.636	288.261	421.300	-1752.748	5.522e+08	2.004e+10
4700.00	58.667	291.485	421.928	-1774.711	5.784e+08	2.058e+10
4750.00	58.700	294.712	422.549	-1796.709	6.054e+08	2.113e+10
4800.00	58.733	297.942	423.163	-1818.741	6.335e+08	2.170e+10
4850.00	58.768	301.174	423.772	-1840.807	6.626e+08	2.226e+10
4900.00	58.804	304.409	424.375	-1862.905	6.926e+08	2.284e+10
4950.00	58.842	307.646	424.972	-1885.037	7.238e+08	2.343e+10
5000.00	58.880	310.886	425.564	-1907.202	7.560e+08	2.403e+10
5050.00	58.920	314.129	426.150	-1929.399	7.894e+08	2.463e+10
5100.00	58.961	317.376	426.731	-1951.628	8.239e+08	2.525e+10
5150.00	59.003	320.625	427.306	-1973.889	8.595e+08	2.587e+10
5200.00	59.047	323.878	427.876	-1996.182	8.964e+08	2.650e+10
5250.00	59.092	327.133	428.442	-2018.505	9.345e+08	2.714e+10
5300.00	59.138	330.393	429.002	-2040.860	9.738e+08	2.779e+10
5350.00	59.185	333.655	429.558	-2063.246	1.014e+09	2.845e+10
5400.00	59.233	336.922	430.108	-2085.662	1.056e+09	2.912e+10
5450.00	59.283	340.192	430.654	-2108.109	1.100e+09	2.980e+10
5500.00	59.334	343.466	431.196	-2130.585	1.144e+09	3.049e+10
5550.00	59.386	346.743	431.733	-2153.091	1.190e+09	3.119e+10
5600.00	59.439	350.025	432.266	-2175.627	1.238e+09	3.190e+10

5650.00	59.493	353.310	432.795	-2198.192	1.287e+09	3.261e+10
5700.00	59.549	356.600	433.319	-2220.786	1.338e+09	3.334e+10
5750.00	59.606	359.894	433.839	-2243.409	1.390e+09	3.407e+10
5800.00	59.664	363.192	434.356	-2266.061	1.443e+09	3.482e+10
5850.00	59.723	366.495	434.868	-2288.741	1.499e+09	3.558e+10
5900.00	59.783	369.802	435.377	-2311.450	1.556e+09	3.634e+10
5950.00	59.845	373.113	435.882	-2334.186	1.614e+09	3.712e+10
6000.00	59.907	376.430	436.383	-2356.950	1.674e+09	3.790e+10
6050.00	59.971	379.751	436.880	-2379.742	1.737e+09	3.869e+10
6100.00	60.036	383.076	437.374	-2402.562	1.800e+09	3.950e+10
6150.00	60.102	386.407	437.864	-2425.409	1.866e+09	4.031e+10
6200.00	60.169	389.743	438.351	-2448.282	1.934e+09	4.114e+10
6250.00	60.236	393.084	438.835	-2471.183	2.003e+09	4.197e+10
6300.00	60.305	396.429	439.315	-2494.111	2.075e+09	4.282e+10
6350.00	60.375	399.780	439.792	-2517.065	2.149e+09	4.367e+10
6400.00	60.446	403.137	440.266	-2540.045	2.224e+09	4.454e+10
6450.00	60.518	406.499	440.736	-2563.052	2.302e+09	4.541e+10
6500.00	60.591	409.866	441.204	-2586.084	2.382e+09	4.630e+10
6550.00	60.665	413.238	441.669	-2609.143	2.464e+09	4.719e+10
6600.00	60.740	416.617	442.130	-2632.228	2.548e+09	4.810e+10
6650.00	60.816	420.000	442.589	-2655.338	2.634e+09	4.901e+10
6700.00	60.892	423.390	443.045	-2678.473	2.723e+09	4.994e+10
6750.00	60.970	426.785	443.498	-2701.634	2.814e+09	5.088e+10
6800.00	61.048	430.186	443.948	-2724.820	2.908e+09	5.182e+10
6850.00	61.127	433.593	444.396	-2748.031	3.004e+09	5.278e+10
6900.00	61.207	437.007	444.840	-2771.267	3.102e+09	5.375e+10
6950.00	61.288	440.426	445.283	-2794.528	3.203e+09	5.473e+10
7000.00	61.369	443.851	445.722	-2817.813	3.307e+09	5.572e+10
7050.00	61.451	447.282	446.159	-2841.123	3.413e+09	5.672e+10
7100.00	61.534	450.719	446.594	-2864.458	3.522e+09	5.773e+10
7150.00	61.618	454.163	447.026	-2887.816	3.634e+09	5.875e+10
7200.00	61.702	457.613	447.456	-2911.198	3.749e+09	5.978e+10
7250.00	61.787	461.069	447.883	-2934.605	3.866e+09	6.083e+10
7300.00	61.873	464.532	448.308	-2958.035	3.987e+09	6.188e+10
7350.00	61.959	468.001	448.731	-2981.489	4.110e+09	6.295e+10
7400.00	62.045	471.477	449.151	-3004.967	4.236e+09	6.402e+10
7450.00	62.133	474.959	449.569	-3028.468	4.366e+09	6.511e+10
7500.00	62.221	478.448	449.985	-3051.993	4.499e+09	6.621e+10
7550.00	62.309	481.943	450.399	-3075.541	4.635e+09	6.732e+10
7600.00	62.398	485.445	450.810	-3099.112	4.774e+09	6.844e+10
7650.00	62.487	488.953	451.220	-3122.706	4.916e+09	6.957e+10
7700.00	62.577	492.469	451.627	-3146.323	5.062e+09	7.071e+10
7750.00	62.667	495.991	452.032	-3169.963	5.211e+09	7.186e+10
7800.00	62.757	499.520	452.436	-3193.625	5.364e+09	7.303e+10
7850.00	62.848	503.055	452.837	-3217.311	5.521e+09	7.420e+10
7900.00	62.940	506.598	453.236	-3241.019	5.681e+09	7.539e+10
7950.00	63.031	510.147	453.634	-3264.749	5.845e+09	7.659e+10
8000.00	63.123	513.703	454.029	-3288.502	6.012e+09	7.780e+10
8050.00	63.215	517.267	454.423	-3312.277	6.184e+09	7.902e+10
8100.00	63.308	520.837	454.814	-3336.073	6.359e+09	8.025e+10
8150.00	63.401	524.414	455.204	-3359.893	6.539e+09	8.150e+10
8200.00	63.493	527.998	455.592	-3383.734	6.722e+09	8.275e+10
8250.00	63.587	531.588	455.979	-3407.597	6.910e+09	8.402e+10
8300.00	63.680	535.186	456.363	-3431.481	7.102e+09	8.530e+10
8350.00	63.773	538.791	456.746	-3455.388	7.298e+09	8.659e+10
8400.00	63.867	542.403	457.127	-3479.316	7.499e+09	8.789e+10
8450.00	63.960	546.022	457.506	-3503.265	7.704e+09	8.921e+10
8500.00	64.054	549.648	457.884	-3527.236	7.913e+09	9.053e+10

8550.00	64.148	553.281	458.260	-3551.229	8.127e+09	9.187e+10
8600.00	64.242	556.921	458.634	-3575.242	8.346e+09	9.322e+10
8650.00	64.336	560.568	459.007	-3599.277	8.569e+09	9.458e+10
8700.00	64.429	564.222	459.378	-3623.333	8.798e+09	9.595e+10
8750.00	64.523	567.883	459.747	-3647.410	9.031e+09	9.734e+10
8800.00	64.617	571.552	460.115	-3671.508	9.269e+09	9.873e+10
8850.00	64.710	575.227	460.482	-3695.626	9.513e+09	1.001e+11
8900.00	64.804	578.909	460.846	-3719.766	9.761e+09	1.016e+11
8950.00	64.897	582.598	461.210	-3743.926	1.002e+10	1.030e+11
9000.00	64.991	586.294	461.572	-3768.107	1.027e+10	1.044e+11
9050.00	65.084	589.998	461.932	-3792.308	1.054e+10	1.059e+11
9100.00	65.177	593.708	462.291	-3816.530	1.081e+10	1.074e+11
9150.00	65.270	597.425	462.648	-3840.772	1.109e+10	1.088e+11
9200.00	65.362	601.149	463.004	-3865.035	1.137e+10	1.103e+11
9250.00	65.455	604.880	463.359	-3889.318	1.165e+10	1.118e+11
9300.00	65.547	608.618	463.712	-3913.621	1.195e+10	1.134e+11
9350.00	65.638	612.363	464.063	-3937.944	1.225e+10	1.149e+11
9400.00	65.730	616.114	464.414	-3962.287	1.255e+10	1.164e+11
9450.00	65.821	619.873	464.763	-3986.651	1.286e+10	1.180e+11
9500.00	65.912	623.638	465.110	-4011.034	1.318e+10	1.196e+11
9550.00	66.002	627.411	465.457	-4035.437	1.351e+10	1.211e+11
9600.00	66.093	631.189	465.801	-4059.859	1.384e+10	1.227e+11
9650.00	66.182	634.975	466.145	-4084.302	1.418e+10	1.243e+11
9700.00	66.272	638.768	466.487	-4108.764	1.452e+10	1.259e+11
9750.00	66.361	642.567	466.828	-4133.245	1.487e+10	1.276e+11
9800.00	66.449	646.372	467.168	-4157.746	1.523e+10	1.292e+11
9850.00	66.537	650.185	467.506	-4182.267	1.559e+10	1.309e+11
9900.00	66.625	654.004	467.843	-4206.807	1.597e+10	1.325e+11
9950.00	66.712	657.829	468.179	-4231.366	1.635e+10	1.342e+11
10000.00	66.799	661.661	468.514	-4255.944	1.673e+10	1.359e+11

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	39.255	3.597	217.852	-18.296	2.562e+03	1.359e+06
150.00	44.099	5.858	234.700	-29.717	5.427e+03	3.745e+06
200.00	47.991	8.432	247.949	-41.956	9.986e+03	7.688e+06
250.00	50.715	11.239	258.970	-54.873	1.696e+04	1.343e+07
298.15	52.513	14.094	268.066	-67.864	2.678e+04	2.086e+07
300.00	52.569	14.206	268.391	-68.372	2.723e+04	2.119e+07
350.00	53.849	17.282	276.596	-82.378	4.183e+04	3.115e+07
400.00	54.754	20.435	283.849	-96.829	6.198e+04	4.349e+07
450.00	55.413	23.643	290.338	-111.679	8.907e+04	5.838e+07
500.00	55.903	26.890	296.203	-126.889	1.247e+05	7.598e+07
550.00	56.278	30.168	301.550	-142.425	1.706e+05	9.642e+07
600.00	56.569	33.470	306.460	-158.261	2.289e+05	1.198e+08
650.00	56.800	36.789	310.997	-174.373	3.017e+05	1.464e+08
700.00	56.985	40.124	315.213	-190.741	3.915e+05	1.762e+08
750.00	57.137	43.470	319.150	-207.348	5.010e+05	2.094e+08
800.00	57.262	46.826	322.842	-224.179	6.331e+05	2.460e+08
850.00	57.366	50.190	326.317	-241.220	7.909e+05	2.863e+08
900.00	57.455	53.561	329.598	-258.459	9.779e+05	3.303e+08
950.00	57.529	56.937	332.707	-275.885	1.198e+06	3.781e+08
1000.00	57.594	60.319	335.659	-293.490	1.454e+06	4.298e+08
1050.00	57.649	63.704	338.471	-311.263	1.752e+06	4.855e+08
1100.00	57.698	67.094	341.154	-329.198	2.095e+06	5.454e+08
1150.00	57.740	70.486	343.719	-347.287	2.489e+06	6.095e+08
1200.00	57.777	73.882	346.177	-365.524	2.938e+06	6.780e+08
1250.00	57.810	77.279	348.537	-383.903	3.447e+06	7.508e+08
1300.00	57.839	80.680	350.805	-402.417	4.023e+06	8.282e+08
1350.00	57.865	84.081	352.988	-421.062	4.671e+06	9.101e+08
1400.00	57.889	87.485	355.093	-439.834	5.398e+06	9.967e+08
1450.00	57.910	90.891	357.125	-458.727	6.211e+06	1.088e+09
1500.00	57.929	94.297	359.088	-477.737	7.115e+06	1.184e+09
1550.00	57.946	97.705	360.988	-496.861	8.119e+06	1.286e+09
1600.00	57.962	101.114	362.828	-516.095	9.230e+06	1.392e+09
1650.00	57.976	104.525	364.612	-535.435	1.046e+07	1.503e+09
1700.00	57.989	107.936	366.343	-554.879	1.181e+07	1.619e+09
1750.00	58.002	111.348	368.024	-574.424	1.329e+07	1.741e+09
1800.00	58.013	114.761	369.658	-594.065	1.491e+07	1.868e+09
1850.00	58.024	118.175	371.247	-613.802	1.668e+07	2.001e+09
1900.00	58.034	121.589	372.795	-633.631	1.861e+07	2.139e+09
1950.00	58.043	125.005	374.303	-653.550	2.071e+07	2.282e+09
2000.00	58.052	128.420	375.772	-673.556	2.299e+07	2.431e+09
2050.00	58.061	131.837	377.206	-693.648	2.547e+07	2.586e+09
2100.00	58.070	135.254	378.605	-713.823	2.814e+07	2.747e+09
2150.00	58.079	138.672	379.972	-734.079	3.103e+07	2.913e+09
2200.00	58.087	142.091	381.307	-754.415	3.415e+07	3.085e+09
2250.00	58.096	145.510	382.612	-774.829	3.750e+07	3.264e+09
2300.00	58.105	148.930	383.889	-795.319	4.110e+07	3.448e+09
2350.00	58.115	152.351	385.139	-815.883	4.497e+07	3.639e+09
2400.00	58.125	155.773	386.363	-836.520	4.912e+07	3.835e+09
2450.00	58.135	159.196	387.561	-857.228	5.355e+07	4.038e+09
2500.00	58.146	162.619	388.736	-878.006	5.830e+07	4.247e+09
2550.00	58.158	166.044	389.887	-898.852	6.336e+07	4.463e+09
2600.00	58.171	169.469	391.017	-919.766	6.876e+07	4.685e+09
2650.00	58.184	172.896	392.125	-940.746	7.451e+07	4.913e+09
2700.00	58.199	176.325	393.213	-961.790	8.063e+07	5.148e+09

2750.00	58.215	179.754	394.281	-982.898	8.713e+07	5.390e+09
2800.00	58.231	183.185	395.330	-1004.068	9.404e+07	5.638e+09
2850.00	58.250	186.618	396.361	-1025.299	1.014e+08	5.893e+09
2900.00	58.269	190.053	397.374	-1046.591	1.091e+08	6.155e+09
2950.00	58.290	193.489	398.370	-1067.942	1.173e+08	6.424e+09
3000.00	58.312	196.928	399.350	-1089.351	1.260e+08	6.700e+09
3050.00	58.336	200.369	400.314	-1110.817	1.352e+08	6.982e+09
3100.00	58.362	203.812	401.263	-1132.340	1.449e+08	7.272e+09
3150.00	58.389	207.258	402.197	-1153.919	1.551e+08	7.569e+09
3200.00	58.419	210.707	403.117	-1175.552	1.659e+08	7.873e+09
3250.00	58.450	214.158	404.023	-1197.239	1.773e+08	8.184e+09
3300.00	58.482	217.613	404.915	-1218.979	1.892e+08	8.502e+09
3350.00	58.517	221.071	405.795	-1240.772	2.018e+08	8.828e+09
3400.00	58.554	224.533	406.662	-1262.616	2.150e+08	9.161e+09
3450.00	58.593	227.998	407.517	-1284.511	2.289e+08	9.502e+09
3500.00	58.634	231.468	408.361	-1306.457	2.435e+08	9.850e+09
3550.00	58.676	234.941	409.193	-1328.452	2.588e+08	1.021e+10
3600.00	58.721	238.419	410.014	-1350.496	2.749e+08	1.057e+10
3650.00	58.769	241.901	410.824	-1372.588	2.917e+08	1.094e+10
3700.00	58.818	245.389	411.624	-1394.728	3.093e+08	1.132e+10
3750.00	58.869	248.881	412.414	-1416.916	3.277e+08	1.170e+10
3800.00	58.923	252.378	413.194	-1439.149	3.469e+08	1.210e+10
3850.00	58.979	255.881	413.964	-1461.429	3.671e+08	1.250e+10
3900.00	59.037	259.389	414.726	-1483.755	3.881e+08	1.291e+10
3950.00	59.097	262.904	415.478	-1506.125	4.101e+08	1.333e+10
4000.00	59.159	266.424	416.222	-1528.540	4.330e+08	1.375e+10
4050.00	59.224	269.951	416.957	-1550.999	4.570e+08	1.419e+10
4100.00	59.290	273.484	417.684	-1573.501	4.819e+08	1.463e+10
4150.00	59.359	277.024	418.404	-1596.047	5.079e+08	1.508e+10
4200.00	59.430	280.571	419.115	-1618.636	5.350e+08	1.554e+10
4250.00	59.503	284.126	419.819	-1641.266	5.633e+08	1.600e+10
4300.00	59.578	287.687	420.515	-1663.939	5.927e+08	1.648e+10
4350.00	59.656	291.256	421.204	-1686.653	6.232e+08	1.696e+10
4400.00	59.735	294.833	421.886	-1709.408	6.551e+08	1.745e+10
4450.00	59.816	298.418	422.562	-1732.204	6.881e+08	1.795e+10
4500.00	59.900	302.012	423.231	-1755.040	7.225e+08	1.846e+10
4550.00	59.985	305.613	423.893	-1777.916	7.582e+08	1.898e+10
4600.00	60.072	309.223	424.549	-1800.831	7.953e+08	1.951e+10
4650.00	60.161	312.842	425.199	-1823.786	8.339e+08	2.004e+10
4700.00	60.252	316.470	425.843	-1846.780	8.738e+08	2.058e+10
4750.00	60.345	320.108	426.481	-1869.813	9.153e+08	2.113e+10
4800.00	60.440	323.754	427.113	-1892.884	9.584e+08	2.170e+10
4850.00	60.536	327.410	427.740	-1915.993	1.003e+09	2.226e+10
4900.00	60.634	331.076	428.362	-1939.140	1.049e+09	2.284e+10
4950.00	60.734	334.752	428.978	-1962.324	1.097e+09	2.343e+10
5000.00	60.835	338.437	429.589	-1985.545	1.147e+09	2.403e+10
5050.00	60.938	342.133	430.194	-2008.803	1.198e+09	2.463e+10
5100.00	61.042	345.839	430.795	-2032.098	1.251e+09	2.525e+10
5150.00	61.148	349.556	431.391	-2055.429	1.306e+09	2.587e+10
5200.00	61.255	353.283	431.983	-2078.797	1.363e+09	2.650e+10
5250.00	61.363	357.021	432.569	-2102.200	1.422e+09	2.714e+10
5300.00	61.473	360.770	433.152	-2125.639	1.483e+09	2.779e+10
5350.00	61.584	364.530	433.729	-2149.113	1.546e+09	2.845e+10
5400.00	61.697	368.302	434.303	-2172.623	1.612e+09	2.912e+10
5450.00	61.810	372.084	434.872	-2196.167	1.679e+09	2.980e+10
5500.00	61.925	375.878	435.437	-2219.747	1.748e+09	3.049e+10
5550.00	62.040	379.683	435.998	-2243.361	1.820e+09	3.119e+10
5600.00	62.157	383.500	436.555	-2267.009	1.895e+09	3.190e+10

5650.00	62.274	387.329	437.108	-2290.691	1.971e+09	3.261e+10
5700.00	62.393	391.169	437.657	-2314.407	2.050e+09	3.334e+10
5750.00	62.512	395.022	438.202	-2338.157	2.132e+09	3.407e+10
5800.00	62.632	398.886	438.744	-2361.941	2.216e+09	3.482e+10
5850.00	62.753	402.762	439.282	-2385.758	2.303e+09	3.558e+10
5900.00	62.874	406.651	439.817	-2409.608	2.392e+09	3.634e+10
5950.00	62.996	410.551	440.348	-2433.491	2.485e+09	3.712e+10
6000.00	63.119	414.464	440.876	-2457.406	2.580e+09	3.790e+10
6050.00	63.242	418.389	441.400	-2481.355	2.678e+09	3.869e+10
6100.00	63.365	422.327	441.921	-2505.336	2.779e+09	3.950e+10
6150.00	63.489	426.276	442.439	-2529.350	2.883e+09	4.031e+10
6200.00	63.614	430.238	442.953	-2553.395	2.991e+09	4.114e+10
6250.00	63.738	434.213	443.465	-2577.473	3.101e+09	4.197e+10
6300.00	63.863	438.200	443.973	-2601.582	3.215e+09	4.282e+10
6350.00	63.988	442.199	444.479	-2625.723	3.332e+09	4.367e+10
6400.00	64.113	446.212	444.981	-2649.896	3.453e+09	4.454e+10
6450.00	64.238	450.236	445.480	-2674.100	3.577e+09	4.541e+10
6500.00	64.363	454.273	445.977	-2698.335	3.705e+09	4.630e+10
6550.00	64.488	458.323	446.471	-2722.601	3.836e+09	4.719e+10
6600.00	64.613	462.385	446.961	-2746.899	3.971e+09	4.810e+10
6650.00	64.738	466.459	447.450	-2771.227	4.111e+09	4.901e+10
6700.00	64.863	470.546	447.935	-2795.586	4.254e+09	4.994e+10
6750.00	64.987	474.645	448.418	-2819.975	4.401e+09	5.088e+10
6800.00	65.112	478.757	448.898	-2844.395	4.552e+09	5.182e+10
6850.00	65.235	482.882	449.375	-2868.845	4.707e+09	5.278e+10
6900.00	65.359	487.018	449.850	-2893.325	4.867e+09	5.375e+10
6950.00	65.482	491.167	450.322	-2917.835	5.031e+09	5.473e+10
7000.00	65.605	495.328	450.792	-2942.375	5.200e+09	5.572e+10
7050.00	65.727	499.502	451.260	-2966.945	5.373e+09	5.672e+10
7100.00	65.848	503.688	451.725	-2991.545	5.551e+09	5.773e+10
7150.00	65.969	507.885	452.187	-3016.174	5.734e+09	5.875e+10
7200.00	66.090	512.095	452.647	-3040.832	5.921e+09	5.978e+10
7250.00	66.209	516.317	453.105	-3065.520	6.114e+09	6.083e+10
7300.00	66.328	520.551	453.561	-3090.237	6.312e+09	6.188e+10
7350.00	66.446	524.796	454.014	-3114.983	6.515e+09	6.295e+10
7400.00	66.564	529.054	454.465	-3139.758	6.723e+09	6.402e+10
7450.00	66.680	533.323	454.913	-3164.561	6.937e+09	6.511e+10
7500.00	66.796	537.603	455.360	-3189.394	7.157e+09	6.621e+10
7550.00	66.911	541.896	455.804	-3214.255	7.382e+09	6.732e+10
7600.00	67.024	546.199	456.246	-3239.144	7.613e+09	6.844e+10
7650.00	67.137	550.514	456.686	-3264.062	7.850e+09	6.957e+10
7700.00	67.249	554.840	457.123	-3289.008	8.093e+09	7.071e+10
7750.00	67.360	559.177	457.559	-3313.982	8.342e+09	7.186e+10
7800.00	67.470	563.526	457.993	-3338.984	8.598e+09	7.303e+10
7850.00	67.578	567.885	458.424	-3364.014	8.860e+09	7.420e+10
7900.00	67.686	572.255	458.853	-3389.072	9.128e+09	7.539e+10
7950.00	67.792	576.636	459.281	-3414.157	9.404e+09	7.659e+10
8000.00	67.897	581.027	459.706	-3439.270	9.686e+09	7.780e+10
8050.00	68.001	585.429	460.130	-3464.411	9.975e+09	7.902e+10
8100.00	68.104	589.841	460.551	-3489.579	1.027e+10	8.025e+10
8150.00	68.205	594.263	460.970	-3514.774	1.057e+10	8.150e+10
8200.00	68.305	598.695	461.388	-3539.996	1.089e+10	8.275e+10
8250.00	68.404	603.137	461.803	-3565.246	1.120e+10	8.402e+10
8300.00	68.502	607.590	462.217	-3590.522	1.153e+10	8.530e+10
8350.00	68.598	612.051	462.629	-3615.825	1.186e+10	8.659e+10
8400.00	68.693	616.523	463.039	-3641.156	1.221e+10	8.789e+10
8450.00	68.786	621.003	463.446	-3666.512	1.256e+10	8.921e+10
8500.00	68.878	625.493	463.853	-3691.895	1.292e+10	9.053e+10

8550.00	68.969	629.992	464.257	-3717.305	1.328e+10	9.187e+10
8600.00	69.058	634.500	464.659	-3742.741	1.366e+10	9.322e+10
8650.00	69.146	639.017	465.060	-3768.203	1.404e+10	9.458e+10
8700.00	69.232	643.543	465.459	-3793.691	1.444e+10	9.595e+10
8750.00	69.317	648.077	465.856	-3819.206	1.484e+10	9.734e+10
8800.00	69.400	652.620	466.251	-3844.746	1.525e+10	9.873e+10
8850.00	69.482	657.171	466.644	-3870.312	1.568e+10	1.001e+11
8900.00	69.562	661.730	467.036	-3895.904	1.611e+10	1.016e+11
8950.00	69.641	666.297	467.426	-3921.521	1.655e+10	1.030e+11
9000.00	69.719	670.871	467.814	-3947.164	1.700e+10	1.044e+11
9050.00	69.794	675.454	468.200	-3972.833	1.746e+10	1.059e+11
9100.00	69.869	680.044	468.585	-3998.527	1.793e+10	1.074e+11
9150.00	69.941	684.641	468.968	-4024.246	1.842e+10	1.088e+11
9200.00	70.013	689.245	469.350	-4049.990	1.891e+10	1.103e+11
9250.00	70.082	693.857	469.729	-4075.759	1.942e+10	1.118e+11
9300.00	70.151	698.475	470.107	-4101.553	1.993e+10	1.134e+11
9350.00	70.217	703.100	470.484	-4127.372	2.046e+10	1.149e+11
9400.00	70.282	707.732	470.858	-4153.216	2.100e+10	1.164e+11
9450.00	70.346	712.370	471.231	-4179.084	2.155e+10	1.180e+11
9500.00	70.408	717.015	471.603	-4204.978	2.212e+10	1.196e+11
9550.00	70.469	721.665	471.972	-4230.895	2.269e+10	1.211e+11
9600.00	70.528	726.322	472.341	-4256.836	2.328e+10	1.227e+11
9650.00	70.585	730.984	472.707	-4282.803	2.388e+10	1.243e+11
9700.00	70.641	735.652	473.072	-4308.793	2.449e+10	1.259e+11
9750.00	70.695	740.326	473.435	-4334.807	2.512e+10	1.276e+11
9800.00	70.748	745.005	473.797	-4360.846	2.576e+10	1.292e+11
9850.00	70.799	749.689	474.157	-4386.908	2.642e+10	1.309e+11
9900.00	70.849	754.378	474.516	-4412.994	2.709e+10	1.325e+11
9950.00	70.898	759.072	474.873	-4439.104	2.777e+10	1.342e+11
10000.00	70.944	763.771	475.228	-4465.237	2.847e+10	1.359e+11

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	41.487	3.823	219.286	-18.400	2.715e+03	1.359e+06
150.00	46.860	6.442	237.177	-30.060	6.104e+03	3.745e+06
200.00	50.485	9.452	251.194	-42.672	1.190e+04	7.688e+06
250.00	52.754	12.713	262.723	-56.076	2.123e+04	1.343e+07
298.15	54.156	16.003	272.143	-69.621	3.489e+04	2.086e+07
300.00	54.199	16.131	272.478	-70.153	3.553e+04	2.119e+07
350.00	55.156	19.652	280.910	-84.811	5.649e+04	3.115e+07
400.00	55.815	23.241	288.321	-99.979	8.612e+04	4.349e+07
450.00	56.285	26.879	294.923	-115.599	1.268e+05	5.838e+07
500.00	56.631	30.552	300.872	-131.627	1.811e+05	7.598e+07
550.00	56.892	34.251	306.283	-148.023	2.522e+05	9.642e+07
600.00	57.094	37.970	311.242	-164.758	3.435e+05	1.198e+08
650.00	57.253	41.704	315.818	-181.803	4.588e+05	1.464e+08
700.00	57.380	45.451	320.066	-199.137	6.023e+05	1.762e+08
750.00	57.484	49.207	324.029	-216.738	7.787e+05	2.094e+08
800.00	57.569	52.972	327.741	-234.591	9.931e+05	2.460e+08
850.00	57.640	56.743	331.234	-252.679	1.251e+06	2.863e+08
900.00	57.700	60.521	334.530	-270.989	1.558e+06	3.303e+08
950.00	57.750	64.302	337.651	-289.509	1.921e+06	3.781e+08
1000.00	57.794	68.088	340.614	-308.229	2.348e+06	4.298e+08
1050.00	57.831	71.878	343.435	-327.138	2.844e+06	4.855e+08
1100.00	57.864	75.670	346.126	-346.228	3.418e+06	5.454e+08
1150.00	57.893	79.465	348.699	-365.490	4.080e+06	6.095e+08
1200.00	57.919	83.263	351.163	-384.917	4.837e+06	6.780e+08
1250.00	57.942	87.063	353.528	-404.502	5.699e+06	7.508e+08
1300.00	57.963	90.864	355.801	-424.240	6.676e+06	8.282e+08
1350.00	57.982	94.668	357.989	-444.124	7.779e+06	9.101e+08
1400.00	58.001	98.473	360.098	-464.149	9.019e+06	9.967e+08
1450.00	58.018	102.280	362.134	-484.310	1.041e+07	1.088e+09
1500.00	58.036	106.089	364.101	-504.602	1.196e+07	1.184e+09
1550.00	58.053	109.900	366.004	-525.021	1.368e+07	1.286e+09
1600.00	58.071	113.713	367.848	-545.563	1.559e+07	1.392e+09
1650.00	58.091	117.528	369.635	-566.225	1.771e+07	1.503e+09
1700.00	58.111	121.345	371.369	-587.002	2.004e+07	1.619e+09
1750.00	58.133	125.165	373.054	-607.891	2.260e+07	1.741e+09
1800.00	58.157	128.987	374.692	-628.890	2.541e+07	1.868e+09
1850.00	58.183	132.814	376.286	-649.994	2.849e+07	2.001e+09
1900.00	58.212	136.643	377.838	-671.203	3.185e+07	2.139e+09
1950.00	58.243	140.477	379.350	-692.512	3.551e+07	2.282e+09
2000.00	58.278	144.316	380.825	-713.919	3.949e+07	2.431e+09
2050.00	58.316	148.160	382.265	-735.423	4.380e+07	2.586e+09
2100.00	58.358	152.009	383.671	-757.020	4.848e+07	2.747e+09
2150.00	58.404	155.865	385.044	-778.709	5.354e+07	2.913e+09
2200.00	58.454	159.728	386.388	-800.488	5.900e+07	3.085e+09
2250.00	58.508	163.598	387.702	-822.355	6.489e+07	3.264e+09
2300.00	58.567	167.476	388.989	-844.307	7.122e+07	3.448e+09
2350.00	58.630	171.364	390.249	-866.345	7.803e+07	3.639e+09
2400.00	58.698	175.261	391.484	-888.465	8.534e+07	3.835e+09
2450.00	58.770	179.168	392.695	-910.666	9.317e+07	4.038e+09
2500.00	58.847	183.086	393.883	-932.947	1.016e+08	4.247e+09
2550.00	58.929	187.016	395.049	-955.307	1.105e+08	4.463e+09
2600.00	59.016	190.959	396.194	-977.744	1.201e+08	4.685e+09
2650.00	59.108	194.915	397.319	-1000.257	1.303e+08	4.913e+09
2700.00	59.205	198.885	398.425	-1022.844	1.412e+08	5.148e+09

2750.00	59.306	202.869	399.512	-1045.505	1.527e+08	5.390e+09
2800.00	59.413	206.870	400.582	-1068.239	1.650e+08	5.638e+09
2850.00	59.524	210.886	401.634	-1091.045	1.781e+08	5.893e+09
2900.00	59.639	214.919	402.671	-1113.921	1.920e+08	6.155e+09
2950.00	59.760	218.970	403.691	-1136.867	2.067e+08	6.424e+09
3000.00	59.884	223.039	404.697	-1159.881	2.223e+08	6.700e+09
3050.00	60.014	227.127	405.687	-1182.964	2.388e+08	6.982e+09
3100.00	60.147	231.234	406.664	-1206.113	2.563e+08	7.272e+09
3150.00	60.285	235.362	407.628	-1229.329	2.747e+08	7.569e+09
3200.00	60.426	239.511	408.578	-1252.611	2.942e+08	7.873e+09
3250.00	60.572	243.681	409.516	-1275.958	3.147e+08	8.184e+09
3300.00	60.721	247.873	410.442	-1299.369	3.364e+08	8.502e+09
3350.00	60.874	252.088	411.356	-1322.844	3.593e+08	8.828e+09
3400.00	61.030	256.326	412.259	-1346.382	3.833e+08	9.161e+09
3450.00	61.190	260.588	413.152	-1369.982	4.087e+08	9.502e+09
3500.00	61.352	264.873	414.033	-1393.645	4.353e+08	9.850e+09
3550.00	61.518	269.183	414.905	-1417.368	4.634e+08	1.021e+10
3600.00	61.686	273.519	415.766	-1441.153	4.928e+08	1.057e+10
3650.00	61.857	277.879	416.618	-1464.998	5.237e+08	1.094e+10
3700.00	62.030	282.265	417.461	-1488.903	5.562e+08	1.132e+10
3750.00	62.206	286.678	418.295	-1512.867	5.902e+08	1.170e+10
3800.00	62.383	291.117	419.120	-1536.891	6.259e+08	1.210e+10
3850.00	62.563	295.582	419.937	-1560.972	6.633e+08	1.250e+10
3900.00	62.744	300.075	420.745	-1585.113	7.025e+08	1.291e+10
3950.00	62.926	304.595	421.545	-1609.310	7.435e+08	1.333e+10
4000.00	63.110	309.142	422.338	-1633.566	7.865e+08	1.375e+10
4050.00	63.295	313.717	423.123	-1657.878	8.314e+08	1.419e+10
4100.00	63.481	318.319	423.901	-1682.247	8.784e+08	1.463e+10
4150.00	63.668	322.950	424.672	-1706.672	9.275e+08	1.508e+10
4200.00	63.855	327.608	425.435	-1731.153	9.788e+08	1.554e+10
4250.00	64.043	332.295	426.192	-1755.690	1.032e+09	1.600e+10
4300.00	64.231	337.010	426.942	-1780.282	1.088e+09	1.648e+10
4350.00	64.418	341.753	427.686	-1804.929	1.147e+09	1.696e+10
4400.00	64.606	346.524	428.423	-1829.631	1.208e+09	1.745e+10
4450.00	64.794	351.323	429.154	-1854.387	1.271e+09	1.795e+10
4500.00	64.981	356.150	429.879	-1879.198	1.337e+09	1.846e+10
4550.00	65.167	361.005	430.598	-1904.062	1.406e+09	1.898e+10
4600.00	65.352	365.888	431.312	-1928.979	1.478e+09	1.951e+10
4650.00	65.537	370.799	432.019	-1953.950	1.553e+09	2.004e+10
4700.00	65.721	375.738	432.721	-1978.974	1.631e+09	2.058e+10
4750.00	65.903	380.703	433.417	-2004.050	1.712e+09	2.113e+10
4800.00	66.084	385.696	434.108	-2029.179	1.797e+09	2.170e+10
4850.00	66.263	390.716	434.794	-2054.360	1.885e+09	2.226e+10
4900.00	66.441	395.763	435.475	-2079.593	1.976e+09	2.284e+10
4950.00	66.616	400.836	436.150	-2104.877	2.071e+09	2.343e+10
5000.00	66.790	405.936	436.820	-2130.213	2.169e+09	2.403e+10
5050.00	66.962	411.061	437.486	-2155.600	2.272e+09	2.463e+10
5100.00	67.132	416.212	438.147	-2181.038	2.379e+09	2.525e+10
5150.00	67.299	421.388	438.802	-2206.527	2.489e+09	2.587e+10
5200.00	67.464	426.589	439.453	-2232.066	2.604e+09	2.650e+10
5250.00	67.627	431.815	440.100	-2257.655	2.723e+09	2.714e+10
5300.00	67.787	437.065	440.741	-2283.293	2.847e+09	2.779e+10
5350.00	67.944	442.339	441.379	-2308.982	2.975e+09	2.845e+10
5400.00	68.099	447.636	442.011	-2334.720	3.108e+09	2.912e+10
5450.00	68.251	452.956	442.640	-2360.507	3.246e+09	2.980e+10
5500.00	68.399	458.298	443.264	-2386.343	3.389e+09	3.049e+10
5550.00	68.545	463.663	443.883	-2412.228	3.538e+09	3.119e+10
5600.00	68.688	469.049	444.499	-2438.161	3.691e+09	3.190e+10

5650.00	68.828	474.456	445.110	-2464.142	3.851e+09	3.261e+10
5700.00	68.964	479.884	445.717	-2490.171	4.016e+09	3.334e+10
5750.00	69.098	485.333	446.320	-2516.248	4.186e+09	3.407e+10
5800.00	69.228	490.801	446.919	-2542.373	4.363e+09	3.482e+10
5850.00	69.355	496.288	447.514	-2568.544	4.546e+09	3.558e+10
5900.00	69.478	501.794	448.104	-2594.763	4.735e+09	3.634e+10
5950.00	69.598	507.319	448.691	-2621.028	4.931e+09	3.712e+10
6000.00	69.715	512.861	449.274	-2647.340	5.134e+09	3.790e+10
6050.00	69.828	518.420	449.853	-2673.698	5.344e+09	3.869e+10
6100.00	69.938	523.996	450.428	-2700.102	5.560e+09	3.950e+10
6150.00	70.044	529.588	451.000	-2726.552	5.785e+09	4.031e+10
6200.00	70.147	535.196	451.567	-2753.048	6.016e+09	4.114e+10
6250.00	70.247	540.819	452.131	-2779.588	6.255e+09	4.197e+10
6300.00	70.343	546.457	452.691	-2806.174	6.503e+09	4.282e+10
6350.00	70.435	552.109	453.248	-2832.805	6.758e+09	4.367e+10
6400.00	70.524	557.774	453.800	-2859.480	7.022e+09	4.454e+10
6450.00	70.610	563.453	454.350	-2886.199	7.295e+09	4.541e+10
6500.00	70.692	569.144	454.895	-2912.963	7.576e+09	4.630e+10
6550.00	70.771	574.847	455.437	-2939.770	7.866e+09	4.719e+10
6600.00	70.846	580.562	455.976	-2966.621	8.166e+09	4.810e+10
6650.00	70.918	586.288	456.511	-2993.515	8.475e+09	4.901e+10
6700.00	70.987	592.024	457.042	-3020.452	8.794e+09	4.994e+10
6750.00	71.052	597.770	457.570	-3047.432	9.123e+09	5.088e+10
6800.00	71.114	603.526	458.095	-3074.455	9.463e+09	5.182e+10
6850.00	71.173	609.291	458.616	-3101.520	9.813e+09	5.278e+10
6900.00	71.228	615.065	459.134	-3128.628	1.017e+10	5.375e+10
6950.00	71.280	620.846	459.648	-3155.777	1.055e+10	5.473e+10
7000.00	71.329	626.635	460.159	-3182.967	1.093e+10	5.572e+10
7050.00	71.375	632.432	460.667	-3210.199	1.132e+10	5.672e+10
7100.00	71.418	638.235	461.172	-3237.473	1.173e+10	5.773e+10
7150.00	71.458	644.044	461.673	-3264.787	1.215e+10	5.875e+10
7200.00	71.495	649.859	462.171	-3292.142	1.258e+10	5.978e+10
7250.00	71.529	655.679	462.666	-3319.537	1.303e+10	6.083e+10
7300.00	71.559	661.504	463.158	-3346.972	1.349e+10	6.188e+10
7350.00	71.587	667.333	463.646	-3374.447	1.396e+10	6.295e+10
7400.00	71.613	673.166	464.132	-3401.962	1.444e+10	6.402e+10
7450.00	71.635	679.003	464.614	-3429.517	1.494e+10	6.511e+10
7500.00	71.655	684.843	465.093	-3457.110	1.546e+10	6.621e+10
7550.00	71.672	690.686	465.569	-3484.742	1.599e+10	6.732e+10
7600.00	71.686	696.531	466.043	-3512.414	1.653e+10	6.844e+10
7650.00	71.698	702.379	466.513	-3540.123	1.709e+10	6.957e+10
7700.00	71.707	708.227	466.980	-3567.871	1.766e+10	7.071e+10
7750.00	71.714	714.077	467.444	-3595.657	1.826e+10	7.186e+10
7800.00	71.719	719.928	467.905	-3623.480	1.886e+10	7.303e+10
7850.00	71.721	725.779	468.363	-3651.342	1.949e+10	7.420e+10
7900.00	71.720	731.631	468.819	-3679.240	2.013e+10	7.539e+10
7950.00	71.718	737.482	469.271	-3707.175	2.079e+10	7.659e+10
8000.00	71.713	743.332	469.721	-3735.147	2.147e+10	7.780e+10
8050.00	71.706	749.182	470.168	-3763.156	2.217e+10	7.902e+10
8100.00	71.697	755.031	470.612	-3791.201	2.289e+10	8.025e+10
8150.00	71.686	760.878	471.053	-3819.282	2.362e+10	8.150e+10
8200.00	71.673	766.723	471.491	-3847.399	2.438e+10	8.275e+10
8250.00	71.658	772.566	471.927	-3875.552	2.515e+10	8.402e+10
8300.00	71.642	778.407	472.360	-3903.740	2.595e+10	8.530e+10
8350.00	71.623	784.245	472.790	-3931.964	2.677e+10	8.659e+10
8400.00	71.603	790.080	473.218	-3960.222	2.761e+10	8.789e+10
8450.00	71.580	795.912	473.643	-3988.515	2.847e+10	8.921e+10
8500.00	71.557	801.740	474.065	-4016.842	2.935e+10	9.053e+10

8550.00	71.531	807.565	474.484	-4045.204	3.026e+10	9.187e+10
8600.00	71.504	813.386	474.901	-4073.600	3.119e+10	9.322e+10
8650.00	71.475	819.203	475.316	-4102.029	3.214e+10	9.458e+10
8700.00	71.445	825.015	475.728	-4130.492	3.312e+10	9.595e+10
8750.00	71.414	830.823	476.137	-4158.989	3.413e+10	9.734e+10
8800.00	71.381	836.625	476.544	-4187.519	3.515e+10	9.873e+10
8850.00	71.347	842.423	476.948	-4216.082	3.621e+10	1.001e+11
8900.00	71.311	848.216	477.350	-4244.677	3.729e+10	1.016e+11
8950.00	71.274	854.003	477.750	-4273.305	3.840e+10	1.030e+11
9000.00	71.236	859.784	478.146	-4301.965	3.953e+10	1.044e+11
9050.00	71.197	865.560	478.541	-4330.658	4.070e+10	1.059e+11
9100.00	71.157	871.330	478.933	-4359.382	4.189e+10	1.074e+11
9150.00	71.115	877.093	479.323	-4388.138	4.311e+10	1.088e+11
9200.00	71.073	882.850	479.710	-4416.925	4.436e+10	1.103e+11
9250.00	71.029	888.601	480.096	-4445.744	4.565e+10	1.118e+11
9300.00	70.985	894.345	480.478	-4474.594	4.696e+10	1.134e+11
9350.00	70.939	900.083	480.859	-4503.475	4.830e+10	1.149e+11
9400.00	70.893	905.813	481.237	-4532.386	4.968e+10	1.164e+11
9450.00	70.846	911.537	481.613	-4561.328	5.109e+10	1.180e+11
9500.00	70.798	917.254	481.987	-4590.300	5.253e+10	1.196e+11
9550.00	70.750	922.963	482.358	-4619.302	5.401e+10	1.211e+11
9600.00	70.700	928.665	482.728	-4648.333	5.552e+10	1.227e+11
9650.00	70.650	934.359	483.095	-4677.396	5.706e+10	1.243e+11
9700.00	70.599	940.046	483.460	-4706.486	5.865e+10	1.259e+11
9750.00	70.548	945.725	483.823	-4735.607	6.026e+10	1.276e+11
9800.00	70.496	951.396	484.183	-4764.756	6.192e+10	1.292e+11
9850.00	70.443	957.060	484.542	-4793.935	6.361e+10	1.309e+11
9900.00	70.390	962.715	484.898	-4823.142	6.534e+10	1.325e+11
9950.00	70.336	968.363	485.253	-4852.378	6.712e+10	1.342e+11
10000.00	70.282	974.002	485.605	-4881.642	6.893e+10	1.359e+11