Absolute energies (hartees), zero point energy corrections (hartrees) and coordinates for structures **2-4**.

transition structure **2**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6		2.473573	1.747430	-0.246910
2	6		2.966064	0.842313	0.717275
3	6		3.011782	-0.552368	0.592479
4	6		2.449501	-1.394388	-0.372088
5	6		1.442436	-1.191091	-1.340714
6	6		0.430286	-0.244149	-1.438596
7	6		0.023620	0.716083	-0.464442
8	6		-0.101022	0.368305	0.981023
9	6		-1.017787	-0.447191	1.533555
10	6		-2.057931	-1.264039	0.898590
11	6		-3.023676	-0.969375	-0.001847
12	6		-3.447347	0.299231	-0.595181
13	6		-3.220730	1.546934	-0.152499
14	1		2.619592	2.809443	-0.050426
15	1		2.608191	1.470831	-1.295401
16	1		3.335392	1.254778	1.655910
17	1		3.616089	-1.062329	1.343536
18	1		2.882136	-2.396036	-0.392964
19	1		1.442575	-1.934695	-2.139372
20	1		-0.077233	-0.192941	-2.401763
21	1		-0.790587	1.362355	-0.810434
22	1		0.627362	0.821906	1.656705
23	1		-0.919055	-0.621783	2.607544
24	1		-2.059916	-2.295939	1.256696
25	1		-3.626805	-1.817547	-0.326648
26	1		-4.074909	0.186493	-1.480303
27	1		-2.643477	1.746165	0.745054
28	1		-3.639631	2.405659	-0.669750
29	1		1.127663	1.517468	-0.362250

NImag = 1 @ -1268.8681 cm^{-1}

E = -504.849984

Zero-point correction = 0.245340

transition structure **3**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6		-1.310647	0.399591	-0.268415
2	6		-1.249644	-0.659189	-1.221945
3	6		-0.757752	-1.950453	-1.039260
4	6		-0.001904	-2.518290	-0.000554
5	6		0.754671	-1.952211	1.038622
6	6		1.248613	-0.661879	1.222071
7	6		1.311628	0.397317	0.269085
8	6		1.738556	0.159829	-1.141755
9	6		2.959415	-0.224934	-1.556031
10	6		4.147971	-0.592457	-0.778291
11	6		4.809172	0.033710	0.222051
12	6		4.632288	1.353873	0.828083
13	6		3.994016	2.425253	0.329203
14	6		-1.737739	0.162163	1.142465
15	6		-2.958390	-0.223415	1.556601
16	6		-4.146551	-0.592068	0.778815
17	6		-4.807889	0.033245	-0.221965
18	6		-4.631486	1.353170	-0.828705
19	6		-3.994335	2.425289	-0.330003
20	1		-1.731749	1.323968	-0.679481
21	1		-1.601825	-0.422957	-2.225942
22	1		-1.011064	-2.648377	-1.838737
23	1		-0.002709	-3.609549	-0.000902
24	1		1.006698	-2.650981	1.837769
25	1		1.600885	-0.426713	2.226287
26	1		1.734271	1.320716	0.680726
27	1		0.983373	0.319663	-1.914042
28	1		3.069578	-0.394850	-2.629693
29	1		4.590966	-1.535543	-1.105952
30	1		5.649597	-0.521332	0.639439
31	1		5.142823	1.474018	1.784601
32	1		3.497717	2.405678	-0.636066
33	1		3.981630	3.367260	0.870440
34	1		-0.982947	0.323150	1.914876
35	1		-3.068649	-0.392960	2.630313
36	1		-4.589068	-1.535259	1.106815
37	1		-5.647950	-0.522445	-0.639229
38	1		-5.141401	1.472362	-1.785674
39	1		-3.982212	3.366988	-0.871783
40	1		-3.498703	2.406613	0.635627
41	1		0.000771	0.669277	0.000185

NImag = 1 @ -1190.8557 cm^{-1}

E = -737.0281839

Zero-point correction = 0.345525

structure **4**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6		1.786482	0.364299	1.807793
2	6		1.589851	-0.939558	1.434028
3	6		1.311329	-1.601281	0.182502
4	6		0.687937	-1.219135	-0.965899
5	6		-0.078101	-0.039629	-1.341020
6	6		-0.978770	0.690552	-0.652337
7	6		-1.458075	0.512205	0.768617
8	6		-1.972492	-0.856208	1.148364
9	6		-2.929219	-1.583508	0.541431
10	6		-3.692335	-1.319947	-0.682459
11	6		-4.389215	-0.241913	-1.112327
12	6		-4.721409	1.024755	-0.461376
13	6		-4.715764	1.316363	0.850207
14	6		1.945909	1.607371	1.100806
15	6		2.348967	1.962129	-0.159355
16	6		2.871188	1.267554	-1.312065
17	6		3.619540	0.141951	-1.502023
18	6		4.331755	-0.738125	-0.590938
19	6		4.669903	-0.512128	0.690937
20	1		1.662889	-1.645223	2.264040
21	1		1.664604	-2.633690	0.176375
22	1		0.748229	-1.951932	-1.773413
23	1		0.034702	0.226293	-2.393320
24	1		-1.443936	1.510915	-1.196524
25	1		-2.257437	1.247037	0.946298
26	1		-1.511828	-1.300705	2.029227
27	1		-3.099357	-2.582922	0.948301
28	1		-3.722708	-2.181889	-1.352897
29	1		-4.814501	-0.335357	-2.111914
30	1		-5.069678	1.798610	-1.146903
31	1		-4.429527	0.587771	1.602357
32	1		-5.034535	2.292475	1.205137
33	1		1.711396	2.465957	1.732662
34	1		2.227728	3.028556	-0.359310
35	1		2.645362	1.800689	-2.237193
36	1		3.783275	-0.111265	-2.550088
37	1		4.673376	-1.668065	-1.046639
38	1		5.255323	-1.238603	1.247720
39	1		4.409703	0.405296	1.204335
40	1		-0.639312	0.770070	1.452653
41	1		1.841358	0.501498	2.889787

NImag = 0

E = -737.0577054

Zero-point correction = 0.350450