Supporting Information

Computational Insights into Non-C_2-Symmetric BINOLate Titanium Catalyzed Hydrocyanation of Aldehydes

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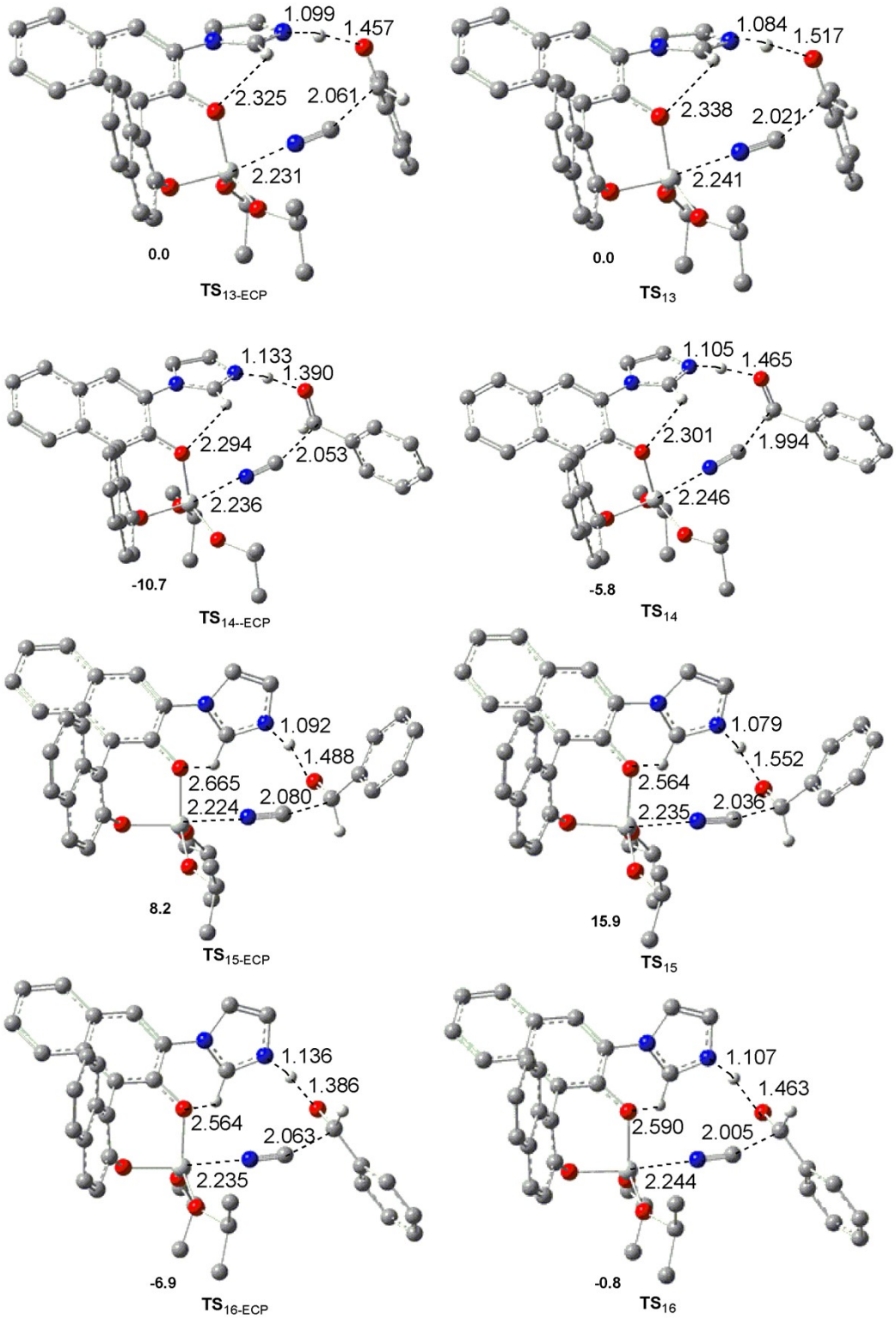
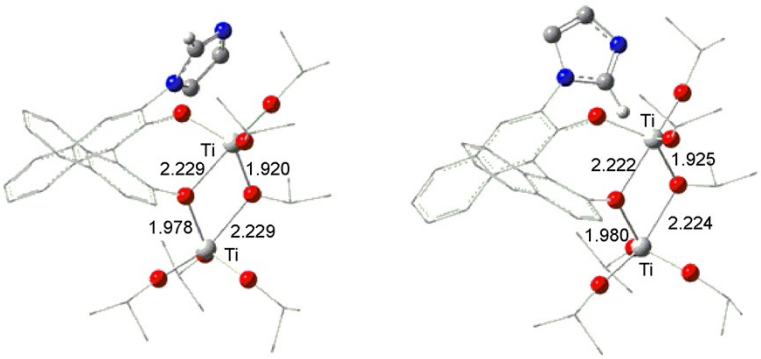


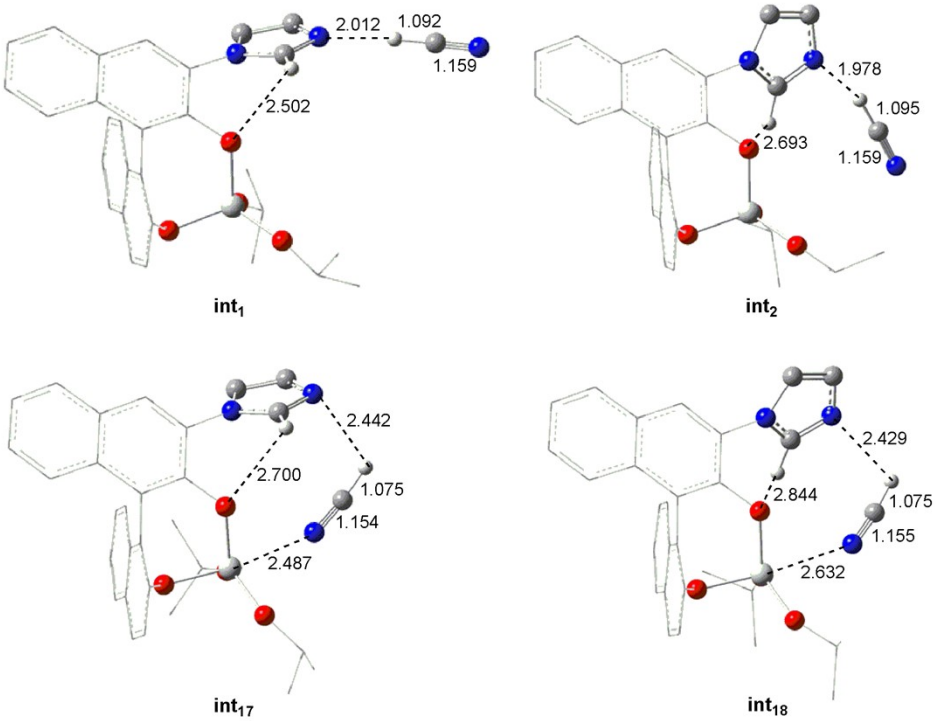
Figure S1. A comparison of $\mathbf{TS_{13}}$-$\mathbf{TS_{16}}$ structures, optimized at B3LYP//LANL2DZ/6-31G* level and B3LYP//6-31G* level, respectively. Selected distances are in Å and relative Gibbs free energies are in kJ/mol.



56.4
3

61.3
4

Figure S2. Structures of dinuclear complex **3** and **4**. (Distances are in Å. for clarity, some hydrogen atoms were omitted and bulky groups are displayed with wireframe mode. relative Gibbs free energies are in kJ/mol. The same as follows.)



int$_1$

int$_2$

int$_{17}$

int$_{18}$

Figure S3. Structures of **int$_1$**, **int$_2$**, **int$_{17}$** and **int$_{18}$**.

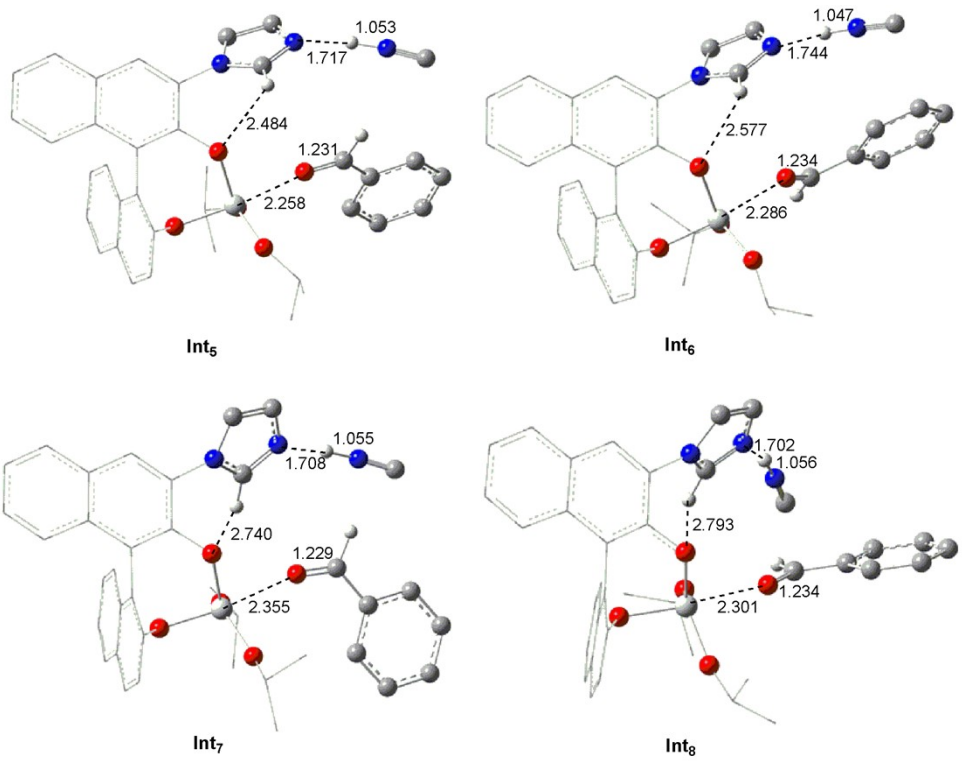


Figure S4. Optimized structure of **int$_5$** - **int$_8$**.

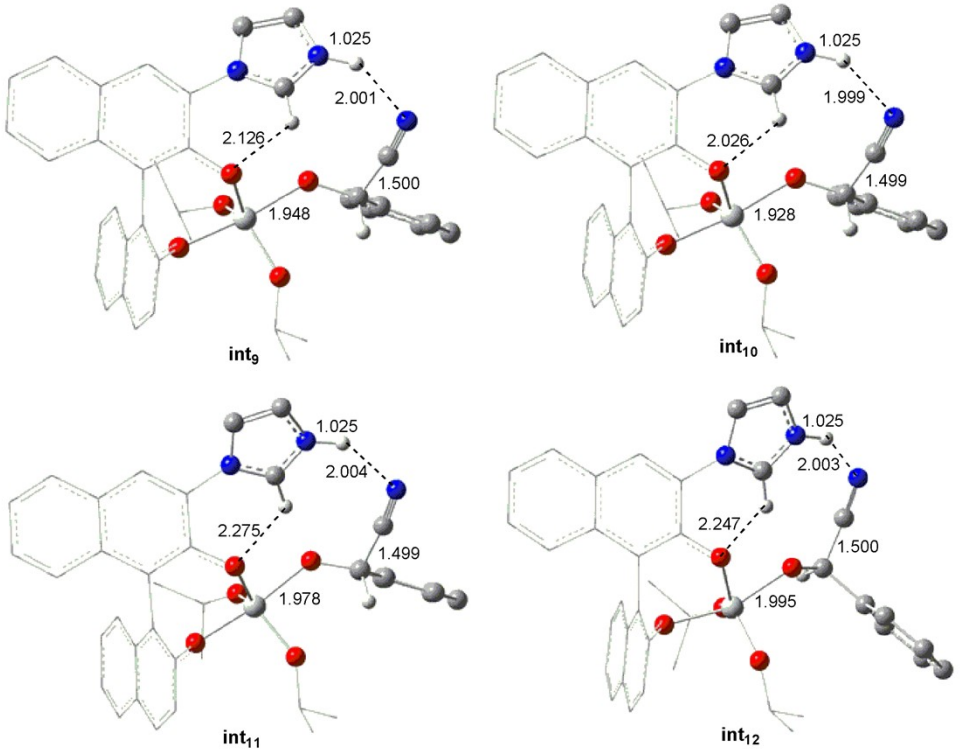


Figure S5. Optimized structure of **int$_9$** - **int$_{12}$**.

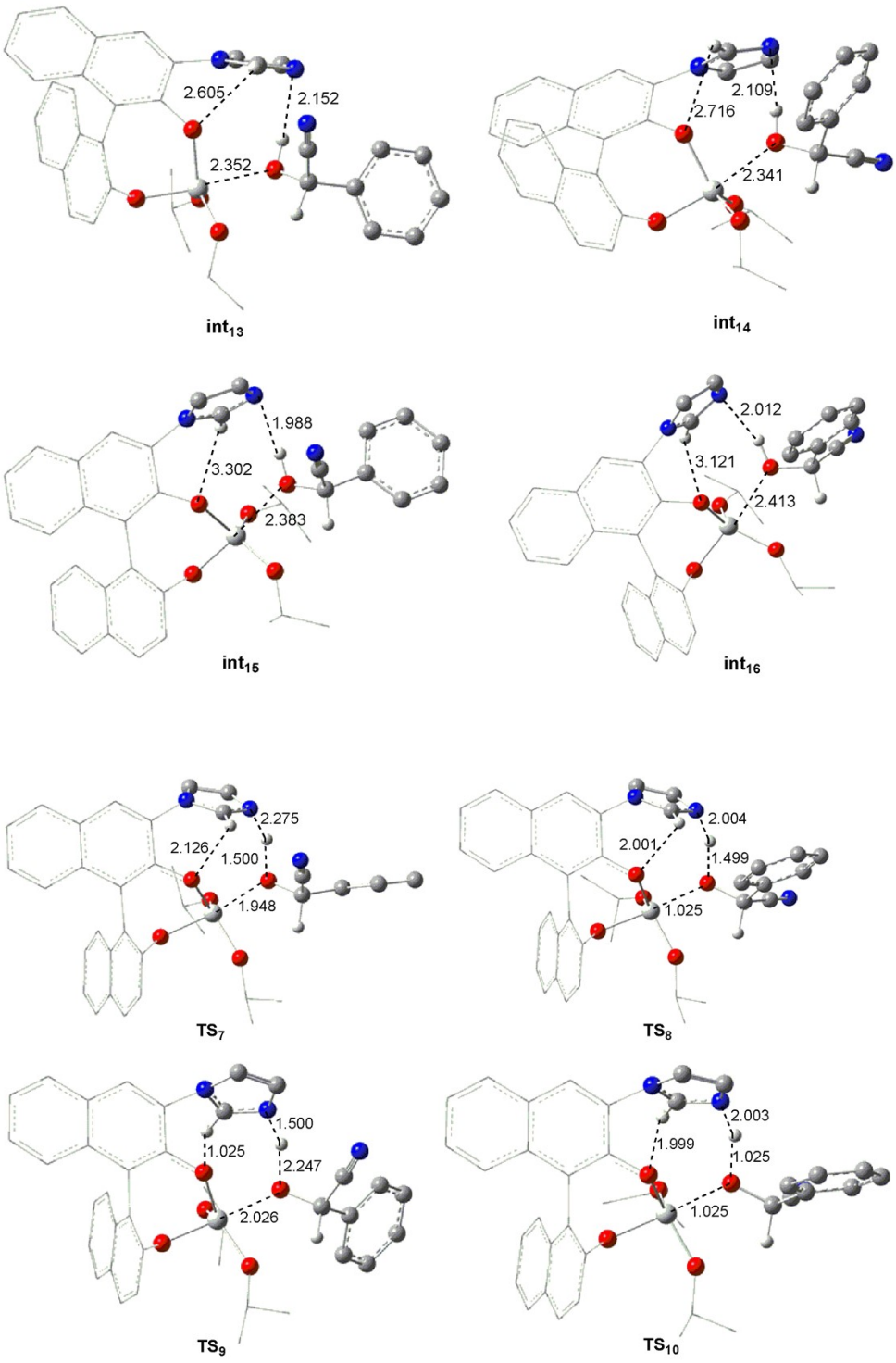


Figure S6. Optimized structure of **int$_{13}$** - **int$_{16}$**, **TS$_7$** - **TS$_{10}$**/.

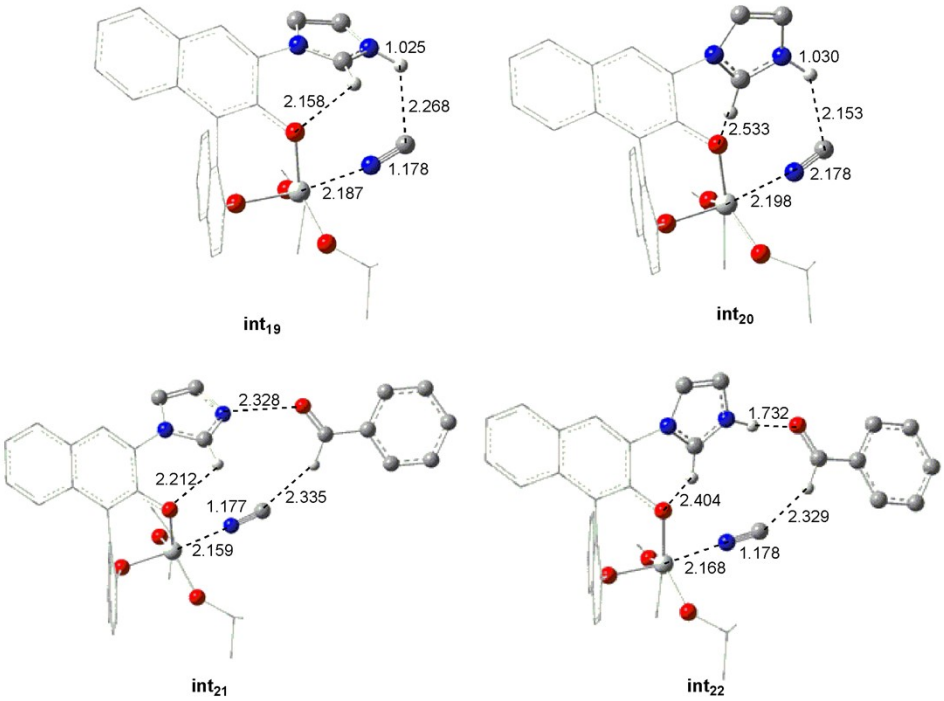


Figure S7. Optimized structure of **int_{19}** - **int_{20}**.

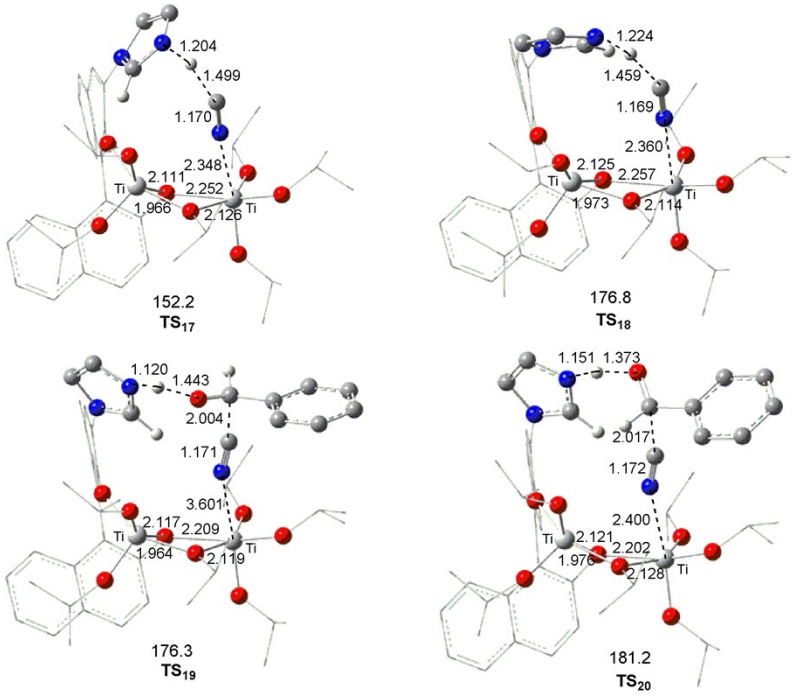


Figure S8. Optimized structure of **TS_{17}** - **TS_{20}**.

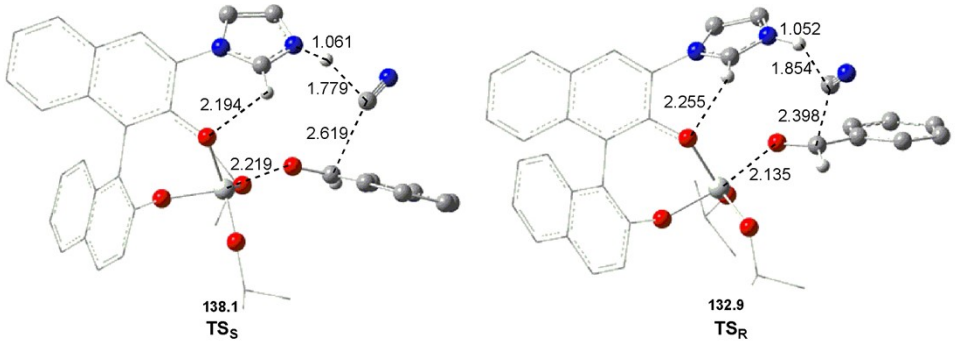


Figure S9. Optimized structure of TS_S - TS_R.

XYZ coordinates, E_{ZPE} (in gas phase) and Gibbs free energies (in CH_2Cl_2)

Reactants, products, and Catalyst

PhCHO

E_{ZPE} B3LYP/6-31G* = -345.59606 (a.u.)
G_{sol}: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -345.44952 (a.u.)

HCN

E_{ZPE}: B3LYP/6-31G* = -93.40615 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -93.45831 (a.u.)

S-Product

E_{ZPE}: B3LYP/6-31G* = -438.87101 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -439.04553 (a.u.)

R-Product

E_{ZPE}: B3LYP/6-31G* = -438.87280 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -439.04454 (a.u.)

$Ti(O^iPr)_4$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.326995	-0.543639	1.558466
2	6	0	-0.050576	-1.646631	2.412912
3	6	0	0.791117	-1.166797	3.595428
4	6	0	-1.369202	-2.285000	2.850012
5	1	0	0.529197	-2.384409	1.837157
6	1	0	1.050175	-2.004945	4.253025
7	1	0	1.719223	-0.704641	3.242816
8	1	0	0.237406	-0.424246	4.181300
9	1	0	-1.970430	-1.567030	3.419546
10	1	0	-1.947786	-2.603548	1.976657
11	1	0	-1.185067	-3.162122	3.481517
12	8	0	-1.635561	0.300769	-0.906242
13	6	0	-3.031268	0.140226	-0.721649
14	6	0	-3.544725	-0.952923	-1.660659
15	6	0	-3.725654	1.483202	-0.953160
16	1	0	-3.208300	-0.174531	0.319542
17	1	0	-4.619139	-1.118538	-1.516807
18	1	0	-3.373522	-0.667593	-2.704910
19	1	0	-3.020570	-1.896239	-1.473642
20	1	0	-3.326876	2.241647	-0.271221
21	1	0	-3.559251	1.824558	-1.981238
22	1	0	-4.805830	1.398562	-0.784490
23	22	0	-0.035331	0.041037	-0.112288
24	8	0	0.926828	-1.200276	-0.990686
25	8	0	0.901312	1.572727	-0.068823
26	6	0	1.274675	2.723737	0.668934

27	6	0	2.757799	3.009829	0.429619
28	6	0	0.379465	3.898238	0.271275
29	1	0	1.124240	2.507028	1.738507
30	6	0	2.103904	-1.351633	-1.771622
31	6	0	2.932625	-2.505451	-1.205691
32	6	0	1.715727	-1.569546	-3.234470
33	1	0	2.689198	-0.422077	-1.692845
34	1	0	2.937508	3.223183	-0.630290
35	1	0	3.086702	3.874052	1.018599
36	1	0	3.365641	2.144757	0.714776
37	1	0	0.626250	4.791870	0.856687
38	1	0	0.508211	4.131451	-0.791768
39	1	0	-0.673760	3.651863	0.441997
40	1	0	3.865645	-2.626185	-1.768651
41	1	0	3.184055	-2.317998	-0.156403
42	1	0	2.368701	-3.443527	-1.263258
43	1	0	1.126054	-2.487455	-3.338968
44	1	0	1.113079	-0.731278	-3.599368
45	1	0	2.608534	-1.655585	-3.865220

E_{ZPE}: B3LYP/6-31G* = -1624.31472 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -1624.65425 (a.u.)

1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.678326	3.351985	0.421452
2	6	0	-1.857925	3.083684	-0.314742
3	6	0	-2.208743	1.725241	-0.607712
4	6	0	-1.372661	0.657552	-0.128158
5	6	0	-0.176193	0.974432	0.518303
6	6	0	0.161577	2.336078	0.810858
7	6	0	-1.775236	-0.768509	-0.331265
8	6	0	-1.010476	-1.637089	-1.112584
9	6	0	-1.451071	-2.955646	-1.403598
10	6	0	-2.624048	-3.428287	-0.876532
11	6	0	-2.973209	-1.283313	0.280556
12	6	0	-3.405175	-2.621264	-0.007169
13	1	0	-0.430791	4.379101	0.673641
14	6	0	-2.692426	4.139106	-0.770005
15	6	0	-3.373474	1.496035	-1.392556
16	8	0	0.189449	-1.249660	-1.636479
17	1	0	-0.830417	-3.565004	-2.053468
18	1	0	-2.961690	-4.436560	-1.104270
19	6	0	-4.591357	-3.120304	0.592532
20	7	0	1.382368	2.636195	1.471968
21	7	0	3.058012	2.569444	2.950153
22	6	0	3.246115	3.629296	2.086982
23	6	0	2.228790	3.697352	1.172684
24	6	0	1.941810	1.999591	2.557520
25	1	0	4.106258	4.279859	2.173899
26	1	0	2.031899	4.355464	0.340564
27	1	0	1.479221	1.132993	3.004463
28	6	0	-3.749625	-0.522655	1.200012
29	8	0	0.694594	0.004145	0.895993
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31	8	0	2.807647	-0.001212	-1.273339
32	8	0	2.194683	-2.427313	0.269867
33	6	0	4.150783	0.347023	-1.597178
34	6	0	2.663131	-3.706853	0.667297
35	6	0	4.238942	1.861365	-1.773223
36	6	0	4.579113	-0.423755	-2.845478
37	1	0	4.783392	0.045255	-0.749916
38	6	0	2.348681	-3.910098	2.148766
39	6	0	4.153708	-3.823092	0.351291
40	1	0	2.109313	-4.450228	0.075684
41	6	0	-3.820975	3.878243	-1.512024

42	6	0	-4.154499	2.541812	-1.833175
43	6	0	-4.889157	-1.040823	1.775371
44	6	0	-5.325258	-2.349403	1.464507
45	1	0	-2.413999	5.162012	-0.527418
46	1	0	-4.449196	4.693424	-1.860180
47	1	0	-5.034511	2.337193	-2.436939
48	1	0	-3.639723	0.478666	-1.654201
49	1	0	-3.427983	0.479802	1.457743
50	1	0	-5.456625	-0.437257	2.478762
51	1	0	-6.228766	-2.744142	1.920923
52	1	0	-4.904076	-4.134461	0.354143
53	1	0	5.272845	2.160401	-1.980903
54	1	0	3.609215	2.183760	-2.610290
55	1	0	3.904618	2.373449	-0.865886
56	1	0	5.617921	-0.188536	-3.103654
57	1	0	4.501594	-1.503836	-2.680935
58	1	0	3.940691	-0.156714	-3.694936
59	1	0	2.653288	-4.912526	2.470526
60	1	0	2.883284	-3.171886	2.756719
61	1	0	1.275654	-3.797337	2.332009
62	1	0	4.522577	-4.823076	0.606126
63	1	0	4.336636	-3.649243	-0.714300
64	1	0	4.724619	-3.086212	0.927406

E_{ZPE}: B3LYP/6-31G* = -2381.51669 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2382.05335 (a.u.)

2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.833723	3.479472	0.221721
2	6	0	-2.021909	3.099104	-0.450922
3	6	0	-2.257734	1.710249	-0.722557
4	6	0	-1.304369	0.732023	-0.276410
5	6	0	-0.124253	1.150297	0.338865
6	6	0	0.099959	2.544193	0.598164
7	6	0	-1.588870	-0.725249	-0.451386
8	6	0	-0.777080	-1.527818	-1.253603
9	6	0	-1.109782	-2.889050	-1.504498
10	6	0	-2.217282	-3.455150	-0.929210
11	6	0	-2.719035	-1.326943	0.207286
12	6	0	-3.038703	-2.704175	-0.043142
13	1	0	-0.641855	4.529016	0.413259
14	6	0	-2.966431	4.068304	-0.888243
15	6	0	-3.427655	1.359333	-1.455412
16	8	0	0.384085	-1.044515	-1.801311
17	1	0	-0.465308	-3.449628	-2.170931
18	1	0	-2.473726	-4.489897	-1.130062
19	6	0	-4.155802	-3.291826	0.610330
20	7	0	1.281077	2.947827	1.276582
21	7	0	3.444466	3.251837	1.730483
22	6	0	2.678292	3.893418	2.681797
23	6	0	1.342823	3.727076	2.423203
24	6	0	2.581355	2.697700	0.909615
25	1	0	3.134465	4.434583	3.500078
26	1	0	0.446171	4.045479	2.932667
27	1	0	2.817154	2.113729	0.031943
28	6	0	-3.525328	-0.610211	1.137557
29	8	0	0.834149	0.268092	0.710472
30	22	0	1.685277	-0.835547	-0.512166
31	8	0	3.104377	-0.047459	-1.231822
32	8	0	2.091802	-2.344043	0.314423
33	6	0	4.548029	-0.014103	-1.279268
34	6	0	1.629173	-3.445405	1.125233
35	6	0	4.955703	0.944252	-2.407676
36	6	0	5.087371	-1.435412	-1.498205
37	1	0	4.897393	0.377431	-0.314908

38	1	0	0.731514	-3.851730	0.642563
39	6	0	1.278416	-2.914211	2.522575
40	6	0	2.736717	-4.507753	1.160609
41	6	0	-4.318273	2.323207	-1.871699
42	6	0	-4.093298	3.691263	-1.580834
43	6	0	-4.920485	-2.565008	1.493677
44	6	0	-4.593302	-1.213839	1.763183
45	1	0	-5.199241	2.035057	-2.433332
46	1	0	-4.805964	4.436145	-1.914385
47	1	0	-2.773679	5.113650	-0.671519
48	1	0	-3.602352	0.317154	-1.684171
49	1	0	-3.280051	0.421787	1.346843
50	1	0	-5.189892	-0.651178	2.471782
51	1	0	-5.767758	-3.022686	1.990449
52	1	0	-4.388110	-4.331277	0.403341
53	1	0	4.538808	1.939657	-2.228730
54	1	0	4.575859	0.566504	-3.362396
55	1	0	6.046972	1.021454	-2.459664
56	1	0	4.733877	-1.815874	-2.462719
57	1	0	4.736539	-2.100463	-0.703206
58	1	0	6.182458	-1.427546	-1.498764
59	1	0	0.520681	-2.128680	2.446931
60	1	0	2.174960	-2.496439	2.991975
61	1	0	0.890759	-3.725193	3.148234
62	1	0	3.632034	-4.087738	1.630272
63	1	0	2.984999	-4.830806	0.144990
64	1	0	2.405940	-5.377127	1.739077

E_{ZPE}: B3LYP/6-31G* = -2381.51513 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2382.05041 (a.u.)

3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.393045	-2.562892	-2.933325
2	6	0	2.639995	-1.949332	-2.662172
3	6	0	2.860505	-1.357559	-1.375070
4	6	0	1.825459	-1.417096	-0.379816
5	6	0	0.583217	-1.961155	-0.710202
6	6	0	0.382556	-2.557045	-2.001607
7	6	0	4.108085	-0.706147	-1.154935
8	6	0	5.079951	-0.670219	-2.131645
9	6	0	4.866882	-1.286273	-3.387043
10	6	0	3.667240	-1.909073	-3.642619
11	1	0	1.233034	-3.044769	-3.893729
12	1	0	3.481133	-2.376166	-4.607100
13	1	0	5.644221	-1.258377	-4.145591
14	1	0	6.021002	-0.163900	-1.933464
15	1	0	4.290880	-0.229239	-0.199256
16	7	0	-0.878486	-3.125572	-2.327078
17	8	0	-0.441986	-1.973633	0.154634
18	22	0	-1.672336	-0.684704	0.759985
19	8	0	-3.171436	-1.612812	0.468229
20	8	0	-1.716508	-0.511323	2.522917
21	6	0	-1.553464	-2.987573	-3.533985
22	6	0	-2.681263	-3.755150	-3.416926
23	7	0	-2.725340	-4.373585	-2.183356
24	6	0	-1.638534	-3.975420	-1.561096
25	1	0	-1.177747	-2.347749	-4.317488
26	1	0	-3.467674	-3.897270	-4.146140
27	1	0	-1.337440	-4.253319	-0.563214
28	6	0	-1.623468	-0.610243	3.932078
29	6	0	-3.023772	-0.536145	4.543563
30	6	0	-0.870413	-1.881963	4.322351
31	1	0	-1.042638	0.259324	4.271808
32	6	0	-4.272864	-2.327538	1.016722
33	6	0	-5.340585	-2.524927	-0.060041

34	6	0	-3.796742	-3.664322	1.588727
35	1	0	-4.684084	-1.715902	1.835231
36	1	0	-3.626568	-1.395725	4.229480
37	1	0	-2.963359	-0.538021	5.638166
38	1	0	-3.534272	0.379091	4.226681
39	1	0	-0.743671	-1.930623	5.410207
40	1	0	-1.422528	-2.772420	4.000758
41	1	0	0.119294	-1.899395	3.857361
42	1	0	-6.205434	-3.052554	0.359270
43	1	0	-5.685338	-1.563980	-0.454950
44	1	0	-4.931734	-3.120143	-0.883001
45	1	0	-3.435646	-4.313266	0.785093
46	1	0	-2.988837	-3.511867	2.311475
47	1	0	-4.624179	-4.173623	2.097019
48	22	0	-0.270614	2.233299	-0.323311
49	8	0	1.414430	2.815185	-0.274747
50	8	0	-2.061061	0.906487	-0.241647
51	8	0	-1.171321	3.515653	0.548753
52	8	0	-0.516859	2.247086	-2.110739
53	6	0	2.630233	3.334903	0.230739
54	6	0	3.673533	3.366171	-0.887268
55	6	0	2.394239	4.712685	0.851678
56	6	0	0.246908	2.588802	-3.262750
57	6	0	0.322590	1.376864	-4.191766
58	6	0	-0.381710	3.805320	-3.943632
59	6	0	-3.266769	1.389595	-0.874240
60	6	0	-4.394385	1.509104	0.149923
61	6	0	-3.617069	0.526796	-2.083426
62	6	0	-2.026261	4.633900	0.682620
63	6	0	-2.229002	4.927304	2.170182
64	6	0	-1.459778	5.833770	-0.078791
65	1	0	2.974653	2.647546	1.016233
66	1	0	3.809312	2.367835	-1.314552
67	1	0	3.358337	4.047623	-1.686313
68	1	0	4.638979	3.712935	-0.499994
69	1	0	3.317314	5.090989	1.306268
70	1	0	2.067575	5.427783	0.087674
71	1	0	1.622253	4.659884	1.625808
72	1	0	1.261612	2.849120	-2.929105
73	1	0	0.939888	1.603193	-5.069365
74	1	0	0.762777	0.519885	-3.672688
75	1	0	-0.679556	1.096929	-4.537666
76	1	0	-0.420096	4.656477	-3.255362
77	1	0	-1.403570	3.578259	-4.269002
78	1	0	0.202748	4.100844	-4.823035
79	1	0	-3.022741	2.395840	-1.234839
80	1	0	-5.280191	1.962412	-0.310741
81	1	0	-4.673416	0.526457	0.540105
82	1	0	-4.080880	2.139478	0.988904
83	1	0	-4.502961	0.928082	-2.590858
84	1	0	-2.783167	0.527832	-2.791188
85	1	0	-3.821769	-0.504094	-1.784004
86	1	0	-3.000262	4.367779	0.242838
87	1	0	-2.934840	5.754431	2.309676
88	1	0	-2.622494	4.044203	2.683962
89	1	0	-1.276408	5.201484	2.638036
90	1	0	-0.485481	6.121549	0.330912
91	1	0	-1.330186	5.588978	-1.138089
92	1	0	-2.136551	6.693017	-0.003797
93	6	0	2.037181	-0.849448	0.983630
94	6	0	3.048629	-1.358061	1.870087
95	6	0	3.281017	-0.712199	3.131070
96	6	0	2.479545	0.403130	3.492317
97	6	0	1.467382	0.832919	2.671007
98	6	0	1.229752	0.194118	1.424856
99	6	0	3.826900	-2.510576	1.563925
100	6	0	4.787801	-2.976694	2.433951
101	6	0	5.033182	-2.317277	3.661145
102	6	0	4.289127	-1.210249	3.998622
103	1	0	3.647350	-3.033313	0.631194

104	1	0	5.360780	-3.863465	2.175975
105	1	0	5.798068	-2.692080	4.335753
106	1	0	4.454488	-0.701403	4.945791
107	1	0	2.664014	0.898749	4.442703
108	1	0	0.822584	1.660437	2.952453
109	8	0	0.156223	0.588902	0.690455

E_{ZPE}: B3LYP/6-31G* = -4005.84865 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -4006.68610 (a.u.)

4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.211278	-2.204216	-2.830776
2	6	0	3.199346	-1.214170	-2.612770
3	6	0	3.168205	-0.459789	-1.393928
4	6	0	2.168762	-0.746146	-0.399790
5	6	0	1.165172	-1.677544	-0.683098
6	6	0	1.216644	-2.423216	-1.910101
7	6	0	4.134460	0.576447	-1.240332
8	6	0	5.078633	0.826774	-2.212485
9	6	0	5.121007	0.055560	-3.397557
10	6	0	4.193751	-0.941994	-3.589718
11	1	0	2.220637	-2.781734	-3.751196
12	1	0	4.199433	-1.534832	-4.501549
13	1	0	5.874978	0.259213	-4.152795
14	1	0	5.798706	1.627574	-2.065966
15	1	0	4.119633	1.180993	-0.341278
16	7	0	0.243831	-3.434347	-2.164261
17	8	0	0.169952	-1.949393	0.168165
18	22	0	-1.351823	-1.100051	0.872512
19	8	0	-2.467767	-2.479307	0.718698
20	8	0	-1.276248	-0.878924	2.630894
21	6	0	0.494001	-4.788396	-2.328614
22	6	0	-0.725422	-5.360816	-2.583954
23	7	0	-1.719926	-4.404622	-2.589683
24	6	0	-1.105222	-3.269965	-2.334452
25	1	0	1.491488	-5.188864	-2.230032
26	1	0	-0.946432	-6.404116	-2.766218
27	1	0	-1.570775	-2.297889	-2.270025
28	6	0	-0.964709	-1.098716	3.996435
29	6	0	-2.229771	-1.509459	4.751049
30	6	0	0.163888	-2.121385	4.124706
31	1	0	-0.611925	-0.135936	4.392719
32	6	0	-3.018548	-3.701797	1.192569
33	6	0	-4.151211	-4.147152	0.266654
34	6	0	-1.917998	-4.758657	1.300699
35	1	0	-3.426621	-3.502896	2.196281
36	1	0	-2.601254	-2.472952	4.383600
37	1	0	-2.020967	-1.605812	5.823008
38	1	0	-3.018130	-0.761502	4.618138
39	1	0	0.455504	-2.237684	5.175015
40	1	0	-0.156695	-3.098868	3.746232
41	1	0	1.040530	-1.799713	3.555180
42	1	0	-4.609068	-5.066769	0.650087
43	1	0	-4.930484	-3.380341	0.204656
44	1	0	-3.762189	-4.341935	-0.738429
45	1	0	-1.496259	-4.972025	0.314129
46	1	0	-1.110689	-4.415650	1.955693
47	1	0	-2.328334	-5.687534	1.714538
48	22	0	-1.112157	2.057697	-0.392291
49	8	0	0.287931	3.154333	-0.532238
50	8	0	-2.358645	0.243955	-0.068663
51	8	0	-2.294693	3.030964	0.543730
52	8	0	-1.510323	1.888243	-2.142422
53	6	0	1.307226	4.068605	-0.174412

54	6	0	2.263876	4.252826	-1.353331
55	6	0	0.684713	5.387053	0.287872
56	6	0	-0.970351	2.324597	-3.386153
57	6	0	-0.404009	1.120709	-4.139687
58	6	0	-2.059447	3.048498	-4.178339
59	6	0	-3.740965	0.314548	-0.483791
60	6	0	-4.671717	0.074466	0.703976
61	6	0	-3.995528	-0.621925	-1.661266
62	6	0	-3.403857	3.892146	0.714580
63	6	0	-3.308175	4.567903	2.083429
64	6	0	-3.482492	4.899374	-0.434146
65	1	0	1.862461	3.625145	0.664328
66	1	0	2.683527	3.290734	-1.662899
67	1	0	1.738515	4.694925	-2.208133
68	1	0	3.089757	4.918451	-1.075445
69	1	0	1.462738	6.082946	0.622966
70	1	0	0.131195	5.857512	-0.533343
71	1	0	-0.008461	5.215425	1.117306
72	1	0	-0.153426	3.028541	-3.170795
73	1	0	0.050230	1.437919	-5.085918
74	1	0	0.362489	0.616224	-3.542901
75	1	0	-1.198224	0.399109	-4.364577
76	1	0	-2.437269	3.910375	-3.618225
77	1	0	-2.898319	2.372755	-4.380629
78	1	0	-1.665647	3.407010	-5.136701
79	1	0	-3.887970	1.343759	-0.831642
80	1	0	-5.715558	0.226803	0.404502
81	1	0	-4.566247	-0.946867	1.081058
82	1	0	-4.440114	0.771720	1.516226
83	1	0	-5.027377	-0.513490	-2.016861
84	1	0	-3.321612	-0.369926	-2.485833
85	1	0	-3.837129	-1.664723	-1.374612
86	1	0	-4.311439	3.268421	0.697548
87	1	0	-4.192277	5.188649	2.270478
88	1	0	-3.238148	3.816574	2.876624
89	1	0	-2.419625	5.207589	2.134209
90	1	0	-2.592701	5.538959	-0.442208
91	1	0	-3.541373	4.378167	-1.395187
92	1	0	-4.368310	5.536989	-0.331234
93	6	0	2.181694	-0.041257	0.914791
94	6	0	3.303494	-0.134043	1.812848
95	6	0	3.323165	0.654277	3.012421
96	6	0	2.211038	1.486340	3.309308
97	6	0	1.111315	1.502820	2.489288
98	6	0	1.085129	0.721690	1.302849
99	6	0	4.402066	-1.009720	1.580611
100	6	0	5.460939	-1.079229	2.459286
101	6	0	5.490135	-0.273728	3.621394
102	6	0	4.437441	0.570917	3.888868
103	1	0	4.393594	-1.640898	0.699374
104	1	0	6.280877	-1.763777	2.258521
105	1	0	6.334526	-0.332784	4.302679
106	1	0	4.435932	1.183917	4.787580
107	1	0	2.232257	2.091774	4.212572
108	1	0	0.236008	2.099610	2.728820
109	8	0	-0.064141	0.686743	0.578550

E_{ZPE}: B3LYP/6-31G* = -4005.84736 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -4006.68424 (a.u.)

Species involved in the bifunctional LALB mechanism

Int_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.615469	3.384160	0.103246

2	6	0	-1.935169	3.187994	-0.371215
3	6	0	-2.443889	1.853656	-0.496006
4	6	0	-1.618434	0.738772	-0.115198
5	6	0	-0.295396	0.975595	0.263807
6	6	0	0.197065	2.314599	0.391481
7	6	0	-2.167701	-0.651877	-0.138755
8	6	0	-1.645435	-1.624943	-0.992898
9	6	0	-2.239724	-2.909905	-1.105564
10	6	0	-3.319900	-3.244695	-0.332221
11	6	0	-3.259239	-1.021679	0.725030
12	6	0	-3.846162	-2.326570	0.615191
13	1	0	-0.241295	4.395679	0.233001
14	6	0	-2.755987	4.290881	-0.728311
15	6	0	-3.756367	1.692264	-1.021915
16	8	0	-0.545102	-1.374645	-1.762163
17	1	0	-1.810756	-3.605766	-1.820055
18	1	0	-3.776711	-4.227260	-0.423060
19	6	0	-4.927443	-2.683550	1.463043
20	7	0	1.546533	2.534892	0.788371
21	7	0	3.466384	2.375312	1.905244
22	6	0	3.576974	3.367832	0.952861
23	6	0	2.405871	3.487273	0.255268
24	6	0	2.245129	1.898916	1.781049
25	1	0	4.491627	3.930626	0.827511
26	1	0	2.105929	4.119345	-0.565738
27	1	0	1.810523	1.104630	2.367519
28	6	0	-3.774611	-0.147930	1.723873
29	8	0	0.554882	-0.046070	0.534677
30	22	0	1.054410	-1.156294	-0.875968
31	8	0	2.194611	-0.383528	-1.986470
32	8	0	1.679909	-2.653034	-0.193532
33	6	0	3.464456	-0.216251	-2.612025
34	6	0	2.124356	-3.949851	0.182331
35	6	0	3.528005	-1.099617	-3.857297
36	1	0	4.231393	-0.544042	-1.895609
37	6	0	3.669332	1.265198	-2.921385
38	6	0	3.612413	-4.086497	-0.135593
39	1	0	1.556429	-4.670496	-0.423712
40	6	0	1.804527	-4.173247	1.659399
41	1	0	4.902485	1.590267	3.074653
42	7	0	6.514872	0.590144	4.285415
43	6	0	5.684731	1.109047	3.665885
44	6	0	-4.026718	4.096379	-1.217426
45	6	0	-4.523072	2.781181	-1.373783
46	6	0	-4.816799	-0.529510	2.540231
47	6	0	-5.410174	-1.805846	2.406392
48	1	0	-2.354151	5.295095	-0.615561
49	1	0	-4.644656	4.946445	-1.492597
50	1	0	-5.519318	2.627134	-1.779251
51	1	0	-4.150023	0.691533	-1.155329
52	1	0	-3.328254	0.831921	1.848776
53	1	0	-5.183761	0.157635	3.297963
54	1	0	-6.235040	-2.092247	3.052836
55	1	0	-5.362276	-3.674853	1.357049
56	1	0	2.749993	-0.807252	-4.571150
57	1	0	3.377883	-2.152216	-3.594119
58	1	0	4.503751	-1.002928	-4.346616
59	1	0	3.595357	1.862176	-2.007240
60	1	0	2.909760	1.614472	-3.629913
61	1	0	4.658700	1.428068	-3.363914
62	1	0	4.196586	-3.370797	0.453543
63	1	0	3.798832	-3.897877	-1.198027
64	1	0	3.962878	-5.097164	0.101982
65	1	0	0.733534	-4.044755	1.844278
66	1	0	2.352853	-3.457142	2.281182
67	1	0	2.090761	-5.186682	1.962623

E_{ZPE}: B3LYP/6-31G* = -2474.93631 (a.u.)

Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2475.50574 (a.u.)

Int_2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.945418	1.247315	-1.073480
2	7	0	-6.727371	0.495157	-0.665256
3	6	0	3.016510	-3.299206	0.710867
4	6	0	3.711463	-2.428999	-0.171520
5	6	0	1.860845	-2.894707	1.325025
6	6	0	1.354339	-1.584153	1.113053
7	6	0	2.038269	-0.654590	0.327741
8	6	0	3.214561	-1.098658	-0.377490
9	6	0	1.582482	0.765996	0.220730
10	6	0	2.431628	1.832902	0.680604
11	6	0	0.341853	1.082237	-0.338900
12	6	0	-0.020552	2.449620	-0.569766
13	6	0	0.820863	3.468536	-0.195646
14	6	0	2.050802	3.195354	0.449869
15	1	0	3.406778	-4.300149	0.878939
16	6	0	4.875399	-2.858723	-0.861069
17	1	0	1.304014	-3.552397	1.985494
18	6	0	3.904088	-0.274412	-1.310801
19	6	0	3.642121	1.597201	1.391499
20	8	0	-0.536520	0.121774	-0.709586
21	1	0	0.522429	4.499139	-0.366357
22	6	0	2.894140	4.248748	0.893520
23	7	0	-1.245635	2.753755	-1.231352
24	22	0	-1.237746	-1.072053	0.533328
25	7	0	-3.417845	2.811974	-1.709009
26	6	0	-2.737726	3.620054	-2.596248
27	6	0	-1.397763	3.604075	-2.318116
28	6	0	-2.498275	2.310033	-0.909993
29	1	0	-3.252798	4.156917	-3.380670
30	1	0	-0.546853	4.074170	-2.786256
31	1	0	-2.674773	1.635630	-0.085274
32	8	0	-2.597534	-0.354174	1.418686
33	8	0	-1.664285	-2.569992	-0.284378
34	6	0	-3.907757	-0.426225	1.995048
35	6	0	-2.009121	-3.781025	-0.945465
36	1	0	-4.626443	-0.236208	1.187823
37	6	0	-4.144694	-1.824618	2.561568
38	6	0	-4.030530	0.671586	3.049010
39	6	0	-3.190932	-3.523679	-1.878783
40	6	0	-0.778270	-4.322455	-1.670742
41	1	0	-2.312335	-4.492970	-0.164267
42	8	0	0.167612	-1.266331	1.712036
43	6	0	4.433223	2.640032	1.820327
44	6	0	4.065558	3.981387	1.562621
45	6	0	5.525788	-2.027131	-1.743636
46	6	0	5.023935	-0.725901	-1.974575
47	1	0	2.587420	5.274442	0.702324
48	1	0	4.701425	4.793932	1.902756
49	1	0	5.348122	2.429154	2.367413
50	1	0	3.936115	0.576623	1.606564
51	1	0	3.530510	0.723523	-1.508897
52	1	0	5.524220	-0.074723	-2.686428
53	1	0	6.413295	-2.368826	-2.268987
54	1	0	5.238860	-3.868271	-0.682902
55	1	0	-3.429704	-2.040003	3.364516
56	1	0	-4.031293	-2.581980	1.778715
57	1	0	-5.158535	-1.903761	2.968877
58	1	0	-3.839574	1.655222	2.608378
59	1	0	-3.310459	0.508967	3.858837
60	1	0	-5.040553	0.676608	3.473425
61	1	0	-2.913327	-2.800077	-2.653187
62	1	0	-4.046125	-3.125481	-1.323540
63	1	0	-3.500246	-4.454242	-2.367990
64	1	0	0.054692	-4.453248	-0.973033

65	1	0	-0.463154	-3.627792	-2.457238
66	1	0	-1.003387	-5.290869	-2.131811
67	1	0	-5.167137	1.931868	-1.426690

E_{ZPE}: B3LYP/6-31G* = -2474.93679 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2475.50217 (a.u.)

TS_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.060685	3.381038	-0.514491
2	6	0	2.311798	3.083256	0.073776
3	6	0	2.611442	1.727003	0.435681
4	6	0	1.675810	0.679048	0.131345
5	6	0	0.427950	1.019611	-0.397164
6	6	0	0.132023	2.387762	-0.705907
7	6	0	2.017898	-0.753544	0.391317
8	6	0	1.257198	-1.529895	1.270051
9	6	0	1.656324	-2.846515	1.624419
10	6	0	2.770150	-3.411313	1.062124
11	6	0	3.142962	-1.370503	-0.263967
12	6	0	3.528193	-2.707045	0.088952
13	1	0	0.836535	4.407036	-0.792981
14	6	0	3.255362	4.112263	0.340126
15	6	0	3.842870	1.483322	1.108142
16	8	0	0.106192	-1.053422	1.824477
17	1	0	1.046484	-3.381519	2.345774
18	1	0	3.073477	-4.418553	1.337463
19	6	0	4.641619	-3.310141	-0.552513
20	7	0	-1.194732	2.728045	-1.133333
21	7	0	-3.230860	2.533471	-1.865908
22	6	0	-3.168648	3.742906	-1.208830
23	6	0	-1.892246	3.876662	-0.752052
24	6	0	-2.046548	1.934643	-1.808530
25	1	0	-4.023213	4.392745	-1.109610
26	1	0	-1.426391	4.651754	-0.166937
27	1	0	-1.863470	0.946561	-2.192818
28	6	0	3.884999	-0.721277	-1.291144
29	8	0	-0.513038	0.095175	-0.652502
30	22	0	-1.349136	-0.940422	0.681535
31	8	0	-2.632764	-0.066317	1.512595
32	8	0	-1.811281	-2.484681	0.000198
33	6	0	-4.012634	0.213005	1.793933
34	6	0	-2.411516	-3.530785	-0.772075
35	6	0	-4.560985	-0.868166	2.721673
36	1	0	-4.543465	0.188976	0.833016
37	6	0	-4.099306	1.611639	2.400817
38	6	0	-3.906972	-3.593182	-0.471483
39	1	0	-1.925056	-4.458851	-0.440898
40	6	0	-2.114607	-3.288245	-2.250731
41	1	0	-4.046868	1.943680	-2.128283
42	7	0	-3.996598	-0.186860	-2.411033
43	6	0	-4.860043	0.076902	-1.647292
44	6	0	4.442882	3.832884	0.973171
45	6	0	4.727671	2.504817	1.371095
46	6	0	4.951405	-1.340339	-1.906125
47	6	0	5.346220	-2.644285	-1.529086
48	1	0	3.011606	5.130256	0.044956
49	1	0	5.155141	4.626551	1.179776
50	1	0	5.655284	2.288569	1.893881
51	1	0	4.076160	0.474196	1.425443
52	1	0	3.593450	0.274539	-1.604851
53	1	0	5.491342	-0.821204	-2.693621
54	1	0	6.192476	-3.119059	-2.017732
55	1	0	4.919462	-4.321053	-0.262992
56	1	0	-4.014733	-0.878398	3.672438
57	1	0	-4.473016	-1.854644	2.255965

58	1	0	-5.620861	-0.684534	2.931005
59	1	0	-3.676284	2.355118	1.716916
60	1	0	-3.550026	1.659871	3.348288
61	1	0	-5.145845	1.876143	2.590463
62	1	0	-4.395080	-2.667191	-0.791859
63	1	0	-4.081330	-3.744390	0.599706
64	1	0	-4.360764	-4.432068	-1.011993
65	1	0	-1.034553	-3.218120	-2.419957
66	1	0	-2.596296	-2.362891	-2.584165
67	1	0	-2.502476	-4.122040	-2.847792

E_{ZPE}: B3LYP/6-31G* = -2474.89123 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2475.47565 (a.u.)

TS_2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.853367	0.892896	-1.665137
2	7	0	-5.111400	0.859396	-0.741682
3	6	0	2.959075	-3.483406	0.570153
4	6	0	3.679893	-2.610019	-0.287316
5	6	0	1.819668	-3.061412	1.201889
6	6	0	1.352726	-1.730261	1.033671
7	6	0	2.063520	-0.801954	0.268145
8	6	0	3.223419	-1.259800	-0.454470
9	6	0	1.639566	0.629753	0.183695
10	6	0	2.508265	1.682211	0.640659
11	6	0	0.398488	0.971999	-0.359815
12	6	0	0.075967	2.350299	-0.583271
13	6	0	0.929936	3.359984	-0.220210
14	6	0	2.155562	3.055887	0.420027
15	1	0	3.315577	-4.501868	0.703917
16	6	0	4.828849	-3.056085	-0.991520
17	1	0	1.243797	-3.721502	1.843013
18	6	0	3.936653	-0.433126	-1.368109
19	6	0	3.718169	1.418220	1.342735
20	8	0	-0.513041	0.044307	-0.717200
21	1	0	0.652549	4.396975	-0.389716
22	6	0	3.022833	4.089430	0.864609
23	7	0	-1.157396	2.655466	-1.248129
24	22	0	-1.289385	-1.024621	0.619403
25	7	0	-3.251515	2.557182	-1.813893
26	6	0	-2.623359	3.326505	-2.767628
27	6	0	-1.305585	3.394933	-2.418985
28	6	0	-2.362176	2.160119	-0.915968
29	1	0	-3.153483	3.747686	-3.606799
30	1	0	-0.461772	3.869237	-2.893469
31	1	0	-2.591455	1.534586	-0.068772
32	8	0	-2.420318	-0.080762	1.590351
33	8	0	-2.034477	-2.423117	-0.134905
34	6	0	-3.708494	0.115133	2.214498
35	6	0	-3.005310	-3.283374	-0.739808
36	1	0	-4.396045	0.389360	1.405401
37	6	0	-4.155016	-1.192322	2.862216
38	6	0	-3.578843	1.260488	3.214588
39	6	0	-3.632112	-2.577188	-1.939657
40	6	0	-2.325398	-4.603237	-1.096556
41	1	0	-3.778052	-3.465873	0.019817
42	8	0	0.194710	-1.389193	1.663240
43	6	0	4.532035	2.442315	1.773079
44	6	0	4.191454	3.793087	1.525534
45	6	0	5.504160	-2.221495	-1.852164
46	6	0	5.041587	-0.899944	-2.046157
47	1	0	2.736909	5.122528	0.681575
48	1	0	4.845976	4.589666	1.867439
49	1	0	5.445104	2.209629	2.314055
50	1	0	3.991191	0.390097	1.548543

51	1	0	3.594246	0.580513	-1.541495
52	1	0	5.559917	-0.244981	-2.741507
53	1	0	6.379747	-2.575855	-2.388826
54	1	0	5.160086	-4.081258	-0.842578
55	1	0	-3.452014	-1.503160	3.644802
56	1	0	-4.224743	-1.988875	2.114052
57	1	0	-5.144757	-1.067837	3.315319
58	1	0	-3.240463	2.175804	2.717587
59	1	0	-2.862803	1.010968	4.006246
60	1	0	-4.551628	1.465687	3.675114
61	1	0	-2.864066	-2.355470	-2.690107
62	1	0	-4.122076	-1.643038	-1.645505
63	1	0	-4.385125	-3.226180	-2.401495
64	1	0	-1.872777	-5.059815	-0.210244
65	1	0	-1.539798	-4.438842	-1.842411
66	1	0	-3.057174	-5.304717	-1.512520
67	1	0	-4.226177	2.146189	-1.746604

E_{ZPE}: B3LYP/6-31G* = -2474.89308 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2475.48242 (a.u.)

Int_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.660706	3.378509	0.098500
2	6	0	-1.970107	3.163071	-0.395468
3	6	0	-2.457108	1.821222	-0.527830
4	6	0	-1.622552	0.718108	-0.132864
5	6	0	-0.308875	0.973806	0.265909
6	6	0	0.161728	2.320019	0.398590
7	6	0	-2.152414	-0.679971	-0.162451
8	6	0	-1.602313	-1.647843	-1.005009
9	6	0	-2.178476	-2.940240	-1.126441
10	6	0	-3.268223	-3.287276	-0.372293
11	6	0	-3.254310	-1.062258	0.682666
12	6	0	-3.822694	-2.374575	0.564308
13	1	0	-0.303093	4.395362	0.233269
14	6	0	-2.801094	4.253996	-0.765777
15	6	0	-3.758422	1.640856	-1.075036
16	8	0	-0.491012	-1.384383	-1.753973
17	1	0	-1.727758	-3.631707	-1.831707
18	1	0	-3.711058	-4.275565	-0.469666
19	6	0	-4.914188	-2.744095	1.393476
20	7	0	1.503941	2.558994	0.812522
21	7	0	3.417151	2.411410	1.933109
22	6	0	3.526335	3.411795	0.989411
23	6	0	2.356757	3.522772	0.288905
24	6	0	2.200522	1.922412	1.802770
25	1	0	4.437274	3.981811	0.873570
26	1	0	2.054677	4.156816	-0.529574
27	1	0	1.774712	1.118940	2.382398
28	6	0	-3.797994	-0.193960	1.671116
29	8	0	0.551474	-0.033502	0.553958
30	22	0	1.086564	-1.164483	-0.828304
31	8	0	2.256841	-0.409642	-1.916868
32	8	0	1.683698	-2.653188	-0.106167
33	6	0	3.524254	-0.219984	-2.540399
34	6	0	2.211621	-3.899440	0.328569
35	6	0	3.598182	-1.090288	-3.794183
36	1	0	4.294391	-0.545674	-1.826626
37	6	0	3.711071	1.266754	-2.835525
38	6	0	3.619747	-4.081415	-0.235812
39	1	0	1.554253	-4.681036	-0.078390
40	6	0	2.167423	-3.949060	1.854807
41	6	0	-4.060656	4.040925	-1.275414
42	6	0	-4.534931	2.718501	-1.439699
43	6	0	-4.849419	-0.587696	2.469711

44	6	0	-5.424333	-1.871474	2.327088
45	1	0	-2.415844	5.263959	-0.646771
46	1	0	-4.686486	4.881801	-1.560668
47	1	0	-5.521992	2.549915	-1.861468
48	1	0	-4.135310	0.634551	-1.214583
49	1	0	-3.366135	0.791498	1.802698
50	1	0	-5.238043	0.095532	3.220126
51	1	0	-6.256735	-2.167528	2.959341
52	1	0	-5.334556	-3.740921	1.281300
53	1	0	2.817569	-0.799364	-4.505778
54	1	0	3.459464	-2.146852	-3.541318
55	1	0	4.573230	-0.978117	-4.281573
56	1	0	3.628520	1.854805	-1.916329
57	1	0	2.948418	1.613175	-3.542166
58	1	0	4.699038	1.445866	-3.274821
59	1	0	4.290485	-3.306734	0.152428
60	1	0	3.608982	-4.019007	-1.329115
61	1	0	4.021752	-5.060035	0.049271
62	1	0	1.145751	-3.793476	2.214950
63	1	0	2.809044	-3.170303	2.281482
64	1	0	2.518275	-4.922868	2.214361
65	1	0	4.684411	1.686098	2.973268
66	6	0	6.221823	0.643196	4.175417
67	7	0	5.407548	1.206056	3.542501

E_{ZPE}: B3LYP/6-31G* = -2474.917374 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2475.49175 (a.u.)

Int_4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-5.800463	1.338424	-1.097902
2	6	0	-6.587093	0.583251	-0.661086
3	1	0	-5.023672	1.954693	-1.425510
4	6	0	3.049630	-3.268164	0.717421
5	6	0	3.736147	-2.388915	-0.162649
6	6	0	1.888293	-2.877761	1.330137
7	6	0	1.366941	-1.572986	1.118739
8	6	0	2.040894	-0.635162	0.334608
9	6	0	3.223762	-1.064432	-0.368687
10	6	0	1.564897	0.778375	0.224605
11	6	0	2.396937	1.859374	0.682644
12	6	0	0.319352	1.073860	-0.335427
13	6	0	-0.063535	2.435526	-0.566449
14	6	0	0.761089	3.468937	-0.195537
15	6	0	1.995556	3.215703	0.449477
16	1	0	3.451123	-4.264678	0.885141
17	6	0	4.906514	-2.804255	-0.850122
18	1	0	1.337940	-3.542691	1.988739
19	6	0	3.905026	-0.231570	-1.300466
20	6	0	3.610611	1.643479	1.394430
21	8	0	-0.544270	0.100311	-0.704895
22	1	0	0.445922	4.494486	-0.366762
23	6	0	2.822635	4.282679	0.891336
24	7	0	-1.297411	2.717630	-1.223332
25	22	0	-1.234213	-1.102162	0.539060
26	7	0	-3.465731	2.719741	-1.698091
27	6	0	-2.811470	3.539421	-2.593500
28	6	0	-1.471737	3.556290	-2.316146
29	6	0	-2.533950	2.244470	-0.895226
30	1	0	-3.342900	4.057043	-3.379334
31	1	0	-0.633614	4.044453	-2.788465
32	1	0	-2.697428	1.570349	-0.068121
33	8	0	-2.603061	-0.398447	1.420082
34	8	0	-1.636490	-2.608792	-0.273644
35	6	0	-3.926312	-0.475394	1.968915
36	6	0	-1.904587	-3.836056	-0.940430

37	1	0	-4.628149	-0.285023	1.147415
38	6	0	-4.169426	-1.875164	2.528905
39	6	0	-4.073649	0.620770	3.021283
40	6	0	-3.190385	-3.694314	-1.752980
41	6	0	-0.694586	-4.217088	-1.792015
42	1	0	-2.051214	-4.595000	-0.158377
43	8	0	0.175679	-1.269487	1.716283
44	6	0	4.385436	2.699064	1.821700
45	6	0	3.997669	4.034278	1.561333
46	6	0	5.548602	-1.964430	-1.730969
47	6	0	5.031513	-0.669247	-1.962294
48	1	0	2.500391	5.303237	0.698408
49	1	0	4.620948	4.856935	1.900283
50	1	0	5.303059	2.503114	2.369689
51	1	0	3.919847	0.627894	1.611518
52	1	0	3.519900	0.761826	-1.499134
53	1	0	5.525213	-0.011756	-2.672897
54	1	0	6.441189	-2.295123	-2.254663
55	1	0	5.281682	-3.809433	-0.671751
56	1	0	-3.470315	-2.089332	3.346120
57	1	0	-4.037882	-2.631498	1.747912
58	1	0	-5.191146	-1.957613	2.915255
59	1	0	-3.879724	1.605683	2.584861
60	1	0	-3.368982	0.460823	3.845151
61	1	0	-5.091983	0.620748	3.425244
62	1	0	-3.069510	-2.928482	-2.527112
63	1	0	-4.027651	-3.405886	-1.109591
64	1	0	-3.440225	-4.643751	-2.239842
65	1	0	0.206682	-4.282803	-1.174542
66	1	0	-0.526137	-3.465690	-2.571330
67	1	0	-0.858957	-5.187430	-2.274219

E_{ZPE}: B3LYP/6-31G* = -2474.918564 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2475.48659 (a.u.)

Int_5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.058102	3.458282	0.170821
2	6	0	3.304886	2.981967	0.639248
3	6	0	3.561901	1.571247	0.624627
4	6	0	2.570621	0.669612	0.104664
5	6	0	1.315840	1.169162	-0.254724
6	6	0	1.080836	2.582992	-0.238627
7	6	0	2.851905	-0.792008	-0.014834
8	6	0	2.058837	-1.711442	0.669080
9	6	0	2.373139	-3.096439	0.675456
10	6	0	3.441927	-3.568713	-0.040760
11	6	0	3.926579	-1.288119	-0.832775
12	6	0	4.231480	-2.690889	-0.830453
13	1	0	1.872467	4.528343	0.142289
14	6	0	4.294574	3.876279	1.128576
15	6	0	4.803172	1.123410	1.161070
16	8	0	0.958551	-1.306084	1.358297
17	1	0	1.741079	-3.757692	1.259844
18	1	0	3.685461	-4.628659	-0.030436
19	6	0	5.300580	-3.177216	-1.628056
20	7	0	-0.194428	3.091938	-0.630030
21	7	0	-2.059419	3.421970	-1.787098
22	6	0	-2.021431	4.316520	-0.736948
23	6	0	-0.877219	4.131548	-0.012193
24	6	0	-0.955080	2.704071	-1.693855
25	1	0	-2.819246	5.025921	-0.569104
26	1	0	-0.493365	4.606851	0.876505
27	1	0	-0.665886	1.894184	-2.343880
28	6	0	4.697252	-0.446837	-1.684613
29	8	0	0.310622	0.365983	-0.646147

30	22	0	-0.590992	-0.928226	0.396756
31	8	0	-1.517099	-0.500867	1.881880
32	8	0	-0.903065	-2.489776	-0.412314
33	6	0	-1.211121	-0.157652	3.234951
34	6	0	-1.774364	-3.565678	-0.716311
35	6	0	-1.904082	-1.148562	4.169335
36	6	0	-1.633036	1.289030	3.489881
37	1	0	-0.123508	-0.248709	3.360519
38	6	0	-2.005688	-4.420138	0.531026
39	6	0	-1.176999	-4.361003	-1.877045
40	1	0	-2.736279	-3.135365	-1.036038
41	1	0	-3.385284	3.101131	-2.830267
42	6	0	5.489933	3.406756	1.619843
43	6	0	5.735560	2.013455	1.645765
44	6	0	5.718847	-0.952855	-2.458224
45	6	0	6.036221	-2.330448	-2.425172
46	1	0	4.081561	4.942850	1.116502
47	1	0	6.238496	4.097962	1.997045
48	1	0	6.670205	1.640170	2.055745
49	1	0	5.006971	0.059903	1.195512
50	1	0	4.463349	0.610690	-1.730983
51	1	0	6.283807	-0.285701	-3.104047
52	1	0	6.848534	-2.716280	-3.035034
53	1	0	5.520266	-4.242389	-1.603923
54	1	0	-1.645599	-0.936476	5.213351
55	1	0	-2.993880	-1.082823	4.066239
56	1	0	-1.593723	-2.173034	3.939763
57	1	0	-1.375969	1.590577	4.512068
58	1	0	-1.126710	1.965331	2.793192
59	1	0	-2.714690	1.404722	3.355604
60	1	0	-2.708948	-5.233785	0.318838
61	1	0	-1.061229	-4.858735	0.872476
62	1	0	-2.416619	-3.811441	1.343724
63	1	0	-1.845483	-5.178920	-2.170206
64	1	0	-1.019978	-3.711310	-2.743653
65	1	0	-0.209438	-4.785084	-1.587207
66	6	0	-5.190128	2.319193	-3.869160
67	7	0	-4.231852	2.773064	-3.364115
68	8	0	-2.387434	-0.247149	-0.789286
69	6	0	-3.527653	0.005386	-1.178571
70	1	0	-3.654867	0.454272	-2.176534
71	6	0	-4.762035	-0.240499	-0.434585
72	6	0	-4.742003	-0.776623	0.867071
73	6	0	-5.985008	0.068153	-1.056949
74	6	0	-5.941748	-1.009482	1.528623
75	1	0	-3.786649	-0.979431	1.340733
76	6	0	-7.181888	-0.170392	-0.385532
77	1	0	-5.989630	0.503869	-2.053612
78	6	0	-7.158979	-0.711171	0.902342
79	1	0	-5.936900	-1.420783	2.534217
80	1	0	-8.128271	0.066746	-0.862307
81	1	0	-8.093288	-0.896976	1.425725

E_{ZPE}: B3LYP/6-31G* = -2820.39369 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.06851 (a.u.)

Int_6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.412037	-3.471122	0.547882
2	6	0	-2.758356	-3.171768	0.864440
3	6	0	-3.250626	-1.845276	0.630001
4	6	0	-2.379015	-0.847024	0.074205
5	6	0	-1.026873	-1.149080	-0.105103
6	6	0	-0.564315	-2.490036	0.092215
7	6	0	-2.892727	0.508617	-0.282706
8	6	0	-2.367775	1.642680	0.334940

9	6	0	-2.920651	2.930070	0.096390
10	6	0	-3.947969	3.092965	-0.796567
11	6	0	-3.921413	0.678773	-1.274311
12	6	0	-4.461709	1.985500	-1.521835
13	1	0	-1.048219	-4.488209	0.664652
14	6	0	-3.624351	-4.161584	1.401751
15	6	0	-4.599368	-1.568256	0.994230
16	8	0	-1.325416	1.551050	1.197887
17	1	0	-2.504716	3.770916	0.643203
18	1	0	-4.371145	4.079199	-0.973090
19	6	0	-5.483479	2.150562	-2.493650
20	7	0	0.796300	-2.811289	-0.193631
21	7	0	2.702896	-3.015168	-1.311714
22	6	0	2.793357	-3.734897	-0.137939
23	6	0	1.625246	-3.625450	0.565557
24	6	0	1.500348	-2.472925	-1.312573
25	1	0	3.689499	-4.279739	0.123132
26	1	0	1.306286	-4.020296	1.517375
27	1	0	1.093385	-1.829440	-2.076618
28	6	0	-4.419177	-0.399391	-2.060299
29	8	0	-0.132557	-0.215690	-0.485220
30	22	0	0.414647	1.239800	0.585343
31	8	0	1.092500	1.123263	2.250769
32	8	0	0.714599	2.728172	-0.347668
33	6	0	0.791285	1.040058	3.642286
34	6	0	0.755876	4.147347	-0.386501
35	6	0	0.207604	2.366566	4.129664
36	1	0	1.750493	0.866442	4.153819
37	6	0	-0.131456	-0.149390	3.910429
38	6	0	2.149993	4.633655	0.011126
39	1	0	0.024507	4.522727	0.345599
40	6	0	0.340616	4.607898	-1.783145
41	1	0	3.869205	-2.855820	-2.598386
42	7	0	4.583507	-2.684822	-3.344871
43	6	0	5.415253	-2.435305	-4.135604
44	8	0	2.511639	0.591454	-0.053365
45	6	0	3.511476	0.631879	0.669549
46	1	0	3.381202	0.895587	1.732350
47	6	0	4.871469	0.365169	0.218484
48	6	0	5.143609	-0.044794	-1.099320
49	6	0	5.924514	0.531002	1.135581
50	6	0	6.455607	-0.283827	-1.491145
51	1	0	4.321679	-0.185310	-1.792518
52	6	0	7.237432	0.300380	0.737287
53	1	0	5.705092	0.844011	2.153954
54	6	0	7.499293	-0.106598	-0.574742
55	1	0	6.660059	-0.626302	-2.500607
56	1	0	8.053277	0.431891	1.442027
57	1	0	8.523728	-0.293743	-0.885478
58	6	0	-4.925849	-3.859560	1.727628
59	6	0	-5.409505	-2.544518	1.530011
60	6	0	-5.401644	-0.203301	-3.006036
61	6	0	-5.951552	1.081378	-3.222401
62	1	0	-3.232568	-5.163965	1.559278
63	1	0	-5.578821	-4.621822	2.143541
64	1	0	-6.431892	-2.301020	1.806423
65	1	0	-4.984618	-0.565142	0.854845
66	1	0	-4.004872	-1.390820	-1.917234
67	1	0	-5.754477	-1.045805	-3.595156
68	1	0	-6.730241	1.221490	-3.967101
69	1	0	-5.883643	3.148642	-2.658418
70	1	0	-0.742897	2.567776	3.626416
71	1	0	0.898591	3.189650	3.916621
72	1	0	0.034234	2.335259	5.211707
73	1	0	0.330237	-1.078713	3.558791
74	1	0	-1.083211	-0.015251	3.387648
75	1	0	-0.329239	-0.249315	4.984001
76	1	0	2.899256	4.265337	-0.698645
77	1	0	2.412175	4.273677	1.012079
78	1	0	2.189275	5.729031	0.018345

79	1	0	-0.656498	4.228496	-2.025813
80	1	0	1.046130	4.232835	-2.532855
81	1	0	0.322686	5.702737	-1.837821

E_{ZPE}: B3LYP/6-31G* = -2820.38061 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.07185 (a.u.)

Int_7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.117101	-3.706909	0.483633
2	6	0	3.945624	-3.009069	-0.435185
3	6	0	2.120457	-3.054591	1.163334
4	6	0	1.922938	-1.657709	0.987798
5	6	0	2.777735	-0.903636	0.184596
6	6	0	3.768096	-1.593891	-0.599048
7	6	0	2.663674	0.584753	0.160218
8	6	0	3.779695	1.404370	0.550635
9	6	0	1.465913	1.197708	-0.218708
10	6	0	1.413353	2.623214	-0.361640
11	6	0	2.502031	3.406599	-0.064324
12	6	0	3.700395	2.829256	0.415634
13	1	0	3.270714	-4.774352	0.624666
14	6	0	4.930140	-3.686667	-1.201737
15	1	0	1.459167	-3.577796	1.847270
16	6	0	4.575617	-0.936155	-1.570151
17	6	0	4.973362	0.863566	1.109064
18	8	0	0.350732	0.495101	-0.487863
19	1	0	2.429843	4.485966	-0.165933
20	6	0	4.805885	3.639473	0.789396
21	7	0	0.233080	3.250332	-0.867060
22	22	0	-0.627786	-0.631456	0.651466
23	7	0	-1.874492	3.904835	-1.083041
24	6	0	-1.107888	4.548730	-2.032538
25	6	0	0.197408	4.161381	-1.913565
26	6	0	-1.043034	3.134361	-0.404571
27	1	0	-1.545683	5.240586	-2.738011
28	1	0	1.088136	4.412162	-2.467725
29	1	0	-1.306548	2.482295	0.412899
30	8	0	-1.558929	0.150627	1.960438
31	8	0	-1.116986	-2.239422	0.022393
32	6	0	-2.707667	0.226252	2.792708
33	6	0	-0.829812	-3.327511	-0.854478
34	1	0	-3.575879	0.407424	2.141305
35	6	0	-2.907292	-1.097788	3.531504
36	6	0	-2.544250	1.410846	3.744881
37	6	0	-1.466252	-4.597184	-0.289893
38	6	0	-1.317313	-2.996620	-2.265610
39	1	0	0.259940	-3.460390	-0.873464
40	8	0	0.885049	-1.073675	1.639301
41	1	0	-3.580757	3.945990	-1.019921
42	6	0	-5.781110	3.643200	-1.179128
43	7	0	-4.629909	3.847363	-1.068587
44	8	0	-2.414554	0.197173	-0.639770
45	6	0	-3.575113	0.418763	-0.978456
46	6	0	-4.725091	-0.456746	-0.730725
47	6	0	-4.563512	-1.740000	-0.175475
48	6	0	-5.679242	-2.541176	0.038018
49	6	0	-6.955949	-2.067948	-0.291486
50	6	0	-7.120934	-0.791807	-0.834820
51	6	0	-6.007526	0.015146	-1.060219
52	1	0	-3.798063	1.355104	-1.516015
53	1	0	-3.564018	-2.087687	0.065532
54	1	0	-5.562076	-3.535426	0.460219
55	1	0	-7.824758	-2.698170	-0.120340
56	1	0	-8.113656	-0.425857	-1.079397
57	1	0	-6.129194	1.019755	-1.458694

58	6	0	5.949917	3.078104	1.305624
59	6	0	6.023364	1.675502	1.476250
60	6	0	5.703166	-3.014067	-2.120079
61	6	0	5.511366	-1.625766	-2.309608
62	1	0	4.722900	4.717313	0.669859
63	1	0	6.788451	3.705753	1.594153
64	1	0	6.917048	1.232818	1.907873
65	1	0	5.046231	-0.206727	1.259671
66	1	0	4.438180	0.126179	-1.736477
67	1	0	6.106257	-1.096799	-3.049618
68	1	0	6.449674	-3.544573	-2.704764
69	1	0	5.053731	-4.757348	-1.054305
70	1	0	-2.044249	-1.308263	4.172950
71	1	0	-3.020828	-1.924515	2.822144
72	1	0	-3.805627	-1.057214	4.158076
73	1	0	-2.398328	2.340163	3.184889
74	1	0	-1.674942	1.259217	4.394103
75	1	0	-3.435154	1.524017	4.373104
76	1	0	-2.558681	-4.507865	-0.267220
77	1	0	-1.112998	-4.782672	0.729479
78	1	0	-1.206398	-5.463020	-0.909781
79	1	0	-0.846042	-2.078513	-2.630978
80	1	0	-2.404161	-2.857318	-2.278286
81	1	0	-1.065696	-3.810239	-2.955789

E_{ZPE}: B3LYP/6-31G* = -2820.39071 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.06320 (a.u.)

Int_8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.272166	-0.785391	-0.482539
2	6	0	-3.422216	-0.387768	-0.280545
3	1	0	-3.668134	0.101960	0.673915
4	6	0	-4.511279	-0.537665	-1.244970
5	6	0	-4.285865	-1.122827	-2.504502
6	6	0	-5.798672	-0.100065	-0.890730
7	6	0	-5.340625	-1.267392	-3.396549
8	1	0	-3.283075	-1.449420	-2.760945
9	6	0	-6.852749	-0.251037	-1.789328
10	1	0	-5.963422	0.364025	0.077852
11	6	0	-6.623622	-0.833173	-3.038015
12	1	0	-5.171952	-1.716011	-4.371335
13	1	0	-7.848633	0.086696	-1.518438
14	1	0	-7.446340	-0.948524	-3.738732
15	1	0	-4.017390	3.041491	0.585209
16	7	0	-4.745329	2.697980	1.268725
17	6	0	-5.493436	2.199473	2.024785
18	6	0	1.846774	3.552679	-0.586225
19	6	0	3.189888	3.210095	-0.304424
20	6	0	3.513187	1.843359	-0.012355
21	6	0	2.493182	0.831890	-0.091813
22	6	0	1.171616	1.214128	-0.338658
23	6	0	0.864882	2.593169	-0.577842
24	6	0	2.823504	-0.604530	0.144623
25	6	0	3.790799	-1.306841	-0.655911
26	6	0	4.181862	-2.639504	-0.292840
27	6	0	3.579936	-3.251102	0.840047
28	6	0	2.189769	-1.292988	1.180884
29	6	0	2.598115	-2.605600	1.545937
30	1	0	1.582266	4.592235	-0.760096
31	6	0	4.202156	4.205635	-0.251438
32	6	0	4.852657	1.557892	0.380250
33	7	0	-0.493880	2.980749	-0.793283
34	6	0	4.365716	-0.747629	-1.832482
35	6	0	5.145139	-3.325833	-1.078024
36	1	0	3.894754	-4.252246	1.125814

37	1	0	2.103639	-3.071867	2.392504
38	8	0	1.160145	-0.729296	1.865449
39	8	0	0.159923	0.331850	-0.387886
40	22	0	-0.485022	-0.809036	0.966845
41	8	0	-0.650262	-2.574731	0.800033
42	8	0	-1.523415	-0.003348	2.184490
43	6	0	-0.612016	-3.820776	0.122154
44	6	0	-2.167022	-0.010114	3.459407
45	6	0	-0.176376	-3.625742	-1.330480
46	6	0	-1.239880	0.642188	4.484448
47	6	0	-1.975677	-4.501724	0.246754
48	1	0	0.141515	-4.434215	0.637481
49	6	0	-2.572096	-1.431224	3.848432
50	1	0	-3.072845	0.603072	3.351265
51	6	0	-1.537470	2.748823	0.048190
52	7	0	-2.654211	3.292796	-0.401724
53	6	0	-2.323554	3.907119	-1.591572
54	6	0	-0.990834	3.728048	-1.849356
55	1	0	-1.436693	2.182706	0.962681
56	1	0	-3.060762	4.431676	-2.182425
57	1	0	-0.358076	4.030792	-2.669044
58	6	0	5.490530	3.884965	0.105574
59	6	0	5.809152	2.546965	0.437306
60	6	0	5.693352	-2.745752	-2.199272
61	6	0	5.286265	-1.446779	-2.582301
62	1	0	3.931537	5.232749	-0.485659
63	1	0	6.257002	4.653734	0.148846
64	1	0	6.820223	2.296402	0.747162
65	1	0	5.116634	0.542586	0.649433
66	1	0	4.059692	0.244174	-2.145871
67	1	0	5.701216	-0.995471	-3.479833
68	1	0	6.426014	-3.283793	-2.794577
69	1	0	5.434794	-4.330883	-0.778907
70	1	0	0.805512	-3.144249	-1.375657
71	1	0	-0.897716	-2.995788	-1.862636
72	1	0	-0.110201	-4.591870	-1.844007
73	1	0	-0.971851	1.655899	4.170176
74	1	0	-0.317849	0.060239	4.589250
75	1	0	-1.732760	0.702356	5.461628
76	1	0	-2.745695	-3.910854	-0.261678
77	1	0	-2.258035	-4.607518	1.299216
78	1	0	-1.948928	-5.499682	-0.206137
79	1	0	-1.686427	-2.066938	3.962956
80	1	0	-3.219029	-1.875311	3.084583
81	1	0	-3.118928	-1.424872	4.798074

E_{ZPE}: B3LYP/6-31G* = -2820.39589 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.06846 (a.u.)

TS_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.772300	3.253793	-0.318860
2	6	0	3.914737	2.553779	0.126412
3	6	0	3.823309	1.138322	0.335368
4	6	0	2.606213	0.443489	0.015599
5	6	0	1.473396	1.173765	-0.362585
6	6	0	1.580199	2.596949	-0.512246
7	6	0	2.528370	-1.040023	0.154562
8	6	0	1.592344	-1.596067	1.026384
9	6	0	1.613232	-2.983761	1.334627
10	6	0	2.512899	-3.817968	0.723523
11	6	0	3.411212	-1.920432	-0.562837
12	6	0	3.410523	-3.323857	-0.261770
13	1	0	2.845943	4.322770	-0.495924
14	6	0	5.131380	3.236933	0.397096
15	6	0	4.966182	0.484044	0.880303

16	8	0	0.635737	-0.825032	1.600888
17	1	0	0.892769	-3.352060	2.057785
18	1	0	2.533087	-4.877802	0.967679
19	6	0	4.289573	-4.190866	-0.962068
20	7	0	0.416657	3.373888	-0.829751
21	7	0	-1.504903	4.014551	-1.642028
22	6	0	-1.010873	5.067594	-0.909433
23	6	0	0.190861	4.679078	-0.396852
24	6	0	-0.645094	3.005287	-1.578460
25	1	0	-1.552922	5.993548	-0.799463
26	1	0	0.884133	5.186487	0.252450
27	1	0	-0.789703	2.030914	-2.012379
28	6	0	4.278058	-1.467079	-1.597280
29	8	0	0.293658	0.599083	-0.628893
30	22	0	-0.851276	-0.429965	0.518022
31	8	0	-1.693046	0.430260	1.851101
32	8	0	-1.350695	-2.115067	0.188898
33	6	0	-1.462911	0.753033	3.222066
34	6	0	-1.970869	-3.155361	-0.541560
35	6	0	-2.438103	-0.031904	4.098605
36	6	0	-1.593710	2.265154	3.401721
37	1	0	-0.435789	0.445037	3.461677
38	6	0	-2.494731	-4.207799	0.436734
39	6	0	-0.988132	-3.729384	-1.563248
40	1	0	-2.829381	-2.721488	-1.077986
41	1	0	-2.499486	3.862326	-2.106209
42	6	0	6.220615	2.564416	0.896758
43	6	0	6.124705	1.175703	1.153665
44	6	0	5.106960	-2.337888	-2.270528
45	6	0	5.125711	-3.714025	-1.945969
46	1	0	5.177322	4.308255	0.214561
47	1	0	7.145041	3.094379	1.108267
48	1	0	6.975604	0.648113	1.576115
49	1	0	4.913564	-0.576570	1.091910
50	1	0	4.271041	-0.416666	-1.866777
51	1	0	5.749959	-1.962812	-3.062540
52	1	0	5.788847	-4.389561	-2.479345
53	1	0	4.279597	-5.249490	-0.711691
54	1	0	-2.245496	0.166584	5.159487
55	1	0	-3.473546	0.253706	3.878513
56	1	0	-2.329890	-1.107401	3.924629
57	1	0	-1.392697	2.547377	4.441908
58	1	0	-0.880530	2.790911	2.758167
59	1	0	-2.604631	2.598266	3.140532
60	1	0	-3.022974	-5.003977	-0.100464
61	1	0	-1.664954	-4.655962	0.994512
62	1	0	-3.188065	-3.752352	1.150933
63	1	0	-1.465922	-4.519932	-2.153773
64	1	0	-0.643725	-2.946961	-2.247734
65	1	0	-0.113000	-4.148612	-1.056309
66	6	0	-4.076091	2.069537	-2.545695
67	7	0	-3.750885	3.197962	-2.624991
68	8	0	-2.348899	0.092166	-0.950074
69	6	0	-3.425185	-0.141978	-1.535230
70	1	0	-3.405763	-0.348830	-2.609166
71	6	0	-4.697041	-0.416137	-0.845091
72	6	0	-4.806084	-0.312297	0.549991
73	6	0	-5.797150	-0.845861	-1.602877
74	6	0	-6.006527	-0.643434	1.174349
75	1	0	-3.952652	0.028941	1.126593
76	6	0	-6.992339	-1.179650	-0.974297
77	1	0	-5.711495	-0.894155	-2.685367
78	6	0	-7.097438	-1.078713	0.416601
79	1	0	-6.094260	-0.562419	2.254504
80	1	0	-7.843256	-1.510149	-1.563253
81	1	0	-8.031816	-1.335630	0.908838

E_{ZPE}: B3LYP/6-31G* = -2820.37602 (a.u.)

Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.06103 (a.u.)

TS_4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.626572	3.167058	-1.097187
2	6	0	3.855912	2.526845	-0.824973
3	6	0	3.845017	1.193543	-0.296186
4	6	0	2.600225	0.487898	-0.164460
5	6	0	1.398047	1.155447	-0.425255
6	6	0	1.435689	2.527039	-0.848621
7	6	0	2.567306	-0.921979	0.321114
8	6	0	1.830793	-1.231074	1.468660
9	6	0	1.944830	-2.511787	2.080159
10	6	0	2.708667	-3.495473	1.507758
11	6	0	3.289047	-1.976511	-0.339846
12	6	0	3.370388	-3.273617	0.269549
13	1	0	2.638637	4.183126	-1.480726
14	6	0	5.089460	3.207002	-1.015374
15	6	0	5.097806	0.636366	0.092664
16	8	0	0.993202	-0.327906	2.029841
17	1	0	1.403799	-2.675522	3.006959
18	1	0	2.796226	-4.469972	1.983028
19	6	0	4.090778	-4.310035	-0.379994
20	7	0	0.217100	3.283938	-0.927668
21	7	0	-1.889893	3.843268	-1.038945
22	6	0	-1.191289	4.986410	-0.727255
23	6	0	0.126275	4.649538	-0.658899
24	6	0	-1.035685	2.829542	-1.148841
25	1	0	-1.682640	5.932766	-0.565700
26	1	0	0.993642	5.234569	-0.405768
27	1	0	-1.302316	1.801966	-1.330598
28	6	0	3.908508	-1.805149	-1.610577
29	8	0	0.208341	0.561495	-0.333217
30	22	0	-0.697023	-0.185868	1.195933
31	8	0	-1.495357	1.023013	2.205815
32	8	0	-1.276474	-1.853897	1.450751
33	6	0	-2.576409	1.497311	3.007893
34	6	0	-1.445419	-3.248910	1.264446
35	6	0	-2.994225	0.418964	4.006555
36	1	0	-3.406134	1.711581	2.321663
37	6	0	-2.137564	2.794003	3.685822
38	6	0	-2.865934	-3.646167	1.670207
39	1	0	-0.733388	-3.748619	1.937086
40	6	0	-1.111605	-3.640511	-0.176177
41	1	0	-2.959059	3.660682	-0.962649
42	6	0	6.280195	2.620886	-0.658987
43	6	0	6.275149	1.328267	-0.082209
44	6	0	4.585375	-2.837080	-2.223419
45	6	0	4.691613	-4.102270	-1.600843
46	1	0	5.069628	4.211275	-1.432998
47	1	0	7.218261	3.150262	-0.800388
48	1	0	7.212528	0.876755	0.231404
49	1	0	5.118075	-0.347926	0.543531
50	1	0	3.830247	-0.844950	-2.108411
51	1	0	5.038928	-2.677170	-3.198213
52	1	0	5.234645	-4.905835	-2.090772
53	1	0	4.147934	-5.282173	0.104992
54	1	0	-2.171625	0.195117	4.695725
55	1	0	-3.266505	-0.505807	3.486937
56	1	0	-3.858266	0.753060	4.592157
57	1	0	-1.844842	3.536408	2.936683
58	1	0	-1.283182	2.611228	4.347182
59	1	0	-2.958952	3.209952	4.280512
60	1	0	-3.602985	-3.190428	0.999250
61	1	0	-3.078421	-3.321405	2.694037
62	1	0	-2.987099	-4.734524	1.620867
63	1	0	-0.086489	-3.348842	-0.424931
64	1	0	-1.795453	-3.151664	-0.878706

65	1	0	-1.200568	-4.725385	-0.306345
66	8	0	-2.290865	-0.098769	-0.368554
67	6	0	-3.509369	-0.341359	-0.244967
68	1	0	-3.952203	-0.444129	0.749920
69	6	0	-4.322079	-0.832909	-1.375426
70	6	0	-3.740079	-1.037841	-2.634357
71	6	0	-5.666570	-1.171960	-1.165950
72	6	0	-4.498561	-1.573861	-3.672437
73	1	0	-2.695438	-0.781327	-2.779091
74	6	0	-6.421744	-1.709611	-2.203708
75	1	0	-6.116648	-0.985967	-0.194329
76	6	0	-5.838147	-1.910110	-3.458684
77	1	0	-4.046708	-1.733331	-4.647622
78	1	0	-7.464408	-1.967068	-2.040202
79	1	0	-6.428277	-2.328562	-4.269730
80	7	0	-4.324460	2.976413	-0.578481
81	6	0	-4.525714	1.891119	-0.171315

E_{ZPE}: B3LYP/6-31G* = -2820.37774 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.07185 (a.u.)

TS_5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.225901	2.920298	-0.990740
2	7	0	-3.832567	4.028160	-1.046048
3	1	0	-2.332707	4.421582	-1.223388
4	6	0	2.241771	-3.978967	0.276003
5	6	0	3.204883	-3.431018	-0.613581
6	6	0	1.373096	-3.166390	0.958125
7	6	0	1.443068	-1.752458	0.816473
8	6	0	2.437523	-1.161480	0.038045
9	6	0	3.298431	-2.004682	-0.746382
10	6	0	2.588481	0.322297	0.053127
11	6	0	3.818353	0.923438	0.491082
12	6	0	1.514189	1.139890	-0.319299
13	6	0	1.726401	2.556189	-0.403308
14	6	0	2.920741	3.137862	-0.051685
15	6	0	3.989736	2.345679	0.421551
16	1	0	2.190243	-5.059197	0.392979
17	6	0	4.062107	-4.263983	-1.379434
18	1	0	0.614633	-3.572351	1.620330
19	6	0	4.235572	-1.489445	-1.686322
20	6	0	4.891389	0.162411	1.039855
21	8	0	0.304290	0.666575	-0.634449
22	1	0	3.036444	4.217237	-0.100211
23	6	0	5.209113	2.938041	0.847954
24	7	0	0.686663	3.402275	-0.916577
25	22	0	-0.921388	-0.355465	0.431337
26	7	0	-1.245967	4.342441	-1.267448
27	6	0	-0.331027	5.014826	-2.043788
28	6	0	0.883705	4.433479	-1.829758
29	6	0	-0.623343	3.373921	-0.605456
30	1	0	-0.615742	5.832836	-2.686261
31	1	0	1.856086	4.628947	-2.250789
32	1	0	-1.102138	2.679514	0.062988
33	8	0	-1.656962	0.481196	1.834965
34	8	0	-1.532204	-1.928092	-0.117775
35	6	0	-1.751051	0.634595	3.248290
36	6	0	-1.812593	-3.207344	-0.657562
37	6	0	-1.877750	-0.734118	3.919436
38	6	0	-0.548975	1.431196	3.756239
39	1	0	-2.668858	1.211423	3.433601
40	6	0	-2.741502	-3.966924	0.290059
41	6	0	-2.395921	-3.056445	-2.063557
42	1	0	-0.854513	-3.741397	-0.725478
43	8	0	0.532664	-0.989616	1.465193

44	8	0	-2.395575	0.582161	-0.864562
45	6	0	-3.552109	0.625408	-1.329297
46	6	0	-4.729801	-0.042625	-0.735613
47	6	0	-4.747952	-0.466876	0.600453
48	6	0	-5.864684	-1.130479	1.102573
49	6	0	-6.963926	-1.384945	0.275909
50	6	0	-6.949544	-0.964746	-1.056128
51	6	0	-5.838470	-0.290062	-1.557223
52	1	0	-3.676641	0.951453	-2.367833
53	1	0	-3.895157	-0.250969	1.233698
54	1	0	-5.883376	-1.447480	2.141972
55	1	0	-7.832449	-1.904564	0.671971
56	1	0	-7.804571	-1.155987	-1.698557
57	1	0	-5.828366	0.057634	-2.587564
58	6	0	4.967802	-3.729195	-2.267131
59	6	0	5.043001	-2.326014	-2.425687
60	6	0	6.056447	0.765366	1.457274
61	6	0	6.228636	2.166522	1.351892
62	1	0	5.314492	4.018338	0.777299
63	1	0	7.156306	2.626805	1.680122
64	1	0	6.852432	0.157289	1.878628
65	1	0	4.776658	-0.909900	1.139809
66	1	0	4.301133	-0.416462	-1.828603
67	1	0	5.742525	-1.902115	-3.141563
68	1	0	5.614573	-4.378120	-2.851234
69	1	0	3.980483	-5.341858	-1.256680
70	1	0	-0.981781	-1.331943	3.725547
71	1	0	-2.748287	-1.274905	3.532210
72	1	0	-1.999346	-0.619888	5.002812
73	1	0	-0.496768	2.405021	3.257308
74	1	0	0.377923	0.884858	3.555671
75	1	0	-0.631149	1.605176	4.835580
76	1	0	-3.697082	-3.441351	0.391366
77	1	0	-2.288069	-4.055001	1.283029
78	1	0	-2.936239	-4.976254	-0.091149
79	1	0	-1.714910	-2.483507	-2.701231
80	1	0	-3.361124	-2.539699	-2.028026
81	1	0	-2.548097	-4.042182	-2.518549

E_{ZPE}: B3LYP/6-31G* = -2820.37292 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.05565 (a.u.)

TS_6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.345782	-0.098395	-0.290050
2	6	0	-3.558635	-0.279599	-0.028690
3	1	0	-3.863415	-0.578692	0.978457
4	6	0	-4.538040	-0.553072	-1.107395
5	6	0	-5.841704	-0.947663	-0.778012
6	6	0	-4.148586	-0.493389	-2.451974
7	6	0	-6.747629	-1.280281	-1.781588
8	1	0	-6.143575	-0.973366	0.266208
9	6	0	-5.057578	-0.823002	-3.455126
10	1	0	-3.133112	-0.193667	-2.690624
11	6	0	-6.356393	-1.217201	-3.122269
12	1	0	-7.757985	-1.584239	-1.522237
13	1	0	-4.754085	-0.776761	-4.497612
14	1	0	-7.063456	-1.475572	-3.906204
15	6	0	-4.357668	1.840944	0.508846
16	7	0	-4.274600	2.994137	0.293515
17	1	0	-3.012754	3.689936	-0.494671
18	6	0	2.476105	3.310298	-0.674268
19	6	0	3.729029	2.734339	-0.365899
20	6	0	3.791452	1.335395	-0.051330
21	6	0	2.603495	0.528306	-0.108273
22	6	0	1.368080	1.137792	-0.356509

23	6	0	1.339012	2.540767	-0.653871
24	6	0	2.657848	-0.937103	0.161572
25	6	0	1.904946	-1.455344	1.217763
26	6	0	2.051754	-2.814440	1.615732
27	6	0	2.879899	-3.658938	0.922447
28	6	0	3.463455	-1.833052	-0.622175
29	6	0	3.583611	-3.207975	-0.226880
30	1	0	2.412299	4.375024	-0.883205
31	6	0	4.907654	3.527154	-0.322942
32	6	0	5.055956	0.812849	0.348043
33	8	0	1.027910	-0.677205	1.888341
34	1	0	1.487605	-3.150991	2.480050
35	1	0	2.993091	-4.695090	1.233570
36	6	0	4.386988	-4.090627	-0.995295
37	7	0	0.081113	3.160991	-0.961131
38	7	0	-2.007004	3.756494	-0.852625
39	6	0	-1.474713	4.383716	-1.956607
40	6	0	-0.163018	4.016228	-2.030093
41	6	0	-1.064801	3.021004	-0.272258
42	1	0	-2.064256	5.021412	-2.595693
43	1	0	0.609487	4.256301	-2.742217
44	1	0	-1.210379	2.417036	0.609823
45	6	0	4.135558	-1.426809	-1.809931
46	8	0	0.208966	0.475141	-0.363248
47	22	0	-0.669812	-0.419834	1.092206
48	8	0	-1.362690	0.727696	2.264839
49	8	0	-1.253639	-2.106850	1.188738
50	6	0	-2.263915	1.000148	3.341882
51	6	0	-1.411601	-3.434356	0.712180
52	6	0	-2.411723	-0.234622	4.229721
53	1	0	-3.229622	1.248038	2.883697
54	6	0	-1.744605	2.216352	4.106511
55	6	0	-1.185425	-3.490963	-0.799724
56	6	0	-2.789154	-3.955707	1.124772
57	1	0	-0.640127	-4.043009	1.205995
58	6	0	6.178257	1.608739	0.393460
59	6	0	6.113435	2.978634	0.043012
60	6	0	5.036342	-3.657769	-2.129085
61	6	0	4.896335	-2.312392	-2.541734
62	1	0	7.009131	3.592362	0.078489
63	1	0	4.832603	4.582909	-0.573869
64	1	0	7.125557	1.180139	0.709478
65	1	0	5.126538	-0.229695	0.632503
66	1	0	4.032273	-0.401397	-2.147237
67	1	0	5.390793	-1.973583	-3.448545
68	1	0	5.644390	-4.344821	-2.711222
69	1	0	4.471178	-5.126173	-0.672622
70	1	0	-1.452793	-0.490768	4.694888
71	1	0	-2.750162	-1.096157	3.644495
72	1	0	-3.143993	-0.047518	5.023522
73	1	0	-1.659758	3.082446	3.442257
74	1	0	-0.758378	2.007358	4.535931
75	1	0	-2.432540	2.477299	4.918852
76	1	0	-0.183222	-3.128397	-1.050978
77	1	0	-1.920982	-2.870276	-1.322404
78	1	0	-1.278016	-4.521331	-1.161959
79	1	0	-3.583891	-3.390768	0.624532
80	1	0	-2.925275	-3.864456	2.207442
81	1	0	-2.896120	-5.011794	0.851238

E_{ZPE}: B3LYP/6-31G* = -2820.37946 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.05984 (a.u.)

Int_9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.331948	3.328621	-0.032007

2	6	0	3.473928	2.740311	0.555639
3	6	0	3.569334	1.308678	0.611397
4	6	0	2.537748	0.493925	0.035464
5	6	0	1.368387	1.099696	-0.438941
6	6	0	1.302719	2.534580	-0.480939
7	6	0	2.669611	-0.987691	-0.049595
8	6	0	1.704305	-1.804606	0.552430
9	6	0	1.902872	-3.217055	0.600860
10	6	0	2.981086	-3.803972	-0.006631
11	6	0	3.761422	-1.598332	-0.760178
12	6	0	3.924520	-3.024021	-0.726801
13	1	0	2.285069	4.410150	-0.124433
14	6	0	4.516281	3.542553	1.095469
15	6	0	4.704962	0.753005	1.269325
16	8	0	0.606442	-1.299244	1.122667
17	1	0	1.169127	-3.809032	1.138485
18	1	0	3.118158	-4.882217	0.040758
19	6	0	5.005745	-3.626741	-1.420455
20	7	0	0.122434	3.157737	-1.018805
21	7	0	-1.669196	3.514795	-2.193247
22	6	0	-1.492624	4.632541	-1.403905
23	6	0	-0.369080	4.413437	-0.667525
24	6	0	-0.701238	2.632178	-1.939312
25	1	0	-2.174168	5.467499	-1.421699
26	1	0	0.107872	5.017309	0.085466
27	1	0	-0.612960	1.641153	-2.346349
28	6	0	4.690366	-0.853077	-1.542228
29	8	0	0.327462	0.405678	-0.894596
30	22	0	-0.959843	-0.534725	0.271299
31	8	0	-1.495641	0.081066	1.886519
32	8	0	-1.629597	-2.125361	-0.290352
33	6	0	-1.021566	0.044543	3.226848
34	6	0	-1.814909	-3.432295	0.234986
35	6	0	-2.118354	-0.520181	4.130604
36	6	0	-0.589432	1.452229	3.640649
37	1	0	-0.147659	-0.620098	3.255493
38	6	0	-3.254722	-3.590120	0.728125
39	1	0	-1.133396	-3.559166	1.089505
40	6	0	-1.447862	-4.450395	-0.845206
41	1	0	-2.471122	3.270830	-2.782392
42	6	0	-3.591466	0.917273	-2.590196
43	7	0	-3.619199	1.744006	-3.408441
44	8	0	-2.340738	0.417473	-0.719854
45	6	0	-3.426324	-0.031464	-1.440933
46	1	0	-3.239558	-1.034617	-1.863435
47	6	0	-4.746404	-0.084824	-0.655377
48	6	0	-5.913328	-0.547973	-1.274454
49	6	0	-4.781865	0.309509	0.683076
50	6	0	-7.109490	-0.613884	-0.561378
51	1	0	-5.889118	-0.857137	-2.318053
52	6	0	-5.981910	0.238557	1.396154
53	1	0	-3.866699	0.643602	1.159800
54	6	0	-7.146075	-0.219288	0.778673
55	1	0	-8.010731	-0.975477	-1.049631
56	1	0	-6.003884	0.540976	2.440228
57	1	0	-8.077112	-0.272849	1.336951
58	6	0	5.687310	1.556281	1.802020
59	6	0	5.605082	2.966912	1.704827
60	6	0	5.722239	-1.469461	-2.216530
61	6	0	5.895272	-2.870968	-2.150161
62	1	0	4.427626	4.624776	1.028074
63	1	0	6.393507	3.587325	2.121697
64	1	0	6.536018	1.102227	2.306465
65	1	0	4.780607	-0.324099	1.357179
66	1	0	4.571086	0.221760	-1.619655
67	1	0	6.407573	-0.870015	-2.810682
68	1	0	6.716119	-3.345083	-2.681406
69	1	0	5.110861	-4.708656	-1.371878
70	1	0	-1.767089	-0.591212	5.167035
71	1	0	-3.006245	0.122875	4.110168

72	1	0	-2.412537	-1.521087	3.797775
73	1	0	-0.204415	1.455033	4.667407
74	1	0	0.202102	1.816368	2.976979
75	1	0	-1.437209	2.145830	3.586117
76	1	0	-3.403643	-4.578670	1.179057
77	1	0	-3.491017	-2.826840	1.476731
78	1	0	-3.961202	-3.479363	-0.102624
79	1	0	-2.102402	-4.331707	-1.716648
80	1	0	-0.412316	-4.305738	-1.167915
81	1	0	-1.557321	-5.474236	-0.467514

E_{ZPE}: B3LYP/6-31G* = -2820.40775 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.08643 (a.u.)

int_{10}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.970559	-2.715869	-1.093472
2	6	0	-4.049752	-2.016090	-0.509619
3	6	0	-3.832207	-0.688341	-0.005971
4	6	0	-2.555025	-0.065103	-0.172601
5	6	0	-1.481087	-0.800576	-0.694821
6	6	0	-1.717162	-2.149148	-1.138141
7	6	0	-2.303260	1.356288	0.201595
8	6	0	-1.270692	1.671036	1.091402
9	6	0	-1.071373	3.016814	1.514275
10	6	0	-1.842202	4.036092	1.021067
11	6	0	-3.061177	2.429838	-0.385886
12	6	0	-2.840889	3.781467	0.045161
13	1	0	-3.153679	-3.710636	-1.489568
14	6	0	-5.332469	-2.618064	-0.387571
15	6	0	-4.921546	-0.052679	0.659375
16	8	0	-0.449810	0.736026	1.605945
17	1	0	-0.289119	3.204248	2.243455
18	1	0	-1.682993	5.058243	1.357530
19	6	0	-3.599933	4.836484	-0.525680
20	7	0	-0.602879	-2.938584	-1.595671
21	7	0	1.393784	-3.539795	-2.218579
22	6	0	0.692420	-4.703838	-1.986554
23	6	0	-0.558078	-4.332385	-1.600982
24	6	0	0.607660	-2.487036	-1.970538
25	1	0	1.133362	-5.680434	-2.104911
26	1	0	-1.401276	-4.930560	-1.303186
27	1	0	0.900996	-1.449052	-1.987721
28	6	0	-4.013372	2.223550	-1.425752
29	8	0	-0.269131	-0.289486	-0.808683
30	22	0	0.961329	-0.254454	0.815140
31	8	0	0.819332	-2.016841	1.181541
32	8	0	2.157450	0.315159	2.074414
33	6	0	1.038382	-2.971425	2.212312
34	6	0	2.309408	1.339431	3.038561
35	6	0	2.538388	-3.159608	2.447093
36	1	0	0.619285	-3.919976	1.841517
37	6	0	0.283946	-2.574415	3.481984
38	6	0	3.092265	0.798928	4.237477
39	1	0	1.301211	1.629747	3.372778
40	6	0	2.990107	2.556983	2.407577
41	1	0	2.402744	-3.434352	-2.366377
42	8	0	2.230485	-0.026841	-0.617607
43	6	0	3.610020	-0.153831	-0.562741
44	1	0	3.973751	-0.245965	0.473342
45	6	0	4.355998	1.000433	-1.240167
46	6	0	3.677246	1.867946	-2.098092
47	6	0	5.722719	1.184598	-1.005087
48	6	0	4.363962	2.914267	-2.717133
49	1	0	2.614564	1.721488	-2.260206
50	6	0	6.408196	2.227572	-1.627708

51	1	0	6.252835	0.512987	-0.332214
52	6	0	5.728779	3.094953	-2.486365
53	1	0	3.829805	3.590228	-3.379718
54	1	0	7.469234	2.366514	-1.437882
55	1	0	6.260813	3.910770	-2.968552
56	6	0	3.937974	-1.437699	-1.264568
57	7	0	4.056163	-2.441673	-1.839364
58	6	0	-6.144495	-0.671153	0.781488
59	6	0	-6.363555	-1.962578	0.241024
60	6	0	-4.528921	4.593920	-1.511475
61	6	0	-4.722939	3.271007	-1.971402
62	1	0	-5.477280	-3.618849	-0.789463
63	1	0	-7.337681	-2.434037	0.336943
64	1	0	-6.952436	-0.163693	1.301979
65	1	0	-4.769523	0.933443	1.082211
66	1	0	-4.169381	1.220393	-1.804926
67	1	0	-5.435841	3.077349	-2.769006
68	1	0	-5.099605	5.411058	-1.944516
69	1	0	-3.420802	5.850107	-0.173072
70	1	0	2.986227	-2.218383	2.780736
71	1	0	3.035027	-3.470588	1.521132
72	1	0	2.720166	-3.926360	3.209668
73	1	0	-0.779588	-2.430813	3.265854
74	1	0	0.681111	-1.636413	3.884456
75	1	0	0.382097	-3.351946	4.248975
76	1	0	4.100621	0.494172	3.932552
77	1	0	2.586383	-0.070778	4.669469
78	1	0	3.185002	1.564337	5.017152
79	1	0	2.409955	2.923476	1.554303
80	1	0	3.993259	2.296844	2.049809
81	1	0	3.084757	3.371037	3.136416

E_{ZPE}: B3LYP/6-31G* = -2820.40910 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.08520 (a.u.)

Int_{11}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.744494	-3.812362	-0.745831
2	6	0	3.725203	-2.930863	-1.272932
3	6	0	1.681840	-3.330677	-0.028621
4	6	0	1.539130	-1.934997	0.229759
5	6	0	2.533054	-1.041695	-0.180074
6	6	0	3.614289	-1.526064	-0.997986
7	6	0	2.455000	0.397969	0.200403
8	6	0	3.506853	1.025162	0.948020
9	6	0	1.341393	1.156341	-0.189527
10	6	0	1.435247	2.589406	-0.089010
11	6	0	2.468208	3.213062	0.571726
12	6	0	3.503998	2.446650	1.150143
13	1	0	2.841870	-4.879524	-0.933495
14	6	0	4.794828	-3.411752	-2.071673
15	1	0	0.920620	-3.996397	0.365867
16	6	0	4.584971	-0.667332	-1.590127
17	6	0	4.563087	0.279568	1.548081
18	8	0	0.231786	0.628080	-0.692193
19	1	0	2.487058	4.294975	0.673276
20	6	0	4.541299	3.058210	1.905643
21	7	0	0.487082	3.399734	-0.806821
22	22	0	-1.058000	-0.509039	0.306181
23	7	0	-1.287369	4.081227	-1.851487
24	6	0	-0.302272	5.007744	-2.121536
25	6	0	0.813063	4.584241	-1.467715
26	6	0	-0.800880	3.115213	-1.063540
27	1	0	-0.467969	5.864690	-2.754322
28	1	0	1.811117	4.987369	-1.439990
29	1	0	-1.365452	2.247835	-0.722224

30	8	0	-1.571258	-0.235475	2.007917
31	8	0	-1.832035	-1.866282	-0.604064
32	6	0	-1.369971	-0.565014	3.375713
33	6	0	-2.028856	-3.270819	-0.528995
34	1	0	-2.192687	-0.084912	3.928172
35	6	0	-1.463125	-2.078010	3.582667
36	6	0	-0.044657	0.018413	3.869034
37	1	0	-1.376945	-3.667642	0.263113
38	6	0	-3.484061	-3.566669	-0.161472
39	6	0	-1.621471	-3.895334	-1.864191
40	8	0	0.462459	-1.523382	0.906570
41	1	0	-2.232659	4.019658	-2.242114
42	6	0	-3.702796	1.747891	-2.039251
43	7	0	-3.740940	2.755038	-2.619349
44	8	0	-2.419113	0.741899	-0.398625
45	6	0	-3.525269	0.521327	-1.195650
46	6	0	-4.828692	0.262892	-0.425212
47	6	0	-4.863896	0.409587	0.962325
48	6	0	-6.051913	0.167324	1.656880
49	6	0	-7.205226	-0.216631	0.971554
50	6	0	-7.168951	-0.364692	-0.417371
51	6	0	-5.983828	-0.126991	-1.112412
52	1	0	-3.360185	-0.326007	-1.883057
53	1	0	-3.953859	0.685585	1.483678
54	1	0	-6.073932	0.277592	2.738193
55	1	0	-8.127379	-0.404656	1.515247
56	1	0	-8.061368	-0.668874	-0.958097
57	1	0	-5.958568	-0.245267	-2.194354
58	6	0	5.546961	2.304347	2.461429
59	6	0	5.547455	0.898995	2.283883
60	6	0	5.604958	-1.164051	-2.372566
61	6	0	5.724242	-2.552174	-2.611869
62	1	0	4.519128	4.137508	2.040901
63	1	0	6.333634	2.779152	3.041132
64	1	0	6.332884	0.301476	2.738953
65	1	0	4.572113	-0.797599	1.430019
66	1	0	4.509010	0.402371	-1.432168
67	1	0	6.323472	-0.478235	-2.814707
68	1	0	6.536352	-2.932236	-3.225721
69	1	0	4.859017	-4.481893	-2.257528
70	1	0	-0.665626	-2.581975	3.029052
71	1	0	-2.429503	-2.453064	3.227723
72	1	0	-1.368774	-2.327409	4.646369
73	1	0	-0.024776	1.103069	3.715632
74	1	0	0.791229	-0.425601	3.321153
75	1	0	0.087611	-0.178972	4.939660
76	1	0	-4.162078	-3.185285	-0.933526
77	1	0	-3.748264	-3.088419	0.787089
78	1	0	-3.644643	-4.646995	-0.062898
79	1	0	-0.575837	-3.665082	-2.089673
80	1	0	-2.246402	-3.501197	-2.674106
81	1	0	-1.740595	-4.985166	-1.834698

E_{ZPE}: B3LYP/6-31G* = -2820.40710 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.08314 (a.u.)

Int_{12}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.332684	0.935493	-0.207798
2	6	0	-3.614930	1.214972	0.229461
3	1	0	-3.688215	1.164825	1.329758
4	6	0	-4.704838	0.323273	-0.374703
5	6	0	-5.865632	0.034947	0.348366
6	6	0	-4.551424	-0.186792	-1.667350
7	6	0	-6.869022	-0.755668	-0.215348
8	1	0	-5.984797	0.424635	1.357295

9	6	0	-5.554171	-0.976397	-2.230775
10	1	0	-3.636062	0.024729	-2.210503
11	6	0	-6.715467	-1.261299	-1.507372
12	1	0	-7.765817	-0.979897	0.356124
13	1	0	-5.429346	-1.370938	-3.235918
14	1	0	-7.494572	-1.878315	-1.947120
15	6	0	-3.896375	2.634389	-0.166321
16	7	0	-3.993685	3.732371	-0.537568
17	1	0	-2.304990	4.429696	-1.358793
18	6	0	2.891608	3.170791	-0.121114
19	6	0	3.965695	2.382325	0.339925
20	6	0	3.795169	0.959874	0.410787
21	6	0	2.554972	0.360338	0.011293
22	6	0	1.456783	1.172994	-0.316949
23	6	0	1.687709	2.588226	-0.447710
24	6	0	2.412561	-1.122210	-0.021827
25	6	0	1.450366	-1.735216	0.782236
26	6	0	1.415497	-3.156912	0.895753
27	6	0	2.261262	-3.945073	0.160289
28	6	0	3.250193	-1.937526	-0.859443
29	6	0	3.178796	-3.367755	-0.758372
30	1	0	3.017916	4.248467	-0.172396
31	6	0	5.194014	2.975095	0.742099
32	6	0	4.884713	0.197499	0.927295
33	8	0	0.561881	-1.015282	1.485566
34	1	0	0.699713	-3.588362	1.589159
35	1	0	2.228711	-5.028107	0.258832
36	6	0	4.011335	-4.172794	-1.578534
37	7	0	0.647348	3.441917	-0.959932
38	7	0	-1.286427	4.325626	-1.390659
39	6	0	-0.346261	5.178816	-1.926764
40	6	0	0.868570	4.623796	-1.666013
41	6	0	-0.678321	3.280685	-0.817074
42	1	0	-0.612314	6.082968	-2.450133
43	1	0	1.859758	4.941448	-1.940254
44	1	0	-1.191756	2.425304	-0.381242
45	6	0	4.144051	-1.391698	-1.824593
46	8	0	0.240319	0.701944	-0.549654
47	22	0	-1.017356	-0.335887	0.587817
48	8	0	-1.768703	-0.014190	2.203955
49	8	0	-1.562606	-1.828799	-0.198762
50	6	0	-1.636202	-0.134071	3.613563
51	6	0	-1.972463	-3.177141	-0.343423
52	6	0	-1.502343	-1.601007	4.026856
53	1	0	-2.568358	0.264694	4.044152
54	6	0	-0.467728	0.723230	4.106375
55	6	0	-2.110817	-3.488662	-1.834178
56	6	0	-3.264371	-3.425484	0.435756
57	1	0	-1.174359	-3.807199	0.073610
58	6	0	6.058042	0.799948	1.319141
59	6	0	6.225643	2.203186	1.218320
60	6	0	4.875053	-3.608514	-2.490053
61	6	0	4.929346	-2.201340	-2.616456
62	1	0	7.160221	2.663021	1.527295
63	1	0	5.297005	4.055978	0.672439
64	1	0	6.865284	0.191127	1.717591
65	1	0	4.771997	-0.875362	1.023974
66	1	0	4.193198	-0.315115	-1.944862
67	1	0	5.594891	-1.752068	-3.349390
68	1	0	5.503508	-4.236619	-3.115663
69	1	0	3.944973	-5.254231	-1.477971
70	1	0	-0.585547	-2.025853	3.609413
71	1	0	-2.357795	-2.180162	3.661953
72	1	0	-1.469935	-1.690163	5.119493
73	1	0	-0.610120	1.768017	3.807011
74	1	0	0.470525	0.360786	3.676579
75	1	0	-0.396155	0.688011	5.200154
76	1	0	-1.171373	-3.277870	-2.354668
77	1	0	-2.902150	-2.875651	-2.278812
78	1	0	-2.362710	-4.545492	-1.982940

79	1	0	-4.076718	-2.805774	0.042483
80	1	0	-3.125526	-3.183866	1.494645
81	1	0	-3.559638	-4.478822	0.358509

E_{ZPE}: B3LYP/6-31G* = -2820.40651 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.08249 (a.u.)

TS_7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.565629	-3.358309	-0.800123
2	6	0	-3.782692	-2.765220	-0.382207
3	6	0	-3.799062	-1.372649	-0.028339
4	6	0	-2.613627	-0.567872	-0.183415
5	6	0	-1.420540	-1.192734	-0.544332
6	6	0	-1.425825	-2.602861	-0.844314
7	6	0	-2.624458	0.899127	0.088537
8	6	0	-1.741178	1.449342	1.024323
9	6	0	-1.881740	2.807518	1.428924
10	6	0	-2.811251	3.628161	0.845893
11	6	0	-3.532009	1.778401	-0.603096
12	6	0	-3.635799	3.153950	-0.208183
13	1	0	-2.531683	-4.417263	-1.042286
14	6	0	-4.965055	-3.542949	-0.260003
15	6	0	-5.014583	-0.850045	0.499268
16	8	0	-0.751029	0.727751	1.593305
17	1	0	-1.228682	3.166992	2.217825
18	1	0	-2.911110	4.662025	1.168856
19	6	0	-4.538959	4.015137	-0.884492
20	7	0	-0.125494	-3.200661	-1.011574
21	7	0	2.040236	-2.761182	-1.096007
22	6	0	1.821996	-3.659726	-0.052189
23	6	0	0.496021	-3.940930	0.008123
24	6	0	0.850799	-2.524933	-1.647553
25	1	0	2.634778	-4.015819	0.561745
26	1	0	-0.082201	-4.567038	0.668709
27	1	0	0.681516	-1.817275	-2.442256
28	8	0	-0.259237	-0.535755	-0.655532
29	22	0	0.862659	0.272208	0.689313
30	8	0	1.448984	-0.610887	2.134129
31	8	0	1.446679	1.958202	0.424098
32	6	0	1.051961	-0.838099	3.484082
33	6	0	1.721493	3.177097	1.105799
34	6	0	0.997721	-2.342355	3.747195
35	1	0	0.045076	-0.413771	3.600122
36	6	0	2.017734	-0.114771	4.422566
37	1	0	1.062308	3.226960	1.984980
38	6	0	1.392106	4.344352	0.176036
39	6	0	3.174833	3.190179	1.583194
40	1	0	2.547655	-1.726018	-0.876001
41	6	0	2.805513	0.153235	-2.750968
42	7	0	2.381458	-0.085638	-3.805893
43	8	0	2.537599	-0.406328	-0.473631
44	6	0	3.272774	0.402452	-1.358658
45	1	0	3.030273	1.451199	-1.134489
46	6	0	4.785870	0.206281	-1.222995
47	6	0	5.659176	0.453809	-2.287676
48	6	0	5.307207	-0.171491	0.019136
49	6	0	7.037742	0.326079	-2.111733
50	1	0	5.263935	0.736811	-3.259950
51	6	0	6.686173	-0.299571	0.192183
52	1	0	4.624146	-0.368840	0.838986
53	6	0	7.555401	-0.050872	-0.871463
54	1	0	7.705788	0.515378	-2.947752
55	1	0	7.081413	-0.595706	1.160576
56	1	0	8.628847	-0.153323	-0.736203
57	6	0	-6.139341	-1.634795	0.625577

58	6	0	-6.126388	-2.992335	0.228518
59	6	0	-4.320229	1.353607	-1.710825
60	6	0	-5.173842	2.218977	-2.359614
61	6	0	-5.299723	3.562714	-1.938159
62	1	0	-4.927710	-4.591133	-0.548198
63	1	0	-7.024134	-3.596554	0.324313
64	1	0	-7.047356	-1.205116	1.040165
65	1	0	-5.045498	0.184742	0.817090
66	1	0	-4.229232	0.331657	-2.060825
67	1	0	-5.751750	1.864911	-3.209398
68	1	0	-5.981759	4.233516	-2.453375
69	1	0	-4.606532	5.051042	-0.559091
70	1	0	0.650886	-2.540528	4.768060
71	1	0	0.308886	-2.827869	3.048742
72	1	0	1.990364	-2.792142	3.626504
73	1	0	1.713072	-0.249366	5.467125
74	1	0	3.035209	-0.505879	4.306091
75	1	0	2.033343	0.958528	4.206346
76	1	0	1.555674	5.300715	0.686855
77	1	0	2.029516	4.316420	-0.715335
78	1	0	0.347272	4.292118	-0.143404
79	1	0	3.864852	3.146825	0.732638
80	1	0	3.385254	4.105751	2.148319
81	1	0	3.376207	2.330571	2.230902

E_{ZPE}: B3LYP/6-31G* = -2820.39029 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.06194 (a.u.)

TS_8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.046126	-0.028997	0.380468
2	7	0	5.984465	-0.322986	0.998306
3	8	0	2.744716	-0.462956	0.058368
4	6	0	3.821160	0.331614	-0.377952
5	1	0	3.591441	1.374916	-0.120715
6	6	0	4.023763	0.238329	-1.893555
7	6	0	2.909726	0.480003	-2.712042
8	6	0	5.253017	-0.059715	-2.486847
9	6	0	3.028150	0.424127	-4.099772
10	1	0	1.950503	0.707073	-2.254273
11	6	0	5.369958	-0.115666	-3.878780
12	1	0	6.122483	-0.250756	-1.864182
13	6	0	4.260712	0.125041	-4.687969
14	1	0	2.159408	0.619734	-4.723180
15	1	0	6.331562	-0.351687	-4.326763
16	1	0	4.353285	0.081627	-5.769883
17	1	0	2.830335	-1.810398	-0.358929
18	6	0	-2.284073	-3.340451	-0.795751
19	6	0	-3.530366	-2.718128	-0.538033
20	6	0	-3.562460	-1.316010	-0.224318
21	6	0	-2.351297	-0.536964	-0.249188
22	6	0	-1.134364	-1.188176	-0.447643
23	6	0	-1.132742	-2.604350	-0.721321
24	6	0	-2.358021	0.935845	-0.013806
25	6	0	-1.582966	1.482471	1.016327
26	6	0	-1.722585	2.858258	1.359810
27	6	0	-2.535870	3.691240	0.637155
28	6	0	-3.140249	1.820529	-0.837258
29	6	0	-3.239315	3.211512	-0.498863
30	1	0	-2.242392	-4.404651	-1.012660
31	6	0	-4.734303	-3.472257	-0.541323
32	6	0	-4.823015	-0.757271	0.133487
33	8	0	-0.711969	0.741670	1.730540
34	1	0	-1.163434	3.221931	2.215754
35	1	0	-2.635141	4.738290	0.914674
36	6	0	-4.019075	4.079925	-1.306576

37	7	0	0.167605	-3.224738	-0.742970
38	7	0	2.337123	-2.823331	-0.608832
39	6	0	2.002330	-3.719536	0.405876
40	6	0	0.672606	-3.979981	0.329664
41	6	0	1.212833	-2.564848	-1.273320
42	1	0	2.744656	-4.087884	1.097018
43	1	0	0.021287	-4.599170	0.925517
44	1	0	1.134515	-1.846172	-2.070341
45	6	0	-3.806270	1.385330	-2.019033
46	8	0	0.043062	-0.550810	-0.425998
47	22	0	1.008881	0.199091	1.089646
48	8	0	1.346603	-0.775901	2.536904
49	8	0	1.713301	1.863885	1.022858
50	6	0	0.982711	-1.179449	3.853002
51	6	0	1.894913	3.013966	1.843513
52	6	0	-0.315276	-1.986194	3.806029
53	6	0	0.884085	0.042720	4.766245
54	1	0	1.798114	-1.825684	4.209156
55	6	0	3.238491	2.930337	2.570565
56	1	0	1.090155	3.023430	2.593065
57	6	0	1.777591	4.262951	0.969960
58	6	0	-5.970170	-1.519205	0.140597
59	6	0	-5.935250	-2.888295	-0.214016
60	6	0	-4.664920	3.618164	-2.430713
61	6	0	-4.542634	2.256617	-2.791918
62	1	0	-6.849846	-3.474566	-0.212735
63	1	0	-6.913812	-1.062686	0.427096
64	1	0	-4.871371	0.287329	0.415356
65	1	0	-4.683494	-4.528724	-0.795242
66	1	0	-3.717225	0.348318	-2.322208
67	1	0	-5.030704	1.892797	-3.692535
68	1	0	-5.254255	4.293811	-3.044553
69	1	0	-4.085828	5.128021	-1.022687
70	1	0	-0.194582	-2.866552	3.165834
71	1	0	-1.124946	-1.370992	3.402121
72	1	0	-0.592955	-2.326456	4.810440
73	1	0	0.083532	0.705564	4.422827
74	1	0	1.827614	0.598540	4.765126
75	1	0	0.668599	-0.264851	5.796145
76	1	0	4.070176	2.945169	1.856748
77	1	0	3.307756	2.006972	3.154635
78	1	0	3.359279	3.780651	3.251924
79	1	0	0.807134	4.287374	0.465692
80	1	0	2.565328	4.269762	0.207760
81	1	0	1.879667	5.169285	1.578645

E_{ZPE}: B3LYP/6-31G* = -2820.38773 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.05937 (a.u.)

TS_9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.129941	3.647786	0.478705
2	6	0	-4.013372	2.950454	-0.386616
3	6	0	-2.068317	3.004807	1.059650
4	6	0	-1.839110	1.615805	0.837931
5	6	0	-2.771275	0.854899	0.124583
6	6	0	-3.828204	1.539838	-0.574298
7	6	0	-2.677966	-0.632998	0.112859
8	6	0	-3.780167	-1.446820	0.565575
9	6	0	-1.502755	-1.263874	-0.296497
10	6	0	-1.484597	-2.702299	-0.393982
11	6	0	-2.555320	-3.484974	-0.063256
12	6	0	-3.729615	-2.877391	0.445082
13	1	0	-3.294519	4.707984	0.657376
14	6	0	-5.060045	3.621296	-1.071634
15	1	0	-1.375806	3.531104	1.708891

16	6	0	-4.696574	0.881092	-1.491155
17	6	0	-4.940127	-0.887942	1.175239
18	8	0	-0.386446	-0.603789	-0.642438
19	1	0	-2.493795	-4.565785	-0.155426
20	6	0	-4.831509	-3.666878	0.869131
21	7	0	-0.242130	-3.252116	-0.876696
22	22	0	0.802172	0.390985	0.501961
23	7	0	1.911530	-2.811140	-1.063727
24	6	0	1.426651	-3.119599	-2.332480
25	6	0	0.098466	-3.390801	-2.226650
26	6	0	0.882395	-2.904409	-0.229415
27	1	0	2.063364	-3.083432	-3.202496
28	1	0	-0.643261	-3.651468	-2.964877
29	1	0	0.905186	-2.598327	0.805951
30	8	0	1.429975	-0.494954	1.938589
31	8	0	1.526034	1.985537	0.025897
32	6	0	2.647977	-0.649343	2.662652
33	6	0	1.223804	3.374343	-0.083046
34	1	0	3.456858	-0.749853	1.925759
35	6	0	2.901645	0.589875	3.521426
36	6	0	2.561121	-1.925309	3.500948
37	6	0	1.693852	4.096488	1.179867
38	6	0	1.871742	3.931236	-1.351592
39	1	0	0.136193	3.485843	-0.171491
40	8	0	-0.730230	1.070809	1.371547
41	1	0	2.476202	-1.831899	-0.840670
42	6	0	3.338643	-0.249171	-2.764096
43	7	0	3.247936	-0.699941	-3.831161
44	8	0	2.497168	-0.449120	-0.561771
45	6	0	3.415478	0.254713	-1.366570
46	6	0	4.839783	0.171352	-0.820294
47	6	0	5.761995	-0.786928	-1.252947
48	6	0	7.032177	-0.855561	-0.676844
49	6	0	7.391741	0.032857	0.337201
50	6	0	6.476271	0.994308	0.772681
51	6	0	5.208995	1.062989	0.195518
52	1	0	3.115019	1.308638	-1.387796
53	1	0	5.494477	-1.472653	-2.052764
54	1	0	7.741606	-1.601623	-1.024996
55	1	0	8.381737	-0.019017	0.782452
56	1	0	6.752166	1.694406	1.556956
57	1	0	4.492059	1.808005	0.531344
58	6	0	-5.985344	-1.680899	1.594285
59	6	0	-5.944522	-3.084872	1.428295
60	6	0	-5.889449	2.947342	-1.938545
61	6	0	-5.692142	1.564019	-2.155186
62	1	0	-4.769333	-4.746763	0.755008
63	1	0	-6.780307	-3.696881	1.755535
64	1	0	-6.850628	-1.220417	2.063522
65	1	0	-4.990271	0.183639	1.322805
66	1	0	-4.555796	-0.176705	-1.682546
67	1	0	-6.329318	1.033301	-2.857942
68	1	0	-6.682536	3.473073	-2.463142
69	1	0	-5.185104	4.689103	-0.905266
70	1	0	2.094093	0.722523	4.250325
71	1	0	2.951218	1.487092	2.896033
72	1	0	3.849752	0.495332	4.063535
73	1	0	2.398442	-2.802906	2.865306
74	1	0	1.733038	-1.858690	4.215428
75	1	0	3.491362	-2.081762	4.059117
76	1	0	2.781121	4.006961	1.291882
77	1	0	1.219459	3.665707	2.067562
78	1	0	1.441347	5.162485	1.133589
79	1	0	1.531003	3.377166	-2.232458
80	1	0	2.964660	3.860160	-1.295993
81	1	0	1.604863	4.985915	-1.486301

E_{ZPE}: B3LYP/6-31G* = -2820.38917 (a.u.)

Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.05953 (a.u.)

TS_{10}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.789914	-0.039641	1.068919
2	7	0	5.480416	-0.221778	1.985144
3	8	0	2.636391	-0.442907	0.178795
4	6	0	3.858983	0.194580	-0.068551
5	1	0	3.679171	1.278819	-0.095688
6	6	0	4.473948	-0.227638	-1.408611
7	6	0	3.612761	-0.421755	-2.496949
8	6	0	5.851930	-0.377978	-1.593478
9	6	0	4.125222	-0.759202	-3.750056
10	1	0	2.542529	-0.314947	-2.348944
11	6	0	6.362987	-0.716157	-2.848727
12	1	0	6.529500	-0.239358	-0.755358
13	6	0	5.502705	-0.907786	-3.930123
14	1	0	3.447198	-0.902997	-4.587662
15	1	0	7.435676	-0.834736	-2.976911
16	1	0	5.901627	-1.171707	-4.906000
17	1	0	2.710391	-1.868286	0.089431
18	6	0	-2.380410	-3.470208	0.273614
19	6	0	-3.621377	-2.807336	0.437651
20	6	0	-3.671647	-1.377509	0.306548
21	6	0	-2.487789	-0.630848	-0.039290
22	6	0	-1.263413	-1.297459	-0.097725
23	6	0	-1.253020	-2.733806	0.036560
24	6	0	-2.549742	0.837561	-0.287218
25	6	0	-3.411054	1.388404	-1.300049
26	6	0	-3.584654	2.809853	-1.394222
27	6	0	-2.884220	3.646008	-0.485545
28	6	0	-1.770999	1.708766	0.481634
29	6	0	-1.997054	3.114553	0.413944
30	1	0	-2.320418	-4.551157	0.366032
31	6	0	-4.798477	-3.534108	0.759608
32	6	0	-4.921821	-0.745123	0.565347
33	7	0	0.046832	-3.338061	-0.129090
34	6	0	-4.088680	0.579966	-2.257129
35	6	0	-4.439419	3.350661	-2.390044
36	1	0	-3.048022	4.720598	-0.525163
37	1	0	-1.450248	3.747117	1.105513
38	8	0	-0.833941	1.256194	1.333924
39	8	0	-0.091502	-0.680602	-0.310444
40	22	0	0.857278	0.490351	0.918264
41	8	0	1.657499	2.046784	0.472366
42	8	0	1.110676	-0.191818	2.548627
43	6	0	1.508116	3.450902	0.299780
44	6	0	1.333949	-0.080224	3.951182
45	6	0	1.560260	4.148589	1.658904
46	6	0	0.012235	0.244372	4.648118
47	1	0	0.526855	3.629887	-0.158230
48	6	0	2.589896	3.954166	-0.657359
49	6	0	2.431375	0.942049	4.241421
50	1	0	1.681025	-1.069553	4.284791
51	7	0	2.203906	-2.881854	-0.045364
52	6	0	1.928639	-3.414439	-1.301647
53	6	0	0.600656	-3.698362	-1.363543
54	6	0	1.053392	-2.856604	0.618311
55	1	0	2.702592	-3.532225	-2.044037
56	1	0	-0.013408	-4.106605	-2.150650
57	1	0	0.913709	-2.384411	1.579702
58	6	0	-5.090027	2.536043	-3.288414
59	6	0	-4.899030	1.136427	-3.222620
60	6	0	-6.042545	-1.475443	0.892871
61	6	0	-5.991196	-2.886467	0.979114
62	1	0	-4.732680	-4.616656	0.842469
63	1	0	-6.885321	-3.449726	1.231027
64	1	0	-6.977544	-0.958926	1.092823

65	1	0	-4.982582	0.334997	0.515226
66	1	0	-3.946986	-0.494700	-2.232587
67	1	0	-5.393270	0.491534	-3.944781
68	1	0	-5.737043	2.962138	-4.050278
69	1	0	-4.561073	4.430815	-2.435456
70	1	0	2.534126	3.986163	2.135282
71	1	0	0.781773	3.754204	2.319873
72	1	0	1.407492	5.228640	1.546914
73	1	0	-0.742745	-0.514137	4.417917
74	1	0	-0.368385	1.214089	4.311394
75	1	0	0.152686	0.277623	5.734870
76	1	0	2.546280	3.411192	-1.607072
77	1	0	3.587423	3.817164	-0.223188
78	1	0	2.451294	5.021793	-0.864112
79	1	0	2.119979	1.941502	3.916886
80	1	0	3.357061	0.676205	3.722406
81	1	0	2.637801	0.979738	5.317416

E_{ZPE}: B3LYP/6-31G* = -2820.38813 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.06054 (a.u.)

Int_{13}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.022250	-3.430289	-0.460560
2	6	0	-3.311996	-2.996888	-0.067501
3	6	0	-3.551870	-1.594649	0.122192
4	6	0	-2.500108	-0.646540	-0.134709
5	6	0	-1.225217	-1.120797	-0.441579
6	6	0	-1.002291	-2.525970	-0.617512
7	6	0	-2.743093	0.823033	-0.029309
8	6	0	-2.015761	1.601692	0.872634
9	6	0	-2.349785	2.964122	1.098470
10	6	0	-3.343471	3.570367	0.374392
11	6	0	-3.729390	1.473485	-0.851875
12	6	0	-4.039669	2.858086	-0.636739
13	1	0	-1.833627	-4.489017	-0.617156
14	6	0	-4.357714	-3.930136	0.163436
15	6	0	-4.837981	-1.206251	0.594311
16	8	0	-0.976748	1.088741	1.583774
17	1	0	-1.794679	3.502915	1.859850
18	1	0	-3.595631	4.612826	0.554172
19	6	0	-5.020630	3.492732	-1.443498
20	7	0	0.326429	-2.972081	-0.879000
21	7	0	2.432171	-2.900808	-1.608282
22	6	0	2.338319	-3.804260	-0.563766
23	6	0	1.053039	-3.862953	-0.098451
24	6	0	1.207233	-2.433420	-1.774226
25	1	0	3.203020	-4.351677	-0.214777
26	1	0	0.587481	-4.413275	0.704292
27	1	0	0.911359	-1.688884	-2.498120
28	6	0	-4.403398	0.805251	-1.913690
29	8	0	-0.173213	-0.288985	-0.587385
30	22	0	0.654961	0.600311	0.849630
31	8	0	1.202345	-0.300936	2.287461
32	8	0	1.367961	2.232913	0.526143
33	6	0	0.799939	-0.705774	3.592740
34	6	0	1.394862	3.541013	1.090951
35	6	0	1.817544	-0.191320	4.609813
36	6	0	0.646926	-2.225764	3.623914
37	1	0	-0.178182	-0.241432	3.786619
38	1	0	0.639300	3.581654	1.889519
39	6	0	1.023426	4.552756	0.007373
40	6	0	2.769039	3.808674	1.706565
41	1	0	2.644362	-1.042767	-0.542571
42	6	0	2.854437	0.665056	-2.467692
43	7	0	2.399436	0.636162	-3.535148

44	8	0	2.624787	-0.115709	-0.217991
45	6	0	3.424701	0.696229	-1.102049
46	1	0	3.294323	1.707729	-0.714016
47	6	0	4.890705	0.304141	-1.080330
48	6	0	5.337795	-0.860547	-1.719298
49	6	0	5.801795	1.106568	-0.385384
50	6	0	6.685581	-1.212144	-1.656910
51	1	0	4.631193	-1.497475	-2.245428
52	6	0	7.150305	0.753500	-0.328187
53	1	0	5.455380	2.009314	0.112102
54	6	0	7.593488	-0.406190	-0.965598
55	1	0	7.027726	-2.115962	-2.153324
56	1	0	7.851976	1.384014	0.210865
57	1	0	8.643944	-0.681514	-0.924742
58	6	0	-5.826286	-2.136980	0.826957
59	6	0	-5.594166	-3.513490	0.597975
60	6	0	-5.339310	1.453748	-2.688953
61	6	0	-5.664516	2.808945	-2.448736
62	1	0	-4.155290	-4.986216	0.000240
63	1	0	-6.385785	-4.235685	0.777078
64	1	0	-6.795153	-1.809108	1.194022
65	1	0	-5.033641	-0.157557	0.782891
66	1	0	-4.160182	-0.230086	-2.123100
67	1	0	-5.828702	0.918338	-3.498286
68	1	0	-6.408975	3.306815	-3.063871
69	1	0	-5.245011	4.540440	-1.255921
70	1	0	1.511804	-0.456807	5.628489
71	1	0	2.804634	-0.626885	4.418159
72	1	0	1.903717	0.898701	4.549311
73	1	0	0.314987	-2.557778	4.614487
74	1	0	-0.094080	-2.550132	2.886054
75	1	0	1.602219	-2.711709	3.395516
76	1	0	1.010567	5.569807	0.416984
77	1	0	1.749816	4.519760	-0.812775
78	1	0	0.033188	4.327823	-0.399616
79	1	0	3.018347	3.040185	2.445844
80	1	0	3.545978	3.809758	0.932119
81	1	0	2.785765	4.785727	2.203204

E_{ZPE}: B3LYP/6-31G* = -2820.40736 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.07891 (a.u.)

Int_{14}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.172266	-3.169150	-1.250755
2	6	0	-3.450318	-2.733367	-0.821841
3	6	0	-3.601419	-1.399550	-0.312932
4	6	0	-2.470358	-0.510668	-0.281886
5	6	0	-1.215706	-1.005119	-0.635566
6	6	0	-1.085408	-2.339908	-1.141895
7	6	0	-2.606668	0.905984	0.166626
8	6	0	-1.879602	1.372619	1.263955
9	6	0	-2.112627	2.671551	1.792830
10	6	0	-2.996369	3.526845	1.187354
11	6	0	-3.475481	1.824215	-0.521076
12	6	0	-3.679573	3.144414	0.003441
13	1	0	-2.048384	-4.172644	-1.649124
14	6	0	-4.572998	-3.602235	-0.869339
15	6	0	-4.885216	-1.023762	0.175268
16	8	0	-0.951683	0.600256	1.883500
17	1	0	-1.571983	2.959208	2.688780
18	1	0	-3.170629	4.517943	1.599736
19	6	0	-4.544244	4.044170	-0.673795
20	7	0	0.225281	-2.802270	-1.464329
21	7	0	2.349692	-2.654242	-2.133149
22	6	0	2.219647	-3.704945	-1.241430

23	6	0	0.923346	-3.811364	-0.812942
24	6	0	1.135289	-2.148151	-2.244950
25	1	0	3.068609	-4.315838	-0.966987
26	1	0	0.428452	-4.476061	-0.121522
27	1	0	0.859208	-1.296738	-2.849813
28	6	0	-4.131422	1.491854	-1.740779
29	8	0	-0.095726	-0.260742	-0.527657
30	22	0	0.689710	0.144629	1.141630
31	8	0	1.168823	-1.156600	2.227454
32	8	0	1.581896	1.714411	1.367635
33	6	0	1.518078	-2.304877	2.984438
34	6	0	1.620697	2.731521	2.368552
35	6	0	2.714754	-1.983936	3.878450
36	1	0	1.807259	-3.082596	2.263333
37	6	0	0.292716	-2.773735	3.769614
38	6	0	2.888580	2.582660	3.210568
39	1	0	0.747540	2.599529	3.023989
40	6	0	1.522283	4.095545	1.685973
41	6	0	4.837437	-0.568795	0.506081
42	7	0	5.581999	-1.298047	1.017144
43	8	0	2.574651	-0.284188	-0.179224
44	6	0	3.859579	0.350830	-0.115898
45	1	0	3.698817	1.183504	0.573011
46	6	0	4.297422	0.880808	-1.469717
47	6	0	3.696344	2.058448	-1.935574
48	6	0	5.226571	0.212996	-2.272644
49	6	0	4.026295	2.563497	-3.191138
50	1	0	2.966090	2.567332	-1.311250
51	6	0	5.557623	0.723164	-3.529367
52	1	0	5.693905	-0.701039	-1.917635
53	6	0	4.960057	1.896657	-3.989385
54	1	0	3.558465	3.477731	-3.545726
55	1	0	6.281701	0.200200	-4.147619
56	1	0	5.220183	2.292390	-4.967386
57	1	0	2.568352	-0.967167	-0.886340
58	6	0	-5.802646	-3.194900	-0.407258
59	6	0	-5.950810	-1.895332	0.131445
60	6	0	-5.174745	3.681091	-1.841574
61	6	0	-4.953032	2.392962	-2.381695
62	1	0	-4.436366	-4.604189	-1.269754
63	1	0	-6.653827	-3.869057	-0.442985
64	1	0	-6.916178	-1.581144	0.519090
65	1	0	-5.017007	-0.035030	0.598150
66	1	0	-3.966440	0.513393	-2.177148
67	1	0	-5.432429	2.111223	-3.315558
68	1	0	-5.830309	4.380180	-2.353452
69	1	0	-4.690510	5.036322	-0.252415
70	1	0	2.456164	-1.190973	4.589968
71	1	0	3.569691	-1.657308	3.278713
72	1	0	3.014327	-2.872069	4.446742
73	1	0	-0.545908	-2.973164	3.094812
74	1	0	-0.019279	-2.005287	4.485381
75	1	0	0.522246	-3.692003	4.322412
76	1	0	3.784169	2.740891	2.597440
77	1	0	2.944259	1.582212	3.652278
78	1	0	2.901006	3.318927	4.022632
79	1	0	0.604585	4.160267	1.093434
80	1	0	2.378943	4.253492	1.020050
81	1	0	1.514324	4.900322	2.430624

E_{ZPE}: B3LYP/6-31G* = -2820.40744 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.08010 (a.u.)

Int_{15}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.476864	3.551429	0.551441

2	6	0	-4.268024	2.792234	-0.349742
3	6	0	-2.395604	2.987538	1.177028
4	6	0	-2.060895	1.623005	0.960186
5	6	0	-2.877706	0.797087	0.185215
6	6	0	-3.960852	1.404122	-0.545855
7	6	0	-2.637362	-0.674376	0.115104
8	6	0	-3.658222	-1.611290	0.509479
9	6	0	-1.407362	-1.169408	-0.319251
10	6	0	-1.230258	-2.579152	-0.509138
11	6	0	-2.225311	-3.474049	-0.217807
12	6	0	-3.455181	-3.019782	0.319948
13	1	0	-3.728046	4.595387	0.723590
14	6	0	-5.341245	3.384221	-1.066432
15	1	0	-1.770637	3.560593	1.854694
16	6	0	-4.736663	0.688619	-1.502276
17	6	0	-4.877645	-1.202439	1.121084
18	8	0	-0.361926	-0.367094	-0.599034
19	1	0	-2.059310	-4.536260	-0.375041
20	6	0	-4.471662	-3.938422	0.693704
21	7	0	0.034375	-3.014066	-1.019423
22	22	0	0.599884	0.580755	0.711625
23	7	0	2.260008	-3.131715	-1.079353
24	6	0	1.760861	-3.184325	-2.370116
25	6	0	0.395259	-3.099350	-2.354752
26	6	0	1.192875	-3.034774	-0.302872
27	1	0	2.417801	-3.263053	-3.224551
28	1	0	-0.346259	-3.078175	-3.138325
29	1	0	1.196015	-2.934035	0.773627
30	8	0	1.348128	-0.359604	2.035287
31	8	0	1.366750	2.146226	0.236106
32	6	0	2.553893	-0.596653	2.755310
33	6	0	1.166627	3.557384	0.296750
34	1	0	3.280639	-1.012022	2.042351
35	6	0	3.102365	0.717454	3.310561
36	6	0	2.272633	-1.625114	3.850199
37	6	0	2.495719	4.237411	0.626059
38	6	0	0.568713	4.042810	-1.023257
39	1	0	0.456452	3.763648	1.109496
40	8	0	-0.938203	1.155180	1.561085
41	1	0	2.515962	-1.196974	-0.703304
42	6	0	3.300810	0.190520	-2.709159
43	7	0	3.186929	-0.036912	-3.841804
44	8	0	2.478435	-0.232043	-0.509082
45	6	0	3.465048	0.473062	-1.264419
46	6	0	4.888181	0.183683	-0.804691
47	6	0	5.349292	-1.134356	-0.679980
48	6	0	6.656403	-1.375613	-0.259017
49	6	0	7.512971	-0.310396	0.031547
50	6	0	7.056595	1.001748	-0.093905
51	6	0	5.746288	1.246798	-0.508654
52	1	0	3.229452	1.527171	-1.099943
53	1	0	4.689437	-1.971087	-0.899324
54	1	0	7.007870	-2.399081	-0.161545
55	1	0	8.531805	-0.504103	0.355889
56	1	0	7.715766	1.834901	0.133834
57	1	0	5.390582	2.270143	-0.603252
58	6	0	-5.838161	-2.118978	1.487705
59	6	0	-5.645034	-3.501994	1.262828
60	6	0	-6.079591	2.655754	-1.970202
61	6	0	-5.760896	1.296438	-2.194589
62	1	0	-4.296378	-4.999299	0.530491
63	1	0	-6.414556	-4.212817	1.550540
64	1	0	-6.754149	-1.774221	1.960030
65	1	0	-5.042484	-0.148668	1.310731
66	1	0	-4.502604	-0.351200	-1.698953
67	1	0	-6.326770	0.724842	-2.925555
68	1	0	-6.894190	3.121262	-2.518125
69	1	0	-5.560446	4.435533	-0.893350
70	1	0	2.385057	1.164866	4.008513
71	1	0	3.286970	1.426642	2.497318

72	1	0	4.045879	0.548480	3.841892
73	1	0	1.871485	-2.549707	3.421956
74	1	0	1.539813	-1.232589	4.563805
75	1	0	3.193273	-1.868637	4.392784
76	1	0	3.225806	4.069690	-0.175075
77	1	0	2.910130	3.847409	1.561306
78	1	0	2.355625	5.318987	0.735572
79	1	0	-0.391145	3.554307	-1.215572
80	1	0	1.245257	3.817652	-1.855751
81	1	0	0.403823	5.126283	-0.995561

E_{ZPE}: B3LYP/6-31G* = -2820.40621 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.07903 (a.u.)

Int_{16}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.075833	-3.451276	0.213979
2	6	0	3.364157	-2.939045	-0.078042
3	6	0	3.532707	-1.523346	-0.243236
4	6	0	2.412088	-0.636768	-0.058172
5	6	0	1.147202	-1.188112	0.146521
6	6	0	1.001033	-2.606323	0.301500
7	6	0	2.592758	0.843859	-0.110120
8	6	0	3.492450	1.513177	0.793890
9	6	0	3.771340	2.910586	0.622932
10	6	0	3.132046	3.615862	-0.430177
11	6	0	1.901449	1.616651	-1.045386
12	6	0	2.212965	2.990901	-1.232373
13	1	0	1.931089	-4.521259	0.335642
14	6	0	4.475003	-3.808559	-0.242437
15	6	0	4.824163	-1.057732	-0.621942
16	7	0	-0.315067	-3.106585	0.549927
17	6	0	4.106705	0.849686	1.894110
18	6	0	4.666507	3.563035	1.511265
19	1	0	3.367302	4.666838	-0.580534
20	1	0	1.704870	3.521107	-2.031640
21	8	0	0.930459	1.084807	-1.831071
22	8	0	0.034149	-0.430033	0.230779
23	22	0	-0.717130	0.498235	-1.231589
24	8	0	-1.556285	2.052892	-0.873223
25	8	0	-1.250001	-0.447422	-2.646552
26	6	0	-1.430585	3.473104	-0.944626
27	6	0	-2.307068	-0.697847	-3.572008
28	1	0	-0.605117	3.702942	-1.631992
29	6	0	-2.634389	0.577062	-4.348643
30	6	0	-1.089551	4.018419	0.441740
31	6	0	-2.720975	4.064545	-1.511523
32	1	0	-3.186471	-0.996197	-2.984341
33	6	0	-1.892692	-1.850165	-4.486069
34	7	0	-2.516299	-3.249103	0.221234
35	6	0	-2.235603	-3.461786	1.559243
36	6	0	-0.888560	-3.366488	1.785843
37	6	0	-1.340242	-3.048330	-0.345734
38	1	0	-3.022411	-3.664683	2.272204
39	1	0	-0.285313	-3.449840	2.676889
40	1	0	-1.169194	-2.813005	-1.386745
41	1	0	-2.872959	-1.292033	-0.077207
42	6	0	-5.081151	0.216405	-0.401868
43	7	0	-6.060486	0.065315	-1.006045
44	8	0	-2.771512	-0.329471	-0.273224
45	6	0	-3.816855	0.427267	0.338743
46	1	0	-3.512413	1.464532	0.165329
47	6	0	-3.946520	0.176294	1.838730
48	6	0	-2.774926	0.043864	2.596085
49	6	0	-5.190247	0.135812	2.476745
50	6	0	-2.853679	-0.120945	3.978511

51	1	0	-1.809040	0.049304	2.100402
52	6	0	-5.263026	-0.027709	3.861426
53	1	0	-6.103707	0.226918	1.895937
54	6	0	-4.096246	-0.154172	4.615427
55	1	0	-1.940372	-0.225042	4.558066
56	1	0	-6.234465	-0.061103	4.346956
57	1	0	-4.154329	-0.282170	5.692999
58	6	0	5.878711	-1.927682	-0.790210
59	6	0	5.712450	-3.317464	-0.586934
60	6	0	5.254853	2.883993	2.553174
61	6	0	4.958330	1.515088	2.748377
62	1	0	4.322066	-4.876254	-0.103144
63	1	0	6.554879	-3.991019	-0.716647
64	1	0	6.849439	-1.540566	-1.088130
65	1	0	4.971959	0.001748	-0.792902
66	1	0	3.884955	-0.197115	2.067161
67	1	0	5.403964	0.981849	3.584036
68	1	0	5.934093	3.395403	3.229595
69	1	0	4.870121	4.620185	1.355664
70	1	0	-1.764874	0.904451	-4.930239
71	1	0	-2.919018	1.381772	-3.662896
72	1	0	-3.468935	0.403435	-5.037040
73	1	0	-0.150708	3.589275	0.804489
74	1	0	-1.883957	3.773664	1.156310
75	1	0	-0.979674	5.108634	0.409030
76	1	0	-3.568478	3.863514	-0.845737
77	1	0	-2.945493	3.637768	-2.494266
78	1	0	-2.625880	5.150851	-1.621990
79	1	0	-1.668039	-2.750309	-3.904495
80	1	0	-1.000330	-1.579766	-5.061395
81	1	0	-2.700815	-2.089724	-5.186330

E_{ZPE}: B3LYP/6-31G* = -2820.40667 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.07843 (a.u.)

Direct C-C bond forming TS

TS_S

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.586491	2.439974	-0.273860
2	7	0	-5.229948	3.391200	-0.018116
3	1	0	-3.156898	3.241397	-0.966135
4	6	0	2.424158	3.298168	-0.946782
5	6	0	3.687280	2.730482	-0.667072
6	6	0	3.760534	1.352407	-0.273347
7	6	0	2.573001	0.542227	-0.271991
8	6	0	1.334476	1.141161	-0.522047
9	6	0	1.282604	2.543323	-0.825572
10	6	0	2.635280	-0.911407	0.059129
11	6	0	3.457384	-1.824565	-0.690375
12	6	0	3.613038	-3.177486	-0.238167
13	6	0	2.926484	-3.594742	0.933516
14	6	0	1.890729	-1.407136	1.131935
15	6	0	2.076875	-2.741844	1.588023
16	1	0	2.365889	4.345063	-1.231263
17	6	0	4.869038	3.518585	-0.721421
18	6	0	5.035465	0.854137	0.122889
19	7	0	0.006434	3.195068	-0.898436
20	6	0	4.108547	-1.456296	-1.901801
21	6	0	4.432608	-4.073745	-0.972844
22	1	0	3.067886	-4.611956	1.291721
23	1	0	1.522318	-3.056588	2.466720
24	8	0	0.972274	-0.641926	1.773756
25	8	0	0.187160	0.457231	-0.517556
26	22	0	-0.704402	-0.458221	0.918920
27	8	0	-1.100411	-2.182933	0.704133

28	8	0	-1.509931	0.369398	2.265209
29	6	0	-1.547852	-3.416430	1.247359
30	6	0	-1.519681	1.058502	3.511364
31	1	0	-2.527991	1.480165	3.624077
32	6	0	-3.008973	-3.299011	1.683498
33	7	0	-2.139442	3.531801	-1.039965
34	6	0	-1.596878	4.680268	-0.509985
35	6	0	-0.252243	4.483910	-0.427319
36	6	0	-1.171055	2.647412	-1.259777
37	1	0	-2.213190	5.516602	-0.220708
38	1	0	0.535003	5.113157	-0.048231
39	1	0	-1.310881	1.637691	-1.602288
40	6	0	-1.258554	0.063036	4.641750
41	6	0	-0.500212	2.196995	3.475112
42	6	0	-1.323127	-4.514728	0.208873
43	1	0	-0.928565	-3.632382	2.131295
44	8	0	-2.437750	-0.038861	-0.400944
45	6	0	-3.659426	-0.006757	-0.148689
46	6	0	-4.661091	-0.519522	-1.097035
47	6	0	-6.022102	-0.492622	-0.755628
48	6	0	-4.256107	-1.109605	-2.303927
49	6	0	-6.966753	-1.046639	-1.613135
50	1	0	-6.330036	-0.003812	0.164269
51	6	0	-5.204726	-1.660668	-3.161629
52	1	0	-3.198759	-1.135336	-2.547941
53	6	0	-6.559066	-1.630004	-2.817331
54	1	0	-8.020535	-1.016880	-1.351332
55	1	0	-4.890808	-2.117485	-4.096176
56	1	0	-7.298475	-2.060002	-3.487898
57	1	0	-3.997127	0.217364	0.867760
58	6	0	6.085331	2.990961	-0.359926
59	6	0	6.159156	1.648498	0.082639
60	6	0	4.883974	-2.355104	-2.601535
61	6	0	5.061906	-3.676338	-2.130526
62	1	0	4.787604	4.555593	-1.039464
63	1	0	6.982804	3.601949	-0.396575
64	1	0	7.114988	1.239548	0.398794
65	1	0	5.114424	-0.168210	0.470901
66	1	0	3.975733	-0.451044	-2.285708
67	1	0	5.360017	-2.045336	-3.528270
68	1	0	5.681866	-4.373658	-2.687257
69	1	0	4.544042	-5.091622	-0.605498
70	1	0	-3.652756	-3.097232	0.819954
71	1	0	-3.129889	-2.484215	2.405691
72	1	0	-3.346119	-4.229668	2.154268
73	1	0	-0.267006	-0.387208	4.526570
74	1	0	-2.008600	-0.734946	4.631296
75	1	0	-1.306142	0.565862	5.614529
76	1	0	-0.731666	2.889965	2.658870
77	1	0	0.507255	1.795866	3.321275
78	1	0	-0.516541	2.758813	4.416058
79	1	0	-0.268948	-4.549789	-0.081772
80	1	0	-1.924355	-4.320868	-0.686378
81	1	0	-1.608917	-5.492063	0.615273

E_{ZPE}: B3LYP/6-31G* = -2820.366844 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.05512 (a.u.)

TS_R

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.438383	-0.053209	-0.369194
2	6	0	3.444892	0.416475	-0.964238
3	1	0	3.342931	1.353671	-1.519622
4	6	0	4.814268	0.034793	-0.541177
5	6	0	5.932963	0.593324	-1.176768
6	6	0	4.992194	-0.821418	0.554030

7	6	0	7.214392	0.292906	-0.725605
8	1	0	5.788469	1.231630	-2.044050
9	6	0	6.277899	-1.122083	1.002294
10	1	0	4.115640	-1.222543	1.052978
11	6	0	7.389283	-0.567036	0.363918
12	1	0	8.078495	0.722344	-1.224798
13	1	0	6.413969	-1.781844	1.855318
14	1	0	8.390995	-0.800881	0.714957
15	6	0	3.593757	-0.452593	-3.097027
16	7	0	3.837027	-0.235310	-4.224608
17	7	0	0.394724	-2.857768	-1.025968
18	7	0	2.323005	-2.696682	-2.015342
19	6	0	1.110658	-2.163842	-1.925586
20	6	0	-1.813013	-3.487848	-0.219617
21	6	0	-3.070491	-3.134648	0.324466
22	6	0	-3.413532	-1.745460	0.451428
23	6	0	-2.503384	-0.733131	-0.008474
24	6	0	-1.230996	-1.112546	-0.440646
25	6	0	-0.916653	-2.506589	-0.563296
26	6	0	-2.870316	0.713319	-0.018565
27	6	0	-4.006471	1.186328	-0.765824
28	6	0	-4.392326	2.566068	-0.678495
29	6	0	-3.619887	3.446920	0.123562
30	6	0	-2.088134	1.642044	0.674049
31	6	0	-2.495112	3.002875	0.767686
32	1	0	-1.563676	-4.537054	-0.354997
33	6	0	-3.986866	-4.131902	0.754948
34	6	0	-4.660932	-1.430542	1.062689
35	6	0	-4.763269	0.348610	-1.634411
36	6	0	-5.519996	3.029707	-1.405264
37	1	0	-3.923819	4.488123	0.204003
38	1	0	-1.885186	3.671423	1.367442
39	8	0	-0.949094	1.287544	1.300583
40	8	0	-0.291486	-0.220517	-0.777757
41	22	0	0.698662	0.823956	0.502730
42	8	0	1.202361	2.440547	-0.081389
43	8	0	1.321856	0.292009	2.101131
44	6	0	1.274531	3.810526	0.297053
45	6	0	0.920985	0.272311	3.465484
46	1	0	-0.116755	0.632787	3.506237
47	1	0	0.620485	3.953103	1.170643
48	6	0	2.420939	-3.753822	-1.135291
49	6	0	1.210691	-3.867741	-0.518639
50	1	0	3.326722	-4.327266	-1.021213
51	1	0	0.859389	-4.545866	0.241507
52	1	0	0.784578	-1.283952	-2.450573
53	1	0	3.063252	-2.123130	-2.494253
54	6	0	0.973430	-1.166462	3.979842
55	6	0	1.816974	1.216793	4.266965
56	6	0	2.710553	4.155492	0.692381
57	6	0	0.753505	4.662816	-0.859328
58	1	0	1.996392	-1.557201	3.926809
59	1	0	0.323538	-1.810909	3.378350
60	1	0	0.637459	-1.216559	5.022203
61	1	0	1.755730	2.234107	3.866137
62	1	0	2.862048	0.889851	4.218783
63	1	0	1.509098	1.242444	5.318953
64	1	0	3.385692	4.019819	-0.160346
65	1	0	3.051683	3.509873	1.508628
66	1	0	2.779800	5.198165	1.023620
67	1	0	-0.275780	4.383308	-1.103882
68	1	0	1.373613	4.514335	-1.750433
69	1	0	0.774243	5.726503	-0.594087
70	6	0	-5.518887	-2.419684	1.488019
71	6	0	-5.189999	-3.786552	1.323140
72	6	0	-6.240462	2.184344	-2.217562
73	6	0	-5.844423	0.832590	-2.338313
74	1	0	-3.710859	-5.177283	0.636154
75	1	0	-5.881445	-4.555730	1.655364
76	1	0	-6.459564	-2.147197	1.958802

77	1	0	-4.926814	-0.389398	1.201061
78	1	0	-4.470922	-0.688160	-1.754991
79	1	0	-6.394648	0.167506	-2.998937
80	1	0	-7.098344	2.552428	-2.773475
81	1	0	-5.797001	4.077808	-1.314884

E_{ZPE}: B3LYP/6-31G* = -2820.36693 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.05711 (a.u.)

Species involved in the Ti-HCN mechanism

Int_{17}

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.303618	3.588899	-0.078156
2	6	0	0.909377	3.687875	0.643346
3	6	0	1.702776	2.508464	0.834446
4	6	0	1.269852	1.255426	0.278405
5	6	0	0.014892	1.178343	-0.333200
6	6	0	-0.749605	2.374031	-0.538980
7	6	0	2.128845	0.038125	0.384054
8	6	0	3.439699	-0.007018	-0.207774
9	6	0	4.278452	-1.151533	0.009061
10	6	0	3.783680	-2.234682	0.783718
11	6	0	2.507090	-2.213994	1.281240
12	6	0	1.667693	-1.089684	1.060615
13	6	0	2.892484	2.634900	1.607941
14	6	0	3.281865	3.849059	2.128222
15	6	0	2.511240	5.014525	1.904685
16	6	0	1.346426	4.929065	1.178800
17	6	0	3.944218	1.033019	-1.039101
18	6	0	5.202243	0.958689	-1.596050
19	6	0	6.035675	-0.157351	-1.352436
20	6	0	5.575228	-1.189604	-0.567437
21	1	0	-0.892427	4.482940	-0.265010
22	1	0	0.733204	5.811395	1.009751
23	1	0	2.834777	5.967285	2.314599
24	1	0	4.190651	3.911345	2.720919
25	1	0	3.492448	1.752688	1.796663
26	1	0	3.316940	1.893009	-1.244399
27	1	0	5.555763	1.765687	-2.232614
28	1	0	7.028329	-0.201158	-1.792235
29	1	0	6.197114	-2.062968	-0.383216
30	1	0	4.427695	-3.093703	0.957567
31	1	0	2.101404	-3.046190	1.847921
32	7	0	-2.004687	2.295675	-1.212288
33	8	0	-0.502130	0.010345	-0.760298
34	8	0	0.394439	-1.144172	1.538645
35	22	0	-0.957420	-1.480050	0.309222
36	8	0	-0.499788	-3.059629	-0.384752
37	8	0	-2.326364	-1.443274	1.438124
38	6	0	-3.212040	2.816250	-0.769706
39	6	0	-4.131858	2.492018	-1.732510
40	7	0	-3.531444	1.791268	-2.759658
41	6	0	-2.261152	1.699160	-2.414990
42	1	0	-3.285205	3.340722	0.170588
43	1	0	-5.188824	2.721643	-1.748894
44	1	0	-1.483648	1.201531	-2.975582
45	6	0	-2.990572	-1.050172	2.630928
46	6	0	-2.381714	-1.801102	3.815430
47	6	0	-2.916431	0.468637	2.789021
48	1	0	-4.043034	-1.348191	2.516124
49	6	0	-0.905733	-4.373478	-0.737619
50	6	0	0.187413	-5.001212	-1.602341
51	6	0	-1.204559	-5.185767	0.522991
52	1	0	-1.827100	-4.284559	-1.332638
53	1	0	-1.322284	-1.544577	3.918885

54	1	0	-2.901538	-1.540184	4.744610
55	1	0	-2.463235	-2.882818	3.666187
56	1	0	-3.477792	0.791962	3.673346
57	1	0	-1.874222	0.787280	2.902556
58	1	0	-3.340077	0.965437	1.909586
59	1	0	-0.110788	-6.002614	-1.934316
60	1	0	0.377637	-4.383247	-2.485444
61	1	0	1.120868	-5.084119	-1.034816
62	1	0	-0.302803	-5.279356	1.139006
63	1	0	-1.981569	-4.695652	1.119285
64	1	0	-1.551886	-6.192231	0.262091
65	1	0	-4.102367	-0.580472	-2.874176
66	7	0	-2.761719	-1.571836	-1.400262
67	6	0	-3.483400	-1.110120	-2.173342

E_{ZPE}: B3LYP/6-31G* = -2474.93088 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2475.49586 (a.u.)

Int_{18}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.430142	3.391020	-0.127031
2	6	0	2.542591	2.822540	0.536343
3	6	0	2.587085	1.401754	0.723395
4	6	0	1.530111	0.576129	0.204216
5	6	0	0.404689	1.183509	-0.362127
6	6	0	0.386572	2.605429	-0.551836
7	6	0	1.631556	-0.912354	0.280955
8	6	0	2.703154	-1.622149	-0.368012
9	6	0	2.839527	-3.037620	-0.172701
10	6	0	1.891800	-3.719043	0.637663
11	6	0	0.831404	-3.048698	1.188312
12	6	0	0.683943	-1.650371	0.987879
13	6	0	3.685807	0.869975	1.457724
14	6	0	4.682155	1.685875	1.945699
15	6	0	4.647063	3.083487	1.727549
16	6	0	3.593007	3.636309	1.038957
17	6	0	3.632635	-0.983423	-1.236838
18	6	0	4.644228	-1.690786	-1.849027
19	6	0	4.792869	-3.079016	-1.625815
20	6	0	3.902648	-3.733605	-0.805486
21	1	0	1.384032	4.466277	-0.277326
22	1	0	3.539296	4.710561	0.877407
23	1	0	5.443235	3.714178	2.113231
24	1	0	5.502914	1.250565	2.509555
25	1	0	3.726312	-0.196570	1.644141
26	1	0	3.529687	0.078649	-1.427847
27	1	0	5.332752	-1.175792	-2.513901
28	1	0	5.599011	-3.624431	-2.108855
29	1	0	3.992384	-4.804450	-0.636291
30	1	0	2.008727	-4.788557	0.796792
31	1	0	0.079842	-3.558194	1.783058
32	7	0	-0.707473	3.213535	-1.237929
33	8	0	-0.661049	0.471167	-0.776434
34	8	0	-0.418106	-1.044862	1.515364
35	22	0	-1.742291	-0.644951	0.283802
36	8	0	-2.159639	-2.233355	-0.389982
37	8	0	-2.910517	0.176445	1.337899
38	6	0	-0.627062	3.954426	-2.407477
39	6	0	-1.916585	4.295403	-2.720416
40	7	0	-2.792459	3.789994	-1.780776
41	6	0	-2.031858	3.153846	-0.910394
42	1	0	0.320963	4.137473	-2.889422
43	1	0	-2.267029	4.874754	-3.564025
44	1	0	-2.376184	2.616463	-0.038602
45	6	0	-3.737573	0.514351	2.438503
46	6	0	-4.357934	-0.754050	3.024767

47	6	0	-2.918931	1.301517	3.462256
48	1	0	-4.540532	1.156937	2.047243
49	6	0	-2.876437	-3.156388	-1.192507
50	6	0	-1.914775	-3.791517	-2.197067
51	6	0	-3.558197	-4.185457	-0.290540
52	1	0	-3.643879	-2.587819	-1.736776
53	1	0	-3.574688	-1.412023	3.418084
54	1	0	-5.045221	-0.505472	3.841587
55	1	0	-4.916668	-1.298669	2.256492
56	1	0	-3.548629	1.605920	4.306300
57	1	0	-2.095416	0.687173	3.841718
58	1	0	-2.494247	2.202328	3.007277
59	1	0	-2.447594	-4.494136	-2.848504
60	1	0	-1.451403	-3.021384	-2.821808
61	1	0	-1.119311	-4.332906	-1.673354
62	1	0	-2.810700	-4.760392	0.267776
63	1	0	-4.218993	-3.689038	0.427794
64	1	0	-4.157485	-4.883076	-0.887010
65	1	0	-4.303422	1.995319	-2.410890
66	7	0	-3.475950	0.119754	-1.542907
67	6	0	-3.952249	1.056754	-2.022106

E_{ZPE}: B3LYP/6-31G* = -24747.92921 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2475.49346 (a.u.)

TS_{11}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.350670	-3.483000	-0.391657
2	6	0	-2.493630	-3.031123	0.308118
3	6	0	-2.621093	-1.631215	0.600848
4	6	0	-1.623568	-0.699776	0.146683
5	6	0	-0.457293	-1.188403	-0.452175
6	6	0	-0.362759	-2.596294	-0.735349
7	6	0	-1.801086	0.770384	0.335614
8	6	0	-2.927738	1.469883	-0.224358
9	6	0	-3.119247	2.860984	0.074374
10	6	0	-2.168759	3.529031	0.892522
11	6	0	-1.056943	2.874446	1.352719
12	6	0	-0.851598	1.499541	1.052722
13	6	0	-3.749229	-1.225634	1.370959
14	6	0	-4.695290	-2.133860	1.789955
15	6	0	-4.581434	-3.505774	1.461374
16	6	0	-3.497038	-3.940971	0.737341
17	6	0	-3.861864	0.852126	-1.104119
18	6	0	-4.928209	1.551558	-1.626283
19	6	0	-5.130591	2.911817	-1.298460
20	6	0	-4.236973	3.547963	-0.467099
21	1	0	-1.250412	-4.536479	-0.640350
22	1	0	-3.382041	-4.994236	0.491034
23	1	0	-5.340501	-4.209286	1.791718
24	1	0	-5.538151	-1.792592	2.384985
25	1	0	-3.850380	-0.181347	1.640273
26	1	0	-3.719888	-0.187380	-1.377384
27	1	0	-5.618431	1.051937	-2.301290
28	1	0	-5.978985	3.451097	-1.710909
29	1	0	-4.366478	4.599207	-0.218716
30	1	0	-2.325999	4.578939	1.129508
31	1	0	-0.302559	3.378011	1.948625
32	7	0	0.852527	-3.066298	-1.333269
33	8	0	0.566050	-0.403982	-0.811843
34	8	0	0.289228	0.920009	1.490488
35	22	0	1.707228	0.696724	0.291222
36	8	0	1.964055	2.390870	-0.189189
37	8	0	2.859086	-0.080956	1.400904
38	6	0	1.722710	-4.022114	-0.808502
39	6	0	2.901489	-3.885004	-1.480424

40	7	0	2.763082	-2.870924	-2.417092
41	6	0	1.519610	-2.410514	-2.297027
42	1	0	1.417202	-4.677578	-0.008569
43	1	0	3.827214	-4.427907	-1.364862
44	1	0	1.128820	-1.550687	-2.813346
45	6	0	4.195286	-0.313594	1.816399
46	6	0	4.607005	0.753344	2.831147
47	6	0	4.292283	-1.732326	2.378166
48	1	0	4.835264	-0.234574	0.926100
49	6	0	2.643831	3.363436	-0.968030
50	6	0	1.655028	3.988613	-1.952515
51	6	0	3.279508	4.394509	-0.034947
52	1	0	3.434526	2.845221	-1.528271
53	1	0	3.967027	0.703483	3.719133
54	1	0	5.648149	0.608603	3.142546
55	1	0	4.512755	1.753330	2.394885
56	1	0	5.323500	-1.962268	2.670964
57	1	0	3.647614	-1.839556	3.257745
58	1	0	3.973803	-2.461289	1.625628
59	1	0	2.154498	4.739917	-2.575524
60	1	0	1.231293	3.221133	-2.608205
61	1	0	0.832529	4.470213	-1.412409
62	1	0	2.508161	4.917665	0.541515
63	1	0	3.963849	3.907067	0.667474
64	1	0	3.846057	5.136006	-0.610235
65	1	0	3.545346	-1.898038	-2.515877
66	7	0	3.283599	0.186054	-1.344143
67	6	0	3.797496	-0.582351	-2.060400

E_{ZPE}: B3LYP/6-31G* = -2474.91236 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2475.47824 (a.u.)

TS_{12}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.530926	-3.424653	-0.128429
2	6	0	-2.631727	-2.854469	0.552705
3	6	0	-2.659496	-1.434186	0.759687
4	6	0	-1.602487	-0.602059	0.249084
5	6	0	-0.475070	-1.205797	-0.318066
6	6	0	-0.489793	-2.629422	-0.531316
7	6	0	-1.690040	0.885277	0.336599
8	6	0	-2.767587	1.613383	-0.280119
9	6	0	-2.872627	3.030727	-0.077246
10	6	0	-1.887403	3.692102	0.704654
11	6	0	-0.822962	3.002070	1.222290
12	6	0	-0.703759	1.600212	1.016461
13	6	0	-3.749303	-0.904592	1.509283
14	6	0	-4.749860	-1.718225	1.991490
15	6	0	-4.731199	-3.112950	1.751991
16	6	0	-3.687279	-3.665682	1.048817
17	6	0	-3.734323	0.996490	-1.124333
18	6	0	-4.751625	1.724254	-1.702516
19	6	0	-4.869135	3.113794	-1.469749
20	6	0	-3.941617	3.748056	-0.674940
21	1	0	-1.497337	-4.496395	-0.306097
22	1	0	-3.645115	-4.737982	0.871258
23	1	0	-5.531123	-3.741176	2.133673
24	1	0	-5.561933	-1.283574	2.568164
25	1	0	-3.776747	0.159162	1.712121
26	1	0	-3.656777	-0.066120	-1.324878
27	1	0	-5.468854	1.224148	-2.348361
28	1	0	-5.679639	3.675706	-1.925832
29	1	0	-4.005914	4.819790	-0.499472
30	1	0	-1.979726	4.763454	0.868439
31	1	0	-0.043946	3.496756	1.793379
32	7	0	0.613750	-3.189325	-1.258391

33	8	0	0.606346	-0.520301	-0.716280
34	8	0	0.391136	0.975353	1.507004
35	22	0	1.789301	0.563778	0.336346
36	8	0	2.243066	2.210811	-0.172375
37	8	0	2.811933	-0.340273	1.495235
38	6	0	0.587228	-3.673151	-2.565534
39	6	0	1.880942	-3.693554	-2.998433
40	7	0	2.696623	-3.238375	-1.974493
41	6	0	1.897891	-2.946885	-0.952396
42	1	0	-0.342643	-3.930761	-3.047352
43	1	0	2.283486	-3.996294	-3.953058
44	1	0	2.217509	-2.481748	-0.033075
45	6	0	4.118741	-0.451373	2.046699
46	6	0	4.516199	0.864057	2.717259
47	6	0	4.139720	-1.633434	3.015811
48	1	0	4.806615	-0.653437	1.212751
49	6	0	2.830789	3.045100	-1.162476
50	6	0	1.787555	3.374087	-2.230326
51	6	0	3.393878	4.292290	-0.481137
52	1	0	3.652473	2.478804	-1.622054
53	1	0	3.834829	1.091523	3.544937
54	1	0	5.536682	0.802787	3.112716
55	1	0	4.472786	1.688845	1.998373
56	1	0	5.145386	-1.774378	3.428475
57	1	0	3.443673	-1.460639	3.844079
58	1	0	3.845322	-2.557698	2.507126
59	1	0	2.222490	4.007544	-3.012444
60	1	0	1.416349	2.455731	-2.697051
61	1	0	0.937259	3.901745	-1.784201
62	1	0	2.590442	4.866210	-0.005880
63	1	0	4.122146	4.015757	0.288405
64	1	0	3.894048	4.935953	-1.214122
65	1	0	3.599138	-2.357780	-2.050517
66	7	0	3.411410	-0.128812	-1.212155
67	6	0	3.917303	-1.024497	-1.767902

E_{ZPE}: B3LYP/6-31G* = -2474.91190 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2475.47512 (a.u.)

Int_{19}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.357054	3.452446	-0.368032
2	6	0	2.511892	3.000144	0.308594
3	6	0	2.652264	1.597576	0.586384
4	6	0	1.663841	0.663499	0.124056
5	6	0	0.492407	1.145421	-0.472232
6	6	0	0.373276	2.558057	-0.711761
7	6	0	1.833036	-0.807198	0.304325
8	6	0	2.963006	-1.513726	-0.237497
9	6	0	3.132237	-2.909445	0.053491
10	6	0	2.154766	-3.572696	0.843531
11	6	0	1.040955	-2.909374	1.285849
12	6	0	0.855170	-1.527712	0.996223
13	6	0	3.786870	1.193995	1.348819
14	6	0	4.728430	2.105167	1.769792
15	6	0	4.604178	3.479476	1.451627
16	6	0	3.513117	3.913505	0.738129
17	6	0	3.922872	-0.900991	-1.093054
18	6	0	4.992996	-1.608397	-1.596698
19	6	0	5.173251	-2.973156	-1.274957
20	6	0	4.253565	-3.604947	-0.468740
21	1	0	1.251945	4.509463	-0.599169
22	1	0	3.389594	4.968289	0.502186
23	1	0	5.360713	4.185109	1.783219
24	1	0	5.576374	1.765541	2.358456
25	1	0	3.895313	0.148088	1.608433

26	1	0	3.798104	0.141653	-1.363247
27	1	0	5.703115	-1.111533	-2.253000
28	1	0	6.024393	-3.519090	-1.672792
29	1	0	4.365029	-4.659696	-0.226228
30	1	0	2.293770	-4.626908	1.073267
31	1	0	0.268045	-3.409799	1.860272
32	7	0	-0.859217	3.039995	-1.271043
33	8	0	-0.508486	0.359329	-0.866600
34	8	0	-0.279415	-0.940470	1.416564
35	22	0	-1.745425	-0.674624	0.252789
36	8	0	-2.123316	-2.384748	-0.084704
37	8	0	-2.804461	0.193862	1.394412
38	6	0	-1.549928	4.186530	-0.877090
39	6	0	-2.758120	4.167076	-1.504359
40	7	0	-2.781877	3.024100	-2.282081
41	6	0	-1.637634	2.357427	-2.119400
42	1	0	-1.128273	4.881492	-0.170197
43	1	0	-3.588684	4.852705	-1.457574
44	1	0	-1.412560	1.391643	-2.531910
45	6	0	-4.151248	0.373573	1.807595
46	6	0	-4.574144	-0.786938	2.708737
47	6	0	-4.269224	1.730701	2.501978
48	1	0	-4.774323	0.375511	0.901785
49	6	0	-2.809445	-3.319339	-0.905835
50	6	0	-1.822471	-3.926719	-1.903299
51	6	0	-3.467139	-4.371804	-0.012843
52	1	0	-3.586333	-2.770338	-1.455048
53	1	0	-3.949525	-0.819551	3.608586
54	1	0	-5.621574	-0.678239	3.013818
55	1	0	-4.464685	-1.739213	2.179736
56	1	0	-5.307063	1.924719	2.797641
57	1	0	-3.640251	1.757949	3.398882
58	1	0	-3.944961	2.532478	1.829855
59	1	0	-2.326759	-4.653035	-2.551678
60	1	0	-1.387644	-3.144661	-2.534182
61	1	0	-1.008093	-4.434148	-1.374269
62	1	0	-2.708879	-4.924272	0.553715
63	1	0	-4.152107	-3.898869	0.698733
64	1	0	-4.037746	-5.086081	-0.617960
65	1	0	-3.595758	2.525791	-2.657053
66	7	0	-3.160770	-0.163641	-1.334339
67	6	0	-3.891388	0.346143	-2.105130

E_{ZPE}: B3LYP/6-31G* = -2474.91563 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2475.49429 (a.u.)

Int_{20}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.556456	-3.378837	-0.109977
2	6	0	-2.650673	-2.805263	0.577078
3	6	0	-2.685157	-1.380825	0.761100
4	6	0	-1.643172	-0.547995	0.224805
5	6	0	-0.515930	-1.149121	-0.348285
6	6	0	-0.529841	-2.575730	-0.536626
7	6	0	-1.726553	0.939119	0.293148
8	6	0	-2.811077	1.666412	-0.310069
9	6	0	-2.893888	3.088892	-0.133409
10	6	0	-1.879476	3.752938	0.608004
11	6	0	-0.811276	3.060438	1.114287
12	6	0	-0.712360	1.651712	0.936867
13	6	0	-3.768463	-0.847120	1.517884
14	6	0	-4.756167	-1.659574	2.026744
15	6	0	-4.731331	-3.058450	1.809592
16	6	0	-3.693721	-3.615678	1.101430
17	6	0	-3.807479	1.045855	-1.116594
18	6	0	-4.831683	1.774585	-1.681457

19	6	0	-4.926323	3.169794	-1.473859
20	6	0	-3.969462	3.807471	-0.717173
21	1	0	-1.517283	-4.453633	-0.268578
22	1	0	-3.646565	-4.690620	0.941402
23	1	0	-5.521464	-3.685540	2.212886
24	1	0	-5.563000	-1.221468	2.608122
25	1	0	-3.799177	0.219628	1.703614
26	1	0	-3.747988	-0.021302	-1.299009
27	1	0	-5.572057	1.270620	-2.297688
28	1	0	-5.741885	3.732879	-1.919420
29	1	0	-4.015587	4.883336	-0.562056
30	1	0	-1.953468	4.828946	0.749791
31	1	0	-0.012187	3.557036	1.655240
32	7	0	0.562725	-3.135552	-1.284903
33	8	0	0.553261	-0.476382	-0.777456
34	8	0	0.376852	1.023797	1.415209
35	22	0	1.818919	0.542978	0.298613
36	8	0	2.399786	2.186597	-0.091306
37	8	0	2.709413	-0.446357	1.503979
38	6	0	0.477299	-3.779183	-2.518334
39	6	0	1.739864	-3.849213	-3.023345
40	7	0	2.575136	-3.260533	-2.090340
41	6	0	1.843430	-2.828074	-1.063197
42	1	0	-0.471921	-4.096195	-2.918526
43	1	0	2.108630	-4.255205	-3.951439
44	1	0	2.224812	-2.292938	-0.210579
45	6	0	4.013014	-0.628560	2.046980
46	6	0	4.464224	0.644710	2.762976
47	6	0	3.986626	-1.842935	2.975434
48	1	0	4.690121	-0.827775	1.203591
49	6	0	3.108912	2.995930	-1.021332
50	6	0	2.136552	3.522868	-2.076948
51	6	0	3.813116	4.116939	-0.256700
52	1	0	3.859654	2.358439	-1.507257
53	1	0	3.795348	0.869470	3.601582
54	1	0	5.483084	0.528864	3.150507
55	1	0	4.450065	1.495055	2.073751
56	1	0	4.985946	-2.039133	3.380992
57	1	0	3.298643	-1.670530	3.810531
58	1	0	3.653960	-2.737328	2.437083
59	1	0	2.663277	4.145585	-2.809766
60	1	0	1.662912	2.691467	-2.609392
61	1	0	1.349954	4.124168	-1.607220
62	1	0	3.081514	4.754869	0.252191
63	1	0	4.491738	3.702659	0.496253
64	1	0	4.398832	4.739406	-0.943373
65	1	0	3.514071	-2.861499	-2.235361
66	7	0	3.294280	-0.179940	-1.160971
67	6	0	4.066500	-0.835078	-1.761906

E_{ZPE}: B3LYP/6-31G* = -2474.91490 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2475.49079 (a.u.)

Int_{21}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.822653	-3.602259	0.254489
2	6	0	-3.220531	-3.403510	0.236583
3	6	0	-3.731304	-2.071016	0.081620
4	6	0	-2.829952	-0.970958	-0.111977
5	6	0	-1.448882	-1.184585	-0.007983
6	6	0	-0.971177	-2.525781	0.172458
7	6	0	-3.336166	0.407968	-0.366628
8	6	0	-4.174127	0.718697	-1.492633
9	6	0	-4.725723	2.037928	-1.622678
10	6	0	-4.400628	3.020239	-0.648381
11	6	0	-3.536646	2.735158	0.376119

12	6	0	-2.972701	1.434283	0.509209
13	6	0	-5.145071	-1.901261	0.150283
14	6	0	-5.987953	-2.975884	0.319575
15	6	0	-5.476156	-4.292152	0.425844
16	6	0	-4.117806	-4.495777	0.388567
17	6	0	-4.464810	-0.219587	-2.523991
18	6	0	-5.269955	0.112580	-3.591982
19	6	0	-5.838543	1.403027	-3.694682
20	6	0	-5.563263	2.342697	-2.727037
21	1	0	-1.434226	-4.613821	0.334674
22	1	0	-3.704926	-5.497325	0.489121
23	1	0	-6.155020	-5.131288	0.549919
24	1	0	-7.060651	-2.811368	0.376753
25	1	0	-5.554401	-0.901093	0.078934
26	1	0	-4.029750	-1.211483	-2.470796
27	1	0	-5.465921	-0.625229	-4.366067
28	1	0	-6.477122	1.651469	-4.538135
29	1	0	-5.976878	3.346474	-2.799478
30	1	0	-4.832781	4.014258	-0.742206
31	1	0	-3.249614	3.484262	1.106947
32	7	0	0.444119	-2.753962	0.287422
33	8	0	-0.544294	-0.213733	-0.111557
34	8	0	-2.087669	1.220717	1.498530
35	22	0	-0.228875	1.266788	1.133234
36	8	0	-0.137655	2.989168	0.656186
37	8	0	0.378954	0.859945	2.760534
38	6	0	1.031546	-3.760458	1.048929
39	6	0	2.378631	-3.657225	0.883548
40	7	0	2.597775	-2.592543	0.036101
41	6	0	1.427337	-2.054622	-0.308448
42	1	0	0.440304	-4.427147	1.653319
43	1	0	3.188646	-4.232997	1.301476
44	1	0	1.282634	-1.173326	-0.908594
45	6	0	1.401832	1.176024	3.694219
46	6	0	1.104029	2.523108	4.353630
47	6	0	1.503752	0.034728	4.706473
48	1	0	2.345026	1.247539	3.133575
49	6	0	0.563777	3.974026	-0.086797
50	6	0	0.087846	3.947816	-1.539771
51	6	0	0.349690	5.334029	0.579082
52	1	0	1.631412	3.716319	-0.055391
53	1	0	0.159468	2.476662	4.907515
54	1	0	1.904351	2.798627	5.050678
55	1	0	1.019049	3.307243	3.594348
56	1	0	2.314438	0.222137	5.420641
57	1	0	0.565304	-0.066671	5.263129
58	1	0	1.704728	-0.912431	4.194772
59	1	0	0.617358	4.701431	-2.135138
60	1	0	0.276549	2.964042	-1.981495
61	1	0	-0.987771	4.150134	-1.593244
62	1	0	-0.712046	5.605260	0.565948
63	1	0	0.685084	5.309232	1.621315
64	1	0	0.913908	6.113146	0.052781
65	1	0	3.534042	-2.244769	-0.264977
66	7	0	1.771138	1.079636	0.342726
67	6	0	2.877172	0.939911	-0.035860
68	6	0	9.562670	0.125008	-2.107904
69	6	0	8.651804	1.146260	-1.827476
70	6	0	7.357508	0.825092	-1.422869
71	6	0	6.973960	-0.519122	-1.298220
72	6	0	7.895153	-1.541714	-1.581628
73	6	0	9.185039	-1.218413	-1.985144
74	6	0	5.601883	-0.826177	-0.873627
75	8	0	5.180513	-1.979185	-0.738088
76	1	0	4.929972	0.027093	-0.672666
77	1	0	10.572155	0.374130	-2.424162
78	1	0	8.950654	2.185880	-1.924863
79	1	0	6.636308	1.608235	-1.201851
80	1	0	7.576537	-2.574530	-1.479772
81	1	0	9.900921	-2.005110	-2.206221

E_{ZPE}: B3LYP/6-31G* = -2820.40073 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.08531 (a.u.)

Int_{22}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.781180	-3.566181	0.426296
2	6	0	-3.148213	-3.354182	0.707452
3	6	0	-3.687973	-2.033480	0.553505
4	6	0	-2.849286	-0.953790	0.115874
5	6	0	-1.469061	-1.162716	-0.023852
6	6	0	-0.977010	-2.509298	0.069951
7	6	0	-3.424176	0.393828	-0.160583
8	6	0	-4.430541	0.595628	-1.167330
9	6	0	-5.023890	1.893764	-1.323501
10	6	0	-4.579649	2.959915	-0.494848
11	6	0	-3.571097	2.772117	0.413464
12	6	0	-2.966782	1.492292	0.568024
13	6	0	-5.060312	-1.844810	0.890834
14	6	0	-5.841313	-2.891821	1.324094
15	6	0	-5.306173	-4.197649	1.444556
16	6	0	-3.983337	-4.417954	1.145214
17	6	0	-4.857444	-0.433719	-2.053951
18	6	0	-5.822999	-0.203851	-3.009997
19	6	0	-6.425194	1.068907	-3.137569
20	6	0	-6.025060	2.093203	-2.309360
21	1	0	-1.365212	-4.565222	0.526613
22	1	0	-3.549867	-5.410512	1.247961
23	1	0	-5.937062	-5.014720	1.783314
24	1	0	-6.881269	-2.712529	1.583672
25	1	0	-5.483526	-0.850346	0.817500
26	1	0	-4.401418	-1.414651	-1.979309
27	1	0	-6.121225	-1.009662	-3.676104
28	1	0	-7.189583	1.236843	-3.891498
29	1	0	-6.465774	3.083440	-2.404596
30	1	0	-5.042293	3.938103	-0.607490
31	1	0	-3.200345	3.582950	1.032183
32	7	0	0.385573	-2.787864	-0.297902
33	8	0	-0.591759	-0.196208	-0.283772
34	8	0	-1.949843	1.361390	1.437665
35	22	0	-0.164743	1.361759	0.822171
36	8	0	-0.124709	3.049263	0.230323
37	8	0	0.622410	1.000328	2.387883
38	6	0	0.783259	-3.894832	-1.042963
39	6	0	2.130240	-3.803296	-1.213734
40	7	0	2.535208	-2.647364	-0.581278
41	6	0	1.475085	-2.045167	-0.039454
42	1	0	0.066491	-4.614412	-1.401190
43	1	0	2.823773	-4.443253	-1.735003
44	1	0	1.496087	-1.106035	0.485154
45	6	0	1.719187	1.381077	3.206922
46	6	0	1.493397	2.788359	3.761103
47	6	0	1.887468	0.336159	4.310452
48	1	0	2.615125	1.383712	2.568717
49	6	0	0.473743	3.976763	-0.662782
50	6	0	-0.215431	3.887313	-2.025080
51	6	0	0.383992	5.374470	-0.048956
52	1	0	1.529522	3.694543	-0.774778
53	1	0	0.594024	2.812453	4.386918
54	1	0	2.349351	3.107229	4.367603
55	1	0	1.362159	3.503732	2.942871
56	1	0	2.756664	0.571869	4.935775
57	1	0	0.996815	0.306349	4.947989
58	1	0	2.032961	-0.659768	3.878371
59	1	0	0.227778	4.600689	-2.730267
60	1	0	-0.108233	2.880347	-2.441268

61	1	0	-1.284289	4.108268	-1.927385
62	1	0	-0.663109	5.673146	0.075642
63	1	0	0.866772	5.394868	0.933778
64	1	0	0.880498	6.109724	-0.693340
65	1	0	3.514974	-2.289263	-0.566697
66	7	0	1.787145	1.136397	-0.094704
67	6	0	2.905727	1.006202	-0.439812
68	6	0	8.853044	1.079365	-1.080448
69	6	0	7.500160	0.761950	-0.975098
70	6	0	7.098658	-0.580084	-0.888630
71	6	0	8.060654	-1.604187	-0.908524
72	6	0	9.408930	-1.284491	-1.014128
73	6	0	9.804385	0.056703	-1.099800
74	6	0	5.665920	-0.881355	-0.773360
75	8	0	5.223328	-2.031094	-0.685274
76	1	0	4.969678	-0.023645	-0.759520
77	1	0	9.166227	2.117207	-1.146825
78	1	0	6.746856	1.545853	-0.957563
79	1	0	7.727864	-2.635234	-0.838941
80	1	0	10.156898	-2.072245	-1.029631
81	1	0	10.859750	0.302952	-1.181687

E_{ZPE}: B3LYP/6-31G* = -2820.39933 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.08368 (a.u.)

TS_{13}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.662961	-3.597076	-0.011822
2	6	0	-2.990307	-3.381611	0.423147
3	6	0	-3.480519	-2.035735	0.521749
4	6	0	-2.647507	-0.932616	0.130064
5	6	0	-1.314830	-1.172367	-0.221903
6	6	0	-0.849772	-2.527051	-0.294149
7	6	0	-3.156763	0.469412	0.150676
8	6	0	-4.290533	0.881353	-0.631515
9	6	0	-4.805510	2.213697	-0.485996
10	6	0	-4.159245	3.109600	0.407855
11	6	0	-3.032765	2.730545	1.089976
12	6	0	-2.506705	1.416773	0.944355
13	6	0	-4.795916	-1.855922	1.039631
14	6	0	-5.579086	-2.930814	1.394722
15	6	0	-5.102399	-4.256178	1.252461
16	6	0	-3.830006	-4.471430	0.779731
17	6	0	-4.922029	0.031974	-1.584416
18	6	0	-6.006562	0.458955	-2.319445
19	6	0	-6.529833	1.761024	-2.145851
20	6	0	-5.932973	2.616883	-1.248161
21	1	0	-1.291627	-4.613462	-0.113763
22	1	0	-3.439033	-5.481856	0.682146
23	1	0	-5.735628	-5.094643	1.528594
24	1	0	-6.575122	-2.758765	1.793732
25	1	0	-5.175801	-0.849316	1.164338
26	1	0	-4.529814	-0.966815	-1.740729
27	1	0	-6.461321	-0.211776	-3.044023
28	1	0	-7.389417	2.084245	-2.726705
29	1	0	-6.311592	3.628069	-1.114628
30	1	0	-4.561944	4.113106	0.526814
31	1	0	-2.507707	3.412729	1.750893
32	7	0	0.523797	-2.761424	-0.636016
33	8	0	-0.448946	-0.200991	-0.528050
34	8	0	-1.367005	1.111492	1.598392
35	22	0	0.275013	1.124538	0.683133
36	8	0	0.335862	2.853472	0.246776
37	8	0	1.324121	0.567341	2.009849
38	6	0	1.364910	-3.691835	-0.034160
39	6	0	2.593679	-3.546890	-0.606870

40	7	0	2.491760	-2.544708	-1.547238
41	6	0	1.246568	-2.080240	-1.543558
42	1	0	1.013996	-4.338084	0.753238
43	1	0	3.521497	-4.062094	-0.415952
44	1	0	0.879896	-1.259763	-2.134105
45	6	0	2.574352	0.710794	2.668445
46	6	0	2.542351	1.947424	3.567137
47	6	0	2.866734	-0.574407	3.442896
48	1	0	3.342141	0.844951	1.892758
49	6	0	0.806722	3.905060	-0.579999
50	6	0	-0.222919	4.184794	-1.675424
51	6	0	1.089478	5.130080	0.290657
52	1	0	1.744552	3.567760	-1.043981
53	1	0	1.772020	1.838433	4.338822
54	1	0	3.511229	2.092919	4.059088
55	1	0	2.314455	2.842016	2.978108
56	1	0	3.846740	-0.515931	3.930708
57	1	0	2.103118	-0.739481	4.211291
58	1	0	2.868399	-1.435000	2.765840
59	1	0	0.125014	4.986697	-2.337397
60	1	0	-0.392064	3.287189	-2.279178
61	1	0	-1.179258	4.484368	-1.233154
62	1	0	0.169546	5.477546	0.774145
63	1	0	1.818208	4.887508	1.071300
64	1	0	1.493309	5.948764	-0.316562
65	1	0	3.271094	-2.042617	-2.109368
66	7	0	2.059999	0.918300	-0.655731
67	6	0	3.061335	0.805181	-1.249756
68	6	0	7.719702	-0.438495	0.498220
69	6	0	7.149543	0.819688	0.275767
70	6	0	6.103593	0.960843	-0.632574
71	6	0	5.609893	-0.152179	-1.324594
72	6	0	6.192284	-1.403888	-1.109114
73	6	0	7.241231	-1.548310	-0.198018
74	6	0	4.528143	-0.011573	-2.373978
75	8	0	4.040894	-1.034468	-2.941928
76	1	0	4.631653	0.902150	-2.978635
77	1	0	8.537210	-0.548269	1.205885
78	1	0	7.522676	1.688560	0.811568
79	1	0	5.650575	1.935729	-0.798712
80	1	0	5.834813	-2.252164	-1.685271
81	1	0	7.691367	-2.525270	-0.040556

E_{ZPE}: B3LYP/6-31G* = -2820.38573 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.06430 (a.u.)

TS_{14}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.273313	-0.014127	0.327110
2	6	0	-3.324598	0.315614	-0.065097
3	6	0	2.487036	3.347792	-0.583503
4	6	0	3.784212	2.824049	-0.382627
5	6	0	3.938095	1.415425	-0.153735
6	6	0	2.791041	0.550972	-0.178300
7	6	0	1.513669	1.110357	-0.291230
8	6	0	1.391161	2.522929	-0.510319
9	6	0	2.932189	-0.926780	-0.031214
10	6	0	3.705456	-1.712875	-0.954128
11	6	0	3.896856	-3.113772	-0.704542
12	6	0	3.289220	-3.700430	0.438309
13	6	0	2.491290	-2.957836	1.268833
14	6	0	2.282855	-1.571977	1.023033
15	6	0	5.252699	0.936455	0.116444
16	6	0	6.336494	1.785148	0.123998
17	6	0	6.179833	3.166474	-0.143546
18	6	0	4.925140	3.671480	-0.387744

19	6	0	4.273897	-1.172362	-2.142840
20	6	0	5.005377	-1.955370	-3.009222
21	6	0	5.218027	-3.327006	-2.739710
22	6	0	4.668167	-3.888527	-1.609654
23	1	0	2.366057	4.407678	-0.791041
24	1	0	4.782714	4.733218	-0.576862
25	1	0	7.045911	3.822359	-0.142203
26	1	0	7.324763	1.389655	0.342662
27	1	0	5.392263	-0.115982	0.331192
28	1	0	4.113856	-0.125092	-2.373888
29	1	0	5.419298	-1.513763	-3.912204
30	1	0	5.801957	-3.932778	-3.427320
31	1	0	4.807132	-4.946116	-1.395523
32	1	0	3.450470	-4.758470	0.633065
33	1	0	1.993660	-3.398068	2.127014
34	7	0	0.078915	3.090973	-0.626897
35	8	0	0.390045	0.386912	-0.239385
36	8	0	1.446111	-0.898705	1.839398
37	22	0	-0.319961	-0.556936	1.292789
38	8	0	-0.905803	-2.236707	1.181162
39	8	0	-0.849514	0.399077	2.701302
40	6	0	-0.331420	4.313391	-0.104316
41	6	0	-1.655241	4.449207	-0.402948
42	7	0	-2.039304	3.324177	-1.100300
43	6	0	-0.987676	2.520973	-1.218516
44	1	0	0.346259	4.945157	0.445599
45	1	0	-2.345883	5.244495	-0.170742
46	1	0	-0.990271	1.545157	-1.670193
47	6	0	-1.884121	0.605072	3.651247
48	6	0	-1.953347	-0.583459	4.611025
49	6	0	-1.626966	1.929088	4.371179
50	1	0	-2.830750	0.675746	3.094862
51	6	0	-1.771308	-3.204179	0.605680
52	6	0	-1.165324	-3.714774	-0.702022
53	6	0	-2.002400	-4.321588	1.623417
54	1	0	-2.727272	-2.706599	0.389890
55	1	0	-1.014203	-0.678168	5.167659
56	1	0	-2.772453	-0.454939	5.328344
57	1	0	-2.119792	-1.512997	4.056882
58	1	0	-2.432485	2.144361	5.083114
59	1	0	-0.679297	1.886489	4.919421
60	1	0	-1.571449	2.751864	3.650735
61	1	0	-1.821638	-4.460730	-1.165480
62	1	0	-1.029118	-2.889771	-1.408859
63	1	0	-0.187815	-4.173042	-0.515789
64	1	0	-1.057807	-4.823022	1.862119
65	1	0	-2.421982	-3.917753	2.550800
66	1	0	-2.700569	-5.066356	1.223769
67	1	0	-3.041247	2.965423	-1.397554
68	6	0	-7.650186	-1.482176	-2.195842
69	6	0	-7.560192	-1.127908	-0.846967
70	6	0	-6.607981	-0.197036	-0.434822
71	6	0	-5.739042	0.382879	-1.364847
72	6	0	-5.835662	0.031623	-2.714308
73	6	0	-6.787482	-0.900118	-3.127677
74	6	0	-4.739282	1.420526	-0.933281
75	8	0	-4.167637	2.130571	-1.821972
76	1	0	-4.990256	1.877022	0.039445
77	1	0	-8.393319	-2.206458	-2.519209
78	1	0	-8.233046	-1.574710	-0.119731
79	1	0	-6.532031	0.078388	0.615457
80	1	0	-5.165381	0.506554	-3.423415
81	1	0	-6.859745	-1.170194	-4.178074

E_{ZPE}: B3LYP/6-31G* = -2820.38797 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.06652 (a.u.)

TS_{15}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.427458	-3.578600	0.517455
2	6	0	-2.827156	-3.399398	0.601906
3	6	0	-3.372459	-2.084423	0.413263
4	6	0	-2.510204	-0.981045	0.088292
5	6	0	-1.124496	-1.175531	0.079150
6	6	0	-0.612412	-2.499647	0.283556
7	6	0	-3.061277	0.377503	-0.185206
8	6	0	-3.996140	0.622754	-1.249681
9	6	0	-4.584920	1.924487	-1.389982
10	6	0	-4.205119	2.954556	-0.487697
11	6	0	-3.254741	2.731202	0.474248
12	6	0	-2.652939	1.449446	0.611675
13	6	0	-4.777577	-1.928847	0.594155
14	6	0	-5.583719	-3.001590	0.901118
15	6	0	-5.041245	-4.300982	1.046776
16	6	0	-3.687298	-4.489310	0.904712
17	6	0	-4.349885	-0.367177	-2.210219
18	6	0	-5.246006	-0.097877	-3.221731
19	6	0	-5.847997	1.176690	-3.333644
20	6	0	-5.515996	2.164255	-2.434219
21	1	0	-0.998352	-4.564364	0.678006
22	1	0	-3.248606	-5.476232	1.034288
23	1	0	-5.691454	-5.138579	1.283211
24	1	0	-6.650456	-2.847007	1.039425
25	1	0	-5.210862	-0.941021	0.497555
26	1	0	-3.891537	-1.347910	-2.148111
27	1	0	-5.488934	-0.873059	-3.944075
28	1	0	-6.557996	1.375114	-4.131936
29	1	0	-5.956038	3.155855	-2.516284
30	1	0	-4.666707	3.934595	-0.586490
31	1	0	-2.930017	3.516249	1.149565
32	7	0	0.807895	-2.695539	0.200502
33	8	0	-0.242237	-0.197418	-0.144774
34	8	0	-1.679484	1.295730	1.534682
35	22	0	0.117054	1.317802	0.979930
36	8	0	0.201265	3.015190	0.427204
37	8	0	0.904619	0.859464	2.527196
38	6	0	1.466150	-3.571870	-0.653906
39	6	0	2.802647	-3.363846	-0.482254
40	7	0	2.943540	-2.377832	0.471421
41	6	0	1.734968	-1.982978	0.860735
42	1	0	0.919144	-4.230541	-1.308587
43	1	0	3.653741	-3.815661	-0.965799
44	1	0	1.526775	-1.203060	1.577172
45	6	0	1.997183	1.144346	3.399605
46	6	0	2.159747	2.653047	3.578004
47	6	0	1.756057	0.420103	4.724348
48	1	0	2.901984	0.739038	2.922487
49	6	0	0.769079	3.974495	-0.452035
50	6	0	0.098170	3.874087	-1.822518
51	6	0	0.620854	5.360465	0.176699
52	1	0	1.836914	3.735399	-0.556334
53	1	0	1.256790	3.084056	4.025967
54	1	0	3.010810	2.871635	4.233245
55	1	0	2.332866	3.137278	2.612184
56	1	0	2.605234	0.566636	5.401659
57	1	0	0.851131	0.802703	5.209115
58	1	0	1.628156	-0.655381	4.561877
59	1	0	0.527172	4.606454	-2.516729
60	1	0	0.239477	2.874241	-2.245834
61	1	0	-0.977617	4.062296	-1.735113
62	1	0	-0.438279	5.617118	0.291545
63	1	0	1.090507	5.386923	1.165351
64	1	0	1.096320	6.121026	-0.453775
65	1	0	3.835133	-1.840922	0.754288
66	6	0	6.693434	-1.103940	-3.514916
67	6	0	6.683186	-1.982772	-2.432138

68	6	0	6.136654	-1.580661	-1.210669
69	6	0	5.591110	-0.300627	-1.064896
70	6	0	5.616453	0.580686	-2.152397
71	6	0	6.161048	0.181676	-3.370213
72	6	0	5.094553	0.117910	0.300460
73	8	0	4.849674	-0.750491	1.189352
74	1	0	5.491307	1.088779	0.632839
75	1	0	7.117391	-1.413787	-4.466431
76	1	0	7.110930	-2.977201	-2.532920
77	1	0	6.156818	-2.242218	-0.349262
78	1	0	5.182204	1.571127	-2.043646
79	1	0	6.166402	0.870001	-4.211203
80	7	0	2.154766	1.127120	0.080952
81	6	0	3.294477	0.967198	-0.130355

E_{ZPE}: B3LYP/6-31G* = -2820.38457 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.05824 (a.u.)

TS_{16}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.361572	-3.472433	-0.094749
2	6	0	-3.638023	-3.017887	0.306998
3	6	0	-3.866772	-1.605519	0.421256
4	6	0	-2.823843	-0.672578	0.092684
5	6	0	-1.543962	-1.153599	-0.208003
6	6	0	-1.353191	-2.570843	-0.329540
7	6	0	-3.077343	0.797294	0.106040
8	6	0	-4.073292	1.404412	-0.735330
9	6	0	-4.355032	2.805777	-0.600665
10	6	0	-3.619059	3.570666	0.344427
11	6	0	-2.620431	2.997564	1.087475
12	6	0	-2.323614	1.612978	0.951393
13	6	0	-5.142038	-1.187087	0.900393
14	6	0	-6.125038	-2.099386	1.210899
15	6	0	-5.901306	-3.489102	1.060312
16	6	0	-4.677368	-3.934502	0.621550
17	6	0	-4.785049	0.683076	-1.735838
18	6	0	-5.730469	1.297473	-2.527988
19	6	0	-6.026470	2.670673	-2.367175
20	6	0	-5.345064	3.404397	-1.422754
21	1	0	-2.171946	-4.539215	-0.181452
22	1	0	-4.479245	-4.999195	0.519382
23	1	0	-6.689078	-4.196419	1.303958
24	1	0	-7.083757	-1.747572	1.582422
25	1	0	-5.329272	-0.128544	1.033373
26	1	0	-4.565442	-0.368535	-1.882774
27	1	0	-6.250887	0.720190	-3.288016
28	1	0	-6.778563	3.142484	-2.993649
29	1	0	-5.547768	4.465847	-1.296904
30	1	0	-3.847466	4.628500	0.454597
31	1	0	-2.027306	3.574591	1.789643
32	7	0	-0.077128	-3.055008	-0.774888
33	8	0	-0.489355	-0.362364	-0.429851
34	8	0	-1.296686	1.105268	1.665171
35	22	0	0.357671	0.833545	0.817723
36	8	0	0.757655	2.536585	0.454703
37	8	0	1.208190	0.006723	2.161772
38	6	0	0.130550	-3.927309	-1.837283
39	6	0	1.479956	-4.055905	-1.985579
40	7	0	2.079155	-3.273734	-1.021055
41	6	0	1.126636	-2.678460	-0.309455
42	1	0	-0.697100	-4.342285	-2.389030
43	1	0	2.054957	-4.629909	-2.695053
44	1	0	1.290788	-1.993854	0.505888
45	6	0	2.403494	0.042929	2.936548
46	6	0	2.501288	1.372509	3.685036

47	6	0	2.409119	-1.161449	3.877630
48	1	0	3.247090	-0.040069	2.235834
49	6	0	1.397187	3.463896	-0.411343
50	6	0	0.562379	3.636173	-1.680770
51	6	0	1.601130	4.777025	0.344473
52	1	0	2.376753	3.043408	-0.678503
53	1	0	1.662917	1.480710	4.382587
54	1	0	3.436897	1.426072	4.253628
55	1	0	2.475365	2.211308	2.981861
56	1	0	3.335670	-1.186960	4.462701
57	1	0	1.560881	-1.109510	4.569234
58	1	0	2.335895	-2.096556	3.312253
59	1	0	1.043727	4.342941	-2.367123
60	1	0	0.449856	2.676856	-2.196682
61	1	0	-0.436009	4.013096	-1.432687
62	1	0	0.635381	5.210161	0.628157
63	1	0	2.185461	4.610657	1.255398
64	1	0	2.136229	5.500504	-0.281749
65	1	0	3.142604	-2.982827	-0.920522
66	7	0	2.180960	0.350490	-0.397965
67	6	0	3.192600	0.006286	-0.873678
68	6	0	7.477130	1.222311	-1.767381
69	6	0	6.304691	0.505648	-2.000767
70	6	0	5.886959	-0.477542	-1.097641
71	6	0	6.656716	-0.745640	0.038065
72	6	0	7.829440	-0.028198	0.272917
73	6	0	8.241221	0.957030	-0.627571
74	6	0	4.646716	-1.282912	-1.365620
75	8	0	4.431435	-2.332827	-0.679649
76	1	0	4.335451	-1.257371	-2.423028
77	1	0	7.796471	1.985062	-2.472643
78	1	0	5.702938	0.713862	-2.883357
79	1	0	6.327279	-1.525669	0.716890
80	1	0	8.425715	-0.240045	1.156723
81	1	0	9.156292	1.514370	-0.444858

E_{ZPE}: B3LYP/6-31G* = -2820.38783 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.06461 (a.u.)

Int_{23}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.503140	-3.589262	-0.052348
2	6	0	-2.836601	-3.422519	0.390056
3	6	0	-3.375072	-2.097118	0.495480
4	6	0	-2.572425	-0.965287	0.119321
5	6	0	-1.234151	-1.164588	-0.229235
6	6	0	-0.717586	-2.498120	-0.331719
7	6	0	-3.133419	0.418281	0.154363
8	6	0	-4.261557	0.797519	-0.652740
9	6	0	-4.837558	2.103704	-0.500263
10	6	0	-4.258968	3.009805	0.428565
11	6	0	-3.138253	2.665307	1.138644
12	6	0	-2.554816	1.378859	0.983799
13	6	0	-4.698309	-1.964867	1.006096
14	6	0	-5.445316	-3.068439	1.353222
15	6	0	-4.919887	-4.374240	1.209269
16	6	0	-3.638155	-4.541883	0.740403
17	6	0	-4.828080	-0.063161	-1.635656
18	6	0	-5.907682	0.329923	-2.396041
19	6	0	-6.490679	1.605959	-2.217932
20	6	0	-5.958911	2.471482	-1.289429
21	1	0	-1.095331	-4.590567	-0.161816
22	1	0	-3.211146	-5.537225	0.639758
23	1	0	-5.523346	-5.236289	1.479790
24	1	0	-6.449322	-2.933530	1.746675
25	1	0	-5.115390	-0.973064	1.132478

26	1	0	-4.389664	-1.042270	-1.792698
27	1	0	-6.313021	-0.347437	-3.143284
28	1	0	-7.346212	1.901748	-2.819044
29	1	0	-6.385527	3.462665	-1.151038
30	1	0	-4.708542	3.992339	0.553619
31	1	0	-2.664362	3.355535	1.829448
32	7	0	0.649932	-2.687140	-0.692662
33	8	0	-0.398203	-0.143072	-0.492524
34	8	0	-1.417480	1.109205	1.673265
35	22	0	0.194701	1.158323	0.748685
36	8	0	0.242453	2.861511	0.225918
37	8	0	1.297110	0.624457	2.032743
38	6	0	1.564596	-3.511838	-0.051142
39	6	0	2.753203	-3.337810	-0.706891
40	7	0	2.593014	-2.432432	-1.736369
41	6	0	1.325435	-2.065692	-1.697992
42	1	0	1.280823	-4.107924	0.801943
43	1	0	3.709168	-3.798684	-0.502592
44	1	0	0.854933	-1.347770	-2.350518
45	6	0	2.498152	0.558582	2.780479
46	6	0	2.462291	1.608887	3.891479
47	6	0	2.669969	-0.863764	3.313953
48	1	0	3.329598	0.784277	2.095766
49	6	0	0.654769	3.979007	-0.537502
50	6	0	-0.382793	4.256743	-1.626038
51	6	0	0.866666	5.171626	0.396321
52	1	0	1.614030	3.722888	-1.013005
53	1	0	1.629846	1.409642	4.575191
54	1	0	3.395969	1.595531	4.465941
55	1	0	2.328749	2.611120	3.470579
56	1	0	3.614469	-0.957629	3.862588
57	1	0	1.846234	-1.117197	3.990653
58	1	0	2.674753	-1.582142	2.488002
59	1	0	-0.075192	5.107160	-2.245938
60	1	0	-0.502776	3.381330	-2.272426
61	1	0	-1.354924	4.483365	-1.175289
62	1	0	-0.074714	5.444024	0.886295
63	1	0	1.599877	4.926966	1.172146
64	1	0	1.231050	6.040732	-0.163809
65	1	0	3.598067	-1.302982	-2.634411
66	7	0	2.168719	1.007056	-0.644495
67	6	0	3.119910	0.786789	-1.267170
68	6	0	7.716824	-0.601746	0.371603
69	6	0	6.941311	0.514615	0.693827
70	6	0	5.835989	0.847096	-0.088773
71	6	0	5.495955	0.064661	-1.198652
72	6	0	6.276852	-1.045491	-1.524164
73	6	0	7.382808	-1.377825	-0.738259
74	6	0	4.314420	0.448185	-2.102789
75	8	0	3.980103	-0.489252	-3.080104
76	1	0	4.574468	1.372573	-2.638284
77	1	0	8.577421	-0.861822	0.981817
78	1	0	7.196583	1.127383	1.554148
79	1	0	5.238745	1.719908	0.167714
80	1	0	6.018341	-1.636627	-2.395975
81	1	0	7.984653	-2.244608	-0.998061

E_{ZPE}: B3LYP/6-31G* = -2820.41503 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.09137 (a.u.)

Int_{24}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.373842	-0.144767	0.126971
2	6	0	3.302699	-0.613490	-0.381744
3	6	0	-2.550880	-3.295752	-0.636474
4	6	0	-3.825317	-2.756241	-0.342965

5	6	0	-3.941814	-1.352818	-0.069801
6	6	0	-2.776903	-0.512561	-0.126899
7	6	0	-1.523694	-1.097754	-0.325432
8	6	0	-1.431535	-2.500540	-0.607904
9	6	0	-2.884011	0.962774	0.078300
10	6	0	-3.670800	1.791856	-0.794625
11	6	0	-3.831003	3.187071	-0.496086
12	6	0	-3.182700	3.727969	0.646664
13	6	0	-2.376532	2.945033	1.431453
14	6	0	-2.201163	1.566261	1.134185
15	6	0	-5.230002	-0.856858	0.281811
16	6	0	-6.328304	-1.686347	0.327559
17	6	0	-6.210928	-3.062522	0.020102
18	6	0	-4.980231	-3.582663	-0.304829
19	6	0	-4.285610	1.296071	-1.979654
20	6	0	-5.029829	2.116994	-2.798500
21	6	0	-5.209503	3.483435	-2.481647
22	6	0	-4.616084	4.001900	-1.353325
23	1	0	-2.458204	-4.351058	-0.878476
24	1	0	-4.868007	-4.641376	-0.527728
25	1	0	-7.087389	-3.703777	0.053017
26	1	0	-7.296101	-1.279031	0.607748
27	1	0	-5.338744	0.192149	0.529681
28	1	0	-4.152479	0.253163	-2.244392
29	1	0	-5.480545	1.709886	-3.699966
30	1	0	-5.804196	4.119023	-3.132126
31	1	0	-4.731213	5.054357	-1.103029
32	1	0	-3.320663	4.781510	0.879451
33	1	0	-1.849383	3.348137	2.290425
34	7	0	-0.147675	-3.083131	-0.830547
35	8	0	-0.381119	-0.388571	-0.279444
36	8	0	-1.350073	0.851359	1.911492
37	22	0	0.345137	0.482532	1.238846
38	8	0	1.009720	2.124036	1.055899
39	8	0	0.977223	-0.531286	2.559718
40	6	0	0.331794	-4.258695	-0.269386
41	6	0	1.606351	-4.410363	-0.744154
42	7	0	1.922879	-3.361750	-1.584811
43	6	0	0.851549	-2.590076	-1.612829
44	1	0	-0.267784	-4.839740	0.413569
45	1	0	2.312019	-5.202239	-0.535841
46	1	0	0.752998	-1.664320	-2.156661
47	6	0	2.007761	-0.904767	3.457072
48	6	0	2.092212	0.111754	4.596470
49	6	0	1.737713	-2.327276	3.947959
50	1	0	2.956109	-0.894591	2.897428
51	6	0	1.805060	3.126659	0.445539
52	6	0	1.115152	3.621983	-0.826103
53	6	0	2.049460	4.245242	1.458856
54	1	0	2.768633	2.668313	0.177424
55	1	0	1.152355	0.131111	5.159227
56	1	0	2.905736	-0.145511	5.284821
57	1	0	2.276963	1.116162	4.200913
58	1	0	2.541848	-2.666873	4.611331
59	1	0	0.791546	-2.365396	4.498971
60	1	0	1.670563	-3.016251	3.099708
61	1	0	1.720970	4.391348	-1.319075
62	1	0	0.967132	2.796103	-1.529563
63	1	0	0.134565	4.046763	-0.585422
64	1	0	1.100871	4.711917	1.746553
65	1	0	2.526712	3.849414	2.361408
66	1	0	2.701472	5.015959	1.031602
67	1	0	3.368552	-2.498214	-2.136211
68	6	0	7.619599	1.633682	-1.562150
69	6	0	7.429484	1.007744	-0.328357
70	6	0	6.413774	0.064293	-0.175091
71	6	0	5.581412	-0.254492	-1.252759
72	6	0	5.771119	0.371734	-2.486985
73	6	0	6.791593	1.311739	-2.639001
74	6	0	4.458185	-1.272116	-1.075014

75	8	0	4.052893	-1.787824	-2.305761
76	1	0	4.800194	-2.060281	-0.382781
77	1	0	8.413876	2.365097	-1.684361
78	1	0	8.075514	1.247301	0.511772
79	1	0	6.272973	-0.428591	0.784923
80	1	0	5.128880	0.104576	-3.318639
81	1	0	6.940303	1.791926	-3.602401

E_{ZPE}: B3LYP/6-31G* = -2820.41543 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.09300 (a.u.)

Int_{25}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.267928	-3.563322	0.665052
2	6	0	-2.672208	-3.412027	0.744825
3	6	0	-3.245686	-2.115118	0.529950
4	6	0	-2.399672	-1.003853	0.185777
5	6	0	-1.012837	-1.177216	0.187134
6	6	0	-0.461067	-2.481540	0.413196
7	6	0	-2.988832	0.329956	-0.135581
8	6	0	-3.908296	0.505313	-1.228452
9	6	0	-4.550572	1.774536	-1.420677
10	6	0	-4.241652	2.845940	-0.539930
11	6	0	-3.306507	2.691692	0.450173
12	6	0	-2.653791	1.442987	0.635715
13	6	0	-4.653615	-1.983886	0.702753
14	6	0	-5.438690	-3.066624	1.031009
15	6	0	-4.868648	-4.349815	1.205426
16	6	0	-3.510191	-4.512490	1.068718
17	6	0	-4.194898	-0.527863	-2.165396
18	6	0	-5.077476	-0.328491	-3.204445
19	6	0	-5.732075	0.914203	-3.368356
20	6	0	-5.466311	1.941894	-2.492463
21	1	0	-0.820151	-4.537409	0.842781
22	1	0	-3.051063	-5.486957	1.219215
23	1	0	-5.501141	-5.196106	1.458749
24	1	0	-6.508910	-2.931635	1.163150
25	1	0	-5.108485	-1.007948	0.584172
26	1	0	-3.696551	-1.485001	-2.061212
27	1	0	-5.269637	-1.134775	-3.907616
28	1	0	-6.431339	1.056648	-4.187793
29	1	0	-5.948704	2.909399	-2.613813
30	1	0	-4.745187	3.800336	-0.676515
31	1	0	-3.034456	3.508215	1.111503
32	7	0	0.954020	-2.662666	0.345080
33	8	0	-0.158290	-0.164050	-0.046124
34	8	0	-1.690839	1.364010	1.591400
35	22	0	0.068091	1.391883	0.991472
36	8	0	0.149637	2.990772	0.207208
37	8	0	0.946039	1.134564	2.526284
38	6	0	1.633550	-3.543912	-0.483432
39	6	0	2.964102	-3.341266	-0.236667
40	7	0	3.119876	-2.364108	0.725567
41	6	0	1.897928	-1.981998	1.049935
42	1	0	1.105468	-4.192299	-1.165075
43	1	0	3.816058	-3.823676	-0.694009
44	1	0	1.642354	-1.217292	1.767728
45	6	0	2.000888	1.455508	3.424930
46	6	0	2.154442	2.971851	3.541590
47	6	0	1.714127	0.787799	4.769871
48	1	0	2.924200	1.030368	3.002728
49	6	0	0.623342	3.899756	-0.772153
50	6	0	-0.128831	3.677603	-2.084879
51	6	0	0.470104	5.323883	-0.236822
52	1	0	1.691769	3.688330	-0.929381
53	1	0	1.236409	3.417647	3.941494

54	1	0	2.983467	3.223979	4.212745
55	1	0	2.355383	3.416716	2.561522
56	1	0	2.537404	0.968450	5.470482
57	1	0	0.790594	1.186365	5.204099
58	1	0	1.596783	-0.293616	4.647096
59	1	0	0.234062	4.364921	-2.858245
60	1	0	0.012095	2.651444	-2.439985
61	1	0	-1.201657	3.845537	-1.941518
62	1	0	-0.587542	5.555695	-0.069228
63	1	0	1.002060	5.437159	0.713410
64	1	0	0.876341	6.049605	-0.951002
65	1	0	4.434243	-1.238690	1.079291
66	6	0	6.231935	-1.375905	-3.637511
67	6	0	6.753022	-1.791589	-2.410709
68	6	0	6.285230	-1.230792	-1.221777
69	6	0	5.288364	-0.250601	-1.252812
70	6	0	4.768112	0.165258	-2.482240
71	6	0	5.238510	-0.396158	-3.670238
72	6	0	4.850872	0.384944	0.071674
73	8	0	5.014700	-0.427570	1.200994
74	1	0	5.462917	1.280600	0.250513
75	1	0	6.595460	-1.814987	-4.562589
76	1	0	7.526233	-2.554571	-2.377270
77	1	0	6.682117	-1.549695	-0.263615
78	1	0	3.986928	0.920855	-2.518679
79	1	0	4.822251	-0.071333	-4.619868
80	7	0	2.327804	1.192214	0.081163
81	6	0	3.436980	0.865075	0.015742

E_{ZPE}: B3LYP/6-31G* = -2820.41449 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.08708 (a.u.)

Int_{26}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.413285	-3.444742	-0.301542
2	6	0	-3.694830	-2.973412	0.067232
3	6	0	-3.886070	-1.566820	0.271362
4	6	0	-2.797195	-0.653633	0.048006
5	6	0	-1.527940	-1.163502	-0.240984
6	6	0	-1.359335	-2.574838	-0.434831
7	6	0	-3.009934	0.820561	0.154908
8	6	0	-3.957106	1.508179	-0.682202
9	6	0	-4.228740	2.899287	-0.454783
10	6	0	-3.531465	3.579558	0.579759
11	6	0	-2.574287	2.936031	1.320022
12	6	0	-2.287401	1.563232	1.089131
13	6	0	-5.166258	-1.138856	0.726795
14	6	0	-6.190719	-2.036311	0.930401
15	6	0	-6.003478	-3.418074	0.690011
16	6	0	-4.775252	-3.872944	0.271771
17	6	0	-4.629007	0.873776	-1.765517
18	6	0	-5.528953	1.559699	-2.551648
19	6	0	-5.816756	2.921244	-2.300888
20	6	0	-5.172822	3.572604	-1.273695
21	1	0	-2.251984	-4.510129	-0.442541
22	1	0	-4.605660	-4.933917	0.102552
23	1	0	-6.822600	-4.113853	0.849186
24	1	0	-7.153302	-1.678448	1.285925
25	1	0	-5.327392	-0.086772	0.928342
26	1	0	-4.415306	-0.167369	-1.979187
27	1	0	-6.020074	1.048673	-3.375754
28	1	0	-6.533784	3.449357	-2.923535
29	1	0	-5.370279	4.624196	-1.077079
30	1	0	-3.754632	4.628334	0.762373
31	1	0	-2.008647	3.448008	2.092064
32	7	0	-0.077038	-3.084805	-0.806114

33	8	0	-0.446131	-0.375950	-0.378252
34	8	0	-1.287121	0.992732	1.808686
35	22	0	0.332191	0.741051	0.928092
36	8	0	0.777045	2.419485	0.523401
37	8	0	1.251942	-0.126317	2.191845
38	6	0	0.201539	-3.884131	-1.904865
39	6	0	1.550474	-4.112338	-1.871968
40	7	0	2.107862	-3.477980	-0.779706
41	6	0	1.104709	-2.875606	-0.165244
42	1	0	-0.574383	-4.181050	-2.593050
43	1	0	2.152631	-4.688747	-2.560147
44	1	0	1.178888	-2.275043	0.728496
45	6	0	2.443634	-0.300213	2.948421
46	6	0	2.989486	1.054944	3.397732
47	6	0	2.141807	-1.232233	4.122184
48	1	0	3.177912	-0.783531	2.286016
49	6	0	1.351876	3.390047	-0.337403
50	6	0	0.381949	3.701071	-1.477849
51	6	0	1.711643	4.626445	0.486752
52	1	0	2.272352	2.956099	-0.755236
53	1	0	2.265253	1.560144	4.047201
54	1	0	3.924839	0.927333	3.954619
55	1	0	3.186465	1.697772	2.533766
56	1	0	3.053555	-1.433380	4.696252
57	1	0	1.401352	-0.777061	4.789116
58	1	0	1.741292	-2.186318	3.764845
59	1	0	0.819106	4.433307	-2.167013
60	1	0	0.148103	2.791885	-2.041561
61	1	0	-0.554602	4.107736	-1.081405
62	1	0	0.808751	5.072394	0.918569
63	1	0	2.389609	4.360502	1.304266
64	1	0	2.204126	5.377509	-0.141864
65	1	0	3.724196	-2.859492	-0.403519
66	7	0	2.302792	0.229339	-0.376183
67	6	0	3.243318	-0.341144	-0.739047
68	6	0	7.048144	1.388043	-2.125089
69	6	0	5.893021	0.607298	-2.127243
70	6	0	5.685760	-0.346069	-1.124405
71	6	0	6.641693	-0.517933	-0.121253
72	6	0	7.799630	0.262526	-0.124188
73	6	0	8.004505	1.216870	-1.121422
74	6	0	4.414060	-1.189607	-1.128964
75	8	0	4.512834	-2.263040	-0.240216
76	1	0	4.209579	-1.523547	-2.159652
77	1	0	7.203783	2.124041	-2.909098
78	1	0	5.152824	0.738805	-2.914273
79	1	0	6.476891	-1.269543	0.642254
80	1	0	8.543536	0.121762	0.655397
81	1	0	8.907043	1.821998	-1.120766

E_{ZPE}: B3LYP/6-31G* = -2820.41541 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2821.08960 (a.u.)

Ts14 and ts16 with different aldehydes

TS14 $_{4\text{-ClC6H4}}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.815434	-0.302213	0.533932
2	6	0	2.859458	-0.703148	0.191927
3	6	0	-3.151579	-3.127953	-0.940553
4	6	0	-4.408524	-2.505324	-0.769994
5	6	0	-4.454184	-1.111389	-0.430702
6	6	0	-3.237423	-0.356054	-0.316287
7	6	0	-2.008586	-1.019823	-0.401430
8	6	0	-1.995551	-2.415653	-0.732904
9	6	0	-3.260972	1.113622	-0.060238

10	6	0	-3.904682	2.031733	-0.960994
11	6	0	-3.990690	3.422105	-0.613185
12	6	0	-3.406666	3.867080	0.603453
13	6	0	-2.729424	2.996903	1.417036
14	6	0	-2.627959	1.619470	1.076376
15	6	0	-5.736913	-0.536689	-0.196508
16	6	0	-6.888462	-1.279862	-0.325145
17	6	0	-6.835203	-2.643582	-0.701580
18	6	0	-5.615998	-3.240913	-0.914883
19	6	0	-4.442093	1.633648	-2.218272
20	6	0	-5.049740	2.540524	-3.059211
21	6	0	-5.161391	3.902032	-2.694618
22	6	0	-4.636053	4.327358	-1.495632
23	1	0	-3.110289	-4.173748	-1.233118
24	1	0	-5.554500	-4.292413	-1.186708
25	1	0	-7.753315	-3.214584	-0.807730
26	1	0	-7.850874	-0.814067	-0.131088
27	1	0	-5.797516	0.503322	0.099868
28	1	0	-4.357932	0.596309	-2.522290
29	1	0	-5.443257	2.205297	-4.015471
30	1	0	-5.648241	4.606640	-3.363346
31	1	0	-4.697242	5.374548	-1.207042
32	1	0	-3.487255	4.918634	0.869925
33	1	0	-2.249482	3.326393	2.332995
34	7	0	-0.732809	-3.090830	-0.825803
35	8	0	-0.831551	-0.410024	-0.224154
36	8	0	-1.907334	0.814525	1.885509
37	22	0	-0.148616	0.354307	1.417756
38	8	0	0.586528	1.977169	1.456982
39	8	0	0.208271	-0.741109	2.778158
40	6	0	-0.468420	-4.389648	-0.402309
41	6	0	0.854385	-4.623627	-0.636820
42	7	0	1.381470	-3.480772	-1.198670
43	6	0	0.416195	-2.572496	-1.297658
44	1	0	-1.234057	-5.002467	0.043756
45	1	0	1.454815	-5.498717	-0.444525
46	1	0	0.535030	-1.563781	-1.650623
47	6	0	1.158714	-1.131236	3.757224
48	6	0	1.169753	-0.115583	4.900430
49	6	0	0.819787	-2.545585	4.228617
50	1	0	2.146339	-1.140643	3.272494
51	6	0	1.608067	2.881516	1.063969
52	6	0	1.168811	3.618954	-0.201076
53	6	0	1.903175	3.827586	2.228162
54	1	0	2.506868	2.289059	0.842624
55	1	0	0.188413	-0.078100	5.386431
56	1	0	1.921062	-0.387027	5.651293
57	1	0	1.404035	0.884685	4.521588
58	1	0	1.558715	-2.897628	4.958013
59	1	0	-0.169783	-2.563357	4.698676
60	1	0	0.811141	-3.238983	3.381070
61	1	0	1.947166	4.317109	-0.530713
62	1	0	0.978230	2.907131	-1.010908
63	1	0	0.247432	4.181466	-0.014681
64	1	0	1.016068	4.421766	2.474734
65	1	0	2.197549	3.262059	3.118571
66	1	0	2.719031	4.512102	1.968325
67	1	0	2.422487	-3.202785	-1.397801
68	6	0	7.499937	0.791960	-1.406727
69	6	0	7.257663	0.361688	-0.101402
70	6	0	6.185028	-0.494756	0.136025
71	6	0	5.360861	-0.916412	-0.911674
72	6	0	5.625684	-0.478958	-2.211878
73	6	0	6.694003	0.378996	-2.467477
74	6	0	4.230659	-1.877947	-0.663534
75	8	0	3.677432	-2.442897	-1.658487
76	1	0	4.346791	-2.438459	0.279919
77	17	0	8.854014	1.871732	-1.719637
78	1	0	7.899817	0.690944	0.708552
79	1	0	5.983894	-0.832771	1.150444

80	1	0	4.990179	-0.829599	-3.018411
81	1	0	6.904569	0.721642	-3.475083

E_{ZPE}: B3LYP/6-31G* = -3279.99381 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -3280.70147 (a.u.)

TS16 $_{4\text{-ClC6H4}}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.013883	-3.383493	-0.120866
2	6	0	-4.264134	-2.852912	0.269528
3	6	0	-4.407609	-1.429423	0.386146
4	6	0	-3.306187	-0.561144	0.071550
5	6	0	-2.055780	-1.118286	-0.221019
6	6	0	-1.950584	-2.544196	-0.344132
7	6	0	-3.466748	0.921609	0.093751
8	6	0	-4.414469	1.597097	-0.750806
9	6	0	-4.608088	3.012348	-0.607217
10	6	0	-3.834240	3.721802	0.350644
11	6	0	-2.881161	3.080691	1.098185
12	6	0	-2.670905	1.681360	0.952604
13	6	0	-5.659925	-0.935477	0.853865
14	6	0	-6.699982	-1.787069	1.150528
15	6	0	-6.559702	-3.187435	0.997596
16	6	0	-5.360586	-3.705419	0.570318
17	6	0	-5.162024	0.929414	-1.762329
18	6	0	-6.060471	1.608123	-2.556642
19	6	0	-6.270176	2.996159	-2.387456
20	6	0	-5.551374	3.678575	-1.432387
21	1	0	-2.888766	-4.459691	-0.208302
22	1	0	-5.226739	-4.779913	0.466537
23	1	0	-7.391668	-3.846072	1.230470
24	1	0	-7.639430	-1.378520	1.513041
25	1	0	-5.784050	0.132048	0.988903
26	1	0	-5.008468	-0.132935	-1.915728
27	1	0	-6.610571	1.070515	-3.324805
28	1	0	-6.985913	3.519016	-3.015973
29	1	0	-5.687713	4.749750	-1.299954
30	1	0	-3.996437	4.791013	0.467762
31	1	0	-2.259972	3.613419	1.811043
32	7	0	-0.701939	-3.104515	-0.778473
33	8	0	-0.953150	-0.391940	-0.432246
34	8	0	-1.683515	1.104005	1.670255
35	22	0	-0.043583	0.739187	0.832109
36	8	0	0.470173	2.415776	0.497057
37	8	0	0.748624	-0.157214	2.167670
38	6	0	-0.538252	-3.987760	-1.839577
39	6	0	0.801751	-4.198717	-1.976556
40	7	0	1.437690	-3.454144	-1.005696
41	6	0	0.517282	-2.801278	-0.301437
42	1	0	-1.384489	-4.351967	-2.398881
43	1	0	1.347504	-4.806434	-2.680946
44	1	0	0.715613	-2.128638	0.516440
45	6	0	1.940713	-0.207037	2.946920
46	6	0	2.129291	1.109293	3.701147
47	6	0	1.859235	-1.412484	3.883102
48	1	0	2.778612	-0.345787	2.248060
49	6	0	1.177589	3.324608	-0.335070
50	6	0	0.354368	3.616845	-1.589906
51	6	0	1.488992	4.584954	0.472591
52	1	0	2.119463	2.839108	-0.626615
53	1	0	1.297333	1.274472	4.395194
54	1	0	3.063374	1.093531	4.274457
55	1	0	2.167058	1.950425	3.001396
56	1	0	2.779920	-1.504765	4.470639
57	1	0	1.014675	-1.303981	4.572602
58	1	0	1.722476	-2.338378	3.314262

59	1	0	0.888891	4.311908	-2.248203
60	1	0	0.163205	2.693426	-2.146575
61	1	0	-0.609516	4.061824	-1.319190
62	1	0	0.561993	5.078862	0.784676
63	1	0	2.065761	4.336166	1.369455
64	1	0	2.073536	5.290738	-0.129082
65	1	0	2.506790	-3.234863	-0.899056
66	7	0	1.754215	0.156046	-0.384907
67	6	0	2.749325	-0.239890	-0.855000
68	6	0	7.090056	0.756030	-1.692605
69	6	0	5.884488	0.101900	-1.935057
70	6	0	5.411335	-0.875502	-1.054171
71	6	0	6.164615	-1.203178	0.076201
72	6	0	7.372661	-0.557788	0.334749
73	6	0	7.822947	0.418360	-0.553752
74	6	0	4.131695	-1.612771	-1.336387
75	8	0	3.856030	-2.648334	-0.654032
76	1	0	3.832559	-1.567393	-2.396703
77	1	0	7.460232	1.515330	-2.373192
78	1	0	5.300765	0.362804	-2.815219
79	1	0	5.795997	-1.977204	0.741322
80	1	0	7.962247	-0.808836	1.210218
81	17	0	9.348184	1.237141	-0.237228

E_{ZPE}: B3LYP/6-31G* = -3279.99364 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -3280.69916 (a.u.)

TS14 $_{4\text{-}CH3C6H4}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.035559	-0.130201	0.425311
2	6	0	3.082032	-0.508055	0.064781
3	6	0	-2.831998	-3.249140	-0.742298
4	6	0	-4.111645	-2.678853	-0.556763
5	6	0	-4.214121	-1.273548	-0.283223
6	6	0	-3.032293	-0.457440	-0.247416
7	6	0	-1.776200	-1.066136	-0.344552
8	6	0	-1.705480	-2.474355	-0.610747
9	6	0	-3.118014	1.019854	-0.056705
10	6	0	-3.833584	1.864721	-0.974309
11	6	0	-3.976588	3.263880	-0.685542
12	6	0	-3.377596	3.790653	0.490469
13	6	0	-2.633259	2.991279	1.317896
14	6	0	-2.473960	1.606194	1.034438
15	6	0	-5.515166	-0.749227	-0.032334
16	6	0	-6.632648	-1.551476	-0.083869
17	6	0	-6.525124	-2.928382	-0.394878
18	6	0	-5.285703	-3.477048	-0.622294
19	6	0	-4.390931	1.384212	-2.193636
20	6	0	-5.068989	2.221651	-3.052545
21	6	0	-5.235230	3.591691	-2.745068
22	6	0	-4.693155	4.096086	-1.584742
23	1	0	-2.749135	-4.305072	-0.985401
24	1	0	-5.181644	-4.536772	-0.844784
25	1	0	-7.417078	-3.546983	-0.440166
26	1	0	-7.609755	-1.122400	0.121253
27	1	0	-5.617336	0.300361	0.214882
28	1	0	-4.265870	0.339102	-2.453908
29	1	0	-5.476259	1.824576	-3.978926
30	1	0	-5.777333	4.240910	-3.427270
31	1	0	-4.796374	5.151313	-1.340771
32	1	0	-3.501787	4.848015	0.713878
33	1	0	-2.141995	3.384347	2.202251
34	7	0	-0.415513	-3.092966	-0.715387
35	8	0	-0.625655	-0.393122	-0.236410
36	8	0	-1.687777	0.875476	1.852025
37	22	0	0.076053	0.476436	1.342589

38	8	0	0.728268	2.134195	1.276001
39	8	0	0.527982	-0.532576	2.741324
40	6	0	-0.072437	-4.352834	-0.234874
41	6	0	1.252104	-4.533788	-0.505366
42	7	0	1.704066	-3.399407	-1.144508
43	6	0	0.691140	-2.547174	-1.254981
44	1	0	-0.791355	-4.976976	0.269613
45	1	0	1.901037	-5.367942	-0.289515
46	1	0	0.746908	-1.554426	-1.664437
47	6	0	1.529564	-0.839636	3.698370
48	6	0	1.574120	0.252021	4.768192
49	6	0	1.240442	-2.224005	4.279357
50	1	0	2.493633	-0.866172	3.168914
51	6	0	1.685903	3.065327	0.795321
52	6	0	1.118620	3.784370	-0.428993
53	6	0	2.052060	4.025306	1.927659
54	1	0	2.579628	2.498445	0.499302
55	1	0	0.617045	0.304945	5.299179
56	1	0	2.366933	0.047485	5.497307
57	1	0	1.767182	1.227684	4.310211
58	1	0	2.018796	-2.513012	4.995427
59	1	0	0.273803	-2.226461	4.795198
60	1	0	1.207210	-2.973543	3.481737
61	1	0	1.847006	4.500399	-0.827645
62	1	0	0.876267	3.063750	-1.216857
63	1	0	0.202627	4.324256	-0.165343
64	1	0	1.172056	4.593715	2.249172
65	1	0	2.439401	3.472627	2.790115
66	1	0	2.821586	4.732851	1.597435
67	1	0	2.737105	-3.068343	-1.395094
68	6	0	7.692136	1.062125	-1.694726
69	6	0	7.459163	0.648963	-0.374795
70	6	0	6.415609	-0.221602	-0.071241
71	6	0	5.572910	-0.697322	-1.080500
72	6	0	5.796585	-0.294028	-2.399283
73	6	0	6.842074	0.577304	-2.698201
74	6	0	4.471543	-1.668730	-0.767518
75	8	0	3.910852	-2.293536	-1.726736
76	1	0	4.619866	-2.187871	0.194780
77	6	0	8.845150	1.979740	-2.028089
78	1	0	8.104509	1.013440	0.421572
79	1	0	6.246409	-0.526997	0.959799
80	1	0	5.146718	-0.678446	-3.178838
81	1	0	7.004269	0.886132	-3.728762
82	1	0	8.640901	2.569010	-2.928275
83	1	0	9.055646	2.675118	-1.208254
84	1	0	9.765880	1.410284	-2.214247

E_{ZPE}: B3LYP/6-31G* = -2859.67896 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2860.3974 (a.u.)

TS16 4-CH3C6H4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.703554	-3.423258	-0.120156
2	6	0	-3.967735	-2.927877	0.272203
3	6	0	-4.149946	-1.509177	0.392104
4	6	0	-3.073054	-0.610522	0.077994
5	6	0	-1.807925	-1.132966	-0.215578
6	6	0	-1.663265	-2.555293	-0.341915
7	6	0	-3.275093	0.867220	0.099722
8	6	0	-4.242126	1.514983	-0.744833
9	6	0	-4.475231	2.924509	-0.602849
10	6	0	-3.720334	3.656602	0.353142
11	6	0	-2.748812	3.043378	1.100147
12	6	0	-2.499643	1.650117	0.956610
13	6	0	-5.414798	-1.050573	0.862044

14	6	0	-6.430984	-1.930788	1.158011
15	6	0	-6.252728	-3.326428	1.001746
16	6	0	-5.040291	-3.810493	0.572058
17	6	0	-4.971283	0.825733	-1.755411
18	6	0	-5.888698	1.478199	-2.550039
19	6	0	-6.137246	2.859962	-2.382144
20	6	0	-5.437282	3.563124	-1.428104
21	1	0	-2.549081	-4.495405	-0.210346
22	1	0	-4.877194	-4.880716	0.465799
23	1	0	-7.066145	-4.008099	1.233991
24	1	0	-7.380817	-1.548767	1.522469
25	1	0	-5.567627	0.012937	0.999477
26	1	0	-4.787823	-0.231971	-1.907997
27	1	0	-6.423647	0.924569	-3.317548
28	1	0	-6.867651	3.361984	-3.010814
29	1	0	-5.603328	4.630246	-1.296641
30	1	0	-3.912049	4.721101	0.468893
31	1	0	-2.141539	3.594255	1.811198
32	7	0	-0.399972	-3.080229	-0.777005
33	8	0	-0.726186	-0.375900	-0.425845
34	8	0	-1.496133	1.102407	1.674187
35	22	0	0.153897	0.779950	0.835670
36	8	0	0.616200	2.470988	0.490970
37	8	0	0.968402	-0.086768	2.177248
38	6	0	-0.210225	-3.952557	-1.842662
39	6	0	1.135775	-4.126122	-1.976371
40	7	0	1.751072	-3.371278	-1.000257
41	6	0	0.811098	-2.748486	-0.295954
42	1	0	-1.045216	-4.335811	-2.406227
43	1	0	1.698524	-4.715366	-2.683236
44	1	0	0.988641	-2.074799	0.525741
45	6	0	2.165306	-0.105888	2.950140
46	6	0	2.328199	1.218539	3.696344
47	6	0	2.115653	-1.307710	3.893216
48	1	0	3.002459	-0.229880	2.247791
49	6	0	1.294333	3.383605	-0.361062
50	6	0	0.480350	3.591776	-1.638606
51	6	0	1.530761	4.684337	0.406781
52	1	0	2.263225	2.934510	-0.620574
53	1	0	1.496438	1.368772	4.394076
54	1	0	3.265513	1.227016	4.264601
55	1	0	2.343193	2.056491	2.991885
56	1	0	3.041563	-1.376647	4.475782
57	1	0	1.272762	-1.214320	4.587031
58	1	0	1.996218	-2.239181	3.329715
59	1	0	0.992075	4.288022	-2.313662
60	1	0	0.343618	2.640558	-2.163548
61	1	0	-0.508324	3.998678	-1.399084
62	1	0	0.575789	5.145020	0.683444
63	1	0	2.099633	4.493528	1.322699
64	1	0	2.094618	5.395401	-0.208354
65	1	0	2.827685	-3.111505	-0.887476
66	7	0	1.964456	0.243202	-0.375534
67	6	0	2.964381	-0.136647	-0.848782
68	6	0	7.292391	0.932163	-1.731273
69	6	0	6.099101	0.255127	-1.967169
70	6	0	5.641870	-0.710686	-1.064841
71	6	0	6.402669	-0.992989	0.072350
72	6	0	7.596317	-0.311973	0.304401
73	6	0	8.063209	0.659412	-0.591209
74	6	0	4.375228	-1.470767	-1.329853
75	8	0	4.122115	-2.510460	-0.638054
76	1	0	4.067874	-1.442630	-2.388285
77	1	0	7.633088	1.683844	-2.440110
78	1	0	5.509245	0.486409	-2.852158
79	1	0	6.049065	-1.754020	0.760649
80	1	0	8.178436	-0.538911	1.195121
81	6	0	9.372734	1.374289	-0.352988
82	1	0	9.638356	1.380018	0.709261
83	1	0	10.196270	0.887112	-0.892449

84	1	0	9.331609	2.413418	-0.697615

E_{ZPE}: B3LYP/6-31G* = -2859.67871 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2860.36733 (a.u.)

TS14 $_{i\text{Pr}}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.574143	-0.477677	-0.146551
2	6	0	-3.624242	-0.263644	-0.618620
3	6	0	1.780267	3.521431	-0.118238
4	6	0	3.107522	3.127924	0.165309
5	6	0	3.413995	1.728545	0.254959
6	6	0	2.393705	0.749114	0.005005
7	6	0	1.072981	1.168498	-0.189766
8	6	0	0.795082	2.574266	-0.258124
9	6	0	2.704677	-0.709731	0.005755
10	6	0	3.660235	-1.285559	-0.901158
11	6	0	4.000371	-2.675447	-0.783101
12	6	0	3.358348	-3.460761	0.212311
13	6	0	2.393404	-2.919147	1.020627
14	6	0	2.038822	-1.546343	0.903362
15	6	0	4.744456	1.372426	0.621104
16	6	0	5.706507	2.331343	0.844030
17	6	0	5.405288	3.708186	0.709931
18	6	0	4.127874	4.093647	0.380615
19	6	0	4.273265	-0.544479	-1.951362
20	6	0	5.181582	-1.128872	-2.807089
21	6	0	5.537097	-2.489889	-2.663929
22	6	0	4.950814	-3.242527	-1.671692
23	1	0	1.547589	4.578266	-0.218148
24	1	0	3.872695	5.147495	0.292889
25	1	0	6.177678	4.452942	0.880390
26	1	0	6.709532	2.027127	1.130952
27	1	0	4.992255	0.324282	0.736256
28	1	0	4.005982	0.497858	-2.085043
29	1	0	5.625784	-0.537324	-3.603632
30	1	0	6.259306	-2.938055	-3.340927
31	1	0	5.199522	-4.295607	-1.558294
32	1	0	3.630601	-4.509561	0.308825
33	1	0	1.869196	-3.513233	1.762256
34	7	0	-0.561612	3.001014	-0.449588
35	8	0	0.051374	0.322073	-0.351243
36	8	0	1.045732	-1.074726	1.685175
37	22	0	-0.685597	-0.882881	0.975546
38	8	0	-1.015151	-2.599472	0.617738
39	8	0	-1.479510	-0.170428	2.403450
40	6	0	-1.161017	4.102772	0.152629
41	6	0	-2.458282	4.129392	-0.266733
42	7	0	-2.638661	3.057772	-1.114286
43	6	0	-1.492896	2.390267	-1.205735
44	1	0	-0.617404	4.735265	0.834599
45	1	0	-3.257249	4.812820	-0.026250
46	1	0	-1.338310	1.477931	-1.753554
47	6	0	-2.647389	-0.151184	3.209748
48	6	0	-2.650738	-1.362882	4.142427
49	6	0	-2.694580	1.176258	3.966955
50	1	0	-3.514148	-0.211763	2.535148
51	6	0	-1.749754	-3.600896	-0.066628
52	6	0	-0.997063	-4.001795	-1.335894
53	6	0	-1.977164	-4.779276	0.881379
54	1	0	-2.721170	-3.168191	-0.345051
55	1	0	-1.784077	-1.331242	4.812202
56	1	0	-3.562266	-1.379901	4.751353
57	1	0	-2.603530	-2.290735	3.562907
58	1	0	-3.607865	1.245253	4.569641
59	1	0	-1.829524	1.266146	4.633436

60	1	0	-2.677688	2.016653	3.264990
61	1	0	-1.549885	-4.772943	-1.885465
62	1	0	-0.867154	-3.135742	-1.992979
63	1	0	-0.005316	-4.393126	-1.083872
64	1	0	-1.019926	-5.220088	1.181518
65	1	0	-2.502594	-4.450671	1.784312
66	1	0	-2.579620	-5.554885	0.394099
67	1	0	-3.551638	2.646583	-1.555574
68	6	0	-6.010997	-0.170515	-2.125969
69	6	0	-5.123889	0.888180	-1.472688
70	8	0	-4.548311	1.741220	-2.205434
71	1	0	-5.452698	1.184112	-0.458731
72	6	0	-6.559951	-1.194437	-1.129947
73	6	0	-7.152232	0.575220	-2.846942
74	1	0	-5.401409	-0.676317	-2.883866
75	1	0	-7.211257	-1.914076	-1.638296
76	1	0	-5.753998	-1.749164	-0.640347
77	1	0	-7.158256	-0.704806	-0.350162
78	1	0	-7.799292	-0.135716	-3.373136
79	1	0	-7.777707	1.126930	-2.132563
80	1	0	-6.751739	1.289261	-3.571601

E_{ZPE}: B3LYP/6-31G* = -2707.27518 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2707.95415 (a.u.)

TS16 $_{iPr}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.671550	3.553556	0.038209
2	6	0	2.987036	3.189220	0.403449
3	6	0	3.331370	1.796843	0.455705
4	6	0	2.361866	0.795932	0.103697
5	6	0	1.041684	1.181548	-0.159312
6	6	0	0.735818	2.582524	-0.220493
7	6	0	2.733436	-0.647681	0.057427
8	6	0	3.760496	-1.141177	-0.819738
9	6	0	4.156643	-2.518907	-0.741206
10	6	0	3.501087	-3.374123	0.185438
11	6	0	2.472419	-2.910914	0.963555
12	6	0	2.062727	-1.550899	0.883269
13	6	0	4.644038	1.464858	0.900548
14	6	0	5.554741	2.441076	1.236011
15	6	0	5.216688	3.812890	1.146079
16	6	0	3.953762	4.174290	0.742138
17	6	0	4.394533	-0.328756	-1.802403
18	6	0	5.372127	-0.835421	-2.630924
19	6	0	5.780338	-2.185062	-2.525992
20	6	0	5.177199	-3.005108	-1.599526
21	1	0	1.395163	4.604088	-0.000863
22	1	0	3.668549	5.222562	0.686696
23	1	0	5.948538	4.571709	1.408481
24	1	0	6.544699	2.154084	1.580347
25	1	0	4.918108	0.420576	0.987727
26	1	0	4.088779	0.706395	-1.905854
27	1	0	5.831060	-0.190756	-3.376258
28	1	0	6.556646	-2.571665	-3.180680
29	1	0	5.467120	-4.050458	-1.516569
30	1	0	3.815788	-4.413242	0.252806
31	1	0	1.939672	-3.558834	1.652117
32	7	0	-0.581613	2.980553	-0.629581
33	8	0	0.050607	0.317511	-0.398235
34	8	0	1.011340	-1.152564	1.628998
35	22	0	-0.677884	-0.989880	0.818688
36	8	0	-0.938452	-2.713812	0.422362
37	8	0	-1.562530	-0.272040	2.203003
38	6	0	-0.871432	3.897073	-1.634060
39	6	0	-2.228186	3.926894	-1.764192

40	7	0	-2.749758	3.040928	-0.845371
41	6	0	-1.744607	2.479736	-0.178912
42	1	0	-0.086458	4.409452	-2.165806
43	1	0	-2.856128	4.494693	-2.432460
44	1	0	-1.844692	1.736240	0.593995
45	6	0	-2.731287	-0.425254	3.002277
46	6	0	-2.680417	-1.758260	3.749427
47	6	0	-2.834572	0.772231	3.946668
48	1	0	-3.593990	-0.424795	2.320056
49	6	0	-1.530494	-3.672017	-0.442439
50	6	0	-0.696485	-3.790669	-1.718505
51	6	0	-1.653435	-4.998176	0.308583
52	1	0	-2.534537	-3.307233	-0.700889
53	1	0	-1.822299	-1.781328	4.430674
54	1	0	-3.594834	-1.906685	4.335541
55	1	0	-2.582107	-2.589524	3.043641
56	1	0	-3.744982	0.706006	4.553501
57	1	0	-1.968973	0.803962	4.617608
58	1	0	-2.868143	1.710150	3.382211
59	1	0	-1.139569	-4.522871	-2.403938
60	1	0	-0.645570	-2.824593	-2.231441
61	1	0	0.324586	-4.107260	-1.478625
62	1	0	-0.662533	-5.377303	0.582686
63	1	0	-2.238508	-4.869096	1.225170
64	1	0	-2.151840	-5.748358	-0.316551
65	1	0	-3.778400	2.673494	-0.752134
66	6	0	-7.616649	0.859518	-1.486283
67	6	0	-6.374041	-0.009342	-1.202251
68	6	0	-5.152641	0.897821	-1.329811
69	8	0	-5.035147	1.889001	-0.557213
70	1	0	-4.742830	0.962177	-2.354601
71	1	0	-8.530527	0.266572	-1.367497
72	6	0	-6.317709	-1.222296	-2.133261
73	1	0	-7.658837	1.711606	-0.802328
74	1	0	-7.603636	1.245648	-2.514156
75	1	0	-6.421556	-0.340625	-0.158309
76	1	0	-5.452269	-1.853670	-1.912315
77	1	0	-7.223760	-1.829460	-2.029183
78	1	0	-6.250652	-0.909326	-3.183528
79	7	0	-2.540847	-0.636857	-0.353847
80	6	0	-3.592377	-0.398965	-0.811529

E_{ZPE}: B3LYP/6-31G* = -2707.27499 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -2707.92187 (a.u.)

Transition states under the catalyzes of 3 and 4

Ts_{17}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.293713	3.309025	-0.059058
2	6	0	-4.015971	2.515168	-0.979425
3	6	0	-3.601218	1.160781	-1.199748
4	6	0	-2.606484	0.570690	-0.340203
5	6	0	-1.935574	1.372196	0.592305
6	6	0	-2.223054	2.788157	0.624981
7	6	0	-4.203477	0.467902	-2.289137
8	6	0	-5.194094	1.048267	-3.050356
9	6	0	-5.650609	2.358154	-2.772757
10	6	0	-5.061239	3.077741	-1.760382
11	1	0	-3.549323	4.360433	0.033173
12	1	0	-5.368321	4.101275	-1.556682
13	1	0	-6.442950	2.797837	-3.371999
14	1	0	-5.626669	0.492471	-3.877903
15	1	0	-3.867232	-0.533360	-2.526291

16	7	0	-1.259077	3.699583	1.184554
17	8	0	-1.072120	0.885444	1.474007
18	22	0	0.429838	-0.335728	1.620355
19	8	0	1.050825	0.541545	3.098296
20	8	0	-0.248086	-1.780953	2.358609
21	6	0	-0.993228	4.963793	0.634318
22	6	0	0.251328	5.321211	1.042726
23	7	0	0.756387	4.317672	1.854679
24	6	0	-0.188993	3.376222	1.937749
25	1	0	-1.687480	5.454437	-0.025469
26	1	0	0.826358	6.202243	0.801346
27	1	0	-0.051396	2.427223	2.423550
28	6	0	-1.305440	-2.681999	2.690809
29	6	0	-0.722371	-3.858144	3.471790
30	6	0	-2.399954	-1.941858	3.456511
31	1	0	-1.712864	-3.045854	1.741454
32	6	0	0.868817	0.360305	4.503305
33	6	0	2.156758	0.727268	5.241046
34	6	0	-0.319044	1.191953	4.995547
35	1	0	0.645979	-0.702850	4.678028
36	1	0	-0.292292	-3.518443	4.421013
37	1	0	-1.508083	-4.590360	3.690443
38	1	0	0.062535	-4.356219	2.894864
39	1	0	-3.248516	-2.610797	3.638489
40	1	0	-2.025237	-1.586026	4.423249
41	1	0	-2.754513	-1.083427	2.879576
42	1	0	2.023997	0.603120	6.322484
43	1	0	2.987960	0.091798	4.923386
44	1	0	2.426304	1.770900	5.043335
45	1	0	-0.111176	2.263729	4.892331
46	1	0	-1.223088	0.955962	4.426391
47	1	0	-0.512686	0.988015	6.055401
48	22	0	2.253682	-0.243565	-1.159003
49	8	0	1.632891	0.678899	-2.576792
50	8	0	2.158972	-0.888138	0.864972
51	8	0	2.369526	-1.962257	-1.752460
52	8	0	4.027929	0.100245	-1.340729
53	6	0	0.557011	1.497322	-3.001293
54	6	0	1.096673	2.872300	-3.401439
55	6	0	-0.186122	0.805145	-4.145640
56	6	0	4.776178	1.140787	-1.959507
57	6	0	5.818670	1.677972	-0.978000
58	6	0	5.415076	0.609970	-3.245100
59	6	0	3.334232	-1.504429	1.442439
60	6	0	2.940199	-2.602030	2.428253
61	6	0	4.255329	-0.453630	2.055395
62	6	0	3.196152	-2.658839	-2.669003
63	6	0	3.464698	-4.068047	-2.135662
64	6	0	2.544183	-2.676273	-4.053689
65	1	0	-0.132748	1.615677	-2.155017
66	1	0	1.625166	3.331044	-2.560154
67	1	0	1.794417	2.780836	-4.242288
68	1	0	0.276943	3.535484	-3.704196
69	1	0	-1.048347	1.403464	-4.463702
70	1	0	0.478094	0.667117	-5.007178
71	1	0	-0.547305	-0.177510	-3.826728
72	1	0	4.083145	1.951818	-2.221935
73	1	0	6.398415	2.486329	-1.440158
74	1	0	5.333842	2.071823	-0.080293
75	1	0	6.512364	0.882228	-0.681815
76	1	0	4.646537	0.230048	-3.925583
77	1	0	6.114399	-0.203822	-3.019325
78	1	0	5.967588	1.406714	-3.758142
79	1	0	3.851676	-1.978159	0.599744
80	1	0	3.838771	-3.128054	2.771895
81	1	0	2.430009	-2.190065	3.305065
82	1	0	2.274337	-3.328086	1.952860
83	1	0	5.147288	-0.936817	2.473279
84	1	0	4.571685	0.260171	1.293532
85	1	0	3.744285	0.092651	2.851772

86	1	0	4.152692	-2.118084	-2.730736
87	1	0	4.142305	-4.613489	-2.803678
88	1	0	3.923686	-4.021770	-1.142414
89	1	0	2.530504	-4.636907	-2.055756
90	1	0	1.595387	-3.225262	-4.024465
91	1	0	2.336867	-1.655951	-4.390386
92	1	0	3.200683	-3.161164	-4.786593
93	6	0	-2.244897	-0.867408	-0.473359
94	6	0	-3.259811	-1.894516	-0.442251
95	6	0	-2.925750	-3.243695	-0.795141
96	6	0	-1.574988	-3.550382	-1.110749
97	6	0	-0.593856	-2.599624	-1.008408
98	6	0	-0.906766	-1.252170	-0.657675
99	6	0	-4.598461	-1.640370	-0.026836
100	6	0	-5.547506	-2.639975	-0.002700
101	6	0	-5.220782	-3.956423	-0.400459
102	6	0	-3.930544	-4.246070	-0.783418
103	1	0	-4.870520	-0.640239	0.290820
104	1	0	-6.557058	-2.412308	0.329712
105	1	0	-5.979782	-4.733900	-0.388169
106	1	0	-3.653082	-5.258353	-1.069544
107	1	0	-1.320376	-4.568225	-1.398968
108	1	0	0.446682	-2.831195	-1.202230
109	8	0	0.114193	-0.372959	-0.466609
110	1	0	1.790462	3.777243	1.559366
111	6	0	2.429514	2.706595	0.727398
112	7	0	2.244684	1.765063	0.057635

E_{ZPE}: B3LYP/6-31G* = -4099.215553 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -4100.07706 (a.u.)

Ts_{18}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.377545	1.004572	-3.136554
2	6	0	-4.037171	-0.171134	-2.704243
3	6	0	-3.610390	-0.792800	-1.482263
4	6	0	-2.641428	-0.144542	-0.629343
5	6	0	-2.026780	1.032494	-1.071078
6	6	0	-2.389397	1.550521	-2.364345
7	6	0	-4.160790	-2.074597	-1.187885
8	6	0	-5.103651	-2.659338	-2.004460
9	6	0	-5.562061	-2.006388	-3.172196
10	6	0	-5.025734	-0.788200	-3.516095
11	1	0	-3.598651	1.423754	-4.114531
12	1	0	-5.335277	-0.283422	-4.428517
13	1	0	-6.314080	-2.475430	-3.800368
14	1	0	-5.495550	-3.640157	-1.748696
15	1	0	-3.821591	-2.602448	-0.306147
16	7	0	-1.457384	2.482993	-2.948306
17	8	0	-1.122267	1.716255	-0.379374
18	22	0	0.419349	1.470471	0.744554
19	8	0	1.007637	3.174963	0.509716
20	8	0	-0.147181	1.555752	2.406300
21	6	0	-1.257229	3.842927	-2.760873
22	6	0	0.024615	4.106849	-3.161352
23	7	0	0.603903	2.920915	-3.581526
24	6	0	-0.315597	1.979122	-3.439291
25	1	0	-2.029621	4.478241	-2.358144
26	1	0	0.563711	5.041337	-3.178296
27	1	0	-0.144123	0.922987	-3.574591
28	6	0	-1.080591	1.517904	3.484318
29	6	0	-0.357320	1.889602	4.777722
30	6	0	-2.267527	2.430422	3.182316
31	1	0	-1.431590	0.482380	3.554107
32	6	0	0.816135	4.408465	1.191467
33	6	0	2.046787	5.299417	1.011779

34	6	0	-0.455686	5.099976	0.693809
35	1	0	0.693785	4.184690	2.263033
36	1	0	0.010346	2.921371	4.735136
37	1	0	-1.041051	1.801303	5.629855
38	1	0	0.494903	1.224977	4.948637
39	1	0	-3.016479	2.347914	3.978010
40	1	0	-1.945875	3.476200	3.116321
41	1	0	-2.737970	2.145585	2.237265
42	1	0	1.907260	6.252832	1.535298
43	1	0	2.944488	4.818627	1.410412
44	1	0	2.213789	5.509907	-0.050969
45	1	0	-0.352122	5.369151	-0.362638
46	1	0	-1.321956	4.440134	0.795397
47	1	0	-0.641754	6.016006	1.267704
48	22	0	2.228754	-1.200801	-0.263788
49	8	0	1.519602	-2.367274	-1.446480
50	8	0	2.206418	0.635352	0.782687
51	8	0	2.416301	-2.181404	1.258424
52	8	0	3.995818	-1.292037	-0.667368
53	6	0	0.405447	-2.565987	-2.295853
54	6	0	0.880324	-2.640683	-3.749596
55	6	0	-0.344061	-3.828440	-1.864263
56	6	0	4.864278	-1.483042	-1.773195
57	6	0	6.265403	-1.000348	-1.392740
58	6	0	4.856573	-2.952220	-2.201389
59	6	0	3.453043	1.074690	1.377870
60	6	0	3.216195	1.638944	2.777203
61	6	0	4.183638	2.042583	0.451411
62	6	0	3.346900	-3.141260	1.726164
63	6	0	3.566263	-2.943800	3.227995
64	6	0	2.856503	-4.551809	1.390447
65	1	0	-0.268750	-1.704701	-2.182609
66	1	0	1.442261	-1.739506	-4.014481
67	1	0	1.535261	-3.507774	-3.895580
68	1	0	0.026183	-2.738321	-4.431075
69	1	0	-1.238174	-3.977159	-2.481518
70	1	0	0.300814	-4.709326	-1.966077
71	1	0	-0.655490	-3.747643	-0.818468
72	1	0	4.490364	-0.868561	-2.604736
73	1	0	6.952880	-1.103293	-2.240975
74	1	0	6.244871	0.051632	-1.091210
75	1	0	6.658051	-1.590380	-0.556102
76	1	0	3.835719	-3.276343	-2.419205
77	1	0	5.259915	-3.586472	-1.402627
78	1	0	5.472074	-3.094492	-3.098045
79	1	0	4.059560	0.168360	1.478725
80	1	0	4.178996	1.869390	3.249060
81	1	0	2.623320	2.557910	2.744682
82	1	0	2.690837	0.911155	3.403066
83	1	0	5.138904	2.341865	0.900621
84	1	0	4.384298	1.563261	-0.508706
85	1	0	3.581463	2.935774	0.271566
86	1	0	4.298152	-2.959679	1.201647
87	1	0	4.322283	-3.643412	3.604651
88	1	0	3.905641	-1.923647	3.436300
89	1	0	2.635132	-3.115076	3.781428
90	1	0	1.914317	-4.765589	1.909177
91	1	0	2.682355	-4.647276	0.314457
92	1	0	3.595577	-5.303173	1.694815
93	6	0	-2.241331	-0.760314	0.665224
94	6	0	-3.235260	-1.094253	1.657036
95	6	0	-2.873816	-1.882746	2.798423
96	6	0	-1.516951	-2.274961	2.948802
97	6	0	-0.556466	-1.843942	2.071633
98	6	0	-0.894586	-1.048393	0.935563
99	6	0	-4.581890	-0.635818	1.578946
100	6	0	-5.511324	-0.963674	2.542789
101	6	0	-5.156100	-1.779011	3.641589
102	6	0	-3.858515	-2.223020	3.762153
103	1	0	-4.875165	-0.002473	0.749127

104	1	0	-6.527651	-0.587607	2.457311
105	1	0	-5.899726	-2.039777	4.389765
106	1	0	-3.560024	-2.833702	4.611649
107	1	0	-1.239484	-2.894309	3.799387
108	1	0	0.488472	-2.095898	2.205536
109	8	0	0.110236	-0.550100	0.165199
110	1	0	1.693354	2.394039	-3.395603
111	6	0	2.386241	1.284913	-2.748010
112	7	0	2.243073	0.399717	-1.997557

E_{ZPE}: B3LYP/6-31G* = -4099.221512 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -4100.08644 (a.u.)

Ts_{19}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.809707	-1.012172	-0.940899
2	7	0	-1.954795	-0.218880	-0.830981
3	6	0	2.221169	-3.612001	-2.039538
4	6	0	3.185243	-2.790053	-2.667551
5	6	0	3.452292	-1.492597	-2.115970
6	6	0	2.835084	-1.087604	-0.878141
7	6	0	1.871498	-1.913615	-0.287432
8	6	0	1.571049	-3.170518	-0.916471
9	6	0	4.315916	-0.637938	-2.861475
10	6	0	4.906078	-1.057043	-4.033286
11	6	0	4.675068	-2.357698	-4.539866
12	6	0	3.822336	-3.201497	-3.868741
13	1	0	1.947117	-4.561361	-2.492401
14	1	0	3.606286	-4.194607	-4.256416
15	1	0	5.154290	-2.676895	-5.461080
16	1	0	5.554304	-0.375843	-4.577990
17	1	0	4.502050	0.365437	-2.500228
18	7	0	0.467383	-3.932158	-0.406425
19	8	0	1.235315	-1.625599	0.842028
20	22	0	0.290322	-0.183613	1.708946
21	8	0	-0.789272	-1.321965	2.612363
22	8	0	1.384452	0.380103	2.967248
23	6	0	0.375621	-5.293049	-0.149075
24	6	0	-0.927589	-5.543173	0.183302
25	7	0	-1.607344	-4.343038	0.128517
26	6	0	-0.747307	-3.396916	-0.221806
27	1	0	1.236538	-5.939145	-0.212475
28	1	0	-1.411207	-6.466707	0.460167
29	1	0	-0.993865	-2.360211	-0.376391
30	6	0	2.653231	0.530426	3.601327
31	6	0	2.460929	1.296619	4.908748
32	6	0	3.303708	-0.837113	3.801190
33	1	0	3.272376	1.127779	2.921659
34	6	0	-0.733695	-2.106910	3.797019
35	6	0	-2.154992	-2.378411	4.293358
36	6	0	0.037732	-3.403599	3.539187
37	1	0	-0.191739	-1.524564	4.559348
38	1	0	1.837708	0.724256	5.605448
39	1	0	3.431194	1.481669	5.384072
40	1	0	1.977185	2.260518	4.723139
41	1	0	4.305924	-0.719292	4.228856
42	1	0	2.706189	-1.453875	4.482855
43	1	0	3.395700	-1.359275	2.844786
44	1	0	-2.133469	-3.007574	5.191351
45	1	0	-2.668777	-1.445123	4.542657
46	1	0	-2.734785	-2.891666	3.518009
47	1	0	-0.499145	-4.031502	2.819801
48	1	0	1.030361	-3.189533	3.134004
49	1	0	0.150524	-3.969866	4.471737
50	8	0	-1.065483	1.210791	1.438975
51	6	0	-2.075674	1.738407	2.333927

52	6	0	-1.502023	1.936972	3.735774
53	6	0	-3.324406	0.861971	2.318754
54	1	0	-2.332750	2.722734	1.927884
55	1	0	-2.243468	2.437028	4.370476
56	1	0	-1.245718	0.979215	4.199830
57	1	0	-0.600748	2.556534	3.702070
58	1	0	-4.098645	1.304710	2.957971
59	1	0	-3.716420	0.780359	1.303344
60	1	0	-3.096826	-0.142218	2.682559
61	6	0	3.180983	0.215488	-0.249019
62	6	0	4.546820	0.539474	0.082857
63	6	0	4.881428	1.864984	0.515791
64	6	0	3.838754	2.820229	0.652329
65	6	0	2.529516	2.470829	0.446793
66	6	0	2.179047	1.154210	0.025273
67	6	0	5.598145	-0.420519	0.039144
68	6	0	6.894297	-0.083566	0.365613
69	6	0	7.222596	1.236534	0.750194
70	6	0	6.228713	2.186095	0.825667
71	1	0	5.367666	-1.441244	-0.244620
72	1	0	7.670946	-0.843312	0.330406
73	1	0	8.249436	1.492932	0.996425
74	1	0	6.458366	3.202194	1.139459
75	1	0	4.091032	3.833300	0.958949
76	1	0	1.721074	3.178760	0.584299
77	8	0	0.862820	0.822235	-0.063684
78	1	0	-2.668775	-4.013155	0.262603
79	22	0	-0.972522	1.954949	-0.542479
80	8	0	-0.492931	1.861885	-2.280559
81	8	0	-0.342315	3.578828	-0.012297
82	8	0	-2.694550	2.499868	-0.675118
83	6	0	0.228547	1.077352	-3.212975
84	6	0	-0.731966	0.524910	-4.269165
85	6	0	1.344285	1.923838	-3.829872
86	6	0	-3.837270	2.445879	-1.514076
87	6	0	-5.062946	2.910185	-0.725280
88	6	0	-3.605723	3.288216	-2.770831
89	6	0	-0.760365	4.918602	-0.208044
90	6	0	-0.453637	5.729535	1.052971
91	6	0	-0.086779	5.500392	-1.453111
92	1	0	0.681904	0.235911	-2.671356
93	1	0	-1.526862	-0.056122	-3.792301
94	1	0	-1.192143	1.342613	-4.836639
95	1	0	-0.197189	-0.124015	-4.973509
96	1	0	1.945450	1.323852	-4.523535
97	1	0	0.920990	2.772979	-4.379659
98	1	0	2.004660	2.313474	-3.049037
99	1	0	-3.986496	1.397681	-1.810698
100	1	0	-5.966071	2.837651	-1.342706
101	1	0	-5.208886	2.291693	0.165178
102	1	0	-4.941135	3.952843	-0.408128
103	1	0	-2.690303	2.968722	-3.275232
104	1	0	-3.505788	4.348541	-2.508252
105	1	0	-4.448547	3.184252	-3.465106
106	1	0	-1.850134	4.904955	-0.365704
107	1	0	-0.815289	6.759843	0.950062
108	1	0	-0.936699	5.278917	1.926396
109	1	0	0.626929	5.762194	1.237395
110	1	0	1.001124	5.534085	-1.320315
111	1	0	-0.304576	4.878998	-2.326828
112	1	0	-0.442737	6.519648	-1.647592
113	6	0	-7.866499	-0.431391	-0.937820
114	6	0	-7.362649	-0.853378	0.294977
115	6	0	-6.138807	-1.519225	0.361662
116	6	0	-7.143067	-0.679398	-2.107582
117	6	0	-5.918911	-1.343384	-2.040225
118	6	0	-5.409356	-1.761564	-0.806149
119	6	0	-4.113002	-2.520751	-0.735895
120	8	0	-3.835833	-3.166546	0.329013
121	1	0	-8.821758	0.084583	-0.988448

122	1	0	-7.926830	-0.666659	1.205064
123	1	0	-5.737372	-1.868403	1.307275
124	1	0	-7.534566	-0.359403	-3.069616
125	1	0	-5.351432	-1.535679	-2.948842
126	1	0	-3.814394	-2.947643	-1.707595

E_{ZPE}: B3LYP/6-31G* = -4444.698899 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -4445.67330 (a.u.)

Ts_{20}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.837113	-0.979080	-0.576654
2	7	0	-1.941903	-0.230198	-0.682384
3	6	0	2.394794	-3.625166	-1.942757
4	6	0	3.401413	-2.802130	-2.496979
5	6	0	3.608189	-1.496915	-1.938678
6	6	0	2.886008	-1.084899	-0.761134
7	6	0	1.874341	-1.909423	-0.248352
8	6	0	1.644047	-3.175344	-0.887857
9	6	0	4.520473	-0.639602	-2.621240
10	6	0	5.209178	-1.063774	-3.735861
11	6	0	5.036477	-2.372914	-4.244247
12	6	0	4.140726	-3.219616	-3.636067
13	1	0	2.169393	-4.585176	-2.399918
14	1	0	3.968001	-4.219241	-4.028603
15	1	0	5.593559	-2.695842	-5.119188
16	1	0	5.890765	-0.379798	-4.234404
17	1	0	4.663768	0.370654	-2.259446
18	7	0	0.503355	-3.942267	-0.475466
19	8	0	1.132334	-1.613649	0.812910
20	22	0	0.189039	-0.132319	1.618185
21	8	0	-1.027577	-1.179052	2.473249
22	8	0	1.254104	0.296053	2.957195
23	6	0	0.430946	-5.243365	-0.001326
24	6	0	-0.897991	-5.523920	0.165007
25	7	0	-1.613843	-4.403669	-0.203925
26	6	0	-0.748518	-3.473995	-0.583380
27	1	0	1.318692	-5.828623	0.178248
28	1	0	-1.379984	-6.423727	0.514171
29	1	0	-1.002795	-2.483816	-0.926410
30	6	0	2.534468	0.342686	3.586590
31	6	0	2.405403	1.105684	4.903687
32	6	0	3.079121	-1.072615	3.769552
33	1	0	3.195905	0.898696	2.912749
34	6	0	-0.965650	-1.943682	3.674625
35	6	0	-2.333471	-1.939681	4.358503
36	6	0	-0.485837	-3.362368	3.364257
37	1	0	-0.235727	-1.462696	4.343306
38	1	0	1.739346	0.576196	5.594734
39	1	0	3.388008	1.206511	5.378839
40	1	0	2.000185	2.107393	4.731873
41	1	0	4.092177	-1.034665	4.185933
42	1	0	2.443744	-1.646684	4.454369
43	1	0	3.117573	-1.593335	2.809125
44	1	0	-2.297616	-2.521266	5.287566
45	1	0	-2.646440	-0.920701	4.605224
46	1	0	-3.092244	-2.385155	3.704203
47	1	0	-1.208364	-3.875562	2.719914
48	1	0	0.476586	-3.336010	2.846203
49	1	0	-0.375178	-3.941989	4.288888
50	8	0	-0.984379	1.435740	1.356017
51	6	0	-1.883758	2.135685	2.242222
52	6	0	-1.228404	2.372079	3.601436
53	6	0	-3.221079	1.407857	2.350246
54	1	0	-2.053692	3.110929	1.771702
55	1	0	-1.881635	2.995019	4.224273

56	1	0	-1.050329	1.428484	4.127150
57	1	0	-0.269229	2.885159	3.484048
58	1	0	-3.912951	1.983468	2.978003
59	1	0	-3.662634	1.291055	1.358877
60	1	0	-3.084994	0.416954	2.790517
61	6	0	3.179555	0.224858	-0.120495
62	6	0	4.513758	0.557875	0.315189
63	6	0	4.805663	1.888369	0.763536
64	6	0	3.748865	2.836409	0.818156
65	6	0	2.461943	2.480805	0.508768
66	6	0	2.155313	1.162596	0.057248
67	6	0	5.570876	-0.395598	0.359958
68	6	0	6.836271	-0.047327	0.781401
69	6	0	7.126129	1.277761	1.179582
70	6	0	6.123270	2.220881	1.173065
71	1	0	5.369390	-1.419617	0.066477
72	1	0	7.618265	-0.801808	0.810708
73	1	0	8.129741	1.542910	1.500804
74	1	0	6.321561	3.240364	1.496933
75	1	0	3.970233	3.850981	1.142959
76	1	0	1.645063	3.188589	0.577447
77	8	0	0.857865	0.815292	-0.158019
78	22	0	-0.945814	1.953247	-0.708082
79	8	0	-0.503265	1.653794	-2.432290
80	8	0	-0.277763	3.613327	-0.378922
81	8	0	-2.662410	2.498158	-0.868067
82	6	0	0.255072	0.793623	-3.263692
83	6	0	-0.669216	0.120876	-4.281421
84	6	0	1.374185	1.592139	-3.936185
85	6	0	-3.886917	2.349881	-1.565225
86	6	0	-4.965916	3.179700	-0.865489
87	6	0	-3.719542	2.748151	-3.032815
88	6	0	-0.627035	4.917244	-0.814060
89	6	0	-0.393167	5.906551	0.329639
90	6	0	0.167448	5.280950	-2.070304
91	1	0	0.708872	0.020772	-2.628786
92	1	0	-1.471841	-0.419549	-3.769971
93	1	0	-1.122730	0.868234	-4.943407
94	1	0	-0.107980	-0.589976	-4.900313
95	1	0	2.002772	0.934893	-4.548801
96	1	0	0.953966	2.373118	-4.581125
97	1	0	2.008157	2.070946	-3.183422
98	1	0	-4.170026	1.288134	-1.516539
99	1	0	-5.936168	3.040163	-1.356649
100	1	0	-5.067026	2.882783	0.182910
101	1	0	-4.709310	4.245272	-0.898424
102	1	0	-2.915474	2.171573	-3.495988
103	1	0	-3.470943	3.813440	-3.114280
104	1	0	-4.649346	2.567684	-3.585625
105	1	0	-1.700386	4.907175	-1.059556
106	1	0	-0.704685	6.917085	0.038701
107	1	0	-0.963819	5.610942	1.216397
108	1	0	0.669163	5.939869	0.599825
109	1	0	1.240677	5.315052	-1.848300
110	1	0	0.003454	4.533366	-2.851894
111	1	0	-0.137721	6.263001	-2.452242
112	1	0	-2.728169	-4.128789	-0.292354
113	6	0	-7.934430	-0.512604	-0.752859
114	6	0	-7.411006	-1.422705	-1.675747
115	6	0	-6.178199	-2.028394	-1.440207
116	6	0	-7.221133	-0.212042	0.409677
117	6	0	-5.985329	-0.815590	0.643758
118	6	0	-5.455733	-1.720737	-0.282165
119	6	0	-4.147766	-2.404776	-0.012993
120	8	0	-3.904228	-3.500695	-0.621455
121	1	0	-8.897571	-0.043667	-0.936771
122	1	0	-7.967991	-1.662548	-2.577792
123	1	0	-5.762810	-2.748595	-2.137657
124	1	0	-7.628052	0.488132	1.134320
125	1	0	-5.428086	-0.583729	1.548395

126	1	0	-3.787052	-2.278030	1.019854

E_{ZPE}: B3LYP/6-31G* = -4444.697940 (a.u.)
Gsol: B3LYP/6-311++G**//(SMD,M06-2X/6-31G*,CH2Cl2) = -4445.67144 (a.u.)

Full citation of reference 14

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