

S1: Total Energies at 298 K^{a,b}

Species	B3LYP/ 6-31G(d,p)	B3LYP/6- 311+G(3df,2p)	QCISD(t)/ 6-31G(d,p)	CBS-Q	ZPEV ^{c,d}	$H_{298}-H_0^d$
	//B3LYP/6-31G(d,p)					
1	-153.7763726	-153.8327944	-153.3595858	-153.5763639	34.21	3.04
2	-613.3980898	-613.4878782	-612.4172794	-612.7538403	29.16	3.50
3	-613.3713415	-613.4612744	-612.3929384	-612.7291569	29.04	3.53
4	-1072.9891572	-1073.1127456	-1071.4474749	-1071.9042343	23.87	4.00
5	-1072.9651549	-1073.0903020	-1071.4262887	-1071.8850174	23.52	4.05
6	-1532.5757154	-1532.7354751	-1530.4754389	-1531.0550914	18.15	4.63
7	-1532.5530561	-1532.7130071	-1530.4554661	-1531.0384812	17.25	4.74
8	-1992.1592477	-1992.3542753	-1989.5009530	-1990.2063224	11.70	5.36
9	-153.1367999	-153.1944241	-152.7254555	-152.9364393	26.60	3.08
10	-612.7334697	-612.8239097	-611.7583488	-612.0886710	21.56	3.39
11	-1072.3213579	-1072.4465143	-1070.7871468	-1071.2385563	15.82	4.04
12	-1531.9084201	-1532.0691432	-1529.8157149	-1530.3919762	9.47	4.76
13	-153.1296835	-153.1863931	-152.7161085	-152.9275051	26.21	2.80
14	-612.7468974	-612.8366266	-611.7695879	-612.1006352	20.88	3.33
15	-612.7363578	-612.8273421	-611.7594842	-612.0912330	21.20	3.34
16	-612.7351836	-612.8260341	-611.7585170	-612.0897341	21.32	3.24
17	-1072.3357832	-1072.4615622	-1070.7979061	-1071.2517825	15.90	3.88
18	-1072.3506236	-1072.4754727	-1070.8108557	-1071.2630213	15.87	3.92
19	-1072.3486141	-1072.4734410	-1070.8093730	-1071.2622151	15.86	3.88
20	-1531.9445624	-1532.1048523	-1529.8449091	-1530.4201720	10.38	4.55
CH ₂ O	-114.4731857	-114.5192283	-114.1775339	-114.3394116	16.44	2.39
CHO	-113.8352467	-113.8820282	-113.5454119	-113.7007926	8.02	2.38
Acetone	-193.0757448	-193.1422867	-192.5399761	-192.8122357	51.52	4.00
C•H ₂ C(=O)CH ₃	-192.4271421	-192.4939379	-191.8946697	-192.1617419	43.34	3.78

a: All calculations are based on B3LYP/6-31G(d,p) optimized structures;

b: Total energies (ZPVE and thermal corrections are included) in hartree, 1 hartree = 627.51 kcal/mol;

c: Scaled by 0.9806;¹⁵;

d: In units of kcal/mol.

S2: Coefficients (kcal/mol) of Truncated Fourier Series Representation Expansions for Internal Rotation Potentials^{a,b,c}

Coef	1	2	3	4	5	6	7
a ₀	5.412E-01	5.258E-01	1.308E+00	1.944E+00	1.970E+00	1.236E+00	1.069E+00
a ₁	3.168E-02	2.932E-02	-4.844E-01	-7.860E-01	-1.112E+00	5.780E-01	3.659E-02
a ₂	-9.993E-04	6.435E-03	4.063E-01	-4.313E-01	-1.461E-02	-1.071E+00	-3.168E-02
a ₃	-5.613E-01	-5.490E-01	-7.696E-01	-6.779E-01	-9.195E-01	-8.532E-01	-1.124E+00
a ₄	-9.486E-04	-8.090E-03	7.307E-02	-1.073E-01	9.266E-02	6.228E-02	2.257E-02
a ₅	-2.846E-02	-2.544E-02	-5.963E-02	2.271E-02	-6.161E-02	5.419E-03	-2.478E-02
a ₆	2.415E-02	2.324E-02	4.682E-02	3.674E-02	6.363E-02	5.686E-02	6.386E-02
a ₇	-4.053E-03	-3.657E-03	-1.337E-02	3.142E-03	-1.851E-02	-1.342E-02	-1.293E-02
b ₁	3.582E-06	3.718E-07	-9.921E-01	-9.851E-08	7.474E-07	-2.241E-06	-1.215E-06
b ₂	-2.677E-06	-1.781E-08	-7.126E-01	1.489E-07	-1.121E-06	3.160E-06	-7.598E-07
b ₃	-1.315E-06	3.094E-07	-2.693E-02	-2.871E-08	3.508E-07	-2.848E-06	2.487E-06
b ₄	4.145E-06	6.285E-07	6.622E-02	-1.499E-07	9.784E-07	2.942E-06	-1.644E-06
b ₅	-2.511E-06	2.464E-07	3.008E-02	1.607E-07	-1.304E-06	-1.039E-07	-1.433E-06
b ₆	-2.648E-06	6.304E-07	1.929E-03	1.026E-08	4.072E-07	-1.347E-06	5.606E-06
b ₇	5.363E-06	9.852E-07	-2.495E-03	-1.423E-07	9.284E-07	3.186E-06	-5.273E-06
Coef	8	9	10	11	12	13	14
a ₀	9.977E-01	2.556E-01	2.935E+00	9.022E-01	4.827E-01	6.663E+00	3.800E+00
a ₁	3.037E-02	1.659E-02	6.643E-01	8.072E-01	1.588E-02	-3.259E-04	8.706E-02
a ₂	2.340E-02	-1.569E-03	7.071E-01	1.976E-01	-4.741E-03	-6.815E+00	-4.261E+00
a ₃	-1.074E+00	-2.720E-01	-3.314E-01	-4.290E-01	-5.321E-01	1.601E-04	-3.288E-02
a ₄	-2.638E-02	-1.173E-04	6.260E-03	-1.529E-02	7.089E-03	1.355E-01	6.262E-01
a ₅	-2.666E-02	-1.223E-02	-3.717E-02	-3.162E-02	-3.914E-03	1.352E-03	-9.385E-02
a ₆	7.873E-02					1.061E-02	-2.456E-01
a ₇	-2.686E-03					6.489E-04	8.982E-02
b ₁	2.172E-09	2.472E-04	1.112E+00	6.191E-05	-3.925E-06	4.996E-04	-1.246E-06
b ₂	2.195E-09	-9.349E-04	-1.251E+00	-7.721E-05	5.514E-06	-4.058E-03	5.093E-07
b ₃	1.984E-09	1.169E-03	2.476E-02	4.124E-05	-1.083E-04	7.503E-04	1.055E-06
b ₄	1.767E-09	-5.961E-04	-4.530E-02	2.588E-05	1.337E-05	-7.167E-04	-9.495E-07
b ₅	2.013E-09	6.731E-04	6.868E-02	-7.093E-05	-1.495E-05	5.000E-04	-6.800E-07
b ₆	2.193E-09					-1.674E-03	1.279E-06
b ₇	2.117E-09					-5.004E-04	1.715E-07
Coef	15	16	17	18	19	20	
a ₀	6.317E+00	7.017E+00	6.496E+00	5.656E+00	5.342E+00	4.576E+00	
a ₁	-3.063E-01	7.237E-01	1.753E-01	-5.941E-01	9.990E-01	2.807E-01	
a ₂	-6.975E+00	-7.425E+00	-7.370E+00	-5.589E+00	-5.382E+00	-5.098E+00	
a ₃	8.830E-02	-4.536E-01	-1.634E-01	-1.821E-02	-3.286E-01	-2.795E-01	
a ₄	1.466E+00	1.071E+00	1.177E+00	8.092E-01	1.039E+00	7.177E-01	
a ₅	-2.593E-01	1.725E-01	-2.602E-02	-1.057E-01	-6.958E-02	-2.769E-02	
a ₆	-6.325E-01	-4.438E-01	-3.289E-01	-3.107E-01	-5.104E-01	-2.604E-01	
a ₇	2.445E-01	-8.128E-02	2.758E-02	1.220E-01	1.852E-01	6.782E-02	
b ₁	1.099E-01	2.896E-02	8.523E-03	-2.792E-04	1.173E-03	4.704E-02	
b ₂	-2.420E-01	-3.337E-02	-3.431E-01	1.291E-04	5.265E-04	-1.260E-01	
b ₃	-3.897E-02	-3.466E-02	8.063E-03	2.055E-04	-1.090E-03	-2.813E-02	
b ₄	4.308E-01	6.422E-02	5.884E-01	-2.533E-04	-7.080E-04	2.216E-01	
b ₅	-8.261E-02	4.537E-02	-3.360E-02	-1.097E-04	5.253E-04	-4.570E-03	
b ₆	-5.251E-01	-9.025E-02	-6.665E-01	2.876E-04	1.136E-03	-2.638E-01	
b ₇	2.186E-01	-5.975E-02	5.575E-02	-7.356E-05	-4.815E-04	4.192E-02	

a: Values of rotational barriers computed at B3LYP/6-31G(d,p) level of theory are used to calculate the coefficients; b: See text for equation II; c: The b_i terms could be omitted when too small, but entropies are slightly reduced.

S3: Thermochemical Properties of Species 1 to 20 at Temperature Range of 5 K to 6000 K

1. CH₃CHO (Ideal Gas)

T (K)	C_p° (cal/mol.K)	S° (cal/mol.K)	$H^\circ - H^\circ(0\text{ K})$ (kcal/mol)
5	8.42	26.91	0.04
50	8.73	45.55	0.40
100	9.74	51.38	0.80
200	10.96	58.47	1.64
298	12.83	63.15	2.64
300	12.87	63.24	2.66
400	15.31	67.22	3.93
500	17.74	70.85	5.45
600	19.95	74.24	7.22
700	21.90	77.43	9.20
800	23.60	80.43	11.36
900	25.08	83.28	13.69
1000	26.37	85.97	16.15
1100	27.50	88.52	18.74
1200	28.48	90.94	21.44
1300	29.33	93.24	24.22
1400	30.07	95.43	27.09
1500	30.72	97.52	30.03
1600	31.29	99.51	33.03
1700	31.78	101.42	36.08
1800	32.22	103.24	39.18
1900	32.61	104.99	42.32
2000	32.95	106.67	45.50
2100	33.25	108.28	48.71
2200	33.52	109.83	51.94
2300	33.76	111.32	55.21
2400	33.98	112.75	58.49
2500	34.17	114.14	61.80
2600	34.35	115.48	65.13
2700	34.51	116.77	68.47
2800	34.65	118.02	71.83
2900	34.78	119.24	75.20
3000	34.89	120.41	78.59
3100	35.00	121.55	81.98
3200	35.10	122.65	85.39
3300	35.19	123.72	88.80
3400	35.27	124.76	92.23
3500	35.34	125.78	95.66
3600	35.41	126.76	99.10
3700	35.47	127.72	102.55
3800	35.53	128.65	106.00
3900	35.58	129.56	109.47
4000	35.63	130.44	112.93
4100	35.67	131.31	116.40
4200	35.71	132.15	119.88
4300	35.75	132.97	123.36
4400	35.78	133.78	126.84
4500	35.82	134.56	130.33
4600	35.84	135.33	133.82
4700	35.87	136.08	137.32
4800	35.89	136.81	140.82
4900	35.92	137.53	144.32
5000	35.94	138.23	147.82
5100	35.96	138.92	151.33
5200	35.97	139.59	154.84
5300	35.99	140.26	158.36
5400	36.00	140.90	161.87
5500	36.01	141.54	165.39
5600	36.03	142.16	168.91
5700	36.04	142.78	172.43
5800	36.05	143.38	175.95
5900	36.06	143.97	179.48
6000	36.06	144.56	183.00

2. CH₃CClO (Ideal Gas)

T (K)	C_p° (cal/mol.K)	S° (cal/mol.K)	$H^\circ - H^\circ(0\text{ K})$ (kcal/mol)
5	8.42	32.06	0.04
50	8.85	50.76	0.40
100	10.35	56.83	0.81
200	13.38	64.93	1.81
298	16.04	70.76	3.09
300	16.09	70.87	3.12
400	18.65	75.80	4.71
500	20.93	80.16	6.56
600	22.89	84.11	8.64
700	24.55	87.73	10.90
800	25.99	91.08	13.31
900	27.22	94.19	15.87
1000	28.28	97.10	18.54
1100	29.21	99.82	21.31
1200	30.01	102.38	24.16
1300	30.70	104.80	27.09
1400	31.31	107.09	30.09
1500	31.83	109.26	33.15
1600	32.29	111.32	36.25
1700	32.70	113.29	39.40
1800	33.06	115.16	42.59
1900	33.37	116.95	45.81
2000	33.65	118.66	49.06
2100	33.89	120.30	52.33
2200	34.11	121.88	55.63
2300	34.31	123.39	58.95
2400	34.48	124.85	62.29
2500	34.64	126.25	65.65
2600	34.78	127.61	69.02
2700	34.91	128.91	72.41
2800	35.02	130.17	75.80
2900	35.12	131.39	79.21
3000	35.22	132.57	82.63
3100	35.30	133.71	86.06
3200	35.38	134.82	89.50
3300	35.45	135.90	92.94
3400	35.51	136.94	96.40
3500	35.57	137.95	99.86
3600	35.62	138.93	103.32
3700	35.67	139.89	106.79
3800	35.71	140.82	110.27
3900	35.75	141.73	113.75
4000	35.78	142.61	117.24
4100	35.81	143.47	120.73
4200	35.84	144.31	124.22
4300	35.87	145.13	127.72
4400	35.89	145.92	131.22
4500	35.92	146.70	134.72
4600	35.94	147.47	138.23
4700	35.95	148.21	141.74
4800	35.97	148.94	145.25
4900	35.98	149.66	148.77
5000	36.00	150.35	152.29
5100	36.01	151.04	155.81
5200	36.02	151.71	159.33
5300	36.03	152.37	162.86
5400	36.04	153.01	166.38
5500	36.04	153.64	169.91
5600	36.05	154.26	173.44
5700	36.06	154.87	176.97
5800	36.06	155.47	180.50
5900	36.07	156.05	184.04
6000	36.07	156.65	187.57

3. CH₂ClCHO (Ideal Gas)

T (K)	C_p° (cal/mol.K)	S° (cal/mol.K)	$H^\circ - H^\circ(0\text{ K})$ (kcal/mol)
5	8.80	34.05	0.04
50	8.77	53.59	0.40
100	10.29	59.48	0.81
200	12.98	67.32	1.79
298	15.85	73.01	3.01
300	15.91	73.12	3.03
400	18.76	78.06	4.56
500	21.23	82.44	6.37
600	23.26	86.40	8.41
700	24.93	89.99	10.66
800	26.33	93.28	13.07
900	27.50	96.31	15.62
1000	28.50	99.12	18.29
1100	29.35	101.74	21.06
1200	30.07	104.20	23.93
1300	30.70	106.51	26.87
1400	31.23	108.69	29.87
1500	31.69	110.75	32.93
1600	32.10	112.71	36.04
1700	32.44	114.57	39.20
1800	32.75	116.35	42.39
1900	33.02	118.04	45.62
2000	33.25	119.67	48.88
2100	33.46	121.22	52.16
2200	33.64	122.72	55.47
2300	33.81	124.16	58.79
2400	33.96	125.54	62.14
2500	34.09	126.88	65.50
2600	34.21	128.17	68.87
2700	34.31	129.41	72.26
2800	34.41	130.62	75.67
2900	34.50	131.79	79.08
3000	34.57	132.92	82.50
3100	34.65	134.02	85.94
3200	34.71	135.09	89.38
3300	34.77	136.13	92.83
3400	34.83	137.14	96.28
3500	34.88	138.12	99.74
3600	34.93	139.08	103.21
3700	34.97	140.01	106.69
3800	35.01	140.92	110.16
3900	35.05	141.81	113.65
4000	35.08	142.68	117.14
4100	35.12	143.52	120.63
4200	35.15	144.35	124.13
4300	35.17	145.16	127.63
4400	35.20	145.95	131.13
4500	35.23	146.73	134.64
4600	35.25	147.49	138.14
4700	35.27	148.23	141.66
4800	35.29	148.96	145.17
4900	35.31	149.68	148.69
5000	35.33	150.38	152.21
5100	35.34	151.06	155.73
5200	35.36	151.74	159.25
5300	35.38	152.40	162.78
5400	35.39	153.05	166.31
5500	35.40	153.69	169.84
5600	35.42	154.32	173.37
5700	35.43	154.94	176.90
5800	35.44	155.55	180.43
5900	35.45	156.14	183.97
6000	35.46	156.74	187.51

4. CH₂ClCClO (Ideal Gas)

T (K)	Cp° (cal/mol.K)	S° (cal/mol.K)	H° - H°(0 K) (kcal/mol)
5	7.95	40.85	0.04
50	8.37	57.59	0.40
100	11.83	62.78	0.85
200	16.85	72.20	2.02
298	20.87	79.68	3.52
300	20.93	79.81	3.55
400	23.26	85.94	5.41
500	24.86	90.93	7.55
600	26.16	95.20	9.90
700	27.28	99.00	12.42
800	28.25	102.45	15.08
900	29.09	105.62	17.86
1000	29.83	108.56	20.73
1100	30.47	111.30	23.69
1200	31.03	113.87	26.72
1300	31.52	116.29	29.81
1400	31.94	118.56	32.95
1500	32.31	120.72	36.13
1600	32.64	122.76	39.35
1700	32.92	124.70	42.61
1800	33.17	126.55	45.89
1900	33.39	128.31	49.21
2000	33.59	130.00	52.54
2100	33.76	131.62	55.89
2200	33.91	133.17	59.26
2300	34.05	134.66	62.65
2400	34.18	136.09	66.05
2500	34.29	137.47	69.46
2600	34.39	138.80	72.89
2700	34.48	140.09	76.32
2800	34.56	141.33	79.77
2900	34.64	142.53	83.22
3000	34.70	143.70	86.68
3100	34.77	144.82	90.15
3200	34.82	145.92	93.62
3300	34.88	146.98	97.10
3400	34.93	148.02	100.59
3500	34.97	149.03	104.08
3600	35.01	150.01	107.57
3700	35.05	150.96	111.07
3800	35.09	151.89	114.57
3900	35.12	152.80	118.08
4000	35.15	153.68	121.59
4100	35.18	154.54	125.10
4200	35.20	155.39	128.62
4300	35.23	156.21	132.13
4400	35.25	157.02	135.66
4500	35.28	157.81	139.18
4600	35.30	158.58	142.71
4700	35.31	159.34	146.23
4800	35.33	160.08	149.76
4900	35.35	160.80	153.29
5000	35.37	161.51	156.83
5100	35.38	162.21	160.36
5200	35.40	162.90	163.90
5300	35.41	163.57	167.44
5400	35.42	164.23	170.98
5500	35.43	164.88	174.52
5600	35.45	165.51	178.06
5700	35.46	166.14	181.60
5800	35.47	166.75	185.15
5900	35.48	167.36	188.69
6000	35.49	167.95	192.24

5. CHCl₂CHO (Ideal Gas)

T (K)	C_p° (cal/mol.K)	S° (cal/mol.K)	$H^\circ - H^\circ(0\text{ K})$ (kcal/mol)
5	7.95	40.46	0.04
50	8.09	57.00	0.40
100	11.90	61.88	0.84
200	17.38	71.57	2.04
298	20.92	79.17	3.57
300	20.98	79.31	3.60
400	23.33	85.50	5.48
500	25.16	90.64	7.61
600	26.67	95.10	9.97
700	27.91	99.06	12.50
800	28.95	102.64	15.17
900	29.82	105.90	17.96
1000	30.56	108.90	20.84
1100	31.18	111.68	23.81
1200	31.71	114.27	26.85
1300	32.16	116.69	29.95
1400	32.55	118.97	33.10
1500	32.88	121.11	36.29
1600	33.17	123.14	39.52
1700	33.42	125.07	42.78
1800	33.64	126.90	46.08
1900	33.83	128.64	49.39
2000	34.00	130.31	52.73
2100	34.15	131.90	56.09
2200	34.28	133.43	59.47
2300	34.39	134.90	62.86
2400	34.50	136.31	66.26
2500	34.59	137.67	69.68
2600	34.67	138.98	73.11
2700	34.75	140.25	76.55
2800	34.82	141.48	80.00
2900	34.88	142.66	83.45
3000	34.93	143.81	86.92
3100	34.98	144.93	90.39
3200	35.03	146.01	93.86
3300	35.07	147.06	97.35
3400	35.11	148.08	100.83
3500	35.15	149.07	104.33
3600	35.18	150.04	107.82
3700	35.21	150.98	111.32
3800	35.24	151.90	114.83
3900	35.27	152.80	118.34
4000	35.29	153.67	121.85
4100	35.31	154.53	125.36
4200	35.33	155.36	128.88
4300	35.35	156.18	132.40
4400	35.37	156.97	135.93
4500	35.39	157.76	139.45
4600	35.41	158.52	142.98
4700	35.42	159.27	146.51
4800	35.44	160.00	150.04
4900	35.45	160.72	153.57
5000	35.46	161.43	157.11
5100	35.47	162.12	160.64
5200	35.49	162.80	164.18
5300	35.50	163.46	167.72
5400	35.51	164.12	171.26
5500	35.51	164.76	174.80
5600	35.52	165.39	178.35
5700	35.53	166.01	181.89
5800	35.54	166.62	185.44
5900	35.55	167.22	188.98
6000	35.56	167.82	192.53

6. CHCl₂CClO (Ideal Gas)

T (K)	C_p° (cal/mol.K)	S° (cal/mol.K)	$H^\circ - H^\circ(0\text{ K})$ (kcal/mol)
5	8.14	41.30	0.04
50	10.36	60.20	0.41
100	13.51	68.30	0.91
200	18.03	79.16	2.31
298	21.78	87.07	4.11
300	21.84	87.21	4.15
400	24.70	93.84	6.34
500	26.78	99.48	8.80
600	28.32	104.39	11.46
700	29.49	108.73	14.27
800	30.41	112.62	17.19
900	31.14	116.14	20.21
1000	31.74	119.37	23.31
1100	32.24	122.34	26.46
1200	32.65	125.09	29.67
1300	33.00	127.66	32.92
1400	33.30	130.06	36.21
1500	33.56	132.32	39.52
1600	33.77	134.46	42.87
1700	33.96	136.47	46.23
1800	34.13	138.39	49.62
1900	34.27	140.21	53.02
2000	34.40	141.94	56.44
2100	34.51	143.60	59.87
2200	34.61	145.19	63.32
2300	34.70	146.71	66.77
2400	34.78	148.17	70.23
2500	34.85	149.58	73.70
2600	34.91	150.93	77.18
2700	34.97	152.24	80.67
2800	35.02	153.50	84.16
2900	35.07	154.72	87.66
3000	35.11	155.89	91.16
3100	35.15	157.04	94.67
3200	35.19	158.15	98.18
3300	35.22	159.22	101.69
3400	35.25	160.26	105.21
3500	35.28	161.28	108.73
3600	35.31	162.27	112.26
3700	35.33	163.23	115.78
3800	35.35	164.17	119.31
3900	35.37	165.08	122.84
4000	35.39	165.97	126.38
4100	35.41	166.84	129.91
4200	35.42	167.69	133.45
4300	35.44	168.52	136.99
4400	35.45	169.33	140.53
4500	35.47	170.12	144.08
4600	35.48	170.90	147.62
4700	35.49	171.66	151.17
4800	35.50	172.40	154.71
4900	35.51	173.13	158.26
5000	35.52	173.85	161.81
5100	35.53	174.55	165.36
5200	35.54	175.23	168.91
5300	35.55	175.91	172.46
5400	35.56	176.57	176.02
5500	35.57	177.22	179.57
5600	35.57	177.86	183.13
5700	35.58	178.49	186.68
5800	35.59	179.10	190.24
5900	35.59	179.71	193.79
6000	35.60	180.31	197.35

7. CCl₃CHO (Ideal Gas)

T (K)	Cp° (cal/mol.K)	S° (cal/mol.K)	H° - H°(0 K) (kcal/mol)
5	8.01	41.11	0.04
50	8.36	57.97	0.40
100	13.33	64.09	0.89
200	19.48	75.31	2.35
298	23.36	83.83	4.25
300	23.42	83.98	4.29
400	26.12	91.05	6.57
500	28.04	96.99	9.10
600	29.47	102.12	11.82
700	30.55	106.62	14.67
800	31.40	110.63	17.64
900	32.07	114.25	20.69
1000	32.61	117.53	23.81
1100	33.05	120.55	27.00
1200	33.41	123.33	30.23
1300	33.71	125.91	33.50
1400	33.96	128.32	36.80
1500	34.17	130.58	40.14
1600	34.35	132.70	43.50
1700	34.50	134.71	46.88
1800	34.63	136.61	50.28
1900	34.74	138.42	53.70
2000	34.84	140.14	57.13
2100	34.92	141.78	60.57
2200	34.99	143.35	64.03
2300	35.06	144.85	67.49
2400	35.12	146.30	70.96
2500	35.17	147.69	74.44
2600	35.21	149.03	77.93
2700	35.25	150.32	81.42
2800	35.29	151.56	84.92
2900	35.32	152.77	88.42
3000	35.35	153.94	91.93
3100	35.38	155.07	95.44
3200	35.40	156.16	98.96
3300	35.42	157.23	102.48
3400	35.44	158.26	106.00
3500	35.46	159.26	109.53
3600	35.48	160.24	113.06
3700	35.50	161.19	116.59
3800	35.51	162.12	120.12
3900	35.52	163.02	123.66
4000	35.54	163.91	127.20
4100	35.55	164.77	130.74
4200	35.56	165.61	134.28
4300	35.57	166.43	137.82
4400	35.58	167.24	141.36
4500	35.59	168.02	144.91
4600	35.59	168.79	148.46
4700	35.60	169.54	152.01
4800	35.61	170.28	155.56
4900	35.62	171.01	159.11
5000	35.62	171.72	162.66
5100	35.63	172.41	166.21
5200	35.63	173.09	169.76
5300	35.64	173.76	173.32
5400	35.64	174.42	176.87
5500	35.65	175.07	180.43
5600	35.65	175.70	183.99
5700	35.66	176.32	187.54
5800	35.66	176.94	191.10
5900	35.66	177.54	194.66
6000	35.67	178.14	198.22

8. CCl₃CClO (Ideal Gas)

T (K)	C_p° (cal/mol.K)	S° (cal/mol.K)	$H^\circ - H^\circ(0\text{ K})$ (kcal/mol)
5	7.97	43.57	0.04
50	9.32	60.88	0.41
100	14.97	68.26	0.95
200	21.95	80.98	2.62
298	26.20	90.58	4.82
300	26.27	90.75	4.87
400	28.89	98.59	7.49
500	30.56	105.09	10.36
600	31.69	110.63	13.39
700	32.50	115.46	16.53
800	33.10	119.74	19.76
900	33.56	123.57	23.05
1000	33.91	127.05	26.38
1100	34.19	130.24	29.76
1200	34.41	133.17	33.16
1300	34.59	135.89	36.59
1400	34.74	138.42	40.04
1500	34.86	140.79	43.50
1600	34.96	143.01	46.98
1700	35.05	145.11	50.46
1800	35.12	147.09	53.96
1900	35.18	148.97	57.46
2000	35.24	150.76	60.98
2100	35.29	152.47	64.49
2200	35.33	154.10	68.02
2300	35.36	155.65	71.54
2400	35.39	157.15	75.07
2500	35.42	158.58	78.61
2600	35.45	159.97	82.15
2700	35.47	161.30	85.69
2800	35.49	162.58	89.23
2900	35.51	163.82	92.78
3000	35.53	165.01	96.32
3100	35.54	166.17	99.87
3200	35.56	167.30	103.42
3300	35.57	168.39	106.98
3400	35.58	169.44	110.53
3500	35.59	170.47	114.09
3600	35.60	171.47	117.64
3700	35.61	172.44	121.20
3800	35.62	173.39	124.76
3900	35.63	174.31	128.32
4000	35.63	175.21	131.88
4100	35.64	176.09	135.44
4200	35.64	176.94	139.00
4300	35.65	177.78	142.56
4400	35.66	178.59	146.13
4500	35.66	179.39	149.69
4600	35.67	180.18	153.25
4700	35.67	180.94	156.82
4800	35.67	181.69	160.39
4900	35.68	182.42	163.95
5000	35.68	183.14	167.52
5100	35.68	183.85	171.08
5200	35.69	184.54	174.65
5300	35.69	185.22	178.22
5400	35.69	185.88	181.79
5500	35.70	186.54	185.36
5600	35.70	187.18	188.92
5700	35.70	187.81	192.49
5800	35.70	188.43	196.06
5900	35.71	189.04	199.63
6000	35.71	189.64	203.20

9. CH₃C•=O (Ideal Gas)

T (K)	C_p° (cal/mol.K)	S° (cal/mol.K)	$H^\circ - H^\circ(0\text{ K})$ (kcal/mol)
5	8.37	29.40	0.04
50	8.13	47.31	0.40
100	9.72	52.86	0.80
200	10.46	59.85	1.65
298	12.08	64.30	2.63
300	12.12	64.38	2.65
400	14.11	68.12	3.85
500	16.04	71.46	5.25
600	17.76	74.53	6.84
700	19.26	77.37	8.59
800	20.57	80.02	10.48
900	21.71	82.50	12.49
1000	22.71	84.83	14.61
1100	23.58	87.03	16.82
1200	24.33	89.11	19.12
1300	24.99	91.08	21.49
1400	25.57	92.95	23.91
1500	26.07	94.73	26.40
1600	26.51	96.42	28.93
1700	26.90	98.04	31.50
1800	27.24	99.59	34.11
1900	27.54	101.06	36.75
2000	27.81	102.48	39.41
2100	28.05	103.84	42.11
2200	28.26	105.15	44.82
2300	28.45	106.41	47.56
2400	28.61	107.62	50.31
2500	28.77	108.79	53.08
2600	28.90	109.92	55.87
2700	29.03	111.01	58.66
2800	29.14	112.06	61.47
2900	29.24	113.08	64.29
3000	29.33	114.07	67.12
3100	29.42	115.02	69.96
3200	29.49	115.95	72.81
3300	29.56	116.85	75.66
3400	29.62	117.73	78.52
3500	29.68	118.58	81.39
3600	29.73	119.40	84.27
3700	29.78	120.21	87.15
3800	29.83	120.99	90.03
3900	29.87	121.75	92.92
4000	29.90	122.50	95.81
4100	29.94	123.22	98.71
4200	29.97	123.92	101.61
4300	30.00	124.61	104.52
4400	30.02	125.29	107.43
4500	30.05	125.94	110.34
4600	30.07	126.58	113.25
4700	30.09	127.21	116.17
4800	30.10	127.83	119.09
4900	30.12	128.43	122.01
5000	30.14	129.01	124.93
5100	30.15	129.59	127.86
5200	30.16	130.15	130.79
5300	30.17	130.70	133.72
5400	30.18	131.24	136.65
5500	30.19	131.77	139.59
5600	30.20	132.29	142.52
5700	30.20	132.80	145.46
5800	30.21	133.30	148.40
5900	30.22	133.79	151.34
6000	30.22	134.29	154.28

10. CH₂ClC•=O (Ideal Gas)

T (K)	Cp° (cal/mol.K)	S° (cal/mol.K)	H° - H°(0 K) (kcal/mol)
5	7.95	36.67	0.04
50	8.12	53.45	0.40
100	10.71	58.80	0.83
200	13.07	66.71	1.82
298	16.21	72.51	3.02
300	16.28	72.62	3.04
400	19.24	77.83	4.52
500	21.39	82.36	6.21
600	22.84	86.23	8.08
700	23.86	89.56	10.10
800	24.65	92.49	12.24
900	25.29	95.12	14.48
1000	25.84	97.53	16.81
1100	26.30	99.75	19.21
1200	26.71	101.81	21.67
1300	27.06	103.74	24.19
1400	27.36	105.56	26.76
1500	27.63	107.27	29.37
1600	27.86	108.90	32.01
1700	28.06	110.44	34.69
1800	28.23	111.90	37.39
1900	28.38	113.30	40.12
2000	28.52	114.64	42.87
2100	28.63	115.92	45.64
2200	28.74	117.15	48.42
2300	28.83	118.34	51.22
2400	28.91	119.47	54.04
2500	28.98	120.57	56.86
2600	29.05	121.63	59.70
2700	29.10	122.65	62.54
2800	29.15	123.64	65.40
2900	29.20	124.60	68.26
3000	29.24	125.53	71.13
3100	29.28	126.43	74.00
3200	29.32	127.30	76.89
3300	29.35	128.15	79.77
3400	29.38	128.98	82.67
3500	29.40	129.79	85.56
3600	29.43	130.57	88.47
3700	29.45	131.34	91.37
3800	29.47	132.08	94.28
3900	29.49	132.81	97.20
4000	29.50	133.52	100.11
4100	29.52	134.22	103.03
4200	29.53	134.90	105.95
4300	29.55	135.56	108.88
4400	29.56	136.21	111.81
4500	29.57	136.85	114.74
4600	29.58	137.48	117.67
4700	29.59	138.09	120.60
4800	29.60	138.69	123.54
4900	29.61	139.27	126.47
5000	29.62	139.85	129.41
5100	29.63	140.42	132.35
5200	29.64	140.97	135.30
5300	29.64	141.52	138.24
5400	29.65	142.05	141.19
5500	29.66	142.58	144.13
5600	29.66	143.10	147.08
5700	29.67	143.61	150.03
5800	29.67	144.11	152.98
5900	29.68	144.60	155.93
6000	29.68	145.09	158.88

11. CHCl₂C•=O (Ideal Gas)

T (K)	C _p ^o (cal/mol.K)	S ^o (cal/mol.K)	H ^o - H ^o (0 K) (kcal/mol)
5	7.95	42.58	0.04
50	8.27	59.07	0.40
100	12.12	64.80	0.85
200	15.97	74.41	2.04
298	18.90	81.34	3.54
300	18.95	81.46	3.58
400	21.11	87.15	5.39
500	22.72	91.94	7.41
600	23.95	96.10	9.59
700	24.91	99.78	11.90
800	25.69	103.07	14.30
900	26.31	106.04	16.78
1000	26.83	108.76	19.32
1100	27.25	111.25	21.92
1200	27.60	113.55	24.56
1300	27.89	115.68	27.25
1400	28.14	117.68	29.96
1500	28.34	119.54	32.70
1600	28.52	121.30	35.47
1700	28.66	122.95	38.25
1800	28.79	124.52	41.06
1900	28.90	126.01	43.88
2000	28.99	127.43	46.71
2100	29.07	128.78	49.55
2200	29.14	130.07	52.41
2300	29.20	131.31	55.28
2400	29.26	132.50	58.15
2500	29.30	133.64	61.03
2600	29.35	134.74	63.92
2700	29.38	135.80	66.82
2800	29.42	136.83	69.72
2900	29.45	137.82	72.63
3000	29.47	138.78	75.54
3100	29.50	139.71	78.45
3200	29.52	140.61	81.37
3300	29.54	141.49	84.29
3400	29.56	142.34	87.22
3500	29.57	143.16	90.15
3600	29.59	143.97	93.08
3700	29.60	144.75	96.01
3800	29.61	145.52	98.95
3900	29.62	146.26	101.89
4000	29.63	146.99	104.83
4100	29.64	147.70	107.77
4200	29.65	148.39	110.72
4300	29.66	149.07	113.66
4400	29.67	149.73	116.61
4500	29.67	150.38	119.56
4600	29.68	151.01	122.51
4700	29.69	151.64	125.46
4800	29.69	152.24	128.41
4900	29.70	152.84	131.37
5000	29.70	153.43	134.32
5100	29.71	154.00	137.28
5200	29.71	154.56	140.24
5300	29.72	155.12	143.19
5400	29.72	155.66	146.15
5500	29.72	156.19	149.11
5600	29.73	156.72	152.07
5700	29.73	157.23	155.03
5800	29.73	157.74	157.99
5900	29.74	158.24	160.95
6000	29.74	158.73	163.92

12. $\text{CCl}_3\text{C}\equiv\text{O}$ (Ideal Gas)

T (K)	C_p° (cal/mol.K)	S° (cal/mol.K)	$H^\circ - H^\circ(0\text{ K})$ (kcal/mol)
5	8.43	41.45	0.04
50	8.73	59.22	0.40
100	13.65	65.86	0.89
200	19.28	77.28	2.35
298	22.62	85.63	4.24
300	22.68	85.79	4.29
400	24.78	92.57	6.52
500	26.15	98.20	8.94
600	27.09	103.00	11.49
700	27.78	107.18	14.12
800	28.28	110.87	16.81
900	28.66	114.17	19.56
1000	28.94	117.14	22.34
1100	29.16	119.85	25.16
1200	29.32	122.32	27.99
1300	29.44	124.60	30.85
1400	29.54	126.71	33.72
1500	29.61	128.68	36.60
1600	29.67	130.53	39.50
1700	29.72	132.26	42.40
1800	29.75	133.89	45.32
1900	29.78	135.44	48.24
2000	29.80	136.91	51.16
2100	29.82	138.31	54.09
2200	29.83	139.64	57.03
2300	29.84	140.91	59.96
2400	29.85	142.14	62.91
2500	29.85	143.31	65.85
2600	29.86	144.44	68.80
2700	29.86	145.52	71.75
2800	29.86	146.57	74.70
2900	29.86	147.58	77.65
3000	29.86	148.56	80.61
3100	29.86	149.50	83.57
3200	29.87	150.42	86.52
3300	29.87	151.31	89.48
3400	29.86	152.17	92.45
3500	29.86	153.01	95.41
3600	29.86	153.83	98.37
3700	29.86	154.62	101.34
3800	29.86	155.40	104.30
3900	29.86	156.15	107.27
4000	29.86	156.88	110.23
4100	29.86	157.60	113.20
4200	29.86	158.30	116.17
4300	29.86	158.99	119.14
4400	29.86	159.66	122.11
4500	29.85	160.31	125.08
4600	29.85	160.95	128.05
4700	29.85	161.58	131.02
4800	29.85	162.20	133.99
4900	29.85	162.80	136.96
5000	29.85	163.39	139.93
5100	29.85	163.97	142.90
5200	29.85	164.53	145.87
5300	29.85	165.09	148.85
5400	29.84	165.64	151.82
5500	29.84	166.18	154.79
5600	29.84	166.70	157.77
5700	29.84	167.22	160.74
5800	29.84	167.73	163.71
5900	29.84	168.23	166.69
6000	29.84	168.73	169.66

13. C•H₂CHO (Ideal Gas)

T (K)	C_p° (cal/mol.K)	S° (cal/mol.K)	$H^\circ - H^\circ(0\text{ K})$ (kcal/mol)
5	7.95	26.00	0.04
50	7.95	44.31	0.40
100	8.15	49.85	0.80
200	10.04	55.99	1.70
298	12.55	60.45	2.80
300	12.60	60.53	2.83
400	15.12	64.50	4.21
500	17.32	68.11	5.84
600	19.15	71.43	7.67
700	20.68	74.50	9.66
800	21.97	77.34	11.79
900	23.08	80.00	14.05
1000	24.04	82.48	16.40
1100	24.87	84.80	18.85
1200	25.59	87.00	21.38
1300	26.22	89.07	23.97
1400	26.77	91.03	26.62
1500	27.25	92.90	29.32
1600	27.67	94.67	32.07
1700	28.04	96.35	34.85
1800	28.37	97.97	37.67
1900	28.66	99.51	40.52
2000	28.91	100.98	43.40
2100	29.14	102.40	46.30
2200	29.34	103.76	49.23
2300	29.52	105.07	52.17
2400	29.69	106.33	55.13
2500	29.83	107.54	58.11
2600	29.97	108.71	61.10
2700	30.09	109.85	64.10
2800	30.19	110.94	67.12
2900	30.29	112.00	70.14
3000	30.38	113.03	73.17
3100	30.47	114.03	76.22
3200	30.54	115.00	79.27
3300	30.61	115.94	82.32
3400	30.68	116.85	85.39
3500	30.74	117.74	88.46
3600	30.79	118.61	91.54
3700	30.84	119.45	94.62
3800	30.89	120.28	97.70
3900	30.93	121.08	100.79
4000	30.97	121.86	103.89
4100	31.01	122.63	106.99
4200	31.05	123.37	110.09
4300	31.08	124.11	113.20
4400	31.11	124.82	116.31
4500	31.14	125.52	119.42
4600	31.17	126.20	122.53
4700	31.19	126.87	125.65
4800	31.22	127.53	128.77
4900	31.24	128.17	131.90
5000	31.26	128.81	135.02
5100	31.28	129.43	138.15
5200	31.30	130.03	141.28
5300	31.32	130.63	144.41
5400	31.33	131.21	147.54
5500	31.35	131.79	150.67
5600	31.37	132.35	153.81
5700	31.38	132.91	156.95
5800	31.39	133.46	160.09
5900	31.41	133.99	163.23
6000	31.42	134.52	166.37

14. C•H₂CClO (Ideal Gas)

T (K)	C_p° (cal/mol.K)	S° (cal/mol.K)	$H^\circ - H^\circ(0\text{ K})$ (kcal/mol)
5	7.95	31.39	0.04
50	7.97	49.70	0.40
100	8.92	55.43	0.81
200	12.85	62.78	1.90
298	16.13	68.54	3.33
300	16.19	68.64	3.36
400	18.73	73.66	5.11
500	20.68	78.05	7.08
600	22.20	81.96	9.23
700	23.43	85.47	11.52
800	24.44	88.67	13.91
900	25.29	91.59	16.40
1000	26.02	94.29	18.96
1100	26.64	96.80	21.60
1200	27.18	99.14	24.29
1300	27.65	101.33	27.03
1400	28.06	103.40	29.82
1500	28.41	105.34	32.64
1600	28.73	107.19	35.50
1700	29.00	108.94	38.38
1800	29.24	110.60	41.30
1900	29.46	112.19	44.23
2000	29.65	113.70	47.19
2100	29.81	115.15	50.16
2200	29.97	116.54	53.15
2300	30.10	117.88	56.15
2400	30.22	119.16	59.17
2500	30.33	120.40	62.20
2600	30.43	121.59	65.23
2700	30.52	122.74	68.28
2800	30.60	123.85	71.34
2900	30.67	124.92	74.40
3000	30.74	125.96	77.47
3100	30.80	126.97	80.55
3200	30.86	127.95	83.63
3300	30.91	128.90	86.72
3400	30.96	129.83	89.81
3500	31.00	130.72	92.91
3600	31.04	131.60	96.01
3700	31.08	132.45	99.12
3800	31.12	133.28	102.23
3900	31.15	134.09	105.34
4000	31.18	134.88	108.46
4100	31.21	135.65	111.58
4200	31.23	136.40	114.70
4300	31.26	137.13	117.83
4400	31.28	137.85	120.95
4500	31.30	138.55	124.08
4600	31.32	139.24	127.21
4700	31.34	139.92	130.35
4800	31.36	140.58	133.48
4900	31.38	141.22	136.62
5000	31.39	141.86	139.76
5100	31.41	142.48	142.90
5200	31.42	143.09	146.04
5300	31.44	143.69	149.18
5400	31.45	144.28	152.33
5500	31.46	144.85	155.47
5600	31.47	145.42	158.62
5700	31.49	145.98	161.77
5800	31.50	146.52	164.92
5900	31.51	147.06	168.07
6000	31.51	147.59	171.22

15. E-C•HClCHO (Ideal Gas)

T (K)	C_p° (cal/mol.K)	S° (cal/mol.K)	$H^\circ - H^\circ(0\text{ K})$ (kcal/mol)
5	7.95	32.17	0.04
50	8.26	50.54	0.40
100	9.80	56.71	0.85
200	12.62	64.39	1.98
298	15.24	69.90	3.34
300	15.29	70.01	3.37
400	17.77	74.74	5.03
500	19.86	78.94	6.91
600	21.56	82.71	8.99
700	22.95	86.14	11.21
800	24.08	89.27	13.57
900	25.03	92.16	16.02
1000	25.83	94.84	18.57
1100	26.51	97.34	21.19
1200	27.09	99.67	23.87
1300	27.59	101.85	26.60
1400	28.02	103.91	29.38
1500	28.40	105.86	32.20
1600	28.72	107.70	35.06
1700	29.00	109.45	37.95
1800	29.25	111.12	40.86
1900	29.47	112.70	43.80
2000	29.66	114.22	46.75
2100	29.83	115.67	49.73
2200	29.99	117.06	52.72
2300	30.12	118.40	55.73
2400	30.24	119.68	58.74
2500	30.35	120.92	61.77
2600	30.45	122.11	64.81
2700	30.54	123.26	67.86
2800	30.62	124.37	70.92
2900	30.69	125.45	73.99
3000	30.76	126.49	77.06
3100	30.82	127.50	80.14
3200	30.88	128.48	83.22
3300	30.93	129.43	86.32
3400	30.98	130.35	89.41
3500	31.02	131.25	92.51
3600	31.06	132.13	95.61
3700	31.10	132.98	98.72
3800	31.13	133.81	101.83
3900	31.16	134.62	104.95
4000	31.19	135.40	108.07
4100	31.22	136.18	111.19
4200	31.25	136.93	114.31
4300	31.27	137.66	117.44
4400	31.30	138.38	120.57
4500	31.32	139.09	123.70
4600	31.34	139.77	126.83
4700	31.36	140.45	129.96
4800	31.37	141.11	133.10
4900	31.39	141.76	136.24
5000	31.41	142.39	139.38
5100	31.42	143.01	142.52
5200	31.43	143.62	145.66
5300	31.45	144.22	148.81
5400	31.46	144.81	151.95
5500	31.47	145.39	155.10
5600	31.48	145.95	158.24
5700	31.49	146.51	161.39
5800	31.50	147.06	164.54
5900	31.51	147.60	167.69
6000	31.52	148.13	170.85

16. Z-C•HClCHO (Ideal Gas)

T (K)	C_p° (cal/mol.K)	S° (cal/mol.K)	$H^\circ - H^\circ(0\text{ K})$ (kcal/mol)
5	7.95	32.64	0.04
50	8.12	50.98	0.40
100	9.38	56.95	0.83
200	12.17	64.30	1.91
298	14.97	69.67	3.24
300	15.02	69.77	3.27
400	17.62	74.45	4.91
500	19.77	78.61	6.78
600	21.50	82.37	8.85
700	22.91	85.79	11.07
800	24.06	88.92	13.42
900	25.02	91.81	15.87
1000	25.82	94.49	18.42
1100	26.51	96.98	21.03
1200	27.09	99.31	23.72
1300	27.60	101.50	26.45
1400	28.03	103.56	29.23
1500	28.40	105.50	32.05
1600	28.73	107.35	34.91
1700	29.01	109.10	37.80
1800	29.26	110.76	40.71
1900	29.48	112.35	43.65
2000	29.67	113.86	46.61
2100	29.84	115.32	49.58
2200	29.99	116.71	52.57
2300	30.13	118.04	55.58
2400	30.25	119.33	58.60
2500	30.36	120.56	61.63
2600	30.46	121.76	64.67
2700	30.55	122.91	67.72
2800	30.63	124.02	70.78
2900	30.70	125.10	73.84
3000	30.77	126.14	76.92
3100	30.83	127.15	80.00
3200	30.88	128.13	83.08
3300	30.93	129.08	86.17
3400	30.98	130.00	89.27
3500	31.02	130.90	92.37
3600	31.06	131.77	95.47
3700	31.10	132.63	98.58
3800	31.14	133.46	101.69
3900	31.17	134.26	104.81
4000	31.20	135.05	107.93
4100	31.23	135.82	111.05
4200	31.25	136.58	114.17
4300	31.28	137.31	117.30
4400	31.30	138.03	120.43
4500	31.32	138.74	123.56
4600	31.34	139.42	126.69
4700	31.36	140.10	129.83
4800	31.38	140.76	132.96
4900	31.39	141.41	136.10
5000	31.41	142.04	139.24
5100	31.42	142.66	142.38
5200	31.44	143.27	145.52
5300	31.45	143.87	148.67
5400	31.46	144.46	151.81
5500	31.47	145.04	154.96
5600	31.48	145.60	158.11
5700	31.49	146.16	161.26
5800	31.50	146.71	164.41
5900	31.51	147.25	167.56
6000	31.52	147.78	170.71

17. C•Cl₂CHO (Ideal Gas)

T (K)	C_p° (cal/mol.K)	S° (cal/mol.K)	$H^\circ - H^\circ(0\text{ K})$ (kcal/mol)
5	7.95	34.94	0.04
50	8.43	53.34	0.40
100	11.08	59.95	0.89
200	15.38	69.06	2.23
298	18.31	75.75	3.88
300	18.37	75.87	3.92
400	20.78	81.49	5.88
500	22.70	86.34	8.06
600	24.21	90.61	10.41
700	25.39	94.43	12.89
800	26.34	97.88	15.48
900	27.10	101.03	18.15
1000	27.72	103.92	20.89
1100	28.24	106.58	23.69
1200	28.67	109.06	26.54
1300	29.03	111.37	29.42
1400	29.34	113.53	32.34
1500	29.60	115.56	35.29
1600	29.82	117.48	38.26
1700	30.01	119.29	41.25
1800	30.18	121.01	44.26
1900	30.32	122.64	47.29
2000	30.45	124.20	50.32
2100	30.56	125.69	53.38
2200	30.66	127.11	56.44
2300	30.75	128.48	59.51
2400	30.83	129.79	62.59
2500	30.90	131.05	65.67
2600	30.96	132.26	68.76
2700	31.02	133.43	71.86
2800	31.07	134.56	74.97
2900	31.11	135.65	78.08
3000	31.16	136.71	81.19
3100	31.19	137.73	84.31
3200	31.23	138.72	87.43
3300	31.26	139.68	90.55
3400	31.29	140.61	93.68
3500	31.32	141.52	96.81
3600	31.34	142.40	99.94
3700	31.37	143.26	103.08
3800	31.39	144.10	106.22
3900	31.41	144.92	109.36
4000	31.43	145.71	112.50
4100	31.44	146.49	115.64
4200	31.46	147.24	118.79
4300	31.48	147.99	121.93
4400	31.49	148.71	125.08
4500	31.50	149.42	128.23
4600	31.51	150.11	131.38
4700	31.53	150.79	134.54
4800	31.54	151.45	137.69
4900	31.55	152.10	140.84
5000	31.56	152.74	144.00
5100	31.57	153.36	147.15
5200	31.57	153.98	150.31
5300	31.58	154.58	153.47
5400	31.59	155.17	156.63
5500	31.60	155.75	159.79
5600	31.60	156.32	162.95
5700	31.61	156.88	166.11
5800	31.62	157.43	169.27
5900	31.62	157.97	172.43
6000	31.63	158.50	175.59

18. E-C•HClCClO (Ideal Gas)

T (K)	C_p° (cal/mol.K)	S° (cal/mol.K)	$H^\circ - H^\circ(0\text{ K})$ (kcal/mol)
5	7.95	36.23	0.04
50	8.94	54.84	0.41
100	11.23	61.74	0.92
200	15.36	70.81	2.25
298	18.65	77.57	3.92
300	18.71	77.70	3.96
400	21.23	83.43	5.96
500	23.11	88.38	8.18
600	24.53	92.72	10.57
700	25.63	96.58	13.08
800	26.50	100.06	15.69
900	27.20	103.22	18.37
1000	27.78	106.12	21.12
1100	28.26	108.79	23.93
1200	28.66	111.26	26.77
1300	29.01	113.57	29.66
1400	29.30	115.73	32.57
1500	29.55	117.76	35.51
1600	29.77	119.67	38.48
1700	29.96	121.48	41.47
1800	30.12	123.20	44.47
1900	30.27	124.83	47.49
2000	30.40	126.39	50.52
2100	30.51	127.87	53.57
2200	30.61	129.29	56.63
2300	30.70	130.66	59.69
2400	30.78	131.96	62.77
2500	30.85	133.22	65.85
2600	30.92	134.43	68.94
2700	30.98	135.60	72.03
2800	31.03	136.73	75.13
2900	31.08	137.82	78.24
3000	31.12	138.87	81.35
3100	31.16	139.89	84.46
3200	31.20	140.88	87.58
3300	31.23	141.84	90.70
3400	31.26	142.78	93.82
3500	31.29	143.68	96.95
3600	31.32	144.56	100.08
3700	31.34	145.42	103.21
3800	31.36	146.26	106.35
3900	31.38	147.07	109.49
4000	31.40	147.87	112.63
4100	31.42	148.64	115.77
4200	31.44	149.40	118.91
4300	31.45	150.14	122.06
4400	31.47	150.86	125.20
4500	31.48	151.57	128.35
4600	31.50	152.26	131.50
4700	31.51	152.94	134.65
4800	31.52	153.60	137.80
4900	31.53	154.25	140.95
5000	31.54	154.89	144.11
5100	31.55	155.52	147.26
5200	31.56	156.13	150.42
5300	31.57	156.73	153.57
5400	31.58	157.32	156.73
5500	31.58	157.90	159.89
5600	31.59	158.47	163.05
5700	31.60	159.03	166.21
5800	31.61	159.58	169.37
5900	31.61	160.12	172.53
6000	31.62	160.65	175.69

19. Z-C•HCICClO (Ideal Gas)

T (K)	C_p° (cal/mol.K)	S° (cal/mol.K)	$H^\circ - H^\circ(0\text{ K})$ (kcal/mol)
5	7.95	36.29	0.04
50	8.87	54.85	0.41
100	10.97	61.67	0.91
200	15.17	70.55	2.21
298	18.58	77.25	3.87
300	18.64	77.38	3.91
400	21.19	83.10	5.91
500	23.10	88.04	8.13
600	24.53	92.38	10.51
700	25.64	96.24	13.02
800	26.51	99.73	15.63
900	27.22	102.89	18.32
1000	27.80	105.79	21.07
1100	28.28	108.46	23.88
1200	28.69	110.93	26.73
1300	29.03	113.24	29.61
1400	29.32	115.41	32.53
1500	29.57	117.44	35.48
1600	29.79	119.35	38.44
1700	29.98	121.16	41.43
1800	30.14	122.88	44.44
1900	30.29	124.51	47.46
2000	30.41	126.07	50.49
2100	30.52	127.56	53.54
2200	30.62	128.98	56.60
2300	30.71	130.34	59.67
2400	30.79	131.65	62.74
2500	30.86	132.91	65.82
2600	30.93	134.12	68.91
2700	30.99	135.29	72.01
2800	31.04	136.42	75.11
2900	31.09	137.51	78.22
3000	31.13	138.56	81.33
3100	31.17	139.58	84.44
3200	31.20	140.57	87.56
3300	31.24	141.53	90.68
3400	31.27	142.46	93.81
3500	31.30	143.37	96.94
3600	31.32	144.25	100.07
3700	31.35	145.11	103.20
3800	31.37	145.95	106.34
3900	31.39	146.76	109.47
4000	31.41	147.56	112.61
4100	31.43	148.33	115.76
4200	31.44	149.09	118.90
4300	31.46	149.83	122.04
4400	31.47	150.55	125.19
4500	31.49	151.26	128.34
4600	31.50	151.95	131.49
4700	31.51	152.63	134.64
4800	31.52	153.30	137.79
4900	31.53	153.95	140.94
5000	31.54	154.58	144.10
5100	31.55	155.21	147.25
5200	31.56	155.82	150.41
5300	31.57	156.42	153.56
5400	31.58	157.01	156.72
5500	31.59	157.59	159.88
5600	31.59	158.16	163.04
5700	31.60	158.72	166.20
5800	31.61	159.27	169.36
5900	31.61	159.81	172.52
6000	31.62	160.34	175.68

20. C•Cl₂CClO (Ideal Gas)

T (K)	C_p° (cal/mol.K)	S° (cal/mol.K)	$H^\circ - H^\circ(0\text{ K})$ (kcal/mol)
5	7.95	37.27	0.04
50	9.83	56.65	0.43
100	12.86	64.34	1.00
200	18.30	75.04	2.58
298	21.79	83.02	4.55
300	21.85	83.17	4.59
400	24.26	89.80	6.91
500	25.97	95.40	9.42
600	27.20	100.25	12.09
700	28.11	104.51	14.85
800	28.79	108.31	17.70
900	29.31	111.73	20.60
1000	29.71	114.83	23.56
1100	30.02	117.68	26.54
1200	30.27	120.30	29.56
1300	30.48	122.73	32.60
1400	30.64	125.00	35.65
1500	30.78	127.12	38.72
1600	30.90	129.11	41.81
1700	30.99	130.98	44.90
1800	31.07	132.76	48.01
1900	31.14	134.44	51.12
2000	31.21	136.04	54.23
2100	31.26	137.56	57.36
2200	31.30	139.02	60.49
2300	31.34	140.41	63.62
2400	31.38	141.74	66.75
2500	31.41	143.02	69.89
2600	31.44	144.26	73.04
2700	31.47	145.44	76.18
2800	31.49	146.59	79.33
2900	31.51	147.69	82.48
3000	31.53	148.76	85.63
3100	31.54	149.80	88.78
3200	31.56	150.80	91.94
3300	31.57	151.77	95.10
3400	31.59	152.71	98.25
3500	31.60	153.63	101.41
3600	31.61	154.52	104.57
3700	31.62	155.38	107.73
3800	31.63	156.23	110.90
3900	31.64	157.05	114.06
4000	31.64	157.85	117.22
4100	31.65	158.63	120.39
4200	31.66	159.39	123.55
4300	31.66	160.14	126.72
4400	31.67	160.87	129.89
4500	31.67	161.58	133.05
4600	31.68	162.28	136.22
4700	31.68	162.96	139.39
4800	31.69	163.62	142.56
4900	31.69	164.28	145.73
5000	31.70	164.92	148.90
5100	31.70	165.55	152.07
5200	31.71	166.16	155.24
5300	31.71	166.76	158.41
5400	31.71	167.36	161.58
5500	31.71	167.94	164.75
5600	31.72	168.51	167.92
5700	31.72	169.07	171.09
5800	31.72	169.62	174.26
5900	31.73	170.17	177.44
6000	31.73	170.70	180.61

Appendix:**"ROTATOR" Program Use****CH₂ClC•=O (10) as an example molecule****(a) Input file: CCICjDO.IR (j indicates Radical site)**

CCICJDO (Title section, molecular name)
 6 (number of atoms)
 (index # atomic #) x y z (standard cartesian coordinate)

1	6	0.005909	0.008618	0.017069
2	6	0.041446	0.065419	1.510744
3	1	1.034211	-0.009861	-0.350777
4	1	-0.477703	0.916436	-0.350275
5	17	-0.872456	-1.424864	-0.707032
6	8	-0.391957	-0.644342	2.350662

1 2 (atom 1 and atom 2; rotation axis, the rotation is about atom 1 – atom 2)
 1 3 (3 atoms in atom 1 group)
 3 4 5 (atoms 3, 4, and 5 are in atom 1 group)
 2 1 (1 atom in atom 2 group)
 6 (atom 6 is in atom 2 group)

V(x)=A+B*COS(nx)+C*SIN(nx) b3lyp/6-31g(d,p) (title section)
 0 0 1 (print option flag)
 1 (print option flag)
 50 (size of matrix)
 5 (number of coefficient sets in Fourier series)
 2.935 (a0)
 0.664 1.112 (a1, b1)
 0.707 -1.251 (a2, b2)
 -0.331 0.025 (a3, b3)
 0.00626 -0.045 (a4, b4)
 -0.037 0.069 (a5, b5)

(b) Output file 1: CCICjDO.CHK
CCICjDO

C	0.0059	0.0086	0.0171
C	0.0414	0.0654	1.5107
H	1.0342	-0.0099	-0.3508
H	-0.4777	0.9164	-0.3503

Cl	-0.8725	-1.4249	-0.7070
O	-0.3920	-0.6443	2.3507

The internal rotation is along the axis of atom ID# 1 (C) and atom ID# 2 (C)

The reduced moment part of Top atom (C) ID# 1 is 98.34 Amu-A²

The reduced moment part of Top atom (C) ID# 2 is 12.07 Amu-A²

Reduced Moment of Inertia = 10.7475 amu*A²

Rotational Constant = 3.1158922747E-16 erg

Rotational Constant = 1.5685317226E+00 cm⁻¹

(c) Output file 2: CCICjDO.DET

Task Name: V(x)=A+B*COS(nx)+C*SIN(nx) b3lyp/6-31g(d,p)

Print File Name: cclcjdo.det

abs(M) = 50 (size of matrix)

abs(K) = 5 (number of coefficient sets in Fourier series)

k	Re (real)	Im (imaginary)
0	1.636125970000000E+0002	
1	3.701491100000000E+0001	-6.198882700000000E+0001
2	3.941196100000000E+0001	6.973743100000000E+0001
3	-1.845171000000000E+0001	-1.393634000000000E+0000
4	3.489660000000000E-0001	2.508541000000000E+0000
5	-2.062578000000000E+0000	-3.846429000000000E+0000

E (eigenenergy)

1	2	3	4	5	6	7	8		
-150.9857	-121.9379	-92.9317	-64.0378	-35.3228	-6.8497	21.3199	49.1254		
9	10	11	12	13	14	15	16		
76.5054	103.3968	129.7330	155.4423	180.4453	188.4945	204.6515	204.9205		
17	18	19	20	21	22	23	24		
219.9174	227.9537	233.6778	246.5075	250.2189	258.7348	270.5958	271.2714		
25	26	27	28	29	30	31	32		
282.2009	290.8521	293.5563	304.5760	308.4687	315.1261	322.1232	326.5223		
33	34	35	36	37	38	39	40		
331.4280	340.3358	341.7613	354.8502	355.0078	370.5327	370.5794	387.6731		
41	42	43	44	45	46	47	48		
387.6900	406.1585	406.1615	425.9082	425.9085	446.8721	446.8721	469.0125		
49	50	51	52	53	54	55	56		
469.0125	492.3006	492.3006	516.7140	516.7140	542.2349	542.2349	568.8488		
57	58	59	60	61	62	63	64		
568.8488	596.5438	596.5438	625.3101	625.3101	655.1392	655.1392	686.0241		
65	66	67	68	69	70	71	72		
686.0241	717.9587	717.9587	750.9378	750.9378	784.9572	784.9572	820.0140		
73	74	75	76	77	78	79	80		
820.0140	856.1086	856.1086	893.2502	893.2502	931.4695	931.4695	970.8435		
81	82	83	84	85	86	87	88		
970.8435	1011.5320	1011.5320	1053.7909	1053.7909	1097.9794	1097.9794	1144.3982		

89	90	91	92	93	94	95	96
1144.3982	1193.5975	1193.5975	1245.1816	1245.1816	1301.1618	1301.1618	1357.2239
97	98	99	100	101			
1357.2239	1429.8939	1429.8939	1481.5038	1481.5038			

(Comment - This table of Output file 2 provides a valuable illustration of near degenerate eigenenergies.)

(d) Output file 3: CCICjDO.SCP

B 3.11589227469909E-0016

Entropy, S298 = 3.840

S298	Cp300	Cp400	Cp500	Cp600	Cp800	Cp1000	Cp1500
3.8400	2.7305	3.3306	3.5049	3.3471	2.7262	2.1726	1.3505