



Fig. 1 Calculated averaged ground state energy $E_{\text{therm}}^{S0}(T, \lambda)$.

RICC2 results:

Optimized ground state geometry:

1.94173447954448	-3.99999837897485	0.00000000000000	c
3.70185257051880	-2.02888366713496	0.00000000000000	c
2.90367656474978	0.47222320987303	0.00000000000000	c
0.31813598497625	1.03759881965605	0.00000000000000	c
-1.45840637077574	-0.91863225343250	0.00000000000000	c
-0.62437535244029	-3.42692762328683	0.00000000000000	c
2.56636000114907	-5.94512221595036	0.00000000000000	h
5.70463559413986	-2.44122096297480	0.00000000000000	h
4.24022322768905	2.01882952616435	0.00000000000000	h
-3.46089093626038	-0.52854331177349	0.00000000000000	h
-2.01047750089535	-4.93063761231714	0.00000000000000	h
-0.27477719678738	3.54936214162664	0.00000000000000	o
-2.89532868979943	4.14551529256358	0.00000000000000	c
-3.82562350963526	3.40171365691415	1.68353482227723	h
-3.00111535653817	6.19300972213297	0.00000000000000	h
-3.82562350963526	3.40171365691415	-1.68353482227723	h

Optimized exited state geometry:

1.95935665387796	-3.99588858987684	0.00000000000000	c
3.79574277771979	-2.04148653155549	0.00000000000000	c
2.95897906273188	0.53223347782830	0.00000000000000	c
0.31298691630125	1.01664074373426	0.00000000000000	c
-1.55942759746061	-0.93773687593137	0.00000000000000	c
-0.68586322936827	-3.49255990096077	0.00000000000000	c
2.58428961964142	-5.94362441589451	0.00000000000000	h
5.78515264864274	-2.49239286264319	0.00000000000000	h
4.24267982709348	2.11819489283523	0.00000000000000	h
-3.55063096208595	-0.51070240588885	0.00000000000000	h
-2.02028726975061	-5.03661446798548	0.00000000000000	h
-0.28808862017892	3.49781591873847	0.00000000000000	o
-2.91664570013995	4.17438011530374	0.00000000000000	c
-3.83660142442356	3.44455738545612	1.68808159063550	h
-2.94504127817702	6.22262613138427	0.00000000000000	h
-3.83660142442356	3.44455738545612	-1.68808159063550	h

ground state vibrational frequencies:

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			-0.00	0.00000	-	-
2			-0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a''	97.83	4.05720	YES	YES
8		a''	210.27	0.20471	YES	YES
9		a'	265.41	2.38674	YES	YES
10		a''	280.79	0.14942	YES	YES
11		a''	414.20	0.00560	YES	YES
12		a'	441.77	0.93793	YES	YES
13		a''	502.96	9.29544	YES	YES
14		a'	550.65	4.89460	YES	YES
15		a'	611.77	0.40378	YES	YES
16		a''	625.80	4.68777	YES	YES
17		a''	747.64	83.21634	YES	YES
18		a'	791.48	12.92165	YES	YES
19		a''	818.94	0.19683	YES	YES
20		a''	866.65	3.68007	YES	YES
21		a''	921.11	0.42234	YES	YES
22		a''	933.78	0.01282	YES	YES
23		a'	1000.11	0.81651	YES	YES
24		a'	1036.58	2.42733	YES	YES
25		a'	1066.20	48.45976	YES	YES
26		a'	1097.56	9.42488	YES	YES
27		a'	1172.03	1.86857	YES	YES
28		a''	1179.20	0.84470	YES	YES

29	a'	1190.77	14.23036	YES	YES
30	a'	1208.29	8.07858	YES	YES
31	a'	1279.95	212.05625	YES	YES
32	a'	1330.80	0.44517	YES	YES
33	a'	1430.08	10.82935	YES	YES
34	a'	1472.75	4.99199	YES	YES
35	a'	1477.94	14.71055	YES	YES
36	a''	1507.14	7.54304	YES	YES
37	a'	1518.84	101.91883	YES	YES
38	a'	1523.91	3.15274	YES	YES
39	a'	1617.03	23.04645	YES	YES
40	a'	1633.50	62.57026	YES	YES
41	a'	3049.76	45.63742	YES	YES
42	a''	3125.79	28.37187	YES	YES
43	a'	3193.52	16.43709	YES	YES
44	a'	3202.16	1.50593	YES	YES
45	a'	3209.55	6.78556	YES	YES
46	a'	3224.22	8.86757	YES	YES
47	a'	3232.67	10.73521	YES	YES
48	a'	3243.98	3.23162	YES	YES

exited state vibrational frequencies:

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			-0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a''	90.20	4.36789	YES	YES
8		a''	142.28	0.01302	YES	YES
9		a''	176.47	0.17960	YES	YES
10		a''	191.72	1.35114	YES	YES
11		a'	263.02	3.74374	YES	YES
12		a''	298.50	4.10279	YES	YES
13		a''	381.88	2.63098	YES	YES
14		a'	426.03	0.33503	YES	YES
15		a''	491.75	13.27519	YES	YES
16		a'	495.04	5.80713	YES	YES
17		a'	527.31	8.78635	YES	YES
18		a''	534.60	0.08942	YES	YES
19		a''	543.51	82.73364	YES	YES
20		a''	602.44	25.70548	YES	YES
21		a'	762.61	3.54405	YES	YES
22		a''	764.68	0.10500	YES	YES
23		a'	951.26	18.47233	YES	YES
24		a'	969.48	1.10796	YES	YES
25		a'	985.09	11.78547	YES	YES
26		a'	1016.39	67.36614	YES	YES
27		a'	1146.29	0.70818	YES	YES

28	a"	1156.28	1.16608	YES	YES
29	a'	1158.88	0.44368	YES	YES
30	a'	1190.81	0.40319	YES	YES
31	a'	1283.29	124.82351	YES	YES
32	a'	1295.81	25.76868	YES	YES
33	a'	1399.71	0.16292	YES	YES
34	a'	1433.77	78.93725	YES	YES
35	a'	1468.58	10.27243	YES	YES
36	a'	1481.64	19.01741	YES	YES
37	a"	1501.31	11.47902	YES	YES
38	a'	1513.82	16.84497	YES	YES
39	a'	1524.86	0.87123	YES	YES
40	a'	1608.69	203.81360	YES	YES
41	a'	3076.62	41.01468	YES	YES
42	a"	3168.63	11.36760	YES	YES
43	a'	3206.56	9.93136	YES	YES
44	a'	3211.28	9.21490	YES	YES
45	a'	3230.58	5.06770	YES	YES
46	a'	3237.06	14.16230	YES	YES
47	a'	3249.96	5.75693	YES	YES
48	a'	3264.99	1.10184	YES	YES