ORGANOMETALLICS
Organometallics, 1998, 17(15), 3240-3253, DOI:10.1021/om9803164

Force field parameters used:

BONDS Ebond = 0.5*K(r-ro)**2

Atoms i - j	K (kcal/molA^2)	ro (Ang)	Source
CA - CA	938.0	1.400	amber95
CT - CT	620.0	1.526	amber95
CT - HC	680.0	1.090	amber95
CA - HA	734.0	1.080	amber95
CA - CT	634.0	1.510	amber95
CT - F	734.0	1.380	amber95

BENDS Ebend = 0.5*k(a-ao)^2

Atoms i - j - k	k (kcal/mol)	ao (deg)	Source	
CA - CA - HA	70.00	120.00	amber95	
CA - CA - CA	126.00	120.00	amber95	
CT - CT - HC	100.00	109.50	amber95	
HC - CT - HC	70.00	109.50	amber95	
CT - CT - CT	80.00	109.50	amber95	
CM - CT - HC	100.00	109.50	amber95	
CA CA N2	140.00	120.10	amber95	N2-CA-CM
CA - CA - CT	140.00	120.0	amber95	
CT - CT - CA	126.00	114.0	amber95	
CA - CT - HC	100.00	109.5	amber95	
CT - CT - F	77.00	109.1	amber95	F-CT-F
CA - CT - F	77.00	109.1	amber95	F-CT-F

TORSIONS Etors=K(1+cos(nt-to))

Atoms i - j - k - l	no. paths	K	per. n	shift to	Source
X - CT - CT - X	9	1.40	3	0.0	amber95
X - CA - CA - X	4	14.50	2	180.0	amber95
X - CT - CM - X	6	0.00	3	0.0	amber95
X - CA - CT - X	6	0.00	2	0.0	amber95
X - N2 - CA - X	4	9.60	2	180.0	amber95

IMPROPER TORSIONS Eimp=K(1-cos(nt-to)) (i is central atom)

Atoms i - j - k - l	K	shift to	per n	Source
CA CA N2 CA	0.00	0.0	2	
CA CA CA HA	1.10	180.0	2	amber95
CA CA CA CT	1.10	180.0	2	amber95

VAN DER WAALS

1-4 scale 0.5 type LJ

atom(s)	emin	rmin	Source
CA	0.0860	3.816	amber95
HA	0.0150	2.918	amber95
CT	0.1094	3.816	amber95
HC	0.0157	2.974	amber95
CM	0.0860	3.816	amber95
Ti	0.0170	3.175	UFF Ti3+4
Zr	0.0690	3.124	UFF Zr3+4
N2	0.1700	3.650	amber95
F	0.0610	3.500	amber95

Geometries (Å)

PART I. Generic Systems

1.1 Titanium Generic systems

Structure 1a

E_{total} = -4.571292 a.u.

Atom	X	Y	Z
Ti	0.0107	0.6173	0.5649
N	1.8637	0.4844	0.6232
C	2.6605	1.0072	-0.5045
C	1.8481	1.1303	-1.7934
C	0.6868	2.1245	-1.7980
N	-0.3831	1.7521	-0.8520
H	2.4546	0.1927	1.4178
H	3.4979	0.3146	-0.6894
H	3.0925	1.9848	-0.2237
H	2.5439	1.4352	-2.5910
H	1.4704	0.1312	-2.0810
H	0.2600	2.1517	-2.8139
H	1.0470	3.1420	-1.5602
H	-1.2540	2.2816	-1.0152
C	-1.3082	-0.0768	1.9687
C	-1.4456	-1.2786	1.0552
H	-0.8347	-0.3022	2.9398
H	-2.2261	0.5195	2.0949
H	-0.7204	-1.2003	0.1469
H	-2.4185	-1.2859	0.5390
C	-1.1261	-2.6375	1.6741
H	-1.1597	-3.4403	0.9252
H	-0.1337	-2.6391	2.1467
H	-1.8741	-2.8549	2.4504

Structure 2a

E_{total} = -4.571067 a.u.

Atom	X	Y	Z
Ti	0.0660	-0.1268	-0.1132
N	1.8473	0.1365	0.3487
C	2.5549	1.3417	-0.1287
C	1.8946	1.9685	-1.3565
C	0.4832	2.5275	-1.1799
N	-0.5084	1.4846	-0.8486
H	2.4317	-0.4313	0.9819
H	3.5848	1.0564	-0.3988
H	2.6172	2.0764	0.6940
H	2.5382	2.7993	-1.6875
H	1.8940	1.2347	-2.1843
H	0.1811	3.0079	-2.1249
H	0.4710	3.3035	-0.3934
H	-1.4761	1.8133	-0.9901
C	-1.1586	-1.5587	0.7003
C	-1.2650	-0.5874	1.8520
H	-2.0984	-1.7137	0.1439
H	-0.6584	-2.5133	0.9289
H	-0.6088	0.3601	1.6638
H	-0.7801	-0.9740	2.7626
C	-2.6577	-0.0339	2.1412
H	-2.6317	0.7518	2.9082
H	-3.1234	0.3778	1.2341
H	-3.2954	-0.8537	2.5033

Stucutre 3a

E_{t0tal} = -5.754734 a.u.

Atom	X	Y	Z
Ti	0.1312	0.0884	0.2991
N	1.9958	0.1539	0.2702
C	2.7889	1.1438	-0.4691
C	1.9438	1.8984	-1.4929
C	0.7808	2.7026	-0.9168
N	-0.1996	1.8551	-0.2261
H	2.5641	-0.3587	0.9643
H	3.6188	0.6354	-0.9898
H	3.2384	1.8548	0.2486
H	2.6042	2.5969	-2.0312
H	1.5658	1.1902	-2.2511
H	0.2773	3.2469	-1.7341
H	1.1581	3.4599	-0.2043
H	-0.9986	2.4033	0.1301
C	-0.7802	-0.5488	2.0214
C	-2.2276	-0.0943	1.8113
H	-0.6810	-1.6570	2.0112
H	-0.3250	-0.1722	2.9547
H	-2.4787	-0.0329	0.7268
H	-2.3444	0.9316	2.1976
C	-3.2676	-1.0128	2.4663
H	-4.2879	-0.6388	2.3002
H	-3.2057	-2.0328	2.0584
H	-3.0916	-1.0704	3.5498
C	-0.9937	-0.7442	-1.9012
C	-0.1694	-1.7092	-1.4335
H	-0.6745	-0.0409	-2.6731
H	-2.0453	-0.6970	-1.6029
H	0.8460	-1.8344	-1.8184
H	-0.5382	-2.4784	-0.7442

Structure 3a'

E_{total} = -5.752124 a.u.

Atom	X	Y	Z
Ti	0.0090	0.0051	0.0511
N	1.8694	-0.0084	0.0468
C	2.7439	1.1773	-0.0127
C	2.0549	2.4369	0.5015
C	0.8074	2.8633	-0.2644
N	-0.2433	1.8320	-0.2555
H	2.3917	-0.8766	-0.1491
H	3.0792	1.3248	-1.0555
H	3.6392	0.9894	0.6032
H	1.8021	2.3086	1.5679
H	2.7813	3.2640	0.4506
H	1.0641	3.0963	-1.3144
H	0.4085	3.7853	0.1912
H	-1.1358	2.2032	-0.6160
C	-0.6120	-0.8622	-1.7691
C	-1.2935	-1.8981	-0.9311
H	-1.2889	-0.2053	-2.3325
H	0.2181	-1.2138	-2.3930
H	-1.1270	-1.6979	0.2041
H	-0.8109	-2.8855	-1.0222
C	-2.8141	-1.9942	-1.0662
H	-3.2484	-2.6957	-0.3402
H	-3.2922	-1.0121	-0.9322
H	-3.0608	-2.3470	-2.0783
C	-0.5407	0.3673	2.5069
C	-0.8413	-0.9426	2.3540
H	0.4760	0.6833	2.7502
H	-1.3179	1.1344	2.5250
H	-0.0765	-1.7161	2.4790
H	-1.8782	-1.2791	2.2725

Strucutre 4a

E_{total} = -5.757577 a.u.

Atom	X	Y	Z
Ti	0.0037	-0.0011	0.0198
N	1.8678	0.0031	-0.0458
C	2.6239	1.2647	-0.2095
C	1.9304	2.4584	0.4425
C	0.5713	2.8595	-0.1269
N	-0.4608	1.8119	0.0364
H	2.4901	-0.8180	-0.0092
H	2.8023	1.4598	-1.2832
H	3.6112	1.1413	0.2639
H	1.8208	2.2605	1.5229
H	2.6001	3.3285	0.3414
H	0.6642	3.1237	-1.1969
H	0.2311	3.7654	0.4002
H	-1.4067	2.2183	0.0959
C	-1.1653	-1.5950	0.7063
C	-0.7472	-1.0942	2.0743
H	-2.2404	-1.4642	0.5013
H	-0.8434	-2.6201	0.4754
H	-0.0818	-0.1550	2.0146
H	-0.0575	-1.8021	2.5602
C	-1.8906	-0.6867	3.0050
H	-1.5138	-0.2589	3.9444
H	-2.5477	0.0536	2.5259
H	-2.4956	-1.5735	3.2422
C	-0.5783	0.0549	-2.4409
C	-0.6711	-1.2526	-2.1103
H	0.3852	0.5048	-2.7014
H	-1.4682	0.6716	-2.5855
H	0.2184	-1.8905	-2.0876
H	-1.6349	-1.7487	-1.9930

Strucutre 5a

E_{total} = -5.752428 a.u.

Atom	X	Y	Z
Ti	-0.0048	-0.0410	0.0011
N	1.8560	0.0151	-0.0129
C	2.6366	1.2673	-0.0999
C	2.1358	2.3149	0.8941
C	0.7075	2.7903	0.6358
N	-0.2740	1.6853	0.6678
H	2.4288	-0.7973	0.2635
H	2.5761	1.6657	-1.1285
H	3.6966	1.0485	0.0970
H	2.2051	1.9047	1.9159
H	2.8010	3.1933	0.8419
H	0.6548	3.2946	-0.3467
H	0.4318	3.5376	1.3955
H	-1.1114	1.9199	1.2226
C	-0.9574	-1.5369	1.0291
C	-2.3668	-0.9503	1.1299
H	-0.9199	-2.4331	0.3717
H	-0.5122	-1.8000	2.0044
H	-2.5696	-0.2495	0.2838
H	-2.4406	-0.3348	2.0416
C	-3.4832	-2.0023	1.1220
H	-4.4731	-1.5306	1.2004
H	-3.4557	-2.5981	0.1977
H	-3.3560	-2.6883	1.9715
C	-1.0603	0.7431	-2.2502
C	-0.2827	-0.3371	-2.4859
H	-0.6855	1.7601	-2.3877
H	-2.1241	0.6417	-2.0165
H	0.7471	-0.2386	-2.8386
H	-0.7009	-1.3505	-2.4542

Strucutre 5a'

E_{total} = -5.751471 a.u.

Atom	X	Y	Z
Ti	0.0224	-0.0096	-0.1330
N	1.8813	0.0273	-0.0917
C	2.7111	1.1955	0.2751
C	2.0762	2.5123	-0.1584
C	0.7216	2.8181	0.4705
N	-0.3023	1.8142	0.1103
H	2.4525	-0.7906	-0.3503
H	3.6900	1.0965	-0.2194
H	2.8944	1.1965	1.3657
H	2.7678	3.3288	0.1083
H	1.9678	2.5133	-1.2562
H	0.3801	3.8031	0.1147
H	0.8100	2.8811	1.5713
H	-1.2394	2.2373	0.0362
C	-0.5567	-0.3880	-2.1308
C	-1.2236	-1.6093	-1.5924
H	-1.2354	0.3858	-2.5140
H	0.2969	-0.5531	-2.7981
H	-1.0823	-1.6903	-0.4348
H	-0.7148	-2.5347	-1.9096
C	-2.7398	-1.7021	-1.7759
H	-3.1658	-2.5695	-1.2528
H	-3.2441	-0.7929	-1.4155
H	-2.9625	-1.8005	-2.8486
C	-0.5077	-0.2662	2.3207
C	-0.7436	-1.5120	1.8464
H	0.4984	0.0458	2.6119
H	-1.3259	0.4185	2.5532
H	0.0661	-2.2439	1.7547
H	-1.7632	-1.8821	1.7111

Strucure 6a

E = -5.758413 a.u.

Atom	X	Y	Z
Ti	-0.0438	-0.2025	-0.1731
N	1.7547	0.0139	0.2752
C	2.4965	1.2424	-0.0678
C	1.8881	1.9895	-1.2527
C	0.4726	2.5348	-1.0737
N	-0.5313	1.4828	-0.8331
H	2.2836	-0.5772	0.9353
H	3.5334	0.9711	-0.3267
H	2.5399	1.9017	0.8187
H	2.5436	2.8469	-1.4757
H	1.9162	1.3401	-2.1446
H	0.1956	3.0860	-1.9881
H	0.4466	3.2575	-0.2370
H	-1.4895	1.8575	-0.9161
C	-1.3333	-1.4831	0.8571
C	-1.2347	-0.4382	1.9489
H	-2.3333	-1.5474	0.3978
H	-0.9629	-2.4797	1.1353
H	-0.5798	0.4571	1.6364
H	-0.6675	-0.8189	2.8128
C	-2.5594	0.1972	2.3761
H	-2.4046	1.0051	3.1046
H	-3.1024	0.6060	1.5112
H	-3.1945	-0.5718	2.8387
C	-0.0703	-1.1909	-2.5197
C	-0.2204	-2.2661	-1.7163
H	0.9250	-0.8023	-2.7564
H	-0.9152	-0.7471	-3.0517

H	0.6501	-2.7635	-1.2762
H	-1.1870	-2.7524	-1.5825

Structure 7a

E_{total} = -5.768320 a.u.

Atom	X	Y	Z
Ti	0.2145	-0.2552	-0.5925
N	1.9286	-0.0536	0.1017
C	2.4554	1.3042	0.3479
C	1.7441	2.3739	-0.4801
C	0.2612	2.6082	-0.1926
N	-0.5735	1.4284	-0.4910
H	2.5720	-0.7853	0.4411
H	3.5246	1.3159	0.0798
H	2.3799	1.5349	1.4258
H	2.2674	3.3273	-0.3040
H	1.8763	2.1475	-1.5549
H	-0.0832	3.4474	-0.8190
H	0.1157	2.8986	0.8636
H	-1.5769	1.6651	-0.5353
C	-0.8178	-2.0253	-0.6991
C	-1.0115	-1.8211	0.7840
H	-0.2317	-2.9106	-0.9905
H	-1.7416	-1.9313	-1.2965
H	-0.5735	-0.7951	1.1277
H	-0.3962	-2.5177	1.3771
C	-2.4584	-1.7865	1.2921
C	-3.1102	-3.1700	1.2138
H	-2.4741	-1.4268	2.3345
H	-3.0409	-1.0644	0.6928
H	-3.0889	-3.5257	0.1697
H	-2.5057	-3.8844	1.7997
C	-4.5464	-3.1647	1.7320
H	-4.5889	-2.8474	2.7848
H	-5.1798	-2.4819	1.1451
H	-4.9862	-4.1699	1.6664

Structure 8a

E = -5.767524 a.u.

Atom	X	Y	Z
Ti	-0.0901	0.0508	-0.1706
N	1.7617	0.0539	-0.2716
C	2.5888	1.1466	0.2939
C	2.0373	2.5258	-0.0671
C	0.6552	2.8302	0.5057
N	-0.3766	1.8799	0.0276
H	2.2997	-0.5925	-0.8686
H	3.6129	1.0508	-0.0967
H	2.6475	1.0309	1.3902
H	2.7385	3.2868	0.3147
H	2.0049	2.6238	-1.1658
H	0.3612	3.8482	0.2077
H	0.6885	2.8122	1.6101
H	-1.2477	2.3516	-0.2572
C	-1.1797	-1.1113	-1.4381
C	-1.1695	-2.1612	-0.2942
H	-0.7055	-1.4896	-2.3565
H	-2.1873	-0.7213	-1.6585
H	-0.2625	-2.7856	-0.3438
H	-2.0244	-2.8458	-0.4326
C	-1.3297	-1.6047	1.1561
C	-2.6242	-0.8230	1.4006
H	-1.2639	-2.4618	1.8472
H	-0.4369	-1.0115	1.5549
H	-2.6972	0.0474	0.7215
H	-3.4623	-1.4820	1.1147
C	-2.7803	-0.3581	2.8446
H	-2.7569	-1.2123	3.5376
H	-1.9756	0.3358	3.1330
H	-3.7370	0.1628	2.9850

Structure 10a

E_{total} = -5.756607 a.u.

Atom	X	Y	Z
Ti	-0.0206	0.0114	-0.0402
N	1.8418	-0.0068	-0.0602
C	2.6988	1.1909	0.0817
C	2.1094	2.4068	-0.6264
C	0.7678	2.8806	-0.0798
N	-0.2824	1.8455	-0.2028
H	2.3951	-0.8620	-0.2146
H	3.6830	0.9670	-0.3585
H	2.8627	1.4128	1.1526
H	2.8276	3.2384	-0.5329
H	1.9999	2.1779	-1.6997
H	0.4473	3.7688	-0.6466
H	0.8693	3.1842	0.9788
H	-1.2133	2.2565	-0.3676
C	-0.2914	-0.0841	2.4455
C	-1.0190	-1.2145	2.2572
H	0.7733	-0.1396	2.6894
H	-0.7819	0.8858	2.5502
H	-2.1098	-1.1194	2.1753
C	-0.4813	-2.6034	2.3632
H	-0.8730	-3.2685	1.5799
H	0.6169	-2.6315	2.3625
H	-0.8283	-3.0315	3.3206
C	-0.5641	-0.8155	-1.9007
C	-1.5832	-1.6024	-1.1378
H	0.2518	-1.4041	-2.3378
H	-0.9607	-0.0833	-2.6121
H	-1.5318	-1.4245	0.0011
H	-1.4540	-2.6934	-1.1918
H	-2.6259	-1.3330	-1.3609

Strucuture 11a

E_{total} = -5.756607

Ti	-0.0206	0.0114	-0.0402
N	1.8418	-0.0068	-0.0602
C	2.6988	1.1909	0.0817
C	2.1094	2.4068	-0.6264
C	0.7678	2.8806	-0.0798
N	-0.2824	1.8455	-0.2028
H	2.3951	-0.8620	-0.2146
H	3.6830	0.9670	-0.3585
H	2.8627	1.4128	1.1526
H	2.8276	3.2384	-0.5329
H	1.9999	2.1779	-1.6997
H	0.4473	3.7688	-0.6466
H	0.8693	3.1842	0.9788
H	-1.2133	2.2565	-0.3676
C	-0.2914	-0.0841	2.4455
C	-1.0190	-1.2145	2.2572
H	0.7733	-0.1396	2.6894
H	-0.7819	0.8858	2.5502
H	-2.1098	-1.1194	2.1753
C	-0.4813	-2.6034	2.3632
H	-0.8730	-3.2685	1.5799
H	0.6169	-2.6315	2.3625
H	-0.8283	-3.0315	3.3206
C	-0.5641	-0.8155	-1.9007
C	-1.5832	-1.6024	-1.1378
H	0.2518	-1.4041	-2.3378
H	-0.9607	-0.0833	-2.6121
H	-1.5318	-1.4245	0.0011
H	-1.4540	-2.6934	-1.1918
H	-2.6259	-1.3330	-1.3609

Strucutre 12a

E_{total} = -4.540195 a.u.

Atom	X	Y	Z
Ti	-0.0041	-0.0535	-0.1510
N	1.8258	0.0616	0.1086
C	2.5634	1.3393	-0.0508
C	2.1191	2.1071	-1.2937
C	0.6680	2.5853	-1.2787
N	-0.2944	1.4637	-1.1690
H	2.4422	-0.7488	0.2800
H	3.6366	1.1107	-0.1350
H	2.4341	1.9566	0.8559
H	2.7649	2.9953	-1.3953
H	2.2845	1.4754	-2.1837
H	0.4630	3.1300	-2.2131
H	0.5034	3.2931	-0.4463
H	-1.1225	1.5786	-1.7758
C	-0.9665	0.3329	2.0727
C	-1.7106	-0.7907	1.9043
C	-1.3988	-2.1195	2.4789
H	-0.0710	0.3224	2.7047
H	-1.3612	1.3092	1.7641
H	-2.6541	-0.7131	1.3481
H	-0.7867	-1.5215	-0.5590
H	-1.4988	-2.9162	1.7270
H	-0.4087	-2.1599	2.9507
H	-2.1568	-2.3368	3.2543

Strucutre 12a'

E_{total} = -4.545981 a.u.

Atom	X	Y	Z
Ti	-0.0058	-0.0902	0.1467
N	1.8195	-0.0336	-0.1842
C	2.6065	1.1822	-0.4354
C	1.7237	2.3696	-0.8123
C	0.7004	2.7845	0.2426
N	-0.2510	1.7022	0.5380
H	2.4099	-0.8457	0.0679
H	3.3239	0.9881	-1.2510
H	3.1957	1.4132	0.4713
H	2.3810	3.2321	-1.0065
H	1.2025	2.1561	-1.7618
H	0.1441	3.6634	-0.1238
H	1.2110	3.0777	1.1779
H	-0.9664	1.9761	1.2339
C	-1.4566	-0.7041	-1.6497
C	-0.3663	-1.0389	-2.3891
C	0.1793	-0.2412	-3.5148
H	-1.9126	-1.4425	-0.9724
H	-2.0336	0.2026	-1.8637
H	0.0987	-2.0198	-2.2186
H	-0.4423	-1.1438	1.4192
H	-0.0663	-0.7772	-4.4504
H	-0.2619	0.7617	-3.5755
H	1.2758	-0.1787	-3.4797

Strucutre TS[3a-8a]

E_{total} = -5.745826 a.u.

Atom	X	Y	Z
Ti	0.0029	0.0072	-0.0242
N	1.8657	0.0042	-0.0078
C	2.6525	1.2517	0.0321
C	1.8507	2.4579	-0.4511
C	0.6272	2.8323	0.3809
N	-0.4176	1.7873	0.3831
H	2.4642	-0.8321	0.0671
H	3.5333	1.1330	-0.6204
H	3.0193	1.4214	1.0609
H	2.5278	3.3270	-0.4561
H	1.5409	2.2930	-1.4987
H	0.1942	3.7547	-0.0400
H	0.9271	3.0503	1.4224
H	-1.3113	2.1611	0.7301
C	-0.6011	-0.4078	-2.1052
C	-0.9985	-1.6315	-1.5328
H	0.3460	-0.3676	-2.6514
H	-1.3671	0.3159	-2.3995
H	-0.3147	-2.4836	-1.5900
H	-2.0572	-1.9004	-1.5156
C	-1.1491	-1.6503	0.6053
C	-2.4681	-1.0076	1.0192
H	-1.1851	-2.7479	0.6132
H	-0.3229	-1.4041	1.3681
H	-2.4394	0.0930	0.8924
H	-3.2536	-1.3607	0.3308
C	-2.8550	-1.3283	2.4677
H	-2.9328	-2.4153	2.6148
H	-2.1104	-0.9381	3.1768
H	-3.8283	-0.8805	2.7132

Strucutre TS[4a-10a]

E_{total} = -5.746363 a.u.

Atom	X	Y	Z
Ti	-0.0058	0.0386	-0.0359
N	1.8595	0.0296	0.0532
C	2.6544	1.2795	0.0851
C	1.9577	2.4026	0.8462
C	0.6412	2.8909	0.2530
N	-0.4012	1.8389	0.2253
H	2.4663	-0.8010	-0.0007
H	2.8818	1.5982	-0.9489
H	3.6146	1.0666	0.5816
H	1.7882	2.0802	1.8883
H	2.6475	3.2620	0.8808
H	0.7994	3.2783	-0.7701
H	0.2697	3.7259	0.8688
H	-1.3483	2.2439	0.2005
C	-0.3706	-0.3624	-2.1460
C	-1.1445	-1.4383	-1.6365
H	0.6150	-0.5806	-2.5669
H	-0.8985	0.4866	-2.5908
H	-0.7090	-2.4426	-1.6457
H	-2.2230	-1.4250	-1.8097
C	-1.5802	-1.4368	0.4013
C	-0.7021	-1.6264	1.6434
H	-2.3210	-0.6188	0.5403
H	-2.1337	-2.3587	0.2022
H	0.0529	-0.8097	1.8347
H	-0.0999	-2.5431	1.5265
C	-1.5354	-1.6773	2.9325
H	-0.8855	-1.8322	3.8051
H	-2.0960	-0.7429	3.0743
H	-2.2525	-2.5080	2.8812

Strucutre TS[3a-11a]

E_{total} = -5.742351 a.u.

Atom	X	Y	Z
Ti	-0.0102	0.0030	-0.0018
N	1.8539	0.0010	0.0047
C	2.6581	1.2406	-0.0066
C	1.9313	2.4061	-0.6705
C	0.6469	2.8680	0.0116
N	-0.3993	1.8243	0.0269
H	2.4460	-0.8355	0.1132
H	3.5874	1.0469	-0.5673
H	2.9432	1.5044	1.0284
H	2.6242	3.2630	-0.6935
H	1.7093	2.1427	-1.7193
H	0.2581	3.7412	-0.5376
H	0.8576	3.1927	1.0470
H	-1.3394	2.2277	0.1518
C	-0.4704	-0.5926	2.1317
C	-1.2156	-1.5922	1.4739
H	0.4989	-0.8436	2.5717
H	-0.9769	0.2820	2.5461
H	-1.1743	-1.4369	-0.0070
H	-2.3073	-1.4488	1.4612
C	-0.7721	-3.0406	1.5072
H	-1.2556	-3.6508	0.7326
H	0.3192	-3.1386	1.4145
H	-1.0564	-3.4607	2.4858
C	-0.4610	-0.5362	-2.1871
C	-1.2297	-1.5023	-1.5287
H	0.5183	-0.7983	-2.5923
H	-0.9339	0.3634	-2.5857
H	-0.8780	-2.5411	-1.5217
H	-2.3216	-1.3947	-1.5137

Strucutre TS[1a-12a]

E_{total} = -4.539234 a.u.

Atom	X	Y	Z
Ti	-0.0061	-0.0043	0.0030
N	1.8468	-0.0526	0.0298
C	2.6453	1.2011	0.0284
C	2.0584	2.2685	-0.8931
C	0.6823	2.8020	-0.5037
N	-0.3572	1.7438	-0.5008
H	2.4346	-0.9002	0.0058
H	3.6618	0.9579	-0.3172
H	2.7358	1.5842	1.0606
H	2.7554	3.1229	-0.9061
H	2.0126	1.8685	-1.9210
H	0.3852	3.5731	-1.2314
H	0.7190	3.2841	0.4899
H	-1.2816	2.0944	-0.7984
C	-0.8031	-0.1706	2.2345
C	-1.3919	-1.3455	1.8554
C	-0.8083	-2.6925	2.0829
H	0.1623	-0.1835	2.7566
H	-1.3891	0.7533	2.2742
H	-2.4299	-1.3224	1.5057
H	-1.0325	-1.3432	-0.3292
H	-1.0320	-3.3863	1.2623
H	0.2712	-2.6638	2.2810
H	-1.2987	-3.1041	2.9855

1.2 Zronium Generic Systems

1.2.1 FO Relativistic Results

Strucutre 1b

E_{total} = -4.593557 a.u.

Atom	X	Y	Z
Zr	0.0174	-0.0039	-0.0091
N	2.0285	-0.0018	0.0146
C	2.6885	1.3232	0.0531
C	1.8078	2.4726	-0.4632
C	0.5765	2.9051	0.3493
N	-0.5088	1.8980	0.3703
H	2.7063	-0.7666	0.1304
H	3.5844	1.2829	-0.5878
H	3.0308	1.5407	1.0805
H	2.4623	3.3579	-0.5258
H	1.5019	2.2604	-1.5086
H	0.1855	3.8266	-0.1120
H	0.8742	3.1568	1.3828
H	-1.3932	2.3003	0.7076
C	-1.3137	-1.7643	-0.0845
C	-1.4224	-1.5305	-1.5777
H	-0.8168	-2.7165	0.1658
H	-2.2731	-1.6815	0.4484
H	-0.7163	-0.6695	-1.9320
H	-2.4044	-1.1168	-1.8542
C	-1.0552	-2.7060	-2.4818
H	-1.0695	-2.4223	-3.5429
H	-0.0610	-3.1067	-2.2382
H	-1.7910	-3.5087	-2.3272

Strucutre 2b

E_{total} = -4.593584 a.u.

Atom	X	Y	Z
Zr	0.0314	0.0141	0.0220
N	2.0403	-0.0489	0.0396
C	2.7304	1.2573	-0.0396
C	1.8438	2.3895	-0.5859
C	0.6655	2.9085	0.2554
N	-0.4407	1.9353	0.3926
H	2.7050	-0.8287	0.1227
H	3.5886	1.1557	-0.7237
H	3.1311	1.5326	0.9523
H	2.5101	3.2524	-0.7508
H	1.4793	2.1136	-1.5976
H	0.2767	3.8082	-0.2489
H	1.0216	3.2205	1.2536
H	-1.3096	2.3894	0.7017
C	-1.2912	-1.7295	0.3068
C	-1.0048	-1.5913	1.7847
H	-2.3506	-1.5711	0.0487
H	-0.9233	-2.6668	-0.1391
H	-0.2917	-0.6891	2.0066
H	-0.3875	-2.4196	2.1653
C	-2.2144	-1.3495	2.6849
H	-1.9177	-1.1416	3.7217
H	-2.8284	-0.5130	2.3210
H	-2.8410	-2.2557	2.6761

Strucutre 3b

E_{total} = -5.783233 a.u.

Atom	X	Y	Z
Zr	0.0175	-0.0602	0.0221
N	2.0389	0.0424	-0.0589
C	2.7730	1.3155	-0.0735
C	1.8793	2.5183	-0.3806
C	0.7824	2.8518	0.6337
N	-0.2540	1.8131	0.7504
H	2.6747	-0.7502	0.1182
H	3.5668	1.2687	-0.8385
H	3.2729	1.4601	0.9012
H	2.5345	3.4016	-0.4503
H	1.4343	2.4031	-1.3879
H	0.3066	3.7981	0.3243
H	1.2356	3.0272	1.6259
H	-0.9946	2.1036	1.4040
C	-1.0669	-1.7525	0.9445
C	-2.3532	-1.0052	1.3073
H	-1.2495	-2.5145	0.1586
H	-0.6063	-2.2702	1.8025
H	-2.4632	-0.0663	0.6944
H	-2.2969	-0.6484	2.3485
C	-3.6443	-1.8070	1.1071
H	-4.5325	-1.2103	1.3597
H	-3.7426	-2.1470	0.0653
H	-3.6316	-2.6988	1.7507
C	-1.1975	0.5424	-2.3183
C	-0.1708	-0.2696	-2.6512
H	-1.1162	1.6288	-2.3800
H	-2.1879	0.1369	-2.0855
H	0.7842	0.1248	-3.0014
H	-0.3015	-1.3569	-2.6999

Strucutre 4b

E_{total} = -5.784167 a.u.

Atom	X	Y	Z
Zr	0.0880	0.0596	-0.0037
N	2.1018	-0.0578	-0.0649
C	2.8584	1.2140	0.0326
C	2.1312	2.3116	0.8234
C	0.8629	2.9527	0.2400
N	-0.3015	2.0371	0.1626
H	2.7298	-0.8615	-0.1888
H	3.1252	1.5823	-0.9756
H	3.8046	1.0100	0.5593
H	1.9068	1.9312	1.8377
H	2.8569	3.1313	0.9581
H	1.0762	3.3807	-0.7574
H	0.5935	3.7941	0.8989
H	-1.1865	2.5591	0.1653
C	-1.3395	-1.6437	0.4494
C	-0.9112	-1.4390	1.8866
H	-2.3968	-1.3818	0.2828
H	-1.1388	-2.6547	0.0728
H	-0.2380	-0.5116	2.0369
H	-0.2361	-2.2431	2.2167
C	-2.0427	-1.2219	2.8942
H	-1.6528	-1.0024	3.8975
H	-2.6963	-0.3941	2.5843
H	-2.6528	-2.1349	2.9461
C	-0.3863	0.1443	-2.6076
C	-0.8652	-1.0858	-2.3093
H	0.6656	0.2907	-2.8717
H	-1.0567	0.9968	-2.7410
H	-0.2157	-1.9644	-2.3100
H	-1.9324	-1.2745	-2.1988

Structure 5b

E_{total} = -5.782516 a.u.

Atom	X	Y	Z
Zr	0.0055	-0.0037	-0.0115
N	2.0165	0.0008	-0.0044
C	2.7294	1.3041	0.0069
C	2.2578	2.2643	-1.0875
C	0.8505	2.8384	-0.9218
N	-0.2099	1.8081	-0.9049
H	2.6431	-0.7830	-0.2280
H	3.8048	1.1146	-0.1262
H	2.6203	1.7817	0.9972
H	2.9553	3.1184	-1.1087
H	2.3315	1.7574	-2.0646
H	0.6596	3.5313	-1.7556
H	0.8043	3.4409	0.0056
H	-1.0564	2.1306	-1.3928
C	-1.0780	-1.7171	-0.9132
C	-1.1988	-2.4208	0.4344
H	-2.0565	-1.4327	-1.3366
H	-0.5168	-2.2942	-1.6645
H	-0.7226	-1.8104	1.2720
H	-0.5876	-3.3366	0.4544
C	-2.6208	-2.7145	0.9089
H	-2.6288	-3.1552	1.9161
H	-3.2375	-1.8033	0.9253
H	-3.0987	-3.4258	0.2197
C	-0.8247	1.4642	2.1442
C	-0.3165	0.3439	2.7005
H	-0.2077	2.3462	1.9638
H	-1.8994	1.5800	1.9797
H	0.7384	0.2704	2.9752
H	-0.9690	-0.4714	3.0195

Strucutre 6b

E_{total} = -5.785449 a.u.

Atom	X	Y	Z
Zr	0.0107	0.0602	0.0139
N	2.0293	0.0245	-0.0175
C	2.7364	1.3228	-0.0092
C	1.8794	2.5023	-0.4940
C	0.6860	2.9652	0.3559
N	-0.4290	1.9950	0.4102
H	2.6850	-0.7606	0.0843
H	3.6084	1.2537	-0.6809
H	3.1227	1.5333	1.0045
H	2.5587	3.3676	-0.5713
H	1.5347	2.3046	-1.5284
H	0.3114	3.9025	-0.0889
H	1.0251	3.2055	1.3800
H	-1.2842	2.4328	0.7759
C	-1.2702	-1.6975	0.6350
C	-0.7614	-1.4031	2.0309
H	-2.3542	-1.5282	0.5368
H	-1.0139	-2.7027	0.2755
H	-0.1308	-0.4363	2.0933
H	-0.0255	-2.1559	2.3520
C	-1.8415	-1.1987	3.0958
H	-1.4079	-0.9079	4.0622
H	-2.5610	-0.4261	2.7884
H	-2.3936	-2.1404	3.2270
C	-0.6419	0.0365	-2.5520
C	-1.1364	-1.1695	-2.1926
H	0.3859	0.1345	-2.9163
H	-1.2900	0.9131	-2.6379
H	-0.5224	-2.0715	-2.2335
H	-2.1940	-1.3127	-1.9727

Structure 7b

E_{total} = -5.790504 a.u.

Atom	X	Y	Z
Zr	0.0086	-0.0643	-0.3066
N	1.8422	-0.0637	0.5226
C	2.5478	1.2380	0.5232
C	2.0168	2.2310	-0.5258
C	0.6173	2.8468	-0.3570
N	-0.4834	1.8726	-0.5268
H	2.3971	-0.7985	0.9790
H	3.6089	1.0553	0.2876
H	2.5085	1.6906	1.5303
H	2.7267	3.0744	-0.5412
H	2.0937	1.7720	-1.5333
H	0.5114	3.6269	-1.1284
H	0.5354	3.3441	0.6261
H	-1.3776	2.3366	-0.7311
C	-1.3885	-1.7667	-0.4078
C	-1.8139	-1.4004	0.9961
H	-0.8927	-2.7504	-0.4654
H	-2.1948	-1.6991	-1.1534
H	-1.1029	-0.6044	1.4727
H	-2.7773	-0.8651	1.0060
C	-1.8270	-2.5425	2.0200
H	-0.8382	-3.0333	2.0370
H	-2.5390	-3.2928	1.6327
C	-2.2357	-2.1217	3.4286
H	-1.5092	-1.3889	3.8226
H	-3.2107	-1.6063	3.3830
C	-2.3333	-3.3122	4.3807
H	-3.0832	-4.0373	4.0291
H	-1.3691	-3.8367	4.4633
H	-2.6276	-2.9876	5.3884

Structure 8b

E_{total} = -5.793156 a.u.

Atom	X	Y	Z
Zr	0.0634	-0.0525	-0.0963
N	2.0727	-0.0465	-0.1381
C	2.7900	1.2577	-0.1344
C	2.1457	2.3236	-1.0243
C	0.7632	2.8459	-0.6247
N	-0.3105	1.8208	-0.7204
H	2.7225	-0.8405	-0.1962
H	3.8109	1.0840	-0.5064
H	2.8903	1.6337	0.9006
H	2.8274	3.1910	-1.0284
H	2.0993	1.9456	-2.0603
H	0.5062	3.6751	-1.3008
H	0.7947	3.2684	0.3966
H	-1.1608	2.1928	-1.1630
C	-1.2006	-1.8152	-0.4746
C	-1.9148	-1.7002	0.9001
H	-0.5842	-2.7318	-0.5223
H	-1.9218	-1.8375	-1.3048
H	-2.1500	-2.7084	1.2783
H	-2.8777	-1.1779	0.7918
C	-1.1154	-0.9984	2.0350
H	-1.0309	0.1215	1.9002
H	-0.0866	-1.4176	2.1261
C	-1.7882	-1.1346	3.4130
H	-2.8234	-0.7651	3.3277
H	-1.8528	-2.2122	3.6369
C	-1.0527	-0.4061	4.5303
H	-0.0208	-0.7728	4.6395
H	-1.0188	0.6796	4.3515
H	-1.5634	-0.5648	5.4905

Strucutre 9b

E_{total} = -5.792486 a.u.

Atom	X	Y	Z
Zr	-0.0696	0.1115	-0.1675
N	1.9372	0.0438	-0.0706
C	2.6570	1.2415	0.4434
C	2.1948	2.5537	-0.1957
C	0.7873	3.0384	0.1508
N	-0.2855	2.1087	-0.2840
H	2.5798	-0.6598	-0.4553
H	3.7290	1.1131	0.2329
H	2.5609	1.2981	1.5428
H	2.8943	3.3427	0.1287
H	2.2885	2.4678	-1.2919
H	0.6292	4.0071	-0.3468
H	0.7073	3.2209	1.2381
H	-1.1089	2.6153	-0.6356
C	-1.2632	-1.2832	-1.3869
C	-2.0156	-1.9560	-0.2115
H	-0.5877	-2.0130	-1.8751
H	-1.9537	-0.8942	-2.1513
H	-2.2840	-2.9852	-0.4967
H	-2.9701	-1.4405	-0.0191
C	-1.2292	-2.0480	1.1322
C	-1.3605	-0.8808	2.1400
H	-1.6006	-2.9290	1.6811
H	-0.1582	-2.3031	0.9565
H	-0.9407	0.1258	1.8366
H	-2.4330	-0.6416	2.2543
C	-0.7342	-1.1936	3.4972
H	-1.2441	-2.0600	3.9439
H	0.3331	-1.4399	3.4035
H	-0.8389	-0.3477	4.1896

Strcuture 11b

E_{total} = -5.790601 a.u.

Atom	X	Y	Z
Zr	-0.1472	-0.0121	-0.2779
N	1.8472	-0.2889	-0.1638
C	2.7062	0.7390	0.4698
C	2.4167	2.1615	-0.0159
C	1.0593	2.7448	0.3765
N	-0.0881	2.0042	-0.1955
H	2.3945	-0.9961	-0.6714
H	3.7582	0.5007	0.2537
H	2.5926	0.6931	1.5682
H	3.1926	2.8208	0.4084
H	2.5225	2.1930	-1.1138
H	1.0176	3.7867	0.0249
H	0.9741	2.7786	1.4788
H	-0.7965	2.6363	-0.5898
C	-1.2499	-0.1613	2.1351
C	-0.3714	-1.1616	2.3813
H	-1.1089	0.8355	2.5582
H	-2.2264	-0.3747	1.6860
H	-0.6170	-2.1736	2.0332
C	0.8415	-1.0497	3.2315
H	1.7109	-1.5440	2.7772
H	1.0841	-0.0099	3.4853
H	0.6366	-1.5870	4.1761
C	-1.1974	-0.9327	-1.9933
C	-1.9212	-1.9526	-1.1098
H	-0.4962	-1.4094	-2.6990
H	-1.8885	-0.2953	-2.5645
H	-1.5374	-1.9939	-0.0510
H	-1.8028	-2.9907	-1.4513
H	-2.9934	-1.7426	-1.0034

Structure 12b

E_{total} = -4.574793 a.u.

Atom	X	Y	Z
Zr	0.0693	-0.2212	-0.0779
N	2.0446	0.1295	-0.0315
C	2.6286	1.4896	0.0773
C	1.8997	2.5260	-0.7771
C	0.4459	2.8085	-0.4009
N	-0.4458	1.6387	-0.6047
H	2.7605	-0.5861	-0.2220
H	3.6795	1.4451	-0.2441
H	2.6314	1.8051	1.1362
H	2.4552	3.4745	-0.6863
H	1.9461	2.2199	-1.8361
H	0.0789	3.6377	-1.0233
H	0.3838	3.1468	0.6489
H	-1.2737	1.8703	-1.1720
C	0.1073	-0.3482	2.6164
C	-1.1808	-0.5422	2.2481
C	-1.7916	-1.8751	1.9582
H	0.7899	-1.1902	2.7695
H	0.4716	0.6395	2.9063
H	-1.8521	0.3270	2.2236
H	-0.5206	-1.6061	-1.1772
H	-2.2332	-1.9368	0.9464
H	-1.0819	-2.7029	2.0919
H	-2.6413	-2.0305	2.6470

Strucutre 12b'

E_{total} = -4.576655 a.u.

Atom	X	Y	Z
Zr	0.0075	0.0063	0.0058
N	2.0204	0.0282	0.0295
C	2.7921	1.2843	0.0561
C	1.9677	2.5136	-0.3315
C	0.8077	2.9021	0.5866
N	-0.2669	1.8936	0.6251
H	2.6114	-0.7839	0.2655
H	3.6393	1.1997	-0.6454
H	3.2186	1.4215	1.0658
H	2.6605	3.3702	-0.3543
H	1.5985	2.4037	-1.3688
H	0.3903	3.8567	0.2254
H	1.1840	3.0733	1.6107
H	-1.0590	2.1994	1.2106
C	-1.0943	-0.1694	-2.3092
C	0.1169	-0.5013	-2.8239
C	0.9563	0.3812	-3.6710
H	-1.7505	-0.9455	-1.8911
H	-1.5398	0.8119	-2.5016
H	0.4638	-1.5390	-2.7184
H	-0.8607	-1.3501	0.9368
H	0.8962	-0.0088	-4.7045
H	0.6024	1.4195	-3.6827
H	2.0176	0.3383	-3.3910

Strucutre TS[3b-8b]

E_{total} = -5.773705 a.u.

Atom	X	Y	Z
Zr	-0.1471	0.0370	-0.0994
N	1.7931	-0.0502	0.4346
C	2.5586	1.2153	0.5149
C	1.9973	2.3331	-0.3720
C	0.6371	2.9444	-0.0126
N	-0.5082	2.0230	-0.2042
H	2.3466	-0.8501	0.7626
H	3.5899	1.0165	0.1802
H	2.6132	1.5586	1.5639
H	2.7288	3.1574	-0.3375
H	1.9752	1.9873	-1.4236
H	0.4872	3.8182	-0.6684
H	0.6558	3.3152	1.0286
H	-1.3957	2.5387	-0.2317
C	-0.4668	-0.8534	-2.2042
C	-1.3943	-1.7301	-1.5626
H	0.4630	-1.2939	-2.5775
H	-0.8783	-0.0481	-2.8215
H	-1.1496	-2.7936	-1.5396
H	-2.4619	-1.5349	-1.6923
C	-1.4932	-1.7994	0.5055
C	-2.0398	-0.8150	1.5474
H	-2.2374	-2.5863	0.3545
H	-0.5683	-2.3071	0.8657
H	-1.4406	0.1289	1.6974
H	-3.0327	-0.4604	1.2230
C	-2.1242	-1.4411	2.9459
H	-2.7814	-2.3217	2.9198
H	-1.1340	-1.7619	3.2978
H	-2.5358	-0.7226	3.6682

Structure TS[4b-10b]

E_{total} = -5.773949 a.u.

Atom	X	Y	Z
Zr	0.0000	0.0001	0.0002
N	2.0146	0.0002	0.0004
C	2.7219	1.3020	-0.0003
C	1.9003	2.4530	0.5897
C	0.6602	2.9420	-0.1675
N	-0.4488	1.9584	-0.2122
H	2.6687	-0.7861	-0.0882
H	3.0467	1.5566	-1.0260
H	3.6303	1.2008	0.6156
H	1.6155	2.2001	1.6280
H	2.5810	3.3168	0.6644
H	0.9388	3.2411	-1.1950
H	0.3007	3.8463	0.3499
H	-1.3492	2.4215	-0.3823
C	-0.7260	-0.9717	-1.9622
C	-1.4734	-1.8435	-1.1151
H	0.1230	-1.3990	-2.5058
H	-1.2746	-0.1943	-2.5040
H	-1.2032	-2.9005	-1.1079
H	-2.5472	-1.6692	-1.0137
C	-1.1124	-1.8739	0.9423
C	-1.3679	-0.8811	2.0812
H	-1.8906	-2.6416	0.9727
H	-0.1368	-2.3943	1.0663
H	-0.7684	0.0751	2.0544
H	-2.4154	-0.5396	2.0418
C	-1.0457	-1.4815	3.4562
H	-1.6652	-2.3727	3.6271
H	0.0102	-1.7784	3.5202
H	-1.2541	-0.7552	4.2539

Strucutre TS[3b-11b]

E_{total} = -5.772452 a.u.

Atom	X	Y	Z
Zr	0.0088	-0.0040	0.0141
N	2.0245	0.0103	0.0213
C	2.7302	1.3133	-0.0279
C	1.9097	2.4418	-0.6610
C	0.6683	2.9465	0.0813
N	-0.4334	1.9573	0.1454
H	2.6849	-0.7664	0.1455
H	3.6417	1.1904	-0.6362
H	3.0508	1.6072	0.9887
H	2.5884	3.3051	-0.7601
H	1.6265	2.1539	-1.6903
H	0.3028	3.8371	-0.4562
H	0.9464	3.2695	1.1016
H	-1.3326	2.4106	0.3480
C	-0.5680	-0.8340	2.1920
C	-1.3533	-1.7519	1.4622
H	0.3689	-1.1737	2.6444
H	-1.0429	0.0290	2.6654
H	-1.2583	-1.5603	-0.0206
H	-2.4306	-1.5316	1.4266
C	-1.0219	-3.2284	1.4562
H	-1.5196	-3.7719	0.6423
H	0.0617	-3.4081	1.3998
H	-1.3767	-3.6557	2.4084
C	-0.6097	-0.6421	-2.2482
C	-1.3372	-1.6209	-1.5622
H	0.3507	-0.8952	-2.7029
H	-1.1195	0.2411	-2.6397
H	-0.9662	-2.6518	-1.5634
H	-2.4287	-1.5351	-1.5126

Strucutre TS[1b-12b]

E_{total} = -4.569956 a.u.

Atom	X	Y	Z
Zr	0.0026	0.0023	-0.0251
N	2.0096	0.0372	-0.0215
C	2.7043	1.3481	0.0204
C	1.8971	2.4963	-0.5925
C	0.6221	2.9536	0.1217
N	-0.4681	1.9473	0.0995
H	2.6785	-0.7404	0.0457
H	3.6377	1.2549	-0.5580
H	2.9857	1.5896	1.0614
H	2.5689	3.3699	-0.6271
H	1.6526	2.2459	-1.6418
H	0.2590	3.8572	-0.3936
H	0.8464	3.2381	1.1656
H	-1.3880	2.3882	0.2268
C	-1.5432	-1.8766	0.3145
C	-1.6702	-2.0113	-1.0444
H	-0.9446	-2.6026	0.8824
H	-2.2958	-1.3081	0.8794
H	-0.3928	-0.3653	-1.8096
H	-2.4395	-1.4283	-1.5587
C	-1.0224	-3.0824	-1.8407
H	-0.7305	-2.7395	-2.8404
H	-0.1647	-3.5379	-1.3286
H	-1.7824	-3.8752	-1.9791

1.2.2 Full QR Results

Structure 1b'

E_{total} = -4.595057 a.u.

Atom	X	Y	Z
Zr	0.0125	0.0024	-0.0361
N	2.0190	0.0197	0.0508
C	2.6755	1.3478	0.0514
C	1.7888	2.4783	-0.4931
C	0.5550	2.9170	0.3091
N	-0.5211	1.9003	0.3444
H	2.6957	-0.7354	0.2201
H	3.5731	1.2943	-0.5856
H	3.0114	1.5946	1.0738
H	2.4369	3.3662	-0.5777
H	1.4861	2.2414	-1.5349
H	0.1579	3.8264	-0.1701
H	0.8479	3.1883	1.3383
H	-1.4047	2.2948	0.6917
C	-1.2998	-1.7664	0.0012
C	-1.4731	-1.5738	-1.4976
H	-0.7882	-2.7126	0.2462
H	-2.2462	-1.6972	0.5587
H	-0.7405	-0.7643	-1.9157
H	-2.4485	-1.1228	-1.7377
C	-1.2097	-2.7917	-2.3805
H	-1.2574	-2.5383	-3.4482
H	-0.2251	-3.2318	-2.1689
H	-1.9747	-3.5518	-2.1662

Structure 2b'

E_{total} = -4.594814 a.u.

Atom	X	Y	Z
Zr	0.0015	0.0013	0.0078
N	2.0100	0.0005	0.0092
C	2.6585	1.3307	-0.0092
C	1.7252	2.4599	-0.4776
C	0.5458	2.8926	0.4099
N	-0.5254	1.8748	0.5073
H	2.7006	-0.7597	0.0416
H	3.5067	1.2951	-0.7115
H	3.0661	1.5651	0.9900
H	2.3582	3.3519	-0.6131
H	1.3467	2.2230	-1.4945
H	0.1179	3.8042	-0.0377
H	0.9077	3.1593	1.4186
H	-1.4026	2.2805	0.8561
C	-1.2727	-1.7921	0.1663
C	-0.9680	-1.7509	1.6485
H	-2.3415	-1.6430	-0.0577
H	-0.9028	-2.6967	-0.3403
H	-0.2940	-0.8308	1.9315
H	-0.3068	-2.5742	1.9598
C	-2.1712	-1.6289	2.5803
H	-1.8691	-1.4774	3.6250
H	-2.8285	-0.7998	2.2809
H	-2.7551	-2.5589	2.5152

Structure 3b'

E_{total} = -5.784731 a.u.

Atom	X	Y	Z
Zr	-0.0005	0.0127	0.0046
N	2.0208	-0.0183	-0.0117
C	2.8258	1.2128	-0.0261
C	2.0076	2.4596	-0.3657
C	0.9094	2.8688	0.6188
N	-0.1969	1.8988	0.7092
H	2.6062	-0.8407	0.1964
H	3.6307	1.1113	-0.7738
H	3.3131	1.3425	0.9567
H	2.7139	3.3028	-0.4303
H	1.5795	2.3599	-1.3822
H	0.5044	3.8411	0.2915
H	1.3473	3.0195	1.6216
H	-0.9389	2.2433	1.3335
C	-1.1852	-1.5923	0.9540
C	-2.4776	-0.7941	1.1669
H	-1.3349	-2.4039	0.2116
H	-0.8148	-2.0658	1.8780
H	-2.5086	0.1165	0.5032
H	-2.4991	-0.3844	2.1896
C	-3.7687	-1.5721	0.8931
H	-4.6582	-0.9413	1.0328
H	-3.7858	-1.9638	-0.1350
H	-3.8374	-2.4293	1.5786
C	-1.1289	0.5918	-2.3648
C	-0.0913	-0.2215	-2.6610
H	-1.0451	1.6777	-2.4295
H	-2.1274	0.1868	-2.1696
H	0.8748	0.1711	-2.9807
H	-0.2200	-1.3088	-2.7133

Strcuture 4b'

E_{total} = -5.785458 a.u.

Atom	X	Y	Z
Zr	0.0003	-0.0058	-0.0156
N	2.0156	0.0042	0.0042
C	2.6940	1.3246	0.0211
C	1.8753	2.4349	0.6947
C	0.5945	2.9442	0.0187
N	-0.5060	1.9492	-0.0238
H	2.6953	-0.7652	-0.0201
H	2.9750	1.6262	-1.0049
H	3.6299	1.2214	0.5927
H	1.6353	2.1238	1.7285
H	2.5452	3.3064	0.7846
H	0.8194	3.3041	-1.0025
H	0.2469	3.8153	0.5969
H	-1.4206	2.4128	-0.0837
C	-1.3371	-1.7380	0.5759
C	-0.9540	-1.3602	1.9936
H	-2.4050	-1.5575	0.3711
H	-1.0799	-2.7734	0.3193
H	-0.3501	-0.3760	2.0631
H	-0.2332	-2.0784	2.4125
C	-2.1200	-1.1238	2.9564
H	-1.7692	-0.7821	3.9396
H	-2.8198	-0.3771	2.5554
H	-2.6685	-2.0673	3.0871
C	-0.4054	-0.1842	-2.6044
C	-0.8311	-1.4060	-2.2032
H	0.6433	-0.0107	-2.8643
H	-1.1138	0.6159	-2.8317
H	-0.1402	-2.2473	-2.1119
H	-1.8900	-1.6390	-2.0987

Structure 5b'

E_{total} = -5.783931 a.u.

Atom	X	Y	Z
Zr	-0.0122	0.0215	0.0193
N	1.9937	-0.0193	-0.0007
C	2.7388	1.2673	-0.0375
C	2.2609	2.2137	-1.1403
C	0.8730	2.8261	-0.9542
N	-0.2144	1.8225	-0.8894
H	2.6007	-0.8234	-0.2028
H	3.8043	1.0483	-0.1979
H	2.6708	1.7674	0.9452
H	2.9774	3.0501	-1.1990
H	2.2975	1.6826	-2.1063
H	0.6785	3.5040	-1.7989
H	0.8622	3.4491	-0.0399
H	-1.0586	2.1564	-1.3722
C	-1.0925	-1.6840	-0.8925
C	-1.1372	-2.4323	0.4385
H	-2.0975	-1.4290	-1.2702
H	-0.5454	-2.2256	-1.6798
H	-0.5795	-1.8699	1.2614
H	-0.5558	-3.3661	0.3853
C	-2.5316	-2.6987	0.9999
H	-2.4877	-3.1691	1.9926
H	-3.1196	-1.7718	1.0812
H	-3.0765	-3.3746	0.3249
C	-0.7869	1.5077	2.1542
C	-0.4797	0.3036	2.6837
H	-0.0381	2.2959	2.0522
H	-1.8201	1.7869	1.9340
H	0.5338	0.0743	3.0230
H	-1.2612	-0.4214	2.9232

Strucutre 6b'

E_{total} = -5.786770 a.u.

Atom	X	Y	Z
Zr	-0.0014	-0.0050	-0.0025
N	2.0153	0.0017	0.0007
C	2.7000	1.3137	0.0027
C	1.8295	2.4687	-0.5136
C	0.6146	2.9188	0.3110
N	-0.4800	1.9236	0.3610
H	2.6856	-0.7675	0.1228
H	3.5842	1.2506	-0.6529
H	3.0640	1.5454	1.0197
H	2.4926	3.3460	-0.5948
H	1.5039	2.2474	-1.5493
H	0.2266	3.8410	-0.1526
H	0.9323	3.1796	1.3367
H	-1.3497	2.3497	0.7047
C	-1.2623	-1.7712	0.6271
C	-0.7709	-1.4434	2.0240
H	-2.3484	-1.6203	0.5211
H	-0.9952	-2.7836	0.2969
H	-0.1533	-0.4665	2.0787
H	-0.0273	-2.1794	2.3655
C	-1.8641	-1.2351	3.0741
H	-1.4447	-0.9234	4.0401
H	-2.5899	-0.4769	2.7467
H	-2.4053	-2.1817	3.2142
C	-0.6058	-0.0663	-2.5634
C	-1.1005	-1.2707	-2.1949
H	0.4243	0.0298	-2.9211
H	-1.2573	0.8053	-2.6703
H	-0.4835	-2.1710	-2.2196
H	-2.1601	-1.4155	-1.9868

Strucutre TS[3b'-8b']

E_{total} = -5.774806 a.u.

Atom	X	Y	Z
Zr	-0.0063	-0.0034	0.0025
N	2.0052	0.0046	0.0206
C	2.7159	1.3052	0.0047
C	1.8945	2.4470	-0.6035
C	0.6538	2.9379	0.1517
N	-0.4570	1.9559	0.1793
H	2.6603	-0.7793	0.1184
H	3.6276	1.1941	-0.6044
H	3.0334	1.5740	1.0283
H	2.5733	3.3114	-0.6897
H	1.6078	2.1782	-1.6384
H	0.2966	3.8476	-0.3580
H	0.9309	3.2265	1.1819
H	-1.3445	2.4130	0.4180
C	-0.8072	-0.7309	-2.0307
C	-1.5141	-1.7116	-1.2703
H	0.0135	-1.0854	-2.6624
H	-1.3916	0.0929	-2.4535
H	-1.2352	-2.7584	-1.4024
H	-2.5847	-1.5663	-1.1064
C	-1.0731	-1.9621	0.7521
C	-1.3329	-1.1029	1.9983
H	-1.8248	-2.7556	0.7234
H	-0.0811	-2.4665	0.8044
H	-0.7405	-0.1448	2.0746
H	-2.3849	-0.7720	1.9970
C	-1.0080	-1.8540	3.2963
H	-1.6222	-2.7628	3.3617
H	0.0495	-2.1497	3.3298
H	-1.2234	-1.2259	4.1716

Structure TS[3b'-11b']

E_{total}= -5.773590

Zr	-0.0011	-0.0027	0.0044
N	2.0115	0.0148	0.0048
C	2.7334	1.3104	-0.0052
C	1.9165	2.4672	-0.5879
C	0.6869	2.9465	0.1884
N	-0.4132	1.9531	0.2306
H	2.6647	-0.7709	0.1058
H	3.6367	1.1995	-0.6274
H	3.0666	1.5643	1.0178
H	2.5993	3.3294	-0.6626
H	1.6193	2.2193	-1.6235
H	0.3146	3.8559	-0.3113
H	0.9785	3.2308	1.2161
H	-1.3064	2.3989	0.4710
C	-0.5797	-0.9384	2.1251
C	-1.3806	-1.8114	1.3555
H	0.3534	-1.3145	2.5563
H	-1.0457	-0.1022	2.6526
H	-1.2922	-1.5510	-0.1140
H	-2.4562	-1.5818	1.3411
C	-1.0609	-3.2881	1.2729
H	-1.5754	-3.7879	0.4416
H	0.0201	-3.4727	1.1908
H	-1.4042	-3.7586	2.2086
C	-0.6240	-0.5208	-2.2738
C	-1.3712	-1.5238	-1.6410
H	0.3280	-0.7712	-2.7471
H	-1.1220	0.3843	-2.6282
H	-1.0202	-2.5600	-1.7029
H	-2.4615	-1.4222	-1.5926

1.3 Generic System of Hafnium

1.3.1 Full QR Results

C2H4_rel

E_{total} = -1.156622 a.u.

Atom	X	Y	Z
C	0.0000	0.0000	0.0057
C	0.0000	0.0000	-1.3257
H	0.0000	0.9292	0.5788
H	0.0000	-0.9292	0.5788
H	0.0000	0.9292	-1.8988
H	0.0000	-0.9292	-1.8988

Strucutre 1c

E_{total} = -4.529847 a.u.

Atom	X	Y	Z
Hf	0.0875	0.0649	-0.3437
N	2.0125	0.0920	0.2999
C	2.6339	1.3481	0.7657
C	1.8253	2.5968	0.3947
C	0.4555	2.7598	1.0607
N	-0.5208	1.7411	0.6258
H	2.5765	-0.7343	0.5335
H	3.6335	1.4369	0.3081
H	2.7706	1.3082	1.8604
H	2.4361	3.4692	0.6779
H	1.7182	2.6635	-0.7060
H	0.0616	3.7562	0.7991
H	0.5685	2.7228	2.1583
H	-1.4464	1.8760	1.0511
C	-0.9915	-1.7422	0.3662
C	-1.7498	-1.8458	-0.9818
H	-0.3069	-2.5961	0.5089
H	-1.6783	-1.6900	1.2209
H	-1.1070	-1.5124	-1.8476
H	-2.6137	-1.1557	-0.9848
C	-2.2287	-3.2538	-1.3524
H	-2.7593	-3.2494	-2.3154
H	-1.3803	-3.9491	-1.4235
H	-2.9148	-3.6244	-0.5773

Strucutre 1c"

E_{total} = -4.519952 a.u.

Atom	X	Y	Z
Hf	-0.0091	0.1742	-0.1161
N	1.9767	0.1469	-0.5787
C	2.8441	1.1228	0.1347
C	2.1627	2.4608	0.4498
C	1.0387	2.5079	1.4915
N	-0.2117	1.8202	1.0706
H	2.5159	-0.4571	-1.2108
H	3.7096	1.3409	-0.5098
H	3.2431	0.6703	1.0615
H	2.9596	3.1303	0.8152
H	1.7938	2.9032	-0.4941
H	0.8004	3.5683	1.6677
H	1.3939	2.0963	2.4544
H	-1.0474	2.2589	1.4760
C	-1.6197	-0.8363	-1.2878
C	-1.5008	0.3517	-2.2427
H	-1.3198	-1.7826	-1.7659
H	-2.6252	-0.9401	-0.8574
H	-0.6289	1.0804	-1.9457
H	-2.3607	1.0343	-2.1519
C	-1.2053	0.0312	-3.7046
H	-1.0499	0.9412	-4.3000
H	-0.3194	-0.6118	-3.8050
H	-2.0672	-0.5134	-4.1191

Strucutre 2c

E_{total} = -4.526559 a.u.

Atom	X	Y	Z
Hf	-0.0134	0.0408	-0.0532
N	1.9797	0.1944	-0.3947
C	2.8076	1.2928	0.1678
C	2.1226	2.6584	0.1294
C	0.8370	2.7823	0.9512
N	-0.2964	1.9937	0.3993
H	2.5139	-0.4270	-1.0127
H	3.7400	1.3521	-0.4124
H	3.0919	1.0452	1.2073
H	2.8416	3.3980	0.5211
H	1.9076	2.9313	-0.9177
H	0.5324	3.8382	0.9883
H	1.0260	2.4754	1.9961
H	-1.0926	2.5723	0.1110
C	-1.1323	-0.5419	-1.8807
C	-1.6142	-1.8506	-1.2038
H	-1.9741	0.1470	-2.0667
H	-0.6102	-0.7312	-2.8271
H	-1.6910	-1.7421	-0.0804
H	-0.8693	-2.6522	-1.3554
C	-2.9944	-2.3443	-1.6508
H	-3.2705	-3.2725	-1.1302
H	-3.7667	-1.5879	-1.4511
H	-2.9785	-2.5432	-2.7321

Strucutre 2c"

E_{total} = -4.524805 a.u.

Atom	X	Y	Z
Hf	-0.0147	-0.0064	-0.0820
N	2.0125	-0.0281	0.1478
C	2.6838	1.2865	0.2023
C	1.8097	2.4407	-0.3119
C	0.6028	2.8789	0.5255
N	-0.4861	1.8808	0.5401
H	2.6496	-0.7989	0.3855
H	3.5891	1.2455	-0.4253
H	3.0094	1.5027	1.2356
H	2.4759	3.3128	-0.4093
H	1.4835	2.2243	-1.3519
H	0.2158	3.8176	0.0956
H	0.9292	3.0992	1.5573
H	-1.3310	2.2341	1.0061
C	-1.2930	-1.7382	0.4796
C	-0.7967	-1.5352	1.9133
H	-2.3748	-1.5495	0.3832
H	-1.0644	-2.7353	0.0777
H	-0.1483	-0.5781	2.0199
H	-0.0714	-2.3139	2.1976
C	-1.8749	-1.3761	2.9816
H	-1.4443	-1.1668	3.9700
H	-2.5757	-0.5684	2.7256
H	-2.4499	-2.3123	3.0415

Strucutre 3c

E = -5.717088 a.u.

Atom	X	Y	Z
Hf	0.0016	0.0300	-0.0570
N	2.0481	-0.0665	0.0805
C	2.8649	1.1554	0.1883
C	2.1033	2.4268	-0.1975
C	0.9460	2.8545	0.7119
N	-0.2012	1.9282	0.6801
H	2.5764	-0.8983	0.3757
H	3.7418	1.0609	-0.4757
H	3.2504	1.2562	1.2193
H	2.8298	3.2555	-0.1987
H	1.7460	2.3488	-1.2421
H	0.6061	3.8517	0.3837
H	1.3141	2.9609	1.7486
H	-0.9694	2.2502	1.2820
C	-1.2363	-1.4594	1.0557
C	-2.5935	-0.7349	0.9999
H	-1.2569	-2.3946	0.4601
H	-0.9405	-1.7362	2.0778
H	-2.5886	0.1000	0.2471
H	-2.7761	-0.2239	1.9590
C	-3.7851	-1.6297	0.6503
H	-4.7211	-1.0540	0.6086
H	-3.6418	-2.1209	-0.3246
H	-3.8974	-2.4189	1.4081
C	-1.1194	0.4105	-2.5505
C	0.0461	-0.2231	-2.8124
H	-1.1948	1.5017	-2.5643
H	-2.0528	-0.1487	-2.4319
H	0.9600	0.3277	-3.0482
H	0.0920	-1.3125	-2.9117

Strucutre 4c

E_{total} = -5.712414 a.u.

Atom	X	Y	Z
Hf	-0.0157	-0.0100	-0.0313
N	2.0289	-0.0222	0.0810
C	2.7242	1.2895	0.0611
C	1.9311	2.4307	0.7112
C	0.6657	2.9562	0.0216
N	-0.4639	1.9940	-0.0075
H	2.6911	-0.8032	0.1487
H	3.0040	1.5660	-0.9727
H	3.6648	1.1868	0.6248
H	1.6826	2.1464	1.7505
H	2.6209	3.2887	0.7829
H	0.9081	3.2896	-1.0046
H	0.3408	3.8506	0.5765
H	-1.3694	2.4783	-0.0253
C	-1.4027	-1.6998	0.5835
C	-1.0198	-1.3358	2.0163
H	-2.4668	-1.5015	0.3787
H	-1.1682	-2.7418	0.3319
H	-0.3322	-0.4067	2.0887
H	-0.3631	-2.1034	2.4549
C	-2.1766	-0.9978	2.9578
H	-1.8153	-0.6748	3.9439
H	-2.8095	-0.2007	2.5418
H	-2.8022	-1.8925	3.0892
C	-0.3162	0.0397	-2.7047
C	-0.6694	-1.2285	-2.3895
H	0.7301	0.3049	-2.8869
H	-1.0655	0.8078	-2.9060
H	0.0804	-2.0208	-2.3021
H	-1.7140	-1.5364	-2.3268

Structure 5c

E_{total} = -5.715582 a.u.

Atom	X	Y	Z
Hf	-0.0030	0.0231	-0.0489
N	2.0313	0.0346	-0.1324
C	2.8457	1.2418	0.1469
C	2.2362	2.5318	-0.4027
C	0.9039	2.9635	0.2129
N	-0.2203	2.0475	-0.1024
H	2.5999	-0.7595	-0.4452
H	3.8347	1.1030	-0.3149
H	3.0144	1.3435	1.2351
H	2.9630	3.3405	-0.2148
H	2.1179	2.4421	-1.4959
H	0.6499	3.9623	-0.1716
H	1.0152	3.0661	1.3082
H	-1.0403	2.5403	-0.4700
C	-0.8166	-0.8563	-1.9703
C	-1.6015	-1.9043	-1.2048
H	-1.4531	-0.1418	-2.5118
H	-0.0520	-1.2611	-2.6440
H	-1.4904	-1.7855	-0.0646
H	-1.1715	-2.9087	-1.3556
C	-3.1130	-1.9160	-1.4437
H	-3.6206	-2.6470	-0.7984
H	-3.5576	-0.9256	-1.2637
H	-3.3106	-2.1837	-2.4921
C	-0.3187	-0.3437	2.6163
C	-1.1812	-1.3238	2.2607
H	0.7269	-0.5679	2.8452
H	-0.6724	0.6687	2.8315
H	-0.8583	-2.3654	2.1827
H	-2.2535	-1.1313	2.1666

Strucutre 6c

E_{total} = -5.717056 a.u.

Atom	X	Y	Z
Hf	-0.0642	-0.0309	-0.0699
N	1.9797	-0.0982	0.1045
C	2.7295	1.1710	0.0720
C	1.9287	2.3447	-0.5071
C	0.7403	2.8814	0.3025
N	-0.3985	1.9473	0.3818
H	2.5561	-0.8682	0.4679
H	3.6318	1.0380	-0.5494
H	3.0749	1.4303	1.0900
H	2.6342	3.1840	-0.6189
H	1.6017	2.1021	-1.5363
H	0.4017	3.8184	-0.1724
H	1.0819	3.1436	1.3213
H	-1.1790	2.3521	0.9153
C	-1.2824	-1.5559	1.0104
C	-0.6823	-1.2211	2.3925
H	-2.3565	-1.2941	0.9724
H	-1.1892	-2.6230	0.7603
H	-0.1520	-0.2269	2.3867
H	0.1110	-1.9437	2.6409
C	-1.7042	-1.1527	3.5296
H	-1.2282	-0.8956	4.4864
H	-2.4805	-0.4028	3.3173
H	-2.1998	-2.1287	3.6383
C	-1.0579	0.3124	-2.5840
C	-0.0830	-0.6170	-2.7143
H	-0.8827	1.3686	-2.8023
H	-2.0891	0.0219	-2.3574
H	0.9242	-0.3538	-3.0476
H	-0.3021	-1.6842	-2.6004

Strucutre 7c

E_{total} = -5.724446 a.u.

Atom	X	Y	Z
Hf	0.0760	0.0303	0.1625
N	2.0653	0.0661	-0.2215
C	2.7699	1.3567	-0.4426
C	2.0453	2.2887	-1.4163
C	0.6966	2.8311	-0.9409
N	-0.3450	1.7835	-0.7632
H	2.6629	-0.7513	-0.3829
H	3.7704	1.1375	-0.8426
H	2.9216	1.8687	0.5255
H	2.7028	3.1572	-1.5906
H	1.9131	1.7732	-2.3821
H	0.3255	3.5573	-1.6787
H	0.8289	3.3822	0.0078
H	-1.2075	1.9861	-1.2801
C	-0.9503	-1.7061	-0.7667
C	-1.8920	-1.8323	0.4566
H	-0.2707	-2.5729	-0.8424
H	-1.5083	-1.6112	-1.7067
H	-1.3709	-1.5599	1.4216
H	-2.7259	-1.1091	0.3704
C	-2.4777	-3.2322	0.7108
H	-1.6491	-3.9511	0.8348
H	-3.0271	-3.5353	-0.1978
C	-3.4062	-3.2826	1.9257
H	-2.8524	-2.9536	2.8236
H	-4.2296	-2.5614	1.7833
C	-3.9840	-4.6751	2.1702
H	-4.5717	-5.0181	1.3053
H	-3.1865	-5.4113	2.3524
H	-4.6474	-4.6742	3.0467

Strucutre 8c

E_{total} = -5.730507 a.u.

Atom	X	Y	Z
Hf	-0.0197	0.0941	0.1193
N	1.9978	-0.0653	-0.0124
C	2.8440	1.1451	-0.1804
C	2.3315	2.1049	-1.2559
C	1.0053	2.8045	-0.9529
N	-0.1498	1.8752	-0.8443
H	2.5245	-0.9401	-0.1071
H	3.8581	0.8176	-0.4521
H	2.9327	1.6759	0.7853
H	3.0930	2.8938	-1.3824
H	2.2517	1.5663	-2.2155
H	0.7958	3.5195	-1.7620
H	1.0985	3.3943	-0.0224
H	-0.9686	2.2010	-1.3702
C	-1.0508	-1.5492	-0.9895
C	-2.1740	-1.7916	0.0532
H	-0.3795	-2.4227	-1.0578
H	-1.4565	-1.3446	-1.9883
H	-2.5567	-2.8208	-0.0712
H	-3.0306	-1.1227	-0.1372
C	-1.7679	-1.6640	1.5388
H	-1.5258	-0.5982	1.8357
H	-0.8640	-2.2687	1.7519
C	-2.8781	-2.0725	2.5183
H	-3.7863	-1.4927	2.2864
H	-3.1187	-3.1297	2.3173
C	-2.4954	-1.8945	3.9831
H	-1.6019	-2.4832	4.2395
H	-2.2934	-0.8392	4.2233
H	-3.3118	-2.2290	4.6380

Strucutre 9c

E_{total} = -5.728164 a.u.

Atom	X	Y	Z
Hf	0.0290	0.0816	0.1401
N	2.0402	-0.0083	-0.1146
C	2.8020	1.2447	-0.3565
C	2.2280	2.0982	-1.4912
C	0.8879	2.7705	-1.1950
N	-0.2075	1.8124	-0.8997
H	2.5625	-0.8509	-0.3781
H	3.8407	0.9729	-0.5950
H	2.8429	1.8375	0.5748
H	2.9529	2.9014	-1.7094
H	2.1393	1.4794	-2.4004
H	0.5973	3.3695	-2.0709
H	1.0044	3.4730	-0.3493
H	-1.0962	2.0967	-1.3285
C	-0.9950	-1.5972	-0.9133
C	-1.9214	-2.0619	0.2410
H	-0.2692	-2.3898	-1.1652
H	-1.5583	-1.3464	-1.8226
H	-2.2609	-3.0889	0.0264
H	-2.8391	-1.4486	0.2690
C	-1.2744	-2.0539	1.6595
C	-1.5796	-0.8339	2.5494
H	-1.6368	-2.9304	2.2207
H	-0.1773	-2.2334	1.5978
H	-1.2242	0.1578	2.1397
H	-2.6736	-0.6915	2.5807
C	-1.0157	-0.9560	3.9622
H	-1.4647	-1.8257	4.4641
H	0.0748	-1.0992	3.9569
H	-1.2456	-0.0658	4.5625

Structure 11c

E_{total} = -5.722940 a.u.

Atom	X	Y	Z
Hf	0.0086	0.0192	0.0056
N	2.0420	0.0396	-0.0914
C	2.8328	1.2918	-0.0112
C	2.2302	2.4456	-0.8145
C	0.8939	2.9853	-0.3043
N	-0.2135	2.0029	-0.3919
H	2.6070	-0.7660	-0.3788
H	3.8421	1.0849	-0.3969
H	2.9540	1.5967	1.0444
H	2.9524	3.2796	-0.7885
H	2.1203	2.1356	-1.8677
H	0.6206	3.8638	-0.9074
H	1.0077	3.3363	0.7380
H	-1.0680	2.4099	-0.7863
C	-0.4981	-0.0562	2.6346
C	-1.1701	-1.2342	2.5753
H	0.5544	-0.0298	2.9384
H	-1.0374	0.8963	2.6149
H	-2.2556	-1.2049	2.4173
C	-0.5823	-2.5716	2.8638
H	-0.9015	-3.3362	2.1412
H	0.5135	-2.5488	2.9256
H	-0.9687	-2.9050	3.8443
C	-0.7608	-1.1462	-1.7656
C	-1.7166	-1.9639	-0.9045
H	0.0175	-1.7515	-2.2487
H	-1.2661	-0.5368	-2.5246
H	-1.6498	-1.7423	0.2083
H	-1.5296	-3.0473	-0.9500
H	-2.7762	-1.7749	-1.1323

Structure 12c

E_{total} = -4.513681 a.u.

Atom	X	Y	Z
Hf	0.1475	-0.0922	-0.0084
N	2.1503	0.1959	-0.1551
C	2.7929	1.5337	-0.1711
C	2.0143	2.5764	-0.9741
C	0.6243	2.9274	-0.4360
N	-0.3489	1.8079	-0.5308
H	2.8041	-0.5636	-0.3821
H	3.7953	1.4294	-0.6117
H	2.9361	1.8916	0.8649
H	2.6116	3.5045	-0.9745
H	1.9253	2.2429	-2.0222
H	0.2249	3.7810	-1.0027
H	0.7034	3.2556	0.6158
H	-1.1550	2.0323	-1.1284
C	-0.2615	-0.6571	2.5419
C	-1.2900	0.2303	2.5563
C	-2.7236	-0.1210	2.3920
H	-0.4568	-1.7340	2.4495
H	0.7440	-0.3585	2.8580
H	-1.0702	1.2812	2.7826
H	-0.4182	-1.3221	-1.2922
H	-3.2467	0.5716	1.7170
H	-2.8790	-1.1591	2.0709
H	-3.2097	0.0017	3.3780

Strucutre TS[3c-8c]

E_{total} = -5.701770 a.u.

Atom	X	Y	Z
Hf	-0.0377	0.0006	-0.0038
N	2.0033	-0.0123	0.0527
C	2.7546	1.2622	0.1128
C	2.0096	2.4453	-0.5113
C	0.7506	2.9595	0.1926
N	-0.3863	2.0119	0.1540
H	2.6222	-0.8261	0.1369
H	3.6965	1.1331	-0.4436
H	3.0244	1.5000	1.1583
H	2.7218	3.2865	-0.5406
H	1.7659	2.2073	-1.5631
H	0.4426	3.8877	-0.3151
H	0.9905	3.2258	1.2388
H	-1.2803	2.4894	0.3134
C	-0.7233	-0.6083	-2.1562
C	-1.5340	-1.5882	-1.5179
H	0.1488	-0.9598	-2.7161
H	-1.2230	0.2712	-2.5741
H	-1.2771	-2.6424	-1.6378
H	-2.6049	-1.3983	-1.4119
C	-1.2849	-1.9621	0.6142
C	-1.5856	-1.1503	1.8791
C	-1.3424	-1.9440	3.1719
H	-2.0922	-2.6816	0.4552
H	-0.3434	-2.5451	0.7118
H	-0.9776	-0.2044	2.0210
H	-2.6258	-0.7873	1.8357
H	-1.9726	-2.8442	3.1781
H	-0.2932	-2.2604	3.2533
H	-1.5931	-1.3365	4.0527

Strucutr TS[4c-10c]

E_{total} = -5.701603 a.u.

Atom	X	Y	Z
Hf	-0.0112	0.0052	-0.0154
N	2.0287	-0.0127	0.0610
C	2.7852	1.2605	0.0630
C	2.0189	2.4309	0.6847
C	0.7911	2.9673	-0.0570
N	-0.3482	2.0216	-0.0984
H	2.6468	-0.8248	-0.0440
H	3.0968	1.5211	-0.9648
H	3.7033	1.1135	0.6544
H	1.7332	2.1684	1.7207
H	2.7312	3.2687	0.7656
H	1.0753	3.2644	-1.0829
H	0.4627	3.8796	0.4664
H	-1.2372	2.5068	-0.2629
C	-0.6137	-0.7633	-2.1493
C	-1.4655	-1.6726	-1.4680
H	0.2827	-1.1622	-2.6328
H	-1.0717	0.0973	-2.6456
H	-1.2326	-2.7384	-1.4938
H	-2.5339	-1.4506	-1.4158
C	-1.2950	-1.9308	0.7054
C	-1.4767	-1.0701	1.9581
H	-2.1813	-2.5562	0.5707
H	-0.4164	-2.5998	0.7960
H	-0.8052	-0.1579	2.0458
H	-2.4929	-0.6437	1.9689
C	-1.1969	-1.8413	3.2584
H	-1.8771	-2.7013	3.3307
H	-0.1655	-2.2202	3.2791
H	-1.3502	-1.1963	4.1348

Strucuure TS[3c-11c]

E_{total} = -5.704194 a.u.

Atom	X	Y	Z
Hf	0.0092	-0.0044	0.0173
N	2.0469	0.0787	-0.0133
C	2.7854	1.3594	-0.0502
C	1.9834	2.5172	-0.6467
C	0.7480	2.9960	0.1172
N	-0.3427	1.9986	0.1625
H	2.6795	-0.7206	0.1038
H	3.6864	1.2241	-0.6704
H	3.1242	1.6287	0.9669
H	2.6698	3.3770	-0.7192
H	1.6927	2.2633	-1.6825
H	0.3721	3.8993	-0.3901
H	1.0348	3.2911	1.1432
H	-1.2404	2.4282	0.4136
C	-0.5938	-0.9177	2.1507
C	-1.4069	-1.8333	1.4283
H	0.3372	-1.2805	2.5988
H	-1.0669	-0.0794	2.6700
H	-1.3519	-1.6346	-0.0317
H	-2.4856	-1.6149	1.4366
C	-1.0691	-3.3091	1.4113
H	-1.6228	-3.8596	0.6392
H	0.0080	-3.4847	1.2741
H	-1.3481	-3.7326	2.3900
C	-0.6997	-0.6821	-2.2093
C	-1.4570	-1.6574	-1.5286
H	0.2381	-0.9682	-2.6931
H	-1.1960	0.2064	-2.6085
H	-1.1213	-2.7001	-1.5715
H	-2.5462	-1.5375	-1.4828

Strucutre TS[1c-12c]

E = -4.502304 a.u.

Atom	X	Y	Z
Hf	-0.0024	0.0015	0.0016
N	2.0348	-0.0085	-0.0060
C	2.7730	1.2778	-0.0096
C	2.0273	2.4172	-0.7085
C	0.7466	2.9569	-0.0660
N	-0.3863	1.9990	-0.0846
H	2.6702	-0.8127	0.0555
H	3.7218	1.1243	-0.5470
H	3.0313	1.5690	1.0253
H	2.7307	3.2643	-0.7669
H	1.8061	2.1157	-1.7483
H	0.4435	3.8513	-0.6317
H	0.9493	3.2830	0.9711
H	-1.2939	2.4788	-0.0818
C	-1.5329	-1.8497	0.0995
C	-1.4441	-1.8668	-1.3002
H	-1.0263	-2.6467	0.6600
H	-2.4359	-1.4337	0.5637
H	-0.3808	-0.5313	-1.7769
H	-2.2277	-1.3553	-1.8702
C	-0.7042	-2.9306	-2.0457
H	-0.3980	-2.6097	-3.0482
H	0.1683	-3.3039	-1.4925
H	-1.4050	-3.7780	-2.1601

1.3.2. Hafnium Generic System pertubatively QR energy correction

C2H4 (D2h)

E_{total} = -1.156776 a.u.

Atom	X	Y	Z
C	-0.6660	0.0000	0.0000
C	0.6660	0.0000	0.0000
H	-1.2386	0.9296	0.0000
H	-1.2386	-0.9296	0.0000
H	1.2386	0.9296	0.0000
H	1.2386	-0.9296	0.0000

Strucutre 1c'

E = -4.503694 a.u.

Atom	X	Y	Z
Hf	0.0193	0.0051	-0.0163
N	2.0951	-0.0105	0.0826
C	2.7525	1.3153	0.0716
C	1.8798	2.4395	-0.5094
C	0.6635	2.9529	0.2790
N	-0.4593	1.9916	0.3500
H	2.7731	-0.7652	0.2496
H	3.6585	1.2500	-0.5530
H	3.0805	1.5874	1.0921
H	2.5455	3.3081	-0.6409
H	1.5617	2.1630	-1.5369
H	0.3094	3.8655	-0.2281
H	0.9779	3.2477	1.2972
H	-1.3232	2.4462	0.6735
C	-1.3872	-1.7838	-0.1004
C	-1.4600	-1.5719	-1.6040
H	-0.9209	-2.7462	0.1674
H	-2.3635	-1.6918	0.3980
H	-0.7552	-0.7077	-1.9659
H	-2.4383	-1.1681	-1.9109
C	-1.0575	-2.7545	-2.4842
H	-1.0450	-2.4836	-3.5489
H	-0.0657	-3.1417	-2.2091
H	-1.7887	-3.5637	-2.3398

Strucutre 2c'

E = -4.505813 a.u.

Atom	X	Y	Z
Hf	0.0132	-0.0025	-0.0242
N	2.0882	-0.0334	0.0669
C	2.7513	1.2890	0.0392
C	1.8742	2.4174	-0.5300
C	0.6771	2.9418	0.2790
N	-0.4450	1.9844	0.3790
H	2.7677	-0.7917	0.2127
H	3.6446	1.2183	-0.6034
H	3.0986	1.5617	1.0521
H	2.5453	3.2787	-0.6820
H	1.5367	2.1399	-1.5518
H	0.3176	3.8531	-0.2273
H	1.0128	3.2411	1.2884
H	-1.3024	2.4449	0.7109
C	-1.3609	-1.7730	0.3680
C	-1.0109	-1.6026	1.8347
H	-2.4271	-1.5893	0.1585
H	-1.0591	-2.7453	-0.0483
H	-0.2785	-0.7065	2.0197
H	-0.3883	-2.4321	2.2062
C	-2.1764	-1.3226	2.7814
H	-1.8320	-1.1076	3.8021
H	-2.7846	-0.4758	2.4310
H	-2.8242	-2.2113	2.8116

Strucutre 3c'

E_{total} = -5.697523 a.u.

Atom	X	Y	Z
Hf	0.0218	-0.0211	0.0424
N	2.1174	0.0145	-0.1206
C	2.8754	1.2743	-0.1753
C	1.9991	2.5020	-0.4441
C	0.9813	2.8941	0.6320
N	-0.1195	1.9271	0.7891
H	2.7508	-0.7789	0.0529
H	3.6353	1.2091	-0.9744
H	3.4252	1.4162	0.7745
H	2.6787	3.3606	-0.5715
H	1.4835	2.3892	-1.4173
H	0.5580	3.8754	0.3550
H	1.5025	3.0299	1.5982
H	-0.8178	2.2716	1.4611
C	-1.1556	-1.6285	1.1508
C	-2.4541	-0.8172	1.1972
H	-1.2601	-2.5428	0.5355
H	-0.8003	-1.9364	2.1457
H	-2.3874	0.1243	0.5663
H	-2.6181	-0.4211	2.2124
C	-3.7062	-1.5513	0.7115
H	-4.5894	-0.8964	0.7232
H	-3.5741	-1.9324	-0.3133
H	-3.9058	-2.4153	1.3624
C	-1.3096	0.3748	-2.3538
C	-0.1449	-0.1956	-2.7389
H	-1.4384	1.4609	-2.3377
H	-2.2009	-0.2325	-2.1649
H	0.7154	0.4030	-3.0476
H	-0.0576	-1.2797	-2.8687

Strucutre 4c'

E = -5.695549 a.u.

Atom	X	Y	Z
Hf	0.0363	0.0151	0.0293
N	2.1184	-0.0092	-0.0664
C	2.8077	1.3035	-0.0001
C	2.0491	2.3839	0.7859
C	0.7578	2.9863	0.2127
N	-0.3945	2.0547	0.1768
H	2.7940	-0.7740	-0.1855
H	3.0384	1.6730	-1.0172
H	3.7741	1.1594	0.5103
H	1.8488	2.0090	1.8081
H	2.7519	3.2260	0.9048
H	0.9509	3.3952	-0.7971
H	0.4904	3.8414	0.8547
H	-1.2828	2.5716	0.1767
C	-1.3823	-1.7582	0.5075
C	-0.9869	-1.5356	1.9582
H	-2.4464	-1.5386	0.3269
H	-1.1425	-2.7650	0.1422
H	-0.2383	-0.6624	2.1126
H	-0.3804	-2.3733	2.3366
C	-2.1271	-1.1999	2.9219
H	-1.7520	-0.9737	3.9297
H	-2.7092	-0.3361	2.5683
H	-2.8073	-2.0613	2.9869
C	-0.4606	0.2109	-2.6572
C	-0.8354	-1.0643	-2.4056
H	0.5793	0.4574	-2.8945
H	-1.1953	1.0125	-2.7595
H	-0.1099	-1.8833	-2.4248
H	-1.8841	-1.3439	-2.2978

Strucutre 5c'

E_{total} = -5.696936 a.u.

Atom	X	Y	Z
Hf	0.0124	-0.0203	-0.0046
N	2.0909	0.0388	0.0607
C	2.8067	1.3342	0.1203
C	2.0513	2.4970	-0.5318
C	0.7615	2.9908	0.1305
N	-0.3627	2.0276	0.0609
H	2.7465	-0.7513	0.0757
H	3.7623	1.2235	-0.4167
H	3.0523	1.5893	1.1682
H	2.7460	3.3538	-0.5457
H	1.8408	2.2441	-1.5869
H	0.4568	3.9107	-0.3938
H	0.9637	3.2700	1.1815
H	-1.2672	2.5133	0.0683
C	-0.5979	-0.7913	-2.1295
C	-1.4289	-1.8231	-1.4400
H	-1.1676	-0.0449	-2.6975
H	0.2545	-1.1725	-2.7030
H	-1.3410	-1.7683	-0.2663
H	-1.0396	-2.8431	-1.5958
C	-2.9382	-1.7549	-1.6793
H	-3.4886	-2.4651	-1.0464
H	-3.3297	-0.7430	-1.4944
H	-3.1411	-1.9989	-2.7325
C	-0.4183	-0.4837	2.6557
C	-1.1640	-1.4854	2.1285
H	0.6229	-0.6433	2.9481
H	-0.8654	0.4769	2.9251
H	-0.7536	-2.4912	2.0005
H	-2.2412	-1.3717	1.9775

Strucutre 6c'

E_{total} = -5.697488 a.u.

Atom	X	Y	Z
Hf	0.0333	0.0042	0.0095
N	2.1189	-0.0166	0.0508
C	2.8166	1.2832	-0.0329
C	1.9705	2.4129	-0.6382
C	0.7723	2.9727	0.1428
N	-0.3691	2.0423	0.2650
H	2.7768	-0.7748	0.2720
H	3.7089	1.1678	-0.6711
H	3.1738	1.5881	0.9684
H	2.6563	3.2617	-0.7951
H	1.6374	2.1173	-1.6531
H	0.4320	3.8779	-0.3885
H	1.1044	3.2978	1.1465
H	-1.2024	2.5345	0.6128
C	-1.2780	-1.7007	0.8335
C	-0.8183	-1.2579	2.2160
H	-2.3633	-1.5761	0.6934
H	-0.9937	-2.7346	0.5928
H	-0.1066	-0.3448	2.1933
H	-0.1606	-2.0103	2.6786
C	-1.9261	-0.8312	3.1804
H	-1.5169	-0.4404	4.1223
H	-2.5684	-0.0572	2.7344
H	-2.5584	-1.7018	3.4076
C	-0.7303	0.0600	-2.6777
C	-0.8826	-1.2413	-2.3514
H	0.2268	0.4399	-3.0492
H	-1.5772	0.7507	-2.6972
H	-0.0502	-1.9473	-2.4393
H	-1.8570	-1.6593	-2.0922

Structure 7c'

E_{total} = -5.700748 a.u.

Atom	X	Y	Z
Hf	0.0240	0.0330	0.0153
N	2.0987	0.0486	-0.0252
C	2.8456	1.3328	-0.1011
C	2.2231	2.3657	-1.0471
C	0.8487	2.9255	-0.6629
N	-0.2570	1.9335	-0.7609
H	2.7303	-0.7615	-0.0511
H	3.8646	1.1180	-0.4578
H	2.9491	1.7692	0.9106
H	2.9210	3.2200	-1.0894
H	2.1682	1.9409	-2.0654
H	0.6177	3.7647	-1.3358
H	0.8884	3.3469	0.3592
H	-1.0386	2.2823	-1.3287
C	-1.1070	-1.7577	-0.8013
C	-1.9922	-1.7418	0.4513
H	-0.4771	-2.6635	-0.8453
H	-1.6940	-1.6797	-1.7267
H	-1.4873	-1.2157	1.3387
H	-2.8980	-1.1323	0.2797
C	-2.3983	-3.1045	1.0344
H	-1.4900	-3.6998	1.2351
H	-2.9586	-3.6389	0.2469
C	-3.2474	-2.9930	2.3002
H	-2.6735	-2.4625	3.0816
H	-4.1361	-2.3739	2.0874
C	-3.6900	-4.3542	2.8328
H	-4.2991	-4.8899	2.0892
H	-2.8232	-4.9868	3.0772
H	-4.2930	-4.2422	3.7449

Structure 8c'

E_{total} = -5.708267 a.u.

Atom	X	Y	Z
Hf	0.0963	0.0001	0.0190
N	2.1441	0.0248	-0.3122
C	2.8861	1.3028	-0.4829
C	2.1459	2.3463	-1.3259
C	0.8389	2.9015	-0.7484
N	-0.2685	1.9084	-0.6994
H	2.7531	-0.7907	-0.4531
H	3.8433	1.0818	-0.9793
H	3.1346	1.7296	0.5067
H	2.8334	3.2007	-1.4536
H	1.9516	1.9326	-2.3314
H	0.5158	3.7489	-1.3720
H	1.0218	3.3097	0.2629
H	-1.1067	2.2410	-1.1919
C	-1.1602	-1.7506	-0.7086
C	-2.0818	-1.7763	0.5417
H	-0.5616	-2.6775	-0.7715
H	-1.7475	-1.6620	-1.6335
H	-2.5176	-2.7860	0.6522
H	-2.9378	-1.0924	0.4108
C	-1.4016	-1.4605	1.8983
H	-1.1366	-0.3656	2.0306
H	-0.4645	-2.0436	2.0121
C	-2.2977	-1.7381	3.1154
H	-3.2455	-1.1910	2.9833
H	-2.5451	-2.8126	3.0972
C	-1.6495	-1.3680	4.4435
H	-0.7115	-1.9217	4.6007
H	-1.4278	-0.2909	4.4986
H	-2.3211	-1.6074	5.2796

Strucutre 9c'

E_{total} = -5.706470 a.u.

Atom	X	Y	Z
Hf	0.0160	0.0356	0.0420
N	2.0897	0.0439	-0.0019
C	2.7969	1.3474	-0.1442
C	2.2459	2.2364	-1.2660
C	0.8559	2.8411	-1.0449
N	-0.2339	1.8336	-0.9657
H	2.7293	-0.7523	-0.1080
H	3.8579	1.1422	-0.3526
H	2.7688	1.8977	0.8144
H	2.9463	3.0808	-1.3896
H	2.2521	1.6681	-2.2132
H	0.6419	3.5209	-1.8842
H	0.8629	3.4615	-0.1292
H	-1.0620	2.1275	-1.4987
C	-1.1723	-1.8019	-0.5803
C	-1.9666	-1.9724	0.7416
H	-0.5097	-2.6739	-0.7352
H	-1.8417	-1.7319	-1.4515
H	-2.3586	-3.0019	0.7985
H	-2.8586	-1.3207	0.7449
C	-1.1533	-1.6995	2.0464
C	-1.3004	-0.3029	2.6857
H	-1.4836	-2.4069	2.8244
H	-0.0798	-1.9655	1.9146
H	-0.9600	0.5774	2.0576
H	-2.3769	-0.0847	2.7933
C	-0.5883	-0.1709	4.0287
H	-1.0180	-0.8893	4.7423
H	0.4869	-0.3842	3.9417
H	-0.7108	0.8354	4.4508

Strucuture 11c'

E_{total} = -5.703575 a.u.

Atom	X	Y	Z
Hf	0.0465	0.0139	-0.0368
N	2.1269	-0.0147	-0.0016
C	2.9089	1.2462	-0.0316
C	2.2782	2.3517	-0.8839
C	0.9699	2.9733	-0.3881
N	-0.1852	2.0442	-0.4224
H	2.7409	-0.8367	0.0076
H	3.8988	1.0232	-0.4594
H	3.0809	1.6193	0.9958
H	3.0169	3.1692	-0.9432
H	2.1302	1.9742	-1.9112
H	0.7398	3.8299	-1.0410
H	1.1104	3.3769	0.6326
H	-1.0567	2.5366	-0.6500
C	-0.4643	0.1436	2.6363
C	-1.1315	-1.0331	2.5230
H	0.5819	0.1664	2.9599
H	-0.9957	1.0989	2.5996
H	-2.2142	-1.0002	2.3465
C	-0.5492	-2.3747	2.8242
H	-0.8579	-3.1446	2.1029
H	0.5464	-2.3515	2.9001
H	-0.9444	-2.7014	3.8032
C	-0.6986	-1.1948	-1.8687
C	-1.6602	-1.9026	-0.9484
H	0.0693	-1.8446	-2.3060
H	-1.1800	-0.5916	-2.6471
H	-1.5662	-1.6099	0.1657
H	-1.5207	-2.9928	-0.8957
H	-2.7190	-1.6797	-1.1480

Structure 12c'

E_{total} = -4.490241 a.u.

Atom	X	Y	Z
Hf	0.0617	-0.1396	-0.0280
N	2.0843	0.1749	-0.0424
C	2.6964	1.5250	0.0275
C	1.9824	2.5660	-0.8394
C	0.5448	2.9057	-0.4357
N	-0.3947	1.7687	-0.5950
H	2.7669	-0.5538	-0.2946
H	3.7433	1.4498	-0.3028
H	2.7181	1.8638	1.0791
H	2.5705	3.4983	-0.7804
H	1.9980	2.2366	-1.8928
H	0.1912	3.7390	-1.0613
H	0.5225	3.2620	0.6102
H	-1.2082	2.0050	-1.1796
C	0.0416	-0.3365	2.7309
C	-1.2510	-0.4974	2.3575
C	-1.8916	-1.8096	2.0478
H	0.7066	-1.1966	2.8671
H	0.4256	0.6399	3.0370
H	-1.9044	0.3867	2.3484
H	-0.5648	-1.4989	-1.1857
H	-2.3666	-1.8292	1.0495
H	-1.1937	-2.6536	2.1324
H	-2.7205	-1.9735	2.7592

Strucuture TS[3c'-8c']

E_{total} = -5.683849 a.u.

Atom	X	Y	Z
Hf	-0.0690	0.0239	-0.0142
N	1.9754	-0.0297	0.3727
C	2.7275	1.2448	0.3309
C	2.0687	2.3329	-0.5277
C	0.7634	2.9791	-0.0443
N	-0.4119	2.0807	-0.0933
H	2.5716	-0.8046	0.6857
H	3.7208	1.0463	-0.1040
H	2.8918	1.6288	1.3551
H	2.8055	3.1488	-0.6115
H	1.9240	1.9484	-1.5562
H	0.5656	3.8410	-0.7027
H	0.9023	3.3776	0.9782
H	-1.2859	2.6178	-0.0544
C	-0.5448	-0.8644	-2.1643
C	-1.4408	-1.7521	-1.4900
H	0.3624	-1.2997	-2.5947
H	-0.9876	-0.0500	-2.7474
H	-1.1886	-2.8150	-1.4810
H	-2.5146	-1.5574	-1.5676
C	-1.5065	-1.8274	0.6072
C	-2.1306	-0.8365	1.5996
C	-2.2811	-1.4241	3.0097
H	-2.2081	-2.6524	0.4570
H	-0.5796	-2.2970	1.0159
H	-1.5635	0.1280	1.7511
H	-3.1112	-0.5141	1.2104
H	-2.9171	-2.3199	2.9760
H	-1.3061	-1.7128	3.4269
H	-2.7465	-0.6940	3.6866

Structure TS[4c'-10c']

E_{total} = -5.683586 a.u.

Atom	X	Y	Z
Hf	-0.0015	-0.0026	-0.0016
N	2.0790	-0.0016	-0.0017
C	2.7897	1.2987	0.0056
C	1.9964	2.4457	0.6453
C	0.7532	2.9866	-0.0740
N	-0.3898	2.0438	-0.1187
H	2.7322	-0.7836	-0.1270
H	3.0849	1.5784	-1.0225
H	3.7175	1.1823	0.5896
H	1.7258	2.1673	1.6824
H	2.6956	3.2940	0.7342
H	1.0238	3.3009	-1.0988
H	0.4364	3.8918	0.4697
H	-1.2733	2.5455	-0.2649
C	-0.7997	-0.9210	-2.0365
C	-1.5635	-1.8116	-1.2182
H	0.0273	-1.3500	-2.6108
H	-1.3391	-0.1139	-2.5433
H	-1.3208	-2.8755	-1.2609
H	-2.6330	-1.6129	-1.1026
C	-1.2203	-1.9552	0.8539
C	-1.5011	-1.0203	2.0386
H	-2.0025	-2.7187	0.8313
H	-0.2550	-2.4927	0.9779
H	-0.8990	-0.0625	2.0801
H	-2.5456	-0.6705	1.9861
C	-1.2237	-1.6872	3.3941
H	-1.8538	-2.5806	3.5061
H	-0.1721	-1.9957	3.4769
H	-1.4508	-0.9973	4.2191

Structure TS[3c'-11c']

E_{total} = -5.685438 a.u.

Atom	X	Y	Z
Hf	0.0070	0.0072	0.0215
N	2.0888	0.0518	0.0231
C	2.7656	1.3673	-0.0339
C	1.9314	2.4787	-0.6842
C	0.6894	3.0046	0.0472
N	-0.4323	2.0404	0.1089
H	2.7662	-0.7084	0.1524
H	3.6843	1.2608	-0.6340
H	3.0740	1.6829	0.9804
H	2.6067	3.3419	-0.8068
H	1.6450	2.1681	-1.7073
H	0.3480	3.8992	-0.4993
H	0.9700	3.3331	1.0654
H	-1.3205	2.5163	0.3050
C	-0.5747	-0.7904	2.2824
C	-1.3202	-1.7675	1.5855
H	0.3806	-1.0699	2.7382
H	-1.0868	0.0652	2.7307
H	-1.2748	-1.6235	0.0775
H	-2.4091	-1.6116	1.5643
C	-0.8940	-3.2203	1.6102
H	-1.3878	-3.8212	0.8354
H	0.1960	-3.3325	1.5151
H	-1.1813	-3.6383	2.5892
C	-0.7034	-0.7815	-2.2309
C	-1.3961	-1.7354	-1.4693
H	0.2460	-1.0448	-2.7050
H	-1.2350	0.0788	-2.6465
H	-1.0140	-2.7624	-1.4446
H	-2.4873	-1.6589	-1.3934

Structure TS[1c'-12c']

E_{total} = -4.483572 a.u.

Atom	X	Y	Z
Hf	0.0063	-0.0067	-0.0104
N	2.0803	0.0305	0.0355
C	2.7647	1.3452	0.0239
C	1.9623	2.4641	-0.6511
C	0.6825	2.9791	0.0201
N	-0.4477	2.0179	-0.0024
H	2.7542	-0.7368	0.1514
H	3.7066	1.2353	-0.5373
H	3.0352	1.6426	1.0545
H	2.6432	3.3284	-0.7242
H	1.7282	2.1637	-1.6898
H	0.3700	3.8841	-0.5244
H	0.9008	3.2869	1.0602
H	-1.3485	2.5032	0.0899
C	-1.4832	-1.9609	0.3335
C	-1.4564	-2.1650	-1.0370
H	-0.8881	-2.6213	0.9809
H	-2.3643	-1.4924	0.7914
H	-0.4126	-0.6300	-1.7960
H	-2.2620	-1.7399	-1.6434
C	-0.6377	-3.2261	-1.6884
H	-0.3413	-2.9629	-2.7102
H	0.2480	-3.5011	-1.0993
H	-1.2794	-4.1255	-1.7482

PART II. The McConville Ssytems

2.1 McConville Titanium system

Structure 1A

E_{total} = -4.532059 a.u.

Atom	X	Y	Z
Ti	-0.0196	-0.0293	0.1845
N	1.7933	-0.0717	-0.2228
C	2.5233	1.2196	-0.1135
C	1.6893	2.4055	-0.5886
C	0.4988	2.7927	0.2808
N	-0.5566	1.7481	0.3068
H	3.4444	1.1799	-0.7104
H	2.8419	1.3735	0.9348
H	2.3578	3.2800	-0.6291
H	1.3444	2.2187	-1.6208
H	0.0806	3.7330	-0.1064
H	0.8354	3.0008	1.3137
C	-1.3126	-1.6220	0.0334
C	-1.2655	-1.2926	-1.4439
H	-0.8936	-2.6097	0.2822
H	-2.2932	-1.4687	0.5121
H	-0.6407	-0.3321	-1.6509
H	-2.2444	-0.9540	-1.8189
C	-0.6426	-2.3530	-2.3473
H	-0.5309	-1.9880	-3.3775
H	0.3468	-2.6639	-1.9809
H	-1.2931	-3.2399	-2.3606
C	2.6560	-1.2483	-0.2626
C	-1.8302	2.2112	0.8460
C	3.5640	-1.4586	-1.3266
C	4.3831	-2.5990	-1.3239
C	4.3078	-3.5277	-0.2818
C	2.5533	-2.2090	0.7663
C	3.3939	-3.3338	0.7581
C	3.5942	-0.5583	-2.5552
H	5.0659	-2.7809	-2.1405
H	4.9448	-4.3998	-0.2869
C	1.6236	-1.9895	1.9513
H	3.3534	-4.0565	1.5589
H	2.8656	0.2390	-2.4286
C	4.9591	0.0961	-2.7880
C	3.1928	-1.2959	-3.8349
H	3.1576	-0.5928	-4.6673
H	3.9156	-2.0808	-4.0578
H	2.2066	-1.7412	-3.7025
H	4.8954	0.7872	-3.6288
H	5.2599	0.6457	-1.8962
H	5.7059	-0.6674	-3.0062
H	0.8264	-1.3204	1.6408
C	0.9468	-3.2663	2.4589
C	2.3328	-1.3259	3.1329
H	0.1927	-3.0074	3.2025
H	0.4661	-3.7819	1.6279
H	1.6835	-3.9272	2.9153
H	1.6215	-1.1575	3.9413
H	3.1376	-1.9697	3.4887
H	2.7495	-0.3694	2.8173
C	-2.6095	3.1819	0.1773
C	-3.8245	3.6033	0.7434
C	-4.2719	3.0704	1.9576
C	-2.3076	1.6489	2.0471
C	-3.5149	2.0898	2.6074
C	-2.2435	3.6906	-1.2105
H	-4.4367	4.3327	0.2340
H	-5.2067	3.4067	2.3818
C	-1.4956	0.6406	2.8456
H	-4.1455	1.9318	3.4701
H	-1.3046	3.2351	-1.5176
C	-3.2739	3.2920	-2.2700
C	-2.0574	5.2092	-1.2666
H	-2.9312	3.6123	-3.2541
H	-3.3932	2.2082	-2.2692
H	-4.2343	3.7601	-2.0534
H	-1.7252	5.5008	-2.2632
H	-2.9998	5.7087	-1.0416
H	-1.3073	5.5134	-0.5367
H	-0.8943	0.1181	2.1073
C	-0.5486	1.2989	3.8507
C	-2.3361	-0.4105	3.5745
H	0.0473	0.5354	4.3502
H	0.1169	1.9868	3.3297
H	-1.1256	1.8504	4.5933
H	-1.6789	-1.1598	4.0165
H	-2.9224	0.0613	4.3632
H	-3.0064	-0.8975	2.8662

Structure 2A

E_{total} = -4.532973 a.u.

Atom	X	Y	Z
Ti	0.0158	0.0120	0.0111
N	1.8761	-0.0209	-0.0055
C	2.5832	1.2797	0.0246
C	1.7187	2.4367	-0.4765
C	0.5158	2.8064	0.3925
N	-0.5225	1.7507	0.4096
H	3.4744	1.2164	-0.6194
H	2.9193	1.5109	1.0491
H	2.3685	3.3260	-0.5250
H	1.3871	2.2377	-1.5125
H	0.0771	3.7352	-0.0041
H	0.8709	3.0115	1.4164
C	-1.1454	-1.6594	0.3236
C	-0.8246	-1.3875	1.7753
H	-2.2142	-1.5658	0.0733
H	-0.7230	-2.5942	-0.0765
H	-0.0877	-0.4949	1.8903
H	-0.2098	-2.1884	2.2166
C	-2.0113	-1.0172	2.6590
H	-1.6899	-0.7211	3.6666
H	-2.5931	-0.1922	2.2231
H	-2.6753	-1.8894	2.7466
C	2.7135	-1.1878	-0.2758
C	-1.8995	2.2255	0.5003
C	2.3480	-2.0385	-1.3424
C	3.1647	-3.1301	-1.6790
C	4.3159	-3.4086	-0.9375
C	3.8703	-1.4828	0.4852
C	4.6605	-2.5923	0.1432
C	1.1619	-1.6998	-2.2365
H	2.9313	-3.7515	-2.5301
H	4.9381	-4.2516	-1.1993
C	4.2340	-0.7119	1.7466
H	5.5422	-2.8322	0.7186
H	0.4382	-1.1459	-1.6468
C	1.5538	-0.8050	-3.4138
C	0.4221	-2.9210	-2.7911
H	0.6642	-0.5380	-3.9847
H	2.0245	0.1043	-3.0399
H	2.2553	-1.3326	-4.0605
H	-0.4893	-2.5964	-3.2939
H	1.0519	-3.4509	-3.5056
H	0.1581	-3.5922	-1.9739
H	3.4060	-0.0574	2.0043
C	4.4328	-1.6151	2.9672
C	5.4897	0.1484	1.5815
H	4.5882	-1.0008	3.8544
H	3.5443	-2.2302	3.1118
H	5.2997	-2.2599	2.8238
H	5.6592	0.7287	2.4887
H	6.3534	-0.4903	1.3951
H	5.3616	0.8294	0.7406
C	-2.8113	1.8102	-0.4948
C	-4.1309	2.2898	-0.4802
C	-4.5577	3.1567	0.5294
C	-2.3413	3.0831	1.5355
C	-3.6678	3.5434	1.5354
C	-2.3476	0.9499	-1.6636
H	-4.8271	2.0126	-1.2570
H	-5.5745	3.5205	0.5367
C	-1.4716	3.4287	2.7351
H	-4.0190	4.1919	2.3242
H	-1.5139	0.3403	-1.3289
C	-3.4069	-0.0228	-2.1896
C	-1.8455	1.7855	-2.8425
H	-2.9534	-0.6932	-2.9202
H	-3.8050	-0.6126	-1.3639
H	-4.2181	0.5261	-2.6676
H	-1.4493	1.1407	-3.6273
H	-2.6193	2.4274	-3.2643
H	-1.0386	2.4084	-2.4564
H	-0.5345	2.8822	2.6841
C	-1.0034	4.8857	2.7617
C	-2.1151	3.0768	4.0789
H	-0.3167	5.0359	3.5951
H	-0.4928	5.1259	1.8296
H	-1.8627	5.5463	2.8789
H	-1.4027	3.2570	4.8842
H	-3.0019	3.6889	4.2429
H	-2.3972	2.0237	4.0815

Structure 3A

E_{total} = -5.716004 a.u.

Atom	X	Y	Z
Ti	-0.0243	0.0889	-0.0977
N	1.8429	-0.0096	-0.0909
C	2.6520	1.2177	0.0196
C	1.8539	2.4754	-0.3093
C	0.6780	2.7974	0.6098
N	-0.4347	1.8262	0.5006
H	3.5165	1.1622	-0.6615
H	3.0576	1.2960	1.0454
H	2.5486	3.3288	-0.2589
H	1.5004	2.4282	-1.3540
H	0.3216	3.8083	0.3597
H	1.0204	2.8351	1.6608
C	-1.1464	-1.5788	0.3316
C	-2.6533	-1.4958	0.0786
H	-0.6816	-2.4576	-0.1627
H	-0.9352	-1.6899	1.4226
H	-2.8444	-1.4435	-1.0068
H	-3.0678	-0.5721	0.5206
C	-3.4203	-2.6975	0.6455
H	-4.4955	-2.6077	0.4323
H	-3.0578	-3.6336	0.1956
H	-3.2887	-2.7718	1.7347
C	-1.1353	0.7954	-2.2977
C	-0.2682	-0.2003	-2.5851
H	-0.9003	1.8373	-2.5236
H	-2.1458	0.5877	-1.9316
H	0.6948	0.0077	-3.0553
H	-0.5526	-1.2519	-2.4738
C	2.6483	-1.2183	0.0486
C	-1.6370	2.3078	1.1774
C	3.4091	-1.6938	-1.0426
C	4.1598	-2.8725	-0.9095
C	4.1641	-3.5786	0.2968
C	3.4140	-3.1094	1.3790
C	2.6454	-1.9399	1.2608
C	3.3948	-0.9933	-2.3930
H	2.7447	-0.1237	-2.3294
C	4.7752	-0.4888	-2.8201
C	2.8402	-1.8807	-3.5105
H	4.6893	0.0644	-3.7556
H	5.1767	0.1705	-2.0506
H	5.4528	-1.3310	-2.9611
H	2.7628	-1.3043	-4.4327
H	1.8505	-2.2421	-3.2305
H	3.4997	-2.7332	-3.6735
C	1.9424	-1.3986	2.4936
H	1.2180	-0.6535	2.1737
C	1.1768	-2.4654	3.2818
C	2.9153	-0.7099	3.4537
H	0.6322	-1.9948	4.0996
H	0.4710	-2.9721	2.6241
H	1.8702	-3.1964	3.6969
H	2.3744	-0.2964	4.3042
H	3.4424	0.0906	2.9353
H	3.6594	-1.4242	3.8070
H	4.7375	-3.2477	-1.7412
H	4.7514	-4.4797	0.3948
H	3.4512	-3.6493	2.3131
C	-2.3813	3.3762	0.6286
C	-3.5229	3.8669	1.2812
C	-3.9249	3.3095	2.4981
C	-3.1887	2.2599	3.0563
C	-2.0537	1.7488	2.4049
C	-2.0633	4.0060	-0.7209
H	-1.1781	3.5238	-1.1288
C	-3.1808	3.8056	-1.7482
C	-1.7576	5.5039	-0.6309
H	-2.8600	4.1879	-2.7175
H	-3.4047	2.7428	-1.8398
H	-4.0796	4.3356	-1.4329
H	-0.9486	5.6706	0.0802
H	-1.4541	5.8748	-1.6101
H	-2.6428	6.0472	-0.3001
C	-1.2532	0.6604	3.0961
H	-0.6637	0.2212	2.2973
C	-0.3000	1.2044	4.1610
C	-2.1109	-0.4451	3.7188
H	0.2655	0.3846	4.6020
H	0.3907	1.9139	3.7060
H	-0.8698	1.7078	4.9423
H	-2.8262	-0.8109	2.9833
H	-1.4744	-1.2692	4.0385
H	-2.6505	-0.0586	4.5833
H	-4.1091	4.6714	0.8625
H	-4.7977	3.6907	3.0073
H	-3.5003	1.8558	4.0077

Strucutre 4A

E_{toalo} = -5.701399 a.u.

Atom	X	Y	Z
Ti	-0.0400	0.1411	0.0912
N	1.8243	0.0724	0.2265
C	2.6419	1.2851	-0.0282
C	2.0270	2.5398	0.5792
C	0.6769	2.9472	-0.0014
N	-0.4178	1.9801	0.2903
H	2.7772	1.4232	-1.1170
H	3.6467	1.1403	0.3985
H	1.9302	2.4035	1.6685
H	2.7272	3.3749	0.4110
H	0.7723	3.0836	-1.0945
H	0.4029	3.9302	0.4124
C	-1.3044	-1.5006	0.4330
C	-0.9206	-1.3376	1.8811
H	-2.3542	-1.2278	0.2241
H	-1.0612	-2.4845	0.0116
H	-0.4156	-0.3265	2.0700
H	-0.1376	-2.0607	2.1545
C	-2.0818	-1.3812	2.8787
H	-1.7346	-1.2124	3.9070
H	-2.8435	-0.6284	2.6304
H	-2.5553	-2.3717	2.8273
C	-0.3714	0.3169	-2.3873
C	-0.5932	-1.0013	-2.1976
H	0.6446	0.7094	-2.5075
H	-1.1994	0.9955	-2.5917
H	0.2291	-1.7157	-2.1235
H	-1.6005	-1.4174	-2.2321
C	2.6483	-1.0732	0.5862
C	-1.6257	2.6685	0.7345
C	2.8629	-1.3821	1.9473
C	3.6865	-2.4659	2.2893
C	4.2994	-3.2376	1.2973
C	3.2916	-1.8337	-0.4140
C	4.1091	-2.9161	-0.0505
C	2.2992	-0.5027	3.0554
H	3.8917	-2.7139	3.3199
H	4.9387	-4.0637	1.5715
C	3.1413	-1.4903	-1.8878
H	4.6135	-3.5063	-0.8010
H	1.4811	0.0827	2.6441
C	1.7397	-1.2827	4.2499
C	3.3308	0.4879	3.5988
H	1.2300	-0.5965	4.9265
H	1.0312	-2.0341	3.9048
H	2.5490	-1.7768	4.7874
H	2.8612	1.1390	4.3365
H	4.1533	-0.0544	4.0657
H	3.7211	1.0958	2.7832
H	2.3218	-0.7833	-1.9936
C	4.3924	-0.8245	-2.4653
C	2.7978	-2.6984	-2.7638
H	4.2167	-0.5519	-3.5061
H	4.6247	0.0746	-1.8948
H	5.2370	-1.5117	-2.4090
H	2.5711	-2.3624	-3.7759
H	3.6399	-3.3896	-2.7974
H	1.9279	-3.2117	-2.3542
C	-2.4319	3.3840	-0.1804
C	-3.5647	4.0758	0.2764
C	-3.9052	4.0647	1.6313
C	-1.9300	2.7274	2.1140
C	-3.0712	3.4210	2.5491
C	-2.0915	3.4661	-1.6591
H	-4.1820	4.6282	-0.4164
H	-4.7745	4.6053	1.9757
C	-0.9272	2.2531	3.1564
H	-3.3059	3.4879	3.6007
H	-0.3072	1.4827	2.7078
C	0.0051	3.3730	3.6250
C	-1.5654	1.6555	4.4137
H	0.7576	2.9655	4.3006
H	0.5013	3.8244	2.7672
H	-0.5708	4.1393	4.1443
H	-0.8002	1.1583	5.0103
H	-2.0258	2.4425	5.0109
H	-2.3300	0.9343	4.1327
H	-1.2285	2.8356	-1.8472
C	-3.2178	2.9608	-2.5642
C	-1.7070	4.8800	-2.1012
H	-2.8699	2.9274	-3.5969
H	-3.5118	1.9581	-2.2532
H	-4.0789	3.6259	-2.4971
H	-1.3741	4.8616	-3.1392
H	-2.5651	5.5459	-2.0091
H	-0.8963	5.2496	-1.4730

Strucutre 5A

E = -5.704326 a.u.

Atom	X	Y	Z
Ti	0.0672	-0.0657	0.0097
N	1.9246	0.0202	-0.1367
C	2.6483	1.3174	-0.1103
C	2.0173	2.3816	-1.0035
C	0.5789	2.7551	-0.6502
N	-0.3440	1.5990	-0.7370
H	3.6931	1.1642	-0.4160
H	2.6868	1.6855	0.9316
H	2.6347	3.2921	-0.9219
H	2.0552	2.0541	-2.0530
H	0.2394	3.5476	-1.3347
H	0.5459	3.1853	0.3677
C	-0.6878	-1.6183	-1.1402
C	-1.1554	-2.3165	0.1119
H	-1.5130	-1.2467	-1.7689
H	0.0630	-2.1497	-1.7403
H	-0.9292	-1.6871	1.0432
H	-0.5599	-3.2233	0.3035
C	-2.6564	-2.6010	0.1891
H	-2.9405	-3.0315	1.1596
H	-3.2445	-1.6848	0.0284
H	-2.9302	-3.3155	-0.6007
C	-0.0040	0.9934	2.4165
C	-1.0521	0.1485	2.4953
H	0.9482	0.7648	2.8980
H	-0.1155	1.9877	1.9828
H	-0.9840	-0.7865	3.0569
H	-2.0400	0.4295	2.1173
C	2.7815	-1.1583	-0.2447
C	-1.4925	1.8401	-1.5988
C	3.5885	-1.3774	-1.3863
C	4.4286	-2.5006	-1.4400
C	4.4717	-3.4158	-0.3858
C	2.8012	-2.1079	0.8009
C	3.6553	-3.2209	0.7310
C	3.4882	-0.5057	-2.6283
H	5.0454	-2.6976	-2.3043
H	5.1236	-4.2752	-0.4387
C	1.9927	-1.8891	2.0664
H	3.7121	-3.9366	1.5372
H	2.6893	0.2134	-2.4811
C	4.7703	0.2735	-2.9321
C	3.1135	-1.3074	-3.8773
H	4.6074	0.9243	-3.7915
H	5.0456	0.8822	-2.0716
H	5.5817	-0.4199	-3.1538
H	2.9522	-0.6291	-4.7151
H	3.9125	-2.0039	-4.1310
H	2.1974	-1.8664	-3.6865
H	1.1452	-1.2610	1.8110
C	1.4175	-3.1700	2.6779
C	2.8023	-1.1726	3.1495
H	0.7193	-2.9107	3.4741
H	0.8903	-3.7384	1.9125
H	2.2186	-3.7811	3.0936
H	2.1790	-1.0094	4.0290
H	3.6658	-1.7782	3.4258
H	3.1473	-0.2106	2.7702
C	-1.5006	1.3704	-2.9308
C	-2.6070	1.6350	-3.7543
C	-3.6974	2.3632	-3.2686
C	-2.5941	2.5761	-1.1124
C	-3.6892	2.8327	-1.9519
C	-0.2734	0.7152	-3.5468
H	-2.6178	1.3015	-4.7810
H	-4.5427	2.5643	-3.9099
C	-2.6357	3.0871	0.3189
H	-4.5363	3.3947	-1.5875
H	0.3589	0.3499	-2.7397
C	-0.5951	-0.4845	-4.4448
C	0.5546	1.7015	-4.3738
H	0.3275	-0.9955	-4.7174
H	-1.2455	-1.1805	-3.9168
H	-1.0944	-0.1496	-5.3538
H	1.4904	1.2334	-4.6782
H	-0.0049	2.0005	-5.2605
H	0.7729	2.5872	-3.7780
H	-1.7624	2.7126	0.8455
C	-2.5901	4.6140	0.4042
C	-3.8581	2.5906	1.0949
H	-2.5556	4.9223	1.4494
H	-1.6991	4.9800	-0.1062
H	-3.4758	5.0394	-0.0683
H	-3.7819	2.9028	2.1367
H	-4.7698	3.0026	0.6623
H	-3.8990	1.5021	1.0502

Strucutre 6A

E= -5.712790 a.u.

Atom	X	Y	Z
Ti	0.0029	0.0975	0.0449
N	1.8688	0.0854	0.2210
C	2.6047	1.3267	-0.0504
C	1.7022	2.3816	-0.6872
C	0.5833	2.9062	0.2107
N	-0.4076	1.8707	0.5484
H	3.4386	1.1089	-0.7402
H	3.0459	1.7411	0.8707
H	2.3328	3.2405	-0.9652
H	1.2865	2.0004	-1.6375
H	0.0727	3.7338	-0.3114
H	1.0571	3.3327	1.1068
C	-1.0495	-1.5822	0.6955
C	-0.6383	-1.1047	2.0725
H	-2.1381	-1.6100	0.5398
H	-0.5856	-2.5314	0.3870
H	-0.0170	-0.1367	2.0295
H	0.0879	-1.7963	2.5282
C	-1.7905	-0.7861	3.0249
H	-1.4276	-0.3532	3.9669
H	-2.5055	-0.0835	2.5731
H	-2.3355	-1.7130	3.2544
C	-0.3374	0.0080	-2.5436
C	-1.0078	-1.1044	-2.1781
H	0.7156	-0.0416	-2.8348
H	-0.8588	0.9554	-2.7050
H	-0.5200	-2.0797	-2.1417
H	-2.0873	-1.0975	-2.0218
C	2.6866	-0.9825	0.7830
C	-1.5830	2.3732	1.2614
C	2.9462	-2.1356	0.0153
C	3.7674	-3.1488	0.5336
C	4.2907	-3.0481	1.8259
C	3.1956	-0.8914	2.0996
C	3.9966	-1.9269	2.6083
C	2.4241	-2.2555	-1.4052
H	4.0252	-4.0184	-0.0520
H	4.9168	-3.8349	2.2199
C	2.8449	0.2695	3.0220
H	4.3942	-1.8737	3.6109
H	1.5954	-1.5620	-1.5127
C	3.4743	-1.8739	-2.4499
C	1.8789	-3.6448	-1.7469
H	3.0339	-1.9147	-3.4463
H	3.8280	-0.8610	-2.2570
H	4.3162	-2.5646	-2.3970
H	1.4281	-3.6256	-2.7394
H	2.6845	-4.3787	-1.7366
H	1.1209	-3.9280	-1.0163
H	2.1053	0.8966	2.5289
C	2.2146	-0.1795	4.3436
C	4.0501	1.1511	3.3598
H	1.9247	0.6944	4.9265
H	1.3297	-0.7819	4.1428
H	2.9277	-0.7703	4.9183
H	3.7231	2.0079	3.9495
H	4.7800	0.5774	3.9312
H	4.5167	1.5061	2.4414
C	-2.8717	2.0411	0.7884
C	-4.0143	2.5403	1.4336
C	-3.8910	3.3835	2.5393
C	-1.4678	3.1535	2.4399
C	-2.6231	3.6675	3.0510
C	-3.0502	1.2454	-0.4904
H	-5.0010	2.3128	1.0598
H	-4.7727	3.7778	3.0227
C	-0.1641	3.2576	3.2218
H	-2.5433	4.2796	3.9370
H	-2.1508	0.6552	-0.6342
C	-4.2206	0.2578	-0.4485
C	-3.2173	2.1424	-1.7182
H	-4.1800	-0.3946	-1.3206
H	-4.1553	-0.3488	0.4548
H	-5.1679	0.7967	-0.4549
H	-3.2697	1.5289	-2.6178
H	-4.1322	2.7281	-1.6259
H	-2.3647	2.8178	-1.7936
H	0.5790	2.6170	2.7540
C	0.3907	4.6844	3.2748
C	-0.2861	2.7525	4.6621
H	1.3641	4.6815	3.7657
H	0.5003	5.0768	2.2641
H	-0.2920	5.3262	3.8320
H	0.6928	2.7768	5.1412
H	-0.9742	3.3815	5.2266
H	-0.6547	1.7271	4.6578

Structure 7A

E_{total} = -5.732815 a.u.

Atom	X	Y	Z
Ti	0.0516	-0.1078	-0.0300
N	1.9099	-0.0069	-0.1174
C	2.5258	1.3317	0.0110
C	1.5786	2.4624	-0.3983
C	0.3769	2.6966	0.5170
N	-0.5749	1.5685	0.4858
H	3.4121	1.3803	-0.6410
H	2.8572	1.5067	1.0482
H	2.1697	3.3927	-0.4075
H	1.2324	2.3024	-1.4363
H	-0.1383	3.6127	0.1872
H	0.7423	2.8677	1.5436
C	-1.0396	-1.8255	0.2876
C	-0.6488	-1.5806	1.7267
H	-0.6492	-2.7537	-0.1564
H	-2.1177	-1.7104	0.0883
H	0.0860	-0.6839	1.8262
H	-0.0054	-2.3856	2.1193
C	-1.7883	-1.2335	2.6884
C	-2.6968	-2.4326	2.9625
H	-1.3678	-0.8610	3.6373
H	-2.3885	-0.4102	2.2623
H	-3.1112	-2.8061	2.0107
H	-2.0925	-3.2543	3.3846
C	-3.8332	-2.0783	3.9185
H	-3.4434	-1.7426	4.8913
H	-4.4590	-1.2708	3.5076
H	-4.4808	-2.9482	4.0958
C	2.8151	-1.0982	-0.4690
C	-1.9780	1.9004	0.7099
C	2.4545	-1.9431	-1.5416
C	3.3208	-2.9727	-1.9444
C	4.5284	-3.1860	-1.2738
C	4.0316	-1.3269	0.2160
C	4.8765	-2.3699	-0.1938
C	1.1988	-1.6664	-2.3588
H	3.0766	-3.6012	-2.7872
H	5.1879	-3.9823	-1.5857
C	4.4096	-0.5700	1.4775
H	5.7991	-2.5596	0.3346
H	0.4626	-1.2093	-1.7055
C	1.4511	-0.6817	-3.5023
C	0.5351	-2.9170	-2.9430
H	0.5145	-0.4699	-4.0186
H	1.8547	0.2479	-3.1008
H	2.1655	-1.1091	-4.2063
H	-0.4230	-2.6458	-3.3870
H	1.1703	-3.3567	-3.7118
H	0.3662	-3.6460	-2.1503
H	3.5457	-0.0887	1.9319
C	4.5585	-1.4433	2.7260
C	5.5833	0.4018	1.3371
H	4.6794	-0.8115	3.6066
H	3.6682	-2.0611	2.8479
H	5.4320	-2.0876	2.6252
H	5.7268	0.9393	2.2746
H	6.4971	-0.1396	1.0917
H	5.3723	1.1194	0.5450
C	-2.9186	1.4865	-0.2580
C	-4.2729	1.8247	-0.1074
C	-4.7014	2.5466	1.0099
C	-2.4180	2.6060	1.8544
C	-3.7786	2.9272	1.9883
C	-2.4618	0.7858	-1.5316
H	-4.9974	1.5499	-0.8587
H	-5.7448	2.8021	1.1216
C	-1.4914	2.9177	3.0207
H	-4.1304	3.4599	2.8591
H	-1.5663	0.2149	-1.3035
C	-3.4736	-0.2129	-2.1015
C	-2.0907	1.7729	-2.6400
H	-3.0146	-0.7676	-2.9202
H	-3.7763	-0.9130	-1.3229
H	-4.3511	0.3129	-2.4776
H	-1.7140	1.2285	-3.5062
H	-2.9688	2.3513	-2.9281
H	-1.3162	2.4507	-2.2807
H	-0.5587	2.3791	2.8747
C	-1.1676	4.4084	3.1471
C	-2.0376	2.4330	4.3672
H	-0.4502	4.5610	3.9537
H	-0.7390	4.7724	2.2138
H	-2.0784	4.9671	3.3637
H	-1.2839	2.5796	5.1411
H	-2.9353	2.9905	4.6339
H	-2.2783	1.3719	4.3017

Structure 8A

E_{total} = -5.729919 a.u.

Atom	X	Y	Z
Ti	-0.0471	-0.0671	-0.3709
N	1.7815	-0.0938	-0.0394
C	2.5849	1.1449	0.0652
C	2.0355	2.2511	-0.8276
C	0.6111	2.7082	-0.5096
N	-0.4299	1.6965	-0.8571
H	3.6218	0.9266	-0.2361
H	2.6117	1.4910	1.1136
H	2.6989	3.1258	-0.7206
H	2.0843	1.9308	-1.8831
H	0.4242	3.6213	-1.0929
H	0.5373	2.9776	0.5581
C	-1.1096	-1.7932	-0.6439
C	-0.9630	-1.9604	0.8847
H	-0.6673	-2.6313	-1.2032
H	-2.1538	-1.6275	-0.9588
H	0.0132	-2.4044	1.1412
H	-1.7213	-2.6758	1.2488
C	-1.1793	-0.6668	1.7281
C	-2.5745	-0.0490	1.6351
H	-0.9382	-0.9207	2.7747
H	-0.4015	0.1595	1.5904
H	-2.8072	0.2474	0.5971
H	-3.3051	-0.8354	1.8932
C	-2.7400	1.1501	2.5630
H	-2.5494	0.8685	3.6094
H	-2.0439	1.9598	2.2960
H	-3.7603	1.5526	2.5052
C	2.5596	-1.3192	0.0846
C	-1.4968	2.2002	-1.7225
C	2.7585	-2.1347	-1.0470
C	3.5338	-3.3003	-0.9378
C	4.0858	-3.6696	0.2933
C	3.0996	-1.7025	1.3306
C	3.8637	-2.8765	1.4238
C	2.2292	-1.7114	-2.4074
H	3.7250	-3.9166	-1.8032
H	4.6792	-4.5685	0.3717
C	2.8079	-0.9142	2.5990
H	4.2800	-3.1826	2.3721
H	1.4000	-1.0268	-2.2469
C	3.2834	-0.9665	-3.2291
C	1.6865	-2.8681	-3.2517
H	2.8539	-0.6415	-4.1764
H	3.6267	-0.0931	-2.6746
H	4.1312	-1.6237	-3.4237
H	1.2249	-2.4748	-4.1572
H	2.4960	-3.5418	-3.5317
H	0.9387	-3.4182	-2.6809
H	2.0851	-0.1350	2.3665
C	2.1712	-1.7682	3.6987
C	4.0505	-0.2306	3.1733
H	1.8976	-1.1342	4.5424
H	1.2740	-2.2506	3.3106
H	2.8728	-2.5310	4.0361
H	3.7713	0.3705	4.0389
H	4.7806	-0.9816	3.4756
H	4.4932	0.4164	2.4160
C	-1.8105	1.4950	-2.9058
C	-2.7972	1.9820	-3.7777
C	-3.4959	3.1526	-3.4757
C	-2.2268	3.3747	-1.4083
C	-3.2144	3.8390	-2.2924
C	-1.0035	0.2824	-3.3375
H	-3.0126	1.4693	-4.7030
H	-4.2548	3.5211	-4.1499
C	-2.0850	4.0989	-0.0754
H	-3.7814	4.7275	-2.0576
H	-0.4716	-0.0997	-2.4726
C	-1.8579	-0.8686	-3.8767
C	0.0451	0.6360	-4.3936
H	-1.2303	-1.7457	-4.0352
H	-2.6383	-1.1134	-3.1566
H	-2.3182	-0.5850	-4.8230
H	0.6076	-0.2556	-4.6677
H	-0.4446	1.0376	-5.2809
H	0.7292	1.3829	-3.9905
H	-1.4207	3.5282	0.5670
C	-1.5135	5.5136	-0.2106
C	-3.4119	4.2045	0.6817
H	-1.3798	5.9507	0.7791
H	-0.5498	5.4781	-0.7173
H	-2.1969	6.1356	-0.7890
H	-3.2335	4.6084	1.6785
H	-4.0994	4.8605	0.1478
H	-3.8586	3.2145	0.7714

Strucutre 11A

E_{total} = -5.710737 a.u.

Atom	X	Y	Z
Ti	0.0664	-0.0365	-0.2919
N	1.9360	0.0007	-0.2414
C	2.6623	1.2282	0.1632
C	2.1513	2.4777	-0.5526
C	0.6847	2.8075	-0.2958
N	-0.2522	1.7489	-0.7553
H	3.7351	1.1088	-0.0523
H	2.5722	1.3661	1.2558
H	2.7509	3.3365	-0.2068
H	2.3232	2.3737	-1.6341
H	0.4380	3.7599	-0.7858
H	0.5349	2.9790	0.7868
C	-0.0334	0.2745	2.2533
C	-0.8401	-0.8053	2.3928
H	1.0432	0.1860	2.4154
H	-0.4537	1.2802	2.1925
H	-1.9259	-0.6484	2.3732
C	-0.3859	-2.1806	2.7305
H	-0.8652	-2.9468	2.1034
H	0.7037	-2.2872	2.6832
H	-0.7049	-2.3985	3.7659
C	-0.6191	-1.3405	-1.7405
C	-1.7563	-1.8004	-0.8540
H	0.1466	-2.1129	-1.9197
H	-0.9266	-0.8678	-2.6829
H	-1.6721	-1.4209	0.2095
H	-1.8013	-2.8917	-0.7201
H	-2.7333	-1.4346	-1.1969
C	2.8103	-1.0244	-0.7988
C	-1.4285	2.2580	-1.4610
C	2.9402	-1.1767	-2.1973
C	3.8167	-2.1450	-2.7116
C	4.5565	-2.9678	-1.8583
C	3.5699	-1.8484	0.0616
C	4.4354	-2.8159	-0.4743
C	2.2560	-0.2305	-3.1706
H	3.9699	-2.2592	-3.7742
H	5.2330	-3.7043	-2.2662
C	3.4576	-1.7312	1.5735
H	5.0249	-3.4521	0.1688
H	1.4631	0.2965	-2.6435
C	3.2293	0.8145	-3.7224
C	1.6144	-0.9365	-4.3697
H	2.6916	1.5349	-4.3373
H	3.7139	1.3365	-2.8979
H	3.9930	0.3249	-4.3269
H	1.0523	-0.2151	-4.9617
H	2.3843	-1.3847	-4.9975
H	0.9390	-1.7172	-4.0226
H	2.5781	-1.1361	1.8057
C	3.2687	-3.0813	2.2720
C	4.6633	-1.0340	2.2068
H	3.0615	-2.9197	3.3301
H	2.4299	-3.6112	1.8202
H	4.1704	-3.6857	2.1744
H	4.5139	-0.9482	3.2833
H	5.5680	-1.6105	2.0121
H	4.7751	-0.0370	1.7816
C	-1.3008	3.0109	-2.6539
C	-2.4437	3.5390	-3.2752
C	-3.7156	3.3017	-2.7499
C	-2.7206	2.0074	-0.9465
C	-3.8526	2.5217	-1.5998
C	0.0152	3.1054	-3.4107
H	-2.3510	4.1241	-4.1781
H	-4.5892	3.7073	-3.2383
C	-2.9006	1.3491	0.4090
H	-4.8419	2.3552	-1.2019
H	0.7546	2.5064	-2.8893
C	-0.0804	2.5296	-4.8260
C	0.5593	4.5327	-3.5162
H	0.9089	2.5082	-5.2826
H	-0.4762	1.5151	-4.7780
H	-0.7407	3.1440	-5.4379
H	1.5475	4.5137	-3.9762
H	-0.1100	5.1406	-4.1252
H	0.6372	4.9742	-2.5234
H	-2.0603	0.6793	0.5602
C	-2.9011	2.3685	1.5505
C	-4.1734	0.5058	0.5403
H	-2.9619	1.8501	2.5076
H	-1.9830	2.9551	1.5175
H	-3.7557	3.0374	1.4465
H	-4.1446	-0.0545	1.4749
H	-5.0528	1.1496	0.5418
H	-4.2415	-0.1928	-0.2926

Structure 12A

E = -4.503875 a.u.

Atom	X	Y	Z
Ti	-0.1710	0.0399	-0.1802
N	1.6511	-0.2310	0.0781
C	2.5412	0.9615	0.0704
C	2.0536	2.0680	-0.8623
C	0.7620	2.7620	-0.4370
N	-0.4121	1.8575	-0.4981
H	3.5402	0.6508	-0.2714
H	2.6445	1.3702	1.0903
H	2.8432	2.8372	-0.8987
H	1.9435	1.6711	-1.8875
H	0.5892	3.6142	-1.1130
H	0.8871	3.1619	0.5839
C	-1.0055	0.2184	2.0785
C	-1.4035	-1.0682	1.8699
C	-0.5829	-2.2703	2.1757
H	-0.0283	0.4309	2.5311
H	-1.7208	1.0417	2.0153
H	-2.4415	-1.2534	1.5750
H	-1.3324	-1.1959	-0.4416
H	-0.6629	-3.0358	1.3913
H	0.4694	-2.0290	2.3738
H	-1.0021	-2.7250	3.0925
C	2.3431	-1.5195	0.0643
C	-1.6527	2.4740	-0.9664
C	1.9625	-2.4890	-0.8903
C	2.6484	-3.7112	-0.9668
C	3.6843	-4.0005	-0.0761
C	3.3727	-1.8312	0.9878
C	4.0350	-3.0668	0.9017
C	0.9052	-2.1939	-1.9414
H	2.3984	-4.4313	-1.7316
H	4.2059	-4.9441	-0.1381
C	3.7077	-0.9370	2.1747
H	4.8169	-3.3163	1.6035
H	0.3952	-1.2764	-1.6702
C	1.5064	-1.9657	-3.3294
C	-0.1634	-3.2854	-2.0464
H	0.7152	-1.7153	-4.0359
H	2.2194	-1.1421	-3.2842
H	2.0179	-2.8676	-3.6662
H	-0.9313	-2.9794	-2.7560
H	0.2848	-4.2181	-2.3883
H	-0.6213	-3.4423	-1.0699
H	2.9680	-0.1442	2.2354
C	3.6275	-1.6710	3.5166
C	5.0927	-0.2915	2.0740
H	3.7707	-0.9604	4.3309
H	2.6467	-2.1358	3.6188
H	4.3986	-2.4390	3.5741
H	5.2548	0.3645	2.9295
H	5.8612	-1.0647	2.0624
H	5.1627	0.2942	1.1582
C	-2.3798	1.8376	-1.9960
C	-3.5561	2.4222	-2.4913
C	-4.0050	3.6459	-1.9888
C	-2.1442	3.6836	-0.4177
C	-3.3059	4.2662	-0.9501
C	-1.8153	0.6223	-2.7146
H	-4.1031	1.9550	-3.2963
H	-4.9003	4.1000	-2.3870
C	-1.5900	4.2683	0.8746
H	-3.6798	5.1974	-0.5511
H	-1.0473	0.1818	-2.0878
C	-2.8502	-0.4751	-2.9755
C	-1.1454	0.9890	-4.0400
H	-2.3541	-1.3537	-3.3868
H	-3.3386	-0.7454	-2.0391
H	-3.5981	-0.1258	-3.6870
H	-0.6968	0.1007	-4.4841
H	-1.8842	1.4027	-4.7267
H	-0.3666	1.7304	-3.8594
H	-0.8583	3.5781	1.2850
C	-0.9060	5.6237	0.6774
C	-2.6561	4.4273	1.9625
H	-0.4768	5.9587	1.6219
H	-0.1116	5.5314	-0.0626
H	-1.6333	6.3584	0.3313
H	-2.1856	4.7520	2.8908
H	-3.3973	5.1670	1.6601
H	-3.1491	3.4693	2.1299

Strucutre TS[3A-8A]

E_{total} = -5.701053 a.u.

Atom	X	Y	Z
Ti	0.0350	0.0798	0.0784
N	1.9006	0.0183	0.0417
C	2.6756	1.2645	-0.1252
C	1.8187	2.4166	-0.6422
C	0.7090	2.8924	0.2907
N	-0.3387	1.8721	0.4971
H	3.4971	1.0988	-0.8395
H	3.1323	1.5452	0.8415
H	2.4897	3.2715	-0.8213
H	1.3871	2.1513	-1.6244
H	0.2471	3.7898	-0.1541
H	1.1478	3.1888	1.2591
C	-0.5398	-0.4097	-2.0142
C	-0.9471	-1.6074	-1.4082
H	0.4287	-0.3815	-2.5208
H	-1.3002	0.2899	-2.3691
H	-0.2577	-2.4561	-1.4018
H	-2.0057	-1.8755	-1.3998
C	-1.1483	-1.5492	0.7410
C	-2.5187	-0.9996	1.1136
H	-1.1078	-2.6472	0.7748
H	-0.3796	-1.2359	1.5344
H	-2.5398	0.1036	1.0583
H	-3.2484	-1.3485	0.3648
C	-2.9682	-1.4348	2.5122
H	-3.0291	-2.5309	2.5743
H	-2.2702	-1.0885	3.2868
H	-3.9615	-1.0227	2.7390
C	2.7354	-1.1229	0.3902
C	-1.5201	2.4318	1.1353
C	3.5525	-1.7328	-0.5855
C	4.3460	-2.8372	-0.2409
C	4.3487	-3.3250	1.0697
C	2.7323	-1.6215	1.7096
C	3.5493	-2.7145	2.0419
C	3.5432	-1.2732	-2.0335
H	4.9561	-3.3212	-0.9894
H	4.9694	-4.1691	1.3315
C	1.9474	-0.9249	2.8107
H	3.5798	-3.0873	3.0547
H	2.7299	-0.5713	-2.2116
C	4.8631	-0.6575	-2.4993
C	2.8852	-2.2677	-2.9914
H	4.7606	-0.3006	-3.5242
H	5.3456	0.1145	-1.9000
H	5.6552	-1.4050	-2.4550
H	2.7672	-1.8095	-3.9737
H	3.5096	-3.1566	-3.0824
H	1.9060	-2.5541	-2.6074
H	1.2103	-0.2724	2.3483
C	1.1837	-1.8892	3.7239
C	2.8392	-0.0410	3.6852
H	0.5575	-1.3204	4.4109
H	0.5497	-2.5537	3.1371
H	1.8856	-2.4887	4.3033
H	2.2338	0.4724	4.4313
H	3.5881	-0.6534	4.1878
H	3.3403	0.6996	3.0621
C	-2.6574	2.7363	0.3595
C	-3.8008	3.2691	0.9747
C	-3.8191	3.5003	2.3537
C	-1.5423	2.6583	2.5287
C	-2.6929	3.1975	3.1259
C	-2.6584	2.5348	-1.1466
H	-4.6734	3.5125	0.3868
H	-4.7004	3.9137	2.8214
C	-0.3507	2.3178	3.4118
H	-2.7206	3.3810	4.1897
H	-1.6966	2.1201	-1.4385
C	-3.7367	1.5564	-1.6193
C	-2.8209	3.8461	-1.9180
H	-3.6485	1.4052	-2.6953
H	-3.6077	0.5997	-1.1141
H	-4.7263	1.9526	-1.3918
H	-2.7414	3.6542	-2.9883
H	-3.7939	4.2879	-1.7026
H	-2.0355	4.5413	-1.6205
H	0.3864	1.7867	2.8131
C	0.3350	3.5602	3.9853
C	-0.7129	1.3978	4.5801
H	1.2259	3.2644	4.5397
H	0.6242	4.2273	3.1736
H	-0.3479	4.0858	4.6531
H	0.1855	1.1479	5.1438
H	-1.4220	1.8931	5.2431
H	-1.1582	0.4822	4.1952

Strucutre TS[3A-11A]

E_{total} = -5.685333 a.u.

Atom	X	Y	Z
Ti	0.0000	0.0018	0.0016
N	1.8796	0.0011	0.0016
C	2.6354	1.2841	-0.0006
C	2.0661	2.3206	-0.9616
C	0.6232	2.7314	-0.6806
N	-0.3424	1.6167	-0.8813
H	3.6835	1.0876	-0.2737
H	2.6497	1.6929	1.0265
H	2.6965	3.2231	-0.8900
H	2.1412	1.9475	-1.9948
H	0.3548	3.5613	-1.3524
H	0.5423	3.1178	0.3522
C	-0.5386	0.6709	2.0932
C	-1.6876	-0.1187	1.8568
H	0.1796	0.3290	2.8436
H	-0.5833	1.7507	1.9395
H	-1.4830	-0.9495	0.7067
H	-2.5506	0.4150	1.4309
C	-2.0620	-1.2550	2.7858
H	-2.7840	-1.9495	2.3360
H	-1.1809	-1.8155	3.1248
H	-2.5359	-0.8131	3.6772
C	-0.3331	-1.8507	-1.2734
C	-1.3971	-2.0188	-0.3775
H	0.5886	-2.4210	-1.1301
H	-0.5203	-1.4877	-2.2826
H	-1.3233	-2.7897	0.3993
H	-2.4183	-1.8085	-0.7191
C	2.7606	-1.1360	0.0059
C	-1.4331	1.9756	-1.7478
C	3.3823	-1.5532	-1.1932
C	4.2595	-2.6495	-1.1819
C	4.5190	-3.3400	0.0054
C	3.9019	-2.9347	1.1921
C	3.0254	-1.8382	1.2001
C	3.1000	-0.8628	-2.5193
H	4.7406	-2.9731	-2.0929
H	5.1947	-4.1825	0.0060
H	4.1147	-3.4693	2.1060
C	2.4193	-1.4037	2.5193
H	2.2777	-0.1677	-2.3758
C	4.2932	-0.0594	-3.0413
C	2.6628	-1.8307	-3.6222
H	4.0109	0.4645	-3.9547
H	4.6002	0.6706	-2.2929
H	5.1272	-0.7291	-3.2520
H	2.4117	-1.2699	-4.5223
H	3.4683	-2.5279	-3.8520
H	1.7866	-2.3886	-3.2927
H	1.7964	-0.5366	2.3300
C	1.5315	-2.4802	3.1456
C	3.4693	-0.9730	3.5456
H	1.0510	-2.0844	4.0405
H	0.7677	-2.7808	2.4283
H	2.1324	-3.3490	3.4146
H	2.9759	-0.5988	4.4428
H	4.1076	-1.8170	3.8076
H	4.0918	-0.1848	3.1215
C	-2.4717	2.8137	-1.2802
C	-3.5117	3.1872	-2.1454
C	-3.5292	2.7515	-3.4724
C	-2.4909	1.9460	-3.9468
C	-1.4431	1.5547	-3.0970
C	-2.5049	3.3293	0.1495
H	-4.3160	3.8258	-1.8117
H	-4.3285	3.0531	-4.1331
H	-2.4961	1.6484	-4.9845
C	-0.2850	0.7705	-3.6907
H	-1.7369	2.8149	0.7178
C	-2.2113	4.8283	0.2435
C	-3.8333	3.0558	0.8603
H	-4.6339	3.6302	0.3942
H	-3.7521	3.3418	1.9092
H	-4.0696	1.9938	0.7966
H	-2.9863	5.3915	-0.2769
H	-2.1849	5.1324	1.2900
H	-1.2455	5.0409	-0.2145
H	0.2715	0.3177	-2.8742
C	-0.7264	-0.3578	-4.6299
C	0.6856	1.6636	-4.4665
H	1.5452	1.0778	-4.7921
H	0.1838	2.0845	-5.3380
H	1.0267	2.4768	-3.8266
H	0.1336	-0.9709	-4.8970
H	-1.4705	-0.9807	-4.1339
H	-1.1591	0.0581	-5.5396

Structure TS[1A-12A]

E_{total} = -4.494016

Ti	-0.0137	0.0026	-0.0038
N	1.8342	-0.0044	-0.0054
C	2.5053	1.3265	0.0016
C	2.0120	2.2304	-1.1282
C	0.5753	2.7069	-0.9718
N	-0.4097	1.5909	-0.9221
H	3.5909	1.1838	-0.1016
H	2.3397	1.8100	0.9805
H	2.6566	3.1248	-1.1589
H	2.1305	1.7067	-2.0914
H	0.3324	3.3845	-1.8026
H	0.4822	3.3091	-0.0475
C	-0.5734	-1.0570	1.9922
C	-1.1872	-1.9993	1.1895
C	-0.5895	-3.3364	0.8979
H	0.4197	-1.2634	2.4076
H	-1.1794	-0.3013	2.5078
H	-2.2634	-1.9058	1.0063
H	-0.9707	-1.3329	-0.5489
H	-0.9550	-3.7666	-0.0418
H	0.5085	-3.3181	0.9025
H	-0.9078	-4.0103	1.7141
C	2.6862	-1.1210	-0.3979
C	-1.7368	2.0024	-1.3744
C	2.3650	-1.8756	-1.5472
C	3.1880	-2.9461	-1.9316
C	4.3015	-3.2971	-1.1631
C	3.8090	-1.4821	0.3819
C	4.6053	-2.5708	-0.0080
C	1.2289	-1.4662	-2.4726
H	2.9813	-3.4959	-2.8377
H	4.9261	-4.1261	-1.4615
C	4.1207	-0.8025	1.7087
H	5.4551	-2.8656	0.5896
H	0.6282	-0.7083	-1.9772
C	1.7402	-0.8506	-3.7768
C	0.2875	-2.6171	-2.8357
H	0.8974	-0.5281	-4.3866
H	2.3708	0.0093	-3.5526
H	2.3229	-1.5867	-4.3311
H	-0.5541	-2.2325	-3.4122
H	0.8170	-3.3627	-3.4286
H	-0.0867	-3.0832	-1.9261
H	3.3938	-0.0131	1.8825
C	4.0017	-1.7565	2.8997
C	5.5077	-0.1552	1.7429
H	4.1728	-1.2093	3.8269
H	3.0004	-2.1875	2.9195
H	4.7367	-2.5569	2.8134
H	5.6475	0.3619	2.6924
H	6.2782	-0.9184	1.6326
H	5.5957	0.5639	0.9287
C	-1.9459	2.4212	-2.7095
C	-3.2215	2.8454	-3.1149
C	-4.2927	2.8397	-2.2174
C	-2.8297	1.9635	-0.4833
C	-4.1005	2.3802	-0.9117
C	-0.8811	2.2371	-3.7832
H	-3.3904	3.1661	-4.1322
H	-5.2707	3.1662	-2.5387
C	-2.6256	1.6201	0.9805
H	-4.9370	2.3809	-0.2293
H	0.0216	1.8446	-3.3204
C	-1.2942	1.2188	-4.8487
C	-0.5019	3.5413	-4.4902
H	-0.4700	1.0614	-5.5446
H	-1.5430	0.2722	-4.3683
H	-2.1624	1.5829	-5.3980
H	0.3387	3.3622	-5.1609
H	-1.3492	3.9122	-5.0671
H	-0.2163	4.2905	-3.7521
H	-1.6920	1.0728	1.0646
C	-2.4973	2.8643	1.8609
C	-3.7256	0.7262	1.5616
H	-2.2906	2.5673	2.8893
H	-1.6780	3.4843	1.4964
H	-3.4241	3.4376	1.8284
H	-3.4552	0.4230	2.5731
H	-4.6713	1.2668	1.5954
H	-3.8397	-0.1618	0.9400

2.2 McConville Zicronium System

Strucutre 1B

E_{total} = -4.553285 a.u.

Atom	X	Y	Z
Zr	0.0576	-0.0156	0.0308
N	2.0671	-0.0319	-0.1196
C	2.6683	1.3264	0.0139
C	1.7943	2.4558	-0.5536
C	0.5434	2.8961	0.2204
N	-0.5518	1.8942	0.1950
H	3.6274	1.3618	-0.5216
H	2.9015	1.5338	1.0751
H	2.4443	3.3446	-0.6090
H	1.5197	2.2194	-1.6010
H	0.1990	3.8393	-0.2281
H	0.8174	3.1299	1.2664
C	-1.2912	-1.7671	0.0297
C	-1.4439	-1.5260	-1.4582
H	-0.8083	-2.7305	0.2600
H	-2.2316	-1.6660	0.5918
H	-0.7351	-0.6772	-1.8369
H	-2.4250	-1.0894	-1.7013
C	-1.1212	-2.6989	-2.3813
H	-1.1624	-2.4042	-3.4387
H	-0.1252	-3.1136	-2.1709
H	-1.8631	-3.4929	-2.2125
C	3.0254	-1.0983	0.1322
C	-1.8077	2.4007	0.7272
C	4.1228	-1.3145	-0.7339
C	5.0366	-2.3432	-0.4540
C	4.8698	-3.1577	0.6697
C	2.8357	-1.9520	1.2401
C	3.7704	-2.9642	1.5109
C	4.2777	-0.5569	-2.0466
H	5.8668	-2.5301	-1.1189
H	5.5798	-3.9443	0.8788
C	1.6930	-1.7292	2.2191
H	3.6568	-3.5977	2.3777
H	3.4689	0.1647	-2.1373
C	5.5971	0.2141	-2.1458
C	4.1648	-1.4724	-3.2681
H	5.6135	0.7945	-3.0685
H	5.6915	0.8907	-1.2965
H	6.4363	-0.4816	-2.1441
H	4.2057	-0.8750	-4.1792
H	4.9828	-2.1929	-3.2736
H	3.2148	-2.0063	-3.2341
H	0.9345	-1.1225	1.7331
C	0.9987	-3.0201	2.6616
C	2.1428	-0.9747	3.4709
H	0.1061	-2.7744	3.2373
H	0.7086	-3.5977	1.7841
H	1.6699	-3.6160	3.2799
H	1.2971	-0.8441	4.1449
H	2.9241	-1.5382	3.9813
H	2.5314	0.0034	3.1863
C	-2.5443	3.3990	0.0505
C	-3.7517	3.8619	0.6003
C	-4.2346	3.3434	1.8070
C	-2.3201	1.8579	1.9224
C	-3.5193	2.3387	2.4669
C	-2.1368	3.9049	-1.3268
H	-4.3300	4.6141	0.0845
H	-5.1625	3.7119	2.2194
C	-1.5511	0.8391	2.7475
H	-4.1575	2.1974	3.3269
H	-1.2150	3.4107	-1.6261
C	-3.1684	3.5657	-2.4056
C	-1.8812	5.4141	-1.3621
H	-2.7961	3.8799	-3.3809
H	-3.3378	2.4887	-2.4186
H	-4.1092	4.0758	-2.1983
H	-1.5214	5.7016	-2.3503
H	-2.8034	5.9532	-1.1446
H	-1.1292	5.6756	-0.6178
H	-0.8798	0.3392	2.0544
C	-0.7042	1.4953	3.8395
C	-2.4292	-0.2386	3.3878
H	-0.1542	0.7333	4.3898
H	0.0022	2.1901	3.3852
H	-1.3501	2.0391	4.5291
H	-1.7968	-0.9918	3.8582
H	-3.0772	0.2071	4.1426
H	-3.0410	-0.7141	2.6213

Structure 2B

E_{total} = -4.554736 a.u.

Atom	X	Y	Z
Zr	0.0356	0.0209	0.0112
N	2.0494	-0.0227	0.0546
C	2.6549	1.3289	0.0269
C	1.6820	2.4179	-0.4623
C	0.5490	2.8648	0.4803
N	-0.5316	1.8608	0.6203
H	3.5142	1.3229	-0.6621
H	3.0285	1.6215	1.0222
H	2.2929	3.3158	-0.6539
H	1.2686	2.1433	-1.4578
H	0.1247	3.7930	0.0657
H	1.0006	3.1104	1.4554
C	-1.2215	-1.7967	0.1674
C	-0.9493	-1.7169	1.6515
H	-2.2872	-1.6786	-0.0829
H	-0.8182	-2.6999	-0.3144
H	-0.2606	-0.8125	1.9250
H	-0.3145	-2.5458	2.0001
C	-2.1714	-1.5327	2.5479
H	-1.8876	-1.3669	3.5958
H	-2.7905	-0.6866	2.2153
H	-2.7876	-2.4421	2.4922
C	2.9853	-1.1057	-0.2179
C	-1.8550	2.4210	0.8687
C	2.7022	-1.9872	-1.2843
C	3.6207	-2.9937	-1.6241
C	4.7928	-3.1627	-0.8825
C	4.1625	-1.2936	0.5455
C	5.0554	-2.3219	0.2023
C	1.4835	-1.7677	-2.1699
H	3.4485	-3.6333	-2.4762
H	5.4929	-3.9418	-1.1459
C	4.4446	-0.4988	1.8129
H	5.9539	-2.4795	0.7800
H	0.7025	-1.3214	-1.5627
C	1.7647	-0.8018	-3.3229
C	0.8894	-3.0521	-2.7556
H	0.8481	-0.6236	-3.8856
H	2.1294	0.1454	-2.9255
H	2.5200	-1.2272	-3.9842
H	-0.0514	-2.8220	-3.2562
H	1.5773	-3.4903	-3.4787
H	0.7007	-3.7663	-1.9539
H	3.5606	0.0821	2.0630
C	4.7093	-1.3891	3.0307
C	5.6232	0.4670	1.6648
H	4.8013	-0.7699	3.9232
H	3.8770	-2.0811	3.1620
H	5.6307	-1.9546	2.8926
H	5.7334	1.0537	2.5771
H	6.5403	-0.0939	1.4837
H	5.4445	1.1397	0.8265
C	-2.9127	2.0445	0.0107
C	-4.1866	2.6127	0.1724
C	-4.4272	3.5335	1.1947
C	-2.1114	3.3328	1.9226
C	-3.3949	3.8835	2.0685
C	-2.6633	1.1223	-1.1741
H	-4.9921	2.3630	-0.5012
H	-5.4094	3.9662	1.3146
C	-1.0844	3.6530	2.9995
H	-3.6027	4.5756	2.8709
H	-1.8513	0.4525	-0.9137
C	-3.8539	0.2313	-1.5405
C	-2.2333	1.8828	-2.4299
H	-3.5472	-0.4922	-2.2962
H	-4.1967	-0.3033	-0.6542
H	-4.6689	0.8353	-1.9389
H	-1.9887	1.1878	-3.2336
H	-2.9981	2.5773	-2.7780
H	-1.3374	2.4441	-2.1640
H	-0.2115	3.0189	2.8752
C	-0.5177	5.0725	2.9092
C	-1.5954	3.4107	4.4225
H	0.2719	5.2008	3.6498
H	-0.1067	5.2441	1.9148
H	-1.3097	5.7977	3.0972
H	-0.7819	3.5588	5.1330
H	-2.4032	4.1041	4.6561
H	-1.9610	2.3871	4.5075

Strucutre 3B

E = -5.745823 a.u.

Atom	X	Y	Z
Zr	0.0665	0.0314	0.2204
N	2.0697	-0.0284	-0.1522
C	2.8298	1.2435	-0.1656
C	1.9715	2.4837	-0.4245
C	0.9718	2.9046	0.6542
N	-0.1378	1.9469	0.8417
H	3.6189	1.2204	-0.9312
H	3.3478	1.3557	0.8050
H	2.6717	3.3264	-0.5480
H	1.4545	2.3873	-1.3985
H	0.5629	3.8869	0.3650
H	1.5056	3.0488	1.6103
C	-1.2080	-1.5723	1.0713
C	-2.4953	-0.7460	1.1562
H	-1.2968	-2.3993	0.3392
H	-0.9258	-2.0225	2.0366
H	-2.4037	0.2203	0.5822
H	-2.6672	-0.4166	2.1930
C	-3.7473	-1.4466	0.6231
H	-4.6277	-0.7892	0.6640
H	-3.6109	-1.7730	-0.4195
H	-3.9560	-2.3439	1.2240
C	-1.2270	0.3734	-2.0985
C	-0.0735	-0.2138	-2.4833
H	-1.3689	1.4531	-2.1700
H	-2.1035	-0.2259	-1.8314
H	0.7606	0.3663	-2.8771
H	0.0257	-1.3039	-2.5278
C	2.9590	-1.1857	-0.1164
C	-1.1372	2.4592	1.7652
C	3.7704	-1.5090	-1.2308
C	4.6112	-2.6322	-1.1791
C	4.6413	-3.4477	-0.0452
C	2.9566	-2.0415	1.0057
C	3.8134	-3.1537	1.0411
C	3.6878	-0.7438	-2.5454
H	5.2290	-2.8898	-2.0266
H	5.2937	-4.3078	-0.0126
C	2.1621	-1.6960	2.2529
H	3.8578	-3.7857	1.9150
H	2.9653	0.0618	-2.4424
C	5.0205	-0.1144	-2.9609
C	3.1914	-1.6153	-3.7019
H	4.8784	0.4821	-3.8623
H	5.3880	0.5284	-2.1612
H	5.7556	-0.8947	-3.1591
H	3.0649	-1.0025	-4.5946
H	3.9099	-2.4085	-3.9089
H	2.2325	-2.0600	-3.4356
H	1.3497	-1.0322	1.9682
C	1.5261	-2.9127	2.9324
C	3.0166	-0.9644	3.2894
H	0.8672	-2.5813	3.7346
H	0.9446	-3.4759	2.2024
H	2.2982	-3.5565	3.3530
H	2.4216	-0.7460	4.1747
H	3.8686	-1.5831	3.5719
H	3.3916	-0.0330	2.8648
C	-2.1433	3.3265	1.2940
C	-3.1228	3.8178	2.1709
C	-3.0964	3.4546	3.5214
C	-1.1224	2.0845	3.1244
C	-2.0989	2.5952	3.9950
C	-2.2512	3.7113	-0.1738
H	-3.9078	4.4727	1.8229
H	-3.8457	3.8372	4.1985
C	-0.0283	1.1942	3.6902
H	-2.0852	2.3351	5.0428
H	-1.4125	3.2718	-0.7101
C	-3.5241	3.1731	-0.8317
C	-2.1807	5.2225	-0.4057
H	-3.5141	3.4074	-1.8964
H	-3.5689	2.0913	-0.7047
H	-4.4025	3.6257	-0.3714
H	-2.1842	5.4290	-1.4762
H	-3.0371	5.7126	0.0575
H	-1.2618	5.6145	0.0305
H	0.4735	0.7597	2.8286
C	1.0074	1.9801	4.4975
C	-0.5517	0.0424	4.5531
H	1.8068	1.3157	4.8237
H	1.4307	2.7703	3.8779
H	0.5323	2.4263	5.3714
H	0.2771	-0.5960	4.8564
H	-1.0399	0.4342	5.4452
H	-1.2660	-0.5490	3.9820

Strucutre 6B

E_{total} = -5.741354 a.u.

Atom	X	Y	Z
Zr	0.0141	-0.0126	-0.0032
N	2.0332	0.0050	0.0113
C	2.6570	1.3374	-0.0010
C	1.6338	2.4510	-0.2738
C	0.6175	2.7609	0.8385
N	-0.3925	1.6996	1.0114
H	3.4222	1.3727	-0.7957
H	3.1683	1.5515	0.9521
H	2.2064	3.3773	-0.4446
H	1.1115	2.2681	-1.2392
H	0.1082	3.7039	0.5754
H	1.1938	2.9499	1.7570
C	-1.1267	-1.9311	0.3246
C	-0.6522	-1.7928	1.7562
H	-2.2215	-1.9059	0.2314
H	-0.7264	-2.8169	-0.1890
H	0.0411	-0.8832	1.9259
H	0.0320	-2.6107	2.0281
C	-1.7563	-1.6168	2.7990
H	-1.3430	-1.4072	3.7948
H	-2.4385	-0.7974	2.5294
H	-2.3516	-2.5399	2.8506
C	-0.6233	0.2952	-2.5914
C	-1.2068	-0.9067	-2.3891
H	0.3970	0.3668	-2.9804
H	-1.2038	1.2211	-2.5466
H	-0.6690	-1.8381	-2.5726
H	-2.2669	-0.9969	-2.1516
C	2.9725	-1.0780	0.2290
C	-1.5336	2.0597	1.8434
C	3.3277	-1.9160	-0.8451
C	4.2564	-2.9481	-0.6413
C	4.7941	-3.1776	0.6298
C	3.4925	-1.3240	1.5186
C	4.4055	-2.3741	1.7078
C	2.7625	-1.6780	-2.2358
H	4.5776	-3.5789	-1.4568
H	5.5031	-3.9783	0.7804
C	3.0469	-0.5084	2.7263
H	4.8166	-2.5767	2.6857
H	1.9205	-0.9953	-2.1474
C	3.7756	-1.0246	-3.1775
C	2.2235	-2.9476	-2.8993
H	3.3044	-0.8180	-4.1386
H	4.1246	-0.0880	-2.7421
H	4.6260	-1.6904	-3.3265
H	1.7470	-2.6908	-3.8456
H	3.0375	-3.6478	-3.0871
H	1.4877	-3.4149	-2.2445
H	2.2480	0.1635	2.4178
C	2.4743	-1.3683	3.8564
C	4.1673	0.3521	3.3152
H	2.0715	-0.7241	4.6383
H	1.6756	-1.9986	3.4681
H	3.2554	-2.0003	4.2789
H	3.7714	0.9630	4.1270
H	4.9626	-0.2869	3.6993
H	4.5749	1.0043	2.5433
C	-2.8377	1.7976	1.3699
C	-3.9540	2.1601	2.1402
C	-3.7870	2.7971	3.3718
C	-1.3700	2.6080	3.1392
C	-2.5001	2.9924	3.8790
C	-3.0644	1.2329	-0.0219
H	-4.9547	1.9887	1.7734
H	-4.6493	3.0884	3.9530
C	-0.0399	2.5391	3.8790
H	-2.3853	3.4280	4.8604
H	-2.1698	0.6886	-0.3105
C	-4.2245	0.2362	-0.1053
C	-3.2948	2.3284	-1.0642
H	-4.2142	-0.2554	-1.0780
H	-4.1176	-0.5164	0.6758
H	-5.1753	0.7542	0.0188
H	-3.4065	1.8800	-2.0515
H	-4.1973	2.8881	-0.8180
H	-2.4417	3.0073	-1.0724
H	0.6769	2.0006	3.2645
C	0.5411	3.9194	4.1985
C	-0.1236	1.7440	5.1849
H	1.5260	3.8067	4.6522
H	0.6334	4.5013	3.2816
H	-0.1165	4.4466	4.8900
H	0.8724	1.6468	5.6176
H	-0.7745	2.2526	5.8960
H	-0.5200	0.7495	4.9789

Structure 7B

E_{total} = -5.749672 a.u.

Atom	X	Y	Z
Zr	-0.2041	0.0215	0.1471
N	1.6944	-0.1212	0.8225
C	2.4681	1.1394	0.6976
C	1.9278	2.1019	-0.3753
C	0.6178	2.8551	-0.1083
N	-0.5787	1.9805	-0.1597
H	3.5036	0.8920	0.4151
H	2.5060	1.6790	1.6588
H	2.7031	2.8737	-0.5123
H	1.8656	1.5803	-1.3530
H	0.5341	3.6403	-0.8738
H	0.6768	3.3699	0.8678
C	-1.7847	-1.5122	0.2668
C	-1.4813	-1.6111	1.7459
H	-1.6844	-2.4709	-0.2632
H	-2.7626	-1.0548	0.0386
H	-0.7659	-0.7634	2.1011
H	-2.3570	-1.4044	2.3808
C	-0.7796	-2.9047	2.1663
H	0.0636	-3.1068	1.4832
H	-1.4979	-3.7276	2.0004
C	-0.2779	-2.9261	3.6063
H	0.3916	-2.0634	3.7723
H	-1.1319	-2.7962	4.2926
C	0.4630	-4.2194	3.9377
H	-0.1896	-5.0954	3.8028
H	1.3413	-4.3522	3.2869
H	0.8139	-4.2199	4.9789
C	2.4831	-1.2882	1.1937
C	-1.8226	2.7338	-0.1515
C	2.4037	-2.4294	0.3679
C	3.1796	-3.5632	0.6532
C	4.0062	-3.5861	1.7793
C	3.3077	-1.3206	2.3444
C	4.0631	-2.4721	2.6217
C	1.5876	-2.3957	-0.9138
H	3.1654	-4.4191	-0.0045
H	4.5994	-4.4617	1.9981
C	3.3229	-0.1950	3.3695
H	4.6928	-2.5138	3.4977
H	0.6151	-1.9486	-0.7242
C	2.2755	-1.6628	-2.0658
C	0.9412	-3.7221	-1.3230
H	1.6341	-1.6300	-2.9466
H	2.7127	-0.6770	-1.9093
H	3.2087	-2.1677	-2.3158
H	0.2287	-3.5478	-2.1298
H	1.7076	-4.4145	-1.6714
H	0.4185	-4.1592	-0.4724
H	2.4932	0.4751	3.1595
C	3.1055	-0.6811	4.8060
C	4.6189	0.6200	3.3433
H	3.0189	0.1784	5.4710
H	2.1900	-1.2685	4.8681
H	3.9472	-1.2939	5.1281
H	4.5445	1.4507	4.0455
H	5.4599	-0.0148	3.6232
H	4.7882	1.0134	2.3416
C	-2.2160	3.4990	-1.2724
C	-3.4099	4.2364	-1.2244
C	-4.2090	4.2220	-0.0769
C	-2.6516	2.6879	0.9883
C	-3.8303	3.4501	1.0258
C	-1.4344	3.4694	-2.5789
H	-3.7271	4.8156	-2.0789
H	-5.1212	4.7993	-0.0455
C	-2.2259	1.9147	2.2260
H	-4.4526	3.4568	1.9079
H	-0.5670	2.8240	-2.4565
C	-2.2460	2.8807	-3.7356
C	-0.9225	4.8482	-3.0046
H	-1.6200	2.8124	-4.6256
H	-2.5913	1.8826	-3.4649
H	-3.1071	3.5140	-3.9494
H	-0.3089	4.7506	-3.9004
H	-1.7634	5.5092	-3.2152
H	-0.3204	5.2785	-2.2044
H	-1.5091	1.1587	1.9182
C	-1.5279	2.8001	3.2601
C	-3.3742	1.1787	2.9219
H	-1.1890	2.1900	4.0977
H	-0.6667	3.2864	2.8023
H	-2.2194	3.5613	3.6221
H	-2.9757	0.5581	3.7248
H	-4.0793	1.8942	3.3444
H	-3.8900	0.5439	2.2012

Structure 8B

E_{total} = -5.754721

Zr	-0.0800	-0.0463	-0.2125
N	1.8982	-0.0883	0.1369
C	2.6171	1.2101	0.2045
C	2.0163	2.2840	-0.7077
C	0.6192	2.8274	-0.3689
N	-0.5064	1.8783	-0.6429
H	3.6596	1.0524	-0.1132
H	2.6486	1.5865	1.2421
H	2.7027	3.1472	-0.6692
H	2.0218	1.9234	-1.7522
H	0.4754	3.7219	-0.9923
H	0.6027	3.1583	0.6845
C	-1.3123	-1.8639	-0.4594
C	-2.0121	-1.6626	0.9092
H	-0.6376	-2.7405	-0.4202
H	-2.0366	-2.0243	-1.2694
H	-2.2222	-2.6415	1.3720
H	-2.9848	-1.1638	0.7780
C	-1.1907	-0.8582	1.9555
H	-1.1570	0.2509	1.7340
H	-0.1456	-1.2366	2.0296
C	-1.7815	-0.9044	3.3744
H	-2.8225	-0.5455	3.3293
H	-1.8228	-1.9651	3.6724
C	-0.9775	-0.1028	4.3896
H	0.0607	-0.4628	4.4511
H	-0.9586	0.9683	4.1366
H	-1.4204	-0.1969	5.3910
C	2.7648	-1.2545	0.1492
C	-1.6103	2.4646	-1.3943
C	2.7487	-2.1282	-0.9573
C	3.6075	-3.2387	-0.9811
C	4.4378	-3.5143	0.1099
C	3.5890	-1.5441	1.2596
C	4.4205	-2.6751	1.2285
C	1.9314	-1.7954	-2.1968
H	3.6546	-3.8777	-1.8499
H	5.0912	-4.3740	0.0887
C	3.5173	-0.7318	2.5450
H	5.0493	-2.9128	2.0736
H	1.1268	-1.1232	-1.9081
C	2.7704	-1.0720	-3.2523
C	1.2689	-3.0062	-2.8598
H	2.1517	-0.8258	-4.1144
H	3.1756	-0.1532	-2.8278
H	3.5927	-1.7125	-3.5720
H	0.6090	-2.6676	-3.6589
H	2.0271	-3.6667	-3.2802
H	0.6831	-3.5531	-2.1215
H	2.7117	-0.0075	2.4557
C	3.1717	-1.5826	3.7701
C	4.8047	0.0422	2.8368
H	3.0509	-0.9382	4.6411
H	2.2372	-2.1147	3.5894
H	3.9659	-2.3033	3.9646
H	4.6782	0.6373	3.7414
H	5.6323	-0.6537	2.9756
H	5.0294	0.7052	2.0014
C	-2.0797	1.7964	-2.5472
C	-3.1027	2.3657	-3.3223
C	-3.6682	3.5905	-2.9612
C	-2.2285	3.6773	-0.9975
C	-3.2451	4.2298	-1.7936
C	-1.3772	0.5557	-3.0762
H	-3.4478	1.8767	-4.2207
H	-4.4560	4.0220	-3.5609
C	-1.9318	4.3541	0.3350
H	-3.7257	5.1512	-1.4999
H	-0.8461	0.0864	-2.2543
C	-2.3317	-0.5022	-3.6368
C	-0.3431	0.8857	-4.1531
H	-1.7828	-1.4258	-3.8222
H	-3.1255	-0.6966	-2.9154
H	-2.7704	-0.1556	-4.5725
H	0.1329	-0.0319	-4.4971
H	-0.8312	1.3750	-4.9963
H	0.4142	1.5516	-3.7391
H	-1.2514	3.7284	0.9046
C	-1.2885	5.7356	0.1824
C	-3.1779	4.5069	1.2116
H	-1.0428	6.1360	1.1662
H	-0.3760	5.6555	-0.4074
H	-1.9796	6.4131	-0.3193
H	-2.8938	4.9093	2.1842
H	-3.8910	5.1825	0.7395
H	-3.6438	3.5312	1.3525

Structure 11B

E_{total} = -5.749191 a.u.

Atom	X	Y	Z
Zr	-0.0653	0.1305	-0.1590
N	1.9342	-0.2291	-0.0170
C	2.8577	0.9386	-0.0201
C	2.4240	2.0978	-0.9214
C	1.1752	2.8779	-0.5075
N	-0.0770	2.0932	-0.6543
H	3.8473	0.6071	-0.3707
H	2.9974	1.3256	1.0060
H	3.2641	2.8131	-0.9345
H	2.2963	1.7325	-1.9546
H	1.1175	3.7727	-1.1460
H	1.3016	3.2339	0.5311
C	-1.1281	0.4273	2.1829
C	0.1136	0.3463	2.7233
H	-1.6332	1.3936	2.0847
H	-1.7326	-0.4760	2.0485
H	0.5392	-0.6448	2.9188
C	0.8917	1.5089	3.2145
H	1.9447	1.4711	2.9032
H	0.4427	2.4676	2.9271
H	0.9048	1.4553	4.3189
C	-1.5391	-1.4177	-0.7663
C	-1.0528	-2.4923	0.2092
H	-1.5141	-1.7541	-1.8151
H	-2.5696	-1.0794	-0.5578
H	-0.2409	-2.1361	0.9027
H	-0.6123	-3.3606	-0.2989
H	-1.8425	-2.8582	0.8813
C	2.6469	-1.4940	-0.1474
C	-1.1514	2.8415	-1.2919
C	2.4016	-2.3201	-1.2656
C	3.1088	-3.5236	-1.4169
C	4.0307	-3.9315	-0.4493
C	3.5799	-1.9114	0.8315
C	4.2619	-3.1281	0.6704
C	1.5170	-1.8481	-2.4074
H	2.9746	-4.1326	-2.2981
H	4.5711	-4.8585	-0.5722
C	3.8106	-1.1265	2.1151
H	4.9716	-3.4582	1.4144
H	0.7906	-1.1429	-2.0124
C	2.3258	-1.1262	-3.4863
C	0.7354	-2.9722	-3.0946
H	1.6626	-0.7975	-4.2846
H	2.8187	-0.2575	-3.0508
H	3.0820	-1.7900	-3.9059
H	0.0604	-2.4320	-3.7587
H	1.2942	-3.7005	-3.6825
H	0.1444	-3.5065	-2.3521
H	3.0799	-0.3250	2.1679
C	3.6001	-1.9656	3.3780
C	5.2026	-0.4935	2.1864
H	3.6684	-1.3291	4.2605
H	2.6020	-2.4039	3.3661
H	4.3485	-2.7556	3.4401
H	5.2851	0.1034	3.0949
H	5.9618	-1.2758	2.2032
H	5.3788	0.1504	1.3250
C	-1.7106	2.3658	-2.4965
C	-2.7230	3.0997	-3.1357
C	-3.2022	4.2861	-2.5735
C	-1.6586	4.0271	-0.7099
C	-2.6749	4.7431	-1.3625
C	-1.1380	1.1452	-3.1975
H	-3.1280	2.7683	-4.0800
H	-3.9814	4.8450	-3.0704
C	-1.2111	4.5069	0.6643
H	-3.0711	5.6478	-0.9260
H	-0.5754	0.5620	-2.4728
C	-2.2029	0.2159	-3.7868
C	-0.1733	1.5342	-4.3191
H	-1.7279	-0.6903	-4.1632
H	-2.9225	-0.0519	-3.0132
H	-2.7225	0.7108	-4.6070
H	0.2049	0.6382	-4.8090
H	-0.6914	2.1507	-5.0540
H	0.6615	2.0977	-3.9020
H	-0.5596	3.7552	1.1017
C	-0.4352	5.8255	0.6164
C	-2.3739	4.6695	1.6470
H	-0.0881	6.0831	1.6172
H	0.4253	5.7212	-0.0439
H	-1.0795	6.6213	0.2421
H	-1.9856	4.9187	2.6348
H	-3.0409	5.4644	1.3135
H	-2.9300	3.7338	1.7088

Structure 12 B

E_{total} = -4.540915 a.u.

Atom	X	Y	Z
Zr	0.4354	-0.2523	-0.0319
N	2.4209	0.0504	0.1023
C	2.8715	1.4736	0.0728
C	2.0870	2.3569	-0.9017
C	0.6470	2.7140	-0.5247
N	-0.2890	1.5539	-0.5464
H	3.9237	1.5012	-0.2465
H	2.8262	1.9181	1.0833
H	2.6360	3.3108	-0.9799
H	2.1033	1.8967	-1.9054
H	0.2916	3.4688	-1.2427
H	0.6394	3.1899	0.4722
C	0.1968	-0.4595	2.5229
C	-0.9977	0.1475	2.3043
C	-2.2703	-0.5611	1.9941
H	0.2733	-1.5560	2.5151
H	1.0566	0.0960	2.9025
H	-1.0640	1.2311	2.4510
H	-0.3542	-1.8574	-0.5610
H	-2.8509	-0.0580	1.2062
H	-2.1270	-1.6197	1.7401
H	-2.9004	-0.5150	2.9031
C	3.5044	-0.9255	0.0177
C	-1.5316	1.8347	-1.2522
C	3.4313	-1.9589	-0.9430
C	4.5196	-2.8263	-1.1282
C	5.6754	-2.6920	-0.3558
C	4.6593	-0.8257	0.8330
C	5.7370	-1.7025	0.6281
C	2.2467	-2.0904	-1.8849
H	4.4811	-3.5955	-1.8853
H	6.5073	-3.3651	-0.5019
C	4.7039	0.0622	2.0705
H	6.6134	-1.6441	1.2565
H	1.4923	-1.3665	-1.5968
C	2.6158	-1.7860	-3.3383
C	1.5893	-3.4715	-1.8288
H	1.7306	-1.8710	-3.9677
H	3.0093	-0.7716	-3.4074
H	3.3710	-2.4903	-3.6874
H	0.7014	-3.4815	-2.4608
H	2.2867	-4.2324	-2.1793
H	1.2996	-3.6943	-0.8018
H	3.7473	0.5653	2.1778
C	4.8949	-0.7366	3.3628
C	5.7953	1.1346	2.0091
H	4.8289	-0.0667	4.2204
H	4.1129	-1.4923	3.4405
H	5.8695	-1.2247	3.3638
H	5.7318	1.7725	2.8910
H	6.7777	0.6631	1.9765
H	5.6625	1.7459	1.1171
C	-1.8501	1.0979	-2.4116
C	-3.0493	1.3526	-3.0956
C	-3.9468	2.3121	-2.6180
C	-2.4545	2.7822	-0.7532
C	-3.6519	3.0182	-1.4479
C	-0.8622	0.1086	-3.0078
H	-3.2836	0.8199	-4.0052
H	-4.8687	2.5022	-3.1475
C	-2.2298	3.5078	0.5659
H	-4.3638	3.7407	-1.0774
H	-0.0708	-0.0682	-2.2850
C	-1.4826	-1.2536	-3.3278
C	-0.1943	0.6537	-4.2719
H	-0.7076	-1.9361	-3.6759
H	-1.9428	-1.6638	-2.4289
H	-2.2394	-1.1483	-4.1050
H	0.5385	-0.0622	-4.6422
H	-0.9456	0.8303	-5.0418
H	0.3094	1.5921	-4.0389
H	-1.3471	3.0940	1.0465
C	-1.9956	5.0096	0.3879
C	-3.3804	3.3150	1.5577
H	-1.7792	5.4642	1.3549
H	-1.1497	5.1712	-0.2801
H	-2.8840	5.4755	-0.0388
H	-3.1209	3.7725	2.5126
H	-4.2897	3.7778	1.1742
H	-3.5552	2.2500	1.7095

Structure TS[3B-8B]

E_{total} = -5.727027 a.u.

Atom	X	Y	Z
Zr	0.0038	-0.0074	0.0013
N	2.0223	-0.0077	-0.0037
C	2.6710	1.3234	0.0072
C	1.7411	2.4506	-0.4627
C	0.5902	2.8841	0.4583
N	-0.4852	1.8751	0.5702
H	3.5412	1.3101	-0.6690
H	3.0515	1.5589	1.0172
H	2.3756	3.3407	-0.6050
H	1.3422	2.2112	-1.4694
H	0.1659	3.8098	0.0329
H	0.9988	3.1373	1.4523
C	-0.5842	-0.3588	-2.2298
C	-1.1986	-1.5388	-1.7523
H	0.3654	-0.4597	-2.7644
H	-1.2254	0.4665	-2.5499
H	-0.7076	-2.4947	-1.9442
H	-2.2894	-1.5913	-1.7302
C	-1.1786	-1.9498	0.3527
C	-2.1194	-1.2066	1.2988
H	-1.6053	-2.9146	0.0616
H	-0.1999	-2.2121	0.8453
H	-1.6890	-0.2460	1.6778
H	-3.0337	-0.9313	0.7444
C	-2.4965	-2.0219	2.5429
H	-3.0043	-2.9493	2.2412
H	-1.6115	-2.2921	3.1341
H	-3.1802	-1.4486	3.1844
C	2.9398	-1.0669	0.3701
C	-1.6871	2.4040	1.1858
C	3.8998	-1.5387	-0.5497
C	4.7796	-2.5622	-0.1653
C	4.7168	-3.1103	1.1198
C	2.8572	-1.6380	1.6567
C	3.7597	-2.6479	2.0294
C	3.9435	-1.0336	-1.9848
H	5.5137	-2.9532	-0.8543
H	5.4036	-3.8923	1.4083
C	1.8778	-1.0982	2.6892
H	3.7415	-3.0773	3.0198
H	3.2027	-0.2454	-2.1036
C	5.3000	-0.4389	-2.3707
C	3.5822	-2.1213	-2.9988
H	5.2471	-0.0307	-3.3802
H	5.5587	0.3598	-1.6754
H	6.0695	-1.2102	-2.3349
H	3.5606	-1.6956	-4.0022
H	4.3186	-2.9244	-2.9635
H	2.5975	-2.5249	-2.7612
H	1.0779	-0.5745	2.1684
C	1.2129	-2.1850	3.5380
C	2.5389	-0.0985	3.6409
H	0.4501	-1.7346	4.1732
H	0.7469	-2.9241	2.8866
H	1.9538	-2.6759	4.1688
H	1.8043	0.2795	4.3504
H	3.3466	-0.5874	4.1861
H	2.9458	0.7362	3.0713
C	-2.8016	2.7152	0.3820
C	-3.9703	3.2198	0.9730
C	-4.0378	3.4070	2.3574
C	-1.7653	2.5660	2.5855
C	-2.9406	3.0765	3.1598
C	-2.7537	2.5359	-1.1258
H	-4.8259	3.4698	0.3632
H	-4.9396	3.7952	2.8073
C	-0.6233	2.1487	3.5003
H	-3.0125	3.2084	4.2292
H	-1.7674	2.1664	-1.3968
C	-3.7736	1.5136	-1.6328
C	-2.9528	3.8476	-1.8881
H	-3.6491	1.3719	-2.7065
H	-3.6156	0.5617	-1.1261
H	-4.7856	1.8648	-1.4309
H	-2.8359	3.6712	-2.9575
H	-3.9497	4.2444	-1.6955
H	-2.2067	4.5726	-1.5621
H	0.1428	1.6601	2.9011
C	0.0365	3.3352	4.2063
C	-1.0555	1.1372	4.5657
H	0.8924	2.9875	4.7854
H	0.3763	4.0588	3.4655
H	-0.6797	3.8153	4.8734
H	-0.1940	0.8379	5.1618
H	-1.8046	1.5802	5.2218
H	-1.4767	0.2569	4.0816

Structure TS[3B-11B]

E = -5.727085 a.u.

Atom	X	Y	Z
Zr	0.0200	-0.0074	0.0107
N	2.0387	0.0138	0.0151
C	2.6524	1.3510	-0.0097
C	1.6059	2.4568	-0.1945
C	0.6390	2.7014	0.9753
N	-0.3597	1.6249	1.1631
H	3.3623	1.4145	-0.8525
H	3.2221	1.5578	0.9109
H	2.1577	3.3975	-0.3462
H	1.0457	2.3059	-1.1397
H	0.1131	3.6498	0.7734
H	1.2628	2.8525	1.8696
C	-0.4772	-1.7119	1.5909
C	-1.1495	-2.3232	0.5083
H	0.4931	-2.1080	1.9066
H	-1.0507	-1.1880	2.3609
H	-1.1336	-1.5032	-0.7306
H	-2.2466	-2.2632	0.5310
C	-0.6105	-3.5976	-0.1029
H	-1.0241	-3.8026	-1.0990
H	0.4874	-3.5934	-0.1615
H	-0.9001	-4.4319	0.5570
C	-0.6671	0.3483	-2.3123
C	-1.2761	-0.8992	-2.1344
H	0.2849	0.4137	-2.8437
H	-1.2733	1.2561	-2.2936
H	-0.8161	-1.7823	-2.5915
H	-2.3681	-0.9517	-2.0578
C	2.9856	-1.0830	0.1173
C	-1.4887	2.0020	2.0080
C	3.1344	-1.9783	-0.9613
C	4.0795	-3.0138	-0.8830
C	4.8286	-3.1999	0.2833
C	3.7185	-1.2916	1.3072
C	4.6376	-2.3505	1.3778
C	2.3448	-1.7746	-2.2435
H	4.2467	-3.6728	-1.7215
H	5.5461	-4.0049	0.3422
C	3.4689	-0.4601	2.5595
H	5.2011	-2.5235	2.2827
H	1.4048	-1.3018	-1.9728
C	3.0590	-0.8540	-3.2356
C	1.9835	-3.0700	-2.9763
H	2.4291	-0.6974	-4.1115
H	3.2587	0.1081	-2.7647
H	4.0025	-1.3052	-3.5435
H	1.3101	-2.8440	-3.8034
H	2.8828	-3.5425	-3.3711
H	1.4856	-3.7538	-2.2895
H	2.6484	0.2281	2.3667
C	3.0357	-1.3043	3.7610
C	4.6828	0.3731	2.9784
H	4.4214	0.9971	3.8334
H	5.5081	-0.2847	3.2512
H	4.9932	1.0115	2.1515
H	2.7886	-0.6505	4.5977
H	2.1560	-1.8906	3.4964
H	3.8405	-1.9773	4.0567
C	-2.8046	1.6988	1.5909
C	-3.9038	2.0957	2.3690
C	-3.7136	2.8157	3.5496
C	-1.3019	2.6232	3.2694
C	-2.4166	3.0460	4.0118
C	-3.0771	1.0418	0.2508
H	-4.9114	1.8912	2.0395
H	-4.5637	3.1351	4.1342
C	0.0376	2.5874	3.9955
H	-2.2811	3.5386	4.9632
H	-2.1607	0.5637	-0.0779
C	-4.1439	-0.0551	0.3139
C	-3.4846	2.0525	-0.8229
H	-4.1635	-0.6018	-0.6288
H	-3.9088	-0.7461	1.1234
H	-5.1258	0.3844	0.4888
H	-3.6130	1.5434	-1.7783
H	-4.4218	2.5332	-0.5417
H	-2.7075	2.8109	-0.9210
H	0.7423	2.0065	3.4062
C	0.6322	3.9791	4.2311
C	-0.0349	1.8699	5.3466
H	1.6219	3.8841	4.6783
H	0.7169	4.5098	3.2831
H	-0.0128	4.5482	4.9008
H	0.9663	1.7868	5.7700
H	-0.6698	2.4254	6.0367
H	-0.4443	0.8694	5.2040

Structure TS[1B-12B]

E = -4.526552 a.u.

Atom	X	Y	Z
Zr	-0.0002	0.0159	-0.0437
N	2.0072	0.0117	-0.0482
C	2.6924	1.3305	-0.0238
C	1.8783	2.4465	-0.6788
C	0.6224	2.9296	0.0464
N	-0.5069	1.9599	-0.0040
H	3.6506	1.2641	-0.5579
H	2.9325	1.6076	1.0191
H	2.5489	3.3179	-0.7552
H	1.6193	2.1589	-1.7149
H	0.3184	3.8751	-0.4224
H	0.8670	3.1681	1.0979
C	-1.6016	-1.8977	0.3934
C	-1.3604	-2.4077	-0.8450
H	-1.1135	-2.3316	1.2762
H	-2.5031	-1.2971	0.5673
H	-0.2561	-0.3346	-1.8377
H	-1.9965	-2.0885	-1.6751
C	-0.3599	-3.4563	-1.1494
H	0.2132	-3.2209	-2.0574
H	0.3162	-3.6694	-0.3099
H	-0.9177	-4.3864	-1.3711
C	2.8997	-1.1090	0.2128
C	-1.7791	2.5566	0.3804
C	3.9420	-1.4423	-0.6834
C	4.7869	-2.5255	-0.3930
C	4.6048	-3.2790	0.7701
C	2.6918	-1.8990	1.3634
C	3.5586	-2.9679	1.6432
C	4.1018	-0.7512	-2.0315
H	5.5740	-2.8015	-1.0791
H	5.2621	-4.1082	0.9866
C	1.6104	-1.5399	2.3715
H	3.4361	-3.5559	2.5401
H	3.3423	0.0215	-2.1264
C	5.4674	-0.0805	-2.2059
C	3.8827	-1.7048	-3.2086
H	5.4920	0.4597	-3.1525
H	5.6386	0.6213	-1.3897
H	6.2556	-0.8335	-2.2013
H	3.9323	-1.1488	-4.1450
H	4.6485	-2.4806	-3.2102
H	2.8999	-2.1688	-3.1207
H	0.8228	-0.9994	1.8515
C	0.9467	-2.7525	3.0309
C	2.1369	-0.6290	3.4820
H	0.0813	-2.4245	3.6073
H	0.6184	-3.4526	2.2626
H	1.6501	-3.2515	3.6972
H	1.3349	-0.3990	4.1824
H	2.9461	-1.1286	4.0150
H	2.5111	0.2979	3.0476
C	-2.3778	3.5910	-0.3774
C	-3.5952	4.1482	0.0496
C	-4.2271	3.6899	1.2104
C	-2.4438	2.0764	1.5277
C	-3.6523	2.6499	1.9475
C	-1.8171	4.0435	-1.7198
H	-4.0666	4.9293	-0.5282
H	-5.1612	4.1311	1.5261
C	-1.8421	1.0165	2.4365
H	-4.3976	2.5946	2.7274
H	-0.9207	3.4683	-1.9411
C	-2.7824	3.7827	-2.8789
C	-1.4363	5.5270	-1.7434
H	-2.3045	4.0515	-3.8212
H	-3.0448	2.7247	-2.9010
H	-3.6882	4.3761	-2.7537
H	-0.9689	5.7701	-2.6978
H	-2.3269	6.1419	-1.6124
H	-0.7343	5.7398	-0.9374
H	-1.2567	0.3827	1.7764
C	-0.9063	1.6003	3.4959
C	-2.8734	0.1272	3.1368
H	-0.4952	0.7961	4.1048
H	-0.0908	2.1355	3.0101
H	-1.4590	2.2889	4.1354
H	-2.3628	-0.6873	3.6512
H	-3.4381	0.7111	3.8640
H	-3.5584	-0.2907	2.3992

PART III New Catalysts

3.1 Backbone modification I

Strucutre 13

E_{total} = -4.532524 a.u.

Atom	X	Y	Z
Zr	0.1110	-0.0787	0.4818
N	2.0808	0.0507	0.1002
C	2.6071	1.4265	-0.1290
C	1.5087	2.4164	-0.6015
C	0.2820	2.8612	0.2400
N	-0.7131	1.7557	0.4106
H	2.0511	3.3440	-0.8529
H	1.1151	2.0431	-1.5695
C	-0.9679	-1.9742	0.8401
C	-1.1203	-2.0509	-0.6640
H	-0.3836	-2.8034	1.2657
H	-1.9369	-1.8839	1.3565
H	-0.7954	-1.0571	-1.1846
H	-0.4154	-2.7679	-1.1098
C	-2.5340	-2.2873	-1.1921
H	-2.8421	-3.3052	-0.9118
H	-3.2500	-1.5846	-0.7442
H	-2.5837	-2.1967	-2.2855
C	3.0637	-0.9789	0.4195
C	3.6446	1.4451	-1.2668
C	3.3748	1.9568	1.0958
C	-0.3019	4.0507	-0.5432
C	0.6800	3.4613	1.5996
C	-2.0125	2.1231	0.9652
C	3.6551	-1.7518	-0.6068
C	4.5889	-2.7485	-0.2817
C	4.9214	-3.0022	1.0516
C	3.3089	-1.3274	1.7675
C	4.2471	-2.3262	2.0720
C	3.2035	-1.6375	-2.0560
H	5.0144	-3.3697	-1.0558
H	5.6359	-3.7750	1.2939
C	2.5286	-0.6995	2.9140
H	4.4453	-2.5928	3.0995
H	2.5254	-0.7924	-2.1490
C	4.3529	-1.4259	-3.0468
C	2.4198	-2.8688	-2.5149
H	3.9470	-1.2128	-4.0359
H	4.9700	-0.5874	-2.7264
H	4.9703	-2.3227	-3.0995
H	2.0253	-2.7017	-3.5174
H	3.0708	-3.7432	-2.5239
H	1.5935	-3.0483	-1.8287
H	1.8627	0.0603	2.5103
C	1.6497	-1.7100	3.6530
C	3.4229	-0.0203	3.9558
H	1.0920	-1.2031	4.4397
H	0.9511	-2.1660	2.9533
H	2.2697	-2.4875	4.0994
H	2.8046	0.5381	4.6591
H	3.9972	-0.7703	4.4998
H	4.1113	0.6652	3.4632
C	-3.0623	2.5526	0.1187
C	-4.3079	2.8955	0.6683
C	-4.5342	2.7844	2.0425
C	-2.2800	1.9175	2.3390
C	-3.5298	2.2749	2.8692
C	-2.9357	2.5179	-1.3987
H	-5.1163	3.2182	0.0293
H	-5.4982	3.0414	2.4559
C	-1.2578	1.2893	3.2766
H	-3.7340	2.1412	3.9212
H	-1.8998	2.3178	-1.6607
C	-3.7596	1.3902	-2.0223
C	-3.3478	3.8257	-2.0837
H	-3.5879	1.3606	-3.0985
H	-3.4561	0.4398	-1.5865
H	-4.8203	1.5521	-1.8294
H	-3.1329	3.7622	-3.1506
H	-4.4145	4.0011	-1.9448
H	-2.7916	4.6599	-1.6576
H	-0.3573	1.0561	2.7123
C	-0.8546	2.2006	4.4400
C	-1.7563	-0.0219	3.8886
H	-0.0532	1.7309	5.0108
H	-0.5061	3.1593	4.0595
H	-1.7098	2.3691	5.0946
H	-0.9722	-0.4651	4.5011
H	-2.6311	0.1655	4.5112
H	-2.0274	-0.7152	3.0953
H	3.6598	2.9961	0.9311
H	2.7606	1.8930	1.9891
H	4.2798	1.3683	1.2470
H	1.4822	4.1871	1.4645
H	-0.1780	3.9672	2.0420
H	1.0123	2.6755	2.2737
H	4.0389	2.4545	-1.3877
H	4.4744	0.7799	-1.0306
H	3.1796	1.1438	-2.2046
H	-1.1988	4.4256	-0.0513
H	0.4296	4.8586	-0.5782
H	-0.5274	3.7549	-1.5664

Strucutre 13[π-complex]

E_{total} = -5.724944 a.u.

Atom	X	Y	Z
Zr	-0.0794	0.0071	-0.0525
N	1.9453	0.0092	0.0332
C	2.5384	1.3733	0.0295
C	1.5107	2.4467	-0.4288
C	0.2996	2.9152	0.4250
N	-0.6001	1.7913	0.7715
H	2.0881	3.3607	-0.6495
H	1.1360	2.1317	-1.4271
C	-0.4519	0.3085	-2.6704
C	-1.1780	-0.8210	-2.5117
H	0.5970	0.2641	-2.9744
H	-0.9394	1.2875	-2.6962
H	-0.7393	-1.8109	-2.6411
H	-2.2582	-0.7869	-2.3764
C	-1.3202	-1.8663	0.1129
C	-1.5098	-1.4820	1.5681
H	-2.2755	-2.0574	-0.3892
H	-0.6640	-2.7504	0.0010
H	-0.6037	-0.9414	1.9877
H	-2.3396	-0.7599	1.6722
C	-1.7662	-2.6654	2.5153
H	-2.7203	-3.1333	2.2346
H	-0.9814	-3.4273	2.4193
H	-1.8267	-2.3432	3.5634
C	2.8754	-1.0959	0.2449
C	3.6774	1.4741	-1.0026
C	3.1878	1.7386	1.3728
C	-0.4336	3.9363	-0.4670
C	0.7691	3.7459	1.6323
C	-1.7995	2.1173	1.5352
C	3.4699	-1.7476	-0.8583
C	4.3680	-2.8092	-0.6733
C	4.6736	-3.2478	0.6173
C	3.1269	-1.6044	1.5417
C	4.0393	-2.6588	1.7151
C	3.1074	-1.4309	-2.2989
H	4.8132	-3.3088	-1.5208
H	5.3590	-4.0695	0.7632
C	2.3717	-1.1124	2.7670
H	4.2397	-3.0465	2.7028
H	2.3934	-0.6121	-2.3397
C	4.2903	-1.1307	-3.2245
C	2.1841	-2.4684	-2.9393
H	3.9196	-0.8127	-4.1991
H	4.9016	-0.3361	-2.7984
H	4.9017	-2.0242	-3.3498
H	1.8372	-2.1085	-3.9083
H	2.7205	-3.4081	-3.0721
H	1.3279	-2.6341	-2.2856
H	1.6774	-0.3321	2.4617
C	1.5440	-2.2293	3.4024
C	3.2716	-0.5476	3.8715
H	0.8913	-1.8173	4.1714
H	0.9450	-2.7081	2.6309
H	2.2013	-2.9745	3.8504
H	2.6540	-0.1321	4.6681
H	3.8989	-1.3394	4.2813
H	3.9117	0.2365	3.4720
C	-3.0374	2.2714	0.8694
C	-4.1932	2.5875	1.5971
C	-4.1348	2.7165	2.9848
C	-1.7516	2.1609	2.9519
C	-2.9288	2.4834	3.6498
C	-3.1749	2.0483	-0.6279
H	-5.1402	2.7157	1.0943
H	-5.0274	2.9503	3.5459
C	-0.5411	1.7983	3.8027
H	-2.9201	2.5304	4.7285
H	-2.1896	1.8511	-1.0406
C	-4.0473	0.8348	-0.9553
C	-3.7545	3.2530	-1.3756
H	-4.0642	0.6746	-2.0334
H	-3.6384	-0.0489	-0.4663
H	-5.0650	1.0008	-0.6015
H	-3.7374	3.0596	-2.4483
H	-4.7829	3.4293	-1.0600
H	-3.1602	4.1411	-1.1645
H	0.2891	1.5682	3.1388
C	-0.0966	2.9119	4.7585
C	-0.7717	0.5539	4.6626
H	0.8389	2.6268	5.2403
H	0.0539	3.8408	4.2115
H	-0.8568	3.0731	5.5228
H	0.1499	0.2915	5.1823
H	-1.5550	0.7450	5.3961
H	-1.0733	-0.2764	4.0288
H	3.5017	2.7826	1.3597
H	2.4821	1.5832	2.1853
H	4.0674	1.1161	1.5345
H	1.4492	4.5286	1.2955

H	-0.0894	4.2186	2.1084
H	1.2884	3.1255	2.3550
H	4.1143	2.4726	-0.9715
H	4.4594	0.7500	-0.7756
H	3.2885	1.2988	-2.0049
H	-1.2878	4.3529	0.0665
H	0.2424	4.7501	-0.7307
H	-0.7730	3.4549	-1.3836

Structure 13[insertion_TS]

E_{total} = -5.710210 a.u.

Atom	X	Y	Z
Zr	0.0000	0.0051	-0.0017
N	2.0188	-0.0007	-0.0069
C	2.6219	1.3573	0.0084
C	1.5881	2.4319	-0.4329
C	0.3918	2.9150	0.4355
N	-0.5482	1.8134	0.7574
H	2.1654	3.3418	-0.6677
H	1.1923	2.1075	-1.4207
C	-0.6524	-0.0971	-2.2499
C	-1.2670	-1.3161	-1.8968
H	0.2639	-0.1413	-2.8457
H	-1.2914	0.7729	-2.4273
H	-0.8104	-2.2487	-2.2299
H	-2.3538	-1.3583	-1.7974
C	-1.1019	-2.0078	0.1576
C	-2.0274	-1.4546	1.2370
H	-1.4946	-2.9462	-0.2463
H	-0.0894	-2.2817	0.5685
H	-1.6334	-0.5183	1.7058
H	-2.9886	-1.1761	0.7744
C	-2.2839	-2.4445	2.3813
H	-2.7579	-3.3537	1.9843
H	-1.3534	-2.7365	2.8858
H	-2.9587	-2.0031	3.1279
C	2.9222	-1.1272	0.1919
C	3.7635	1.4730	-1.0205
C	3.2730	1.6875	1.3602
C	-0.2955	3.9857	-0.4359
C	0.8796	3.6962	1.6698
C	-1.7376	2.1624	1.5236
C	3.5120	-1.7697	-0.9214
C	4.3919	-2.8459	-0.7263
C	4.6673	-3.3139	0.5608
C	3.1240	-1.6724	1.4817
C	4.0150	-2.7434	1.6566
C	3.1284	-1.4072	-2.3483
H	4.8438	-3.3419	-1.5724
H	5.3374	-4.1488	0.7029
C	2.3448	-1.1890	2.6959
H	4.1854	-3.1555	2.6401
H	2.5242	-0.5036	-2.3309
C	4.3300	-1.1430	-3.2610
C	2.2740	-2.4935	-3.0043
H	3.9727	-0.7922	-4.2293
H	4.9555	-0.3672	-2.8209
H	4.9419	-2.0310	-3.4196
H	1.9372	-2.1555	-3.9846
H	2.8572	-3.4076	-3.1175
H	1.4068	-2.6990	-2.3775
H	1.6778	-0.3856	2.3895
C	1.4710	-2.2955	3.2903
C	3.2321	-0.6634	3.8296
H	0.8514	-1.9368	4.1109
H	0.8251	-2.6961	2.5111
H	2.1033	-3.1011	3.6635
H	2.6072	-0.2453	4.6189
H	3.8318	-1.4758	4.2401
H	3.8985	0.1118	3.4558
C	-2.9634	2.4164	0.8627
C	-4.1137	2.7214	1.6071
C	-4.0731	2.7426	3.0028
C	-1.7242	2.1066	2.9394
C	-2.8864	2.4171	3.6633
C	-3.0985	2.3261	-0.6497
H	-5.0488	2.9250	1.1068
H	-4.9650	2.9684	3.5685
C	-0.5049	1.6434	3.7264
H	-2.8812	2.3834	4.7427
H	-2.1163	2.1404	-1.0736
C	-3.9999	1.1725	-1.0941
C	-3.6429	3.6060	-1.2924
H	-4.0060	1.1093	-2.1825
H	-3.6213	0.2378	-0.6856
H	-5.0170	1.3341	-0.7365
H	-3.6178	3.5085	-2.3780
H	-4.6707	3.7771	-0.9727
H	-3.0323	4.4584	-0.9977
H	0.3084	1.4458	3.0324
C	-0.0149	2.6697	4.7541
C	-0.7531	0.3440	4.4944
H	0.9231	2.3280	5.1925
H	0.1463	3.6336	4.2744
H	-0.7563	2.7886	5.5443
H	0.1529	0.0547	5.0266
H	-1.5611	0.4814	5.2129
H	-1.0239	-0.4456	3.7972
H	3.6102	2.7243	1.3652
H	2.5599	1.5348	2.1665
H	4.1354	1.0404	1.5183
H	1.5888	4.4643	1.3606
H	0.0332	4.1829	2.1540
H	1.3688	3.0387	2.3804
H	4.2165	2.4627	-0.9549
H	4.5333	0.7292	-0.8169
H	3.3742	1.3410	-2.0292
H	-1.1414	4.4152	0.0998
H	0.4103	4.7849	-0.6643
H	-0.6342	3.5457	-1.3732

Structure 13[termination_TS]

E = -5.705812 a.u.

Atom	X	Y	Z
Zr	-0.0005	0.0001	-0.0003
N	2.0269	-0.0006	-0.0030
C	2.6250	1.3625	-0.0011
C	1.5654	2.4622	-0.2795
C	0.4525	2.8434	0.7323
N	-0.3916	1.6755	1.0775
H	2.1217	3.3928	-0.4788
H	1.0917	2.2273	-1.2551
C	-0.7795	-1.5810	1.5868
C	-1.2689	-2.2738	0.4554
H	0.1180	-1.9432	2.0894
H	-1.4877	-1.0323	2.2156
H	-1.2105	-1.4650	-0.7620
H	-2.3623	-2.2966	0.3432
C	-0.5600	-3.5183	-0.0309
H	-0.8421	-3.7987	-1.0544
H	0.5345	-3.4232	0.0291
H	-0.8493	-4.3496	0.6332
C	-0.7139	0.3871	-2.3073
C	-1.3828	-0.8292	-2.1270
H	0.2079	0.4133	-2.8904
H	-1.2768	1.3218	-2.2572
H	-0.9986	-1.7252	-2.6258
H	-2.4714	-0.8237	-2.0009
C	2.9647	-1.1200	-0.0759
C	3.6482	1.5297	-1.1385
C	3.4061	1.6513	1.2862
C	-0.3886	3.9168	0.0169
C	1.0647	3.5541	1.9534
C	-1.4791	1.8940	2.0238
C	3.3131	-1.6706	-1.3328
C	4.2512	-2.7113	-1.4142
C	4.8291	-3.2387	-0.2583
C	3.4887	-1.7216	1.0966
C	4.4299	-2.7587	0.9906
C	2.6547	-1.2069	-2.6214
H	4.5226	-3.1281	-2.3726
H	5.5432	-4.0459	-0.3276
C	2.9883	-1.3760	2.4925
H	4.8367	-3.2178	1.8792
H	2.0456	-0.3349	-2.4018
C	3.6503	-0.8066	-3.7154
C	1.7264	-2.2720	-3.2069
H	3.1103	-0.3803	-4.5612
H	4.3488	-0.0657	-3.3285
H	4.2085	-1.6800	-4.0522
H	1.1936	-1.8661	-4.0671
H	2.3063	-3.1372	-3.5287
H	1.0094	-2.5844	-2.4487
H	2.2059	-0.6237	2.4097
C	2.3837	-2.5948	3.1984
C	4.0736	-0.8473	3.4377
H	3.6239	-0.5380	4.3814
H	4.8196	-1.6199	3.6247
H	4.5632	0.0272	3.0165
H	1.8753	-2.2799	4.1095
H	1.6735	-3.0908	2.5384
H	3.1700	-3.3042	3.4570
C	-2.8029	2.0518	1.5535
C	-3.8555	2.2494	2.4606
C	-3.6161	2.2516	3.8364
C	-1.2572	1.8127	3.4218
C	-2.3250	2.0115	4.3118
C	-3.1386	1.9786	0.0738
H	-4.8656	2.3843	2.1032
H	-4.4324	2.3927	4.5293
C	0.0890	1.4149	4.0149
H	-2.1634	1.9538	5.3779
H	-2.2134	1.8689	-0.4835
C	-4.0114	0.7685	-0.2638
C	-3.8440	3.2309	-0.4551
H	-4.1658	0.7164	-1.3417
H	-3.5155	-0.1412	0.0738
H	-4.9775	0.8553	0.2336
H	-3.9698	3.1506	-1.5351
H	-4.8231	3.3344	0.0127
H	-3.2464	4.1137	-0.2310
H	0.8155	1.3291	3.2108
C	0.6259	2.4204	5.0404
C	0.0526	0.0577	4.7219
H	1.6438	2.1479	5.3202
H	0.6275	3.4236	4.6172
H	-0.0024	2.4160	5.9311
H	1.0508	-0.1953	5.0795
H	-0.6327	0.0962	5.5688
H	-0.2814	-0.7109	4.0289
H	3.7159	2.6964	1.3043
H	2.7874	1.4414	2.1562
H	4.2987	1.0285	1.3121
H	0.1991	3.9613	2.4755
H	1.7598	3.1743	2.6988
H	1.5671	4.3770	1.4450
H	4.1082	2.5163	-1.0757
H	4.4339	0.7787	-1.0580
H	3.1499	1.4453	-2.1030
H	-1.1781	4.2745	0.6775
H	0.2426	4.7607	-0.2632
H	-0.8318	3.4998	-0.8870

3.1.2 Backbone modification 2

Strucutre 14

E = -4.503908 a.u.

Atom	X	Y	Z
Zr	0.1520	-0.0677	0.6962
N	1.9456	-0.0475	-0.2144
C	2.5627	1.3280	-0.1631
C	1.5152	2.4383	-0.5375
C	0.2951	2.9474	0.2970
N	-0.6089	1.7973	0.6412
H	2.0992	3.3401	-0.7854
H	1.0944	2.0972	-1.5018
C	-1.1423	-1.8351	0.9576
C	-1.0743	-1.9564	-0.5499
H	-0.7860	-2.7244	1.4953
H	-2.1552	-1.5680	1.3078
H	-0.8419	-0.9330	-1.0375
H	-0.2215	-2.5828	-0.8632
C	-2.3430	-2.4221	-1.2686
H	-2.5292	-3.4705	-0.9955
H	-3.2149	-1.8338	-0.9553
H	-2.2379	-2.3565	-2.3598
C	2.7290	-1.1705	-0.7305
C	3.6401	1.5445	-1.2469
C	3.3208	1.5842	1.1772
C	-0.3763	3.9316	-0.6813
C	0.6895	3.7986	1.5506
C	-1.9374	2.0549	1.2024
C	2.9568	-1.3155	-2.1226
C	3.7379	-2.3795	-2.6019
C	4.2484	-3.3396	-1.7269
C	3.1129	-2.2362	0.1206
C	3.9014	-3.2861	-0.3762
C	2.2110	-0.4750	-3.1521
H	3.9127	-2.4972	-3.6607
H	4.8345	-4.1640	-2.1054
C	2.6464	-2.3353	1.5640
H	4.2224	-4.0834	0.2776
H	1.7723	0.3857	-2.6563
C	3.0929	0.0384	-4.2966
C	1.0461	-1.2411	-3.7829
H	2.5233	0.7368	-4.9100
H	3.9677	0.5475	-3.8935
H	3.4216	-0.7937	-4.9191
H	0.4996	-0.5863	-4.4619
H	1.4228	-2.1022	-4.3354
H	0.3714	-1.5858	-3.0006
H	1.9886	-1.4963	1.7748
C	1.8337	-3.6068	1.8198
C	3.7857	-2.3355	2.5899
H	1.3785	-3.5586	2.8094
H	1.0534	-3.6988	1.0657
H	2.4814	-4.4819	1.7651
H	3.3699	-2.3471	3.5976
H	4.4119	-3.2169	2.4513
H	4.3997	-1.4457	2.4722
C	-3.0371	2.4069	0.3802
C	-4.2911	2.6614	0.9586
C	-4.4857	2.5196	2.3341
C	-2.1814	1.7795	2.5710
C	-3.4406	2.0473	3.1303
C	-2.9740	2.3213	-1.1389
H	-5.1342	2.9260	0.3380
H	-5.4573	2.7053	2.7674
C	-1.1141	1.1821	3.4771
H	-3.6186	1.8732	4.1811
H	-1.9449	2.1488	-1.4388
C	-3.7692	1.1316	-1.6768
C	-3.4882	3.5722	-1.8618
H	-3.6203	1.0447	-2.7533
H	-3.4196	0.2225	-1.1919
H	-4.8307	1.2647	-1.4670
H	-3.3114	3.4724	-2.9330
H	-4.5575	3.6912	-1.6875
H	-2.9706	4.4579	-1.4971
H	-0.2446	0.9498	2.8733

C	-0.6638	2.1125	4.6067
C	-1.5534	-0.1314	4.1296
H	0.1239	1.6306	5.1856
H	-0.2761	3.0411	4.1938
H	-1.5054	2.3369	5.2622
H	-0.7126	-0.5734	4.6647
H	-2.3678	0.0525	4.8303
H	-1.8928	-0.8262	3.3639
H	3.4701	2.6555	1.2710
C	2.5661	1.1252	2.4249
C	4.7193	0.9536	1.2428
C	1.8137	4.8174	1.2948
C	-0.4436	4.6643	2.1287
H	1.0245	3.1292	2.3362
H	4.1908	2.4611	-1.0348
H	4.3438	0.7135	-1.2800
H	3.1776	1.6736	-2.2213
H	-1.3049	4.3126	-0.2626
H	0.2846	4.7736	-0.8821
H	-0.5727	3.4426	-1.6337
H	2.9106	1.6951	3.2879
H	1.5037	1.2797	2.2905
H	2.7477	0.0732	2.6132
H	5.1089	1.0340	2.2578
H	4.6746	-0.0955	0.9556
H	5.4017	1.4779	0.5749
H	-0.0983	5.1421	3.0460
H	-0.7264	5.4449	1.4223
H	-1.3169	4.0666	2.3650
H	2.0880	5.2939	2.2361
H	2.6978	4.3307	0.8861
H	1.4781	5.5873	0.6007

Structure 14[π-complex]

E_{total} = -5.68274 a.u.

Atom	X	Y	Z
Zr	0.0677	0.1057	0.2839
N	2.0961	0.2322	0.2269
C	2.5937	1.6033	-0.1004
C	1.4077	2.4821	-0.6627
C	0.1346	3.0712	0.0543
N	-0.6175	1.9739	0.7243
H	1.8753	3.3356	-1.1804
H	1.0164	1.8793	-1.5146
C	-0.4721	-0.1746	-2.3475
C	-1.0464	-1.3112	-1.8953
H	0.5557	-0.1693	-2.7160
H	-1.0797	0.7104	-2.5566
H	-0.5003	-2.2525	-1.8350
H	-2.1162	-1.3645	-1.7020
C	-1.0229	-1.7813	0.8743
C	-1.3121	-1.0775	2.1866
H	-1.9360	-2.1835	0.4220
H	-0.2876	-2.6004	0.9934
H	-0.4425	-0.4294	2.5083
H	-2.1648	-0.3843	2.0707
C	-1.6190	-2.0055	3.3747
H	-2.5519	-2.5458	3.1598
H	-0.8273	-2.7515	3.5174
H	-1.7493	-1.4394	4.3066
C	3.0601	-0.8565	0.4263
C	3.5151	1.5816	-1.3399
C	3.4777	2.2985	0.9859
C	-0.6835	3.5942	-1.1472
C	0.4187	4.3225	0.9424
C	-1.8349	2.2843	1.4748
C	3.6347	-1.5501	-0.6717
C	4.5919	-2.5543	-0.4550
C	4.9522	-2.9313	0.8384
C	3.3277	-1.3533	1.7281
C	4.2907	-2.3561	1.9229
C	3.1227	-1.3885	-2.0943
H	5.0294	-3.0806	-1.2901
H	5.6773	-3.7161	0.9958
C	2.5603	-0.8875	2.9531
H	4.5120	-2.7137	2.9175
H	2.4352	-0.5512	-2.1207
C	4.2182	-1.1430	-3.1393
C	2.3329	-2.6164	-2.5530
H	3.7587	-0.9342	-4.1056
H	4.8338	-0.2935	-2.8480
H	4.8529	-2.0245	-3.2309
H	1.8691	-2.4164	-3.5191
H	2.9979	-3.4756	-2.6426
H	1.5592	-2.8426	-1.8202
H	1.8401	-0.1342	2.6489
C	1.7712	-2.0287	3.5935
C	3.4463	-0.3064	4.0599
H	1.1247	-1.6329	4.3769
H	1.1689	-2.5197	2.8306
H	2.4533	-2.7602	4.0268
H	2.8199	0.1321	4.8370
H	4.0602	-1.0937	4.4976
H	4.1021	0.4592	3.6526
C	-3.1058	2.1411	0.8660
C	-4.2746	2.4125	1.5947
C	-4.2081	2.7786	2.9397
C	-1.7845	2.5681	2.8663
C	-2.9669	2.8320	3.5754
C	-3.2701	1.6372	-0.5580
H	-5.2430	2.3172	1.1266
H	-5.1131	2.9732	3.4960
C	-0.4879	2.5455	3.6629
H	-2.9298	3.0597	4.6303
H	-2.2848	1.4771	-0.9842
C	-4.0077	0.2980	-0.6190
C	-4.0243	2.6107	-1.4699
H	-4.0384	-0.0575	-1.6490
H	-3.4878	-0.4325	-0.0007
H	-5.0270	0.4154	-0.2509
H	-4.0104	2.2370	-2.4939
H	-5.0583	2.7069	-1.1384
H	-3.5523	3.5914	-1.4421
H	0.3230	2.3423	2.9746
C	-0.1843	3.8601	4.3912
C	-0.4449	1.4557	4.7370
H	0.8097	3.8095	4.8362
H	-0.2180	4.6945	3.6948
H	-0.9196	4.0288	5.1779
H	0.5337	1.4543	5.2178
H	-1.2138	1.6394	5.4875
H	-0.6147	0.4832	4.2855
H	3.7055	3.2971	0.6172
C	2.8388	2.4872	2.3599
C	4.8534	1.6483	1.2133
C	1.4962	5.2635	0.3821
C	-0.7921	5.2478	1.1636
H	0.7501	3.9831	1.9128
H	3.9309	2.5758	-1.5075
H	4.3377	0.8852	-1.1960
H	2.9513	1.3051	-2.2294
H	-1.6378	3.9932	-0.8119
H	-0.1351	4.3780	-1.6689
H	-0.8727	2.7861	-1.8517
H	2.3934	3.4738	2.4222
H	2.0889	1.7246	2.5336
H	3.5996	2.4369	3.1375
H	5.4023	2.2184	1.9630
H	4.7487	0.6263	1.5634
H	5.4402	1.6580	0.2963
H	-0.5313	6.0134	1.8942
H	-1.0659	5.7456	0.2335
H	-1.6492	4.6945	1.5367
H	1.6424	6.0956	1.0710
H	2.4439	4.7451	0.2725
H	1.1890	5.6590	-0.5858

Structure 14[insertion_TS]

E_{total} = -5.678049 a.u.

Atom	X	Y	Z
Zr	-0.0044	-0.0144	0.0016
N	2.0219	-0.0067	0.0057
C	2.6066	1.3657	-0.0012
C	1.4901	2.4131	-0.4017
C	0.2082	2.9250	0.3653
N	-0.6667	1.7730	0.7178
H	2.0269	3.3266	-0.7047
H	1.1099	2.0230	-1.3747
C	-0.6707	-0.0609	-2.2673
C	-1.2559	-1.2932	-1.9437
H	0.2406	-0.0638	-2.8703
H	-1.3213	0.8091	-2.3932
H	-0.7759	-2.2128	-2.2789
H	-2.3371	-1.3655	-1.8171
C	-1.0817	-2.0314	0.1402
C	-2.0536	-1.5334	1.2019
H	-1.4268	-2.9688	-0.3070
H	-0.0751	-2.2796	0.5773
H	-1.7048	-0.5885	1.6841
H	-3.0149	-1.2847	0.7228
C	-2.2966	-2.5436	2.3313
H	-2.7448	-3.4596	1.9208
H	-1.3644	-2.8179	2.8422
H	-2.9884	-2.1263	3.0763
C	2.8908	-1.1874	-0.0237
C	3.5799	1.5605	-1.1854
C	3.4815	1.7418	1.2390
C	-0.4664	3.7768	-0.7331
C	0.4997	3.9016	1.5463
C	-1.8793	1.9827	1.5020
C	3.4592	-1.6525	-1.2391
C	4.3243	-2.7585	-1.2392
C	4.5910	-3.4576	-0.0624
C	3.0465	-2.0020	1.1295
C	3.9216	-3.0998	1.1075
C	3.0241	-1.1249	-2.5989
H	4.7596	-3.1110	-2.1622
H	5.2463	-4.3159	-0.0744
C	2.2695	-1.7700	2.4169
H	4.0692	-3.6972	1.9948
H	2.3897	-0.2565	-2.4523
C	4.1831	-0.7275	-3.5221
C	2.1826	-2.1510	-3.3611
H	3.7864	-0.2633	-4.4252
H	4.8418	-0.0212	-3.0197
H	4.7592	-1.6100	-3.8002
H	1.7931	-1.7022	-4.2751
H	2.7922	-3.0180	-3.6166
H	1.3515	-2.4738	-2.7356
H	1.5712	-0.9514	2.2607
C	1.4452	-2.9902	2.8398
C	3.1620	-1.4467	3.6203
H	0.8150	-2.7289	3.6899
H	0.8192	-3.3224	2.0145
H	2.1067	-3.8074	3.1274
H	2.5427	-1.1596	4.4702
H	3.7545	-2.3212	3.8891
H	3.8397	-0.6323	3.3788
C	-3.1337	2.1750	0.8712
C	-4.2978	2.3076	1.6448
C	-4.2465	2.2089	3.0364
C	-1.8510	1.8074	2.9093
C	-3.0280	1.9407	3.6621
C	-3.2945	2.1831	-0.6404
H	-5.2538	2.4632	1.1675
H	-5.1495	2.3008	3.6216
C	-0.5732	1.4537	3.6549
H	-3.0053	1.8208	4.7351
H	-2.3127	2.0975	-1.0925
C	-4.1210	1.0022	-1.1531
C	-3.9475	3.4614	-1.1769
H	-4.1312	1.0069	-2.2432
H	-3.6789	0.0712	-0.8046
H	-5.1438	1.0725	-0.7827
H	-3.9188	3.4565	-2.2667
H	-4.9848	3.5172	-0.8470
H	-3.4128	4.3361	-0.8092
H	0.2422	1.4605	2.9419
C	-0.2280	2.4444	4.7719
C	-0.5908	0.0604	4.2862
H	0.7571	2.2105	5.1762
H	-0.2193	3.4600	4.3794
H	-0.9668	2.3789	5.5706
H	0.3422	-0.1097	4.8236
H	-1.4273	-0.0270	4.9795
H	-0.6844	-0.6916	3.5073
H	3.7806	2.7809	1.1142
C	2.8036	1.6553	2.6045
C	4.8060	0.9651	1.3423
C	1.6588	4.8751	1.2821
C	-0.6713	4.8189	1.9431
H	0.7524	3.3160	2.4180
H	4.0618	2.5360	-1.1101
H	4.3512	0.7941	-1.1779
H	3.0418	1.5298	-2.1314
H	-1.4088	4.1816	-0.3741
H	0.1814	4.6025	-1.0256
H	-0.6572	3.1663	-1.6153
H	2.3167	2.5952	2.8328
H	2.0819	0.8475	2.6176
H	3.5496	1.4913	3.3813
H	5.3509	1.2947	2.2270
H	4.6270	-0.1029	1.4214
H	5.4351	1.1626	0.4758
H	-0.4061	5.3680	2.8466
H	-0.8757	5.5397	1.1517
H	-1.5715	4.2460	2.1454
H	1.8184	5.4945	2.1649
H	2.5778	4.3345	1.0765
H	1.4261	5.5221	0.4368

Structure 14[termination_TS]

E_{total} = -5.672100 a.u.

Atom	X	Y	Z
Zr	-0.0057	-0.0012	-0.0052
N	2.0364	-0.0070	0.0028
C	2.5789	1.3864	-0.0029
C	1.4285	2.4346	-0.2724
C	0.2497	2.8642	0.6726
N	-0.5325	1.6554	1.0638
H	1.9293	3.3666	-0.5762
H	0.9579	2.1060	-1.2247
C	-0.8208	-1.6094	1.5381
C	-1.2228	-2.3143	0.3809
H	0.0528	-1.9252	2.1089
H	-1.5947	-1.0859	2.1060
H	-1.1633	-1.4793	-0.8093
H	-2.3087	-2.3861	0.2252
C	-0.4425	-3.5101	-0.1187
H	-0.7518	-3.8199	-1.1256
H	0.6437	-3.3356	-0.1210
H	-0.6350	-4.3535	0.5648
C	-0.7174	0.3970	-2.3356
C	-1.3418	-0.8434	-2.1677
H	0.1947	0.4652	-2.9280
H	-1.3180	1.3075	-2.2910
H	-0.9248	-1.7241	-2.6672
H	-2.4300	-0.8788	-2.0464
C	2.9649	-1.1182	-0.2561
C	3.4828	1.6505	-1.2256
C	3.4619	1.7711	1.2209

C	-0.6124	3.7571	-0.2443
C	0.7130	3.7729	1.8583
C	-1.6916	1.8556	1.9336
C	3.3546	-1.4667	-1.5789
C	4.2713	-2.5010	-1.8255
C	4.7625	-3.2837	-0.7855
C	3.4041	-1.9985	0.7750
C	4.3026	-3.0441	0.5057
C	2.6315	-0.9140	-2.7943
H	4.5855	-2.7234	-2.8342
H	5.4512	-4.0919	-0.9829
C	2.8998	-1.9191	2.2075
H	4.6388	-3.6921	1.3012
H	1.9881	-0.1041	-2.4689
C	3.5604	-0.3708	-3.8871
C	1.7395	-1.9709	-3.4488
H	2.9660	0.1144	-4.6615
H	4.2544	0.3541	-3.4642
H	4.1297	-1.1853	-4.3346
H	1.1354	-1.5113	-4.2312
H	2.3540	-2.7586	-3.8852
H	1.0871	-2.4097	-2.6949
H	2.2054	-1.0861	2.2898
C	2.1592	-3.1880	2.6436
C	4.0212	-1.7479	3.2419
H	3.5868	-1.5539	4.2230
H	4.6238	-2.6546	3.2941
H	4.6701	-0.9194	2.9655
H	1.6888	-3.0231	3.6133
H	1.3972	-3.4442	1.9117
H	2.8574	-4.0214	2.7225
C	-2.9929	1.9112	1.3823
C	-4.0751	2.2490	2.2105
C	-3.9203	2.2514	3.5989
C	-1.6328	1.4934	3.3047
C	-2.7021	1.8411	4.1459
C	-3.2618	1.6973	-0.0951
H	-5.0462	2.4602	1.7883
H	-4.7544	2.4914	4.2415
C	-0.4136	0.8457	3.9436
H	-2.6093	1.7495	5.2179
H	-2.3114	1.5389	-0.5921
C	-4.1193	0.4553	-0.3446
C	-3.9545	2.8799	-0.7804
H	-4.2503	0.3071	-1.4165
H	-3.6272	-0.4173	0.0838
H	-5.0969	0.5792	0.1217
H	-4.0141	2.6951	-1.8532
H	-4.9620	3.0046	-0.3836
H	-3.3893	3.7943	-0.6083
H	0.2602	0.5352	3.1511
C	0.3403	1.7679	4.9078
C	-0.7520	-0.4113	4.7529
H	1.2520	1.2759	5.2473
H	0.6014	2.6998	4.4140
H	-0.2866	1.9940	5.7704
H	0.1696	-0.9007	5.0690
H	-1.3348	-0.1429	5.6341
H	-1.3319	-1.1043	4.1464
H	3.5800	2.8512	1.1938
C	2.8502	1.4375	2.5757
C	4.8895	1.2046	1.1967
C	1.7027	4.8787	1.4525
C	-0.4008	4.5577	2.5743
H	1.2036	3.1590	2.6007
H	3.9420	2.6358	-1.1369
H	4.2743	0.9057	-1.2901
H	2.8888	1.6465	-2.1376
H	-1.4900	4.1149	0.2909
H	-0.0366	4.6127	-0.5952
H	-0.9402	3.1887	-1.1133
H	3.0727	2.2375	3.2819
H	1.7797	1.3233	2.4659
H	3.2657	0.5195	2.9674
H	5.3937	1.4548	2.1303
H	4.8709	0.1237	1.0802
H	5.4568	1.6440	0.3770
H	2.0366	5.4075	2.3455
H	2.5771	4.4654	0.9588
H	1.2215	5.5925	0.7844
H	0.0189	5.0572	3.4477
H	-0.8189	5.3153	1.9118
H	-1.1958	3.9029	2.9132

3.2 Increase bulky substitutes on aryl ring

3.2.1 Flouirne System

Structure 15

E = -4.532990 a.u.

Atom	X	Y	Z
Zr	-0.0330	-0.0253	0.1878
N	1.9547	-0.0861	-0.1040
C	2.6124	1.2521	-0.0724
C	1.7336	2.3979	-0.5959
C	0.5489	2.8856	0.2470
N	-0.5695	1.9078	0.3343
H	3.5157	1.2227	-0.6965
H	2.9571	1.4829	0.9521
H	2.4031	3.2666	-0.7094
H	1.3800	2.1540	-1.6163
H	0.1801	3.8097	-0.2220
H	0.8953	3.1629	1.2600
C	-1.4088	-1.7563	0.0452
C	-1.4092	-1.4865	-1.4430
H	-0.9514	-2.7250	0.3067
H	-2.4005	-1.6651	0.5121
H	-0.7015	-0.5997	-1.7294
H	-2.3734	-1.0799	-1.7836
C	-0.9381	-2.6283	-2.3406
H	-0.8621	-2.3176	-3.3913
H	0.0398	-3.0138	-2.0178
H	-1.6652	-3.4506	-2.2705
C	2.9066	-1.1886	-0.1062
C	-1.7630	2.5001	0.9156
C	3.7102	-1.4482	-1.2480
C	4.6713	-2.4704	-1.1955
C	4.8144	-3.2622	-0.0554
C	3.0137	-2.0309	1.0296
C	3.9811	-3.0504	1.0442
C	3.5257	-0.7466	-2.5974
H	5.3009	-2.6718	-2.0492
H	5.5547	-4.0482	-0.0311
C	2.1687	-1.8207	2.2868
H	4.1104	-3.6814	1.9096
F	2.3804	0.0213	-2.6463
C	4.7048	0.1557	-2.9771
C	3.3193	-1.7393	-3.7470
H	4.4961	0.6562	-3.9231
H	4.8658	0.9066	-2.2050
H	5.6094	-0.4437	-3.0817
H	3.1091	-1.1963	-4.6691
H	4.2137	-2.3452	-3.8900
H	2.4757	-2.3913	-3.5181
F	0.8748	-1.5103	1.9346
C	2.0109	-3.0709	3.1601
C	2.6961	-0.7024	3.1899
H	1.2914	-2.8732	3.9553
H	1.6474	-3.9001	2.5522
H	2.9662	-3.3393	3.6112
H	2.0460	-0.5910	4.0581
H	3.7049	-0.9463	3.5238
H	2.7193	0.2380	2.6429
C	-2.5929	3.3640	0.1571
C	-3.7231	3.9356	0.7655
C	-4.0525	3.6406	2.0909
C	-2.1057	2.1926	2.2535
C	-3.2521	2.7637	2.8265
C	-2.3784	3.6503	-1.3317
H	-4.3660	4.5994	0.2072
H	-4.9300	4.0801	2.5415
C	-1.2494	1.2878	3.1347
H	-3.5215	2.5383	3.8475
F	-1.4474	2.8059	-1.9029
C	-3.6395	3.4017	-2.1671
C	-1.9147	5.0852	-1.6017
H	-3.4119	3.5332	-3.2254
H	-3.9899	2.3822	-2.0028
H	-4.4253	4.1020	-1.8852
H	-1.7654	5.2053	-2.6751
H	-2.6976	5.7707	-1.2766
H	-0.9897	5.3499	-1.0907
F	0.0879	1.2579	2.7929
C	-0.8829	1.8850	4.4986
C	-1.7908	-0.1308	3.3089
H	-0.1720	1.2368	5.0131
H	-0.4384	2.8719	4.3630
H	-1.7781	1.9793	5.1132
H	-1.1033	-0.7187	3.9175
H	-2.7652	-0.0946	3.7964
H	-1.8969	-0.5991	2.3336

Structure 15 [π-complex]

E_{total} = -5.710835 a.u.

Atom	X	Y	Z
Zr	0.1288	0.0765	0.1277
N	2.1507	0.0436	-0.1573
C	2.8793	1.3307	-0.0105
C	2.0286	2.5668	-0.3183
C	0.9494	2.9667	0.6902
N	-0.1305	1.9676	0.8361
H	3.7507	1.3495	-0.6824
H	3.2821	1.4070	1.0152
H	2.7231	3.4205	-0.3823
H	1.5863	2.4711	-1.3296
H	0.5174	3.9264	0.3594
H	1.4228	3.1598	1.6696
C	-1.1991	-1.5957	0.7660
C	-2.4249	-0.7527	1.1320
H	-1.4043	-2.2411	-0.1111
H	-0.8810	-2.2664	1.5822
H	-2.3783	0.2609	0.6500
H	-2.4307	-0.5416	2.2132
C	-3.7700	-1.3624	0.7247
H	-4.6084	-0.7000	0.9840
H	-3.8092	-1.5558	-0.3584
H	-3.9144	-2.3246	1.2375
C	-1.2911	0.2491	-2.2021
C	-0.2104	-0.4865	-2.5312
H	-1.3710	1.2958	-2.4996
H	-2.1757	-0.2080	-1.7484
H	0.6137	-0.0550	-3.0994
H	-0.1740	-1.5664	-2.3479
C	3.0828	-1.0833	-0.1912
C	-1.1853	2.4471	1.7187
C	3.8774	-1.3228	-1.3468
C	4.7816	-2.3975	-1.3558
C	4.9137	-3.2384	-0.2516
C	3.2045	-1.9587	0.9204
C	4.1286	-3.0159	0.8789
C	3.7688	-0.5305	-2.6537
H	5.3843	-2.5945	-2.2298
H	5.6187	-4.0563	-0.2719
C	2.4663	-1.7379	2.2365
H	4.2621	-3.6652	1.7304
F	2.8050	0.4532	-2.6323
C	5.0739	0.1813	-3.0242
C	3.3630	-1.4171	-3.8359
H	4.9319	0.7590	-3.9380
H	5.3667	0.8541	-2.2183
H	5.8660	-0.5502	-3.1843
H	3.2349	-0.8053	-4.7293
H	4.1305	-2.1673	-4.0257
H	2.4215	-1.9179	-3.6088
F	1.2715	-1.1001	2.0151
C	2.0564	-3.0286	2.9543
C	3.2766	-0.8918	3.2224
H	1.4138	-2.7870	3.8016
H	1.5092	-3.6729	2.2656
H	2.9376	-3.5538	3.3223
H	2.7174	-0.7622	4.1491
H	4.2225	-1.3880	3.4407
H	3.4813	0.0859	2.7878
C	-2.2776	3.1672	1.1725
C	-3.3286	3.5830	2.0073
C	-3.3179	3.2876	3.3711
C	-1.1599	2.1717	3.1105
C	-2.2330	2.5957	3.9096
C	-2.3930	3.4962	-0.3147
H	-4.1723	4.1188	1.5988
H	-4.1344	3.6016	4.0045
C	0.0044	1.4911	3.8287
H	-2.2329	2.3840	4.9684
F	-1.3276	3.1920	-1.1357
C	-3.5833	2.7773	-0.9583
C	-2.5827	4.9984	-0.5513
H	-3.6295	3.0158	-2.0213
H	-3.4680	1.7004	-0.8389
H	-4.5120	3.0904	-0.4813
H	-2.6269	5.2006	-1.6220
H	-3.5080	5.3406	-0.0882
H	-1.7425	5.5432	-0.1201
F	1.0674	1.2466	2.9912
C	0.6020	2.3667	4.9344
C	-0.3795	0.1432	4.4461
H	1.4865	1.8826	5.3497
H	0.8871	3.3334	4.5183
H	-0.1273	2.5188	5.7298
H	0.4904	-0.3037	4.9276
H	-1.1651	0.2840	5.1885
H	-0.7390	-0.5281	3.6676

Structure 15[insertion_TS]

E_{total} = -5.707532 a.u.

Atom	X	Y	Z
Zr	-0.0001	-0.0001	-0.0006
N	2.0186	-0.0002	0.0018
C	2.6432	1.3473	0.0007
C	1.7401	2.4316	-0.6074
C	0.5509	2.9394	0.2192
N	-0.5067	1.9236	0.4373
H	3.5689	1.3135	-0.5963
H	2.9344	1.6437	1.0232
H	2.3806	3.3098	-0.7907
H	1.3933	2.1074	-1.6089
H	0.1144	3.7943	-0.3261
H	0.9289	3.3322	1.1786
C	-0.5742	-0.5078	-2.2070
C	-1.2258	-1.6365	-1.6578
H	0.3609	-0.6750	-2.7475
H	-1.1938	0.3090	-2.5863
H	-0.7728	-2.6189	-1.8037
H	-2.3168	-1.6511	-1.6197
C	-1.1115	-1.9818	0.4580
C	-1.8390	-1.2177	1.5656
H	-1.6735	-2.8866	0.2106
H	-0.1006	-2.3398	0.7830
H	-1.3599	-0.2395	1.8441
H	-2.8498	-0.9518	1.2111
C	-1.9291	-2.0133	2.8747
H	-2.4635	-2.9576	2.6990
H	-0.9319	-2.2530	3.2683
H	-2.4773	-1.4433	3.6375
C	2.9878	-1.0641	0.2093
C	-1.6697	2.4915	1.1004
C	3.7667	-1.5361	-0.8775
C	4.7436	-2.5210	-0.6590
C	4.9662	-3.0370	0.6188
C	3.1755	-1.6280	1.4968
C	4.1818	-2.5896	1.6827
C	3.5378	-1.1093	-2.3262
H	5.3302	-2.8967	-1.4841
H	5.7262	-3.7872	0.7794
C	2.3758	-1.1888	2.7214
H	4.3678	-3.0032	2.6619
F	2.8026	0.0436	-2.5073
C	4.7765	-0.5244	-3.0133
C	2.9178	-2.2094	-3.1911
H	4.5184	-0.1728	-4.0131
H	5.1632	0.3097	-2.4268
H	5.5485	-1.2893	-3.0969
H	2.7400	-1.8331	-4.1988
H	3.5919	-3.0647	-3.2407
H	1.9705	-2.5252	-2.7535
F	1.1366	-0.7286	2.3417
C	2.0532	-2.3285	3.6940
C	3.0659	-0.0809	3.5220
H	1.3767	-1.9670	4.4690
H	1.5723	-3.1449	3.1545
H	2.9650	-2.6925	4.1671
H	2.4350	0.2182	4.3594
H	4.0211	-0.4434	3.9025
H	3.2434	0.7831	2.8841
C	-2.8365	2.7813	0.3495
C	-3.9650	3.3114	0.9965
C	-3.9451	3.5782	2.3659
C	-1.6591	2.7449	2.4981
C	-2.7970	3.2977	3.1077
C	-2.9429	2.5143	-1.1508
H	-4.8687	3.5205	0.4451
H	-4.8171	3.9915	2.8510
C	-0.4775	2.4294	3.4178
H	-2.8018	3.5032	4.1676
F	-1.7035	2.5199	-1.7566
C	-3.6043	1.1664	-1.4423
C	-3.7168	3.5924	-1.9182
H	-3.5953	0.9712	-2.5149
H	-3.0606	0.3779	-0.9243
H	-4.6347	1.1776	-1.0860
H	-3.6542	3.3955	-2.9889
H	-4.7657	3.5906	-1.6229
H	-3.2829	4.5710	-1.7109
F	0.5157	1.7173	2.7862
C	0.1919	3.6908	3.9709
C	-0.8662	1.5409	4.6041
H	1.0543	3.4146	4.5783
H	0.5228	4.3228	3.1470
H	-0.5159	4.2478	4.5850
H	0.0242	1.2837	5.1785
H	-1.5685	2.0634	5.2532
H	-1.3291	0.6252	4.2372

Structure 15[termination_TS]

E_{total} = -5.69621 a.u.

Atom	X	Y	Z
Zr	0.00420	-0.00120	0.00650
N	2.03680	0.00050	0.00250
C	2.68840	1.33430	0.00090
C	1.76720	2.46580	-0.47040
C	0.61750	2.90060	0.44610
N	-0.46640	1.89450	0.57800
H	3.55030	1.30910	-0.68680
H	3.08020	1.58090	1.00330
H	2.40710	3.35320	-0.60200
H	1.37470	2.23280	-1.47890
H	0.19420	3.82580	0.01980
H	1.03330	3.15970	1.43520
C	-0.65610	-1.19880	1.97810
C	-1.21620	-2.11040	1.05380
H	0.26330	-1.47720	2.49730
H	-1.31650	-0.51150	2.51220
H	-1.16500	-1.63460	-0.30860
H	-2.31450	-2.11580	0.99210
C	-0.56930	-3.46250	0.83920
H	-0.90610	-3.95560	-0.08230
H	0.52900	-3.39660	0.83120
H	-0.85150	-4.10980	1.68570
C	-0.70400	-0.29720	-2.33670
C	-1.32710	-1.43000	-1.80530
H	0.21710	-0.40700	-2.90590
H	-1.30300	0.57730	-2.58330
H	-0.89520	-2.41700	-2.00510
H	-2.41740	-1.43390	-1.68920
C	3.01720	-1.08090	0.06250
C	-1.66970	2.47970	1.16250
C	3.46920	-1.70570	-1.13030
C	4.38170	-2.77100	-1.05980
C	4.90480	-3.18890	0.16270
C	3.56580	-1.50290	1.30430
C	4.50740	-2.54480	1.33350
C	3.01530	-1.29760	-2.52960
H	4.70150	-3.27650	-1.95860
H	5.61970	-3.99750	0.20120
C	3.22270	-0.86690	2.64910
H	4.93900	-2.86540	2.26960
F	2.38600	-0.07210	-2.54350
C	4.18260	-1.10520	-3.50310
C	2.06850	-2.32620	-3.15150
H	3.79590	-0.73230	-4.45200
H	4.86400	-0.35860	-3.09410
H	4.75040	-2.01320	-3.70550
H	1.60720	-2.04050	-4.09710
H	2.54430	-3.29940	-3.27370
H	1.29990	-2.40700	-2.38400
F	2.12100	-0.05150	2.56540
C	2.86330	-1.89420	3.72880
C	4.35740	0.00750	3.18970
H	2.50360	-1.38340	4.62250
H	2.06450	-2.54410	3.37130
H	3.73370	-2.49700	3.98690
H	4.04660	0.47410	4.12490
H	5.23860	-0.60700	3.37450
H	4.61650	0.78780	2.47430
C	-2.75020	2.86930	0.32750
C	-3.91340	3.41410	0.89550
C	-4.01230	3.61920	2.27060
C	-1.77340	2.70150	2.56370
C	-2.94130	3.27460	3.09380
C	-2.73050	2.73540	-1.19270
H	-4.74990	3.69190	0.27240
H	-4.90770	4.05030	2.69350
C	-0.67730	2.35330	3.56970
H	-3.02880	3.45530	4.15440
F	-1.44680	2.60880	-1.67810
C	-3.55660	1.53860	-1.66930
C	-3.25010	3.97980	-1.92180
H	-3.46370	1.42800	-2.75000
H	-3.20140	0.63410	-1.17720
H	-4.60540	1.68960	-1.41310
H	-3.11140	3.85860	-2.99660
H	-4.31080	4.12510	-1.71930
H	-2.69440	4.85660	-1.58820
F	0.28060	1.53420	3.02260
C	0.04820	3.59290	4.10140
C	-1.19280	1.56260	4.77790
H	0.85640	3.29060	4.76800
H	0.46330	4.16330	3.27100
H	-0.65210	4.22380	4.64940
H	-0.35180	1.25010	5.39770
H	-1.86170	2.17970	5.37730
H	-1.73060	0.67850	4.43570

3.2.2 Increase bulky on aryl-ring II

Strucutre 16

E_{total} = -3.876770 a.u.

Atom	X	Y	Z
Zr	0.0435	-0.0380	0.1239
N	2.0500	-0.0699	-0.0537
C	2.6562	1.2973	-0.0703
C	1.8479	2.3453	-0.8452
C	0.5717	2.8852	-0.1929
N	-0.5127	1.8789	-0.0979
H	3.6541	1.2375	-0.5218
H	2.8233	1.6595	0.9613
H	2.5150	3.2135	-0.9773
H	1.6213	1.9680	-1.8592
H	0.2248	3.7441	-0.7815
H	0.8144	3.2793	0.8112
C	-1.4094	-1.7097	0.0041
C	-1.1519	-1.6719	-1.4853
H	-1.1834	-2.6875	0.4532
H	-2.4264	-1.3919	0.2867
H	-0.3847	-0.8406	-1.7770
H	-2.0274	-1.3234	-2.0537
C	-0.5600	-2.9413	-2.0906
H	-0.2849	-2.7992	-3.1442
H	0.3315	-3.2733	-1.5384
H	-1.3104	-3.7432	-2.0308
C	3.0454	-1.1158	0.1200
C	-1.8446	2.4456	0.0353
C	3.9440	-1.4364	-0.9258
C	4.8561	-2.4922	-0.7545
C	4.8952	-3.2126	0.4435
C	3.0689	-1.8691	1.3132
C	4.0002	-2.9049	1.4712
C	3.8358	-0.7794	-2.2997
H	5.5270	-2.7955	-1.5435
H	5.5988	-4.0230	0.5642
C	2.1168	-1.5865	2.4614
H	4.0236	-3.4780	2.3865
C	2.5342	-0.9369	-3.0934
C	5.0673	-0.8388	-3.2132
C	4.6513	0.4842	-2.5860
H	5.9886	-1.2287	-2.7822
H	4.8685	-0.8878	-4.2839
H	2.6455	-0.5073	-4.0890
H	2.2921	-1.9957	-3.1848
H	1.7212	-0.4254	-2.5808
C	0.9026	-2.4957	2.6408
C	2.7881	-1.3103	3.8102
C	2.0566	-0.1900	3.0864
H	0.2125	-2.0672	3.3677
H	0.4003	-2.6091	1.6844
H	1.2305	-3.4762	2.9865
H	2.2603	-1.6885	4.6860
H	3.8737	-1.2140	3.7836
C	-2.5061	2.9979	-1.0860
C	-3.8394	3.4232	-0.9588
C	-4.5080	3.3221	0.2653
C	-2.5257	2.3374	1.2659
C	-3.8516	2.7816	1.3746
C	-1.8552	3.0265	-2.4651
H	-4.3774	3.8108	-1.8104
H	-5.5331	3.6512	0.3508
C	-1.8350	1.8102	2.5127
H	-4.3752	2.7069	2.3163
C	-1.4866	1.7027	-3.1422
C	-2.3592	4.0742	-3.4659
C	-0.9822	4.2280	-2.8353
H	-1.1662	1.8812	-4.1687
H	-0.6727	1.2242	-2.6004
H	-2.3548	1.0436	-3.1467
H	-2.3224	3.7891	-4.5174
H	-3.0717	4.8101	-3.0946
C	-1.8018	0.3048	2.7801
C	-2.0222	2.6340	3.7905
C	-0.6720	2.6233	3.0855
H	-2.5648	3.5724	3.6755
H	-2.0375	2.0673	4.7216
H	-1.4593	0.1100	3.7964
H	-2.8014	-0.1107	2.6518
H	-1.1171	-0.1730	2.0843
H	4.1905	1.1863	-3.2811
H	5.3107	0.8105	-1.7817
H	2.7330	0.5550	2.6726
H	1.1065	0.0795	3.5455
H	-0.9305	5.0174	-2.0853
H	-0.1520	4.0083	-3.5069
H	0.0938	2.0498	3.6061
H	-0.4480	3.5558	2.5682

Structure 16[π-complex]

E = -5.061287 a.u.

Atom	X	Y	Z
Zr	0.2099	0.0225	0.1247
N	2.1902	0.1750	-0.3723
C	2.8112	1.4891	-0.0352
C	1.8926	2.6971	-0.2158
C	0.8081	2.8969	0.8398
N	-0.2806	1.8863	0.8077
H	3.7049	1.6557	-0.6412
H	3.1723	1.4736	1.0099
H	2.5381	3.5901	-0.1672
H	1.4539	2.6955	-1.2309
H	0.3736	3.9009	0.7126
H	1.2982	2.9064	1.8267
C	-1.0840	-1.7303	0.6055
C	-2.3888	-0.9299	0.6514
H	-1.1303	-2.5808	-0.0920
H	-0.8130	-2.1442	1.5959
H	-2.2449	0.1077	0.2325
H	-2.6979	-0.7451	1.6928
C	-3.5508	-1.5494	-0.1265
H	-4.4459	-0.9122	-0.0893
H	-3.2898	-1.7071	-1.1836
H	-3.8062	-2.5289	0.3034
C	-0.8897	0.3780	-2.3607
C	-0.4366	-0.8905	-2.3969
H	-0.2360	1.2329	-2.5476
H	-1.9563	0.5853	-2.2676
H	0.6144	-1.1210	-2.6023
H	-1.1199	-1.7366	-2.3176
C	3.2082	-0.8058	-0.7538
C	-1.4303	2.3851	1.5551
C	4.0478	-0.6016	-1.8875
C	4.9435	-1.6141	-2.2763
C	5.0719	-2.7907	-1.5383
C	3.3345	-2.0143	-0.0290
C	4.2705	-2.9844	-0.4150
C	3.9010	0.5954	-2.8314
H	5.5289	-1.5207	-3.1773
H	5.7700	-3.5544	-1.8477
C	2.5396	-2.3114	1.2262
H	4.3701	-3.8976	0.1533
C	2.5627	0.8292	-3.5346
C	5.0680	0.8895	-3.7885
C	4.7877	1.8298	-2.6287
H	5.9946	0.3355	-3.6455
H	4.8039	1.3163	-4.7562
H	2.6465	1.6533	-4.2434
H	2.2685	-0.0750	-4.0672
H	1.8047	1.0789	-2.7976
C	1.5683	-3.4926	1.1964
C	3.4296	-2.4247	2.4703
C	2.4296	-1.2888	2.3619
H	0.9304	-3.4776	2.0802
H	0.9552	-3.4351	0.2981
H	2.1306	-4.4264	1.1779
H	3.1485	-3.2131	3.1689
H	4.4687	-2.1319	2.3181
C	-2.4713	3.0744	0.8849
C	-3.5572	3.5846	1.6125
C	-3.6329	3.4183	2.9961
C	-1.5152	2.2176	2.9597
C	-2.6212	2.7240	3.6612
C	-2.5566	3.1996	-0.6297
H	-4.3607	4.0921	1.0991
H	-4.4805	3.8019	3.5445
C	-0.4887	1.4266	3.7553
H	-2.7083	2.5731	4.7268
C	-3.6295	2.3763	-1.3475
C	-2.6458	4.6486	-1.1218
C	-1.4337	3.8060	-1.4807
H	-3.5007	2.4489	-2.4277
H	-3.5561	1.3338	-1.0438
H	-4.6171	2.7513	-1.0784
H	-3.3253	4.8241	-1.9562
H	-2.4425	5.4113	-0.3697
C	-0.5681	-0.0959	3.7172
C	-0.2000	1.9182	5.1721
C	0.8718	2.0474	4.0957
H	-0.6241	2.8818	5.4547
H	0.0331	1.1543	5.9140
H	0.1335	-0.5287	4.4303
H	-1.5797	-0.4153	3.9677
H	-0.3187	-0.4334	2.7152
H	4.3316	2.7784	-2.9129
H	5.5102	1.7564	-1.8154
H	2.8862	-0.3179	2.1800
H	1.5769	-1.4128	3.0245
H	-0.5387	4.1435	-0.9677
H	-1.4141	3.5015	-2.5271
H	1.6415	1.5128	3.5388
H	0.8940	3.0927	3.7891

Structure 16[insertion_TS]

E_{total} = -5.064150 a.u.

Atom	X	Y	Z
Zr	0.0000	-0.0013	-0.0005
N	2.0222	-0.0005	-0.0020
C	2.5425	1.4081	0.0008
C	1.9145	2.3052	-1.0712
C	0.5668	2.9177	-0.7036
N	-0.4997	1.9244	-0.4342
H	3.6296	1.3821	-0.1384
H	2.3978	1.8748	0.9927
H	2.6005	3.1517	-1.2422
H	1.8492	1.7582	-2.0281
H	0.2485	3.5802	-1.5255
H	0.7256	3.5562	0.1769
C	-0.4094	-1.4484	-1.7946
C	-1.1534	-2.1843	-0.8465
H	0.5752	-1.8336	-2.0741
H	-0.9379	-0.9030	-2.5787
H	-0.7026	-3.0862	-0.4280
H	-2.2395	-2.2292	-0.9346
C	-1.5024	-1.3604	1.1054
C	-2.8333	-0.6172	1.1665
H	-1.6059	-2.3840	1.4889
H	-0.7695	-0.8883	1.8467
H	-2.7382	0.4333	0.8315
H	-3.5356	-1.0977	0.4652
C	-3.4382	-0.6278	2.5753
H	-3.6299	-1.6599	2.9034
H	-2.7680	-0.1567	3.3084
H	-4.3925	-0.0827	2.5862
C	3.0832	-0.9763	0.2101
C	-1.7969	2.5694	-0.2902
C	4.1287	-1.1270	-0.7395
C	5.0995	-2.1257	-0.5487
C	5.0824	-2.9378	0.5870
C	3.0576	-1.8252	1.3400
C	4.0625	-2.7854	1.5268
C	4.1328	-0.3787	-2.0721
H	5.8563	-2.3103	-1.2954
H	5.8368	-3.6986	0.7225
C	1.9947	-1.7264	2.4170
H	4.0455	-3.4245	2.3975
C	2.9962	-0.6370	-3.0659
C	5.4775	-0.2680	-2.8061
C	4.8527	0.9698	-2.1833
H	6.3674	-0.5962	-2.2703
H	5.4324	-0.2720	-3.8953
H	3.1754	-0.0934	-3.9937
H	2.9376	-1.7041	-3.2800
H	2.0509	-0.3043	-2.6423
C	1.0031	-2.8832	2.5515
C	2.5563	-1.3652	3.7972
C	1.6559	-0.3816	3.0706
H	0.1953	-2.6102	3.2308
H	0.5930	-3.1234	1.5715
H	1.5185	-3.7607	2.9423
H	2.0858	-1.8797	4.6354
H	3.6128	-1.0958	3.8046
C	-2.7829	2.3916	-1.2875
C	-4.0488	2.9754	-1.1394
C	-4.3563	3.7203	-0.0001
C	-2.1099	3.3280	0.8666
C	-3.3954	3.8817	1.0006
C	-2.5522	1.5502	-2.5302
H	-4.8021	2.8356	-1.9008
H	-5.3397	4.1512	0.1171
C	-1.1381	3.4699	2.0376
H	-3.6748	4.4262	1.8890
C	-3.3112	0.2268	-2.6469
C	-2.6684	2.3283	-3.8445
C	-1.3216	1.7639	-3.4195
H	-2.9846	-0.3204	-3.5314
H	-3.1266	-0.3746	-1.7593
H	-4.3804	0.4251	-2.7221
H	-3.1338	1.7903	-4.6707
H	-2.7455	3.4108	-3.7406
C	-0.6792	2.2119	2.7779
C	-1.3905	4.6214	3.0132
C	-0.1803	4.6689	2.0898
H	-2.1317	5.3707	2.7380
H	-1.1140	4.4488	4.0534
H	0.0170	2.4781	3.5735
H	-1.5443	1.7116	3.2106
H	-0.1811	1.5369	2.0848
H	4.4264	1.6683	-2.9035
H	5.3665	1.3087	-1.2838
H	2.1820	0.4850	2.6740
H	0.6579	-0.3053	3.5012
H	-0.6219	2.5361	-3.1081
H	-1.0049	0.9018	-4.0063
H	0.8466	4.3121	2.0133
H	-0.3938	5.3390	1.2565

16[termination_TS]

E_{total} = -5.049927 a.u.

Atom	X	Y	Z
Zr	-0.0032	-0.0036	-0.0046
N	2.0432	-0.0086	-0.0102
C	2.5505	1.3824	-0.0043
C	1.5291	2.4020	-0.5415
C	0.4373	2.8645	0.4341
N	-0.4735	1.7872	0.8604
H	3.4483	1.4451	-0.6396
H	2.8332	1.7011	1.0111
H	2.0864	3.3119	-0.8138
H	1.0987	2.0428	-1.4981
H	-0.1377	3.6680	-0.0583
H	0.9570	3.3173	1.2861
C	-0.4572	-1.4752	1.8144
C	-1.1997	-2.1987	0.8560
H	0.5227	-1.8558	2.1135
H	-0.9762	-0.8499	2.5464
H	-1.3060	-1.4890	-0.4459
H	-2.2929	-2.1512	0.9551
C	-0.6783	-3.5198	0.3352
H	-1.1573	-3.8283	-0.6034
H	0.4126	-3.5063	0.1945
H	-0.8998	-4.2905	1.0916
C	-0.8456	0.1031	-2.2913
C	-1.6053	-0.9928	-1.8764
H	0.0119	-0.0574	-2.9397
H	-1.2813	1.1009	-2.3206
H	-1.3717	-1.9829	-2.2801
H	-2.6660	-0.8537	-1.6507
C	3.1084	-1.0037	-0.1329
C	-1.4800	2.2203	1.8346
C	3.2166	-1.7897	-1.3045
C	4.1607	-2.8235	-1.3945
C	5.0336	-3.0835	-0.3400
C	4.0449	-1.2363	0.9114
C	4.9745	-2.2847	0.8013
C	2.4148	-1.5011	-2.5549
H	4.2322	-3.4200	-2.2923
H	5.7530	-3.8851	-0.4193
C	4.0375	-0.4867	2.2351
H	5.6509	-2.5013	1.6145
C	1.2811	-2.4592	-2.9179
C	3.2988	-1.3107	-3.7959
C	2.5293	-0.1299	-3.2367
H	4.3723	-1.2565	-3.6130
H	2.8934	-1.6959	-4.7319
H	0.7106	-2.0697	-3.7611
H	1.6970	-3.4312	-3.1838
H	0.6291	-2.5814	-2.0556
C	3.1174	-0.9976	3.3440
C	5.4321	-0.2345	2.8312
C	4.6074	0.9349	2.3324
H	3.2266	-0.3847	4.2387
H	2.0858	-0.9596	3.0049
H	3.3757	-2.0294	3.5830
H	5.4985	-0.3012	3.9174
H	6.2789	-0.4754	2.1887
C	-2.8609	2.0913	1.5471
C	-3.8287	2.4249	2.5061
C	-3.4549	2.8852	3.7659
C	-1.1086	2.7203	3.1153
C	-2.1007	3.0252	4.0643
C	-3.3931	1.6786	0.1912
H	-4.8790	2.3293	2.2722
H	-4.2052	3.1259	4.5044
C	0.3397	2.8000	3.5862
H	-1.8367	3.3493	5.0586
C	-4.3068	2.7501	-0.4201
C	-4.0976	0.3267	0.0790
C	-2.9803	2.4273	-1.0805
H	-4.4168	0.1515	-0.9485
H	-3.4159	-0.4612	0.3912
H	-4.9715	0.3152	0.7304
H	-5.1711	2.3806	-0.9726
H	-4.3138	3.7152	0.0871
C	1.1456	1.5073	3.6789
C	0.6426	3.7164	4.7827
C	1.1257	4.1015	3.3942
H	-0.1478	4.3808	5.1290
H	1.4546	3.4032	5.4393
H	2.1283	1.7103	4.1033
H	0.6183	0.7963	4.3150
H	1.2655	1.0800	2.6854
H	1.7035	0.1732	-3.8783
H	3.1655	0.6001	-2.7377
H	4.9646	1.3593	1.3941
H	4.1889	1.5535	3.1258
H	2.1968	3.9728	3.2353
H	0.5627	4.9133	2.9330
H	-2.2290	3.2057	-0.9520
H	-3.1005	1.8836	-2.0167

3.3 Bridge systems

3.3.1 6-carbon bridge

Structure 17

E_{total} = -4.543415 a.u.

Atom	X	Y	Z
Zr	0.0046	0.0019	-0.0004
N	2.0303	-0.0052	0.0013
C	2.5559	1.3948	0.0050
C	1.6709	2.4056	-0.7455
C	0.3959	2.9356	-0.0768
N	-0.6537	1.9026	0.0578
H	3.5382	1.4351	-0.4789
H	2.7189	1.7428	1.0416
H	2.3021	3.2917	-0.9231
H	1.4323	2.0110	-1.7551
H	0.0290	3.7708	-0.6916
H	0.6483	3.3580	0.9123
C	-1.3890	-1.7193	-0.0233
C	-1.3689	-1.5808	-1.5300
H	-1.0095	-2.6928	0.3242
H	-2.3700	-1.5062	0.4296
H	-0.6280	-0.7466	-1.8825
H	-2.3146	-1.1754	-1.9210
C	-0.9287	-2.8136	-2.3157
H	-0.8307	-2.5973	-3.3881
H	0.0305	-3.2043	-1.9472
H	-1.6877	-3.5992	-2.1872
C	3.0091	-0.9899	0.4643
C	-1.9073	2.4003	0.6061
C	4.2982	-1.1078	-0.1162
C	5.2302	-2.0058	0.4306
C	4.8923	-2.8208	1.5138
C	2.6570	-1.8721	1.5125
C	3.5984	-2.7691	2.0363
C	4.6737	-0.4314	-1.4300
H	6.2109	-2.1062	-0.0103
H	5.6130	-3.5181	1.9148
C	1.2598	-1.9026	2.0997
H	3.3243	-3.4290	2.8464
H	3.8237	0.1423	-1.7917
C	5.8726	0.5149	-1.3055
C	4.9849	-1.4400	-2.5391
H	6.0338	1.0283	-2.2537
H	5.6822	1.2533	-0.5269
H	6.7677	-0.0512	-1.0475
H	5.1645	-0.9111	-3.4754
H	5.8691	-2.0229	-2.2812
H	4.1354	-2.1114	-2.6668
H	0.5721	-1.4446	1.4018
H	0.9605	-2.9459	2.2026
C	1.0741	-1.2248	3.4579
C	1.4657	0.2546	3.4158
H	0.0221	-1.3119	3.7299
H	1.6718	-1.7355	4.2133
C	-2.7371	3.2754	-0.1300
C	-3.9452	3.7208	0.4312
C	-4.3346	3.3052	1.7091
C	-2.3149	1.9687	1.8860
C	-3.5201	2.4299	2.4343
C	-2.4228	3.6653	-1.5672
H	-4.5945	4.3774	-0.1289
H	-5.2645	3.6557	2.1322
C	-1.4130	1.1035	2.7463
H	-3.8173	2.1218	3.4261
H	-1.5122	3.1591	-1.8812
C	-3.5162	3.2311	-2.5460
C	-2.2020	5.1699	-1.7421
H	-3.1565	3.4341	-3.5550
H	-3.5208	2.1534	-2.3801
H	-4.5339	3.6104	-2.4518
H	-1.9078	5.3956	-2.7673
H	-3.1216	5.7070	-1.5091
H	-1.4149	5.5036	-1.0659
H	-0.8669	0.4148	2.1065
C	-0.4244	1.9297	3.5800
H	-2.0300	0.5104	3.4217
C	0.5913	1.0852	4.3603
H	0.1219	2.6007	2.9181
H	-0.9887	2.5381	4.2872
H	2.5129	0.3512	3.7031
H	1.3463	0.6404	2.4062
H	1.2350	1.7621	4.9224
H	0.0731	0.4355	5.0661

Strucutre 17[π-complex]

E_{total} = -5.730067 a.u.

Atom	X	Y	Z
Zr	-0.0183	0.0228	0.0609
N	2.0074	0.0438	-0.0259
C	2.7331	1.3299	-0.0486
C	1.8657	2.5093	-0.4924
C	0.6965	2.9438	0.3974
N	-0.4293	1.9797	0.4624
H	3.5938	1.2784	-0.7332
H	3.1434	1.5351	0.9567
H	2.5376	3.3808	-0.5606
H	1.5075	2.3362	-1.5248
H	0.3449	3.9148	0.0177
H	1.0659	3.1312	1.4225
C	-1.2075	-1.6600	0.8800
C	-2.5963	-1.1006	0.5541
H	-0.9865	-2.5859	0.3145
H	-1.0748	-1.8928	1.9503
H	-2.5267	-0.1371	-0.0308
H	-3.1101	-0.7946	1.4790
C	-3.4940	-2.0381	-0.2559
H	-4.4580	-1.5680	-0.4988
H	-3.0144	-2.3385	-1.1998
H	-3.6927	-2.9537	0.3201
C	-0.9772	0.7451	-2.4378
C	-0.3209	-0.4331	-2.5126
H	-0.4854	1.6899	-2.6704
H	-2.0509	0.7910	-2.2405
H	0.7213	-0.4856	-2.8335
H	-0.8579	-1.3819	-2.3993
C	2.8921	-1.0898	0.2181
C	-1.5871	2.5458	1.1482
C	3.7703	-1.5508	-0.7880
C	4.5972	-2.6578	-0.5343
C	4.5574	-3.3104	0.7027
C	2.8426	-1.7662	1.4530
C	3.6793	-2.8643	1.6954
C	3.7761	-0.9454	-2.1848
H	5.2627	-3.0263	-1.3010
H	5.1991	-4.1589	0.8886
C	1.9763	-1.2506	2.5788
H	3.6580	-3.3611	2.6543
H	3.0517	-0.1346	-2.2203
C	5.1340	-0.3589	-2.5787
C	3.3540	-1.9482	-3.2616
H	5.0557	0.1233	-3.5534
H	5.4419	0.3795	-1.8384
H	5.8817	-1.1506	-2.6283
H	3.2915	-1.4453	-4.2269
H	4.0805	-2.7584	-3.3243
H	2.3766	-2.3607	-3.0102
H	1.1233	-0.7331	2.1485
H	1.5962	-2.0918	3.1587
C	2.7275	-0.2965	3.5131
C	1.8569	0.9047	3.8802
H	3.0398	-0.8264	4.4133
H	3.6144	0.0738	2.9981
C	-2.3427	3.5861	0.5589
C	-3.4594	4.1047	1.2365
C	-3.8437	3.5913	2.4792
C	-1.9963	2.0181	2.3903
C	-3.1152	2.5443	3.0505
C	-2.0542	4.0898	-0.8501
H	-4.0487	4.8929	0.7920
H	-4.7058	3.9943	2.9898
C	-1.1883	0.9455	3.0858
H	-3.4172	2.1562	4.0122
H	-1.1995	3.5586	-1.2627
C	-3.2549	3.7592	-1.7412
C	-1.7609	5.5902	-0.9266
H	-3.0249	4.0207	-2.7743
H	-3.4693	2.6920	-1.6830
H	-4.1312	4.3208	-1.4174
H	-1.5286	5.8648	-1.9557
H	-2.6286	6.1577	-0.5904
H	-0.9080	5.8289	-0.2913
H	-0.4108	0.6021	2.4109
C	-0.5378	1.4151	4.3905
H	-1.8358	0.0968	3.3058
C	0.6465	0.5112	4.7354
H	-0.1859	2.4418	4.2823
H	-1.2764	1.3742	5.1912
H	2.4560	1.6303	4.4310
H	1.5221	1.3766	2.9570
H	0.9051	0.6281	5.7880
H	0.3658	-0.5264	4.5540

Structure 17[insertion_TS]

E_{total} = -5.717031 a.u.

Atom	X	Y	Z
Zr	0.0497	-0.0212	-0.0040
N	2.0640	0.0106	-0.0782
C	2.7188	1.3353	-0.0405
C	1.7763	2.4710	-0.4567
C	0.6068	2.8480	0.4672
N	-0.5191	1.8687	0.4875
H	3.5737	1.3447	-0.7358
H	3.1245	1.5379	0.9670
H	2.4007	3.3757	-0.5409
H	1.3934	2.2804	-1.4784
H	0.2269	3.8181	0.1085
H	0.9868	3.0162	1.4917
C	-0.6050	-0.2562	-2.2354
C	-1.0516	-1.5336	-1.8394
H	0.3202	-0.1904	-2.8153
H	-1.3471	0.5264	-2.4189
H	-0.4461	-2.4024	-2.1039
H	-2.1247	-1.7286	-1.7906
C	-1.0082	-2.0462	0.2569
C	-2.1997	-1.5237	1.0458
H	-1.1633	-3.0830	-0.0621
H	-0.0763	-2.1116	0.8991
H	-2.1073	-0.4382	1.2869
H	-3.0924	-1.5820	0.4001
C	-2.4457	-2.2835	2.3533
H	-2.6332	-3.3464	2.1425
H	-1.5777	-2.2197	3.0254
H	-3.3207	-1.8777	2.8804
C	2.9846	-1.0989	0.0996
C	-1.6517	2.4206	1.2111
C	3.8164	-1.5196	-0.9596
C	4.6751	-2.6155	-0.7732
C	4.7101	-3.2927	0.4512
C	3.0101	-1.7959	1.3245
C	3.8785	-2.8825	1.4986
C	3.7426	-0.8710	-2.3344
H	5.3074	-2.9547	-1.5803
H	5.3755	-4.1327	0.5860
C	2.1899	-1.3228	2.5073
H	3.9165	-3.3994	2.4463
H	3.0162	-0.0614	-2.3027
C	5.0747	-0.2641	-2.7814
C	3.2614	-1.8406	-3.4164
H	4.9428	0.2459	-3.7358
H	5.4177	0.4545	-2.0370
H	5.8228	-1.0491	-2.8939
H	3.1565	-1.3109	-4.3635
H	3.9781	-2.6532	-3.5359
H	2.2939	-2.2530	-3.1291
H	1.2959	-0.8539	2.1017
H	1.8816	-2.1790	3.1076
C	2.9403	-0.3245	3.3958
C	2.0733	0.8974	3.6993
H	3.2488	-0.8078	4.3231
H	3.8304	0.0143	2.8650
C	-2.4756	3.3993	0.6143
C	-3.5676	3.9175	1.3300
C	-3.8445	3.4729	2.6276
C	-1.9438	1.9667	2.5135
C	-3.0347	2.4965	3.2169
C	-2.2723	3.8383	-0.8293
H	-4.2143	4.6544	0.8773
H	-4.6865	3.8771	3.1699
C	-1.0574	0.9501	3.2023
H	-3.2493	2.1575	4.2197
H	-1.3865	3.3460	-1.2259
C	-3.4350	3.4281	-1.7360
C	-2.0524	5.3464	-0.9738
H	-3.2108	3.7022	-2.7671
H	-3.5771	2.3488	-1.6765
H	-4.3499	3.9299	-1.4204
H	-1.8372	5.5869	-2.0151
H	-2.9452	5.8859	-0.6576
H	-1.2092	5.6531	-0.3549
H	-0.3681	0.5301	2.4738
C	-0.2531	1.5089	4.3784
H	-1.6802	0.1368	3.5729
C	0.9284	0.5809	4.6675
H	0.1181	2.5063	4.1396
H	-0.8989	1.5672	5.2548
H	2.6940	1.6803	4.1357
H	1.6693	1.2710	2.7600
H	1.2772	0.7343	5.6889
H	0.6053	-0.4543	4.5546

Structure 17[termination_TS]

E_{total} = -5.714343 a.u.

Atom	X	Y	Z
Zr	-0.0008	0.0007	-0.0028
N	2.0173	0.0016	-0.0004
C	2.7174	1.3030	0.0019
C	1.8000	2.4927	-0.3016
C	0.6954	2.8342	0.7048
N	-0.3992	1.8359	0.7452
H	3.5080	1.2927	-0.7677
H	3.2111	1.4690	0.9747
H	2.4520	3.3784	-0.3656
H	1.3588	2.3794	-1.3094
H	0.2775	3.8117	0.4101
H	1.1375	2.9560	1.7104
C	-0.7293	-1.6279	1.5928
C	-1.3775	-2.2248	0.4846
H	0.1754	-2.1016	1.9874
H	-1.3352	-1.0844	2.3223
H	-1.2646	-1.4381	-0.7479
H	-2.4702	-2.1069	0.4534
C	-0.8727	-3.5370	-0.0750
H	-1.2842	-3.7637	-1.0674
H	0.2260	-3.5704	-0.1256
H	-1.1925	-4.3392	0.6105
C	-0.5795	0.2895	-2.3395
C	-1.3335	-0.8729	-2.1300
H	0.3759	0.2225	-2.8633
H	-1.0809	1.2594	-2.3564
H	-0.9783	-1.8140	-2.5647
H	-2.4253	-0.7898	-2.0658
C	2.9270	-1.1213	0.1430
C	-1.4916	2.2769	1.5938
C	3.4804	-1.7308	-1.0001
C	4.3437	-2.8286	-0.8537
C	4.6614	-3.3168	0.4193
C	3.2414	-1.6221	1.4232
C	4.1102	-2.7144	1.5560
C	3.1328	-1.2412	-2.3966
H	4.7644	-3.3097	-1.7243
H	5.3262	-4.1615	0.5239
C	2.6558	-0.9937	2.6715
H	4.3543	-3.0964	2.5364
H	2.5136	-0.3505	-2.3105
C	4.3639	-0.8454	-3.2141
C	2.3309	-2.2700	-3.1955
H	4.0418	-0.4269	-4.1678
H	4.9211	-0.0822	-2.6703
H	5.0263	-1.6888	-3.4098
H	1.9991	-1.8334	-4.1378
H	2.7995	-3.2336	-3.3963
H	1.4668	-2.4210	-2.5481
H	1.7064	-0.5379	2.4055
H	2.4514	-1.7736	3.4053
C	3.5471	0.0715	3.3153
C	2.7081	1.2912	3.7050
H	4.0542	-0.3375	4.1895
H	4.2964	0.3872	2.5894
C	-2.5354	3.0532	1.0526
C	-3.5943	3.4635	1.8789
C	-3.6136	3.1135	3.2345
C	-1.5142	1.9253	2.9582
C	-2.5751	2.3452	3.7731
C	-2.5606	3.4111	-0.4258
H	-4.4082	4.0459	1.4733
H	-4.4319	3.4324	3.8631
C	-0.3965	1.1022	3.5658
H	-2.5952	2.0764	4.8191
H	-1.6093	3.1235	-0.8695
C	-3.6516	2.6592	-1.1907
C	-2.7258	4.9112	-0.6810
H	-3.5871	2.8978	-2.2525
H	-3.5137	1.5860	-1.0567
H	-4.6339	2.9456	-0.8145
H	-2.6522	5.1105	-1.7503
H	-3.6973	5.2485	-0.3197
H	-1.9378	5.4565	-0.1612
H	0.2618	0.7729	2.7675
C	0.4460	1.8305	4.6154
H	-0.8271	0.2142	4.0285
C	1.7361	1.0435	4.8636
H	0.6933	2.8333	4.2656
H	-0.1233	1.9033	5.5422
H	3.3554	2.1358	3.9416
H	3.1513	2.2810	3.8152
H	2.1981	1.3752	5.7937
H	1.4984	-0.0174	4.9442

3.3.2 8-Carbon Bridge system

Structure 18

E_{total} = -4.542246 a.u.

Atom	X	Y	Z
Zr	0.1284	-0.0386	0.0822
N	2.1473	-0.0926	-0.0703
C	2.7241	1.2841	-0.0033
C	1.8210	2.3761	-0.5984
C	0.6159	2.8763	0.2068
N	-0.4637	1.8693	0.3256
H	3.6675	1.3281	-0.5599
H	2.9797	1.5425	1.0411
H	2.4677	3.2563	-0.7488
H	1.4969	2.0759	-1.6165
H	0.2375	3.7753	-0.3013
H	0.9492	3.1975	1.2100
C	-1.3081	-1.7184	0.0366
C	-1.4003	-1.4611	-1.4523
H	-0.9363	-2.7265	0.2743
H	-2.2445	-1.5175	0.5807
H	-0.6620	-0.6206	-1.7966
H	-2.3592	-1.0003	-1.7348
C	-1.0600	-2.6348	-2.3669
H	-1.0362	-2.3317	-3.4225
H	-0.0879	-3.0780	-2.1078
H	-1.8303	-3.4102	-2.2457
C	3.1253	-1.1267	0.2584
C	-1.6696	2.3932	0.9501
C	4.3516	-1.2591	-0.4396
C	5.2940	-2.2129	-0.0175
C	5.0342	-3.0517	1.0705
C	2.8467	-2.0362	1.3017
C	3.7994	-2.9755	1.7199
C	4.6282	-0.5339	-1.7514
H	6.2253	-2.3278	-0.5520
H	5.7684	-3.7824	1.3772
C	1.5234	-2.0753	2.0467
H	3.9418	-3.7664	2.4417
H	3.7785	0.1001	-1.9942
C	5.8808	0.3472	-1.7065
C	4.7716	-1.4983	-2.9319
H	5.9744	0.8982	-2.6426
H	5.8053	1.0548	-0.8811
H	6.7665	-0.2723	-1.5650
H	4.8867	-0.9320	-3.8563
H	5.6433	-2.1377	-2.7916
H	3.8778	-2.1187	-3.0032
H	0.7894	-1.5399	1.4558
C	0.9832	-3.4980	2.2169
C	1.5425	-1.4306	3.4358
C	1.7865	0.0792	3.3482
H	0.5632	-1.5964	3.8809
H	2.2855	-1.8715	4.1010
C	-2.4742	3.3473	0.2867
C	-3.6202	3.8511	0.9220
C	-3.9701	3.4181	2.2043
C	-2.0451	1.9295	2.2297
C	-3.1855	2.4610	2.8545
C	-2.2042	3.7662	-1.1523
H	-4.2501	4.5702	0.4195
H	-4.8492	3.8167	2.6886
C	-1.1639	0.9520	2.9966
H	-3.4654	2.1497	3.8493
H	-1.3193	3.2454	-1.5119
C	-3.3403	3.3761	-2.1012
C	-1.9468	5.2681	-1.3025
H	-3.0656	3.6288	-3.1255
H	-3.5161	2.3022	-2.0336
H	-4.2528	3.9082	-1.8321
H	-1.6843	5.4932	-2.3364
H	-2.8408	5.8284	-1.0284
H	-1.1244	5.5657	-0.6521
H	-0.6429	0.3406	2.2640
C	-0.1142	1.6965	3.8423
C	-1.9609	-0.0151	3.8802
C	1.0044	0.8256	4.4351
H	0.3530	2.4557	3.2160
H	-0.6231	2.2111	4.6578
H	2.8531	0.2744	3.4615
H	1.4704	0.4499	2.3762
H	1.6949	1.4787	4.9691
H	0.5866	0.1193	5.1523
H	-0.0266	-3.4646	2.6267
H	0.9270	-3.9901	1.2457
H	1.6271	-4.0716	2.8838
H	-1.3033	-0.7802	4.2880
H	-2.4257	0.5244	4.7051
H	-2.7328	-0.4995	3.2819

Structure 18'

E_{total} = -4.541533a.u.

Atom	X	Y	Z
Zr	-0.0618	0.0421	0.1641
N	1.8741	0.0122	-0.3593
C	2.6578	1.2241	0.0053
C	1.8599	2.5196	-0.1169
C	0.7334	2.7637	0.8865
N	-0.4992	1.9526	0.6357
H	3.5360	1.3108	-0.6484
H	3.0501	1.1301	1.0355
H	2.5837	3.3388	0.0252
H	1.4673	2.6203	-1.1454
H	0.4815	3.8307	0.8322
H	1.1053	2.5948	1.9153
C	-1.3056	-0.8073	-1.4523
C	-1.6168	-1.9509	-0.5010
H	-0.7747	-1.1274	-2.3588
H	-2.1972	-0.2170	-1.7135
H	-1.2611	-1.7357	0.5799
H	-1.0268	-2.8500	-0.7402
C	-3.0893	-2.3126	-0.3133
H	-3.2261	-3.0608	0.4795
H	-3.6928	-1.4266	-0.0709
H	-3.4676	-2.7287	-1.2574
C	2.6943	-1.1710	-0.5810
C	-1.6626	2.5042	1.3205
C	3.6242	-1.2417	-1.6441
C	4.4086	-2.3965	-1.8039
C	4.2779	-3.4793	-0.9277
C	2.5415	-2.2825	0.2750
C	3.3404	-3.4226	0.1085
C	3.7146	-0.1595	-2.7120
H	5.1108	-2.4670	-2.6214
H	4.8894	-4.3595	-1.0632
C	1.5956	-2.2606	1.4669
H	3.5484	-4.3978	0.5236
H	3.0079	0.6325	-2.4741
C	5.1048	0.4750	-2.8106
C	3.3228	-0.6720	-4.1002
H	5.0844	1.2910	-3.5333
H	5.3992	0.8670	-1.8372
H	5.8326	-0.2705	-3.1312
H	3.3302	0.1539	-4.8117
H	4.0263	-1.4367	-4.4299
H	2.3203	-1.0986	-4.0591
H	0.7151	-1.7019	1.1681
C	1.0959	-3.6484	1.8808
C	2.2012	-1.5578	2.6929
C	1.3684	-0.3559	3.1511
H	2.3500	-2.2572	3.5161
H	3.1706	-1.2021	2.3434
C	-2.1742	3.7827	0.9924
C	-3.2674	4.2986	1.7074
C	-3.8575	3.5627	2.7388
C	-2.2941	1.7457	2.3320
C	-3.3748	2.2876	3.0454
C	-1.6649	4.5791	-0.2027
H	-3.6741	5.2668	1.4557
H	-4.6951	3.9708	3.2851
C	-1.7782	0.3691	2.7198
H	-3.8408	1.7286	3.8428
H	-0.8567	4.0277	-0.6784
C	-2.7364	4.7724	-1.2787
C	-1.1227	5.9599	0.1798
H	-2.3033	5.2811	-2.1402
H	-3.1153	3.7994	-1.5921
H	-3.5592	5.3696	-0.8853
H	-0.7002	6.4443	-0.7007
H	-1.9268	6.5784	0.5787
H	-0.3455	5.8540	0.9364
H	-1.1735	0.0056	1.8985
C	-0.8895	0.3868	3.9720
C	-2.8957	-0.6612	2.9173
C	0.1224	-0.7655	3.9437
H	-0.3472	1.3315	4.0245
H	-1.5185	0.2993	4.8582
H	1.9853	0.2827	3.7836
H	1.0734	0.2192	2.2768
H	0.4225	-1.0106	4.9626
H	-0.3401	-1.6424	3.4939
H	0.3304	-3.5585	2.6511
H	0.6261	-4.1418	1.0296
H	1.9210	-4.2554	2.2538
H	-2.4685	-1.6582	3.0225
H	-3.4723	-0.4246	3.8114
H	-3.5572	-0.6480	2.0520

Structure **18**[π-complex]

E_{total} = -5.727594 a.u.

Atom	X	Y	Z
Zr	-0.0258	-0.0139	0.0963
N	2.0069	0.0596	-0.1625
C	2.6202	1.4172	-0.1497
C	1.6687	2.5685	-0.4796
C	0.5923	2.9261	0.5434
N	-0.4290	1.5740	0.7061
H	3.4547	1.4828	-0.8598
H	3.0641	1.5936	0.8473
H	2.3025	3.4638	-0.5928
H	1.2070	2.4128	-1.4737
H	0.1202	3.6653	0.2143
H	1.0712	3.1396	1.5154
C	-1.3070	-1.6639	0.8596
C	-2.6415	-0.9261	0.7051
H	-1.2591	-2.5879	0.2557
H	-1.1082	-1.9477	1.9074
H	-2.5097	0.0693	0.1894
H	-3.0425	-0.6462	1.6921
C	-3.7023	-1.6922	-0.0856
H	-4.6140	-1.0948	-0.2280
H	-3.3304	-1.9929	-1.0774
H	-3.9733	-2.6122	0.4530
C	-1.0819	0.2314	-2.3198
C	0.1480	-0.2375	-2.6254
H	-1.3210	1.2952	-2.3796
H	-1.9170	-0.4553	-2.1488
H	0.9572	0.4247	-2.9326
H	0.3525	-1.3119	-2.6841
C	3.0438	-0.9632	-0.0131
C	-1.5308	2.3106	1.5508
C	4.1116	-1.0650	-0.9404
C	5.1546	-1.9749	-0.7065
C	5.1554	-2.7926	0.4248
C	3.0052	-1.8617	1.0775
C	4.0734	-2.7444	1.3060
C	4.0957	-0.5502	-2.2870
H	5.9710	-2.0829	-1.4051
H	5.9649	-3.4871	0.5946
C	1.8425	-1.8888	2.0518
H	4.0716	-3.4073	2.1583
H	3.2226	0.2954	-2.3396
C	5.3347	0.5173	-2.5316
C	3.9620	-1.5255	-3.4591
H	5.2207	1.3614	-3.4694
H	5.4522	1.2311	-1.7165
H	6.2243	-0.1102	-2.5876
H	3.8786	-0.7583	-4.3924
H	4.8344	-1.5775	-3.5055
H	3.0661	-1.5321	-3.3248
H	1.0414	-1.2832	1.6424
C	1.2798	-3.5009	2.2444
C	2.1643	-1.3360	3.4428
C	2.3985	0.1778	3.4174
H	1.3215	-1.5547	4.0947
H	3.0446	-1.3338	3.8501
C	-2.4902	3.2155	1.0455
C	-3.5498	3.6369	1.8637
C	-3.6598	3.1706	3.1768
C	-1.6617	1.5151	2.8661
C	-2.7189	2.2644	3.6749
C	-2.4644	3.6787	-0.4046
H	-4.2957	4.3184	1.4824
H	-4.4735	3.5049	3.8034
C	-0.6214	0.3781	3.4619
H	-2.8153	1.9252	4.6950
H	-1.5889	3.2582	-0.8945
C	-3.6775	3.1381	-1.1982
C	-2.3730	5.2003	-0.5469
H	-3.5762	5.4833	-2.2428
H	-3.7339	2.1008	-1.1383
H	-4.5912	3.6193	-0.7889
H	-2.2806	5.4649	-1.6004
H	-3.2676	5.6682	-0.1359
H	-1.4979	5.5651	-0.0091
H	-0.1630	0.3358	2.6384
C	0.4788	1.6651	4.1954
C	-1.2325	-0.1689	4.4019
C	1.7179	0.3577	4.6116
H	0.8123	2.4720	3.5443
H	0.0471	2.1208	5.0869
H	3.4713	0.5679	3.4515
H	2.0023	0.6032	2.4977
H	2.4301	1.5481	5.0637
H	1.4468	0.1170	5.3638
H	0.3968	-1.2626	2.8823
H	1.0039	-1.7179	1.2758
H	2.0254	-1.6422	2.7140
H	-0.4858	-0.9089	4.6808
H	-1.6054	0.5799	5.3069
H	-2.0547	-0.8756	3.8969

Structure **18**[insertion_TS]

E_{total} = -5.722305 a.u.

Atom	X	Y	Z
Zr	0.0157	-0.0094	-0.0017
N	2.0396	-0.0134	-0.0011
C	2.6369	1.3483	0.0032
C	1.6812	2.4424	-0.4935
C	0.5246	2.8815	0.4154
N	-0.5320	1.8567	0.5688
H	3.5164	1.3734	-0.6572
H	2.9997	1.6082	1.0138
H	2.2983	3.3413	-0.6548
H	1.2933	2.1758	-1.4970
H	0.0891	3.7890	-0.0348
H	0.9302	3.1737	1.4001
C	-0.5719	-0.1067	-2.2706
C	-1.1631	-1.3390	-1.9406
H	0.3840	-0.1199	-2.8033
H	-1.2201	0.7545	-2.4564
H	-0.6386	-2.2595	-2.2026
H	-2.2516	-1.4232	-1.9292
C	-1.2609	-1.9083	0.1579
C	-2.4383	-1.3144	0.9207
H	-1.4872	-2.9138	-0.2145
H	-0.3792	-2.0828	0.8457
H	-2.1973	-0.3173	1.3537
H	-3.2659	-1.1373	0.2129
C	-2.9195	-2.2171	2.0632
H	-3.2410	-3.1901	1.6640
H	-2.1229	-2.3970	2.7988
H	-3.7734	-1.7615	2.5839
C	3.0211	-1.0280	0.3527
C	-1.6978	2.3805	1.2556
C	4.1115	-1.3027	-0.5063
C	5.0771	-2.2493	-0.1286
C	4.9691	-2.9292	1.0871
C	2.8892	-1.7547	1.5579
C	3.8739	-2.6879	1.9205
C	4.2026	-0.7113	-1.9075
H	5.9010	-2.4800	-0.7874
H	5.7158	-3.6563	1.3700
C	1.7295	-1.5287	2.5176
H	3.7969	-3.2284	2.8521
H	3.3650	-0.0349	-2.0634
C	5.4895	0.0840	-2.1457
C	4.0903	-1.7780	-2.9997
H	5.4582	0.5434	-3.1339
H	5.5833	0.8651	-1.3914
H	6.3534	-0.5779	-2.0849
H	4.0849	-1.3007	-3.9798
H	4.9333	-2.4664	-2.9395
H	3.1615	-2.3338	-2.8687
H	0.9718	-0.9294	2.0191
C	1.0464	-2.8344	2.9370
C	2.1310	-0.8060	3.8107
C	2.1617	0.7169	3.6398
H	1.4178	-1.0637	4.5928
H	3.1160	-1.1500	4.1270
C	-2.6304	3.1750	0.5567
C	-3.7528	3.6826	1.2298
C	-3.9521	3.4029	2.5858
C	-1.9077	2.0853	2.6189
C	-3.0308	2.6104	3.2785
C	-2.4951	3.4224	-0.9389
H	-4.4811	4.2801	0.7018
H	-4.8171	3.7984	3.0976
C	-0.8957	1.2642	3.4031
H	-3.1931	2.4152	4.3277
H	-1.5628	2.9810	-1.2853
C	-3.6143	2.7611	-1.7461
C	-2.4444	4.9092	-1.2991
H	-3.4339	2.9068	-2.8114
H	-3.6336	1.6925	-1.5301
H	-4.5759	3.2000	-1.4796
H	-2.2705	5.0210	-2.3695
H	-3.3867	5.3900	-1.0360
H	-1.6314	5.3883	-0.7535
H	-0.3585	0.6455	2.6881
C	0.1205	2.1636	4.1260
C	-1.5442	0.3083	4.4108
C	1.3231	1.4173	4.7177
H	0.4936	2.9078	3.4241
H	-0.3905	2.6944	4.9297
H	3.1935	1.0602	3.7156
H	1.7832	0.9859	2.6560
H	1.9576	2.1418	5.2285
H	0.9775	0.6980	5.4591
H	0.1295	-2.6085	3.4815
H	0.8027	-3.4232	2.0530
H	1.7088	-3.4138	3.5802
H	-0.8055	-0.4014	4.7806
H	-1.9535	0.8693	5.2508
H	-2.3471	-0.2430	3.9240

Structure **18**[termination_TS]

E = 5.708648 a.u.

Atom	X	Y	Z
Zr	-0.0010	-0.0022	-0.0059
N	2.0165	-0.0008	-0.0013
C	2.7085	1.3055	0.0024
C	1.7698	2.5001	-0.2094
C	0.6919	2.7935	0.8415
N	-0.3607	1.7550	0.9263
H	3.4509	1.3304	-0.8133
H	3.2651	1.4380	0.9455
H	2.4120	3.3940	-0.2564
H	1.2979	2.4290	-1.2068
H	0.2308	3.7565	0.5646
H	1.1633	2.9368	1.8292
C	-0.7648	-1.7520	1.4166
C	-1.4171	-2.2423	0.2594
H	0.1247	-2.2766	1.7775
H	-1.3638	-1.2518	2.1803
H	-1.2671	-1.3606	-0.9023
H	-2.5059	-2.0913	0.2280
C	-0.9433	-3.5176	-0.4016
H	-1.3388	-3.6433	-1.4182
H	0.1544	-3.5844	-0.4322
H	-1.3063	-4.3642	0.2045
C	-0.5493	0.4877	-2.3235
C	-1.3035	-0.6898	-2.2280
H	0.4176	0.4653	-2.8295
H	-1.0549	1.4538	-2.2789
H	-0.9335	-1.5907	-2.7308
H	-2.3972	-0.6142	-2.1881
C	2.9458	-1.1146	0.0624
C	-1.4781	2.1962	1.7425
C	3.5219	-1.6081	-1.1260
C	4.4352	-2.6721	-1.0682
C	4.7848	-3.2372	0.1623
C	3.2788	-1.7020	1.3029
C	4.2097	-2.7531	1.3422
C	3.1422	-1.0332	-2.4821
H	4.8753	-3.0634	-1.9735
H	5.4937	-4.0511	0.2011
C	2.6617	-1.2043	2.6036
H	4.4931	-3.2019	2.2822
H	2.4924	-0.1750	-2.3267
C	4.3469	-0.5309	-3.2812
C	2.3604	-2.0279	-3.3425
H	4.0042	-0.0605	-4.2031
H	4.8950	0.2021	-2.6889
H	5.0071	-1.3628	-3.5264
H	2.0462	-1.5453	-4.2681
H	2.9866	-2.8887	-3.5781
H	1.4783	-2.3634	-2.7968
H	1.7126	-0.7386	2.3476
C	2.3395	-2.3329	3.5905
C	3.5291	-0.1489	3.3094
C	2.7350	1.1289	3.6036
H	3.9507	-0.5487	4.2320
H	4.3521	0.1143	2.6446
C	-2.4934	2.9871	1.1659
C	-3.5534	3.4489	1.9618
C	-3.6023	3.1388	3.3249
C	-1.5379	1.8681	3.1145
C	-2.5977	2.3519	3.8984
C	-2.4827	3.3226	-0.3181
H	-4.3417	4.0461	1.5281
H	-4.4181	3.5013	3.9326
C	-0.4718	1.0012	3.7669
H	-2.6493	2.1204	4.9517
H	-1.5382	2.9904	-0.7430
C	-3.5919	2.6039	-1.0890
C	-2.5828	4.8238	-0.5988
H	-3.5007	2.8225	-2.1532
H	-3.5007	1.5283	-0.9361
H	-4.5674	2.9366	-0.7338
H	-2.4828	5.0030	-1.6695
H	-3.5458	5.2056	-0.2599
H	-1.7825	5.3454	-0.0735
H	0.0811	0.5109	2.9691
C	0.5274	1.8056	4.6145
C	-1.0711	-0.1056	4.6449
C	1.8366	1.0371	4.8417
H	0.7544	2.7481	4.1157
H	0.0717	2.0321	5.5787
H	3.4325	1.9540	3.7488
H	2.1247	1.3562	2.7344
H	2.3682	1.4740	5.6872
H	1.6160	-0.0009	5.0774
H	1.7515	-1.9463	4.4209
H	1.7655	-3.1085	3.0839
H	3.2606	-2.7657	3.9806
H	-0.3026	-0.8284	4.9148
H	-1.4915	0.3241	5.5540
H	-1.8623	-0.6193	4.1002