

Supporting Information

A DFT Study on the Mechanisms of Stereoselective C(2)-Vinylation of 1-Substituted Imidazoles with 3-Phenyl-2-propynenitrile

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Cartesian Coordinates of B3LYP/6-31G(d, p) Model Structures

Table 1 The ZPE (zero-point energies), E (electronic energies), E' (sum of electronic and zero-point energies), H (sum of electronic and thermal enthalpies), G (sum of electronic and thermal free energies) of SP (stationary points) at B3LYP/6-31G (d, p) level (unit: a.u.).

SP	ZPE	E	E'	H	G
R1	0.099141	-265.536287	-265.437146	-265.430802	-265.466164
R2	0.109431	-400.651939	-400.542508	-400.533499	-400.576087
(E)-M1	0.211443	-666.159603	-665.948160	-665.933277	-665.990540
(E)-M2	0.211662	-666.192757	-665.981095	-665.966409	-666.022658
(E)-M3	0.426458	-1332.360814	-1331.934356	-1331.905344	-1331.994763
(E)-TS1	0.209737	-666.149583	-665.939846	-665.924877	-665.982966
(E)-TS2	0.207558	-666.145956	-665.938398	-665.923916	-665.979781
(E)-TS3	0.209282	-666.130556	-665.921274	-665.906894	-665.962514
(E)-TS4	0.424825	-1332.351518	-1331.926693	-1331.897825	-1331.986005
(E)-TS5	0.425794	-1332.349964	-1331.924170	-1331.895858	-1331.982041
(E)-P	0.212757	-666.243409	-666.030653	-666.016163	-666.071822
(Z)-M1	0.211364	-666.160490	-665.949127	-665.934144	-665.992103
(Z)-M2	0.424895	-1332.355438	-1331.930543	-1331.900037	-1331.995595
(Z)-M3	0.422431	-1332.351597	-1331.927034	-1331.896660	-1331.991240

(Z)-M4	0.423986	-1332.384221	-1331.960236	-1331.929504	-1332.026239
(Z)-M5	0.211623	-666.189204	-665.977581	-665.962887	-666.019148
(Z)-M6	0.425672	-1332.360230	-1331.934558	-1331.905301	-1331.994155
(Z)-TS1	0.209779	-666.156370	-665.946591	-665.931598	-665.990154
(Z)-TS2	0.419387	-1332.333906	-1331.914519	-1331.884460	-1331.977609
(Z)-TS3	0.419915	-1332.346979	-1331.927064	-1331.896922	-1331.991002
(Z)-TS4	0.209500	-666.133524	-665.924025	-665.909741	-665.964763
(Z)-TS5	0.424338	-1332.349989	-1331.925651	-1331.896612	-1331.984896
(Z)-TS6	0.425625	-1332.354679	-1331.929054	-1331.900586	-1331.987213
(Z)-P	0.212803	-666.245409	-666.032607	-666.018160	-666.073488

Table 2 The E (single-point energies) of SP (stationary points) at B3LYP/6-31G (d, p) level in different solvent using PCM method (unit: a.u.).

SP	E _{Water}	E _{Ethanol}	E _{DMSO}	E _{THF}	E _{CCl4}
R1	-265.548257	-265.547618	-265.542967	-265.541783	-265.539192
R2	-400.660244	-400.659854	-400.656954	-400.656150	-400.654270
(E)-M1	-666.194979	-666.193047	-666.183076	-666.179181	-666.170263
(E)-M2	-666.209253	-666.208240	-666.201766	-666.200167	-666.196688
(E)-M3	-1332.390007	-1332.387586	-1332.376110	-1332.373232	-1332.367300
(E)-TS1	-666.176424	-666.175010	-666.167151	-666.164305	-666.157710
(E)-TS2	-666.169292	-666.168011	-666.161097	-666.158550	-666.152791
(E)-TS3	-666.150067	-666.148806	-666.142248	-666.140216	-666.135712
(E)-TS4	-1332.376371	-1332.374349	-1332.363938	-1332.361675	-1332.356764
(E)-TS5	-1332.385273	-1332.382941	-1332.370366	-1332.366703	-1332.358805
(E)-P	-666.262291	-666.260948	-666.253736	-666.251837	-666.247815
(Z)-M1	-666.192464	-666.190548	-666.180486	-666.177064	-666.169411
(Z)-M2	-1332.392242	-1332.389504	-1332.375425	-1332.371717	-1332.363925
(Z)-M3	-1332.386685	-1332.383445	-1332.370804	-1332.367083	-1332.359498
(Z)-M4	-1332.414611	-1332.411398	-1332.401298	-1332.398075	-1332.391359
(Z)-M5	-666.208387	-666.206979	-666.199906	-666.197978	-666.193844
(Z)-M6	-1332.391405	-1332.388006	-1332.375692	-1332.372643	-1332.366799
(Z)-TS1	-666.181471	-666.179967	-666.171730	-666.169124	-666.163262
(Z)-TS2	-1332.377340	-1332.374124	-1332.360145	-1332.355380	-1332.345178
(Z)-TS3	-1332.386110	-1332.382551	-1332.370188	-1332.365943	-1332.356869
(Z)-TS4	-666.149196	-666.148236	-666.141752	-666.140268	-666.137098
(Z)-TS5	-1332.377234	-1332.374073	-1332.363519	-1332.360954	-1332.355691
(Z)-TS6	-1332.387392	-1332.384759	-1332.372149	-1332.368947	-1332.362075
(Z)-P	-666.262131	-666.260961	-666.254180	-666.252496	-666.249052

R1

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

1	6	0	-0.200198	-1.084834	-0.000006
2	1	0	0.206061	-2.087899	-0.000028
3	6	0	-0.225910	1.115382	-0.000018
4	1	0	0.158949	2.123971	-0.000016
5	6	0	-1.501621	0.607402	0.000048
6	1	0	-2.433881	1.155171	0.000090
7	7	0	-1.477574	-0.769046	-0.000095
8	7	0	0.611182	0.016798	-0.000031
9	6	0	2.062685	0.029429	0.000072
10	1	0	2.448977	0.534724	0.890576
11	1	0	2.425844	-0.999959	-0.000338
12	1	0	2.449063	0.535452	-0.889978

R2

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

1	6	0	2.474166	-1.210512	0.000000
2	6	0	1.082744	-1.217516	0.000000
3	6	0	0.373797	-0.000004	0.000001
4	6	0	1.082739	1.217514	0.000000
5	6	0	2.474160	1.210517	0.000000
6	6	0	3.171547	0.000004	0.000000
7	1	0	3.016020	-2.150953	0.000000
8	1	0	0.534073	-2.152995	0.000000
9	1	0	0.534061	2.152989	0.000000
10	1	0	3.016011	2.150959	0.000000
11	1	0	4.257097	0.000007	0.000001
12	6	0	-1.048816	-0.000005	0.000000
13	6	0	-2.266407	-0.000002	0.000000
14	6	0	-3.633960	0.000000	-0.000001
15	7	0	-4.802439	0.000002	-0.000001

(E)-M1

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

1	6	0	-3.575969	-0.592474	-0.699574
2	6	0	-2.418116	0.180640	-0.740303

3	6	0	-1.282743	-0.181153	0.006537
4	6	0	-1.354947	-1.342496	0.800005
5	6	0	-2.513677	-2.117539	0.835571
6	6	0	-3.629015	-1.748222	0.082539
7	1	0	-4.440302	-0.291038	-1.284203
8	1	0	-2.386231	1.082681	-1.341129
9	1	0	-0.507317	-1.627400	1.417814
10	1	0	-2.548387	-3.004296	1.462676
11	1	0	-4.532475	-2.350191	0.111096
12	6	0	-0.092191	0.704833	-0.005099
13	6	0	0.057116	2.034151	0.067691
14	6	0	-1.033210	2.901097	0.166551
15	7	0	-1.856029	3.737914	0.237495
16	1	0	0.674275	-1.959987	-0.885615
17	6	0	1.463682	-1.304613	-0.559833
18	6	0	2.816812	-1.486030	-0.528561
19	7	0	1.200885	-0.034154	-0.081803
20	1	0	3.424617	-2.328775	-0.817252
21	7	0	3.365445	-0.316775	-0.032907
22	6	0	2.362922	0.540346	0.232697
23	6	0	4.783558	-0.059604	0.197267
24	1	0	2.419348	1.561602	0.580166
25	1	0	5.344792	-0.223593	-0.725191
26	1	0	4.907418	0.977281	0.509221
27	1	0	5.166811	-0.718792	0.980005

(E)-M2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.448634	-0.751208	-0.756564
2	6	0	-2.320529	0.064954	-0.820050
3	6	0	-1.209280	-0.194645	-0.003291
4	6	0	-1.250691	-1.292566	0.874416
5	6	0	-2.382068	-2.102068	0.938295
6	6	0	-3.483347	-1.834714	0.121832
7	1	0	-4.299737	-0.539693	-1.396400
8	1	0	-2.296067	0.902702	-1.508116
9	1	0	-0.400887	-1.495696	1.518292
10	1	0	-2.406145	-2.938939	1.629785
11	1	0	-4.363905	-2.468234	0.171137
12	6	0	-0.019700	0.690145	-0.039500

13	6	0	-0.063845	2.043251	0.006473
14	6	0	-1.251074	2.803130	0.175137
15	7	0	-2.191878	3.479669	0.301476
16	1	0	0.710977	-1.827667	-1.059536
17	6	0	1.490910	-1.200901	-0.660717
18	6	0	2.827670	-1.388208	-0.592428
19	7	0	1.249818	0.061427	-0.098423
20	1	0	3.434810	-2.222474	-0.909361
21	7	0	3.356362	-0.240223	0.002386
22	6	0	2.416535	0.686872	0.323106
23	6	0	4.771588	-0.046723	0.280245
24	1	0	0.875424	2.586115	-0.027047
25	1	0	5.357402	-0.103342	-0.642527
26	1	0	4.885076	0.941564	0.723665
27	1	0	5.137718	-0.804362	0.980302

(E)-M3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.119959	-0.189118	-0.400555
2	6	0	-0.484324	-0.753445	0.888173
3	7	0	-0.658742	1.204933	-0.629613
4	6	0	-0.694214	2.178099	0.336128
5	6	0	1.932438	0.174444	0.856834
6	7	0	0.824945	-0.642604	1.318222
7	6	0	-4.853992	-0.530080	-1.276373
8	6	0	-3.462989	-0.657599	-1.328382
9	6	0	-2.666556	-0.121501	-0.313935
10	6	0	-3.282191	0.576078	0.737043
11	6	0	-4.669226	0.704933	0.785479
12	6	0	-5.462370	0.145132	-0.219865
13	1	0	-5.458906	-0.960931	-2.068940
14	1	0	-2.992609	-1.173362	-2.156244
15	1	0	-2.663042	1.049923	1.492249
16	1	0	-5.130284	1.250660	1.604090
17	1	0	-6.543515	0.244238	-0.182571
18	6	0	-0.575202	-1.091205	-1.476912
19	6	0	-0.924055	-2.442860	-1.495020
20	7	0	-1.241474	-3.577785	-1.499095
21	1	0	-0.378309	1.091205	-2.776475
22	6	0	-0.392950	1.715119	-1.899068

23	6	0	-0.214460	3.048014	-1.734147
24	1	0	0.025530	3.818999	-2.449940
25	7	0	-0.399626	3.302303	-0.376434
26	6	0	-0.256800	4.615616	0.233047
27	1	0	1.043353	1.770396	1.866188
28	1	0	-0.584470	4.537694	1.269433
29	1	0	0.786060	4.947534	0.205568
30	1	0	-0.879487	5.349168	-0.288032
31	1	0	5.665859	-2.478950	-1.964989
32	6	0	4.914298	-1.942242	-1.393935
33	6	0	3.646950	-2.493479	-1.206985
34	6	0	5.212081	-0.696714	-0.836332
35	6	0	2.682661	-1.807667	-0.472652
36	1	0	3.399648	-3.460354	-1.633650
37	6	0	4.253978	-0.003122	-0.104780
38	1	0	6.198758	-0.262568	-0.965085
39	6	0	2.964284	-0.542372	0.083160
40	1	0	1.703025	-2.252099	-0.351459
41	1	0	4.519244	0.953088	0.325930
42	6	0	1.917807	1.450675	1.306648
43	6	0	2.844300	2.482266	1.002444
44	6	0	1.070158	-1.580672	2.318329
45	7	0	3.574210	3.350552	0.733811
46	1	0	2.036935	-1.654310	2.786923
47	6	0	-0.072420	-2.264352	2.515810
48	7	0	-1.026490	-1.757669	1.643581
49	1	0	0.432203	-0.858043	-1.805012
50	1	0	-0.304735	-3.064524	3.198404
51	6	0	-2.363991	-2.371274	1.573137
52	1	0	-2.335385	-3.255989	2.209642
53	1	0	-3.127198	-1.682733	1.932698
54	1	0	-2.581962	-2.683196	0.554233

(E)-TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.707559	-0.548663	-0.769626
2	6	0	-2.560920	0.241653	-0.766022
3	6	0	-1.457319	-0.100964	0.037191
4	6	0	-1.542257	-1.251826	0.841088
5	6	0	-2.692110	-2.039888	0.833251

6	6	0	-3.777146	-1.694820	0.025495
7	1	0	-4.548666	-0.269316	-1.397390
8	1	0	-2.505696	1.135458	-1.378645
9	1	0	-0.713698	-1.510522	1.492485
10	1	0	-2.744633	-2.919929	1.468112
11	1	0	-4.671825	-2.310285	0.020488
12	6	0	-0.313869	0.804612	0.060469
13	6	0	0.022154	2.033170	0.096660
14	6	0	-0.536680	3.286417	0.166673
15	7	0	-0.934515	4.390685	0.218368
16	1	0	0.622567	-2.273432	-0.576888
17	6	0	1.419366	-1.576100	-0.373656
18	6	0	2.775304	-1.762765	-0.397400
19	7	0	1.168346	-0.266203	-0.031661
20	1	0	3.377402	-2.630404	-0.620361
21	7	0	3.340778	-0.542408	-0.067669
22	6	0	2.332212	0.330134	0.141241
23	6	0	4.765670	-0.249724	0.036361
24	1	0	2.423136	1.381988	0.378548
25	1	0	5.264912	-0.462323	-0.912071
26	1	0	4.892117	0.806712	0.273953
27	1	0	5.221044	-0.849887	0.828153

(E)-TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.656686	-0.324114	-0.713168
2	6	0	-2.430961	0.336607	-0.717678
3	6	0	-1.337013	-0.176913	0.001434
4	6	0	-1.514986	-1.368100	0.729998
5	6	0	-2.743209	-2.027696	0.729723
6	6	0	-3.817741	-1.511263	0.004502
7	1	0	-4.488685	0.089147	-1.275550
8	1	0	-2.311788	1.259698	-1.273989
9	1	0	-0.700153	-1.761369	1.330540
10	1	0	-2.862938	-2.940305	1.306659
11	1	0	-4.774284	-2.025282	0.004215
12	6	0	-0.065566	0.568708	0.019887
13	6	0	0.228827	1.876101	0.102167
14	6	0	-0.704827	2.911771	0.204492
15	7	0	-1.398213	3.854108	0.279130

16	1	0	0.724369	-2.275136	-0.564207
17	6	0	1.480138	-1.537065	-0.354709
18	6	0	2.842059	-1.632737	-0.367746
19	7	0	1.184750	-0.231869	-0.021272
20	1	0	3.487524	-2.473683	-0.570237
21	7	0	3.334031	-0.369225	-0.053728
22	6	0	2.310402	0.479107	0.161000
23	6	0	4.744670	-0.015913	0.055441
24	1	0	1.779321	1.644741	0.231408
25	1	0	5.262565	-0.240946	-0.880267
26	1	0	4.814418	1.051968	0.258977
27	1	0	5.215042	-0.570891	0.871481

(E)-TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.514964	-0.050954	0.712933
2	6	0	2.209840	0.434298	0.763819
3	6	0	1.178570	-0.229705	0.082201
4	6	0	1.477707	-1.388928	-0.643936
5	6	0	2.784646	-1.870140	-0.695796
6	6	0	3.806484	-1.203878	-0.017638
7	1	0	4.303357	0.472877	1.244978
8	1	0	1.985657	1.329511	1.333820
9	1	0	0.673927	-1.898587	-1.162115
10	1	0	3.005141	-2.765816	-1.269202
11	1	0	4.824495	-1.580384	-0.058429
12	6	0	-0.205759	0.316902	0.160496
13	6	0	-0.514861	1.643829	-0.050414
14	6	0	0.372880	2.585925	-0.613564
15	7	0	1.067228	3.403494	-1.076835
16	1	0	-2.401442	0.346670	2.763859
17	6	0	-2.350907	-0.016194	1.748601
18	6	0	-3.344790	-0.215808	0.842431
19	7	0	-1.161775	-0.476669	1.167126
20	1	0	-4.416397	-0.110133	0.941924
21	7	0	-2.759819	-0.682448	-0.328185
22	6	0	-1.416294	-0.859972	-0.125052
23	6	0	-3.450067	-0.909462	-1.588721
24	1	0	-1.521257	1.994349	0.158394
25	1	0	-3.812263	0.034411	-2.008346

26	1	0	-2.739568	-1.359542	-2.281246
27	1	0	-4.295570	-1.589473	-1.450549

(E)-TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.301247	-0.096508	0.609973
2	6	0	0.523869	-0.872047	-0.989272
3	7	0	0.628610	1.193439	0.793576
4	6	0	0.572066	2.179975	-0.165455
5	6	0	-1.894251	-0.130858	-0.954475
6	7	0	-0.837776	-1.082416	-1.115787
7	6	0	5.116017	-0.001620	0.883093
8	6	0	3.770077	-0.246133	1.168549
9	6	0	2.770342	0.113085	0.256619
10	6	0	3.145152	0.761918	-0.930711
11	6	0	4.487046	1.012532	-1.209645
12	6	0	5.480662	0.624496	-0.306749
13	1	0	5.875397	-0.300111	1.599822
14	1	0	3.500938	-0.717753	2.105403
15	1	0	2.370927	1.091865	-1.612207
16	1	0	4.757073	1.517533	-2.132920
17	1	0	6.526766	0.817435	-0.526959
18	6	0	0.944253	-1.051597	1.599044
19	6	0	1.575920	-2.296095	1.741392
20	7	0	2.086556	-3.345624	1.859905
21	1	0	0.193812	1.033061	2.925500
22	6	0	0.166012	1.639576	2.036953
23	6	0	-0.218435	2.924645	1.858796
24	1	0	-0.636800	3.634661	2.555570
25	7	0	0.036552	3.225443	0.523307
26	6	0	-0.248485	4.516065	-0.087169
27	1	0	-0.822690	1.273262	-2.098352
28	1	0	0.179415	4.508125	-1.089041
29	1	0	-1.326988	4.684022	-0.157730
30	1	0	0.209197	5.321024	0.496077
31	1	0	-6.118953	-1.799035	1.919793
32	6	0	-5.267811	-1.465090	1.334087
33	6	0	-3.984517	-1.923727	1.637398
34	6	0	-5.452995	-0.582662	0.268361
35	6	0	-2.892847	-1.499902	0.884377

36	1	0	-3.831224	-2.613316	2.461819
37	6	0	-4.364804	-0.153647	-0.487335
38	1	0	-6.449292	-0.232961	0.016202
39	6	0	-3.065145	-0.595298	-0.180821
40	1	0	-1.899363	-1.862598	1.123946
41	1	0	-4.527380	0.516525	-1.323020
42	6	0	-1.737472	1.072073	-1.553156
43	6	0	-2.623409	2.175359	-1.423644
44	6	0	-1.104840	-2.365876	-1.604252
45	7	0	-3.305678	3.118613	-1.365809
46	1	0	-2.108918	-2.711864	-1.782735
47	6	0	0.091694	-2.947153	-1.823248
48	7	0	1.071900	-2.028869	-1.465895
49	1	0	-0.034288	-0.968544	2.057765
50	1	0	0.338112	-3.922311	-2.211423
51	6	0	2.495888	-2.366373	-1.577502
52	1	0	2.576928	-3.232262	-2.236596
53	1	0	3.046603	-1.532413	-2.006503
54	1	0	2.908171	-2.619278	-0.600726

(E)-TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.252318	-0.119113	-0.445076
2	6	0	-0.718372	-0.814190	0.842103
3	7	0	-0.374554	1.052849	-0.716207
4	6	0	0.644607	1.443014	0.070914
5	6	0	1.755187	-0.080612	1.022595
6	7	0	0.550412	-0.853559	1.360924
7	6	0	-4.927869	0.938913	-0.886445
8	6	0	-3.684933	0.344583	-1.120851
9	6	0	-2.661705	0.462753	-0.176880
10	6	0	-2.889153	1.210728	0.987103
11	6	0	-4.127019	1.807958	1.217407
12	6	0	-5.154274	1.668067	0.280190
13	1	0	-5.719456	0.827499	-1.621507
14	1	0	-3.511024	-0.223291	-2.026932
15	1	0	-2.087541	1.336016	1.710964
16	1	0	-4.288141	2.385828	2.122896
17	1	0	-6.120927	2.130242	0.457784
18	6	0	-1.125224	-1.060747	-1.595815

19	6	0	-1.991263	-2.135390	-1.788875
20	7	0	-2.736848	-3.032472	-1.958214
21	1	0	-1.342420	1.781513	-2.508338
22	6	0	-0.577611	1.936932	-1.766471
23	6	0	0.334282	2.928786	-1.600355
24	1	0	0.513355	3.823533	-2.175983
25	7	0	1.082797	2.604925	-0.471544
26	6	0	2.148574	3.441139	0.073143
27	1	0	1.906756	0.484421	3.074007
28	1	0	2.646061	2.910393	0.882761
29	1	0	2.878650	3.673531	-0.706297
30	1	0	1.734106	4.375625	0.462746
31	1	0	4.515879	-1.964853	-3.234141
32	6	0	3.953707	-1.580577	-2.388477
33	6	0	2.945655	-2.347580	-1.806299
34	6	0	4.235086	-0.315617	-1.871259
35	6	0	2.221919	-1.854117	-0.720494
36	1	0	2.714497	-3.334604	-2.195035
37	6	0	3.512452	0.180100	-0.788265
38	1	0	5.022416	0.290913	-2.308627
39	6	0	2.494102	-0.582087	-0.195582
40	1	0	1.441406	-2.469001	-0.289159
41	1	0	3.761459	1.155888	-0.392651
42	6	0	2.463203	0.309202	2.157929
43	6	0	3.790789	0.775026	2.147687
44	6	0	0.618892	-1.834527	2.347048
45	7	0	4.888184	1.181664	2.177994
46	1	0	1.540028	-2.031651	2.866487
47	6	0	-0.606495	-2.393086	2.439194
48	7	0	-1.432305	-1.753060	1.530779
49	1	0	-0.124970	-1.157671	-1.999933
50	1	0	-0.974642	-3.181505	3.074740
51	6	0	-2.858782	-2.097956	1.420591
52	1	0	-3.000774	-3.034243	1.960951
53	1	0	-3.474292	-1.316770	1.869587
54	1	0	-3.134837	-2.253858	0.381006

(E)-P

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.472259	-0.438586	-0.534506

2	6	0	-2.260735	0.227004	-0.706046
3	6	0	-1.106183	-0.204580	-0.032088
4	6	0	-1.195029	-1.332512	0.802476
5	6	0	-2.409278	-1.988779	0.980609
6	6	0	-3.552375	-1.543839	0.313396
7	1	0	-4.352399	-0.095383	-1.069520
8	1	0	-2.206524	1.072515	-1.381988
9	1	0	-0.308149	-1.691295	1.312398
10	1	0	-2.462229	-2.852338	1.636778
11	1	0	-4.497872	-2.061128	0.447226
12	6	0	0.182305	0.513546	-0.186542
13	6	0	0.281782	1.871256	-0.278281
14	6	0	-0.776151	2.804128	-0.097911
15	7	0	-1.588033	3.627227	0.052205
16	1	0	3.063860	-2.847732	-1.204859
17	6	0	2.740251	-1.905812	-0.784354
18	6	0	3.498282	-0.976266	-0.110463
19	7	0	1.443961	-1.492111	-0.868261
20	1	0	4.539362	-0.957071	0.175030
21	7	0	2.644188	0.048548	0.221462
22	6	0	1.396797	-0.306850	-0.268278
23	6	0	3.024243	1.183482	1.055983
24	1	0	1.238839	2.325950	-0.510859
25	1	0	3.409614	2.014111	0.456112
26	1	0	2.162287	1.529888	1.626009
27	1	0	3.802493	0.863680	1.751853

(Z)-M1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.029354	0.541156	0.213377
2	6	0	-2.732879	1.038327	0.266765
3	6	0	-1.631823	0.222022	-0.057870
4	6	0	-1.884992	-1.105169	-0.447713
5	6	0	-3.189077	-1.601567	-0.499300
6	6	0	-4.267461	-0.784513	-0.165823
7	1	0	-4.862078	1.189232	0.472304
8	1	0	-2.530320	2.065706	0.549822
9	1	0	-1.064573	-1.754427	-0.738143
10	1	0	-3.358700	-2.629026	-0.809672
11	1	0	-5.281504	-1.171521	-0.203842

12	6	0	-0.281462	0.818271	-0.006676
13	6	0	0.009471	2.124386	0.011117
14	6	0	1.319356	2.587689	0.029991
15	7	0	2.411945	3.030294	-0.000920
16	1	0	0.132777	-1.464741	1.689362
17	6	0	0.944674	-1.219723	1.025229
18	6	0	2.198631	-1.741769	0.915614
19	7	0	0.819055	-0.217859	0.074464
20	1	0	2.691383	-2.527029	1.466450
21	7	0	2.833412	-1.052224	-0.103286
22	6	0	1.974942	-0.137180	-0.588250
23	6	0	4.221722	-1.217616	-0.523849
24	1	0	2.203727	0.588600	-1.349912
25	1	0	4.416729	-2.266623	-0.756039
26	1	0	4.394791	-0.615039	-1.415277
27	1	0	4.896404	-0.882488	0.267455

(Z)-M2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.941131	-0.301943	1.602980
2	6	0	2.603900	0.042590	1.750022
3	6	0	2.071077	1.171019	1.097176
4	6	0	2.936004	1.944246	0.303206
5	6	0	4.280638	1.597721	0.161050
6	6	0	4.790636	0.472860	0.805889
7	1	0	4.325532	-1.181966	2.110720
8	1	0	1.937258	-0.544062	2.372134
9	1	0	2.568179	2.832536	-0.199939
10	1	0	4.928964	2.214103	-0.455600
11	1	0	5.836438	0.202478	0.692985
12	6	0	0.645542	1.502200	1.302646
13	6	0	-0.188728	0.896469	2.159877
14	6	0	-1.523053	1.256454	2.329698
15	7	0	-2.668151	1.406713	2.570841
16	1	0	-0.153895	4.175696	1.869789
17	6	0	-0.266762	3.857932	0.846809
18	6	0	-0.817111	4.481337	-0.234214
19	7	0	0.156930	2.612038	0.428760
20	1	0	-1.268825	5.454553	-0.336152
21	7	0	-0.726821	3.604013	-1.299185

22	6	0	-0.134413	2.477639	-0.870640
23	6	0	-1.263759	3.815955	-2.648681
24	1	0	0.043433	1.583677	-1.464030
25	1	0	-1.769989	4.781013	-2.665080
26	1	0	-0.449171	3.822570	-3.375998
27	1	0	-1.973162	3.015376	-2.879199
28	1	0	3.907219	-4.312918	-0.711034
29	6	0	2.984070	-3.751127	-0.819444
30	6	0	1.821056	-4.178230	-0.182041
31	6	0	2.948654	-2.592418	-1.602621
32	6	0	0.635121	-3.454885	-0.318220
33	1	0	1.830703	-5.079541	0.424595
34	6	0	1.769150	-1.873142	-1.744124
35	1	0	3.848731	-2.247553	-2.103490
36	6	0	0.587602	-2.286864	-1.099145
37	1	0	-0.259131	-3.815864	0.179335
38	1	0	1.726196	-0.978808	-2.355498
39	6	0	-0.644782	-1.496033	-1.298158
40	6	0	-0.793748	-0.463913	-2.141454
41	7	0	-1.781034	-1.930417	-0.430705
42	6	0	-1.990159	0.230903	-2.305075
43	6	0	-2.965504	-2.502434	-0.850545
44	6	0	-1.893424	-1.626017	0.867875
45	7	0	-2.903208	0.940288	-2.538746
46	1	0	-3.111107	-2.807036	-1.873432
47	6	0	-3.798926	-2.544434	0.228356
48	7	0	-3.112621	-1.991999	1.294250
49	1	0	-1.130774	-1.131202	1.462986
50	1	0	-4.810264	-2.903241	0.328387
51	6	0	-3.642618	-1.754297	2.642412
52	1	0	-4.692079	-2.048185	2.651672
53	1	0	-3.092371	-2.355440	3.369446
54	1	0	-3.547127	-0.690161	2.879089

(Z)-M3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.916245	-2.291086	-1.899446
2	6	0	0.934658	-1.313023	-1.761005
3	6	0	-0.395077	-1.693213	-1.506627
4	6	0	-0.718676	-3.056498	-1.378649

5	6	0	0.268926	-4.024868	-1.530661
6	6	0	1.587375	-3.643524	-1.792922
7	1	0	2.947245	-1.990902	-2.052954
8	1	0	1.192813	-0.255071	-1.771369
9	1	0	-1.743838	-3.357317	-1.182777
10	1	0	0.011411	-5.076065	-1.443242
11	1	0	2.359172	-4.400137	-1.897779
12	6	0	-1.433251	-0.658188	-1.402854
13	6	0	-1.419476	0.496108	-2.104215
14	6	0	-2.376286	1.541440	-1.992516
15	7	0	-3.167384	2.395849	-1.972126
16	1	0	-4.267411	-0.647050	-1.673705
17	6	0	-3.863785	-0.817708	-0.690140
18	6	0	-4.473504	-0.992859	0.512061
19	7	0	-2.495942	-0.898948	-0.459699
20	1	0	-5.518179	-0.998564	0.776613
21	7	0	-3.475825	-1.179253	1.455334
22	6	0	-2.287664	-1.113917	0.853887
23	6	0	-3.658480	-1.176623	2.912253
24	1	0	-1.307019	-1.089443	1.356449
25	1	0	-4.653366	-1.559011	3.141404
26	1	0	-2.904098	-1.819329	3.365844
27	1	0	-3.526230	-0.148109	3.261681
28	1	0	5.510868	-2.340241	0.953782
29	6	0	4.625240	-1.713156	1.008720
30	6	0	4.583389	-0.488393	0.343418
31	6	0	3.514893	-2.117408	1.758091
32	6	0	3.448070	0.321407	0.416913
33	1	0	5.440517	-0.153606	-0.235396
34	6	0	2.386622	-1.310137	1.836887
35	1	0	3.535509	-3.064536	2.291319
36	6	0	2.322388	-0.074880	1.161558
37	1	0	3.429733	1.262993	-0.118099
38	1	0	1.527419	-1.602559	2.430982
39	6	0	1.104043	0.764109	1.293571
40	6	0	0.038120	0.387797	2.031251
41	7	0	1.160973	2.045615	0.594162
42	6	0	-1.092245	1.185747	2.223157
43	6	0	1.195171	3.277806	1.237239
44	6	0	1.086617	2.165491	-0.771447
45	7	0	-2.149016	1.651481	2.473303
46	1	0	1.241611	3.367969	2.310708
47	6	0	1.151716	4.219832	0.262581
48	7	0	1.089768	3.523946	-0.941610

49	1	0	-0.615688	0.656645	-2.811272
50	1	0	1.155799	5.297430	0.320732
51	6	0	0.983225	4.160093	-2.242335
52	1	0	1.785477	4.891618	-2.384213
53	1	0	1.071894	3.381768	-3.000209
54	1	0	0.018824	4.666604	-2.356666

(Z)-M4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.625561	1.761944	3.554310
2	6	0	0.121562	0.589651	2.998924
3	6	0	-0.836138	0.636745	1.968735
4	6	0	-1.283348	1.894230	1.525806
5	6	0	-0.782540	3.065460	2.090130
6	6	0	0.173874	3.005356	3.104818
7	1	0	1.359886	1.705233	4.352378
8	1	0	0.452563	-0.371306	3.377258
9	1	0	-2.009522	1.949582	0.722887
10	1	0	-1.137291	4.027023	1.731178
11	1	0	0.558928	3.918894	3.548382
12	6	0	-1.358708	-0.606383	1.367713
13	6	0	-0.672979	-1.773795	1.357587
14	6	0	-1.249150	-3.011232	0.953088
15	7	0	-1.697263	-4.055633	0.698180
16	1	0	-3.859931	0.155232	2.404382
17	6	0	-3.816351	-0.134348	1.366557
18	6	0	-4.784757	-0.228439	0.426228
19	7	0	-2.633602	-0.538620	0.738318
20	1	0	-5.844114	-0.030877	0.488123
21	7	0	-4.159031	-0.670814	-0.739523
22	6	0	-2.819409	-0.874680	-0.592068
23	6	0	-4.850734	-0.901093	-1.997877
24	1	0	-0.435780	-1.340183	-2.031107
25	1	0	-5.301856	0.023913	-2.371740
26	1	0	-4.113230	-1.261858	-2.713577
27	1	0	-5.634247	-1.655316	-1.876132
28	1	0	-0.246602	4.617602	-2.814533
29	6	0	0.071916	3.616205	-2.540166
30	6	0	0.907077	3.422036	-1.438510
31	6	0	-0.344625	2.516358	-3.293745

32	6	0	1.324408	2.139484	-1.090118
33	1	0	1.231187	4.270755	-0.843673
34	6	0	0.074421	1.233700	-2.951844
35	1	0	-0.984158	2.659477	-4.159644
36	6	0	0.909651	1.024513	-1.839542
37	1	0	1.955222	1.992977	-0.220392
38	1	0	-0.224256	0.386975	-3.560744
39	6	0	1.343467	-0.338371	-1.472043
40	6	0	0.603179	-1.442789	-1.727186
41	7	0	2.588105	-0.461287	-0.794747
42	6	0	1.092081	-2.770284	-1.567248
43	6	0	3.803654	0.048076	-1.264758
44	6	0	2.714790	-1.114034	0.419990
45	7	0	1.468918	-3.871337	-1.520232
46	1	0	3.894478	0.579627	-2.198477
47	6	0	4.731443	-0.300560	-0.344094
48	7	0	4.050580	-0.993524	0.657513
49	1	0	0.383402	-1.789858	1.617971
50	1	0	5.796170	-0.125062	-0.319799
51	6	0	4.687710	-1.542943	1.843919
52	1	0	5.146071	-0.750495	2.444515
53	1	0	3.915642	-2.042585	2.427469
54	1	0	5.457153	-2.270096	1.567080

(Z)-M5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.906189	0.391476	0.449979
2	6	0	2.609441	0.898414	0.500179
3	6	0	1.540285	0.184944	-0.067186
4	6	0	1.800762	-1.058096	-0.670738
5	6	0	3.098626	-1.561063	-0.719976
6	6	0	4.155157	-0.838790	-0.161009
7	1	0	4.720431	0.951927	0.899300
8	1	0	2.414285	1.840429	1.002910
9	1	0	0.984401	-1.615066	-1.118455
10	1	0	3.286341	-2.516660	-1.200295
11	1	0	5.165372	-1.235373	-0.196252
12	6	0	0.168095	0.742667	-0.055002
13	6	0	-0.057917	2.065965	-0.235700
14	6	0	-1.308429	2.733677	-0.119101

15	7	0	-2.261968	3.391366	0.004885
16	1	0	-0.053860	-1.419599	1.711068
17	6	0	-0.888640	-1.216537	1.060093
18	6	0	-2.096902	-1.812276	0.951212
19	7	0	-0.895036	-0.169670	0.124874
20	1	0	-2.514552	-2.650285	1.488456
21	7	0	-2.789810	-1.121740	-0.045738
22	6	0	-2.082721	-0.094521	-0.590567
23	6	0	-4.134110	-1.460283	-0.487812
24	1	0	0.786049	2.700881	-0.484545
25	1	0	-4.843623	-1.386930	0.342234
26	1	0	-4.409504	-0.746752	-1.263164
27	1	0	-4.166665	-2.475729	-0.895626

(Z)-M6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.137548	-0.294574	-0.791067
2	6	0	-0.566183	-1.238651	0.303749
3	7	0	-0.340273	0.986884	-0.817712
4	6	0	-0.471309	1.964839	0.140348
5	6	0	1.566246	-0.138224	1.212648
6	7	0	0.665793	-1.234491	0.911208
7	6	0	-4.738599	0.930891	-1.276649
8	6	0	-3.429604	0.520622	-1.526795
9	6	0	-2.597438	0.103232	-0.479700
10	6	0	-3.095897	0.145091	0.828116
11	6	0	-4.409520	0.546450	1.076959
12	6	0	-5.238789	0.936748	0.026052
13	1	0	-5.366509	1.248678	-2.104186
14	1	0	-3.045154	0.541082	-2.540276
15	1	0	-2.460082	-0.113654	1.667160
16	1	0	-4.773633	0.567974	2.099932
17	1	0	-6.259251	1.253819	0.220727
18	6	0	-1.056023	-1.073551	-2.065987
19	6	0	0.100396	-1.726819	-2.475382
20	7	0	1.092432	-2.270259	-2.811552
21	1	0	0.629236	0.765996	-2.753819
22	6	0	0.437112	1.396324	-1.902960
23	6	0	0.833031	2.660029	-1.621728
24	1	0	1.449020	3.344442	-2.184819

25	7	0	0.271712	2.979688	-0.382685
26	6	0	0.418148	4.267435	0.273382
27	1	0	1.802080	1.569745	2.435243
28	1	0	-0.142237	4.225672	1.207119
29	1	0	1.471000	4.483730	0.486169
30	1	0	0.016654	5.072341	-0.351290
31	1	0	6.308781	-0.041637	-1.301673
32	6	0	5.349463	-0.064386	-0.793244
33	6	0	4.309986	-0.851922	-1.284903
34	6	0	5.153803	0.691156	0.367949
35	6	0	3.078586	-0.884799	-0.632916
36	1	0	4.437983	-1.443398	-2.185701
37	6	0	3.929795	0.662388	1.024061
38	1	0	5.962891	1.293627	0.769910
39	6	0	2.864217	-0.115814	0.523827
40	1	0	2.287671	-1.493765	-1.054115
41	1	0	3.813117	1.229255	1.941862
42	6	0	1.185233	0.713252	2.191808
43	6	0	0.014385	0.542559	2.978656
44	6	0	0.874525	-2.454584	1.554021
45	7	0	-0.898052	0.387330	3.685804
46	1	0	1.783147	-2.650776	2.097608
47	6	0	-0.234003	-3.198947	1.360769
48	7	0	-1.113490	-2.450032	0.600653
49	1	0	-1.968579	-1.269899	-2.608505
50	1	0	-0.481073	-4.194776	1.689796
51	6	0	-2.352276	-3.001052	0.057257
52	1	0	-2.414692	-4.046895	0.358013
53	1	0	-3.214689	-2.451679	0.433640
54	1	0	-2.308956	-2.909875	-1.032432

(Z)-TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.078604	0.452735	0.395465
2	6	0	-2.799669	0.997718	0.415650
3	6	0	-1.698805	0.268964	-0.078665
4	6	0	-1.928981	-1.014923	-0.601378
5	6	0	-3.214522	-1.556525	-0.619144
6	6	0	-4.294053	-0.829565	-0.118540
7	1	0	-4.912253	1.029852	0.785222

8	1	0	-2.621043	1.993340	0.806445
9	1	0	-1.102548	-1.581704	-1.015250
10	1	0	-3.371265	-2.548279	-1.034035
11	1	0	-5.293505	-1.254175	-0.131451
12	6	0	-0.389943	0.917366	-0.056971
13	6	0	0.027077	2.137662	-0.017033
14	6	0	1.281572	2.707247	-0.004535
15	7	0	2.339506	3.221704	-0.020133
16	1	0	0.117535	-1.760952	1.451205
17	6	0	0.963080	-1.414151	0.878790
18	6	0	2.258110	-1.851274	0.870980
19	7	0	0.846749	-0.374006	-0.020831
20	1	0	2.754506	-2.633629	1.423603
21	7	0	2.933337	-1.058452	-0.040089
22	6	0	2.046469	-0.178106	-0.552347
23	6	0	4.353449	-1.129721	-0.365834
24	1	0	2.302192	0.605831	-1.246835
25	1	0	4.591451	-2.091293	-0.827587
26	1	0	4.595672	-0.326790	-1.062130
27	1	0	4.951031	-1.001475	0.539554

(Z)-TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.596236	2.934253	-2.769696
2	6	0	-0.272947	1.598746	-2.554870
3	6	0	0.748023	1.240906	-1.652846
4	6	0	1.445607	2.267848	-0.992301
5	6	0	1.125290	3.604537	-1.218238
6	6	0	0.104169	3.944926	-2.105877
7	1	0	-1.385078	3.189667	-3.471456
8	1	0	-0.787798	0.811399	-3.094651
9	1	0	2.222781	2.022959	-0.276189
10	1	0	1.668433	4.381474	-0.688909
11	1	0	-0.141083	4.987846	-2.283115
12	6	0	1.054157	-0.183096	-1.452471
13	6	0	0.220934	-1.212609	-1.728787
14	6	0	0.711363	-2.540145	-1.701450
15	7	0	1.072542	-3.649836	-1.778058
16	1	0	3.777081	0.044261	-2.370471
17	6	0	3.619782	-0.357030	-1.382921

18	6	0	4.496673	-0.851740	-0.465671
19	7	0	2.352806	-0.467198	-0.833395
20	1	0	5.568268	-0.965229	-0.500806
21	7	0	3.747699	-1.250428	0.632033
22	6	0	2.452948	-1.010623	0.388696
23	6	0	4.254104	-1.874932	1.854160
24	1	0	1.601665	-1.191869	1.086966
25	1	0	4.985833	-1.219686	2.331588
26	1	0	3.413439	-2.039020	2.528184
27	1	0	4.716160	-2.834989	1.614784
28	1	0	-0.287230	4.690624	2.727662
29	6	0	-0.444965	3.648027	2.466508
30	6	0	-1.451154	3.288688	1.570903
31	6	0	0.350640	2.646979	3.034167
32	6	0	-1.661161	1.949587	1.240307
33	1	0	-2.077231	4.053891	1.120267
34	6	0	0.138567	1.311327	2.712487
35	1	0	1.128158	2.910740	3.746813
36	6	0	-0.867306	0.932061	1.799610
37	1	0	-2.441459	1.695450	0.531478
38	1	0	0.725822	0.522064	3.170108
39	6	0	-1.061637	-0.501971	1.494036
40	6	0	-0.213200	-1.482590	1.869974
41	7	0	-2.286922	-0.792124	0.722131
42	6	0	-0.548651	-2.830985	1.657784
43	6	0	-3.553878	-0.955804	1.261560
44	6	0	-2.297905	-1.044779	-0.608427
45	7	0	-0.724264	-3.989784	1.578372
46	1	0	-3.749053	-0.811860	2.311909
47	6	0	-4.373588	-1.323394	0.241769
48	7	0	-3.580624	-1.371101	-0.897905
49	1	0	-1.109860	-1.077592	-1.416849
50	1	0	-5.425226	-1.563564	0.228192
51	6	0	-4.046466	-1.761247	-2.221459
52	1	0	-4.819882	-1.073358	-2.575545
53	1	0	-3.199960	-1.734978	-2.906771
54	1	0	-4.451397	-2.776556	-2.197125

(Z)-TS3

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

1	6	0	-0.061510	0.288927	-1.932526
2	6	0	2.730686	-0.963081	-0.746905
3	1	0	0.525428	-0.606127	-2.125369
4	6	0	-2.653189	-3.235315	-1.977214
5	6	0	-1.915501	-2.063364	-2.107787
6	6	0	-2.056896	-1.020494	-1.173047
7	6	0	-2.971220	-1.178893	-0.117203
8	6	0	-3.713064	-2.351076	0.004228
9	6	0	-3.558383	-3.382087	-0.923355
10	1	0	-2.534133	-4.028859	-2.708557
11	1	0	-1.241210	-1.939514	-2.948685
12	1	0	-3.071502	-0.400793	0.630974
13	1	0	-4.404840	-2.462785	0.833308
14	1	0	-4.140874	-4.293454	-0.828089
15	6	0	-1.269460	0.212083	-1.328331
16	6	0	0.547010	1.522199	-2.299481
17	7	0	1.006177	2.519536	-2.687064
18	1	0	-3.714241	1.545085	-1.858633
19	6	0	-3.056472	1.993949	-1.132612
20	6	0	-3.165484	3.140473	-0.413144
21	7	0	-1.837402	1.419406	-0.782895
22	1	0	-3.941493	3.889086	-0.393430
23	7	0	-2.017543	3.235137	0.365595
24	6	0	-1.214068	2.186771	0.141539
25	6	0	-1.687336	4.322981	1.287485
26	1	0	-0.128866	1.978257	0.696369
27	1	0	-2.449111	4.397684	2.066943
28	1	0	-0.718924	4.104860	1.737115
29	1	0	-1.625747	5.265981	0.740066
30	1	0	-1.927511	-3.103024	3.443354
31	6	0	-1.226813	-2.431770	2.954717
32	6	0	-0.307267	-2.923586	2.027264
33	6	0	-1.222939	-1.067994	3.260777
34	6	0	0.604959	-2.069496	1.408970
35	1	0	-0.299261	-3.981736	1.780127
36	6	0	-0.308663	-0.213831	2.650068
37	1	0	-1.916036	-0.674041	4.000083
38	6	0	0.621095	-0.693287	1.703517
39	1	0	1.300110	-2.458222	0.673923
40	1	0	-0.263523	0.835681	2.921710
41	6	0	1.588364	0.250807	1.093606
42	6	0	1.381282	1.588420	1.099119
43	7	0	2.760679	-0.358219	0.486045
44	6	0	2.359555	2.493613	0.640695

45	6	0	4.038976	-0.319945	1.033272
46	7	0	3.085437	3.364841	0.340776
47	1	0	4.248094	0.137120	1.987212
48	6	0	4.855433	-0.923454	0.134387
49	7	0	4.042290	-1.306225	-0.928997
50	1	0	5.920003	-1.099279	0.155180
51	6	0	4.525784	-1.966228	-2.128180
52	1	0	5.239079	-1.331748	-2.664651
53	1	0	5.013020	-2.916387	-1.884020
54	1	0	3.664799	-2.157058	-2.768302

(Z)-TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.618436	0.906168	0.838876
2	6	0	-2.242271	1.049823	0.672103
3	6	0	-1.513833	0.114348	-0.078050
4	6	0	-2.189238	-0.972876	-0.646667
5	6	0	-3.566200	-1.113301	-0.479353
6	6	0	-4.286079	-0.175398	0.262031
7	1	0	-4.167532	1.636538	1.425888
8	1	0	-1.722317	1.881110	1.137578
9	1	0	-1.627737	-1.700364	-1.220924
10	1	0	-4.077825	-1.957369	-0.932670
11	1	0	-5.358337	-0.288104	0.392607
12	6	0	-0.046612	0.310198	-0.258093
13	6	0	0.434778	1.562690	-0.597590
14	6	0	1.800020	1.901409	-0.690605
15	7	0	2.931757	2.190595	-0.748247
16	1	0	1.997806	-1.379645	-2.400091
17	6	0	1.917855	-1.192167	-1.340824
18	6	0	2.881152	-1.148721	-0.383467
19	7	0	0.691708	-1.019088	-0.689522
20	1	0	3.944069	-1.331220	-0.449451
21	7	0	2.268266	-0.823364	0.817505
22	6	0	0.912302	-0.782507	0.642209
23	6	0	2.961891	-0.516797	2.061192
24	1	0	-0.280869	2.361454	-0.752652
25	1	0	3.539887	0.404245	1.949319
26	1	0	2.210029	-0.384343	2.838528
27	1	0	3.628744	-1.336519	2.343144

(Z)-TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.314105	-0.181058	-0.891156
2	6	0	-0.527371	-1.231366	0.562848
3	7	0	-0.518142	1.046574	-0.878716
4	6	0	-0.588789	1.958957	0.155154
5	6	0	1.678005	-0.194229	1.172579
6	7	0	0.820154	-1.292409	0.846631
7	6	0	-5.072592	0.456980	-1.091832
8	6	0	-3.749753	0.176553	-1.439942
9	6	0	-2.751529	0.088209	-0.459429
10	6	0	-3.103841	0.318226	0.878417
11	6	0	-4.426711	0.592894	1.224540
12	6	0	-5.417694	0.661925	0.242962
13	1	0	-5.829423	0.516622	-1.868886
14	1	0	-3.484818	0.036456	-2.482303
15	1	0	-2.341555	0.287956	1.646471
16	1	0	-4.677742	0.761318	2.267746
17	1	0	-6.446366	0.879215	0.516532
18	6	0	-1.183729	-1.038401	-2.017126
19	6	0	0.012942	-1.364346	-2.666960
20	7	0	1.006377	-1.640300	-3.229162
21	1	0	0.352657	0.996191	-2.888605
22	6	0	0.199060	1.544278	-1.976108
23	6	0	0.612762	2.781967	-1.624159
24	1	0	1.194664	3.506683	-2.172952
25	7	0	0.123870	3.007653	-0.336292
26	6	0	0.330826	4.235596	0.411735
27	1	0	1.900144	1.570831	2.297744
28	1	0	-0.268092	4.171212	1.319660
29	1	0	1.386158	4.364433	0.677828
30	1	0	0.010527	5.103343	-0.173705
31	1	0	6.463296	0.045905	-1.254748
32	6	0	5.495668	-0.007318	-0.764511
33	6	0	4.411445	-0.600051	-1.412468
34	6	0	5.334987	0.506650	0.525241
35	6	0	3.168887	-0.675822	-0.786205
36	1	0	4.519862	-1.001632	-2.415050
37	6	0	4.098182	0.431956	1.157483

38	1	0	6.178815	0.949456	1.045886
39	6	0	2.991899	-0.145575	0.503758
40	1	0	2.338598	-1.123926	-1.319574
41	1	0	3.994880	0.793731	2.175682
42	6	0	1.288031	0.695134	2.114841
43	6	0	0.141142	0.553508	2.943480
44	6	0	1.224452	-2.609494	1.097713
45	7	0	-0.739753	0.438207	3.696907
46	1	0	2.242680	-2.855203	1.349378
47	6	0	0.114671	-3.370884	1.003601
48	7	0	-0.943285	-2.521169	0.700747
49	1	0	-2.022227	-1.687202	-2.237145
50	1	0	-0.025422	-4.431322	1.141421
51	6	0	-2.281097	-3.029151	0.420329
52	1	0	-2.443489	-3.924450	1.023182
53	1	0	-3.023820	-2.279573	0.682186
54	1	0	-2.378345	-3.280765	-0.640265

(Z)-TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.243892	-0.358467	0.852001
2	6	0	-0.703416	1.067715	0.527643
3	7	0	-0.292854	-1.335238	0.222894
4	6	0	0.406865	-1.077457	-0.900623
5	6	0	1.447222	0.894871	-0.956897
6	7	0	0.443137	1.515490	-0.068565
7	6	0	-4.789100	-1.613896	0.029676
8	6	0	-3.581822	-1.395480	0.694470
9	6	0	-2.612143	-0.543471	0.150378
10	6	0	-2.867241	0.062094	-1.088793
11	6	0	-4.076882	-0.154146	-1.750041
12	6	0	-5.044224	-0.990444	-1.192171
13	1	0	-5.529459	-2.275838	0.469742
14	1	0	-3.384667	-1.897628	1.634407
15	1	0	-2.122398	0.699019	-1.556743
16	1	0	-4.254346	0.330061	-2.705622
17	1	0	-5.984777	-1.160284	-1.708075
18	6	0	-1.313350	-0.568801	2.324163
19	6	0	-0.178965	-0.390222	3.116930
20	7	0	0.794153	-0.246698	3.765480

21	1	0	-0.691108	-3.037641	1.485947
22	6	0	-0.197981	-2.665886	0.604055
23	6	0	0.601686	-3.259763	-0.318117
24	1	0	0.936201	-4.281759	-0.406476
25	7	0	0.963732	-2.270738	-1.228668
26	6	0	1.845682	-2.479883	-2.367654
27	1	0	2.395737	1.357260	-2.819542
28	1	0	1.787250	-1.604623	-3.013332
29	1	0	2.879203	-2.621154	-2.038640
30	1	0	1.522086	-3.357754	-2.933361
31	1	0	5.932750	-0.834823	1.503490
32	6	0	5.029257	-0.488127	1.010789
33	6	0	3.909019	-0.131730	1.758800
34	6	0	4.977022	-0.403455	-0.383305
35	6	0	2.750036	0.315174	1.125004
36	1	0	3.910758	-0.205396	2.841452
37	6	0	3.818115	0.032584	-1.019302
38	1	0	5.841463	-0.680234	-0.980034
39	6	0	2.684607	0.407160	-0.273067
40	1	0	1.901254	0.570725	1.746200
41	1	0	3.801684	0.072280	-2.102911
42	6	0	1.508172	1.472982	-2.212837
43	6	0	0.369122	2.024851	-2.833982
44	6	0	0.555843	2.889508	0.131459
45	7	0	-0.587601	2.481613	-3.328325
46	1	0	1.391595	3.439971	-0.262315
47	6	0	-0.535542	3.288721	0.817039
48	7	0	-1.308362	2.168017	1.047677
49	1	0	-2.279286	-0.555061	2.806672
50	1	0	-0.838672	4.264737	1.157921
51	6	0	-2.549369	2.214999	1.819343
52	1	0	-2.792276	3.264475	1.987855
53	1	0	-3.358369	1.739524	1.265409
54	1	0	-2.402377	1.690412	2.764762

(Z)-P

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.740370	0.852063	-0.375095
2	6	0	-2.382700	1.140047	-0.487745
3	6	0	-1.414338	0.249677	0.009222

4	6	0	-1.848255	-0.950211	0.598951
5	6	0	-3.206311	-1.233907	0.715887
6	6	0	-4.157435	-0.333523	0.232706
7	1	0	-4.472480	1.546780	-0.775742
8	1	0	-2.067317	2.044483	-0.998036
9	1	0	-1.115356	-1.658973	0.967001
10	1	0	-3.522536	-2.162239	1.181992
11	1	0	-5.216124	-0.560208	0.316908
12	6	0	0.030359	0.578531	-0.065054
13	6	0	0.429723	1.880752	0.017583
14	6	0	1.746377	2.354836	-0.223464
15	7	0	2.814514	2.781794	-0.415610
16	1	0	1.925233	-3.224245	-1.658823
17	6	0	1.834251	-2.338028	-1.046291
18	6	0	2.727705	-1.858058	-0.115319
19	7	0	0.740273	-1.527949	-1.117109
20	1	0	3.676145	-2.231433	0.240443
21	7	0	2.174780	-0.708805	0.392559
22	6	0	0.964133	-0.539409	-0.255855
23	6	0	2.742167	0.044769	1.507209
24	1	0	-0.302215	2.649853	0.243120
25	1	0	3.490939	0.758992	1.158413
26	1	0	1.949501	0.592060	2.017428
27	1	0	3.195399	-0.655580	2.212001

IRC Structures of (Z)-TS2 at B3LYP/6-31G(d, p) Level (IRC-point 8 is transition state)

Table 3 The C2—H3 and H3—C4' bond lengths (unit: Å), E (electronic energies, unit: a.u.) of IRC-point n (n=1-15) at B3LYP/6-31G (d, p) level.

	C2—H3	H3—C4'	E
IRC-point 1	1.142	1.711	-1332.341369
IRC-point 2	1.159	1.677	-1332.340596
IRC-point 3	1.192	1.632	-1332.339505
IRC-point 4	1.235	1.581	-1332.338051
IRC-point 5	1.283	1.530	-1332.336483
IRC-point 6	1.333	1.478	-1332.335122
IRC-point 7	1.384	1.425	-1332.334223
IRC-point 8	1.437	1.374	-1332.333907
IRC-point 9	1.491	1.322	-1332.334192
IRC-point 10	1.541	1.277	-1332.334870

IRC-point 11	1.592	1.233	-1332.335784
IRC-point 12	1.640	1.197	-1332.336703
IRC-point 13	1.684	1.169	-1332.337520
IRC-point 14	1.722	1.153	-1332.338221
IRC-point 15	1.758	1.141	-1332.338816

IRC-point 1

C	-0.59562400	2.93483000	-2.76949000
C	-0.27273000	1.59975600	-2.55463200
C	0.74927100	1.24013500	-1.65409000
C	1.44647700	2.26693800	-0.99415700
C	1.12656600	3.60450500	-1.21951300
C	0.10544400	3.94603200	-2.10599700
H	-1.38429300	3.19136100	-3.47170800
H	-0.78452700	0.80721900	-3.09020700
H	2.22581800	2.02163100	-0.28022600
H	1.67110700	4.38135600	-0.69083900
H	-0.13941500	4.98919800	-2.28306200
C	1.05007600	-0.18841600	-1.45471000
C	0.23558000	-1.21644700	-1.75267300
C	0.71330700	-2.53640800	-1.70172100
N	1.06813500	-3.65204400	-1.77836400
H	3.77384900	0.04237300	-2.37177500
C	3.61871300	-0.35939800	-1.38406500
C	4.49754400	-0.85516800	-0.46826900
N	2.35497800	-0.46483900	-0.83086200
H	5.56881700	-0.97117400	-0.50459400
N	3.75038000	-1.25339800	0.62991400
C	2.45566800	-1.01030800	0.38541400
C	4.25538300	-1.87770800	1.85053400
H	1.61236700	-1.19208900	1.08026500
H	4.98783700	-1.22370300	2.32903300
H	3.41529300	-2.04126300	2.52543900
H	4.71685200	-2.83869300	1.61313500
H	-0.28175200	4.69038800	2.72668800
C	-0.44091200	3.64788700	2.46657500
C	-1.44774500	3.28963000	1.57173100
C	0.35447300	2.64643700	3.03369400
C	-1.65875600	1.95064600	1.24144600
H	-2.07267800	4.05503600	1.12037700
C	0.14155500	1.31107800	2.71228700
H	1.13322400	2.90948400	3.74499500
C	-0.86531000	0.93356700	1.80016700
H	-2.44000500	1.70078200	0.53169600

H	0.72981500	0.52184600	3.16826300
C	-1.05442600	-0.49972500	1.49724300
C	-0.21545600	-1.48447500	1.87181900
N	-2.28361300	-0.78963600	0.72489700
C	-0.54802700	-2.83113100	1.65790500
C	-3.54900100	-0.95326400	1.26069200
C	-2.31358600	-1.04533000	-0.59153800
N	-0.72582700	-3.98946400	1.57863200
H	-3.73988300	-0.80712600	2.31109900
C	-4.36992100	-1.32072400	0.24072300
N	-3.58170200	-1.37044500	-0.89942400
H	-1.39993000	-1.05485600	-1.27647700
H	-5.42115600	-1.56034100	0.22339500
C	-4.04753900	-1.76013200	-2.22338900
H	-4.81957600	-1.06909900	-2.57135000
H	-3.20218400	-1.73588100	-2.91042200
H	-4.45219700	-2.77450200	-2.19320300

IRC-point 2

C	-0.59582900	2.93481900	-2.76937600
C	-0.27294100	1.59964500	-2.55466400
C	0.74890900	1.24040100	-1.65380500
C	1.44638000	2.26708800	-0.99383400
C	1.12648700	3.60446500	-1.21925300
C	0.10528400	3.94579900	-2.10586800
H	-1.38463900	3.19127500	-3.47140100
H	-0.78526200	0.80812300	-3.09118200
H	2.22525300	2.02168000	-0.27944600
H	1.67080200	4.38135200	-0.69045800
H	-0.13959600	4.98895000	-2.28292100
C	1.05063400	-0.18753500	-1.45428300
C	0.23143900	-1.21544400	-1.74561000
C	0.71211100	-2.53679000	-1.70160900
N	1.06888500	-3.65150600	-1.77880900
H	3.77441000	0.04259500	-2.37208600
C	3.61875900	-0.35908000	-1.38440700
C	4.49720300	-0.85460800	-0.46830800
N	2.35447500	-0.46581900	-0.83198900
H	5.56855200	-0.97004000	-0.50433300
N	3.74968100	-1.25296600	0.62983500
C	2.45485300	-1.01062000	0.38555300
C	4.25518100	-1.87737700	1.85065900
H	1.61064000	-1.19203400	1.08084700
H	4.98760800	-1.22316300	2.32886200

H	3.41513500	-2.04110600	2.52557100
H	4.71673000	-2.83817900	1.61274100
H	-0.28231100	4.69033400	2.72710600
C	-0.44119400	3.64784800	2.46670300
C	-1.44801600	3.28943400	1.57179800
C	0.35424000	2.64640600	3.03379900
C	-1.65889700	1.95042000	1.24142500
H	-2.07324500	4.05482400	1.12076600
C	0.14136800	1.31096300	2.71229000
H	1.13277200	2.90948800	3.74535500
C	-0.86546500	0.93312800	1.80005700
H	-2.44017700	1.69985500	0.53198300
H	0.72938900	0.52173900	3.16862900
C	-1.05604600	-0.50033000	1.49652200
C	-0.21470100	-1.48396700	1.87105800
N	-2.28388000	-0.79025500	0.72352500
C	-0.54806700	-2.83107300	1.65774400
C	-3.54965100	-0.95366500	1.26094000
C	-2.30718300	-1.04509100	-0.59685100
N	-0.72539000	-3.98950900	1.57843700
H	-3.74087000	-0.80793400	2.31145600
C	-4.37033200	-1.32098300	0.24120900
N	-3.58044800	-1.37011600	-0.89907800
H	-1.37277300	-1.05994000	-1.28224600
H	-5.42169000	-1.56069800	0.22420300
C	-4.04772700	-1.75995300	-2.22235200
H	-4.81996400	-1.06947500	-2.57131400
H	-3.20249500	-1.73535600	-2.90949900
H	-4.45232000	-2.77448000	-2.19328000

IRC-point 3

C	-0.59590100	2.93478500	-2.76935400
C	-0.27299200	1.59951500	-2.55469800
C	0.74867000	1.24057500	-1.65357600
C	1.44629900	2.26721900	-0.99352100
C	1.12638500	3.60444200	-1.21901200
C	0.10516000	3.94561400	-2.10579800
H	-1.38478200	3.19109300	-3.47126300
H	-0.78587800	0.80899300	-3.09206800
H	2.22477400	2.02182100	-0.27873600
H	1.67048900	4.38133100	-0.69009400
H	-0.13975300	4.98873800	-2.28285700
C	1.05133400	-0.18663700	-1.45394300
C	0.22830600	-1.21462800	-1.74078000

C	0.71152500	-2.53736500	-1.70163700
N	1.06956400	-3.65112900	-1.77892800
H	3.77498300	0.04283400	-2.37204200
C	3.61891100	-0.35875500	-1.38438900
C	4.49700400	-0.85412500	-0.46805000
N	2.35406100	-0.46640600	-0.83263700
H	5.56840800	-0.96911100	-0.50386500
N	3.74915600	-1.25256600	0.63003000
C	2.45428400	-1.01079600	0.38600300
C	4.25496000	-1.87705600	1.85110000
H	1.60890500	-1.19202700	1.08179000
H	4.98730700	-1.22264600	2.32908900
H	3.41484500	-2.04088100	2.52589400
H	4.71657900	-2.83769900	1.61276900
H	-0.28301700	4.69033200	2.72737500
C	-0.44167000	3.64784400	2.46675400
C	-1.44842500	3.28928200	1.57173800
C	0.35378700	2.64643600	3.03389900
C	-1.65917600	1.95025400	1.24129200
H	-2.07386000	4.05466100	1.12089900
C	0.14100600	1.31094200	2.71231800
H	1.13211200	2.90959800	3.74569000
C	-0.86570300	0.93282800	1.79996600
H	-2.44035900	1.69896200	0.53206000
H	0.72881300	0.52169600	3.16895000
C	-1.05738300	-0.50076700	1.49591500
C	-0.21420600	-1.48360700	1.87062000
N	-2.28441400	-0.79069000	0.72284400
C	-0.54820300	-2.83104900	1.65765900
C	-3.55052200	-0.95403300	1.26117900
C	-2.30267800	-1.04487800	-0.60106000
N	-0.72514600	-3.98956700	1.57830700
H	-3.74242500	-0.80871600	2.31171700
C	-4.37101200	-1.32130500	0.24155300
N	-3.58007300	-1.37003400	-0.89874200
H	-1.33450000	-1.06432800	-1.29620100
H	-5.42246400	-1.56109700	0.22518400
C	-4.04767800	-1.75993600	-2.22182700
H	-4.82010300	-1.07001900	-2.57189800
H	-3.20230400	-1.73498100	-2.90872900
H	-4.45230100	-2.77460700	-2.19387700
IRC-point 4			
C	-0.59596600	2.93471500	-2.76938400

C	-0.27300400	1.59936900	-2.55472900
C	0.74849000	1.24068500	-1.65339700
C	1.44618900	2.26734100	-0.99325100
C	1.12622200	3.60444100	-1.21882200
C	0.10499900	3.94545700	-2.10577800
H	-1.38487100	3.19085000	-3.47122400
H	-0.78637500	0.80967600	-3.09276700
H	2.22434500	2.02201400	-0.27814200
H	1.67013100	4.38133100	-0.68980400
H	-0.13996500	4.98854700	-2.28285900
C	1.05196800	-0.18583600	-1.45363700
C	0.22600900	-1.21402900	-1.73738700
C	0.71127400	-2.53796300	-1.70164400
N	1.07017600	-3.65082400	-1.77886500
H	3.77546900	0.04308900	-2.37184000
C	3.61907800	-0.35842500	-1.38421000
C	4.49688200	-0.85366000	-0.46767200
N	2.35373200	-0.46674000	-0.83299700
H	5.56833200	-0.96828900	-0.50332800
N	3.74876600	-1.25216100	0.63033900
C	2.45389400	-1.01085600	0.38652000
C	4.25476700	-1.87669000	1.85164200
H	1.60731800	-1.19201500	1.08280300
H	4.98700800	-1.22210100	2.32947200
H	3.41455100	-2.04057900	2.52628900
H	4.71645900	-2.83719800	1.61300700
H	-0.28378600	4.69036600	2.72752200
C	-0.44224300	3.64786700	2.46674900
C	-1.44890500	3.28915500	1.57161700
C	0.35324000	2.64651200	3.03397400
C	-1.65952200	1.95011500	1.24112300
H	-2.07449900	4.05451300	1.12088300
C	0.14057500	1.31098300	2.71235200
H	1.13138600	2.90977800	3.74596200
C	-0.86598100	0.93262000	1.79989200
H	-2.44055900	1.69817300	0.53203200
H	0.72822200	0.52171700	3.16921900
C	-1.05843900	-0.50108400	1.49544300
C	-0.21388100	-1.48334100	1.87037700
N	-2.28495500	-0.79102400	0.72252800
C	-0.54832300	-2.83103300	1.65764200
C	-3.55131700	-0.95438500	1.26135200
C	-2.30010800	-1.04476300	-0.60382900
N	-0.72495700	-3.98961900	1.57826200

H	-3.74392000	-0.80941400	2.31187300
C	-4.37164200	-1.32167400	0.24175300
N	-3.58005800	-1.37012500	-0.89847400
H	-1.29114100	-1.06782500	-1.31610500
H	-5.42315700	-1.56153900	0.22602800
C	-4.04752100	-1.76007300	-2.22157000
H	-4.82014400	-1.07064000	-2.57260300
H	-3.20195100	-1.73481300	-2.90817200
H	-4.45220600	-2.77487400	-2.19453900

IRC-point 5

C	-0.59604300	2.93461600	-2.76944300
C	-0.27300600	1.59921800	-2.55475900
C	0.74834200	1.24075900	-1.65325000
C	1.44605200	2.26746100	-0.99301300
C	1.12600800	3.60445800	-1.21866900
C	0.10480000	3.94531900	-2.10578900
H	-1.38495400	3.19057600	-3.47125000
H	-0.78678500	0.81018700	-3.09331600
H	2.22394000	2.02223800	-0.27764300
H	1.66972500	4.38134500	-0.68957600
H	-0.14023000	4.98837000	-2.28290300
C	1.05252400	-0.18513100	-1.45334900
C	0.22431100	-1.21358500	-1.73485800
C	0.71120600	-2.53852400	-1.70161700
N	1.07075200	-3.65055800	-1.77871200
H	3.77588600	0.04336800	-2.37157200
C	3.61924200	-0.35808800	-1.38395100
C	4.49680800	-0.85319300	-0.46723500
N	2.35346800	-0.46692200	-0.83318400
H	5.56828800	-0.96751700	-0.50276000
N	3.74846700	-1.25174400	0.63070600
C	2.45361100	-1.01083500	0.38704200
C	4.25460100	-1.87628200	1.85222000
H	1.60590100	-1.19198000	1.08378800
H	4.98672900	-1.22152400	2.32993000
H	3.41428900	-2.04022000	2.52670900
H	4.71637600	-2.83667100	1.61336000
H	-0.28459400	4.69042800	2.72759600
C	-0.44287000	3.64790100	2.46670900
C	-1.44942700	3.28903800	1.57146600
C	0.35264300	2.64661500	3.03402900
C	-1.65990200	1.94998300	1.24093900
H	-2.07515400	4.05436300	1.12078300

C	0.14011300	1.31105400	2.71238600
H	1.13063200	2.90999800	3.74618900
C	-0.86628400	0.93246100	1.79982600
H	-2.44076500	1.69747400	0.53195000
H	0.72764500	0.52178100	3.16945200
C	-1.05930200	-0.50133200	1.49506800
C	-0.21365800	-1.48313200	1.87023900
N	-2.28545000	-0.79131100	0.72238600
C	-0.54841200	-2.83102100	1.65766600
C	-3.55200300	-0.95473400	1.26146000
C	-2.29886800	-1.04473100	-0.60552600
N	-0.72477800	-3.98966300	1.57827100
H	-3.74524900	-0.81004200	2.31194500
C	-4.37217100	-1.32207800	0.24184000
N	-3.58016000	-1.37031900	-0.89827300
H	-1.24643000	-1.07065700	-1.33937500
H	-5.42370600	-1.56201000	0.22669000
C	-4.04730000	-1.76031100	-2.22145800
H	-4.82011000	-1.07130100	-2.57329400
H	-3.20155800	-1.73479300	-2.90774000
H	-4.45205000	-2.77524200	-2.19516500

IRC-point 6

C	-0.59614000	2.93450100	-2.76951100
C	-0.27301700	1.59905700	-2.55479300
C	0.74820100	1.24080100	-1.65310200
C	1.44590100	2.26759600	-0.99278500
C	1.12576600	3.60447700	-1.21853100
C	0.10456900	3.94518200	-2.10581300
H	-1.38501800	3.19028400	-3.47128700
H	-0.78714300	0.81062500	-3.09379100
H	2.22354900	2.02246400	-0.27714400
H	1.66931400	4.38138700	-0.68934700
H	-0.14051100	4.98819400	-2.28295700
C	1.05301100	-0.18446000	-1.45307700
C	0.22289800	-1.21324400	-1.73245500
C	0.71119900	-2.53904000	-1.70157600
N	1.07133400	-3.65028400	-1.77853000
H	3.77628700	0.04365000	-2.37124900
C	3.61941400	-0.35773500	-1.38366800
C	4.49675100	-0.85270800	-0.46678300
N	2.35321600	-0.46705300	-0.83334800
H	5.56828200	-0.96675300	-0.50216000
N	3.74820000	-1.25130400	0.63108900

C	2.45338200	-1.01078300	0.38756100
C	4.25445800	-1.87584000	1.85281000
H	1.60439900	-1.19195300	1.08486600
H	4.98644700	-1.22092600	2.33042300
H	3.41402100	-2.03984400	2.52716700
H	4.71630500	-2.83612300	1.61376300
H	-0.28543300	4.69047500	2.72764100
C	-0.44352600	3.64794100	2.46665700
C	-1.44997300	3.28891800	1.57130500
C	0.35202500	2.64673000	3.03407700
C	-1.66029800	1.94984900	1.24075400
H	-2.07582500	4.05420500	1.12065500
C	0.13964100	1.31114000	2.71241900
H	1.12985200	2.91023100	3.74640000
C	-0.86659100	0.93231600	1.79976800
H	-2.44100700	1.69678300	0.53182800
H	0.72705700	0.52186100	3.16968000
C	-1.06011100	-0.50156400	1.49472100
C	-0.21345300	-1.48294400	1.87014500
N	-2.28594700	-0.79159900	0.72227800
C	-0.54847700	-2.83101000	1.65770700
C	-3.55261300	-0.95508700	1.26154200
C	-2.29807700	-1.04477300	-0.60663900
N	-0.72458100	-3.98970700	1.57830200
H	-3.74654800	-0.81064600	2.31197400
C	-4.37263100	-1.32250400	0.24188400
N	-3.58021800	-1.37055300	-0.89812500
H	-1.20229200	-1.07270200	-1.36556800
H	-5.42424200	-1.56249700	0.22723100
C	-4.04705900	-1.76061000	-2.22137900
H	-4.82008400	-1.07196900	-2.57401400
H	-3.20104600	-1.73481500	-2.90740900
H	-4.45188100	-2.77565300	-2.19579800

IRC-point 7

C	-0.59619300	2.93439700	-2.76959600
C	-0.27298800	1.59891800	-2.55482900
C	0.74810500	1.24086500	-1.65298200
C	1.44575600	2.26771400	-0.99256000
C	1.12553900	3.60451000	-1.21839200
C	0.10437700	3.94506700	-2.10584000
H	-1.38507000	3.18999900	-3.47135100
H	-0.78746000	0.81101900	-3.09423100
H	2.22317900	2.02270500	-0.27670400

H	1.66889000	4.38142800	-0.68914700
H	-0.14079600	4.98803300	-2.28302800
C	1.05352000	-0.18382900	-1.45279500
C	0.22152300	-1.21287800	-1.73059300
C	0.71126000	-2.53955900	-1.70152800
N	1.07187300	-3.65005500	-1.77832200
H	3.77664600	0.04393900	-2.37090400
C	3.61957700	-0.35740300	-1.38333000
C	4.49670300	-0.85225400	-0.46627600
N	2.35301200	-0.46712500	-0.83339200
H	5.56826000	-0.96602900	-0.50155700
N	3.74794900	-1.25089400	0.63151800
C	2.45316500	-1.01071000	0.38808600
C	4.25428300	-1.87542000	1.85343000
H	1.60310300	-1.19192700	1.08582600
H	4.98615700	-1.22034400	2.33093900
H	3.41374500	-2.03945800	2.52762500
H	4.71623500	-2.83558600	1.61420600
H	-0.28627100	4.69054800	2.72765700
C	-0.44420000	3.64797900	2.46659100
C	-1.45052900	3.28881100	1.57112100
C	0.35137500	2.64684200	3.03412000
C	-1.66070800	1.94972900	1.24054500
H	-2.07649100	4.05406100	1.12048500
C	0.13913400	1.31122400	2.71244900
H	1.12906500	2.91046900	3.74658800
C	-0.86693000	0.93219400	1.79969200
H	-2.44121500	1.69615200	0.53167400
H	0.72648500	0.52195100	3.16986700
C	-1.06084900	-0.50175900	1.49439700
C	-0.21333400	-1.48277600	1.87005800
N	-2.28640000	-0.79184500	0.72218000
C	-0.54857000	-2.83099800	1.65773300
C	-3.55322600	-0.95542200	1.26154800
C	-2.29779400	-1.04475100	-0.60769300
N	-0.72444400	-3.98974400	1.57831900
H	-3.74772200	-0.81122800	2.31194800
C	-4.37309900	-1.32291400	0.24183800
N	-3.58040900	-1.37079700	-0.89801800
H	-1.15545800	-1.07604600	-1.38803500
H	-5.42471200	-1.56299900	0.22772100
C	-4.04679200	-1.76089100	-2.22141400
H	-4.82000900	-1.07262000	-2.57472600
H	-3.20059500	-1.73489000	-2.90711800

H	-4.45167300	-2.77606400	-2.19641400
IRC-point 8			
C	-0.59623500	2.93425300	-2.76969600
C	-0.27294700	1.59874600	-2.55487000
C	0.74802300	1.24090600	-1.65284600
C	1.44560800	2.26784800	-0.99230100
C	1.12529100	3.60453700	-1.21823800
C	0.10417000	3.94492600	-2.10587700
H	-1.38507700	3.18966800	-3.47145600
H	-0.78779800	0.81139900	-3.09465100
H	2.22278100	2.02295800	-0.27618900
H	1.66843400	4.38147400	-0.68890800
H	-0.14108200	4.98784600	-2.28311400
C	1.05415700	-0.18309600	-1.45247100
C	0.22093400	-1.21260900	-1.72878700
C	0.71136200	-2.54014500	-1.70145000
N	1.07254100	-3.64983600	-1.77805800
H	3.77708100	0.04426000	-2.37047100
C	3.61978200	-0.35703100	-1.38292100
C	4.49667300	-0.85174100	-0.46567100
N	2.35280600	-0.46719900	-0.83339500
H	5.56826800	-0.96523000	-0.50080600
N	3.74769900	-1.25042900	0.63203300
C	2.45294800	-1.01062400	0.38869600
C	4.25410300	-1.87493300	1.85416000
H	1.60166500	-1.19187000	1.08696600
H	4.98583200	-1.21968800	2.33158800
H	3.41343800	-2.03902100	2.52818400
H	4.71615900	-2.83499000	1.61478400
H	-0.28722900	4.69062400	2.72766300
C	-0.44496400	3.64802700	2.46650800
C	-1.45115300	3.28868800	1.57090300
C	0.35064000	2.64697900	3.03416700
C	-1.66116100	1.94958700	1.24030700
H	-2.07723000	4.05389100	1.12026700
C	0.13856700	1.31132700	2.71248700
H	1.12815800	2.91073900	3.74681300
C	-0.86730600	0.93206100	1.79961000
H	-2.44145900	1.69545000	0.53147800
H	0.72582200	0.52206300	3.17010800
C	-1.06163700	-0.50197100	1.49403600
C	-0.21320100	-1.48259000	1.86997400
N	-2.28692200	-0.79212400	0.72213100

C	-0.54865200	-2.83098500	1.65778400
C	-3.55387800	-0.95580300	1.26156000
C	-2.29790500	-1.04477800	-0.60842700
N	-0.72426500	-3.98978400	1.57837200
H	-3.74905300	-0.81185900	2.31190900
C	-4.37358800	-1.32339300	0.24176900
N	-3.58062400	-1.37110000	-0.89790500
H	-1.10986000	-1.07759200	-1.41684900
H	-5.42522600	-1.56356300	0.22819100
C	-4.04646600	-1.76124600	-2.22145900
H	-4.81988200	-1.07335700	-2.57554500
H	-3.19996000	-1.73497700	-2.90677100
H	-4.45139800	-2.77655500	-2.19712600

IRC-point 9

C	-0.59624600	2.93410900	-2.76980400
C	-0.27287800	1.59857400	-2.55491500
C	0.74796000	1.24095000	-1.65270400
C	1.44547100	2.26798400	-0.99202100
C	1.12505800	3.60456200	-1.21806500
C	0.10398800	3.94478400	-2.10591100
H	-1.38504200	3.18933800	-3.47158000
H	-0.78812500	0.81179700	-3.09508700
H	2.22238000	2.02321200	-0.27563700
H	1.66798500	4.38151900	-0.68864100
H	-0.14133800	4.98766100	-2.28320000
C	1.05486100	-0.18231900	-1.45212800
C	0.22061400	-1.21235300	-1.72700100
C	0.71147100	-2.54075600	-1.70137000
N	1.07324700	-3.64962300	-1.77778700
H	3.77755800	0.04458900	-2.36999000
C	3.62000400	-0.35665100	-1.38247100
C	4.49664400	-0.85121800	-0.46501400
N	2.35260400	-0.46728000	-0.83337800
H	5.56828000	-0.96441800	-0.49997700
N	3.74743300	-1.24995800	0.63259200
C	2.45271400	-1.01054200	0.38934200
C	4.25389900	-1.87444200	1.85494300
H	1.60018200	-1.19180500	1.08814300
H	4.98547400	-1.21902500	2.33230200
H	3.41309500	-2.03858200	2.52878600
H	4.71605800	-2.83439100	1.61542100
H	-0.28823000	4.69069700	2.72767100
C	-0.44576300	3.64807400	2.46642000

C	-1.45180100	3.28856100	1.57066600
C	0.34986500	2.64711400	3.03422000
C	-1.66163000	1.94944100	1.24004600
H	-2.07798900	4.05371700	1.12002800
C	0.13796500	1.31142700	2.71252500
H	1.12719600	2.91100700	3.74706100
C	-0.86770500	0.93192100	1.79951300
H	-2.44171200	1.69473400	0.53125300
H	0.72510900	0.52217400	3.17037000
C	-1.06246300	-0.50218900	1.49364300
C	-0.21307800	-1.48239700	1.86987200
N	-2.28747500	-0.79240700	0.72206300
C	-0.54875200	-2.83097300	1.65782200
C	-3.55456800	-0.95619300	1.26154300
C	-2.29807600	-1.04479500	-0.60918300
N	-0.72409700	-3.98982500	1.57840800
H	-3.75045600	-0.81251000	2.31183600
C	-4.37410500	-1.32388000	0.24166100
N	-3.58086000	-1.37140400	-0.89781700
H	-1.06455900	-1.07909200	-1.44570600
H	-5.42577000	-1.56413400	0.22862800
C	-4.04611400	-1.76159700	-2.22154200
H	-4.81972300	-1.07409900	-2.57644100
H	-3.19926300	-1.73504200	-2.90642600
H	-4.45109100	-2.77704500	-2.19791200

IRC-point 10

C	-0.59620100	2.93396500	-2.76991400
C	-0.27277600	1.59840600	-2.55496800
C	0.74793100	1.24099600	-1.65256000
C	1.44537000	2.26811700	-0.99171700
C	1.12486300	3.60458300	-1.21787600
C	0.10385800	3.94463500	-2.10594100
H	-1.38494300	3.18901300	-3.47171600
H	-0.78844300	0.81220200	-3.09551600
H	2.22200800	2.02344000	-0.27504300
H	1.66757300	4.38155400	-0.68834200
H	-0.14153200	4.98746600	-2.28327800
C	1.05566800	-0.18150500	-1.45176700
C	0.22094400	-1.21214700	-1.72535700
C	0.71157700	-2.54139300	-1.70128200
N	1.07399600	-3.64944400	-1.77751300
H	3.77807400	0.04491300	-2.36948600
C	3.62025300	-0.35628600	-1.38199100

C	4.49661900	-0.85071400	-0.46430200
N	2.35241700	-0.46738500	-0.83332400
H	5.56829400	-0.96361800	-0.49908300
N	3.74715700	-1.24950400	0.63319200
C	2.45246500	-1.01048300	0.39002800
C	4.25366900	-1.87397100	1.85577100
H	1.59868800	-1.19173300	1.08933300
H	4.98509000	-1.21838800	2.33307000
H	3.41272600	-2.03816100	2.52942600
H	4.71593300	-2.83381400	1.61611400
H	-0.28923600	4.69076600	2.72768400
C	-0.44656200	3.64812000	2.46633100
C	-1.45244100	3.28843800	1.57041500
C	0.34907800	2.64724500	3.03427800
C	-1.66209400	1.94929800	1.23976600
H	-2.07873700	4.05354700	1.11977100
C	0.13734900	1.31152000	2.71256700
H	1.12620800	2.91126300	3.74732700
C	-0.86811000	0.93177700	1.79940600
H	-2.44195900	1.69401200	0.53099600
H	0.72436500	0.52227700	3.17064900
C	-1.06331200	-0.50241500	1.49322200
C	-0.21296200	-1.48219700	1.86974200
N	-2.28806600	-0.79268500	0.72199100
C	-0.54887500	-2.83095900	1.65784900
C	-3.55529600	-0.95657400	1.26151400
C	-2.29832900	-1.04478900	-0.60993300
N	-0.72394800	-3.98986400	1.57843400
H	-3.75191600	-0.81316200	2.31175200
C	-4.37465600	-1.32435400	0.24153000
N	-3.58113500	-1.37169300	-0.89774200
H	-1.02373900	-1.07979700	-1.47475800
H	-5.42634800	-1.56469200	0.22904700
C	-4.04574600	-1.76192300	-2.22164900
H	-4.81952600	-1.07482200	-2.57738800
H	-3.19849700	-1.73506300	-2.90604200
H	-4.45075400	-2.77751000	-2.19874900

IRC-point 11

C	-0.59606600	2.93380500	-2.77004100
C	-0.27260500	1.59822200	-2.55503000
C	0.74795200	1.24106500	-1.65239700
C	1.44530400	2.26825400	-0.99134200
C	1.12471000	3.60459200	-1.21763300

C	0.10379800	3.94445900	-2.10596300
H	-1.38475300	3.18866100	-3.47187800
H	-0.78879900	0.81269500	-3.09600400
H	2.22161700	2.02366800	-0.27432500
H	1.66716600	4.38158300	-0.68796000
H	-0.14166500	4.98724300	-2.28335700
C	1.05674600	-0.18051900	-1.45131100
C	0.22226300	-1.21196800	-1.72365800
C	0.71167900	-2.54216800	-1.70116800
N	1.07490000	-3.64930100	-1.77720700
H	3.77871300	0.04525600	-2.36886800
C	3.62055800	-0.35590300	-1.38140500
C	4.49659000	-0.85017600	-0.46343400
N	2.35223200	-0.46754900	-0.83321300
H	5.56831100	-0.96273700	-0.49798700
N	3.74682100	-1.24902600	0.63392600
C	2.45214600	-1.01045400	0.39084700
C	4.25337200	-1.87347700	1.85676500
H	1.59699300	-1.19164900	1.09067900
H	4.98462200	-1.21770500	2.33400100
H	3.41226700	-2.03771800	2.53020300
H	4.71575800	-2.83320200	1.61695900
H	-0.29036600	4.69084000	2.72771000
C	-0.44745400	3.64816800	2.46623000
C	-1.45314700	3.28830300	1.57011400
C	0.34818300	2.64738200	3.03435400
C	-1.66260000	1.94913700	1.23942600
H	-2.07955500	4.05336400	1.11946800
C	0.13663900	1.31161200	2.71261700
H	1.12507100	2.91153200	3.74765400
C	-0.86857800	0.93160400	1.79926500
H	-2.44221000	1.69319400	0.53066500
H	0.72349800	0.52238500	3.17098600
C	-1.06432300	-0.50268100	1.49270800
C	-0.21284000	-1.48195200	1.86954400
N	-2.28879200	-0.79299200	0.72188700
C	-0.54904800	-2.83094200	1.65786300
C	-3.55618700	-0.95699000	1.26147300
C	-2.29864800	-1.04473100	-0.61084600
N	-0.72381200	-3.98990300	1.57844100
H	-3.75364800	-0.81391000	2.31165000
C	-4.37534800	-1.32486400	0.24137300
N	-3.58151200	-1.37198400	-0.89766500
H	-0.98433500	-1.07953000	-1.50785700

H	-5.42706700	-1.56530200	0.22952600
C	-4.04532000	-1.76224300	-2.22178900
H	-4.81926500	-1.07560000	-2.57852000
H	-3.19754400	-1.73501100	-2.90553500
H	-4.45033600	-2.77798600	-2.19975300

IRC-point 12

C	-0.59578900	2.93363000	-2.77018600
C	-0.27232100	1.59802200	-2.55510000
C	0.74807000	1.24118600	-1.65222000
C	1.44529500	2.26837900	-0.99087800
C	1.12464300	3.60457800	-1.21730600
C	0.10386700	3.94425900	-2.10596400
H	-1.38442400	3.18830800	-3.47207400
H	-0.78917500	0.81331700	-3.09655900
H	2.22120600	2.02387700	-0.27346200
H	1.66679400	4.38160700	-0.68745500
H	-0.14168000	4.98700200	-2.28341800
C	1.05824600	-0.17930800	-1.45070200
C	0.22524500	-1.21182100	-1.72206400
C	0.71177200	-2.54311500	-1.70101600
N	1.07601500	-3.64925900	-1.77688400
H	3.77951300	0.04560200	-2.36807800
C	3.62091000	-0.35552000	-1.38067700
C	4.49655300	-0.84961400	-0.46236900
N	2.35208700	-0.46780500	-0.83298600
H	5.56833800	-0.96178800	-0.49660900
N	3.74640100	-1.24854600	0.63483300
C	2.45171400	-1.01047100	0.39180900
C	4.25298000	-1.87298400	1.85796300
H	1.59514300	-1.19154100	1.09214200
H	4.98404400	-1.21700100	2.33514300
H	3.41168800	-2.03728200	2.53115600
H	4.71550800	-2.83259000	1.61800100
H	-0.29162400	4.69090700	2.72776500
C	-0.44843700	3.64821400	2.46612200
C	-1.45390700	3.28814900	1.56975500
C	0.34716900	2.64751200	3.03445600
C	-1.66313200	1.94895400	1.23901600
H	-2.08042800	4.05316500	1.11911400
C	0.13581500	1.31168200	2.71267100
H	1.12376100	2.91179100	3.74806600
C	-0.86912200	0.93138800	1.79907300
H	-2.44244400	1.69229900	0.53023700

H	0.72247500	0.52249800	3.17140300
C	-1.06553900	-0.50300300	1.49208600
C	-0.21272800	-1.48164000	1.86921400
N	-2.28969800	-0.79333200	0.72172000
C	-0.54929100	-2.83090900	1.65784600
C	-3.55729900	-0.95744500	1.26141200
C	-2.29904100	-1.04456200	-0.61203800
N	-0.72370200	-3.98994100	1.57840800
H	-3.75568900	-0.81477900	2.31151500
C	-4.37625000	-1.32539900	0.24120700
N	-3.58206600	-1.37225300	-0.89758100
H	-0.95069900	-1.07771000	-1.54471800
H	-5.42798600	-1.56597000	0.23006700
C	-4.04484200	-1.76251500	-2.22196300
H	-4.81890800	-1.07639900	-2.57987900
H	-3.19635800	-1.73481900	-2.90483400
H	-4.44979900	-2.77843500	-2.20096600

IRC-point 13

C	-0.59535800	2.93344400	-2.77034700
C	-0.27193200	1.59782500	-2.55518900
C	0.74830400	1.24138600	-1.65205700
C	1.44535400	2.26849900	-0.99032700
C	1.12466300	3.60455300	-1.21690600
C	0.10407800	3.94402900	-2.10594700
H	-1.38393600	3.18795900	-3.47229500
H	-0.78952400	0.81402200	-3.09717700
H	2.22081300	2.02402600	-0.27245400
H	1.66647000	4.38162000	-0.68683100
H	-0.14155500	4.98672800	-2.28345600
C	1.06023900	-0.17789700	-1.44991400
C	0.22980200	-1.21167300	-1.72075100
C	0.71187900	-2.54426200	-1.70080700
N	1.07734900	-3.64937300	-1.77659200
H	3.78041100	0.04595600	-2.36713800
C	3.62131400	-0.35515100	-1.37980900
C	4.49649200	-0.84904700	-0.46109600
N	2.35201900	-0.46813400	-0.83258300
H	5.56834000	-0.96078600	-0.49494800
N	3.74590000	-1.24807900	0.63591300
C	2.45117700	-1.01054400	0.39292200
C	4.25248200	-1.87249900	1.85934700
H	1.59315700	-1.19138600	1.09365400
H	4.98334500	-1.21629500	2.33648900

H	3.41099500	-2.03686000	2.53228700
H	4.71517300	-2.83198000	1.61925900
H	-0.29299600	4.69096500	2.72783900
C	-0.44949900	3.64825700	2.46600100
C	-1.45470900	3.28798600	1.56933400
C	0.34604800	2.64763700	3.03457700
C	-1.66368300	1.94875400	1.23853100
H	-2.08134000	4.05295000	1.11870000
C	0.13488800	1.31173000	2.71273000
H	1.12229400	2.91202700	3.74855800
C	-0.86974700	0.93113100	1.79882100
H	-2.44266800	1.69136800	0.52969500
H	0.72131500	0.52260000	3.17190700
C	-1.06695700	-0.50336900	1.49136000
C	-0.21263400	-1.48126100	1.86873500
N	-2.29079000	-0.79369700	0.72146400
C	-0.54960600	-2.83086300	1.65779300
C	-3.55863300	-0.95793100	1.26134300
C	-2.29949200	-1.04427700	-0.61349800
N	-0.72362400	-3.98996800	1.57834000
H	-3.75796200	-0.81574900	2.31138800
C	-4.37737900	-1.32594900	0.24104800
N	-3.58281200	-1.37248200	-0.89749400
H	-0.92337600	-1.07454600	-1.58418500
H	-5.42912200	-1.56669500	0.23063900
C	-4.04434500	-1.76272600	-2.22215500
H	-4.81846800	-1.07718300	-2.58143100
H	-3.19497100	-1.73447400	-2.90392900
H	-4.44914400	-2.77885000	-2.20234800

IRC-point 14

C	-0.59471300	2.93329100	-2.77049000
C	-0.27140900	1.59768400	-2.55528400
C	0.74876300	1.24177200	-1.65195100
C	1.44549300	2.26863600	-0.98964500
C	1.12479300	3.60454600	-1.21636600
C	0.10449800	3.94379800	-2.10585100
H	-1.38323200	3.18769500	-3.47249300
H	-0.78973500	0.81482000	-3.09781400
H	2.22045700	2.02407300	-0.27127800
H	1.66620400	4.38165200	-0.68599100
H	-0.14123100	4.98644900	-2.28338500
C	1.06298600	-0.17624800	-1.44889900
C	0.23633200	-1.21147600	-1.72030800

C	0.71213600	-2.54561500	-1.70052600
N	1.07894300	-3.64981800	-1.77625600
H	3.78133300	0.04636100	-2.36599800
C	3.62174700	-0.35479900	-1.37874700
C	4.49638500	-0.84848300	-0.45955100
N	2.35215300	-0.46848600	-0.83181800
H	5.56829800	-0.95975000	-0.49290000
N	3.74528800	-1.24766900	0.63720800
C	2.45050700	-1.01068600	0.39418800
C	4.25182700	-1.87205600	1.86091500
H	1.59112600	-1.19116400	1.09512000
H	4.98246900	-1.21563900	2.33806700
H	3.41016200	-2.03650100	2.53361000
H	4.71471500	-2.83141900	1.62077500
H	-0.29450300	4.69096100	2.72798800
C	-0.45065000	3.64825100	2.46590300
C	-1.45554800	3.28778400	1.56887900
C	0.34479500	2.64769000	3.03474100
C	-1.66424600	1.94851400	1.23797000
H	-2.08228200	4.05269000	1.11824900
C	0.13382300	1.31169100	2.71279000
H	1.12062800	2.91214400	3.74916800
C	-0.87048700	0.93079400	1.79847800
H	-2.44289600	1.69048700	0.52901100
H	0.71996700	0.52264700	3.17249700
C	-1.06860800	-0.50380500	1.49050700
C	-0.21261900	-1.48081700	1.86793800
N	-2.29213700	-0.79410500	0.72100800
C	-0.55000100	-2.83079900	1.65762000
C	-3.56025100	-0.95849100	1.26124200
C	-2.30009000	-1.04375800	-0.61535400
N	-0.72358200	-3.98998300	1.57815400
H	-3.76033600	-0.81689500	2.31127400
C	-4.37886200	-1.32652400	0.24093800
N	-3.58391300	-1.37261700	-0.89742600
H	-0.90426600	-1.06999800	-1.62393600
H	-5.43058100	-1.56754800	0.23118400
C	-4.04390500	-1.76279900	-2.22237000
H	-4.81797300	-1.07785600	-2.58318600
H	-3.19341900	-1.73386100	-2.90273700
H	-4.44834000	-2.77917700	-2.20390800
IRC-point 15			
C	-0.59394600	2.93316200	-2.77063300

C	-0.27078600	1.59758400	-2.55539400
C	0.74942900	1.24227400	-1.65190900
C	1.44568800	2.26881400	-0.98889000
C	1.12498500	3.60458500	-1.21572800
C	0.10504500	3.94358900	-2.10571400
H	-1.38240700	3.18751100	-3.47268700
H	-0.78977800	0.81562000	-3.09847800
H	2.22012700	2.02409200	-0.27003600
H	1.66594100	4.38174400	-0.68501300
H	-0.14079400	4.98620400	-2.28326500
C	1.06624200	-0.17453100	-1.44780100
C	0.24354000	-1.21116700	-1.72071900
C	0.71261300	-2.54715100	-1.70021000
N	1.08067500	-3.65052500	-1.77594900
H	3.78217300	0.04679900	-2.36466200
C	3.62220800	-0.35446400	-1.37750800
C	4.49625200	-0.84792800	-0.45780300
N	2.35249900	-0.46875600	-0.83072200
H	5.56823100	-0.95873600	-0.49056400
N	3.74461500	-1.24731100	0.63866400
C	2.44979100	-1.01086200	0.39558500
C	4.25106100	-1.87163200	1.86260400
H	1.58902500	-1.19092700	1.09660100
H	4.98146800	-1.21499700	2.33979600
H	3.40922400	-2.03616800	2.53506200
H	4.71417200	-2.83088300	1.62247700
H	-0.29610400	4.69093100	2.72816800
C	-0.45187300	3.64821800	2.46580900
C	-1.45642500	3.28756200	1.56838700
C	0.34343800	2.64768900	3.03491600
C	-1.66483400	1.94825500	1.23734100
H	-2.08325400	4.05240900	1.11774100
C	0.13264300	1.31159200	2.71283600
H	1.11882900	2.91217900	3.74983700
C	-0.87133000	0.93040900	1.79806400
H	-2.44314200	1.68969300	0.52821500
H	0.71849000	0.52264800	3.17312300
C	-1.07039500	-0.50425300	1.48956200
C	-0.21269800	-1.48033900	1.86688300
N	-2.29366700	-0.79452700	0.72040700
C	-0.55043900	-2.83071400	1.65734300
C	-3.56202700	-0.95911400	1.26111400
C	-2.30083700	-1.04310000	-0.61736500
N	-0.72355400	-3.98996800	1.57790400

H	-3.76263900	-0.81815300	2.31117500
C	-4.38058300	-1.32712400	0.24086900
N	-3.58526800	-1.37267200	-0.89738700
H	-0.88658300	-1.06557000	-1.66188300
H	-5.43225200	-1.56850400	0.23167500
C	-4.04358300	-1.76278600	-2.22259600
H	-4.81755000	-1.07845200	-2.58503200
H	-3.19185600	-1.73308100	-2.90139100
H	-4.44751100	-2.77946200	-2.20552800

IRC Structures of (Z)-TS3 at B3LYP/6-31G(d, p) Level (IRC-point 4 is transition state)

Table 4 The C2'—H3' and H3'—C4 bond lengths (unit: Å), E (electronic energies, unit: a.u.) of IRC-point n (n=1-13) at B3LYP/6-31G (d, p) level.

	C2'—H3'	H3'—C4	E
IRC-point 1	1.188	1.696	-1332.347060
IRC-point 2	1.199	1.673	-1332.347030
IRC-point 3	1.207	1.655	-1332.347005
IRC-point 4	1.237	1.611	-1332.346979
IRC-point 5	1.285	1.551	-1332.347092
IRC-point 6	1.332	1.500	-1332.347510
IRC-point 7	1.380	1.448	-1332.348435
IRC-point 8	1.430	1.397	-1332.349965
IRC-point 9	1.481	1.345	-1332.352070
IRC-point 10	1.532	1.295	-1332.354610
IRC-point 11	1.583	1.246	-1332.357328
IRC-point 12	1.633	1.200	-1332.359906
IRC-point 13	1.680	1.162	-1332.362076

IRC-point 1

C	-0.05968800	0.28767000	-1.92788700
C	2.72887100	-0.96400300	-0.75058600
H	0.53279900	-0.60625600	-2.11197600
C	-2.65413000	-3.23755000	-1.97408800
C	-1.91640800	-2.06579000	-2.10585100
C	-2.05767500	-1.02252600	-1.17162200
C	-2.97092800	-1.18018100	-0.11469800
C	-3.71266500	-2.35221200	0.00780800
C	-3.55874100	-3.38350300	-0.91962900
H	-2.53541500	-4.03165600	-2.70484100
H	-1.24211800	-1.94227700	-2.94680100
H	-3.06970000	-0.40265700	0.63434100

H	-4.40325000	-2.46384700	0.83784600
H	-4.14109500	-4.29483500	-0.82340300
C	-1.27061600	0.20935000	-1.32958700
C	0.54589500	1.52146600	-2.29810400
N	1.00128600	2.51964100	-2.68796100
H	-3.72177000	1.54367200	-1.85980600
C	-3.06264100	1.99321000	-1.13553700
C	-3.17125700	3.14020000	-0.41536500
N	-1.84320400	1.41850600	-0.78959000
H	-3.94780900	3.88806000	-0.39390800
N	-2.02267400	3.23704200	0.36119200
C	-1.22414200	2.18869500	0.13114200
C	-1.68508800	4.32154000	1.28580500
H	-0.18376500	1.98779200	0.66738400
H	-2.44699700	4.39845000	2.06463100
H	-0.71803400	4.09442500	1.73457100
H	-1.61726600	5.26456700	0.73948700
H	-1.92707600	-3.10190300	3.44337500
C	-1.22572400	-2.43059100	2.95568900
C	-0.30565000	-2.92158400	2.02851500
C	-1.22111500	-1.06672400	3.26237700
C	0.60790900	-2.06730200	1.41187900
H	-0.29760900	-3.97958300	1.78042300
C	-0.30622600	-0.21256300	2.65290300
H	-1.91460500	-0.67284700	4.00151800
C	0.62548200	-0.69123000	1.70759000
H	1.30387500	-2.45675800	0.67800800
H	-0.26032300	0.83738300	2.92307900
C	1.59416600	0.25407500	1.09988800
C	1.40043400	1.59293000	1.12642000
N	2.76051400	-0.35952400	0.48191200
C	2.37130100	2.49498900	0.65170800
C	4.03961700	-0.32106100	1.02670100
N	3.08831000	3.36850400	0.33443500
H	4.24928700	0.13630200	1.98034400
C	4.85519800	-0.92454800	0.12717800
N	4.04057800	-1.30729000	-0.93505500
H	5.91977600	-1.10051600	0.14639200
C	4.52343000	-1.96724600	-2.13423200
H	5.23645600	-1.33288100	-2.67129800
H	5.01101900	-2.91734200	-1.89031100
H	3.66229700	-2.15852200	-2.77408500

IRC-point 2

C	-0.06019800	0.28842000	-1.93015100
C	2.73064600	-0.96340300	-0.74913300
H	0.53025900	-0.60581000	-2.11816100
C	-2.65259400	-3.23694000	-1.97599800
C	-1.91518500	-2.06492100	-2.10701100
C	-2.05682300	-1.02210700	-1.17231000
C	-2.97065200	-1.18037600	-0.11599000
C	-3.71219200	-2.35264200	0.00572400
C	-3.55753000	-3.38362200	-0.92191500
H	-2.53340100	-4.03066200	-2.70710200
H	-1.24078800	-1.94095800	-2.94780800
H	-3.07010200	-0.40300400	0.63309600
H	-4.40328200	-2.46468000	0.83529500
H	-4.13964500	-4.29517300	-0.82630200
C	-1.26967800	0.20997500	-1.32902500
C	0.54631300	1.52213000	-2.29893800
N	1.00334900	2.51999400	-2.68765100
H	-3.71847100	1.54372600	-1.85939400
C	-3.06024400	1.99299600	-1.13414400
C	-3.16954600	3.13978800	-0.41408600
N	-1.84126400	1.41826100	-0.78665600
H	-3.94605300	3.88773900	-0.39356900
N	-2.02184300	3.23621000	0.36381200
C	-1.22255700	2.18784000	0.13527100
C	-1.68689600	4.32191200	1.28766800
H	-0.17170400	1.98546800	0.67528900
H	-2.44827400	4.39689700	2.06728000
H	-0.71872500	4.09868800	1.73576900
H	-1.62281800	5.26502400	0.74098500
H	-1.92636300	-3.10345400	3.44366400
C	-1.22571900	-2.43193900	2.95525600
C	-0.30590800	-2.92298100	2.02778400
C	-1.22187800	-1.06799400	3.26136100
C	0.60666800	-2.06849400	1.41011600
H	-0.29746900	-3.98109700	1.78026800
C	-0.30780400	-0.21357700	2.65092200
H	-1.91515900	-0.67425700	4.00073100
C	0.62334100	-0.69230100	1.70518300
H	1.30245600	-2.45758900	0.67586300
H	-0.26236200	0.83636000	2.92113900
C	1.59118200	0.25293800	1.09654600
C	1.39344500	1.59121600	1.11646800
N	2.76022400	-0.35898600	0.48334600
C	2.36559800	2.49450300	0.64628800

C	4.03850200	-0.31944000	1.03017600
N	3.08515900	3.36830400	0.33645700
H	4.24664400	0.13814800	1.98406000
C	4.85566600	-0.92238900	0.13165000
N	4.04272100	-1.30573800	-0.93167800
H	5.92035700	-1.09750500	0.15233700
C	4.52673200	-1.96544800	-2.13049300
H	5.23987600	-1.33077800	-2.66702400
H	5.01445700	-2.91540000	-1.88632600
H	3.66601100	-2.15686200	-2.77083500

IRC-point 3

C	-0.06067600	0.28861900	-1.93135400
C	2.73082300	-0.96318800	-0.74803400
H	0.52826700	-0.60597600	-2.12156200
C	-2.65269600	-3.23625600	-1.97660000
C	-1.91521200	-2.06424900	-2.10740900
C	-2.05678500	-1.02144600	-1.17265300
C	-2.97087400	-1.17977600	-0.11658600
C	-3.71251000	-2.35202500	0.00496800
C	-3.55776000	-3.38301500	-0.92263200
H	-2.53349600	-4.02989500	-2.70779900
H	-1.24082900	-1.94033100	-2.94822100
H	-3.07067700	-0.40219800	0.63222600
H	-4.40388400	-2.46395400	0.83432700
H	-4.13997800	-4.29452100	-0.82716400
C	-1.26937900	0.21068300	-1.32872200
C	0.54670200	1.52214400	-2.29926000
N	1.00466500	2.51982000	-2.68736800
H	-3.71622300	1.54411200	-1.85899200
C	-3.05831100	1.99329100	-1.13337100
C	-3.16757300	3.14000900	-0.41359200
N	-1.83945000	1.41857000	-0.78491200
H	-3.94382200	3.88827000	-0.39345800
N	-2.01996400	3.23581700	0.36476800
C	-1.21948700	2.18740400	0.13785600
C	-1.68710300	4.32251300	1.28775700
H	-0.16062800	1.98356600	0.68084500
H	-2.44871000	4.39715600	2.06723600
H	-0.71874300	4.10162800	1.73645800
H	-1.62436200	5.26546500	0.74057000
H	-1.92682100	-3.10335200	3.44360200
C	-1.22619700	-2.43193900	2.95503700
C	-0.30649600	-2.92330500	2.02757500

C	-1.22235900	-1.06803600	3.26106700
C	0.60588900	-2.06897300	1.40957800
H	-0.29819900	-3.98145900	1.78028400
C	-0.30825500	-0.21373100	2.65044200
H	-1.91553300	-0.67422400	4.00046500
C	0.62233000	-0.69275600	1.70436400
H	1.30145000	-2.45792600	0.67503100
H	-0.26280900	0.83608900	2.92105600
C	1.58980000	0.25211900	1.09504100
C	1.38846100	1.59000500	1.10901900
N	2.76038700	-0.35870800	0.48453900
C	2.36269200	2.49395500	0.64344300
C	4.03859900	-0.31951600	1.03171300
N	3.08508900	3.36690900	0.33849000
H	4.24698100	0.13793900	1.98561800
C	4.85562600	-0.92267500	0.13313700
N	4.04272300	-1.30583200	-0.93029800
H	5.92027700	-1.09802400	0.15394500
C	4.52647100	-1.96565000	-2.12922700
H	5.23966700	-1.33109900	-2.66581100
H	5.01399600	-2.91570700	-1.88511200
H	3.66559900	-2.15682100	-2.76942800

IRC-point 4

C	-0.06151000	0.28892700	-1.93252600
C	2.73068600	-0.96308100	-0.74690500
H	0.52542800	-0.60612700	-2.12536900
C	-2.65318900	-3.23531500	-1.97721400
C	-1.91550100	-2.06336400	-2.10778700
C	-2.05689600	-1.02049400	-1.17304700
C	-2.97122000	-1.17889300	-0.11720300
C	-3.71306400	-2.35107600	0.00422800
C	-3.55838300	-3.38208700	-0.92335500
H	-2.53413300	-4.02885900	-2.70855700
H	-1.24121000	-1.93951400	-2.94868500
H	-3.07150200	-0.40079300	0.63097400
H	-4.40484000	-2.46278500	0.83330800
H	-4.14087400	-4.29345400	-0.82808900
C	-1.26946000	0.21208300	-1.32833100
C	0.54701000	1.52219900	-2.29948100
N	1.00617700	2.51953600	-2.68706400
H	-3.71424100	1.54508500	-1.85863300
C	-3.05647200	1.99394900	-1.13261200
C	-3.16548400	3.14047300	-0.41314400

N	-1.83740200	1.41940600	-0.78289500
H	-3.94149300	3.88908600	-0.39343100
N	-2.01754300	3.23513700	0.36559500
C	-1.21406800	2.18677100	0.14153900
C	-1.68733600	4.32298100	1.28748500
H	-0.12886600	1.97825700	0.69636900
H	-2.44911100	4.39768400	2.06694300
H	-0.71892400	4.10486000	1.73711500
H	-1.62574700	5.26598100	0.74006600
H	-1.92751100	-3.10302400	3.44335400
C	-1.22681300	-2.43177000	2.95471700
C	-0.30726700	-2.92358600	2.02726400
C	-1.22293900	-1.06799400	3.26077700
C	0.60495900	-2.06949600	1.40897000
H	-0.29926100	-3.98173600	1.78012700
C	-0.30866300	-0.21383100	2.65006800
H	-1.91603600	-0.67404100	4.00008300
C	0.62109500	-0.69328700	1.70351700
H	1.30011000	-2.45822200	0.67392300
H	-0.26352300	0.83568100	2.92171000
C	1.58836400	0.25080700	1.09360600
C	1.38128200	1.58842000	1.09911900
N	2.76067900	-0.35821900	0.48604500
C	2.35955500	2.49361300	0.64069500
C	4.03897600	-0.31994500	1.03327200
N	3.08543700	3.36484100	0.34077600
H	4.24809400	0.13712000	1.98721200
C	4.85543300	-0.92345400	0.13438700
N	4.04229000	-1.30622500	-0.92899700
H	5.92000300	-1.09927900	0.15518000
C	4.52578400	-1.96622800	-2.12818000
H	5.23907900	-1.33174800	-2.66465100
H	5.01302000	-2.91638700	-1.88401900
H	3.66479900	-2.15705800	-2.76830200

IRC-point 5

C	-0.06229300	0.28912000	-1.93312400
C	2.73030700	-0.96321400	-0.74645600
H	0.52303900	-0.60600900	-2.12792000
C	-2.65388100	-3.23460200	-1.97748900
C	-1.91596900	-2.06271500	-2.10792400
C	-2.05711600	-1.01976600	-1.17325500
C	-2.97153800	-1.17816600	-0.11747000
C	-3.71359400	-2.35026800	0.00394500

C	-3.55910900	-3.38130700	-0.92364500
H	-2.53506000	-4.02808000	-2.70895300
H	-1.24186900	-1.93890800	-2.94888800
H	-3.07211700	-0.39947100	0.62991600
H	-4.40572000	-2.46178700	0.83283300
H	-4.14190900	-4.29257000	-0.82855400
C	-1.26987600	0.21353100	-1.32799100
C	0.54698700	1.52225000	-2.29954400
N	1.00707700	2.51927700	-2.68696500
H	-3.71381500	1.54638000	-1.85845800
C	-3.05589500	1.99466400	-1.13229600
C	-3.16456000	3.14100300	-0.41300700
N	-1.83652300	1.42027100	-0.78182000
H	-3.94060200	3.88973600	-0.39367700
N	-2.01618900	3.23472400	0.36584400
C	-1.20896100	2.18621800	0.14452900
C	-1.68741400	4.32306100	1.28703800
H	-0.08083400	1.97037900	0.71997600
H	-2.44912700	4.39829900	2.06671400
H	-0.71929000	4.10679400	1.73729800
H	-1.62627700	5.26644400	0.73988900
H	-1.92805000	-3.10263600	3.44309900
C	-1.22720000	-2.43150000	2.95448900
C	-0.30782200	-2.92369700	2.02701600
C	-1.22327400	-1.06787600	3.26065300
C	0.60435900	-2.06980600	1.40855100
H	-0.30011000	-3.98175300	1.77987500
C	-0.30877200	-0.21380000	2.64990600
H	-1.91634100	-0.67377400	3.99975600
C	0.62022800	-0.69362100	1.70300700
H	1.29900400	-2.45836700	0.67309800
H	-0.26438700	0.83522500	2.92279700
C	1.58761300	0.24944600	1.09288500
C	1.37531500	1.58725400	1.09170700
N	2.76089900	-0.35775400	0.48704900
C	2.35797300	2.49394000	0.63923700
C	4.03940000	-0.32048200	1.03401600
N	3.08583700	3.36310200	0.34205600
H	4.24926400	0.13609700	1.98789500
C	4.85516300	-0.92427800	0.13475400
N	4.04166800	-1.30669400	-0.92845500
H	5.91968500	-1.10050300	0.15551300
C	4.52504100	-1.96690400	-2.12793000
H	5.23839900	-1.33236900	-2.66413900

H	5.01205300	-2.91708400	-1.88361100
H	3.66400200	-2.15743500	-2.76803400

IRC-point 6

C	-0.06270900	0.28918900	-1.93329300
C	2.72998400	-0.96348200	-0.74655200
H	0.52221500	-0.60661300	-2.12896000
C	-2.65448500	-3.23423500	-1.97746000
C	-1.91642000	-2.06242400	-2.10788400
C	-2.05732100	-1.01941300	-1.17326700
C	-2.97176500	-1.17775400	-0.11745100
C	-3.71397800	-2.34977000	0.00401700
C	-3.55966800	-3.38084300	-0.92359300
H	-2.53581700	-4.02772100	-2.70903300
H	-1.24221300	-1.93855400	-2.94915800
H	-3.07240400	-0.39848700	0.62960400
H	-4.40618700	-2.46116400	0.83275400
H	-4.14256000	-4.29189300	-0.82856300
C	-1.27034900	0.21426800	-1.32782800
C	0.54689100	1.52231100	-2.29963000
N	1.00735900	2.51909700	-2.68702100
H	-3.71483800	1.54731700	-1.85879900
C	-3.05622200	1.99518900	-1.13234700
C	-3.16459200	3.14148500	-0.41308200
N	-1.83627000	1.42096300	-0.78132000
H	-3.94082700	3.89001200	-0.39418900
N	-2.01548100	3.23430900	0.36573400
C	-1.20744300	2.18632000	0.14541700
C	-1.68741000	4.32319900	1.28674000
H	-0.03737400	1.96232900	0.74168100
H	-2.44862000	4.39904700	2.06704800
H	-0.71874000	4.10679200	1.73715900
H	-1.62594600	5.26690900	0.74027600
H	-1.92823200	-3.10223400	3.44298500
C	-1.22739200	-2.43125600	2.95445300
C	-0.30812600	-2.92365600	2.02692100
C	-1.22333700	-1.06772500	3.26062600
C	0.60402400	-2.06995300	1.40839600
H	-0.30059400	-3.98177400	1.77971700
C	-0.30880300	-0.21373700	2.64989800
H	-1.91638500	-0.67344700	3.99961400
C	0.61987000	-0.69375500	1.70276900
H	1.29866000	-2.45851200	0.67243300
H	-0.26481900	0.83539800	2.92351100

C	1. 58742700	0. 24873200	1. 09270700
C	1. 37256700	1. 58673300	1. 08854700
N	2. 76096600	-0. 35760900	0. 48733000
C	2. 35729700	2. 49374700	0. 63892700
C	4. 03957400	-0. 32089400	1. 03407500
N	3. 08650300	3. 36266900	0. 34210300
H	4. 24998900	0. 13561500	1. 98836200
C	4. 85494300	-0. 92483700	0. 13461600
N	4. 04122200	-1. 30707800	-0. 92846700
H	5. 91933200	-1. 10124700	0. 15536700
C	4. 52451800	-1. 96743200	-2. 12810400
H	5. 23792300	-1. 33287300	-2. 66418600
H	5. 01141100	-2. 91760200	-1. 88368700
H	3. 66349700	-2. 15779800	-2. 76815000

IRC-point 7

C	-0. 06308200	0. 28918300	-1. 93341300
C	2. 72968600	-0. 96369900	-0. 74673100
H	0. 52085300	-0. 60589500	-2. 12963600
C	-2. 65499900	-3. 23393700	-1. 97742800
C	-1. 91680900	-2. 06216800	-2. 10784700
C	-2. 05752000	-1. 01915200	-1. 17327300
C	-2. 97194500	-1. 17741300	-0. 11737500
C	-3. 71427800	-2. 34938500	0. 00411000
C	-3. 56013000	-3. 38046600	-0. 92351200
H	-2. 53653700	-4. 02739500	-2. 70899500
H	-1. 24295500	-1. 93834500	-2. 94892200
H	-3. 07260200	-0. 39794900	0. 62905500
H	-4. 40668200	-2. 46069800	0. 83288900
H	-4. 14326800	-4. 29159000	-0. 82849800
C	-1. 27067500	0. 21503700	-1. 32763800
C	0. 54670100	1. 52227000	-2. 29965000
N	1. 00751700	2. 51901100	-2. 68710200
H	-3. 71528600	1. 54845900	-1. 85850400
C	-3. 05661300	1. 99561000	-1. 13238000
C	-3. 16471700	3. 14183500	-0. 41313500
N	-1. 83658900	1. 42134800	-0. 78130500
H	-3. 94117700	3. 89033700	-0. 39452000
N	-2. 01551100	3. 23441200	0. 36563100
C	-1. 20570000	2. 18619000	0. 14633700
C	-1. 68724500	4. 32310600	1. 28655200
H	0. 00684900	1. 95464700	0. 76377900
H	-2. 44826200	4. 39951300	2. 06716200
H	-0. 71938000	4. 10732300	1. 73674300

H	-1.62576500	5.26734100	0.74039400
H	-1.92845800	-3.10203600	3.44300100
C	-1.22746600	-2.43107100	2.95440100
C	-0.30833600	-2.92365500	2.02682000
C	-1.22337000	-1.06762200	3.26064800
C	0.60384600	-2.07003700	1.40819500
H	-0.30095300	-3.98155800	1.77961000
C	-0.30869300	-0.21364100	2.64983400
H	-1.91632500	-0.67324000	3.99947300
C	0.61957500	-0.69384200	1.70257100
H	1.29789100	-2.45848600	0.67231400
H	-0.26546600	0.83483900	2.92413000
C	1.58733100	0.24786200	1.09259000
C	1.37014900	1.58629200	1.08594800
N	2.76096400	-0.35740500	0.48754800
C	2.35746400	2.49449400	0.63843400
C	4.03975300	-0.32120400	1.03406500
N	3.08653700	3.36173000	0.34226500
H	4.25044100	0.13484900	1.98789000
C	4.85474200	-0.92526500	0.13438800
N	4.04081700	-1.30735800	-0.92856300
H	5.91921700	-1.10185300	0.15513500
C	4.52407300	-1.96784400	-2.12838900
H	5.23744100	-1.33322200	-2.66431200
H	5.01084900	-2.91799500	-1.88384300
H	3.66297400	-2.15807200	-2.76840500

IRC-point 8

C	-0.06346800	0.28921500	-1.93350000
C	2.72937900	-0.96394200	-0.74695600
H	0.52013200	-0.60625000	-2.13042500
C	-2.65554300	-3.23367400	-1.97731700
C	-1.91725000	-2.06196100	-2.10773800
C	-2.05773700	-1.01891300	-1.17324000
C	-2.97213400	-1.17710300	-0.11726600
C	-3.71459300	-2.34900400	0.00428900
C	-3.56061800	-3.38012400	-0.92334400
H	-2.53726300	-4.02717600	-2.70894200
H	-1.24336800	-1.93811000	-2.94907400
H	-3.07280300	-0.39715400	0.62883600
H	-4.40705300	-2.46021300	0.83297900
H	-4.14384500	-4.29109500	-0.82834800
C	-1.27105800	0.21571200	-1.32745400
C	0.54652300	1.52226800	-2.29972700

N	1.00760300	2.51886200	-2.68721400
H	-3.71631300	1.54926700	-1.85871300
C	-3.05702700	1.99601900	-1.13241300
C	-3.16490200	3.14222700	-0.41319500
N	-1.83688800	1.42175000	-0.78127300
H	-3.94155300	3.89053400	-0.39494400
N	-2.01549200	3.23445000	0.36547600
C	-1.20466000	2.18623000	0.14688600
C	-1.68715200	4.32311100	1.28629300
H	0.05194200	1.94660300	0.78671300
H	-2.44784600	4.40009900	2.06735200
H	-0.71896500	4.10739300	1.73663600
H	-1.62551700	5.26765400	0.74067400
H	-1.92852900	-3.10168200	3.44298600
C	-1.22754200	-2.43085200	2.95441000
C	-0.30853300	-2.92360000	2.02676500
C	-1.22336000	-1.06746900	3.26067900
C	0.60364000	-2.07009500	1.40806400
H	-0.30128900	-3.98152900	1.77950500
C	-0.30860000	-0.21355600	2.64979100
H	-1.91626400	-0.67294400	3.99941100
C	0.61932700	-0.69389500	1.70239300
H	1.29758200	-2.45865800	0.67179900
H	-0.26599900	0.83492500	2.92479100
C	1.58727600	0.24707100	1.09247500
C	1.36816600	1.58592000	1.08366300
N	2.76095700	-0.35723900	0.48769400
C	2.35735200	2.49478000	0.63810000
C	4.03989800	-0.32153100	1.03393000
N	3.08685400	3.36119200	0.34218300
H	4.25100000	0.13445600	1.98804400
C	4.85454200	-0.92568900	0.13410900
N	4.04041300	-1.30765600	-0.92870600
H	5.91891600	-1.10241400	0.15484200
C	4.52360400	-1.96828400	-2.12870500
H	5.23696000	-1.33360700	-2.66451700
H	5.01027400	-2.91841300	-1.88403700
H	3.66248700	-2.15838100	-2.76864200

IRC-point 9

C	-0.06382000	0.28921700	-1.93359000
C	2.72908000	-0.96417500	-0.74720600
H	0.51914700	-0.60610900	-2.13107700
C	-2.65607600	-3.23341700	-1.97722100

C	-1.91766800	-2.06175100	-2.10765900
C	-2.05795000	-1.01867800	-1.17320700
C	-2.97231900	-1.17679700	-0.11714200
C	-3.71489000	-2.34864200	0.00445600
C	-3.56108400	-3.37978300	-0.92318900
H	-2.53797700	-4.02691600	-2.70887500
H	-1.24395600	-1.93789600	-2.94900800
H	-3.07297000	-0.39652900	0.62848900
H	-4.40746400	-2.45976500	0.83314000
H	-4.14447200	-4.29072800	-0.82820100
C	-1.27144500	0.21637600	-1.32726700
C	0.54633000	1.52226800	-2.29978900
N	1.00767400	2.51875000	-2.68732100
H	-3.71709900	1.55025300	-1.85862000
C	-3.05748300	1.99640200	-1.13245900
C	-3.16510500	3.14260500	-0.41322800
N	-1.83721000	1.42214100	-0.78124600
H	-3.94201900	3.89076600	-0.39533900
N	-2.01550100	3.23448800	0.36534300
C	-1.20378900	2.18629600	0.14736300
C	-1.68702700	4.32308300	1.28609700
H	0.09711300	1.93855100	0.80991800
H	-2.44742700	4.40065900	2.06758700
H	-0.71904100	4.10750800	1.73631200
H	-1.62525700	5.26808100	0.74092500
H	-1.92864000	-3.10142400	3.44300300
C	-1.22759200	-2.43065400	2.95440200
C	-0.30871000	-2.92356800	2.02669200
C	-1.22333500	-1.06734300	3.26071000
C	0.60346900	-2.07017200	1.40790000
H	-0.30159800	-3.98139200	1.77940100
C	-0.30849800	-0.21346400	2.64975700
H	-1.91615400	-0.67269600	3.99931900
C	0.61910100	-0.69395300	1.70221300
H	1.29707500	-2.45870200	0.67150400
H	-0.26653800	0.83470800	2.92535600
C	1.58722900	0.24627600	1.09236300
C	1.36632600	1.58552500	1.08149600
N	2.76094800	-0.35707200	0.48781800
C	2.35730100	2.49513000	0.63776800
C	4.04005200	-0.32183100	1.03381000
N	3.08713100	3.36063900	0.34211900
H	4.25146900	0.13388900	1.98779600
C	4.85434100	-0.92609200	0.13380200

N	4.04001700	-1.30793200	-0.92887700
H	5.91871800	-1.10296200	0.15452700
C	4.52314600	-1.96869000	-2.12905000
H	5.23647200	-1.33396500	-2.66474300
H	5.00971300	-2.91879400	-1.88427100
H	3.66198100	-2.15866500	-2.76892900

IRC-point 10

C	-0.06421600	0.28923500	-1.93366700
C	2.72878700	-0.96436000	-0.74751900
H	0.51832500	-0.60628000	-2.13180800
C	-2.65657400	-3.23322500	-1.97707300
C	-1.91809000	-2.06159300	-2.10753100
C	-2.05815900	-1.01849500	-1.17314500
C	-2.97247300	-1.17656700	-0.11697500
C	-3.71513800	-2.34836200	0.00469800
C	-3.56149800	-3.37953300	-0.92296700
H	-2.53865400	-4.02675200	-2.70878200
H	-1.24443200	-1.93769100	-2.94907800
H	-3.07311400	-0.39583800	0.62827600
H	-4.40777300	-2.45940800	0.83333100
H	-4.14497500	-4.29038000	-0.82798500
C	-1.27187900	0.21703500	-1.32705100
C	0.54606100	1.52227700	-2.29986100
N	1.00764200	2.51865200	-2.68745700
H	-3.71828400	1.55107900	-1.85873900
C	-3.05806700	1.99673400	-1.13248300
C	-3.16545900	3.14293800	-0.41324800
N	-1.83767900	1.42248300	-0.78127300
H	-3.94264300	3.89084600	-0.39576900
N	-2.01569200	3.23452500	0.36518200
C	-1.20337600	2.18642800	0.14763900
C	-1.68701100	4.32302400	1.28588600
H	0.14146500	1.93123000	0.83575100
H	-2.44703900	4.40120400	2.06787100
H	-0.71884900	4.10735000	1.73603700
H	-1.62507400	5.26840600	0.74128200
H	-1.92858800	-3.10115900	3.44302400
C	-1.22754000	-2.43047900	2.95441900
C	-0.30878100	-2.92353000	2.02662000
C	-1.22322300	-1.06722900	3.26075800
C	0.60336100	-2.07022800	1.40774000
H	-0.30179100	-3.98134200	1.77927600
C	-0.30834600	-0.21338400	2.64972700

H	-1.91598100	-0.67245900	3.99928300
C	0.61893900	-0.69398500	1.70202900
H	1.29678200	-2.45881000	0.67103000
H	-0.26713800	0.83470700	2.92594800
C	1.58721000	0.24541400	1.09223700
C	1.36529000	1.58494300	1.07953000
N	2.76094500	-0.35683400	0.48788500
C	2.35729100	2.49560600	0.63739600
C	4.04022800	-0.32205500	1.03358800
N	3.08735500	3.36015600	0.34194600
H	4.25205200	0.13353700	1.98775100
C	4.85416300	-0.92638900	0.13340600
N	4.03962900	-1.30812200	-0.92912500
H	5.91848000	-1.10337400	0.15410300
C	4.52269600	-1.96900900	-2.12948600
H	5.23597700	-1.33420000	-2.66506900
H	5.00918800	-2.91907700	-1.88458400
H	3.66149500	-2.15887500	-2.76927600

IRC-point 11

C	-0.06463600	0.28924800	-1.93375400
C	2.72849600	-0.96451900	-0.74785400
H	0.51729800	-0.60622400	-2.13255600
C	-2.65705800	-3.23304400	-1.97693300
C	-1.91849700	-2.06143600	-2.10741400
C	-2.05836100	-1.01831500	-1.17308200
C	-2.97261500	-1.17635200	-0.11679600
C	-3.71536200	-2.34811200	0.00494200
C	-3.56188500	-3.37930300	-0.92274700
H	-2.53932300	-4.02656900	-2.70868500
H	-1.24500900	-1.93748900	-2.94904200
H	-3.07324800	-0.39522200	0.62796300
H	-4.40809400	-2.45909000	0.83355700
H	-4.14548900	-4.29011300	-0.82777000
C	-1.27234200	0.21773900	-1.32681700
C	0.54575800	1.52230500	-2.29992500
N	1.00759100	2.51857200	-2.68758600
H	-3.71939800	1.55203400	-1.85867800
C	-3.05872700	1.99704800	-1.13250900
C	-3.16587000	3.14325200	-0.41325000
N	-1.83818500	1.42283700	-0.78128000
H	-3.94338700	3.89092400	-0.39620000
N	-2.01592400	3.23453100	0.36503300
C	-1.20282200	2.18652700	0.14803000

C	-1.68702900	4.32291600	1.28569400
H	0.18508100	1.92446100	0.86243000
H	-2.44667500	4.40172800	2.06819600
H	-0.71893500	4.10722600	1.73565300
H	-1.62493900	5.26878400	0.74164700
H	-1.92850800	-3.10095000	3.44304900
C	-1.22743700	-2.43032300	2.95442100
C	-0.30881000	-2.92351400	2.02652800
C	-1.22307700	-1.06714600	3.26080700
C	0.60329200	-2.07029900	1.40754400
H	-0.30193600	-3.98124200	1.77913300
C	-0.30817200	-0.21330900	2.64970100
H	-1.91575900	-0.67226400	3.99922300
C	0.61877600	-0.69403000	1.70183100
H	1.29639800	-2.45884500	0.67062000
H	-0.26778400	0.83453100	2.92655500
C	1.58720600	0.24448700	1.09209400
C	1.36440700	1.58423400	1.07743700
N	2.76096000	-0.35654600	0.48795500
C	2.35722200	2.49612400	0.63701000
C	4.04044200	-0.32223900	1.03337800
N	3.08758400	3.35968600	0.34180000
H	4.25264700	0.13309400	1.98749400
C	4.85399000	-0.92665000	0.13297700
N	4.03923600	-1.30827100	-0.92939600
H	5.91829600	-1.10375300	0.15364500
C	4.52224500	-1.96928100	-2.12996000
H	5.23546500	-1.33437900	-2.66542000
H	5.00866700	-2.91930400	-1.88493700
H	3.66099400	-2.15904400	-2.76967100

IRC-point 12

C	-0.06513500	0.28927800	-1.93384700
C	2.72821100	-0.96461000	-0.74825000
H	0.51615900	-0.60622000	-2.13343900
C	-2.65749800	-3.23292300	-1.97676700
C	-1.91889000	-2.06131600	-2.10727400
C	-2.05854500	-1.01817000	-1.17300000
C	-2.97271700	-1.17621100	-0.11657900
C	-3.71551900	-2.34795500	0.00523800
C	-3.56220300	-3.37916100	-0.92248600
H	-2.53995500	-4.02643900	-2.70858100
H	-1.24558500	-1.93728700	-2.94903300
H	-3.07337200	-0.39459600	0.62763800

H	-4.40834900	-2.45887800	0.83381900
H	-4.14591400	-4.28992800	-0.82751900
C	-1.27288500	0.21851900	-1.32654000
C	0.54536200	1.52236200	-2.29998900
N	1.00745600	2.51851800	-2.68772700
H	-3.72080100	1.55298800	-1.85864500
C	-3.05957500	1.99731300	-1.13252100
C	-3.16646700	3.14350900	-0.41323400
N	-1.83883300	1.42318700	-0.78128600
H	-3.94437700	3.89087100	-0.39667100
N	-2.01632100	3.23447900	0.36487500
C	-1.20228900	2.18661000	0.14849200
C	-1.68719500	4.32272200	1.28548800
H	0.22645000	1.91924200	0.89217000
H	-2.44637100	4.40221800	2.06858900
H	-0.71908700	4.10695600	1.73521100
H	-1.62494300	5.26911700	0.74210600
H	-1.92826600	-3.10078700	3.44306500
C	-1.22719500	-2.43020400	2.95442000
C	-0.30871300	-2.92351800	2.02641100
C	-1.22283000	-1.06711000	3.26086500
C	0.60330700	-2.07037300	1.40730800
H	-0.30193900	-3.98117300	1.77894400
C	-0.30793800	-0.21325300	2.64968100
H	-1.91544600	-0.67212200	3.99917400
C	0.61864200	-0.69407800	1.70161200
H	1.29610200	-2.45886000	0.67009500
H	-0.26854400	0.83435200	2.92725900
C	1.58724100	0.24341200	1.09191100
C	1.36430700	1.58317200	1.07523200
N	2.76100900	-0.35612900	0.48800500
C	2.35708100	2.49679700	0.63655700
C	4.04072900	-0.32232100	1.03311700
N	3.08779200	3.35926700	0.34162400
H	4.25338600	0.13274000	1.98725000
C	4.85384200	-0.92679000	0.13245400
N	4.03883900	-1.30830600	-0.92973400
H	5.91812400	-1.10399800	0.15308000
C	4.52179600	-1.96943400	-2.13053400
H	5.23492800	-1.33439800	-2.66586000
H	5.00817700	-2.91939500	-1.88538100
H	3.66049300	-2.15910700	-2.77015500

IRC-point 13

C	-0.06577000	0.28933900	-1.93394800
C	2.72794500	-0.96457200	-0.74871400
H	0.51479900	-0.60623200	-2.13452800
C	-2.65784900	-3.23290200	-1.97657500
C	-1.91924000	-2.06125400	-2.10710800
C	-2.05869400	-1.01808100	-1.17289200
C	-2.97274600	-1.17619700	-0.11631700
C	-3.71555900	-2.34795700	0.00560000
C	-3.56239400	-3.37917100	-0.92217500
H	-2.54050400	-4.02639200	-2.70847800
H	-1.24616900	-1.93709500	-2.94904700
H	-3.07349000	-0.39399700	0.62725800
H	-4.40850000	-2.45885100	0.83412800
H	-4.14618800	-4.28990600	-0.82722800
C	-1.27355500	0.21941700	-1.32620000
C	0.54481800	1.52247300	-2.30005100
N	1.00719400	2.51850700	-2.68787800
H	-3.72258700	1.55395700	-1.85861400
C	-3.06072400	1.99749500	-1.13251700
C	-3.16737000	3.14366600	-0.41319700
N	-1.83968900	1.42353500	-0.78127800
H	-3.94576200	3.89062200	-0.39720300
N	-2.01698900	3.23432100	0.36469900
C	-1.20172600	2.18665200	0.14910700
C	-1.68761800	4.32238000	1.28526100
H	0.26247900	1.91699900	0.92675800
H	-2.44619300	4.40262000	2.06907900
H	-0.71942100	4.10647900	1.73465500
H	-1.62519400	5.26937400	0.74268700
H	-1.92777600	-3.10072500	3.44306600
C	-1.22672900	-2.43015600	2.95440500
C	-0.30840300	-2.92356100	2.02624500
C	-1.22242000	-1.06715700	3.26093500
C	0.60346600	-2.07044400	1.40700400
H	-0.30171400	-3.98114700	1.77868500
C	-0.30760800	-0.21323600	2.64966600
H	-1.91500200	-0.67208400	3.99914000
C	0.61854600	-0.69414400	1.70136200
H	1.29590900	-2.45881500	0.66943300
H	-0.26948200	0.83411700	2.92813000
C	1.58736200	0.24207500	1.09166300
C	1.36552900	1.58150800	1.07282400
N	2.76112700	-0.35550800	0.48801500
C	2.35681000	2.49771400	0.63599600

C	4.04112900	-0.32222500	1.03279600
N	3.08798400	3.35895500	0.34142500
H	4.25435700	0.13249600	1.98696500
C	4.85374000	-0.92672400	0.13180200
N	4.03844200	-1.30814600	-0.93017400
H	5.91800600	-1.10402200	0.15234900
C	4.52136400	-1.96937900	-2.13125800
H	5.23436800	-1.33414100	-2.66643000
H	5.00775200	-2.91925400	-1.88596000
H	3.66000300	-2.15898700	-2.77077400