1, 298 K, dichloromethane, B3LYP/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.085363	0.862245	0.000001
2	6	0	4.198968	-1.842783	0.000002
3	6	0	6.003379	-0.196414	0.000002
4	6	0	3.727579	0.545995	-0.000000
5	6	0	3.290362	-0.785731	0.000000
6	6	0	5.565449	-1.532035	0.000002
7	6	0	1.791156	-0.830053	-0.000001
8	6	0	1.326429	0.573824	-0.000002
9	6	0	2.533542	1.444162	-0.000001
10	8	0	2.562770	2.672958	-0.000002
11	8	0	1.137985	-1.873927	-0.000001
12	6	0	0.079484	1.166345	-0.000001
13	6	0	-1.268886	0.689465	-0.000001
14	6	0	-4.039287	-0.060586	0.000000
15	6	0	-1.667751	-0.676112	-0.000002
16	6	0	-2.310539	1.659318	0.000000
17	6	0	-3.646236	1.311451	0.000001
18	6	0	-2.999626	-1.040464	-0.000002
19	7	0	-5.351733	-0.420606	0.000001
20	6	0	-6.398607	0.597536	0.000005
21	6	0	-5.734614	-1.830080	-0.000002
22	1	0	5.419985	1.898985	0.000000
23	1	0	3.855021	-2.876394	0.000002
24	1	0	7.072936	0.014923	0.000003
25	1	0	6.302724	-2.335248	0.000004
26	1	0	0.153059	2.259425	-0.000001
27	1	0	-0.898821	-1.445007	-0.000003
28	1	0	-2.044603	2.717203	0.000001
29	1	0	-4.394206	2.098879	0.000002
30	1	0	-3.247952	-2.098137	-0.000002
31	1	0	-6.335503	1.236690	-0.893116
32	1	0	-7.372859	0.103908	0.000008
33	1	0	-6.335497	1.236689	0.893126
34	1	0	-5.355323	-2.347968	-0.893172
35	1	0	-5.355325	-2.347972	0.893166
36	1	0	-6.824526	-1.900481	-0.000004

TSA2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.086985	0.510572	0.000008
2	6	0	-3.788560	-2.025368	-0.000046
3	6	0	-5.825378	-0.676402	-0.000017
4	6	0	-3.693717	0.412297	0.000006
5	6	0	-3.052564	-0.838683	-0.000021
6	6	0	-5.183436	-1.929819	-0.000044
7	6	0	-1.569393	-0.656575	-0.000017
8	6	0	-1.331481	0.823777	0.000016
9	6	0	-2.672896	1.497508	0.000030
10	8	0	-2.887534	2.701505	0.000056

11	8	0	-0.738859	-1.552664	-0.000037
12	6	0	-0.168871	1.505769	0.000033
13	6	0	1.202940	0.942144	0.000022
14	6	0	3.875444	-0.077138	0.000001
15	6	0	1.884922	0.695907	1.200837
16	6	0	1.884924	0.695959	-1.200803
17	6	0	3.188386	0.200723	-1.208240
18	6	0	3.188384	0.200671	1.208254
19	7	0	5.154273	-0.610781	-0.000010
20	6	0	5.905180	-0.661502	-1.246308
21	6	0	5.905177	-0.661565	1.246288
22	1	0	-5.578823	1.482325	0.000029
23	1	0	-3.288187	-2.992775	-0.000066
24	1	0	-6.914677	-0.636030	-0.000016
25	1	0	-5.787691	-2.837082	-0.000063
26	1	0	-0.264300	2.598589	0.000058
27	1	0	1.391994	0.891466	2.153636
28	1	0	1.391997	0.891559	-2.153594
29	1	0	3.666706	0.029690	-2.168766
30	1	0	3.666703	0.029596	2.168773
31	1	0	6.086759	0.340975	-1.674395
32	1	0	6.872302	-1.136862	-1.058655
33	1	0	5.378474	-1.265113	-1.997900
34	1	0	6.086764	0.340892	1.674421
35	1	0	5.378463	-1.265204	1.997851
36	1	0	6.872294	-1.136925	1.058616

TSA1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.080572	0.464298	0.000024
2	6	0	3.740011	-2.049611	-0.000086
3	6	0	5.799030	-0.734844	-0.000018
4	6	0	3.685845	0.389325	0.000011
5	6	0	3.023935	-0.850793	-0.000044
6	6	0	5.136283	-1.977378	-0.000073
7	6	0	1.544022	-0.644166	-0.000046
8	6	0	1.330640	0.839916	0.000019
9	6	0	2.683110	1.491292	0.000050
10	8	0	2.917448	2.691588	0.000098
11	8	0	0.698976	-1.526644	-0.000093
12	6	0	0.180047	1.542029	0.000055
13	6	0	-1.201962	1.004000	0.000038
14	6	0	-3.897889	0.047632	0.000012
15	6	0	-1.885437	0.761877	1.200813
16	6	0	-1.885450	0.761979	-1.200750
17	6	0	-3.196879	0.288219	-1.208092
18	6	0	-3.196865	0.288116	1.208128
19	7	0	-5.215444	-0.383314	0.000001
20	6	0	-5.813006	-0.843472	-1.245661
21	6	0	-5.812985	-0.843592	1.245629
22	1	0	5.588733	1.427612	0.000066
23	1	0	3.223521	-3.008519	-0.000128
24	1	0	6.888843	-0.712604	-0.000009
25	1	0	5.725309	-2.894598	-0.000104
26	1	0	0.295049	2.632973	0.000104
27	1	0	-1.384038	0.934386	2.153629
28	1	0	-1.384061	0.934569	-2.153558

29	1	0	-3.670571	0.105303	-2.168702
30	1	0	-3.670548	0.105119	2.168728
31	1	0	-5.293060	-1.722612	-1.667314
32	1	0	-6.856017	-1.115470	-1.059241
33	1	0	-5.807794	-0.046470	-2.001487
34	1	0	-5.293019	-1.722761	1.667198
35	1	0	-5.807779	-0.046658	2.001526
36	1	0	-6.855993	-1.115594	1.059196

TSD2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.069810	0.924974	0.000006
2	6	0	4.252256	-1.803777	-0.000058
3	6	0	6.012164	-0.109383	-0.000021
4	6	0	3.719121	0.574067	-0.000000
5	6	0	3.315831	-0.769368	-0.000032
6	6	0	5.608068	-1.457390	-0.000052
7	6	0	1.823184	-0.860281	-0.000031
8	6	0	1.314247	0.540507	0.000004
9	6	0	2.510500	1.444756	0.000023
10	8	0	2.501598	2.669777	0.000053
11	8	0	1.195913	-1.914762	-0.000057
12	6	0	0.067667	1.100581	0.000024
13	6	0	-1.287418	0.581422	0.000016
14	6	0	-4.004223	-0.226058	0.000010
15	6	0	-2.336329	1.533983	0.000050
16	6	0	-1.634743	-0.789464	-0.000022
17	6	0	-2.972479	-1.177067	-0.000025
18	6	0	-3.669850	1.139808	0.000048
19	7	0	-5.369232	-0.686161	0.000006
20	6	0	-6.098347	-0.308747	1.215633
21	6	0	-6.098360	-0.308686	-1.215593
22	1	0	5.377401	1.969814	0.000030
23	1	0	3.934835	-2.845628	-0.000082
24	1	0	7.076049	0.128157	-0.000017
25	1	0	6.366188	-2.240719	-0.000072
26	1	0	0.110650	2.195027	0.000052
27	1	0	-2.090494	2.596455	0.000079
28	1	0	-0.846140	-1.537094	-0.000048
29	1	0	-3.239703	-2.233162	-0.000054
30	1	0	-4.453952	1.896132	0.000075
31	1	0	-5.535692	-0.634541	2.098665
32	1	0	-6.282120	0.780659	1.297407
33	1	0	-7.070615	-0.818855	1.216979
34	1	0	-5.535715	-0.634438	-2.098648
35	1	0	-7.070629	-0.818791	-1.216954
36	1	0	-6.282132	0.780724	-1.297312

TSD1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.081514	0.774361	0.000000
2	6	0	4.114741	-1.905101	0.000001

3	6	0	5.965411	-0.310373	0.000001
4	6	0	3.713553	0.498438	-0.000000
5	6	0	3.236731	-0.820691	0.000000
6	6	0	5.487592	-1.634052	0.000002
7	6	0	1.741332	-0.829163	-0.000001
8	6	0	1.310487	0.597565	-0.000002
9	6	0	2.554800	1.434435	-0.000001
10	8	0	2.613427	2.658062	-0.000002
11	8	0	1.056868	-1.847539	-0.000001
12	6	0	0.096990	1.226130	-0.000001
13	6	0	-1.285032	0.783900	-0.000000
14	6	0	-4.043161	0.131220	0.000001
15	6	0	-2.278073	1.792657	0.000005
16	6	0	-1.708773	-0.566677	-0.000005
17	6	0	-3.064328	-0.880385	-0.000004
18	6	0	-3.632581	1.471507	0.000006
19	7	0	-5.454159	-0.158647	0.000002
20	6	0	-5.894205	-0.851727	-1.215727
21	6	0	-5.894201	-0.851739	1.215726
22	1	0	5.446193	1.800685	-0.000001
23	1	0	3.740307	-2.927817	0.000002
24	1	0	7.040761	-0.131824	0.000001
25	1	0	6.201369	-2.458005	0.000002
26	1	0	0.200919	2.316516	0.000000
27	1	0	-1.974655	2.839903	0.000008
28	1	0	-0.961882	-1.356166	-0.000008
29	1	0	-3.366939	-1.927192	-0.000008
30	1	0	-4.390609	2.253598	0.000011
31	1	0	-5.569642	-0.288308	-2.098741
32	1	0	-5.506843	-1.886367	-1.296344
33	1	0	-6.991268	-0.897892	-1.218451
34	1	0	-5.569634	-0.288330	2.098744
35	1	0	-6.991264	-0.897903	1.218454
36	1	0	-5.506840	-1.886380	1.296330

TSDA

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.063314	-0.514992	-0.094931
2	6	0	3.758447	2.014360	0.042672
3	6	0	5.797943	0.673922	-0.068063
4	6	0	3.670311	-0.422218	-0.052113
5	6	0	3.025951	0.825767	0.015862
6	6	0	5.152900	1.923980	-0.000055
7	6	0	1.544824	0.638509	0.049432
8	6	0	1.311130	-0.841800	-0.002520
9	6	0	2.653904	-1.510887	-0.067421
10	8	0	2.869207	-2.713020	-0.122171
11	8	0	0.708872	1.527466	0.106915
12	6	0	0.150706	-1.524617	0.002210
13	6	0	-1.221096	-0.960289	0.064404
14	6	0	-3.861912	0.034748	0.179290
15	6	0	-1.853832	-0.760322	1.299867
16	6	0	-1.925132	-0.670358	-1.115044
17	6	0	-3.229687	-0.174911	-1.056188
18	6	0	-3.160121	-0.264551	1.352412
19	7	0	-5.208001	0.545902	0.284247
20	6	0	-6.210853	-0.355987	-0.288270

21	6	0	-5.344631	1.911183	-0.230406
22	1	0	5.557626	-1.484007	-0.147648
23	1	0	3.255784	2.979105	0.095212
24	1	0	6.886889	0.637825	-0.100065
25	1	0	5.754538	2.832727	0.019310
26	1	0	0.237238	-2.616293	-0.045334
27	1	0	-1.323755	-0.985678	2.225200
28	1	0	-1.448829	-0.825775	-2.083219
29	1	0	-3.754256	0.050120	-1.984710
30	1	0	-3.648614	-0.102825	2.312935
31	1	0	-6.095414	-1.357262	0.144030
32	1	0	-7.212517	0.017146	-0.035458
33	1	0	-6.146655	-0.441047	-1.391568
34	1	0	-6.343786	2.290112	0.023688
35	1	0	-4.597518	2.559486	0.242911
36	1	0	-5.222344	1.980264	-1.329803

1, 298 K, dichloromethane, B3LYP/aug-cc-pVTZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.061621	0.863081	-0.000059
2	6	0	4.190975	-1.828416	-0.002401
3	6	0	5.978926	-0.185551	-0.001704
4	6	0	3.712739	0.544685	0.000361
5	6	0	3.283024	-0.781522	-0.000749
6	6	0	5.548633	-1.514986	-0.002886
7	6	0	1.788794	-0.832024	0.000052
8	6	0	1.321159	0.564385	0.001430
9	6	0	2.520202	1.436365	0.001761
10	8	0	2.545609	2.658781	0.002898
11	8	0	1.141958	-1.872275	-0.000498
12	6	0	0.080104	1.148799	0.001683
13	6	0	-1.262436	0.675205	0.001430
14	6	0	-4.023830	-0.058961	0.000142
15	6	0	-1.666688	-0.681093	0.002404
16	6	0	-2.295794	1.643525	0.000107
17	6	0	-3.624914	1.303856	-0.000724
18	6	0	-2.992158	-1.036910	0.002025
19	7	0	-5.332981	-0.412210	-0.000840
20	6	0	-6.375052	0.606912	-0.008415
21	6	0	-5.723017	-1.816895	0.005455
22	1	0	5.389920	1.893214	0.000835
23	1	0	3.853334	-2.855505	-0.003315
24	1	0	7.038960	0.028459	-0.002099
25	1	0	6.282598	-2.309259	-0.004199
26	1	0	0.150162	2.234374	0.001949
27	1	0	-0.908733	-1.448899	0.003204
28	1	0	-2.026851	2.692198	-0.000194
29	1	0	-4.365037	2.087653	-0.001359
30	1	0	-3.244828	-2.085275	0.002408
31	1	0	-6.303996	1.243353	-0.892951
32	1	0	-7.344511	0.120755	-0.017746
33	1	0	-6.319632	1.241776	0.878546
34	1	0	-5.354785	-2.337795	-0.880889

35	1	0	-5.344361	-2.331990	0.890629
36	1	0	-6.805625	-1.882361	0.012385

TSA2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.065029	0.511197	0.000008
2	6	0	-3.780572	-2.011899	-0.000046
3	6	0	-5.802553	-0.666799	-0.000017
4	6	0	-3.679987	0.411376	0.000006
5	6	0	-3.045302	-0.834301	-0.000021
6	6	0	-5.167201	-1.914413	-0.000044
7	6	0	-1.566456	-0.657834	-0.000017
8	6	0	-1.326244	0.817057	0.000016
9	6	0	-2.661408	1.491384	0.000030
10	8	0	-2.873129	2.689277	0.000056
11	8	0	-0.742801	-1.551434	-0.000036
12	6	0	-0.169907	1.491437	0.000033
13	6	0	1.197831	0.930625	0.000021
14	6	0	3.860219	-0.077204	0.000001
15	6	0	1.877723	0.687435	1.193552
16	6	0	1.877724	0.687485	-1.193518
17	6	0	3.174945	0.198777	-1.201170
18	6	0	3.174943	0.198726	1.201183
19	7	0	5.137500	-0.602709	-0.000010
20	6	0	5.888797	-0.654034	-1.242546
21	6	0	5.888793	-0.654097	1.242526
22	1	0	-5.550824	1.476792	0.000028
23	1	0	-3.286120	-2.973138	-0.000066
24	1	0	-6.882933	-0.623861	-0.000017
25	1	0	-5.768301	-2.813191	-0.000062
26	1	0	-0.260225	2.576801	0.000058
27	1	0	1.388228	0.879665	2.139382
28	1	0	1.388230	0.879756	-2.139341
29	1	0	3.651251	0.029434	-2.153805
30	1	0	3.651249	0.029342	2.153812
31	1	0	6.076660	0.341193	-1.664221
32	1	0	6.846354	-1.131949	-1.056721
33	1	0	5.365238	-1.246569	-1.993628
34	1	0	6.076665	0.341110	1.664246
35	1	0	5.365227	-1.246660	1.993580
36	1	0	6.846346	-1.132014	1.056683

TSA1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.058864	0.465333	0.000022
2	6	0	3.732892	-2.036185	-0.000087
3	6	0	5.776796	-0.724698	-0.000021
4	6	0	3.672351	0.388448	0.000011
5	6	0	3.017207	-0.846572	-0.000043
6	6	0	5.120938	-1.961651	-0.000074
7	6	0	1.541484	-0.645915	-0.000044
8	6	0	1.325429	0.832735	0.000020

9	6	0	2.671602	1.484998	0.000050
10	8	0	2.902778	2.679265	0.000099
11	8	0	0.703591	-1.526237	-0.000089
12	6	0	0.180979	1.527171	0.000055
13	6	0	-1.197065	0.992256	0.000038
14	6	0	-3.883592	0.050008	0.000011
15	6	0	-1.878605	0.753723	1.193550
16	6	0	-1.878617	0.753824	-1.193487
17	6	0	-3.183726	0.286577	-1.201048
18	6	0	-3.183715	0.286475	1.201084
19	7	0	-5.196893	-0.379156	0.000000
20	6	0	-5.797810	-0.835340	-1.241990
21	6	0	-5.797791	-0.835458	1.241957
22	1	0	5.560710	1.422679	0.000064
23	1	0	3.222577	-2.989111	-0.000128
24	1	0	6.857731	-0.699574	-0.000013
25	1	0	5.707106	-2.870236	-0.000106
26	1	0	0.290881	2.610722	0.000105
27	1	0	-1.380754	0.922994	2.139391
28	1	0	-1.380774	0.923173	-2.139319
29	1	0	-3.655660	0.105801	-2.153737
30	1	0	-3.655640	0.105620	2.153762
31	1	0	-5.291548	-1.715067	-1.658139
32	1	0	-6.836311	-1.094712	-1.057173
33	1	0	-5.784480	-0.048282	-1.996717
34	1	0	-5.291511	-1.715213	1.658023
35	1	0	-5.784467	-0.048466	1.996752
36	1	0	-6.836289	-1.094832	1.057127

TSD2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.058741	0.775640	-0.000001
2	6	0	-4.107925	-1.890726	0.000004
3	6	0	-5.942148	-0.299068	0.000001
4	6	0	-3.699552	0.497391	-0.000001
5	6	0	-3.230280	-0.816403	0.000002
6	6	0	-5.472009	-1.616815	0.000003
7	6	0	-1.739776	-0.831269	0.000001
8	6	0	-1.305700	0.588332	-0.000001
9	6	0	-2.542387	1.427051	-0.000003
10	8	0	-2.597347	2.644379	-0.000005
11	8	0	-1.061765	-1.846256	0.000003
12	6	0	-0.098073	1.208596	-0.000002
13	6	0	1.278345	0.769084	-0.000002
14	6	0	4.026405	0.131140	-0.000000
15	6	0	2.263315	1.775533	-0.000004
16	6	0	1.706944	-0.572079	0.000001
17	6	0	3.055870	-0.877991	0.000001
18	6	0	3.611177	1.461981	-0.000003
19	7	0	5.434286	-0.152916	0.000000
20	6	0	5.882168	-0.838055	1.213711
21	6	0	5.882168	-0.838060	-1.213708
22	1	0	-5.416957	1.795527	-0.000003
23	1	0	-3.739918	-2.907088	0.000005
24	1	0	-7.008093	-0.117693	0.000001
25	1	0	-6.182726	-2.431756	0.000005
26	1	0	-0.198017	2.291596	-0.000004

27	1	0	1.957412	2.813450	-0.000005
28	1	0	0.970411	-1.359641	0.000002
29	1	0	3.360609	-1.915796	0.000003
30	1	0	4.359591	2.241882	-0.000005
31	1	0	5.564493	-0.277156	2.091325
32	1	0	5.500000	-1.865471	1.300926
33	1	0	6.971400	-0.882740	1.210955
34	1	0	5.564494	-0.277164	-2.091324
35	1	0	6.971400	-0.882745	-1.210952
36	1	0	5.500001	-1.865476	-1.300919

TSD1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.046240	0.924890	0.000006
2	6	0	4.243451	-1.789756	-0.000055
3	6	0	5.987394	-0.099629	-0.000019
4	6	0	3.704391	0.572344	-0.000001
5	6	0	3.308095	-0.765274	-0.000031
6	6	0	5.590406	-1.441217	-0.000049
7	6	0	1.820648	-0.862017	-0.000031
8	6	0	1.309190	0.531585	0.000003
9	6	0	2.497880	1.437000	0.000021
10	8	0	2.485833	2.655532	0.000050
11	8	0	1.199371	-1.912600	-0.000056
12	6	0	0.069114	1.084078	0.000021
13	6	0	-1.280696	0.568487	0.000014
14	6	0	-3.988741	-0.222028	0.000010
15	6	0	-2.320884	1.519874	0.000051
16	6	0	-1.634162	-0.793004	-0.000025
17	6	0	-2.965937	-1.171596	-0.000028
18	6	0	-3.648480	1.134555	0.000049
19	7	0	-5.351957	-0.674046	0.000007
20	6	0	-6.080613	-0.301838	1.213791
21	6	0	-6.080627	-0.301776	-1.213748
22	1	0	5.347848	1.962930	0.000029
23	1	0	3.931971	-2.824871	-0.000078
24	1	0	7.041770	0.140051	-0.000014
25	1	0	6.344842	-2.215844	-0.000067
26	1	0	0.108935	2.170923	0.000049
27	1	0	-2.071388	2.573002	0.000081
28	1	0	-0.856342	-1.539669	-0.000053
29	1	0	-3.235187	-2.218773	-0.000058
30	1	0	-4.423291	1.888808	0.000078
31	1	0	-5.527376	-0.633301	2.091171
32	1	0	-6.256827	0.780086	1.302560
33	1	0	-7.049328	-0.801785	1.210026
34	1	0	-5.527402	-0.633195	-2.091153
35	1	0	-7.049344	-0.801721	-1.209997
36	1	0	-6.256840	0.780153	-1.302460

TSDA

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	5.042074	-0.515858	-0.093822
2	6	0	3.751583	2.001013	0.041037
3	6	0	5.776036	0.663993	-0.068074
4	6	0	3.657306	-0.421288	-0.051316
5	6	0	3.019611	0.821588	0.015356
6	6	0	5.137788	1.908426	-0.001390
7	6	0	1.542771	0.640282	0.048756
8	6	0	1.306467	-0.834588	-0.001973
9	6	0	2.642933	-1.504562	-0.065826
10	8	0	2.855095	-2.700682	-0.119167
11	8	0	0.713845	1.527000	0.104981
12	6	0	0.152195	-1.509549	0.002957
13	6	0	-1.215633	-0.948137	0.064147
14	6	0	-3.847068	0.033314	0.176900
15	6	0	-1.846865	-0.749733	1.291856
16	6	0	-1.917556	-0.663160	-1.108592
17	6	0	-3.216233	-0.174716	-1.050959
18	6	0	-3.147179	-0.260843	1.343409
19	7	0	-5.191327	0.538348	0.280133
20	6	0	-6.193150	-0.364015	-0.285430
21	6	0	-5.336169	1.902388	-0.226650
22	1	0	5.530243	-1.478831	-0.145427
23	1	0	3.254979	2.959724	0.092446
24	1	0	6.856073	0.625110	-0.099871
25	1	0	5.736439	2.808607	0.017114
26	1	0	0.233739	-2.593832	-0.043432
27	1	0	-1.320208	-0.970659	2.210413
28	1	0	-1.444434	-0.817023	-2.069249
29	1	0	-3.737670	0.046057	-1.972737
30	1	0	-3.632159	-0.101110	2.296712
31	1	0	-6.081122	-1.356605	0.148414
32	1	0	-7.187664	0.008502	-0.037660
33	1	0	-6.129668	-0.455904	-1.380115
34	1	0	-6.332495	2.269901	0.021312
35	1	0	-4.602644	2.551409	0.249249
36	1	0	-5.209100	1.978347	-1.316924

2, 298 K, dichloromethane, B3LYP/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.696023	-0.405126	-0.236178
2	6	0	3.361632	-2.900824	-0.023084
3	6	0	5.404685	-1.613395	-0.282159
4	6	0	3.303361	-0.450391	-0.088253
5	6	0	2.661834	-1.699224	0.010948
6	6	0	4.752521	-2.849819	-0.173852
7	6	0	1.194936	-1.499424	0.141129
8	6	0	0.958004	-0.032624	0.058264
9	6	0	2.270130	0.613971	0.009479
10	6	0	2.556672	1.971097	0.114200
11	8	0	0.381236	-2.411204	0.265171
12	6	0	-0.240928	0.653068	-0.115053
13	6	0	-1.625165	0.309392	-0.084887
14	6	0	-4.469420	-0.104163	-0.060058

15	6	0	-2.193975	-0.939155	0.302290
16	6	0	-2.545359	1.340975	-0.443678
17	6	0	-3.909846	1.153972	-0.441321
18	6	0	-3.557886	-1.139128	0.317832
19	7	0	-5.811308	-0.306502	-0.051582
20	6	0	-6.366948	-1.598348	0.348152
21	6	0	-6.726352	0.768281	-0.431669
22	6	0	1.592772	2.988615	0.397840
23	6	0	3.875428	2.510760	0.005422
24	7	0	0.870167	3.867019	0.653637
25	7	0	4.923106	3.014227	-0.081619
26	1	0	5.240225	0.529361	-0.324138
27	1	0	2.833072	-3.849492	0.062853
28	1	0	6.487206	-1.587094	-0.404735
29	1	0	5.332823	-3.771727	-0.208490
30	1	0	-0.108775	1.706118	-0.358459
31	1	0	-1.532018	-1.751076	0.585550
32	1	0	-2.153718	2.317043	-0.732047
33	1	0	-4.553754	1.979809	-0.728589
34	1	0	-3.935085	-2.109177	0.628719
35	1	0	-6.010176	-2.404861	-0.308177
36	1	0	-7.455449	-1.552233	0.275141
37	1	0	-6.099485	-1.843940	1.386065
38	1	0	-6.624999	1.634015	0.238773
39	1	0	-6.544245	1.099013	-1.464266
40	1	0	-7.751978	0.399615	-0.364820

TSA1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.503958	-0.937899	-0.000007
2	6	0	2.647383	-3.087450	0.000011
3	6	0	4.934120	-2.267449	-0.000004
4	6	0	3.123257	-0.677260	-0.000001
5	6	0	2.219573	-1.761338	0.000007
6	6	0	4.021523	-3.336112	0.000005
7	6	0	0.827075	-1.258796	0.000011
8	6	0	0.922594	0.246638	0.000001
9	6	0	2.365598	0.593320	-0.000002
10	6	0	2.921178	1.855953	-0.000002
11	8	0	-0.185713	-1.938285	0.000019
12	6	0	-0.139877	1.086283	-0.000008
13	6	0	-1.573908	0.702168	-0.000006
14	6	0	-4.370383	0.107441	-0.000003
15	6	0	-2.282536	0.554412	1.201003
16	6	0	-2.282533	0.554386	-1.201013
17	6	0	-3.644271	0.255659	-1.208233
18	6	0	-3.644274	0.255685	1.208226
19	7	0	-5.732040	-0.149227	-0.000002
20	6	0	-6.386081	-0.522807	-1.246266
21	6	0	-6.386086	-0.522774	1.246268
22	6	0	2.167263	3.073212	0.000000
23	6	0	4.331854	2.102631	-0.000004
24	7	0	1.618592	4.100200	0.000002
25	7	0	5.465463	2.367162	-0.000005
26	1	0	5.243252	-0.143953	-0.000014
27	1	0	1.921328	-3.899299	0.000017
28	1	0	6.003260	-2.477609	-0.000009

29	1	0	4.392151	-4.360875	0.000007
30	1	0	0.050745	2.159737	-0.000018
31	1	0	-1.763562	0.662971	2.153774
32	1	0	-1.763556	0.662925	-2.153786
33	1	0	-4.138338	0.138649	-2.168796
34	1	0	-4.138344	0.138696	2.168790
35	1	0	-5.983674	-1.459192	-1.673058
36	1	0	-6.280382	0.270557	-1.998654
37	1	0	-7.454889	-0.660086	-1.058478
38	1	0	-5.983687	-1.459151	1.673083
39	1	0	-6.280384	0.270607	1.998638
40	1	0	-7.454894	-0.660051	1.058481

TSA2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.525271	-0.888074	0.078810
2	6	0	2.711440	-3.067143	-0.094109
3	6	0	4.979378	-2.209502	0.058712
4	6	0	3.142026	-0.650946	0.013039
5	6	0	2.259541	-1.749305	-0.070115
6	6	0	4.088063	-3.292497	-0.028154
7	6	0	0.859406	-1.270377	-0.119040
8	6	0	0.926183	0.233722	-0.025462
9	6	0	2.362082	0.605868	0.011299
10	6	0	2.893863	1.878605	0.018344
11	8	0	-0.138824	-1.964536	-0.214400
12	6	0	-0.151483	1.049617	0.055129
13	6	0	-1.577169	0.636221	0.039179
14	6	0	-4.356275	-0.034527	0.020764
15	6	0	-2.264854	0.367736	1.231478
16	6	0	-2.303608	0.593633	-1.159607
17	6	0	-3.659053	0.268111	-1.175762
18	6	0	-3.620118	0.040468	1.229857
19	7	0	-5.692584	-0.398919	0.007714
20	6	0	-6.423716	-0.473582	1.264530
21	6	0	-6.462947	-0.241344	-1.217667
22	6	0	2.116497	3.080488	-0.018129
23	6	0	4.299389	2.151341	0.050014
24	7	0	1.547138	4.095638	-0.050040
25	7	0	5.427830	2.435854	0.076668
26	1	0	5.248316	-0.082085	0.147349
27	1	0	2.001680	-3.890593	-0.160641
28	1	0	6.050553	-2.401823	0.111836
29	1	0	4.477120	-4.310294	-0.042804
30	1	0	0.019171	2.122423	0.149642
31	1	0	-1.736351	0.411845	2.184240
32	1	0	-1.805750	0.816812	-2.103704
33	1	0	-4.170868	0.251565	-2.134081
34	1	0	-4.100935	-0.157352	2.183937
35	1	0	-6.465015	0.497488	1.790151
36	1	0	-5.969107	-1.210630	1.940475
37	1	0	-7.447763	-0.799075	1.060202
38	1	0	-6.519916	0.810465	-1.551489
39	1	0	-6.030388	-0.837102	-2.032979
40	1	0	-7.480339	-0.604446	-1.046000

TSD1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.633869	-0.554474	0.305769
2	6	0	-3.181875	-2.964720	-0.085098
3	6	0	-5.273256	-1.798868	0.330525
4	6	0	-3.248599	-0.518393	0.088706
5	6	0	-2.546301	-1.725931	-0.097211
6	6	0	-4.562497	-2.993592	0.133486
7	6	0	-1.101536	-1.448840	-0.287821
8	6	0	-0.932948	0.030981	-0.107264
9	6	0	-2.289225	0.604110	-0.008471
10	6	0	-2.633264	1.941286	-0.090713
11	8	0	-0.248415	-2.296089	-0.514616
12	6	0	0.210434	0.744320	0.157849
13	6	0	1.628531	0.436833	0.138059
14	6	0	4.442709	0.085568	0.181241
15	6	0	2.229798	-0.677021	-0.496450
16	6	0	2.479634	1.377429	0.770959
17	6	0	3.858485	1.197716	0.803899
18	6	0	3.610866	-0.840955	-0.474690
19	7	0	5.874218	-0.059703	0.227702
20	6	0	6.499210	0.020948	-1.097386
21	6	0	6.301172	-1.255211	0.963531
22	6	0	-1.707459	2.997616	-0.368611
23	6	0	-3.976624	2.417842	0.034206
24	7	0	-1.014332	3.900142	-0.617075
25	7	0	-5.048229	2.862368	0.135005
26	1	0	-5.218981	0.345574	0.464726
27	1	0	-2.610454	-3.879115	-0.238905
28	1	0	-6.347797	-1.838458	0.506951
29	1	0	-5.092393	-3.945619	0.153240
30	1	0	0.034921	1.764060	0.498765
31	1	0	1.605481	-1.406829	-1.000110
32	1	0	2.044016	2.256986	1.245395
33	1	0	4.502184	1.921044	1.302379
34	1	0	4.049767	-1.702406	-0.977194
35	1	0	6.259653	-0.841996	-1.749051
36	1	0	7.589143	0.060176	-0.971065
37	1	0	6.176235	0.939511	-1.601671
38	1	0	7.391069	-1.219707	1.091284
39	1	0	5.836591	-1.261831	1.956808
40	1	0	6.045958	-2.202192	0.448847

TSD2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.667524	-0.392105	0.370975
2	6	0	-3.366675	-2.878741	-0.070479
3	6	0	-5.375855	-1.598239	0.408197
4	6	0	-3.288921	-0.433529	0.115601
5	6	0	-2.662155	-1.677996	-0.095014
6	6	0	-4.740131	-2.830326	0.186394
7	6	0	-1.209912	-1.482347	-0.325329

8	6	0	-0.951810	-0.015891	-0.142508
9	6	0	-2.270012	0.633122	-0.003459
10	6	0	-2.539942	1.988162	-0.069543
11	8	0	-0.413663	-2.375174	-0.582014
12	6	0	0.237665	0.630131	0.090757
13	6	0	1.635178	0.243366	0.031437
14	6	0	4.425955	-0.262990	-0.005660
15	6	0	2.155391	-0.904767	-0.610758
16	6	0	2.555702	1.140305	0.632928
17	6	0	3.921764	0.887311	0.627624
18	6	0	3.527208	-1.143036	-0.627002
19	7	0	5.832621	-0.565942	-0.048823
20	6	0	6.400730	-0.820034	1.279835
21	6	0	6.608840	0.430257	-0.795737
22	6	0	-1.563980	2.993027	-0.366036
23	6	0	-3.850425	2.538839	0.094143
24	7	0	-0.828162	3.857397	-0.627132
25	7	0	-4.891956	3.042697	0.226262
26	1	0	-5.195921	0.538748	0.549894
27	1	0	-2.852769	-3.823261	-0.244008
28	1	0	-6.445654	-1.577637	0.614213
29	1	0	-5.322848	-3.750686	0.216825
30	1	0	0.130028	1.657525	0.436527
31	1	0	1.478648	-1.603378	-1.090162
32	1	0	2.181483	2.044989	1.112870
33	1	0	4.600178	1.591679	1.107319
34	1	0	3.925496	-2.024147	-1.128777
35	1	0	6.436600	0.081878	1.921920
36	1	0	7.426187	-1.193202	1.159142
37	1	0	5.810686	-1.589626	1.791698
38	1	0	7.634295	0.057803	-0.918707
39	1	0	6.169578	0.568990	-1.790809
40	1	0	6.659240	1.415530	-0.292177

TSDA

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.506935	-0.892100	-0.036798
2	6	0	-2.678900	-3.066363	-0.001586
3	6	0	-4.954385	-2.215866	-0.039709
4	6	0	-3.123176	-0.649785	-0.015555
5	6	0	-2.233633	-1.745950	0.002223
6	6	0	-4.056041	-3.296502	-0.022713
7	6	0	-0.835962	-1.261282	0.024965
8	6	0	-0.912572	0.245436	0.027127
9	6	0	-2.350512	0.611150	-0.008494
10	6	0	-2.886874	1.881202	-0.036168
11	8	0	0.171312	-1.948639	0.039888
12	6	0	0.161875	1.066249	0.066674
13	6	0	1.589316	0.653187	0.106084
14	6	0	4.337710	0.013242	0.181061
15	6	0	2.319188	0.510932	-1.084156
16	6	0	2.248067	0.489529	1.332757
17	6	0	3.608194	0.167819	1.365212
18	6	0	3.677727	0.189954	-1.044991
19	7	0	5.740383	-0.317120	0.265445
20	6	0	6.610665	0.733227	-0.269865
21	6	0	6.055658	-1.630108	-0.303947

22	6	0	-2.111282	3.084665	-0.039230
23	6	0	-4.293369	2.148926	-0.068159
24	7	0	-1.538383	4.098220	-0.044594
25	7	0	-5.422743	2.429381	-0.094076
26	1	0	-5.235405	-0.088270	-0.050181
27	1	0	-1.964005	-3.887891	0.012069
28	1	0	-6.026026	-2.412076	-0.055506
29	1	0	-4.440242	-4.316199	-0.025890
30	1	0	-0.000476	2.143757	0.072627
31	1	0	1.822639	0.645050	-2.045230
32	1	0	1.697984	0.606649	2.266353
33	1	0	4.118709	0.032927	2.318345
34	1	0	4.223512	0.077625	-1.981625
35	1	0	6.529899	0.853281	-1.368761
36	1	0	7.654447	0.487466	-0.032117
37	1	0	6.364675	1.691785	0.202740
38	1	0	7.097873	-1.881707	-0.065252
39	1	0	5.404557	-2.391015	0.142830
40	1	0	5.938014	-1.671008	-1.405313

3, 298 K, dichloromethane, B3LYP/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.410382	-0.095977	-1.088047
2	6	0	-3.041712	-2.540932	-0.662100
3	6	0	-4.975288	-1.314041	-1.485093
4	6	0	-3.145375	-0.101405	-0.492055
5	6	0	-2.463989	-1.328247	-0.278215
6	6	0	-4.298653	-2.521492	-1.278211
7	6	0	-1.176762	-1.031641	0.371937
8	6	0	-0.976133	0.415390	0.286202
9	6	0	-2.290249	1.002355	-0.008818
10	6	0	-2.697659	2.318402	0.158773
11	6	0	-0.433274	-1.920919	1.131177
12	6	0	0.203312	1.155413	0.274022
13	6	0	1.559076	0.797216	0.019560
14	6	0	4.330125	0.299347	-0.535424
15	6	0	1.995226	-0.429320	-0.557757
16	6	0	2.563961	1.777935	0.262737
17	6	0	3.899392	1.543687	0.018826
18	6	0	3.320491	-0.669444	-0.839723
19	7	0	5.639550	0.050598	-0.782107
20	6	0	6.655983	1.055775	-0.474323
21	6	0	6.059555	-1.220131	-1.371990
22	6	0	-1.892143	3.334348	0.759558
23	6	0	-3.999500	2.792111	-0.190558
24	7	0	-1.281017	4.193901	1.255239
25	7	0	-5.043191	3.235509	-0.459050
26	6	0	0.613631	-1.503344	2.008732
27	7	0	1.442197	-1.203974	2.770173
28	6	0	-0.718124	-3.318627	1.207179
29	7	0	-0.905458	-4.465579	1.290766
30	1	0	-4.957390	0.824867	-1.262310
31	1	0	-2.531463	-3.487935	-0.513686
32	1	0	-5.953151	-1.317490	-1.965366

33	1	0	-4.751342	-3.458114	-1.602152
34	1	0	0.072679	2.230273	0.388662
35	1	0	1.268006	-1.190709	-0.829438
36	1	0	2.266570	2.744970	0.669412
37	1	0	4.618739	2.325662	0.242345
38	1	0	3.591112	-1.612166	-1.305893
39	1	0	7.639560	0.650566	-0.720002
40	1	0	6.644907	1.314171	0.593855
41	1	0	5.616775	-1.362382	-2.368338
42	1	0	7.146398	-1.218524	-1.475931
43	1	0	6.500938	1.972414	-1.061684
44	1	0	5.774024	-2.067531	-0.732960

TSA2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.368641	0.248976	-1.143297
2	6	0	2.811810	2.595682	-0.783047
3	6	0	4.822319	1.488023	-1.602779
4	6	0	3.119039	0.181874	-0.516063
5	6	0	2.342533	1.359565	-0.325502
6	6	0	4.050485	2.645689	-1.429249
7	6	0	1.117294	1.001971	0.408264
8	6	0	0.999987	-0.471825	0.287716
9	6	0	2.375303	-0.963405	0.016363
10	6	0	2.836007	-2.233219	0.270984
11	6	0	0.350885	1.848604	1.171398
12	6	0	-0.090018	-1.222796	-0.019838
13	6	0	-1.516185	-0.853466	-0.153979
14	6	0	-4.304797	-0.351112	-0.558195
15	6	0	-2.048800	-0.682261	-1.447046
16	6	0	-2.412405	-0.820916	0.925172
17	6	0	-3.771564	-0.585234	0.735198
18	6	0	-3.399067	-0.420228	-1.650756
19	7	0	-5.639650	-0.071947	-0.748418
20	6	0	-6.565286	-0.161343	0.372344
21	6	0	-6.181288	0.002278	-2.098135
22	6	0	2.040427	-3.232755	0.920926
23	6	0	4.167341	-2.658638	-0.038125
24	7	0	1.443325	-4.072789	1.461614
25	7	0	5.240746	-3.039341	-0.277343
26	6	0	-0.557471	1.415299	2.189051
27	7	0	-1.228082	1.160933	3.104976
28	6	0	0.524087	3.271777	1.154826
29	7	0	0.618838	4.431442	1.161493
30	1	0	4.977742	-0.637287	-1.294308
31	1	0	2.231654	3.505651	-0.664441
32	1	0	5.785419	1.552259	-2.107677
33	1	0	4.418840	3.599908	-1.804334
34	1	0	0.138572	-2.238244	-0.354441
35	1	0	-1.391241	-0.743791	-2.315028
36	1	0	-2.052487	-1.005546	1.934146
37	1	0	-4.418825	-0.588080	1.607630
38	1	0	-3.748633	-0.277846	-2.669553
39	1	0	-7.563281	0.128049	0.032429
40	1	0	-6.273281	0.523436	1.181068
41	1	0	-6.089638	-0.954961	-2.639770
42	1	0	-7.240959	0.265043	-2.041197

43	1	0	-6.622166	-1.182281	0.787685
44	1	0	-5.673634	0.780360	-2.685868

TSA1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.350823	0.328217	-1.151082
2	6	0	2.791546	2.655974	-0.694104
3	6	0	4.804924	1.587834	-1.552364
4	6	0	3.099869	0.230587	-0.530609
5	6	0	2.321846	1.398607	-0.301550
6	6	0	4.033979	2.737485	-1.329481
7	6	0	1.078538	1.004097	0.372192
8	6	0	0.979377	-0.464283	0.238314
9	6	0	2.357935	-0.938337	-0.033642
10	6	0	2.865705	-2.200740	0.189352
11	6	0	0.291259	1.801216	1.172862
12	6	0	-0.121379	-1.267968	0.124596
13	6	0	-1.530841	-0.952730	-0.063433
14	6	0	-4.299120	-0.526914	-0.472442
15	6	0	-1.996661	0.230722	-0.677154
16	6	0	-2.479211	-1.932324	0.302106
17	6	0	-3.842643	-1.711186	0.121176
18	6	0	-3.356346	0.434299	-0.883703
19	7	0	-5.715224	-0.344995	-0.654909
20	6	0	-6.247917	0.783159	0.117362
21	6	0	-6.107612	-0.278193	-2.066680
22	6	0	2.119185	-3.257476	0.801382
23	6	0	4.215428	-2.566728	-0.112845
24	7	0	1.555364	-4.142942	1.304733
25	7	0	5.303372	-2.911332	-0.342754
26	6	0	-0.731274	1.279837	2.026776
27	7	0	-1.539828	0.900053	2.772281
28	6	0	0.494921	3.211087	1.308657
29	7	0	0.622438	4.360656	1.439307
30	1	0	4.964236	-0.547069	-1.340872
31	1	0	2.206068	3.557240	-0.537361
32	1	0	5.769730	1.674184	-2.050707
33	1	0	4.404813	3.707533	-1.658730
34	1	0	0.079230	-2.337999	0.087052
35	1	0	-1.290611	0.979763	-1.029395
36	1	0	-2.139633	-2.867861	0.746965
37	1	0	-4.571227	-2.461711	0.424281
38	1	0	-3.689288	1.347816	-1.375019
39	1	0	-5.901041	1.768939	-0.250086
40	1	0	-5.955423	0.680244	1.169015
41	1	0	-5.714227	-1.151733	-2.600221
42	1	0	-7.203528	-0.298727	-2.129620
43	1	0	-7.344085	0.764393	0.058726
44	1	0	-5.751857	0.637442	-2.578762

TSD2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-4.409790	-0.095489	-1.105376
2	6	0	-2.996084	-2.530873	-0.744820
3	6	0	-4.951689	-1.311302	-1.532110
4	6	0	-3.143657	-0.096383	-0.508595
5	6	0	-2.439076	-1.318118	-0.327128
6	6	0	-4.252626	-2.514008	-1.357081
7	6	0	-1.160227	-1.023841	0.331003
8	6	0	-0.967354	0.438129	0.231396
9	6	0	-2.317226	1.007812	0.002728
10	6	0	-2.736394	2.293865	0.270164
11	6	0	-0.412674	-1.890746	1.096207
12	6	0	0.181368	1.169913	0.110427
13	6	0	1.561353	0.763560	-0.119354
14	6	0	4.282244	0.157444	-0.609417
15	6	0	1.928480	-0.428270	-0.778831
16	6	0	2.585099	1.663181	0.253145
17	6	0	3.924145	1.354917	0.033415
18	6	0	3.267465	-0.718641	-1.024000
19	7	0	5.651787	-0.197883	-0.874542
20	6	0	6.317636	0.731627	-1.793711
21	6	0	6.430531	-0.409998	0.351000
22	6	0	-1.909109	3.281712	0.893315
23	6	0	-4.064888	2.755133	0.006834
24	7	0	-1.276855	4.113127	1.407434
25	7	0	-5.132295	3.175556	-0.190947
26	6	0	0.659412	-1.458987	1.939389
27	7	0	1.506254	-1.150329	2.675157
28	6	0	-0.709081	-3.286500	1.204021
29	7	0	-0.913396	-4.427394	1.310847
30	1	0	-4.968765	0.822487	-1.258106
31	1	0	-2.466864	-3.471806	-0.625412
32	1	0	-5.929106	-1.321165	-2.012968
33	1	0	-4.691159	-3.448211	-1.706137
34	1	0	0.051997	2.251526	0.101920
35	1	0	1.164940	-1.115596	-1.136435
36	1	0	2.320909	2.605006	0.734681
37	1	0	4.693759	2.057800	0.349903
38	1	0	3.547826	-1.631185	-1.548380
39	1	0	6.483203	1.736681	-1.358537
40	1	0	5.718398	0.840645	-2.705590
41	1	0	5.913940	-1.131070	0.995464
42	1	0	7.409348	-0.826443	0.079167
43	1	0	7.295343	0.315300	-2.069577
44	1	0	6.600607	0.519679	0.928631

TSD1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.177155	0.165185	-1.410907
2	6	0	2.657946	2.534706	-1.028432
3	6	0	4.574081	1.373758	-1.989182
4	6	0	3.000563	0.138873	-0.653345
5	6	0	2.246009	1.329080	-0.451862
6	6	0	3.820251	2.541893	-1.805450
7	6	0	1.115534	1.017658	0.437889
8	6	0	0.969360	-0.458463	0.383572
9	6	0	2.316328	-0.971701	0.016296

10	6	0	2.799552	-2.226155	0.298789
11	6	0	0.487214	1.897024	1.284990
12	6	0	-0.138889	-1.215060	0.166762
13	6	0	-1.568953	-0.862225	0.041431
14	6	0	-4.317877	-0.340569	-0.381471
15	6	0	-2.156770	-1.064052	-1.225950
16	6	0	-2.387079	-0.440072	1.098315
17	6	0	-3.746104	-0.187032	0.884976
18	6	0	-3.504380	-0.785050	-1.438872
19	7	0	-5.720523	-0.055533	-0.552451
20	6	0	-5.968316	1.073968	-1.453430
21	6	0	-6.505540	-1.236207	-0.925600
22	6	0	2.062624	-3.184115	1.069082
23	6	0	4.098134	-2.671862	-0.106101
24	7	0	1.507398	-3.987690	1.701701
25	7	0	5.146650	-3.066179	-0.421115
26	6	0	-0.249396	1.496264	2.444695
27	7	0	-0.768194	1.248118	3.456025
28	6	0	0.684866	3.315049	1.207187
29	7	0	0.804603	4.471520	1.167173
30	1	0	4.770625	-0.730093	-1.571553
31	1	0	2.088035	3.450517	-0.903225
32	1	0	5.477968	1.405553	-2.596248
33	1	0	4.142692	3.470413	-2.275310
34	1	0	0.069639	-2.243527	-0.135732
35	1	0	-1.546199	-1.427964	-2.053023
36	1	0	-1.981449	-0.344883	2.099718
37	1	0	-4.379782	0.129746	1.712515
38	1	0	-3.926761	-0.928500	-2.432939
39	1	0	-5.706429	0.859790	-2.508738
40	1	0	-5.389912	1.944336	-1.121012
41	1	0	-6.313028	-2.046720	-0.212560
42	1	0	-7.572712	-0.981459	-0.880516
43	1	0	-7.035002	1.331922	-1.414400
44	1	0	-6.285094	-1.606142	-1.946593

TSDA

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.265829	0.234341	-1.256698
2	6	0	2.681190	2.570912	-0.943319
3	6	0	4.673123	1.456123	-1.798897
4	6	0	3.046821	0.178039	-0.571334
5	6	0	2.259024	1.351861	-0.403446
6	6	0	3.887178	2.607879	-1.649755
7	6	0	1.084581	1.010280	0.415846
8	6	0	0.969997	-0.467745	0.338400
9	6	0	2.345822	-0.951833	0.046550
10	6	0	2.835164	-2.199901	0.346243
11	6	0	0.391181	1.869345	1.232560
12	6	0	-0.107966	-1.242834	0.046320
13	6	0	-1.534813	-0.917504	-0.160866
14	6	0	-4.263141	-0.441810	-0.741486
15	6	0	-2.044057	-1.121710	-1.459880
16	6	0	-2.421304	-0.516356	0.849917
17	6	0	-3.768872	-0.286376	0.561439
18	6	0	-3.383464	-0.864045	-1.748086
19	7	0	-5.643533	-0.203092	-1.082197

20	6	0	-6.565625	-1.130958	-0.419631
21	6	0	-6.044984	1.194516	-0.894257
22	6	0	2.072771	-3.176765	1.066490
23	6	0	4.162831	-2.618778	0.013444
24	7	0	1.496782	-3.994363	1.661453
25	7	0	5.234812	-2.991288	-0.243839
26	6	0	-0.405512	1.443909	2.342722
27	7	0	-0.979660	1.177052	3.318787
28	6	0	0.566608	3.291524	1.180449
29	7	0	0.666761	4.450360	1.159395
30	1	0	4.885035	-0.647919	-1.389846
31	1	0	2.087375	3.474671	-0.844318
32	1	0	5.610803	1.511128	-2.350506
33	1	0	4.218857	3.547039	-2.091170
34	1	0	0.139262	-2.262946	-0.255453
35	1	0	-1.381697	-1.469951	-2.252846
36	1	0	-2.074879	-0.421685	1.873419
37	1	0	-4.437567	0.011763	1.368375
38	1	0	-3.766564	-1.000801	-2.758657
39	1	0	-6.631445	-0.977166	0.675561
40	1	0	-6.247317	-2.163386	-0.607493
41	1	0	-5.349894	1.852673	-1.429396
42	1	0	-7.049112	1.335206	-1.315930
43	1	0	-7.569956	-0.995713	-0.842563
44	1	0	-6.073336	1.503693	0.169255

4, 248 K, dichloromethane, B3LYP/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.837229	-0.952822	0.047879
2	6	0	-4.979599	1.760700	0.007770
3	6	0	-6.766838	0.096402	0.053952
4	6	0	-4.483412	-0.622485	0.021728
5	6	0	-4.060362	0.713354	0.001881
6	6	0	-6.343179	1.436014	0.034181
7	6	0	-2.560717	0.771563	-0.024529
8	6	0	-2.082817	-0.625251	-0.018708
9	6	0	-3.278172	-1.507161	0.009819
10	8	0	-3.296220	-2.737223	0.022086
11	8	0	-1.919768	1.823964	-0.046424
12	6	0	-0.826754	-1.207046	-0.033198
13	6	0	0.514578	-0.721427	-0.058136
14	6	0	3.265014	0.042541	-0.079289
15	6	0	1.561914	-1.684740	-0.064424
16	6	0	0.902961	0.645744	-0.074829
17	6	0	2.228089	1.035614	-0.094800
18	6	0	2.899724	-1.344259	-0.083843
19	7	0	4.581324	0.412673	-0.047072
20	6	0	4.987280	1.816132	-0.169566
21	6	0	5.657681	-0.576046	-0.161677
22	6	0	2.591433	2.505786	-0.141721
23	6	0	3.969561	2.752501	0.469857
24	6	0	3.972166	-2.413607	-0.116161
25	6	0	5.276633	-1.899458	0.490845

26	1	0	-6.160854	-1.992988	0.063091
27	1	0	-4.646552	2.797829	-0.007724
28	1	0	-7.833946	-0.126309	0.074265
29	1	0	-7.088649	2.231676	0.039506
30	1	0	-0.892176	-2.300561	-0.022052
31	1	0	1.295759	-2.743513	-0.054552
32	1	0	0.124048	1.405463	-0.073666
33	1	0	5.964780	1.917226	0.317965
34	1	0	5.125682	2.073880	-1.234776
35	1	0	6.545753	-0.149864	0.320924
36	1	0	5.908967	-0.734127	-1.225715
37	1	0	1.821006	3.091222	0.376063
38	1	0	2.594345	2.850268	-1.188838
39	1	0	3.941695	2.574771	1.554755
40	1	0	4.287792	3.790984	0.311914
41	1	0	3.618840	-3.307140	0.414749
42	1	0	4.155493	-2.720970	-1.158660
43	1	0	5.159393	-1.751343	1.574162
44	1	0	6.089530	-2.621431	0.340616

TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.817771	-0.000010	0.451366
2	6	0	4.461307	0.000029	-2.053841
3	6	0	6.528679	0.000005	-0.752324
4	6	0	4.422570	-0.000005	0.385221
5	6	0	3.752857	0.000014	-0.850543
6	6	0	5.858033	0.000024	-1.990570
7	6	0	2.273977	0.000015	-0.634518
8	6	0	2.070053	-0.000008	0.850705
9	6	0	3.426400	-0.000019	1.493330
10	8	0	3.668824	-0.000036	2.692188
11	8	0	1.424301	0.000031	-1.512501
12	6	0	0.924276	-0.000018	1.561319
13	6	0	-0.462525	-0.000012	1.035858
14	6	0	-3.138982	-0.000002	0.091092
15	6	0	-1.145619	-1.200958	0.806603
16	6	0	-1.145623	1.200939	0.806639
17	6	0	-2.463351	1.223544	0.342661
18	6	0	-2.463347	-1.223554	0.342625
19	7	0	-4.434851	0.000004	-0.440096
20	6	0	-5.214219	1.232169	-0.379419
21	6	0	-5.214215	-1.232167	-0.379457
22	6	0	-3.156442	2.556539	0.126185
23	6	0	-4.366463	2.427952	-0.800658
24	6	0	-3.156435	-2.556545	0.126110
25	6	0	-4.366454	-2.427934	-0.800731
26	1	0	6.332075	-0.000025	1.411426
27	1	0	3.938665	0.000044	-3.009440
28	1	0	7.618619	0.000002	-0.736937
29	1	0	6.441077	0.000036	-2.911621
30	1	0	1.049053	-0.000035	2.651366
31	1	0	-0.638781	-2.151045	0.983647
32	1	0	-0.638788	2.151021	0.983712
33	1	0	-6.073880	1.113295	-1.052035
34	1	0	-5.617756	1.398153	0.640005
35	1	0	-6.073875	-1.113274	-1.052072

36	1	0	-5.617754	-1.398182	0.639960
37	1	0	-2.437994	3.284461	-0.275318
38	1	0	-3.486091	2.956062	1.099347
39	1	0	-4.037121	2.284159	-1.840005
40	1	0	-4.975402	3.341321	-0.769226
41	1	0	-2.437984	-3.284454	-0.275412
42	1	0	-3.486084	-2.956095	1.099260
43	1	0	-4.037112	-2.284109	-1.840073
44	1	0	-4.975391	-3.341306	-0.769327

GS, Sz 248K,

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.848286	-0.942624	0.044143
2	6	0	-4.998979	1.746733	0.008352
3	6	0	-6.780715	0.097014	0.049596
4	6	0	-4.495325	-0.620436	0.018844
5	6	0	-4.076279	0.709293	0.003772
6	6	0	-6.359804	1.428826	0.031902
7	6	0	-2.572656	0.769734	-0.019758
8	6	0	-2.089069	-0.624458	-0.013344
9	6	0	-3.286081	-1.502418	0.007532
10	8	0	-3.308676	-2.721712	0.012112
11	8	0	-1.935257	1.810307	-0.038029
12	6	0	-0.827830	-1.205248	-0.024007
13	6	0	0.520432	-0.722840	-0.060082
14	6	0	3.278922	0.045170	-0.081947
15	6	0	1.572546	-1.684261	-0.053284
16	6	0	0.912733	0.643332	-0.072043
17	6	0	2.239782	1.034112	-0.097977
18	6	0	2.911573	-1.340542	-0.081327
19	7	0	4.592923	0.413160	-0.060906
20	6	0	4.988913	1.814264	-0.161626
21	6	0	5.660860	-0.575697	-0.166490
22	6	0	2.610376	2.503607	-0.142026
23	6	0	3.977843	2.753699	0.463265
24	6	0	3.987290	-2.407042	-0.106002
25	6	0	5.292305	-1.899370	0.484095
26	1	0	-6.172374	-1.975777	0.057355
27	1	0	-4.672537	2.778827	-0.004640
28	1	0	-7.842411	-0.122708	0.068090
29	1	0	-7.100900	2.218748	0.036117
30	1	0	-0.893444	-2.303271	-0.003148
31	1	0	1.310919	-2.746786	-0.034693
32	1	0	0.138277	1.409026	-0.066180
33	1	0	5.944986	1.905298	0.329619
34	1	0	5.137047	2.075078	-1.202749
35	1	0	6.541929	-0.138966	0.285246
36	1	0	5.892802	-0.741107	-1.208971
37	1	0	1.854469	3.092205	0.362332
38	1	0	2.618306	2.837067	-1.174043
39	1	0	3.947346	2.589943	1.534757
40	1	0	4.295611	3.788759	0.298661
41	1	0	3.645500	-3.293308	0.420043
42	1	0	4.165091	-2.714852	-1.131114
43	1	0	5.188618	-1.758185	1.553226
44	1	0	6.090479	-2.625977	0.324245

TS Sz 248 K

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.815062	-0.000006	0.439796
2	6	0	-4.465199	0.000035	-2.053780
3	6	0	-6.522165	0.000018	-0.762432
4	6	0	-4.429659	-0.000008	0.380026
5	6	0	-3.761772	0.000012	-0.852114
6	6	0	-5.849866	0.000038	-1.994566
7	6	0	-2.289577	0.000004	-0.626152
8	6	0	-2.082650	-0.000020	0.864062
9	6	0	-3.440822	-0.000029	1.494958
10	8	0	-3.693490	-0.000050	2.684441
11	8	0	-1.448126	0.000017	-1.491022
12	6	0	-0.929750	-0.000032	1.563786
13	6	0	0.460911	-0.000020	1.032397
14	6	0	3.152792	-0.000000	0.093834
15	6	0	1.152779	1.200505	0.806822
16	6	0	1.152776	-1.200551	0.806784
17	6	0	2.475321	-1.225375	0.350306
18	6	0	2.475315	1.225364	0.350349
19	7	0	4.450942	0.000012	-0.422440
20	6	0	5.215876	-1.239173	-0.386806
21	6	0	5.215874	1.239198	-0.386757
22	6	0	3.165617	-2.560630	0.121623
23	6	0	4.370448	-2.435227	-0.802030
24	6	0	3.165617	2.560645	0.121741
25	6	0	4.370434	2.435260	-0.801956
26	1	0	-6.324438	-0.000021	1.398060
27	1	0	-3.946171	0.000051	-3.006770
28	1	0	-7.600713	0.000020	-0.752638
29	1	0	-6.419719	0.000056	-2.918092
30	1	0	-1.045316	-0.000050	2.650723
31	1	0	0.645130	2.152656	0.980644
32	1	0	0.645231	-2.152521	0.980540
33	1	0	6.067885	-1.122145	-1.053771
34	1	0	5.618148	-1.419947	0.616811
35	1	0	6.067886	1.122194	-1.053743
36	1	0	5.618101	1.419923	0.616738
37	1	0	2.454246	-3.278798	-0.279696
38	1	0	3.490687	-2.966559	1.078376
39	1	0	4.041657	-2.297921	-1.830387
40	1	0	4.976900	-3.345929	-0.772432
41	1	0	2.454272	3.278780	-0.279553
42	1	0	3.490549	2.966372	1.078099
43	1	0	4.041679	2.298004	-1.830204
44	1	0	4.976893	3.345978	-0.772322

5, 298 K, dichloromethane, B3LYP/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-5.487367	0.923491	-0.037020
2	6	0	-4.631975	-1.790500	0.057175
3	6	0	-6.416761	-0.123998	-0.009490
4	6	0	-4.132882	0.592054	-0.017126
5	6	0	-3.710973	-0.743997	0.029203
6	6	0	-5.994069	-1.464270	0.037025
7	6	0	-2.213755	-0.807944	0.043308
8	6	0	-1.729963	0.592739	-0.003789
9	6	0	-2.931059	1.477088	-0.037736
10	8	0	-2.944548	2.704318	-0.076152
11	8	0	-1.573230	-1.856766	0.089751
12	6	0	-0.481777	1.172068	-0.021820
13	6	0	0.869817	0.681934	-0.011987
14	6	0	3.613160	-0.077823	-0.004829
15	6	0	1.251110	-0.680771	0.003899
16	6	0	1.907505	1.646612	-0.021753
17	6	0	3.253884	1.305601	-0.022267
18	6	0	2.584461	-1.072802	0.010242
19	7	0	4.954737	-0.453832	-0.001128
20	6	0	5.922517	0.117142	0.922922
21	6	0	5.489905	-1.445579	-0.921272
22	1	0	-5.809826	1.963384	-0.072988
23	1	0	-4.299862	-2.827272	0.093598
24	1	0	-7.483813	0.098969	-0.024058
25	1	0	-6.740708	-2.258461	0.057718
26	1	0	-0.544973	2.265254	-0.053288
27	1	0	0.471314	-1.437014	0.050146
28	1	0	1.636487	2.702422	-0.070710
29	1	0	6.488188	-0.700371	1.397892
30	1	0	6.647644	0.783992	0.428159
31	1	0	5.412149	0.668755	1.716842
32	1	0	5.757406	-2.392630	-0.424616
33	1	0	4.772609	-1.650309	-1.720415
34	1	0	6.402204	-1.042357	-1.389223
35	6	0	2.904936	-2.544045	0.159198
36	1	0	3.239717	-3.008313	-0.778328
37	1	0	3.700048	-2.698176	0.900878
38	1	0	2.013185	-3.086908	0.492528
39	6	0	4.287948	2.400169	-0.165879
40	1	0	4.808109	2.626814	0.774631
41	1	0	5.053079	2.120122	-0.902078
42	1	0	3.808129	3.325506	-0.505601

TSA

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.477748	-0.505354	0.067118
2	6	0	4.171560	2.001498	-0.288793
3	6	0	6.212429	0.672385	-0.098376
4	6	0	4.084162	-0.412597	0.052341
5	6	0	3.439272	0.824141	-0.123381
6	6	0	5.566672	1.911409	-0.274258
7	6	0	1.956914	0.639134	-0.098981
8	6	0	1.723530	-0.826765	0.110030
9	6	0	3.066679	-1.490243	0.204211
10	8	0	3.284342	-2.681691	0.373101
11	8	0	1.122733	1.522612	-0.226012
12	6	0	0.563100	-1.504350	0.209414

13	6	0	-0.812385	-0.952653	0.133511
14	6	0	-3.467805	0.008042	0.004316
15	6	0	-1.490565	-0.894462	-1.089996
16	6	0	-1.477970	-0.539118	1.293459
17	6	0	-2.797045	-0.069674	1.251233
18	6	0	-2.799850	-0.404325	-1.176687
19	7	0	-4.792871	0.491727	-0.062566
20	6	0	-5.149118	1.817022	0.401628
21	6	0	-5.876161	-0.314694	-0.586905
22	1	0	5.972686	-1.465888	0.203514
23	1	0	3.668177	2.957758	-0.424501
24	1	0	7.301827	0.635884	-0.091847
25	1	0	6.168050	2.811744	-0.400657
26	1	0	0.658172	-2.585732	0.364634
27	1	0	-0.978678	-1.202067	-2.002627
28	1	0	-0.969612	-0.603632	2.256302
29	1	0	-5.696466	2.363772	-0.386551
30	1	0	-5.793541	1.799405	1.299924
31	1	0	-4.246420	2.391183	0.634111
32	1	0	-6.290157	0.084661	-1.531070
33	1	0	-5.532900	-1.338859	-0.765694
34	1	0	-6.704886	-0.364882	0.141723
35	6	0	-3.452440	-0.268810	-2.532660
36	1	0	-4.192677	-1.059326	-2.723413
37	1	0	-3.979270	0.691289	-2.614987
38	1	0	-2.699769	-0.324116	-3.328308
39	6	0	-3.496485	0.290740	2.541147
40	1	0	-3.564381	1.377860	2.691768
41	1	0	-4.522975	-0.099663	2.548768
42	1	0	-2.957149	-0.126803	3.399933

TSD

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.487716	0.882369	-0.000001
2	6	0	4.596599	-1.822979	-0.000004
3	6	0	6.401962	-0.177114	-0.000005
4	6	0	4.128120	0.568079	0.000000
5	6	0	3.688562	-0.763710	-0.000001
6	6	0	5.961510	-1.513548	-0.000006
7	6	0	2.193276	-0.813456	0.000002
8	6	0	1.723203	0.599962	0.000004
9	6	0	2.942840	1.470942	0.000004
10	8	0	2.968500	2.696141	0.000006
11	8	0	1.538218	-1.851164	0.000003
12	6	0	0.491926	1.195799	0.000004
13	6	0	-0.878385	0.721148	0.000002
14	6	0	-3.616194	0.004048	-0.000003
15	6	0	-1.270878	-0.633875	0.000005
16	6	0	-1.891511	1.705800	-0.000001
17	6	0	-3.245332	1.370923	-0.000004
18	6	0	-2.617989	-1.004378	0.000004
19	7	0	-5.024227	-0.276465	-0.000006
20	6	0	-5.596724	-0.816143	-1.226487
21	6	0	-5.596731	-0.816119	1.226483
22	1	0	5.823475	1.918540	-0.000000
23	1	0	4.250999	-2.855853	-0.000005
24	1	0	7.471896	0.031715	-0.000007

25	1	0	6.698192	-2.317127	-0.000009
26	1	0	0.568866	2.288494	0.000004
27	1	0	-0.501356	-1.401506	0.000009
28	1	0	-1.604670	2.758229	-0.000003
29	1	0	-5.479088	-1.910935	-1.338906
30	1	0	-6.674710	-0.597147	-1.245605
31	1	0	-5.136776	-0.329493	-2.095065
32	1	0	-5.479088	-1.910908	1.338927
33	1	0	-5.136794	-0.329447	2.095053
34	1	0	-6.674719	-0.597130	1.245586
35	6	0	-2.963654	-2.477435	0.000013
36	1	0	-3.550344	-2.758373	0.883778
37	1	0	-3.550361	-2.758381	-0.883738
38	1	0	-2.048614	-3.080386	0.000007
39	6	0	-4.295357	2.456294	-0.000010
40	1	0	-4.946663	2.379116	-0.880692
41	1	0	-4.946673	2.379115	0.880664
42	1	0	-3.825478	3.447272	-0.000006

TSDA

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.467121	-0.509686	-0.060360
2	6	0	4.157233	2.017235	0.069218
3	6	0	6.199943	0.679862	-0.015243
4	6	0	4.073516	-0.418632	-0.039817
5	6	0	3.426670	0.828059	0.024243
6	6	0	5.552363	1.928761	0.048764
7	6	0	1.944989	0.638885	0.033199
8	6	0	1.714082	-0.841186	-0.029613
9	6	0	3.058252	-1.508098	-0.077143
10	8	0	3.276640	-2.709748	-0.135015
11	8	0	1.108569	1.528023	0.082165
12	6	0	0.555106	-1.527364	-0.043922
13	6	0	-0.819788	-0.970260	0.001392
14	6	0	-3.463570	0.009288	0.079483
15	6	0	-1.506323	-0.678423	-1.182245
16	6	0	-1.470094	-0.783582	1.226257
17	6	0	-2.781694	-0.293174	1.279932
18	6	0	-2.820122	-0.186595	-1.164355
19	7	0	-4.805696	0.511872	0.207870
20	6	0	-5.023775	1.917668	-0.101636
21	6	0	-5.891888	-0.369996	-0.193801
22	1	0	5.963443	-1.477849	-0.109993
23	1	0	3.652619	2.981143	0.118656
24	1	0	7.289320	0.645100	-0.029611
25	1	0	6.152453	2.838119	0.082745
26	1	0	0.647678	-2.618662	-0.093709
27	1	0	-1.009401	-0.827271	-2.141543
28	1	0	-0.947297	-1.013973	2.154963
29	1	0	-5.145229	2.131857	-1.181573
30	1	0	-5.938039	2.262274	0.404939
31	1	0	-4.182676	2.513367	0.273212
32	1	0	-6.097214	-0.373062	-1.282289
33	1	0	-5.667082	-1.398063	0.115390
34	1	0	-6.817875	-0.057374	0.312245
35	6	0	-3.496090	0.119191	-2.483144
36	1	0	-4.412328	-0.469599	-2.618409

37	1	0	-3.774646	1.177942	-2.561928
38	1	0	-2.824494	-0.111664	-3.318491
39	6	0	-3.450026	-0.090099	2.619473
40	1	0	-3.725832	0.962408	2.770516
41	1	0	-4.378643	-0.671560	2.693624
42	1	0	-2.781982	-0.393555	3.434891

6a, 298 K, benzene, B3LYP/aug-cc-pVTZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.345556	0.361610	0.019524
2	1	0	2.395504	1.442929	0.076076
3	6	0	1.152990	-0.291463	-0.025733
4	1	0	1.188447	-1.377728	-0.084038
5	6	0	-0.137220	0.297645	-0.001405
6	1	0	-0.207918	1.375270	0.061025
7	6	0	-1.265647	-0.473240	-0.051458
8	1	0	-1.152808	-1.550740	-0.085754
9	6	0	3.587298	-0.362066	-0.006141
10	8	0	4.707705	0.133094	0.030973
11	1	0	3.477711	-1.465099	-0.065248
12	7	0	-2.543439	-0.052757	-0.077455
13	6	0	-2.862448	1.362822	-0.006085
14	1	0	-3.914606	1.503220	-0.240322
15	1	0	-2.668512	1.770985	0.990629
16	1	0	-2.270038	1.921891	-0.729926
17	6	0	-3.641004	-0.993718	0.076574
18	1	0	-4.084553	-0.929064	1.074667
19	1	0	-4.419066	-0.789114	-0.659655
20	1	0	-3.278887	-2.007538	-0.074703

TS1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.337582	0.567817	-0.132431
2	1	0	2.314118	1.638337	0.051419
3	6	0	1.204308	-0.145166	-0.226290
4	1	0	1.285864	-1.211463	-0.425271
5	6	0	-0.132586	0.365299	-0.074902
6	1	0	-0.246410	1.421139	0.134061
7	6	0	-1.217443	-0.440276	-0.188105
8	1	0	-1.061495	-1.498897	-0.364515
9	6	0	3.692160	-0.025596	-0.285724
10	8	0	4.367514	-0.442588	0.627951
11	1	0	4.100265	-0.063097	-1.316781
12	7	0	-2.531872	-0.083946	-0.137682
13	6	0	-2.895698	1.284200	0.172831
14	1	0	-3.959498	1.421384	-0.009605
15	1	0	-2.685088	1.542880	1.218042
16	1	0	-2.346633	1.973671	-0.467713

17	6	0	-3.528569	-1.102364	0.147296
18	1	0	-3.711467	-1.213291	1.223007
19	1	0	-4.471073	-0.844321	-0.335405
20	1	0	-3.194113	-2.061491	-0.243135

TS1b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.374442	0.769849	0.034874
2	1	0	2.306348	1.850644	0.080158
3	6	0	1.249373	0.003713	-0.007419
4	1	0	1.400728	-1.071448	-0.054011
5	6	0	-0.088533	0.466151	0.005984
6	1	0	-0.268083	1.532054	0.056736
7	6	0	-1.134861	-0.415670	-0.040126
8	1	0	-0.912416	-1.475976	-0.063726
9	6	0	3.700835	0.198110	0.021343
10	8	0	3.978929	-0.996274	-0.027358
11	1	0	4.522460	0.939813	0.059427
12	7	0	-2.447234	-0.126233	-0.072008
13	6	0	-2.908617	1.250405	-0.018838
14	1	0	-3.969955	1.279715	-0.251399
15	1	0	-2.755305	1.688789	0.971931
16	1	0	-2.377594	1.857472	-0.751781
17	6	0	-3.446899	-1.172913	0.066696
18	1	0	-3.923194	-1.138957	1.050850
19	1	0	-4.220185	-1.060260	-0.694257
20	1	0	-2.978048	-2.145889	-0.056110

TS1c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.334190	0.521190	0.263933
2	1	0	2.311145	1.605595	0.326523
3	6	0	1.202612	-0.191430	0.148903
4	1	0	1.283684	-1.274938	0.097239
5	6	0	-0.131776	0.342881	0.080292
6	1	0	-0.245157	1.418345	0.124969
7	6	0	-1.214018	-0.463897	-0.049548
8	1	0	-1.061926	-1.537548	-0.065017
9	6	0	3.685457	-0.095038	0.332425
10	8	0	4.398013	-0.297317	-0.624715
11	1	0	4.053990	-0.364699	1.343679
12	7	0	-2.517004	-0.095700	-0.201315
13	6	0	-2.884741	1.303942	-0.124240
14	1	0	-3.917126	1.420595	-0.447249
15	1	0	-2.791272	1.702383	0.893794
16	1	0	-2.250480	1.896091	-0.783181
17	6	0	-3.563370	-1.061095	0.088696
18	1	0	-3.880814	-1.025426	1.138003
19	1	0	-4.432882	-0.865604	-0.538760
20	1	0	-3.204373	-2.065687	-0.125838

TS2a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.201511	0.178940	-0.219953
2	1	0	2.043563	0.462650	-1.253661
3	6	0	1.201045	0.155537	0.669294
4	1	0	1.455707	-0.135487	1.688980
5	6	0	-0.201058	0.528424	0.395164
6	1	0	-0.438011	1.583171	0.469385
7	6	0	-1.145119	-0.371641	0.069854
8	1	0	-0.881882	-1.423120	0.035948
9	6	0	3.560257	-0.185828	0.175311
10	8	0	4.520011	-0.194797	-0.570064
11	1	0	3.676014	-0.469455	1.240027
12	7	0	-2.450145	-0.127405	-0.287139
13	6	0	-2.954699	1.226769	-0.198021
14	1	0	-3.946906	1.269646	-0.643042
15	1	0	-3.022871	1.582616	0.839253
16	1	0	-2.303565	1.905781	-0.748575
17	6	0	-3.421594	-1.185485	-0.062043
18	1	0	-3.796240	-1.200223	0.969917
19	1	0	-4.270846	-1.054130	-0.732151
20	1	0	-2.966090	-2.151538	-0.273236

TS2b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.057127	0.136885	-0.033875
2	1	0	-1.721073	1.159161	-0.160456
3	6	0	-1.198333	-0.915075	0.062657
4	1	0	-1.665920	-1.890754	0.168689
5	6	0	0.228181	-0.941938	0.045818
6	1	0	0.694568	-1.915550	0.088993
7	6	0	1.012927	0.177715	-0.004428
8	1	0	0.542887	1.153133	0.004467
9	6	0	-3.477585	-0.074530	0.021958
10	8	0	-4.336267	0.797256	-0.052608
11	1	0	-3.781945	-1.134964	0.141704
12	7	0	2.354355	0.222990	-0.069520
13	6	0	3.142455	-0.997315	-0.074939
14	1	0	4.173827	-0.754587	-0.316853
15	1	0	3.119287	-1.495168	0.899146
16	1	0	2.763256	-1.690228	-0.826090
17	6	0	3.069537	1.480651	0.077432
18	1	0	3.575100	1.537624	1.045541
19	1	0	3.818206	1.583839	-0.709030
20	1	0	2.371123	2.310159	0.003670

TS2c

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	2.194469	-0.347131	0.585510
2	1	0	1.901621	-0.783185	1.533576
3	6	0	1.295462	-0.148011	-0.385416
4	1	0	1.666180	0.290698	-1.309986
5	6	0	-0.133578	-0.511778	-0.309247
6	1	0	-0.381176	-1.532243	-0.577539
7	6	0	-1.090790	0.356584	0.058825
8	1	0	-0.815088	1.380527	0.285888
9	6	0	3.614818	0.013581	0.437290
10	8	0	4.120887	0.496335	-0.556309
11	1	0	4.239497	-0.185368	1.328602
12	7	0	-2.431748	0.102691	0.239155
13	6	0	-2.944871	-1.202029	-0.122336
14	1	0	-3.981169	-1.281773	0.200449
15	1	0	-2.902457	-1.385735	-1.204877
16	1	0	-2.370182	-1.981932	0.377416
17	6	0	-3.353667	1.214895	0.073036
18	1	0	-3.603417	1.401529	-0.979839
19	1	0	-4.278020	1.010163	0.612712
20	1	0	-2.911704	2.121131	0.484011

TS3a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.361350	0.000001	-0.381341
2	1	0	2.421074	0.000003	-1.463358
3	6	0	1.178595	-0.000001	0.262722
4	1	0	1.185963	-0.000003	1.349491
5	6	0	-0.112283	0.000001	-0.377169
6	1	0	-0.151307	0.000003	-1.460264
7	6	0	-1.260301	-0.000001	0.310481
8	1	0	-1.238578	-0.000003	1.406197
9	6	0	3.615013	-0.000001	0.355730
10	8	0	4.720702	0.000000	-0.153611
11	1	0	3.508696	-0.000003	1.458664
12	7	0	-2.537020	0.000001	-0.309364
13	6	0	-3.290276	1.209627	0.033745
14	1	0	-4.241971	1.197255	-0.496672
15	1	0	-3.496743	1.288722	1.112612
16	1	0	-2.732910	2.091098	-0.277809
17	6	0	-3.290276	-1.209627	0.033741
18	1	0	-3.496744	-1.288726	1.112607
19	1	0	-4.241971	-1.197252	-0.496677
20	1	0	-2.732910	-2.091097	-0.277816

TS3b = GS

TS3c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.224604	-0.000000	-0.356800

2	1	0	-2.160537	0.000008	-1.438686
3	6	0	-1.123142	-0.000007	0.418312
4	1	0	-1.253211	-0.000014	1.497623
5	6	0	0.233353	-0.000005	-0.066089
6	1	0	0.380284	-0.000002	-1.140760
7	6	0	1.290628	-0.000004	0.758601
8	1	0	1.122801	-0.000005	1.833867
9	6	0	-3.554637	-0.000002	0.231528
10	8	0	-4.594323	0.000007	-0.401709
11	1	0	-3.575782	-0.000013	1.339136
12	7	0	2.659728	-0.000000	0.355990
13	6	0	3.065643	1.216823	-0.346045
14	1	0	4.149648	1.212038	-0.463422
15	1	0	2.613087	1.315250	-1.343892
16	1	0	2.790045	2.090800	0.242267
17	6	0	3.065650	-1.216815	-0.346057
18	1	0	2.613100	-1.315232	-1.343908
19	1	0	4.149655	-1.212026	-0.463427
20	1	0	2.790051	-2.090799	0.242243

6b, 225 K, dichloromethane, B3LYP/aug-cc-pVTZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.530254	0.390523	-0.017066
2	1	0	3.540316	1.465256	-0.159839
3	6	0	2.356752	-0.308206	0.005655
4	1	0	2.427593	-1.383694	0.155177
5	6	0	1.056514	0.223279	-0.148559
6	1	0	0.953118	1.288516	-0.303249
7	6	0	-0.041383	-0.597053	-0.105438
8	1	0	0.126216	-1.660437	0.024643
9	6	0	4.784171	-0.276323	0.148770
10	8	0	5.895216	0.257171	0.145366
11	1	0	4.710682	-1.372721	0.291586
12	7	0	-1.338555	-0.265354	-0.191592
13	6	0	-1.805802	1.097381	-0.432597
14	1	0	-1.046792	1.807970	-0.118120
15	1	0	-1.985932	1.237806	-1.503463
16	6	0	-2.365872	-1.294629	-0.352959
17	1	0	-1.970532	-2.249500	-0.011892
18	1	0	-2.625515	-1.387701	-1.412880
19	6	0	-3.087825	1.357320	0.350454
20	1	0	-3.511537	2.316517	0.060052
21	1	0	-2.868900	1.378403	1.424374
22	6	0	-3.611386	-0.927652	0.440435
23	1	0	-4.416249	-1.625705	0.219102
24	1	0	-3.397926	-0.961516	1.515235
25	8	0	-4.077366	0.369884	0.083164

TS2a (TSCC(C))

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	3.375385	-0.211315	-0.238389
2	1	0	3.142425	-0.598836	-1.223128
3	6	0	2.437816	-0.068959	0.707536
4	1	0	2.763600	0.321217	1.671700
5	6	0	1.014679	-0.434514	0.563852
6	1	0	0.768686	-1.470619	0.764389
7	6	0	0.069380	0.449626	0.206934
8	1	0	0.348788	1.485771	0.048864
9	6	0	4.760456	0.159339	0.029027
10	8	0	5.671258	0.065349	-0.774826
11	1	0	4.952842	0.550657	1.045512
12	7	0	-1.266474	0.210627	-0.042003
13	6	0	-1.819228	-1.102712	0.258419
14	1	0	-1.153636	-1.870833	-0.134907
15	1	0	-1.902066	-1.253021	1.344343
16	6	0	-2.191521	1.312594	0.227441
17	1	0	-1.759013	2.238167	-0.152845
18	1	0	-2.350701	1.431462	1.308159
19	6	0	-3.184212	-1.262831	-0.396275
20	1	0	-3.654270	-2.185882	-0.062181
21	1	0	-3.069322	-1.300319	-1.486182
22	6	0	-3.527192	1.055110	-0.448420
23	1	0	-4.250669	1.815610	-0.160505
24	1	0	-3.407153	1.073885	-1.538322
25	8	0	-4.068454	-0.201559	-0.049127

TS1c (TSCC(O))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.528185	0.591002	0.132647
2	1	0	3.468861	1.658550	-0.060511
3	6	0	2.420463	-0.162849	0.222263
4	1	0	2.536666	-1.222688	0.436718
5	6	0	1.068618	0.300193	0.048898
6	1	0	0.923935	1.349720	-0.171882
7	6	0	0.013855	-0.543653	0.161345
8	1	0	0.210335	-1.593517	0.351531
9	6	0	4.900235	0.050587	0.310430
10	8	0	5.602357	-0.349401	-0.593811
11	1	0	5.298124	0.037134	1.344141
12	7	0	-1.318060	-0.250016	0.097889
13	6	0	-1.767863	1.081985	-0.286923
14	1	0	-1.127630	1.828268	0.180108
15	1	0	-1.700018	1.210502	-1.375239
16	6	0	-2.247357	-1.322446	-0.257642
17	1	0	-1.907829	-2.251203	0.199875
18	1	0	-2.266230	-1.466103	-1.345845
19	6	0	-3.199994	1.309557	0.177814
20	1	0	-3.581558	2.243032	-0.231475
21	1	0	-3.229351	1.366568	1.272488
22	6	0	-3.648478	-0.990319	0.227614
23	1	0	-4.360022	-1.727480	-0.139551
24	1	0	-3.676515	-0.985393	1.323852
25	8	0	-4.073398	0.276699	-0.267203

TS3a (TSCN)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.864767	3.070052	-0.000000
2	1	0	2.850676	2.620154	-0.000000
3	6	0	0.744510	2.319966	-0.000000
4	1	0	-0.215585	2.828742	-0.000000
5	6	0	0.716400	0.880146	-0.000000
6	1	0	1.658993	0.345399	-0.000000
7	6	0	-0.427048	0.183637	0.000000
8	1	0	-1.385992	0.710526	-0.000000
9	6	0	1.788685	4.518731	-0.000000
10	8	0	2.753535	5.267477	-0.000000
11	1	0	0.763931	4.935032	-0.000000
12	7	0	-0.468732	-1.233636	0.000000
13	6	0	-1.135300	-1.755793	1.206833
14	1	0	-0.593306	-1.408901	2.086522
15	1	0	-2.171609	-1.390829	1.277823
16	6	0	-1.135300	-1.755793	-1.206833
17	1	0	-0.593306	-1.408901	-2.086522
18	1	0	-2.171609	-1.390829	-1.277823
19	6	0	-1.135300	-3.275081	1.174888
20	1	0	-1.691637	-3.670900	2.022750
21	1	0	-0.105402	-3.647852	1.222393
22	6	0	-1.135300	-3.275081	-1.174888
23	1	0	-1.691637	-3.670900	-2.022750
24	1	0	-0.105402	-3.647852	-1.222393
25	8	0	-1.771494	-3.771495	0.000000

TSCN,CC(C)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.420714	0.226864	0.212421
2	1	0	3.209008	1.259155	0.499482
3	6	0	2.467692	-0.723993	0.202927
4	1	0	2.761490	-1.739380	-0.090524
5	6	0	1.055593	-0.515719	0.596277
6	1	0	0.823323	-0.554642	1.664988
7	6	0	0.055727	-0.300747	-0.263949
8	1	0	0.249923	-0.255997	-1.347834
9	6	0	4.800196	-0.095904	-0.174648
10	8	0	5.716840	0.709884	-0.195992
11	1	0	4.975812	-1.159546	-0.461276
12	7	0	-1.294187	-0.114655	0.162971
13	6	0	-1.814875	1.202352	-0.244008
14	1	0	-1.179476	1.982955	0.194755
15	1	0	-1.794627	1.320412	-1.346999
16	6	0	-2.174346	-1.182127	-0.345203
17	1	0	-1.801995	-2.148539	0.019435
18	1	0	-2.176887	-1.208894	-1.454397
19	6	0	-3.245908	1.366106	0.255577
20	1	0	-3.673828	2.308493	-0.107514
21	1	0	-3.258344	1.368125	1.359889
22	6	0	-3.596234	-0.958100	0.157594

23	1	0	-4.278075	-1.699902	-0.275945
24	1	0	-3.621498	-1.047084	1.258105
25	8	0	-4.090199	0.323247	-0.233370

TSCN,CC(O)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.573633	-0.263384	0.559386
2	1	0	-3.503066	-0.317438	1.650725
3	6	0	-2.466415	-0.185602	-0.200840
4	1	0	-2.567375	-0.140616	-1.289857
5	6	0	-1.112136	-0.146384	0.332673
6	1	0	-0.986941	-0.185861	1.417491
7	6	0	-0.016744	-0.061961	-0.441523
8	1	0	-0.118105	-0.017320	-1.538556
9	6	0	-4.958972	-0.290280	-0.001056
10	8	0	-5.640729	0.702235	-0.164627
11	1	0	-5.372520	-1.293573	-0.258625
12	7	0	1.305664	-0.024066	0.089539
13	6	0	2.102681	-1.182308	-0.354370
14	1	0	1.599829	-2.101689	-0.026737
15	1	0	2.189371	-1.211213	-1.460127
16	6	0	1.998181	1.227507	-0.268154
17	1	0	1.418433	2.074188	0.122155
18	1	0	2.078911	1.342253	-1.368713
19	6	0	3.496196	-1.113324	0.260471
20	1	0	4.125456	-1.925811	-0.123086
21	1	0	3.424568	-1.202688	1.358909
22	6	0	3.393962	1.235687	0.344852
23	1	0	3.949417	2.124914	0.022529
24	1	0	3.318143	1.239487	1.446585
25	8	0	4.156417	0.105780	-0.081384

7, 215 K, dichloromethane, B3LYP/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.234346	-0.646657	-0.000039
2	6	0	5.160769	1.989506	-0.000019
3	6	0	7.076279	0.474080	-0.000038
4	6	0	4.857894	-0.428266	-0.000030
5	6	0	4.327822	0.872118	-0.000020
6	6	0	6.546130	1.775395	-0.000028
7	6	0	2.828964	0.800300	-0.000012
8	6	0	2.478908	-0.632881	-0.000017
9	6	0	3.731494	-1.416489	-0.000029
10	6	0	1.227344	-1.212270	-0.000013
11	6	0	-0.025252	-0.549409	-0.000002
12	6	0	-1.202536	-1.264186	0.000002
13	6	0	-2.544819	-0.752793	0.000012
14	6	0	-5.261930	0.166263	0.000030
15	6	0	-2.859562	0.631457	0.000020

16	6	0	-3.637546	-1.655805	0.000013
17	6	0	-4.952366	-1.224927	0.000022
18	6	0	-4.165043	1.081824	0.000029
19	8	0	3.850237	-2.641080	-0.000036
20	8	0	2.072371	1.771891	-0.000002
21	7	0	-6.551937	0.608313	0.000039
22	6	0	-7.657712	-0.343886	0.000040
23	6	0	-6.846108	2.038009	0.000047
24	1	0	6.640786	-1.657496	-0.000046
25	1	0	4.746048	2.997012	-0.000011
26	1	0	8.158023	0.338024	-0.000044
27	1	0	7.225034	2.628534	-0.000027
28	1	0	1.211837	-2.307190	-0.000018
29	1	0	-0.025517	0.539347	0.000003
30	1	0	-1.118067	-2.355525	-0.000004
31	1	0	-2.058364	1.369383	0.000020
32	1	0	-3.435720	-2.727996	0.000007
33	1	0	-5.746637	-1.965860	0.000023
34	1	0	-4.347045	2.152643	0.000035
35	1	0	-7.633871	-0.986433	0.893031
36	1	0	-7.633880	-0.986424	-0.892958
37	1	0	-8.600699	0.207415	0.000048
38	1	0	-6.436051	2.532721	0.893179
39	1	0	-7.929585	2.176148	0.000053
40	1	0	-6.436060	2.532729	-0.893085

TS, C-CAr1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.224759	0.477270	-0.000004
2	6	0	5.007354	-2.098064	0.000016
3	6	0	7.001347	-0.686787	0.000005
4	6	0	4.836650	0.334796	-0.000002
5	6	0	4.235617	-0.935529	0.000008
6	6	0	6.399786	-1.958920	0.000015
7	6	0	2.746733	-0.792320	0.000007
8	6	0	2.468239	0.670346	-0.000004
9	6	0	3.775860	1.385577	-0.000010
10	6	0	1.267881	1.314048	-0.000009
11	6	0	-0.040309	0.708126	-0.000004
12	6	0	-1.162410	1.466377	-0.000011
13	6	0	-2.545002	0.924985	-0.000007
14	6	0	-5.225833	-0.084848	-0.000000
15	6	0	-3.225987	0.665293	1.200046
16	6	0	-3.225986	0.665274	-1.200056
17	6	0	-4.528651	0.167057	-1.208321
18	6	0	-4.528651	0.167076	1.208317
19	8	0	3.953761	2.598123	-0.000020
20	8	0	1.939161	-1.715043	0.000015
21	7	0	-6.534844	-0.539270	0.000003
22	6	0	-7.127970	-1.003391	-1.246228
23	6	0	-7.127973	-1.003367	1.246241
24	1	0	6.685746	1.464139	-0.000012
25	1	0	4.538086	-3.081028	0.000024
26	1	0	8.088845	-0.611548	0.000004
27	1	0	7.031847	-2.847086	0.000021
28	1	0	1.305230	2.408111	-0.000018
29	1	0	-0.107425	-0.379309	0.000004

30	1	0	-1.046885	2.556614	-0.000020
31	1	0	-2.727369	0.846759	2.152919
32	1	0	-2.727368	0.846726	-2.152932
33	1	0	-4.998265	-0.027090	-2.168783
34	1	0	-4.998266	-0.027056	2.168782
35	1	0	-6.595172	-1.872377	-1.672772
36	1	0	-7.136990	-0.203265	-1.998808
37	1	0	-8.166016	-1.292893	-1.058712
38	1	0	-6.595180	-1.872348	1.672801
39	1	0	-8.166021	-1.292867	1.058730
40	1	0	-7.136990	-0.203228	1.998807

TS, C-C3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.119758	0.248577	0.330276
2	6	0	-4.637578	-2.158734	-0.022676
3	6	0	-6.746807	-0.999269	0.395400
4	6	0	-4.744453	0.275953	0.088702
5	6	0	-4.012602	-0.911695	-0.085572
6	6	0	-6.013981	-2.189028	0.221605
7	6	0	-2.572835	-0.595987	-0.331693
8	6	0	-2.457768	0.896006	-0.271799
9	6	0	-3.831198	1.447892	-0.028554
10	6	0	-1.365244	1.675179	-0.408672
11	6	0	0.027361	1.238993	-0.631785
12	6	0	0.912083	1.016477	0.358709
13	6	0	2.320467	0.626524	0.226523
14	6	0	5.091755	-0.121990	0.083375
15	6	0	2.958447	0.388821	-1.008122
16	6	0	3.106368	0.465538	1.383151
17	6	0	4.449271	0.100380	1.327560
18	6	0	4.296714	0.023484	-1.086603
19	8	0	-4.141900	2.627458	0.060068
20	8	0	-1.689391	-1.409518	-0.558586
21	7	0	6.429649	-0.453055	0.007813
22	6	0	7.166059	-0.756790	1.226177
23	6	0	7.006285	-0.852164	-1.268280
24	1	0	-6.682654	1.171489	0.463277
25	1	0	-4.067378	-3.076746	-0.158221
26	1	0	-7.819005	-1.056744	0.583222
27	1	0	-6.531948	-3.146466	0.279049
28	1	0	-1.551924	2.756364	-0.366240
29	1	0	0.326944	1.153874	-1.680694
30	1	0	0.563523	1.132240	1.389235
31	1	0	2.399386	0.485418	-1.939099
32	1	0	2.650393	0.628894	2.361375
33	1	0	4.995427	-0.012244	2.260207
34	1	0	4.727431	-0.153366	-2.068529
35	1	0	6.758158	-1.635145	1.756723
36	1	0	7.153662	0.097521	1.917720
37	1	0	8.208823	-0.962900	0.969404
38	1	0	6.536050	-1.764183	-1.675906
39	1	0	8.073194	-1.047655	-1.129707
40	1	0	6.907180	-0.051498	-2.014677

TS, C-N1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.232374	0.683091	-0.000005
2	6	0	-5.186776	-1.966085	0.000087
3	6	0	-7.084398	-0.427904	0.000038
4	6	0	-4.857198	0.449876	-0.000002
5	6	0	-4.340990	-0.856979	0.000044
6	6	0	-6.567911	-1.736201	0.000084
7	6	0	-2.844754	-0.808302	0.000036
8	6	0	-2.473923	0.628598	-0.000018
9	6	0	-3.726530	1.427756	-0.000042
10	6	0	-1.226935	1.192582	-0.000043
11	6	0	0.026029	0.503524	-0.000021
12	6	0	1.203316	1.194593	-0.000051
13	6	0	2.551361	0.644842	-0.000033
14	6	0	5.217341	-0.317948	-0.000003
15	6	0	2.821724	-0.741771	0.000021
16	6	0	3.648204	1.534257	-0.000072
17	6	0	4.959193	1.062777	-0.000057
18	6	0	4.132348	-1.209830	0.000035
19	8	0	-3.825811	2.650760	-0.000087
20	8	0	-2.098193	-1.783436	0.000068
21	7	0	6.554125	-0.855698	0.000015
22	6	0	7.304430	-0.523109	1.215368
23	6	0	7.304430	-0.523194	-1.215361
24	1	0	-6.627829	1.698088	-0.000041
25	1	0	-4.782771	-2.977708	0.000123
26	1	0	-8.164585	-0.280991	0.000036
27	1	0	-7.256576	-2.581307	0.000117
28	1	0	-1.194291	2.286819	-0.000083
29	1	0	0.004642	-0.584897	0.000019
30	1	0	1.145626	2.286972	-0.000092
31	1	0	2.003252	-1.459987	0.000051
32	1	0	3.462098	2.609054	-0.000113
33	1	0	5.784796	1.773859	-0.000087
34	1	0	4.337681	-2.279635	0.000077
35	1	0	6.723749	-0.815917	2.098324
36	1	0	7.551506	0.553756	1.298282
37	1	0	8.245545	-1.088880	1.216713
38	1	0	8.245543	-1.088969	-1.216667
39	1	0	7.551511	0.553664	-1.298348
40	1	0	6.723748	-0.816061	-2.098296

TS, C-N2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.215836	0.555765	-0.000002
2	6	0	-5.064846	-2.049282	-0.000001
3	6	0	-7.022675	-0.588478	-0.000003
4	6	0	-4.832439	0.377909	0.000000
5	6	0	-4.264180	-0.907159	0.000000
6	6	0	-6.454084	-1.874973	-0.000002
7	6	0	-2.771125	-0.798326	0.000002

8	6	0	-2.458305	0.652264	0.000002
9	6	0	-3.741990	1.400459	0.000001
10	6	0	-1.234669	1.265382	0.000002
11	6	0	0.044276	0.625902	0.000002
12	6	0	1.194042	1.361970	0.000001
13	6	0	2.562060	0.864334	0.000000
14	6	0	5.262820	0.003585	-0.000002
15	6	0	2.884464	-0.512533	0.000005
16	6	0	3.623773	1.793308	-0.000006
17	6	0	4.952466	1.369124	-0.000007
18	6	0	4.209728	-0.932482	0.000005
19	8	0	-3.890601	2.618446	0.000001
20	8	0	-1.985898	-1.742670	0.000003
21	7	0	6.647644	-0.393850	-0.000003
22	6	0	7.035087	-1.117723	-1.215195
23	6	0	7.035093	-1.117708	1.215196
24	1	0	-6.651443	1.554157	-0.000002
25	1	0	-4.620784	-3.043975	-0.000001
26	1	0	-8.107895	-0.484981	-0.000004
27	1	0	-7.108257	-2.747040	-0.000003
28	1	0	-1.245110	2.360017	0.000001
29	1	0	0.064941	-0.462505	0.000003
30	1	0	1.094901	2.451403	-0.000001
31	1	0	2.092243	-1.259741	0.000010
32	1	0	3.398993	2.860520	-0.000009
33	1	0	5.766804	2.092680	-0.000012
34	1	0	4.431208	-1.999337	0.000009
35	1	0	6.755064	-0.531203	-2.098419
36	1	0	6.569952	-2.119940	-1.296438
37	1	0	8.125437	-1.248120	-1.217436
38	1	0	8.125442	-1.248104	1.217434
39	1	0	6.569959	-2.119925	1.296451
40	1	0	6.755071	-0.531180	2.098414

TS, C-CAr, C-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.209368	-0.507963	-0.083709
2	6	0	-5.007892	2.071558	0.051439
3	6	0	-6.992731	0.650855	-0.048365
4	6	0	-4.822326	-0.358311	-0.050615
5	6	0	-4.229149	0.914135	0.016138
6	6	0	-6.399037	1.925067	0.018354
7	6	0	-2.740162	0.779637	0.038707
8	6	0	-2.452256	-0.680904	-0.019201
9	6	0	-3.756025	-1.402620	-0.075815
10	6	0	-1.248936	-1.317075	-0.022579
11	6	0	0.054336	-0.700717	0.030546
12	6	0	1.182227	-1.447867	0.022783
13	6	0	2.558306	-0.888497	0.075761
14	6	0	5.185278	0.155705	0.174961
15	6	0	3.199777	-0.679539	1.306522
16	6	0	3.249610	-0.575232	-1.106631
17	6	0	4.546264	-0.057319	-1.056531
18	6	0	4.497995	-0.161178	1.352162
19	8	0	-3.925457	-2.614740	-0.132018
20	8	0	-1.937881	1.705005	0.094158
21	7	0	6.523007	0.690055	0.271869

22	6	0	6.631774	2.059620	-0.237866
23	6	0	7.536851	-0.191733	-0.312658
24	1	0	-6.664214	-1.496298	-0.135494
25	1	0	-4.544743	3.056043	0.103054
26	1	0	-8.079532	0.570032	-0.072767
27	1	0	-7.036435	2.809001	0.044413
28	1	0	-1.277674	-2.410232	-0.070188
29	1	0	0.110293	0.386315	0.077959
30	1	0	1.087859	-2.538110	-0.025170
31	1	0	2.680773	-0.918407	2.234975
32	1	0	2.767658	-0.733105	-2.071819
33	1	0	5.058795	0.183565	-1.987865
34	1	0	4.990969	0.005673	2.309563
35	1	0	5.878124	2.693243	0.245044
36	1	0	6.498746	2.131519	-1.335824
37	1	0	7.626477	2.454510	0.009232
38	1	0	8.533807	0.197631	-0.065844
39	1	0	7.465323	-0.272837	-1.415775
40	1	0	7.442203	-1.196773	0.115896

TS, C-C, CN

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.106533	-0.252714	0.379446
2	6	0	-4.633274	2.138979	-0.097672
3	6	0	-6.736660	0.995179	0.387748
4	6	0	-4.732579	-0.288222	0.131229
5	6	0	-4.005044	0.891974	-0.103960
6	6	0	-6.008352	2.177177	0.152314
7	6	0	-2.566606	0.569114	-0.343518
8	6	0	-2.448376	-0.919123	-0.220726
9	6	0	-3.817950	-1.462508	0.062872
10	6	0	-1.356436	-1.699713	-0.343075
11	6	0	0.028224	-1.264093	-0.612015
12	6	0	0.928832	-0.991399	0.347624
13	6	0	2.333635	-0.592726	0.154691
14	6	0	5.054821	0.182220	-0.096659
15	6	0	2.929166	-0.432470	-1.111783
16	6	0	3.132869	-0.354933	1.289311
17	6	0	4.470845	0.025723	1.169013
18	6	0	4.265256	-0.052159	-1.232260
19	8	0	-4.122615	-2.637281	0.211070
20	8	0	-1.683464	1.371615	-0.607319
21	7	0	6.432256	0.575080	-0.275064
22	6	0	7.382167	-0.412987	0.243478
23	6	0	6.715022	1.920895	0.231381
24	1	0	-6.666061	-1.169553	0.559915
25	1	0	-4.066537	3.050780	-0.280961
26	1	0	-7.807968	1.058819	0.578503
27	1	0	-6.528950	3.134782	0.165784
28	1	0	-1.531364	-2.779397	-0.253372
29	1	0	0.306439	-1.222095	-1.669249
30	1	0	0.607956	-1.060136	1.390468
31	1	0	2.348887	-0.603644	-2.017952
32	1	0	2.695687	-0.470668	2.282322
33	1	0	5.059448	0.201352	2.069493
34	1	0	4.716819	0.070284	-2.216456
35	1	0	7.158277	-1.398311	-0.182857

36	1	0	7.368134	-0.497949	1.348509
37	1	0	8.397735	-0.126219	-0.061352
38	1	0	7.729008	2.211696	-0.074806
39	1	0	6.656712	1.996251	1.335641
40	1	0	6.004452	2.634472	-0.202842

7, 298 K, dichloromethane, B3LYP/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.234346	-0.646657	-0.000039
2	6	0	5.160769	1.989506	-0.000019
3	6	0	7.076279	0.474080	-0.000038
4	6	0	4.857894	-0.428266	-0.000030
5	6	0	4.327822	0.872118	-0.000020
6	6	0	6.546130	1.775395	-0.000028
7	6	0	2.828964	0.800300	-0.000012
8	6	0	2.478908	-0.632881	-0.000017
9	6	0	3.731494	-1.416489	-0.000029
10	6	0	1.227344	-1.212270	-0.000013
11	6	0	-0.025252	-0.549409	-0.000002
12	6	0	-1.202536	-1.264186	0.000002
13	6	0	-2.544819	-0.752793	0.000012
14	6	0	-5.261930	0.166263	0.000030
15	6	0	-2.859562	0.631457	0.000020
16	6	0	-3.637546	-1.655805	0.000013
17	6	0	-4.952366	-1.224927	0.000022
18	6	0	-4.165043	1.081824	0.000029
19	8	0	3.850237	-2.641080	-0.000036
20	8	0	2.072371	1.771891	-0.000002
21	7	0	-6.551937	0.608313	0.000039
22	6	0	-7.657712	-0.343886	0.000040
23	6	0	-6.846108	2.038009	0.000047
24	1	0	6.640786	-1.657496	-0.000046
25	1	0	4.746048	2.997012	-0.000011
26	1	0	8.158023	0.338024	-0.000044
27	1	0	7.225034	2.628534	-0.000027
28	1	0	1.211837	-2.307190	-0.000018
29	1	0	-0.025517	0.539347	0.000003
30	1	0	-1.118067	-2.355525	-0.000004
31	1	0	-2.058364	1.369383	0.000020
32	1	0	-3.435720	-2.727996	0.000007
33	1	0	-5.746637	-1.965860	0.000023
34	1	0	-4.347045	2.152643	0.000035
35	1	0	-7.633871	-0.986433	0.893031
36	1	0	-7.633880	-0.986424	-0.892958
37	1	0	-8.600699	0.207415	0.000048
38	1	0	-6.436051	2.532721	0.893179
39	1	0	-7.929585	2.176148	0.000053
40	1	0	-6.436060	2.532729	-0.893085

TS C-C2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.122675	0.338764	0.000000
2	6	0	4.638245	-2.089638	0.000000
3	6	0	6.773257	-0.902996	-0.000000
4	6	0	4.729021	0.343381	0.000001
5	6	0	3.997223	-0.852369	0.000001
6	6	0	6.040141	-2.101695	-0.000000
7	6	0	2.528193	-0.546736	0.000001
8	6	0	2.400622	0.921752	0.000001
9	6	0	3.771652	1.492532	0.000001
10	6	0	1.309895	1.777231	-0.000000
11	6	0	-0.100979	1.604706	-0.000001
12	6	0	-0.798988	0.414203	-0.000001
13	6	0	-2.226033	0.253699	-0.000001
14	6	0	-5.059423	-0.204890	-0.000000
15	6	0	-3.153098	1.329779	-0.000001
16	6	0	-2.772168	-1.055688	-0.000001
17	6	0	-4.135253	-1.290033	-0.000000
18	6	0	-4.517479	1.117725	-0.000001
19	8	0	4.083505	2.682296	0.000001
20	8	0	1.647063	-1.409432	-0.000000
21	7	0	-6.405911	-0.417009	0.000000
22	6	0	-6.938626	-1.775831	0.000001
23	6	0	-7.334900	0.709031	0.000001
24	1	0	6.686759	1.270863	0.000000
25	1	0	4.066363	-3.016862	0.000000
26	1	0	7.862781	-0.942943	-0.000001
27	1	0	6.572584	-3.053141	-0.000001
28	1	0	1.622162	2.826970	0.000001
29	1	0	-0.663231	2.539802	-0.000001
30	1	0	-0.210749	-0.505063	-0.000001
31	1	0	-2.793375	2.357955	-0.000002
32	1	0	-2.091270	-1.907870	-0.000001
33	1	0	-4.490737	-2.316396	-0.000000
34	1	0	-5.179335	1.979156	-0.000001
35	1	0	-6.617249	-2.332451	0.893074
36	1	0	-6.617249	-2.332452	-0.893071
37	1	0	-8.029878	-1.728837	0.000002
38	1	0	-7.203762	1.337847	0.893187
39	1	0	-8.357087	0.324176	0.000004
40	1	0	-7.203766	1.337845	-0.893186

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.232374	0.683091	-0.000005
2	6	0	-5.186776	-1.966085	0.000087
3	6	0	-7.084398	-0.427904	0.000038
4	6	0	-4.857198	0.449876	-0.000002
5	6	0	-4.340990	-0.856979	0.000044
6	6	0	-6.567911	-1.736201	0.000084
7	6	0	-2.844754	-0.808302	0.000036
8	6	0	-2.473923	0.628598	-0.000018
9	6	0	-3.726530	1.427756	-0.000042
10	6	0	-1.226935	1.192582	-0.000043
11	6	0	0.026029	0.503524	-0.000021

12	6	0	1.203316	1.194593	-0.000051
13	6	0	2.551361	0.644842	-0.000033
14	6	0	5.217341	-0.317948	-0.000003
15	6	0	2.821724	-0.741771	0.000021
16	6	0	3.648204	1.534257	-0.000072
17	6	0	4.959193	1.062777	-0.000057
18	6	0	4.132348	-1.209830	0.000035
19	8	0	-3.825811	2.650760	-0.000087
20	8	0	-2.098193	-1.783436	0.000068
21	7	0	6.554125	-0.855698	0.000015
22	6	0	7.304430	-0.523109	1.215368
23	6	0	7.304430	-0.523194	-1.215361
24	1	0	-6.627829	1.698088	-0.000041
25	1	0	-4.782771	-2.977708	0.000123
26	1	0	-8.164585	-0.280991	0.000036
27	1	0	-7.256576	-2.581307	0.000117
28	1	0	-1.194291	2.286819	-0.000083
29	1	0	0.004642	-0.584897	0.000019
30	1	0	1.145626	2.286972	-0.000092
31	1	0	2.003252	-1.459987	0.000051
32	1	0	3.462098	2.609054	-0.000113
33	1	0	5.784796	1.773859	-0.000087
34	1	0	4.337681	-2.279635	0.000077
35	1	0	6.723749	-0.815917	2.098324
36	1	0	7.551506	0.553756	1.298282
37	1	0	8.245545	-1.088880	1.216713
38	1	0	8.245543	-1.088969	-1.216667
39	1	0	7.551511	0.553664	-1.298348
40	1	0	6.723748	-0.816061	-2.098296

TS C-N2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.215836	0.555765	-0.000002
2	6	0	-5.064846	-2.049282	-0.000001
3	6	0	-7.022675	-0.588478	-0.000003
4	6	0	-4.832439	0.377909	-0.000000
5	6	0	-4.264180	-0.907159	0.000000
6	6	0	-6.454084	-1.874973	-0.000002
7	6	0	-2.771125	-0.798326	0.000002
8	6	0	-2.458305	0.652264	0.000002
9	6	0	-3.741990	1.400459	0.000001
10	6	0	-1.234669	1.265382	0.000002
11	6	0	0.044276	0.625902	0.000002
12	6	0	1.194042	1.361970	0.000001
13	6	0	2.562060	0.864334	0.000000
14	6	0	5.262820	0.003585	-0.000002
15	6	0	2.884464	-0.512533	0.000005
16	6	0	3.623773	1.793308	-0.000006
17	6	0	4.952466	1.369124	-0.000007
18	6	0	4.209728	-0.932482	0.000005
19	8	0	-3.890601	2.618446	0.000001
20	8	0	-1.985898	-1.742670	0.000003
21	7	0	6.647644	-0.393850	-0.000003
22	6	0	7.035087	-1.117723	-1.215195
23	6	0	7.035093	-1.117708	1.215196
24	1	0	-6.651443	1.554157	-0.000002
25	1	0	-4.620784	-3.043975	-0.000001

26	1	0	-8.107895	-0.484981	-0.000004
27	1	0	-7.108257	-2.747040	-0.000003
28	1	0	-1.245110	2.360017	0.000001
29	1	0	0.064941	-0.462505	0.000003
30	1	0	1.094901	2.451403	-0.000001
31	1	0	2.092243	-1.259741	0.000010
32	1	0	3.398993	2.860520	-0.000009
33	1	0	5.766804	2.092680	-0.000012
34	1	0	4.431208	-1.999337	0.000009
35	1	0	6.755064	-0.531203	-2.098419
36	1	0	6.569952	-2.119940	-1.296438
37	1	0	8.125437	-1.248120	-1.217436
38	1	0	8.125442	-1.248104	1.217434
39	1	0	6.569959	-2.119925	1.296451
40	1	0	6.755071	-0.531180	2.098414

TS C-CAr1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.224759	0.477270	-0.000004
2	6	0	5.007354	-2.098064	0.000016
3	6	0	7.001347	-0.686787	0.000005
4	6	0	4.836650	0.334796	-0.000002
5	6	0	4.235617	-0.935529	0.000008
6	6	0	6.399786	-1.958920	0.000015
7	6	0	2.746733	-0.792320	0.000007
8	6	0	2.468239	0.670346	-0.000004
9	6	0	3.775860	1.385577	-0.000010
10	6	0	1.267881	1.314048	-0.000009
11	6	0	-0.040309	0.708126	-0.000004
12	6	0	-1.162410	1.466377	-0.000011
13	6	0	-2.545002	0.924985	-0.000007
14	6	0	-5.225833	-0.084848	0.000000
15	6	0	-3.225987	0.665293	1.200046
16	6	0	-3.225986	0.665274	-1.200056
17	6	0	-4.528651	0.167057	-1.208321
18	6	0	-4.528651	0.167076	1.208317
19	8	0	3.953761	2.598123	-0.000020
20	8	0	1.939161	-1.715043	0.000015
21	7	0	-6.534844	-0.539270	0.000003
22	6	0	-7.127970	-1.003391	-1.246228
23	6	0	-7.127973	-1.003367	1.246241
24	1	0	6.685746	1.464139	-0.000012
25	1	0	4.538086	-3.081028	0.000024
26	1	0	8.088845	-0.611548	0.000004
27	1	0	7.031847	-2.847086	0.000021
28	1	0	1.305230	2.408111	-0.000018
29	1	0	-0.107425	-0.379309	0.000004
30	1	0	-1.046885	2.556614	-0.000020
31	1	0	-2.727369	0.846759	2.152919
32	1	0	-2.727368	0.846726	-2.152932
33	1	0	-4.998265	-0.027090	-2.168783
34	1	0	-4.998266	-0.027056	2.168782
35	1	0	-6.595172	-1.872377	-1.672772
36	1	0	-7.136990	-0.203265	-1.998808
37	1	0	-8.166016	-1.292893	-1.058712
38	1	0	-6.595180	-1.872348	1.672801
39	1	0	-8.166021	-1.292867	1.058730

40	1	0	-7.136990	-0.203228	1.998807

TS C-CAr2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.232592	0.512846	-0.000001
2	6	0	-5.043858	-2.075850	0.000001
3	6	0	-7.022060	-0.642518	-0.000000
4	6	0	-4.846145	0.354964	-0.000001
5	6	0	-4.259272	-0.921954	0.000001
6	6	0	-6.434657	-1.921259	0.000001
7	6	0	-2.768889	-0.795326	0.000002
8	6	0	-2.474129	0.664179	0.000001
9	6	0	-3.773732	1.393874	-0.000001
10	6	0	-1.266669	1.294464	-0.000000
11	6	0	0.034588	0.673812	0.000000
12	6	0	1.165393	1.419022	-0.000002
13	6	0	2.541072	0.860138	-0.000002
14	6	0	5.202632	-0.198952	-0.000000
15	6	0	3.221840	0.599923	1.200056
16	6	0	3.221839	0.599917	-1.200058
17	6	0	4.518682	0.086756	-1.208377
18	6	0	4.518683	0.086762	1.208376
19	8	0	-3.938173	2.608317	-0.000002
20	8	0	-1.971685	-1.726994	0.000003
21	7	0	6.474318	-0.748912	0.000001
22	6	0	7.224628	-0.809407	-1.246390
23	6	0	7.224629	-0.809403	1.246391
24	1	0	-6.682576	1.504781	-0.000002
25	1	0	-4.585509	-3.063954	0.000002
26	1	0	-8.108651	-0.555204	-0.000001
27	1	0	-7.076499	-2.802380	0.000001
28	1	0	-1.291724	2.388873	-0.000002
29	1	0	0.089379	-0.414322	0.000003
30	1	0	1.062796	2.510575	-0.000005
31	1	0	2.731006	0.801501	2.152940
32	1	0	2.731004	0.801490	-2.152943
33	1	0	4.993901	-0.093192	-2.168864
34	1	0	4.993903	-0.093180	2.168864
35	1	0	7.417904	0.190604	-1.674957
36	1	0	6.690873	-1.407189	-1.997681
37	1	0	8.186071	-1.295982	-1.058421
38	1	0	7.417906	0.190610	1.674954
39	1	0	8.186070	-1.295980	1.058424
40	1	0	6.690873	-1.407180	1.997686

TS C-C1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.125897	0.275257	0.324784
2	6	0	-4.663906	-2.142505	-0.040719
3	6	0	-6.764324	-0.967367	0.378048
4	6	0	-4.749503	0.292114	0.088534

5	6	0	-4.027572	-0.900680	-0.091828
6	6	0	-6.041484	-2.162288	0.197961
7	6	0	-2.584100	-0.596044	-0.330148
8	6	0	-2.456466	0.894588	-0.261116
9	6	0	-3.825586	1.456734	-0.017141
10	6	0	-1.357229	1.665223	-0.392505
11	6	0	0.031341	1.217898	-0.618633
12	6	0	0.914882	0.982477	0.369897
13	6	0	2.319002	0.578472	0.234348
14	6	0	5.077866	-0.213626	0.085075
15	6	0	3.101274	0.392499	1.389723
16	6	0	2.959964	0.364118	-1.003012
17	6	0	4.294021	-0.015564	-1.084746
18	6	0	4.440143	0.013311	1.330913
19	8	0	-4.126129	2.638308	0.079553
20	8	0	-1.706639	-1.415957	-0.557316
21	7	0	6.394566	-0.620274	0.008803
22	6	0	7.062479	-0.674911	-1.283774
23	6	0	7.211137	-0.646543	1.213594
24	1	0	-6.680975	1.202185	0.462623
25	1	0	-4.101461	-3.064557	-0.181131
26	1	0	-7.837716	-1.016658	0.561303
27	1	0	-6.568216	-3.115449	0.245991
28	1	0	-1.534573	2.747691	-0.343437
29	1	0	0.328980	1.134223	-1.668203
30	1	0	0.568066	1.095085	1.401367
31	1	0	2.647564	0.554107	2.369290
32	1	0	2.408735	0.498423	-1.933965
33	1	0	4.731020	-0.159614	-2.069250
34	1	0	4.987228	-0.105663	2.262227
35	1	0	7.117627	0.314174	-1.771447
36	1	0	6.547492	-1.365964	-1.965849
37	1	0	8.081308	-1.045530	-1.141302
38	1	0	7.317807	0.352834	1.670950
39	1	0	8.208064	-1.017251	0.959718
40	1	0	6.782987	-1.323914	1.966070

TS C-C3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.119758	0.248577	0.330276
2	6	0	-4.637578	-2.158734	-0.022676
3	6	0	-6.746807	-0.999269	0.395400
4	6	0	-4.744453	0.275953	0.088702
5	6	0	-4.012602	-0.911695	-0.085572
6	6	0	-6.013981	-2.189028	0.221605
7	6	0	-2.572835	-0.595987	-0.331693
8	6	0	-2.457768	0.896006	-0.271799
9	6	0	-3.831198	1.447892	-0.028554
10	6	0	-1.365244	1.675179	-0.408672
11	6	0	0.027361	1.238993	-0.631785
12	6	0	0.912083	1.016477	0.358709
13	6	0	2.320467	0.626524	0.226523
14	6	0	5.091755	-0.121990	0.083375
15	6	0	2.958447	0.388821	-1.008122
16	6	0	3.106368	0.465538	1.383151
17	6	0	4.449271	0.100380	1.327560
18	6	0	4.296714	0.023484	-1.086603

19	8	0	-4.141900	2.627458	0.060068
20	8	0	-1.689391	-1.409518	-0.558586
21	7	0	6.429649	-0.453055	0.007813
22	6	0	7.166059	-0.756790	1.226177
23	6	0	7.006285	-0.852164	-1.268280
24	1	0	-6.682654	1.171489	0.463277
25	1	0	-4.067378	-3.076746	-0.158221
26	1	0	-7.819005	-1.056744	0.583222
27	1	0	-6.531948	-3.146466	0.279049
28	1	0	-1.551924	2.756364	-0.366240
29	1	0	0.326944	1.153874	-1.680694
30	1	0	0.563523	1.132240	1.389235
31	1	0	2.399386	0.485418	-1.939099
32	1	0	2.650393	0.628894	2.361375
33	1	0	4.995427	-0.012244	2.260207
34	1	0	4.727431	-0.153366	-2.068529
35	1	0	6.758158	-1.635145	1.756723
36	1	0	7.153662	0.097521	1.917720
37	1	0	8.208823	-0.962900	0.969404
38	1	0	6.536050	-1.764183	-1.675906
39	1	0	8.073194	-1.047655	-1.129707
40	1	0	6.907180	-0.051498	-2.014677

TS C-CAr, C-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.209369	-0.507965	-0.083715
2	6	0	5.007895	2.071557	0.051443
3	6	0	6.992733	0.650853	-0.048370
4	6	0	4.822327	-0.358312	-0.050617
5	6	0	4.229151	0.914134	0.016141
6	6	0	6.399039	1.925064	0.018354
7	6	0	2.740163	0.779638	0.038714
8	6	0	2.452257	-0.680903	-0.019199
9	6	0	3.756024	-1.402619	-0.075817
10	6	0	1.248935	-1.317073	-0.022578
11	6	0	-0.054336	-0.700715	0.030549
12	6	0	-1.182228	-1.447865	0.022778
13	6	0	-2.558306	-0.888496	0.075759
14	6	0	-5.185280	0.155705	0.174961
15	6	0	-3.249607	-0.575217	-1.106632
16	6	0	-3.199782	-0.679552	1.306519
17	6	0	-4.498001	-0.161191	1.352160
18	6	0	-4.546260	-0.057304	-1.056531
19	8	0	3.925455	-2.614740	-0.132022
20	8	0	1.937884	1.705006	0.094169
21	7	0	-6.523010	0.690053	0.271870
22	6	0	-6.631778	2.059620	-0.237860
23	6	0	-7.536850	-0.191735	-0.312666
24	1	0	6.664214	-1.496300	-0.135503
25	1	0	4.544747	3.056042	0.103062
26	1	0	8.079533	0.570029	-0.072774
27	1	0	7.036439	2.808998	0.044414
28	1	0	1.277673	-2.410230	-0.070191
29	1	0	-0.110292	0.386318	0.077970
30	1	0	-1.087860	-2.538108	-0.025183
31	1	0	-2.767650	-0.733079	-2.071821
32	1	0	-2.680782	-0.918430	2.234972

33	1	0	-4.990979	0.005649	2.309562
34	1	0	-5.058789	0.183590	-1.987864
35	1	0	-6.498748	2.131523	-1.335818
36	1	0	-5.878131	2.693243	0.245055
37	1	0	-7.626484	2.454506	0.009237
38	1	0	-7.465315	-0.272837	-1.415782
39	1	0	-8.533808	0.197627	-0.065856
40	1	0	-7.442203	-1.196777	0.115887

8, 225 K, dichloromethane, B3LYP/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.666668	-0.605782	0.000000
2	6	0	-4.162639	-3.011385	0.000009
3	6	0	-6.299001	-1.857375	0.000003
4	6	0	-4.266825	-0.560570	0.000001
5	6	0	-3.540503	-1.767881	0.000006
6	6	0	-5.562623	-3.049754	0.000008
7	6	0	-3.302027	0.576346	-0.000002
8	6	0	-1.960602	0.014573	0.000001
9	6	0	-2.085512	-1.465414	0.000006
10	8	0	-1.184300	-2.301929	0.000010
11	6	0	-3.674312	1.918571	-0.000006
12	6	0	-2.753991	3.010828	-0.000008
13	6	0	-5.029892	2.368021	-0.000008
14	7	0	-6.112589	2.800668	-0.000010
15	7	0	-2.053056	3.942612	-0.000010
16	6	0	-0.747826	0.700605	-0.000001
17	6	0	0.544251	0.134323	0.000001
18	6	0	1.660888	0.951820	-0.000002
19	6	0	3.034706	0.556821	-0.000001
20	6	0	5.819072	-0.125693	0.000000
21	6	0	3.466936	-0.798021	0.000003
22	6	0	4.047649	1.552352	-0.000005
23	6	0	5.391911	1.235973	-0.000004
24	6	0	4.804146	-1.134075	0.000004
25	7	0	7.138925	-0.454001	0.000000
26	6	0	8.160516	0.589956	-0.000004
27	6	0	7.557338	-1.853791	0.000005
28	1	0	-6.276189	0.291820	-0.000004
29	1	0	-3.569028	-3.924948	0.000013
30	1	0	-7.387972	-1.899353	0.000003
31	1	0	-6.083555	-4.007123	0.000011
32	1	0	-0.777861	1.789529	-0.000005
33	1	0	0.639152	-0.948262	0.000004
34	1	0	1.484130	2.031856	-0.000006
35	1	0	2.731548	-1.601266	0.000006
36	1	0	3.752920	2.602518	-0.000008
37	1	0	6.120752	2.040976	-0.000007
38	1	0	5.078384	-2.184933	0.000007
39	1	0	9.146458	0.120514	-0.000004
40	1	0	8.080792	1.226813	-0.893251
41	1	0	8.080795	1.226818	0.893240
42	1	0	7.191284	-2.380378	0.893464
43	1	0	7.191284	-2.380384	-0.893450

44	1	0	8.648594	-1.896414	0.000006

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.608166	-0.775130	0.000007
2	6	0	-3.966223	-3.091936	-0.000008
3	6	0	-6.164503	-2.058864	0.000005
4	6	0	-4.210714	-0.648441	0.000001
5	6	0	-3.415431	-1.813130	-0.000006
6	6	0	-5.359027	-3.208912	-0.000002
7	6	0	-3.326015	0.542582	0.000001
8	6	0	-1.935564	0.058394	-0.000002
9	6	0	-1.982155	-1.439845	-0.000010
10	8	0	-1.037593	-2.219148	-0.000017
11	6	0	-3.764269	1.855301	0.000001
12	6	0	-2.901435	2.996411	-0.000005
13	6	0	-5.144842	2.231502	0.000004
14	7	0	-6.248784	2.602360	0.000007
15	7	0	-2.252172	3.963428	-0.000010
16	6	0	-0.784665	0.803992	0.000004
17	6	0	0.565237	0.301293	0.000002
18	6	0	1.615236	1.159954	0.000011
19	6	0	3.039416	0.743218	0.000008
20	6	0	5.798430	-0.024535	0.000002
21	6	0	3.740190	0.545556	-1.200478
22	6	0	3.740190	0.545537	1.200491
23	6	0	5.081776	0.164929	1.208430
24	6	0	5.081776	0.164949	-1.208423
25	7	0	7.141573	-0.362754	-0.000001
26	6	0	7.774334	-0.770434	1.246577
27	6	0	7.774336	-0.770408	-1.246587
28	1	0	-6.268434	0.085717	0.000013
29	1	0	-3.320632	-3.969251	-0.000013
30	1	0	-7.248916	-2.165146	0.000010
31	1	0	-5.825199	-4.193917	-0.000003
32	1	0	-0.865950	1.890008	0.000013
33	1	0	0.730027	-0.773593	-0.000008
34	1	0	1.403806	2.235724	0.000021
35	1	0	3.227630	0.682615	-2.153301
36	1	0	3.227630	0.682581	2.153316
37	1	0	5.567016	0.013931	2.168828
38	1	0	5.567015	0.013966	-2.168824
39	1	0	8.833508	-0.968378	1.058451
40	1	0	7.713909	0.028922	1.997610
41	1	0	7.320062	-1.681890	1.675215
42	1	0	7.320066	-1.681856	-1.675244
43	1	0	7.713909	0.028964	-1.997603
44	1	0	8.833510	-0.968353	-1.058464

TS C-C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-5.408158	-1.017651	0.268776
2	6	0	-3.512311	-3.113024	-0.020235
3	6	0	-5.792331	-2.359014	0.347858
4	6	0	-4.054439	-0.717570	0.043564
5	6	0	-3.130245	-1.775314	-0.096530
6	6	0	-4.860042	-3.400847	0.206549
7	6	0	-3.345322	0.574346	-0.087877
8	6	0	-1.912782	0.268334	-0.316696
9	6	0	-1.773657	-1.231892	-0.333586
10	8	0	-0.759482	-1.879417	-0.536125
11	6	0	-3.928309	1.821263	0.005384
12	6	0	-3.215890	3.057490	-0.112509
13	6	0	-5.326209	2.028604	0.236376
14	7	0	-6.451796	2.260652	0.421584
15	7	0	-2.697986	4.096963	-0.196694
16	6	0	-0.887946	1.132610	-0.515590
17	6	0	0.534174	0.780992	-0.706754
18	6	0	1.424841	0.702697	0.299730
19	6	0	2.862486	0.429354	0.198082
20	6	0	5.685572	-0.102745	0.115485
21	6	0	3.643511	0.383692	1.368389
22	6	0	3.537268	0.209866	-1.020244
23	6	0	4.902286	-0.044393	-1.070033
24	6	0	5.012679	0.130504	1.341649
25	7	0	7.035483	-0.384923	0.072703
26	6	0	7.722630	-0.451057	-1.209218
27	6	0	7.833676	-0.275684	1.285069
28	1	0	-6.161620	-0.245192	0.381467
29	1	0	-2.771816	-3.903558	-0.134596
30	1	0	-6.840535	-2.599810	0.522522
31	1	0	-5.194438	-4.435777	0.274363
32	1	0	-1.112560	2.199473	-0.562999
33	1	0	0.849026	0.661128	-1.747506
34	1	0	1.057183	0.849704	1.319366
35	1	0	3.163678	0.555900	2.333581
36	1	0	2.988393	0.240648	-1.961699
37	1	0	5.364287	-0.198782	-2.041449
38	1	0	5.556219	0.115752	2.282466
39	1	0	8.771043	-0.709434	-1.036956
40	1	0	7.287279	-1.229369	-1.851851
41	1	0	7.686632	0.507622	-1.755584
42	1	0	7.839891	0.750358	1.692903
43	1	0	7.460025	-0.952759	2.066414
44	1	0	8.864381	-0.562778	1.059561

TS C-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.626600	-0.695179	-0.000022
2	6	0	-4.051785	-3.057292	0.000094
3	6	0	-6.220137	-1.963316	0.000016
4	6	0	-4.227076	-0.608677	-0.000002
5	6	0	-3.465406	-1.795114	0.000055
6	6	0	-5.448253	-3.135137	0.000074
7	6	0	-3.304389	0.556583	-0.000033
8	6	0	-1.935437	0.033027	0.000005
9	6	0	-2.021694	-1.458313	0.000064
10	8	0	-1.097661	-2.264888	0.000112

11	6	0	-3.708135	1.883335	-0.000088
12	6	0	-2.814710	2.999669	-0.000120
13	6	0	-5.076977	2.296970	-0.000121
14	7	0	-6.170511	2.698650	-0.000150
15	7	0	-2.137477	3.947748	-0.000148
16	6	0	-0.755653	0.748320	-0.000015
17	6	0	0.564704	0.208424	0.000013
18	6	0	1.646775	1.046847	-0.000017
19	6	0	3.050401	0.674006	-0.000002
20	6	0	5.816788	0.062508	0.000019
21	6	0	4.023458	1.696842	-0.000042
22	6	0	3.495886	-0.668957	0.000049
23	6	0	4.853267	-0.966235	0.000060
24	6	0	5.384309	1.394836	-0.000032
25	7	0	7.231518	-0.206681	0.000030
26	6	0	7.682983	-0.892420	-1.215605
27	6	0	7.682984	-0.892315	1.215723
28	1	0	-6.262107	0.184077	-0.000066
29	1	0	-3.431571	-3.952792	0.000138
30	1	0	-7.307222	-2.038169	0.000001
31	1	0	-5.941907	-4.106705	0.000103
32	1	0	-0.809721	1.836094	-0.000059
33	1	0	0.681678	-0.871825	0.000056
34	1	0	1.451866	2.123125	-0.000059
35	1	0	3.701605	2.738739	-0.000082
36	1	0	2.774924	-1.485009	0.000081
37	1	0	5.171631	-2.008105	0.000100
38	1	0	6.130220	2.188430	-0.000064
39	1	0	8.780632	-0.921558	-1.218052
40	1	0	7.312136	-1.933185	-1.296452
41	1	0	7.349915	-0.334080	-2.098641
42	1	0	8.780633	-0.921452	1.218172
43	1	0	7.349916	-0.333898	2.098711
44	1	0	7.312137	-1.933072	1.296661

TS C-CAr, C-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.603904	-0.744017	-0.044781
2	6	0	3.979108	-3.072467	0.012563
3	6	0	6.169333	-2.023624	-0.041555
4	6	0	4.205756	-0.627224	-0.018826
5	6	0	3.419067	-1.797582	0.009562
6	6	0	5.372363	-3.179396	-0.013401
7	6	0	3.313406	0.557505	-0.015688
8	6	0	1.925967	0.063588	0.020231
9	6	0	1.983706	-1.435058	0.033763
10	8	0	1.044602	-2.220184	0.059771
11	6	0	3.740885	1.872991	-0.045042
12	6	0	2.868730	3.007073	-0.046975
13	6	0	5.118298	2.259463	-0.079137
14	7	0	6.219144	2.638142	-0.107173
15	7	0	2.210928	3.968222	-0.050661
16	6	0	0.770973	0.800592	0.041014
17	6	0	-0.574961	0.285116	0.073239
18	6	0	-1.631703	1.132949	0.087243
19	6	0	-3.051892	0.697900	0.115748
20	6	0	-5.763460	-0.102290	0.166593

21	6	0	-3.718891	0.508460	1.335986
22	6	0	-3.758572	0.488304	-1.080323
23	6	0	-5.097548	0.090640	-1.053834
24	6	0	-5.059488	0.110354	1.357294
25	7	0	-7.145723	-0.512038	0.238621
26	6	0	-7.376980	-1.849676	-0.313433
27	6	0	-8.067753	0.477664	-0.325069
28	1	0	6.257723	0.121439	-0.066910
29	1	0	3.340136	-3.954318	0.034656
30	1	0	7.254274	-2.122302	-0.061423
31	1	0	5.845717	-4.160951	-0.011877
32	1	0	0.843170	1.887123	0.031812
33	1	0	-0.728310	-0.791446	0.084294
34	1	0	-1.440923	2.211504	0.075506
35	1	0	-3.187863	0.668454	2.274455
36	1	0	-3.256528	0.633176	-2.037198
37	1	0	-5.622567	-0.071124	-1.995151
38	1	0	-5.573912	-0.041490	2.305846
39	1	0	-8.406113	-2.157250	-0.084012
40	1	0	-7.242135	-1.900702	-1.412381
41	1	0	-6.689664	-2.564982	0.154098
42	1	0	-9.098749	0.175328	-0.096892
43	1	0	-7.884287	1.456080	0.135086
44	1	0	-7.978730	0.585084	-1.424629

9, 242 K, dichloromethane, B3LYP/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.332136	-0.161850	-1.118799
2	6	0	-4.161762	2.401097	-0.824786
3	6	0	-5.993527	0.985446	-1.575246
4	6	0	-4.070950	-0.025375	-0.531941
5	6	0	-3.487281	1.260453	-0.382422
6	6	0	-5.414621	2.250684	-1.432835
7	6	0	-3.132583	-1.032057	0.005447
8	6	0	-1.887524	-0.327351	0.312102
9	6	0	-2.184567	1.099804	0.290773
10	6	0	-1.476048	2.107207	0.932887
11	6	0	-3.416702	-2.376112	0.208044
12	6	0	-2.533526	-3.281730	0.872870
13	6	0	-4.650434	-2.989762	-0.168022
14	7	0	-5.634391	-3.543353	-0.457300
15	7	0	-1.855795	-4.053972	1.422917
16	6	0	-0.635380	-0.950418	0.318500
17	6	0	0.642008	-0.381847	0.177295
18	6	0	1.763914	-1.195214	0.120535
19	6	0	3.122514	-0.802460	-0.057138
20	6	0	5.885957	-0.127677	-0.407686
21	6	0	3.545290	0.549535	-0.196792
22	6	0	4.135880	-1.799060	-0.099339
23	6	0	5.468862	-1.486499	-0.267999
24	6	0	4.871075	0.881496	-0.366631
25	7	0	7.194057	0.197494	-0.571450
26	6	0	8.218744	-0.844285	-0.599910

27	6	0	7.602717	1.594105	-0.711850
28	6	0	-0.456452	1.850640	1.899572
29	6	0	-1.794722	3.494459	0.809464
30	7	0	-2.003359	4.638005	0.727060
31	7	0	0.346737	1.689163	2.727854
32	1	0	-5.804944	-1.131132	-1.239807
33	1	0	-3.732718	3.393263	-0.724140
34	1	0	-6.969629	0.886655	-2.048932
35	1	0	-5.940932	3.131513	-1.799265
36	1	0	-0.643306	-2.039428	0.329498
37	1	0	0.754211	0.693660	0.071087
38	1	0	1.595597	-2.270848	0.223899
39	1	0	2.811755	1.353599	-0.166965
40	1	0	3.848636	-2.845843	0.006218
41	1	0	6.198005	-2.290782	-0.291429
42	1	0	5.138882	1.929230	-0.465254
43	1	0	9.196162	-0.375538	-0.730840
44	1	0	8.054606	-1.541892	-1.433970
45	1	0	8.686066	1.633397	-0.842420
46	1	0	7.132090	2.060152	-1.589360
47	1	0	7.340338	2.178638	0.181869
48	1	0	8.231976	-1.415384	0.339689

TS C-C1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.918722	1.414483	1.048620
2	6	0	-4.918705	-1.414585	1.048526
3	6	0	-5.968199	0.696496	1.652356
4	6	0	-3.874012	0.708249	0.459129
5	6	0	-3.874004	-0.708300	0.459082
6	6	0	-5.968191	-0.696651	1.652310
7	6	0	-2.647577	1.162687	-0.252750
8	6	0	-1.926095	0.000023	-0.635114
9	6	0	-2.647564	-1.162676	-0.252828
10	6	0	-2.299317	-2.501594	-0.509105
11	6	0	-2.299346	2.501626	-0.508939
12	6	0	-1.193060	2.868505	-1.327877
13	6	0	-3.029970	3.618005	-0.017157
14	7	0	-3.589515	4.568618	0.367394
15	7	0	-0.315678	3.224183	-2.011884
16	6	0	-0.586846	0.000051	-1.258926
17	6	0	0.567064	0.000035	-0.538982
18	6	0	1.834778	0.000062	-1.193819
19	6	0	3.092579	0.000042	-0.601542
20	6	0	5.728326	-0.000009	0.509996
21	6	0	3.305384	-0.000009	0.821860
22	6	0	4.263685	0.000071	-1.436516
23	6	0	5.526525	0.000047	-0.915612
24	6	0	4.561126	-0.000033	1.357719
25	7	0	6.960969	-0.000040	1.034426
26	6	0	8.148507	-0.000020	0.169599
27	6	0	7.164781	-0.000099	2.489409
28	6	0	-1.193023	-2.868406	-1.328063
29	6	0	-3.029930	-3.618014	-0.017402
30	7	0	-3.589467	-4.568659	0.367082
31	7	0	-0.315634	-3.224030	-2.012090

32	1	0	-4.943818	2.500049	1.055380
33	1	0	-4.943788	-2.500152	1.055213
34	1	0	-6.787242	1.241146	2.121659
35	1	0	-6.787227	-1.241342	2.121576
36	1	0	-0.511826	0.000087	-2.350254
37	1	0	0.513481	-0.000002	0.549100
38	1	0	1.807966	0.000100	-2.286024
39	1	0	2.450827	-0.000030	1.495139
40	1	0	4.131352	0.000113	-2.518249
41	1	0	6.378032	0.000070	-1.588222
42	1	0	4.674007	-0.000073	2.437104
43	1	0	9.039170	-0.000064	0.799210
44	1	0	8.167236	0.895389	-0.464931
45	1	0	8.236520	-0.000111	2.691753
46	1	0	6.722118	0.895325	2.944147
47	1	0	6.722111	-0.895557	2.944074
48	1	0	8.167206	-0.895371	-0.465013

TS C-C2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.382992	0.337181	-0.959995
2	6	0	-3.783273	2.650931	-0.576135
3	6	0	-5.875518	1.608191	-1.265703
4	6	0	-4.074413	0.221988	-0.475600
5	6	0	-3.274579	1.382602	-0.274747
6	6	0	-5.083306	2.750327	-1.079801
7	6	0	-3.288272	-0.962013	-0.116307
8	6	0	-1.889632	-0.490720	0.051905
9	6	0	-1.978264	0.970620	0.286186
10	6	0	-1.113754	1.754044	1.011474
11	6	0	-3.732179	-2.247617	0.082889
12	6	0	-2.883368	-3.298139	0.562425
13	6	0	-5.092261	-2.645952	-0.118254
14	7	0	-6.187842	-3.006537	-0.273130
15	7	0	-2.240736	-4.180551	0.966001
16	6	0	-0.827004	-1.214031	-0.384570
17	6	0	0.566521	-0.799333	-0.629623
18	6	0	1.586660	-0.933684	0.241153
19	6	0	3.003462	-0.659969	-0.000493
20	6	0	5.806031	-0.144582	-0.354117
21	6	0	3.929083	-0.845671	1.045127
22	6	0	3.521775	-0.215219	-1.234973
23	6	0	4.875018	0.035321	-1.416012
24	6	0	5.289359	-0.601320	0.886374
25	7	0	7.145079	0.114634	-0.524932
26	6	0	7.653994	0.522434	-1.826450
27	6	0	8.082074	-0.144358	0.558465
28	6	0	-0.086653	1.240934	1.866751
29	6	0	-1.269202	3.174999	1.122527
30	7	0	-1.349272	4.331141	1.226535
31	7	0	0.695630	0.918290	2.665059
32	1	0	-6.010079	-0.535229	-1.117877
33	1	0	-3.188744	3.549866	-0.445210
34	1	0	-6.886253	1.710775	-1.658746
35	1	0	-5.484350	3.731126	-1.332924
36	1	0	-1.067825	-2.216892	-0.750491

37	1	0	0.757799	-0.502822	-1.666056
38	1	0	1.355757	-1.287423	1.247268
39	1	0	3.570023	-1.192799	2.015175
40	1	0	2.855659	-0.063048	-2.084438
41	1	0	5.214552	0.372284	-2.391763
42	1	0	5.950077	-0.765915	1.733122
43	1	0	8.730477	0.695404	-1.749131
44	1	0	7.183900	1.457750	-2.166386
45	1	0	9.088137	0.132970	0.233547
46	1	0	7.837206	0.450363	1.451721
47	1	0	8.094011	-1.208562	0.846661
48	1	0	7.483795	-0.248466	-2.596182

TS C-CAr

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.235971	0.141785	-1.251269
2	6	0	-3.840530	2.578749	-0.841122
3	6	0	-5.756249	1.354036	-1.714165
4	6	0	-4.000386	0.147062	-0.594083
5	6	0	-3.304074	1.370011	-0.386216
6	6	0	-5.065861	2.557333	-1.514231
7	6	0	-3.202546	-0.953957	-0.033466
8	6	0	-1.880817	-0.379859	0.295331
9	6	0	-2.064714	1.081294	0.349508
10	6	0	-1.326641	1.970296	1.102182
11	6	0	-3.617829	-2.249138	0.193377
12	6	0	-2.817209	-3.221437	0.873624
13	6	0	-4.911627	-2.735317	-0.175357
14	7	0	-5.951770	-3.174139	-0.459641
15	7	0	-2.206175	-4.039417	1.432975
16	6	0	-0.709479	-1.088435	0.218395
17	6	0	0.637015	-0.590519	0.126650
18	6	0	1.683492	-1.443256	0.002351
19	6	0	3.096906	-1.018175	-0.147719
20	6	0	5.834483	-0.234314	-0.442202
21	6	0	3.926277	-0.838388	0.971001
22	6	0	3.657432	-0.795083	-1.415579
23	6	0	4.988202	-0.406678	-1.566744
24	6	0	5.258588	-0.450900	0.835427
25	7	0	7.166108	0.113500	-0.585373
26	6	0	7.660799	0.531286	-1.889364
27	6	0	7.937955	0.489730	0.590678
28	6	0	-0.350836	1.556363	2.063482
29	6	0	-1.564245	3.381801	1.097053
30	7	0	-1.717958	4.535433	1.112295
31	7	0	0.416425	1.262052	2.887595
32	1	0	-5.788106	-0.777327	-1.421595
33	1	0	-3.320774	3.521814	-0.700691
34	1	0	-6.709523	1.360298	-2.241350
35	1	0	-5.486475	3.489436	-1.889973
36	1	0	-0.795609	-2.168568	0.104300
37	1	0	0.825246	0.481002	0.111240
38	1	0	1.475471	-2.519030	0.015519
39	1	0	3.523367	-0.994370	1.972021
40	1	0	3.042316	-0.919829	-2.307445
41	1	0	5.362633	-0.235675	-2.572325

42	1	0	5.847814	-0.314185	1.738021
43	1	0	8.732597	0.735408	-1.813165
44	1	0	7.158332	1.442026	-2.261647
45	1	0	8.965832	0.705606	0.285736
46	1	0	7.530054	1.382514	1.097444
47	1	0	7.972065	-0.332510	1.318604
48	1	0	7.525549	-0.264362	-2.634910

TS C-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.277984	0.205123	-1.219207
2	6	0	4.121290	-2.368247	-0.927397
3	6	0	5.918435	-0.931452	-1.723948
4	6	0	4.042300	0.054276	-0.580964
5	6	0	3.466193	-1.236798	-0.432111
6	6	0	5.345929	-2.201972	-1.582817
7	6	0	3.131102	1.049905	0.009305
8	6	0	1.879159	0.337164	0.316538
9	6	0	2.194936	-1.096648	0.295257
10	6	0	1.530702	-2.094795	0.982974
11	6	0	3.417570	2.377712	0.264936
12	6	0	2.530845	3.253413	0.967442
13	6	0	4.654172	3.000043	-0.092509
14	7	0	5.642428	3.552499	-0.365200
15	7	0	1.846752	3.997804	1.545498
16	6	0	0.637620	0.941610	0.297329
17	6	0	-0.647350	0.340839	0.174592
18	6	0	-1.767908	1.124248	0.102225
19	6	0	-3.141075	0.688777	-0.071884
20	6	0	-5.855519	-0.041596	-0.420672
21	6	0	-3.517482	-0.668986	-0.186032
22	6	0	-4.157674	1.668731	-0.134619
23	6	0	-5.492101	1.311060	-0.306193
24	6	0	-4.851298	-1.022559	-0.357977
25	7	0	-7.220408	-0.463687	-0.599056
26	6	0	-7.797767	-0.008609	-1.868486
27	6	0	-8.076803	-0.129024	0.544107
28	6	0	0.518606	-1.830325	1.958202
29	6	0	1.889180	-3.476897	0.895286
30	7	0	2.137423	-4.613297	0.843639
31	7	0	-0.277680	-1.658409	2.789896
32	1	0	5.741765	1.178594	-1.343614
33	1	0	3.694794	-3.362223	-0.831793
34	1	0	6.873278	-0.823394	-2.237098
35	1	0	5.857827	-3.073254	-1.989975
36	1	0	0.629064	2.030405	0.265027
37	1	0	-0.733759	-0.739467	0.094073
38	1	0	-1.628865	2.205593	0.181218
39	1	0	-2.765080	-1.454256	-0.138034
40	1	0	-3.888201	2.721788	-0.046501
41	1	0	-6.254211	2.088253	-0.350850
42	1	0	-5.139951	-2.069168	-0.444525
43	1	0	-8.773578	-0.492646	-2.006290
44	1	0	-7.144491	-0.305124	-2.697831
45	1	0	-8.249842	0.958976	0.659480
46	1	0	-9.051507	-0.616150	0.409362

47	1	0	-7.624299	-0.510139	1.467318
48	1	0	-7.948826	1.087881	-1.913676

TS C-CAr, C-N

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.193334	0.114120	-1.320996
2	6	0	-3.823200	2.559686	-0.875783
3	6	0	-5.710316	1.323652	-1.794319
4	6	0	-3.973407	0.126505	-0.635173
5	6	0	-3.290067	1.353778	-0.409534
6	6	0	-5.032342	2.531165	-1.577143
7	6	0	-3.181883	-0.970220	-0.058286
8	6	0	-1.870248	-0.387877	0.298778
9	6	0	-2.066721	1.072289	0.354615
10	6	0	-1.354382	1.962693	1.129370
11	6	0	-3.593002	-2.267827	0.159386
12	6	0	-2.798846	-3.235673	0.853588
13	6	0	-4.876673	-2.761373	-0.234512
14	7	0	-5.908614	-3.205650	-0.539184
15	7	0	-2.192231	-4.050093	1.422739
16	6	0	-0.693510	-1.087189	0.243608
17	6	0	0.651002	-0.575798	0.181545
18	6	0	1.707469	-1.417060	0.083339
19	6	0	3.120173	-0.973489	-0.035074
20	6	0	5.816449	-0.157558	-0.267021
21	6	0	3.911534	-0.789311	1.109197
22	6	0	3.693630	-0.751224	-1.298261
23	6	0	5.025769	-0.345647	-1.411458
24	6	0	5.244514	-0.383642	0.990214
25	7	0	7.196068	0.260414	-0.338471
26	6	0	7.360477	1.604082	-0.899441
27	6	0	8.059505	-0.719087	-1.003435
28	6	0	-0.395140	1.551052	2.108302
29	6	0	-1.606187	3.371868	1.128429
30	7	0	-1.772633	4.523590	1.147825
31	7	0	0.358702	1.257094	2.944763
32	1	0	-5.735364	-0.808320	-1.505290
33	1	0	-3.312834	3.505852	-0.722166
34	1	0	-6.651180	1.324680	-2.343365
35	1	0	-5.450126	3.460987	-1.961565
36	1	0	-0.768337	-2.167589	0.124343
37	1	0	0.827304	0.497820	0.168219
38	1	0	1.520554	-2.495682	0.093174
39	1	0	3.483552	-0.957608	2.097207
40	1	0	3.093639	-0.893635	-2.197340
41	1	0	5.446788	-0.174314	-2.402099
42	1	0	5.855930	-0.235223	1.879822
43	1	0	8.406597	1.915722	-0.777875
44	1	0	6.723421	2.311152	-0.354582
45	1	0	7.856454	-0.819212	-2.088397
46	1	0	9.106907	-0.411627	-0.881999
47	1	0	7.930972	-1.701920	-0.534177
48	1	0	7.109086	1.663956	-1.977241

10, 298 K, dichloromethane, B3LYP/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.336213	-0.412411	-0.000001
2	6	0	-2.502140	-1.140128	0.000000
3	6	0	-3.855165	-0.647794	0.000000
4	6	0	-6.589145	0.226038	-0.000001
5	6	0	-4.194020	0.729709	0.000000
6	6	0	-4.932639	-1.567602	0.000000
7	6	0	-6.255558	-1.158608	0.000000
8	6	0	-5.507965	1.158664	0.000000
9	7	0	-7.888135	0.646755	-0.000002
10	6	0	-8.976605	-0.324196	0.000001
11	6	0	-8.205322	2.070773	0.000002
12	1	0	-1.365199	0.679233	-0.000002
13	1	0	-2.403119	-2.230001	0.000002
14	1	0	-3.406893	1.482802	0.000001
15	1	0	-4.713616	-2.636484	0.000001
16	1	0	-7.036812	-1.913353	0.000000
17	1	0	-5.707099	2.226535	0.000001
18	1	0	-8.942103	-0.966828	0.892851
19	1	0	-8.942105	-0.966830	-0.892847
20	1	0	-9.929363	0.210293	0.000001
21	1	0	-7.803518	2.572911	0.893032
22	1	0	-9.290939	2.191611	0.000003
23	1	0	-7.803520	2.572914	-0.893026
24	6	0	-0.058648	-1.032833	0.000000
25	6	0	1.149182	-0.362167	-0.000001
26	1	0	-0.036927	-2.127612	0.000000
27	1	0	1.165177	0.727759	-0.000002
28	6	0	2.379984	-1.060136	-0.000001
29	6	0	3.651244	-0.521927	-0.000001
30	1	0	2.331027	-2.154166	-0.000001
31	6	0	6.036085	-0.401884	0.000001
32	6	0	7.403973	-0.668578	0.000002
33	6	0	8.284953	0.421881	0.000002
34	6	0	7.801033	1.740975	0.000001
35	6	0	6.423906	2.003583	0.000000
36	6	0	5.552138	0.916380	0.000000
37	1	0	7.774906	-1.693009	0.000003
38	1	0	9.361228	0.247676	0.000004
39	1	0	8.509570	2.569698	0.000002
40	1	0	6.044687	3.024903	-0.000001
41	6	0	4.051353	0.897568	-0.000002
42	8	0	3.329981	1.895775	-0.000003
43	6	0	4.874976	-1.349165	0.000000
44	8	0	4.949908	-2.577550	0.000000

1, 298 K, dichloromethane, M062X/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-5.066991	0.864493	-0.000000
2	6	0	-4.183945	-1.838115	0.000000
3	6	0	-5.981227	-0.191567	-0.000001
4	6	0	-3.714199	0.543489	-0.000000
5	6	0	-3.280471	-0.781506	0.000000
6	6	0	-5.545320	-1.524946	-0.000000
7	6	0	-1.780880	-0.832640	0.000001
8	6	0	-1.312083	0.572206	0.000002
9	6	0	-2.520029	1.442696	0.000001
10	8	0	-2.549104	2.660448	0.000001
11	8	0	-1.141009	-1.871387	0.000003
12	6	0	-0.079364	1.167344	0.000001
13	6	0	1.271691	0.687288	-0.000000
14	6	0	4.025295	-0.061349	-0.000009
15	6	0	1.661358	-0.673736	0.000001
16	6	0	2.305135	1.654913	-0.000003
17	6	0	3.639089	1.308237	-0.000006
18	6	0	2.990281	-1.040440	-0.000002
19	7	0	5.331245	-0.421529	-0.000019
20	6	0	6.368986	0.596626	0.000016
21	6	0	5.702866	-1.827248	0.000002
22	1	0	-5.396913	1.901831	-0.000001
23	1	0	-3.837293	-2.869994	0.000001
24	1	0	-7.049669	0.018614	-0.000001
25	1	0	-6.283724	-2.325300	-0.000000
26	1	0	-0.155993	2.260439	0.000001
27	1	0	0.893607	-1.442158	0.000007
28	1	0	2.036687	2.711487	-0.000001
29	1	0	4.389334	2.092567	-0.000006
30	1	0	3.240107	-2.097032	0.000002
31	1	0	6.298023	1.233211	0.892599
32	1	0	7.343762	0.106811	0.000005
33	1	0	6.298031	1.233259	-0.892533
34	1	0	5.317013	-2.338090	0.892638
35	1	0	5.316962	-2.338124	-0.892591
36	1	0	6.791113	-1.903779	-0.000031

2, 298 K, dichloromethane, M062X/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.653265	-0.473219	-0.251258
2	6	0	3.225350	-2.918655	-0.092192
3	6	0	5.310939	-1.704503	-0.323306
4	6	0	3.264185	-0.474868	-0.102923
5	6	0	2.577990	-1.694045	-0.030299
6	6	0	4.613728	-2.914467	-0.241226
7	6	0	1.114201	-1.445965	0.103778
8	6	0	0.938907	0.031431	0.053392
9	6	0	2.271727	0.624174	0.017255
10	6	0	2.585977	1.954257	0.167494
11	8	0	0.270460	-2.320126	0.168531
12	6	0	-0.217768	0.736822	-0.207492
13	6	0	-1.599643	0.388021	-0.135581

14	6	0	-4.411755	-0.087643	-0.053346
15	6	0	-2.138471	-0.713443	0.576965
16	6	0	-2.523093	1.264251	-0.762952
17	6	0	-3.879697	1.039342	-0.745136
18	6	0	-3.494121	-0.943345	0.625830
19	7	0	-5.740807	-0.326998	-0.026646
20	6	0	-6.266693	-1.469195	0.706153
21	6	0	-6.660126	0.572258	-0.707672
22	6	0	1.623867	2.968001	0.487059
23	6	0	3.924711	2.457741	0.093137
24	7	0	0.885109	3.815079	0.770261
25	7	0	4.990289	2.909766	0.034674
26	1	0	5.231433	0.442032	-0.322693
27	1	0	2.658413	-3.845834	-0.027582
28	1	0	6.392334	-1.718522	-0.446697
29	1	0	5.159642	-3.854717	-0.296080
30	1	0	-0.063537	1.751589	-0.576248
31	1	0	-1.471163	-1.380241	1.111705
32	1	0	-2.142446	2.142870	-1.284019
33	1	0	-4.538782	1.736783	-1.251907
34	1	0	-3.860124	-1.788775	1.199857
35	1	0	-5.853148	-2.408549	0.316634
36	1	0	-7.350987	-1.492568	0.590136
37	1	0	-6.030173	-1.394792	1.776072
38	1	0	-6.606139	1.585512	-0.287071
39	1	0	-6.435269	0.622293	-1.781162
40	1	0	-7.676749	0.197291	-0.583294

3, 298 K, dichloromethane, M062X/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.402860	-0.256625	-1.052351
2	6	0	-2.901655	-2.611667	-0.575759
3	6	0	-4.906000	-1.512650	-1.397341
4	6	0	-3.133875	-0.183671	-0.479206
5	6	0	-2.389732	-1.360204	-0.241259
6	6	0	-4.165532	-2.673727	-1.165628
7	6	0	-1.106545	-0.977968	0.373288
8	6	0	-0.973693	0.474050	0.216211
9	6	0	-2.329589	0.978496	-0.046116
10	6	0	-2.798632	2.255095	0.124630
11	6	0	-0.320969	-1.784009	1.152633
12	6	0	0.160915	1.247384	0.120534
13	6	0	1.525253	0.876372	-0.105769
14	6	0	4.282716	0.301941	-0.539922
15	6	0	1.939161	-0.353981	-0.669696
16	6	0	2.532144	1.829359	0.175156
17	6	0	3.869630	1.556406	-0.007869
18	6	0	3.265966	-0.635162	-0.894646
19	7	0	5.589911	0.014969	-0.725101
20	6	0	6.608781	0.992964	-0.375525
21	6	0	5.987884	-1.264699	-1.292169
22	6	0	-2.011811	3.316668	0.678785
23	6	0	-4.147491	2.639627	-0.166999

24	7	0	-1.401828	4.190635	1.132942
25	7	0	-5.228315	2.991673	-0.390802
26	6	0	0.754146	-1.272591	1.949387
27	7	0	1.604647	-0.877301	2.628540
28	6	0	-0.574536	-3.183215	1.326578
29	7	0	-0.750935	-4.317691	1.480899
30	1	0	-4.996263	0.629384	-1.252726
31	1	0	-2.335503	-3.523823	-0.413314
32	1	0	-5.887967	-1.583803	-1.860832
33	1	0	-4.574839	-3.640321	-1.452959
34	1	0	0.006863	2.325674	0.142790
35	1	0	1.196301	-1.087819	-0.975739
36	1	0	2.240874	2.803014	0.569298
37	1	0	4.602488	2.315664	0.245188
38	1	0	3.530871	-1.581399	-1.355674
39	1	0	7.591673	0.564839	-0.576263
40	1	0	6.551688	1.252867	0.689674
41	1	0	5.588258	-1.388580	-2.307800
42	1	0	7.076797	-1.304355	-1.340276
43	1	0	6.497129	1.909872	-0.970136
44	1	0	5.635225	-2.096372	-0.668262

4, 298 K, dichloromethane, M062X/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.817762	-0.953003	0.044407
2	6	0	-4.961316	1.757450	0.009240
3	6	0	-6.742627	0.094237	0.051488
4	6	0	-4.468610	-0.619042	0.019697
5	6	0	-4.047790	0.709874	0.002425
6	6	0	-6.319888	1.431397	0.034116
7	6	0	-2.547934	0.774034	-0.022657
8	6	0	-2.067022	-0.624637	-0.019172
9	6	0	-3.264425	-1.505888	0.007167
10	8	0	-3.283281	-2.724592	0.017499
11	8	0	-1.919287	1.820310	-0.041798
12	6	0	-0.826354	-1.209695	-0.033354
13	6	0	0.518109	-0.721422	-0.056621
14	6	0	3.254368	0.042511	-0.073417
15	6	0	1.557878	-1.681572	-0.062485
16	6	0	0.898007	0.640879	-0.073179
17	6	0	2.220807	1.030915	-0.091217
18	6	0	2.893250	-1.339276	-0.079899
19	7	0	4.566547	0.413547	-0.037773
20	6	0	4.962018	1.809939	-0.188318
21	6	0	5.633344	-0.572123	-0.176632
22	6	0	2.580538	2.498349	-0.135935
23	6	0	3.956069	2.737613	0.472334
24	6	0	3.964159	-2.405180	-0.109279
25	6	0	5.259789	-1.882312	0.496941
26	1	0	-6.137554	-1.993501	0.057774
27	1	0	-4.625071	2.792745	-0.004382
28	1	0	-7.808799	-0.126523	0.070844
29	1	0	-7.065866	2.224717	0.040241

30	1	0	-0.895119	-2.303300	-0.023536
31	1	0	1.293339	-2.740570	-0.053656
32	1	0	0.122404	1.402922	-0.073472
33	1	0	5.949548	1.919984	0.272894
34	1	0	5.063366	2.060877	-1.257797
35	1	0	6.532185	-0.145610	0.281749
36	1	0	5.852743	-0.743952	-1.244057
37	1	0	1.810409	3.076195	0.387306
38	1	0	2.584036	2.842741	-1.180551
39	1	0	3.934164	2.534808	1.551197
40	1	0	4.272434	3.776260	0.327894
41	1	0	3.609082	-3.293391	0.425663
42	1	0	4.150625	-2.710618	-1.149249
43	1	0	5.131635	-1.709596	1.573614
44	1	0	6.073510	-2.603051	0.362434

6, 298 K, dichloromethane, M062X/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.332085	0.373549	0.014243
2	1	0	2.387680	1.454542	0.056992
3	6	0	1.149880	-0.280846	-0.022672
4	1	0	1.186441	-1.368444	-0.066419
5	6	0	-0.146353	0.308010	-0.007189
6	1	0	-0.224825	1.385793	0.039517
7	6	0	-1.259666	-0.475701	-0.047556
8	1	0	-1.137303	-1.553388	-0.074072
9	6	0	3.571587	-0.367542	-0.002331
10	8	0	4.686454	0.117005	0.028772
11	1	0	3.450336	-1.467866	-0.047444
12	7	0	-2.534282	-0.059271	-0.069491
13	6	0	-2.828925	1.356237	-0.000477
14	1	0	-3.899110	1.502669	-0.116764
15	1	0	-2.514620	1.779166	0.957772
16	1	0	-2.312057	1.889373	-0.799261
17	6	0	-3.637844	-0.988000	0.067175
18	1	0	-4.107677	-0.899841	1.049773
19	1	0	-4.390945	-0.792492	-0.696254
20	1	0	-3.274171	-2.004889	-0.054736

7, 298 K, dichloromethane, M062X/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.213185	-0.635295	-0.000043
2	6	0	5.123696	1.990714	-0.000028
3	6	0	7.043074	0.488613	-0.000045
4	6	0	4.839485	-0.422330	-0.000034

5	6	0	4.303730	0.868143	-0.000025
6	6	0	6.505453	1.784072	-0.000038
7	6	0	2.805085	0.792112	-0.000009
8	6	0	2.461968	-0.645577	-0.000019
9	6	0	3.722205	-1.420968	-0.000036
10	6	0	1.226335	-1.224604	-0.000013
11	6	0	-0.029015	-0.547964	0.000002
12	6	0	-1.189873	-1.265743	0.000005
13	6	0	-2.538320	-0.751737	0.000019
14	6	0	-5.237896	0.167873	0.000048
15	6	0	-2.842720	0.626754	0.000030
16	6	0	-3.622683	-1.651307	0.000018
17	6	0	-4.936215	-1.219797	0.000030
18	6	0	-4.145237	1.081105	0.000044
19	8	0	3.847406	-2.632973	-0.000049
20	8	0	2.051700	1.751302	0.000008
21	7	0	-6.522508	0.611175	0.000071
22	6	0	-7.619030	-0.340985	0.000024
23	6	0	-6.803783	2.036326	0.000035
24	1	0	6.622452	-1.644085	-0.000050
25	1	0	4.699052	2.993169	-0.000021
26	1	0	8.124578	0.361641	-0.000052
27	1	0	7.179440	2.639408	-0.000040
28	1	0	1.206800	-2.319269	-0.000021
29	1	0	-0.024899	0.540098	0.000010
30	1	0	-1.103244	-2.356508	-0.000004
31	1	0	-2.038000	1.360242	0.000028
32	1	0	-3.419775	-2.722657	0.000005
33	1	0	-5.733244	-1.956813	0.000025
34	1	0	-4.327272	2.151316	0.000049
35	1	0	-7.587921	-0.982028	0.892284
36	1	0	-7.587931	-0.981939	-0.892302
37	1	0	-8.562791	0.206641	0.000059
38	1	0	-6.387012	2.523785	0.892454
39	1	0	-7.885122	2.181979	0.000067
40	1	0	-6.387066	2.523737	-0.892438

8, 298 K, dichloromethane, M062X/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.650298	-0.598989	-0.000002
2	6	0	-4.140238	-2.997877	0.000009
3	6	0	-6.273587	-1.850298	0.000001
4	6	0	-4.253624	-0.554103	-0.000000
5	6	0	-3.528639	-1.753507	0.000005
6	6	0	-5.535685	-3.038368	0.000007
7	6	0	-3.292579	0.585791	-0.000003
8	6	0	-1.946692	0.027839	0.000000
9	6	0	-2.071795	-1.452725	0.000005
10	8	0	-1.181525	-2.284493	0.000010
11	6	0	-3.663146	1.911087	-0.000005
12	6	0	-2.736055	3.002431	-0.000003
13	6	0	-5.025040	2.353825	-0.000006
14	7	0	-6.107623	2.768020	-0.000008

15	7	0	-2.021338	3.915060	-0.000002
16	6	0	-0.744144	0.703953	-0.000002
17	6	0	0.549236	0.122423	0.000000
18	6	0	1.648364	0.943879	-0.000003
19	6	0	3.028618	0.551029	-0.000002
20	6	0	5.797401	-0.126217	-0.000000
21	6	0	3.453637	-0.797973	0.000004
22	6	0	4.031036	1.545238	-0.000007
23	6	0	5.374878	1.231757	-0.000006
24	6	0	4.788963	-1.134879	0.000005
25	7	0	7.112541	-0.452792	0.000000
26	6	0	8.122363	0.592837	-0.000006
27	6	0	7.521448	-1.848082	0.000007
28	1	0	-6.264531	0.294755	-0.000008
29	1	0	-3.539929	-3.906128	0.000013
30	1	0	-7.361065	-1.896815	-0.000001
31	1	0	-6.055065	-3.995068	0.000010
32	1	0	-0.758627	1.793088	-0.000006
33	1	0	0.644436	-0.959084	0.000004
34	1	0	1.466996	2.023047	-0.000008
35	1	0	2.716561	-1.599204	0.000008
36	1	0	3.732402	2.593714	-0.000012
37	1	0	6.104618	2.035146	-0.000010
38	1	0	5.066062	-2.184371	0.000010
39	1	0	9.109945	0.129538	-0.000006
40	1	0	8.034011	1.227266	-0.892605
41	1	0	8.034014	1.227274	0.892587
42	1	0	7.149704	-2.369097	0.892807
43	1	0	7.149704	-2.369106	-0.892788
44	1	0	8.611368	-1.895456	0.000007

9, 298 K, dichloromethane, M062X/aug-cc-pVDZ

GS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.305962	-0.084043	-1.140923
2	6	0	-4.055129	2.438636	-0.837523
3	6	0	-5.921871	1.083119	-1.598920
4	6	0	-4.050515	0.016990	-0.544542
5	6	0	-3.430259	1.277140	-0.390125
6	6	0	-5.304178	2.325986	-1.452845
7	6	0	-3.147555	-1.021663	-0.004820
8	6	0	-1.873745	-0.361383	0.285100
9	6	0	-2.136027	1.074192	0.290203
10	6	0	-1.417636	2.034078	0.957607
11	6	0	-3.471812	-2.334927	0.221687
12	6	0	-2.591882	-3.252200	0.883133
13	6	0	-4.743187	-2.900949	-0.116046
14	7	0	-5.758000	-3.396113	-0.375800
15	7	0	-1.903507	-4.010421	1.425048
16	6	0	-0.647702	-0.998864	0.238709
17	6	0	0.635078	-0.421323	0.102895
18	6	0	1.740557	-1.233593	0.039833
19	6	0	3.105936	-0.827761	-0.105865
20	6	0	5.851479	-0.123701	-0.400809

21	6	0	3.515128	0.526311	-0.154013
22	6	0	4.114062	-1.813086	-0.201172
23	6	0	5.445829	-1.486675	-0.346589
24	6	0	4.838329	0.875921	-0.296643
25	7	0	7.153993	0.215732	-0.542225
26	6	0	8.170736	-0.819375	-0.638931
27	6	0	7.547509	1.615459	-0.583673
28	6	0	-0.375926	1.714756	1.887567
29	6	0	-1.744728	3.428285	0.905924
30	7	0	-1.975491	4.563203	0.877275
31	7	0	0.449257	1.478296	2.665453
32	1	0	-5.805838	-1.038138	-1.272036
33	1	0	-3.590344	3.414653	-0.739574
34	1	0	-6.894949	1.018116	-2.081643
35	1	0	-5.798603	3.220979	-1.825518
36	1	0	-0.661524	-2.087881	0.201851
37	1	0	0.744329	0.655252	0.010714
38	1	0	1.571844	-2.311645	0.112109
39	1	0	2.776133	1.321286	-0.067925
40	1	0	3.828514	-2.864260	-0.159309
41	1	0	6.180341	-2.282616	-0.415945
42	1	0	5.104327	1.927844	-0.323380
43	1	0	9.146225	-0.345613	-0.756129
44	1	0	7.990820	-1.467596	-1.507178
45	1	0	8.630608	1.672963	-0.699757
46	1	0	7.077727	2.132310	-1.431281
47	1	0	7.267942	2.132107	0.344458
48	1	0	8.189499	-1.440592	0.266971
