

Absolute energy values G

	G absolute values				
		Zr/Et	Hf/Et	Zr/Pro	Hf/Pro
Precursor		-1354.1054	-1356.4407	-1354.1054	-1356.4407
Cation	1	-473.2094	-475.5415	-473.2094	-475.5415
1st	2a	-551.7762	-554.1064	-591.0729	-593.4038
	2b			-591.0720	-593.4022
1st TS	3a	-551.7593	-554.0901	-591.0480	-593.3788
	3b			-591.0402	-593.3700
1st bprod	4a	-551.7912	-554.1193	-591.0759	-593.4042
	4b			-591.0729	-593.4007
2nd pi complex	5a	-630.3422	-632.6715	-708.9178	-711.2479
	5e			-708.9201	-711.2504
	5f	-630.3407	-632.6941	-708.9192	-711.2437
	5g			-708.9167	-711.2387
2nd TS	6a	-630.3333	-632.6623	-708.9022	-711.2326
	6b			-708.898021	-711.2281
	6c			-708.9022	-711.2326
	6d			-708.8980	-711.2882
	6e			-708.8992	-711.2275
	6f			-708.8954	-711.2251
	6g			-708.8932	-711.2213
TS elimination	8a	-551.7765	-554.1050	-591.0658	-593.3946
	8b			-591.0639	-593.3878
TS transfer	7a	-630.3211	-632.6464	-708.8934	-711.2181
	7b			-708.8902	-711.2140
Hydrogenolysis pi complex	9a	-552.9554	-555.2821	-592.2407	-594.5681
	9b			-592.2382	-594.5648
TS hydrogenolysis	10a	-552.9507	-555.2790	-592.2360	-594.5643
	10b			-592.2356	-594.5634
2nd bprod	11a	-630.3668	-632.6941	-708.9347	-711.2623
	11b			-708.9347	-711.2632
Elimination product	12a	-551.7821	-554.1121	-591.07795	-593.4087
	12b			-591.0738	-593.4011
Transfer product	13a	-630.3525	-632.6809	-708.9277	-711.2520

	13b			-708.9212	-711.2465
		Zr/But	Hf/But	Zr/Hex	Hf/Hex
Precursor		-1354.1054	-1356.4407	-1354.1054	-1356.4407
Cation	1	-473.2094	-475.5415	-473.2094	-475.5415
1st	2a	-630.3596	-632.6913	-708.9348	-711.2660
	2b	-630.3594	-632.6900	-708.9341	-711.2641
1st TS	3a	-630.3352	-632.6662	-708.9101	-711.2410
	3b	-630.3278	-632.6574	-708.8987	-711.2293
1st bprod	4a	-630.3620	-632.6903	-708.9358	-711.2641
	4b	-630.3604	-632.6883	-708.9341	-711.2613
2nd pi complex	5a	-787.4918	-789.8231	-944.6394	-946.9684
	5e	-787.4932	-789.8231	-944.6412	-946.9709
	5f	-787.4903	-789.8156	-944.6390	-946.9631
	5g	-787.4889	-789.811786	-944.6366	-946.9622
2nd TS	6a	-787.4741	-789.8045	-944.6228	-946.9526
	6b	-787.4694	-789.7999	not located	-946.9451
	6c	-787.4737	-789.8035	-944.6228	-946.9527
	6d	-787.4698	-789.8000	-944.6181	-946.9484
	6e	-787.4707	-789.8000	-944.6189	-946.9480
	6f	-787.4624	-789.7890	-944.6105	-946.9395
	6g	-787.4609	-789.7891	-944.6099	-946.9378
TS elimination	8a	-630.3515	-632.6811	-708.9247	-711.2540
	8b	-630.3523	-632.6759	-708.9278	-711.2483
TS transfer	7a	-787.4644	-789.7914	-944.6130	-946.9399
	7b	-787.4636	-789.7881	-944.6101	-946.9349
Hydrogenolysis pi complex	9a	-631.5247	-633.8516	-710.0994	-712.4259
	9b	-631.5256	-633.8517	-710.1003	-712.4266
TS hydrogenolysis	10a	-631.5202	-633.8483	-710.0948	-712.4230
	10b	-631.5223	-633.8500	-710.0983	-712.4246
2nd bprod	11a	-787.5036	-789.8318	-944.6517	-946.9791
	11b	-787.5033	-789.8309	-944.6552	-946.9818
Elimination product	12a	-630.3623	-632.6922	-708.9359	-711.2679
	12b	-630.3607	-632.6889	-708.9364	-711.2643
Transfer product	13a	-787.4993	-789.8239	-944.6456	-946.9692
	13b	-787.4949	-789.8192	-944.6428	-946.9674

Absolute energy values E

		Zr/Et	Hf/Et	Zr/Pro	Hf/Pro
Precursor		-1354.2359	-1356.5698	-1354.2359	-1356.5698
Cation	1	-473.3728	-475.7028	-473.3728	-475.7028
1st	2a	-551.9910	-554.32131	-591.3138	-593.6444
	2b			-591.3132	-593.6435
1st TS	3a	-551.9780	-554.30787	-591.2944	-593.6248
	3b			-591.2869	-593.6163
1st bprod	4a	-552.0094	-554.337792	-591.3222	-593.6506
	4b			-591.3188	-593.6466
2nd pi complex	5a	-630.6115	-632.940988	-709.2395	-711.5693
	5e			-709.2431	-711.5727
	5f	-630.6113	-632.935028	-709.2433	-711.5673
	5g			-709.2412	-711.5637
2nd TS	6a	-630.6053	-632.934445	-709.2298	-711.5597
	6b			-709.2255	-711.5553
	6c			-709.2298	-711.5597
	6d			-709.2255	-711.5553
	6e			-709.2252	-711.5539
	6f			-709.2294	-711.5525
	6g			-709.2213	-711.5490
TS elimination	8a	-551.9927	-554.320934	-591.3091	-593.6376
	8b			-591.3076	-593.6305
TS transfer	7a	-630.5908	-632.91547	-709.2171	-711.5418
	7b			-709.2142	-711.5386
Hydrogenolysis pi complex	9a	-553.1918	-634.1466	-592.5042	-594.8313
	9b			-592.5020	-594.8286
TS hydrogenolysis	10a	-553.1873	-634.1438	-592.4997	-594.8279
	10b			-592.4988	-594.8264
2nd bprod	11a	-630.6374	-632.9660	-709.2602	-711.5886
	11b			-709.2598	-711.5872
Elimination product	12a	-551.9962	-554.3258	-591.3168	-593.6468
	12b			-591.3154	-593.6430
	13a	-630.6199	-632.9498	-709.2504	-711.5744
	13b			-709.2445	-711.5686

		Zr/But	Hf/But	Zr/Hex	Hf/Hex
Precursor		-1354.2359	-1356.5698	-1354.2359	-1356.5698
Cation	1	-473.3728	-475.7028	-473.3728	-475.7028
1st	2a	-630.6276	-632.9583	-709.2553	-711.5862
	2b	-630.6271	-632.9576	-709.2542	-711.5854
1st TS	3a	-630.6083	-632.9388	-709.2355	-711.5660
	3b	-630.6006	-632.9301	-709.2251	-711.5547
1st bprod	4a	-630.6351	-632.9635	-709.2618	-711.5902
	4b	-630.6324	-632.9600	-709.2593	-711.5870
2nd pi complex	5a	-787.8654	-790.1952	-945.1194	-947.4491
	5e	-787.8691	-790.1989	-945.1230	-947.4520
	5f	-787.8685	-790.1923	-945.1225	-947.4463
	5g	-787.8668	-790.1907	-945.1210	-947.4448
2nd TS	6a	-787.8552	-790.1851	-945.1088	-947.4388
	6b	-787.8506	-790.1803	not located	-947.4327
	6c	-787.8545	-790.1845	-945.1081	-947.4381
	6d	-787.8510	-790.1808	-945.1047	-947.4346
	6e	-787.8511	-790.1798	-945.1046	-947.4333
	6f	-787.8448	-790.1736	-945.0988	-947.4276
	6g	-787.8434	-790.1707	-945.0975	-947.4249
TS elimination	8a	-630.6213	-632.9500	-709.2483	-711.5769
	8b	-630.6229	-632.9447	-709.2509	-711.5707
TS transfer	7a	-787.8396	-790.1680	-945.0935	-947.4189
	7b	-787.8418	-790.1660	-945.0930	-947.4173
Hydrogenolysis pi complex	9a	-631.8160	-634.1430	-710.4427	-712.7697
	9b	-631.8154	-634.1420	-710.4432	-712.7698
TS hydrogenolysis	10a	-631.8114	-634.1396	-710.4382	-712.7663
	10b	-631.8120	-634.1396	-710.4399	-712.7676
2nd b product	11a	-787.8836	-790.2118	-945.1367	-947.4649
	11b	-787.8846	-790.2120	-945.1378	-947.4652
Elimination product	12a	-630.6289	-632.9589	-709.2561	-711.5860
	12b	-630.6305	-632.9582	-709.2586	-711.5863
Transfer product	13a	-787.8765	-790.2005	-945.1275	-947.4514
	13b	-787.8717	-790.1958	-945.1210	-947.4496

Coordinates

Zr Dichloride precursor

C	-2.31936200	0.31633300	1.06616600
C	-2.56765300	-0.18695300	-0.23255300
C	-2.11030100	0.77780400	-1.17434200
C	-1.56214100	1.86606000	-0.45532800
C	-1.67143100	1.57269000	0.93705300
C	2.10793500	0.78243100	1.17469500
C	2.56731700	-0.18616100	0.23777000
C	2.32157300	0.31169000	-1.06344600
C	1.67340300	1.56865000	-0.94083400
C	1.56158300	1.86787600	0.45002700
H	-2.53050900	-0.19459200	1.99488600
H	-3.00469000	-1.14711400	-0.47181700
H	-2.14978900	0.67799200	-2.25080800
H	-1.14340100	2.76659000	-0.88468300
H	-1.36102000	2.21426600	1.75185700
H	2.14539900	0.68711400	2.25165400
H	3.00380400	-1.14533800	0.48190100
H	2.53446100	-0.20311200	-1.98962100
H	1.36451700	2.20680000	-1.75891100
H	1.14212400	2.77024100	0.87478400
Zr	0.00002700	-0.09586000	0.00000300
Cl	0.05255300	-1.67454000	1.87699800
Cl	-0.05299600	-1.67492900	-1.87668100

Cation/Zr

1

H	-2.40798900	1.35917500	1.50275100
C	-2.23769900	0.50178900	0.86535600
C	-2.53040800	0.42117100	-0.51843400
C	-1.67602000	-0.74614800	1.26688700
C	-2.18369500	-0.88737900	-0.97081200
H	-2.96799200	1.20780600	-1.12171800
C	-1.66654600	-1.61161300	0.13046700
H	-1.38873900	-1.01937300	2.27466600
H	-2.31851700	-1.26987000	-1.97717700
H	-1.34577500	-2.64505200	0.11917400
C	0.00200000	2.44074700	0.10478200
H	-0.92770800	2.90197700	-0.25165000
H	0.84848800	2.88574400	-0.43980500
H	0.12113400	2.73294000	1.15697100
C	1.73757400	-0.55362100	1.31449700
C	2.30481500	0.59606900	0.69165400
C	1.64259000	-1.58633900	0.33232600
H	1.50157900	-0.65491400	2.36674300
C	2.50565000	0.29221200	-0.67788200
H	2.53965200	1.53336900	1.17699200
C	2.10360700	-1.06155000	-0.89756800
H	1.29385100	-2.59611600	0.50430700
H	2.92976900	0.95824500	-1.42085200
H	2.16660900	-1.60147600	-1.83631300
Zr	-0.00138900	0.23438800	-0.29754300

1st π -complex

Zr/Et

2a

H	5.83758600	1.26008100	1.57536200
C	5.98285400	0.45825200	0.86449700
C	5.61398300	0.47959400	-0.50196600
C	6.57033600	-0.80809300	1.13844600
C	5.94409200	-0.78610600	-1.07017700
H	5.12179900	1.29844100	-1.01125400
C	6.53622100	-1.58086300	-0.06156000

H	6.90993400	-1.15411000	2.10602300
H	5.74142700	-1.10287100	-2.08581100
H	6.86071800	-2.60734900	-0.16979100
C	8.17036500	2.44627300	0.31411700
H	7.27427100	2.95596900	-0.06540500
H	9.05735300	2.97420700	-0.06179000
H	8.16730100	2.56643900	1.40458300
C	9.81999800	-0.60400400	1.26737100
C	10.44096900	0.57480200	0.77273900
C	9.79435400	-1.56719600	0.21261600
H	9.49887600	-0.77041800	2.28776000
C	10.75827200	0.35911100	-0.59027200
H	10.64155700	1.47297900	1.33989900
C	10.36621700	-0.97175600	-0.93234000
H	9.42603300	-2.58185800	0.28673000
H	11.27383600	1.05695200	-1.23723700
H	10.50830600	-1.45359800	-1.89265500
Zr	8.19136400	0.30853800	-0.41755100
H	9.57366300	0.51568500	-3.43291200
C	8.93352100	1.28024700	-3.00161000
H	9.42176500	2.17618000	-2.62595800
C	7.58849100	1.18981000	-3.05865800
H	6.95399500	2.01078700	-2.73413400
H	7.09654900	0.35017400	-3.54157500

Zr/Pro

2a

C	3.65924800	-1.28615700	0.32847800
H	3.29982400	-2.28535900	0.58767900
H	3.73673300	-0.68224800	1.23986800
C	2.80374100	-0.61801200	-0.69571000
H	3.08396200	0.40068800	-0.96231600
C	1.76352500	-1.19175500	-1.34696100
H	1.53149900	-2.24403500	-1.20695700
H	1.30518400	-0.69453600	-2.20631100
H	-0.46594800	-3.22343000	0.21845600
C	-1.11339200	-2.37132400	0.05158100
C	-1.81929400	-1.66072400	1.05354200
C	-1.45064100	-1.80685400	-1.21322000
C	-2.56581200	-0.63290100	0.41523400
H	-1.79847500	-1.86709100	2.11452900
C	-2.34764000	-0.73644100	-0.99132700
H	-1.10200800	-2.15185700	-2.17940100
H	-3.24221300	0.05577100	0.90476600
H	-2.81066300	-0.12442700	-1.75428700
H	1.32440900	2.07771500	-1.98531200
C	0.67793600	2.14442000	-1.11776500
C	-0.73826900	2.16280500	-1.14250100
C	1.09967800	2.26441500	0.23667900
C	-1.19423500	2.30171200	0.20298800
H	-1.36081100	2.12714000	-2.02710600
C	-0.05461100	2.37656700	1.04958700
H	2.12328800	2.30182200	0.58714400
H	-2.22502400	2.40644800	0.51493400
H	-0.06590500	2.50230000	2.12384700
C	0.62989500	-0.36373100	2.15069600
H	-0.06346400	-0.11819500	2.96494100
H	1.54420300	0.21717200	2.32466300
H	0.86813700	-1.43255800	2.24603900
H	4.67955500	-1.37439900	-0.06998100
Zr	-0.16157600	0.01542400	0.06692500

2b

C	2.18071000	-0.16507500	1.33599000
C	2.87948600	0.43206700	0.34081500
H	2.24781300	-1.23785300	1.50217500
H	1.73861900	0.43235400	2.13500100
C	3.72452200	-0.26472500	-0.67530400
H	2.88573600	1.52072100	0.29879300

H	3.66889900	-1.35336300	-0.59409200
H	3.46201200	0.03955700	-1.69597000
H	0.08726100	-3.04736500	1.33578600
C	-0.30904300	-2.56696200	0.44975100
C	-1.64827300	-2.13940900	0.26949500
C	0.40914100	-2.28631700	-0.74479900
C	-1.75425400	-1.57009000	-1.02858900
H	-2.44821900	-2.23454400	0.99110000
C	-0.47806900	-1.66687700	-1.65946200
H	1.44844000	-2.52455300	-0.93456400
H	-2.65941200	-1.18896000	-1.48348300
H	-0.24207500	-1.36660900	-2.67214000
C	-1.11770800	0.00007600	2.31813300
H	-2.21283800	0.05175100	2.36471000
H	-0.73448700	0.86045600	2.88382700
H	-0.81723400	-0.91939000	2.83780200
C	0.37106000	2.11694400	-1.09844000
C	0.08527100	2.54080800	0.23590600
C	-0.82213300	1.61587400	-1.66324000
H	1.32417000	2.19677700	-1.60673900
C	-1.29143400	2.31827800	0.48186600
H	0.78284900	3.00590700	0.92241000
C	-1.84983200	1.71704600	-0.67918000
H	-0.94112300	1.23938000	-2.67074300
H	-1.82572100	2.56330200	1.38882600
H	-2.89041300	1.45107800	-0.81641300
H	4.77072300	0.03714500	-0.52852900
Zr	-0.24804200	-0.00039100	0.22611500

Zr/But

2a

C	-1.74828000	-0.54470600	-1.36922400
C	-2.59311200	0.14253400	-0.56272800
H	-1.78090300	-1.62967700	-1.41260900
H	-1.20452500	-0.03524500	-2.16952100
C	-3.57348900	-0.46540400	0.39009800
H	-2.61939600	1.23043300	-0.64175900
C	-5.02371000	-0.17078700	-0.05600900
H	-3.41148900	-1.54658500	0.46371700
H	-3.41826400	-0.03919500	1.38971600
H	-5.72290600	-0.60097500	0.66661200
H	-5.21551500	0.90613600	-0.11049600
H	-5.23319400	-0.60761400	-1.03715400
H	-0.99192900	2.86394400	0.73412500
C	-0.05440900	2.52552900	0.31160500
C	1.13385500	2.26789700	1.03889900
C	0.21280800	2.30187900	-1.06697800
C	2.13462500	1.86548900	0.11295300
H	1.25814000	2.36812700	2.10882300
C	1.56311800	1.88666000	-1.19400500
H	-0.48277700	2.45250000	-1.88441500
H	3.16693800	1.64316500	0.34922400
H	2.08168000	1.67661800	-2.12064400
C	-0.39731500	-0.11516900	2.16039000
H	0.35481100	-0.05622400	2.95774300
H	-0.92515700	-1.07000600	2.28881000
H	-1.10650800	0.70483500	2.32981400
C	1.17133900	-2.08750300	-1.24602000
C	0.63486500	-2.55622400	-0.01020400
C	2.34394200	-1.35055300	-0.96359400
H	0.76539400	-2.27937500	-2.23225600
C	1.48988100	-2.12384200	1.03334700
H	-0.24727300	-3.17313500	0.10950000
C	2.53422700	-1.35490400	0.45079000
H	2.99500800	-0.88504900	-1.69199000
H	1.37218400	-2.34245400	2.08545700
H	3.36847600	-0.91476800	0.98200200
Zr	0.45067900	0.00022900	0.06648500

2b

C	1.81399000	-0.18969000	1.46727700
C	2.57326900	0.36690500	0.49240900
H	1.84361900	-1.26035000	1.65791200
H	1.35039300	0.43461900	2.23283300
C	3.45854700	-0.36874100	-0.46559800
H	2.61381300	1.45473000	0.43061600
C	4.93952600	0.01252100	-0.24356000
H	3.32772400	-1.45063500	-0.35298600
H	3.17999600	-0.10561300	-1.49593900
H	5.56800100	-0.51639700	-0.96556900
H	5.10039200	1.08726600	-0.37897900
H	5.27032600	-0.26034500	0.76310900
H	-0.35227400	-3.04672000	1.36027600
C	-0.67843300	-2.56103500	0.44892100
C	-1.99230600	-2.10195900	0.17990100
C	0.12334000	-2.30143000	-0.69576500
C	-1.99867400	-1.53498100	-1.12343900
H	-2.84036800	-2.17582300	0.84701900
C	-0.68597000	-1.66220700	-1.66774400
H	1.16727500	-2.56369300	-0.81487100
H	-2.86240800	-1.13385600	-1.63770100
H	-0.37556900	-1.36850100	-2.66218300
C	-1.51809900	0.01485700	2.27071100
H	-2.61330600	0.08274000	2.26465900
H	-1.14932200	0.86754000	2.85709800
H	-1.25650800	-0.91068800	2.80045200
C	0.16967300	2.10681400	-1.07315400
C	-0.16567700	2.53832800	0.24705100
C	-1.00727300	1.62701900	-1.68853900
H	1.14554500	2.16613300	-1.53927900
C	-1.55545400	2.34053200	0.43390700
H	0.51015500	2.99175600	0.96245900
C	-2.07427100	1.74833700	-0.74985500
H	-1.08912200	1.24957500	-2.69942900
H	-2.12401600	2.59688600	1.31654900
H	-3.11253600	1.49996900	-0.93093900
Zr	-0.54287300	0.00374400	0.22474400

Zr/Hex

2a

C	-1.86942800	0.30613200	-0.75048300
C	-1.01604100	-0.44594800	-1.48912500
H	-0.40202600	0.01360500	-2.26866700
H	-1.10932300	-1.52812300	-1.51342000
H	1.86380900	2.29955700	2.19518200
C	1.81092400	2.21801000	1.11782900
C	2.85841600	1.79011900	0.25754000
C	0.68614600	2.52792300	0.31420800
C	2.38081500	1.84991500	-1.08565200
H	3.86324200	1.52728600	0.56100700
C	1.04116800	2.31272900	-1.04613500
H	-0.26575300	2.89518600	0.67608600
H	2.95402100	1.63143600	-1.97742800
H	0.40951400	2.49657400	-1.90755100
H	1.45440400	-2.26933300	-2.25166700
C	1.82038100	-2.10641200	-1.24485700
C	3.00406200	-1.41645800	-0.89647800
C	1.20975600	-2.57199400	-0.04311300
C	3.12726300	-1.44776000	0.52489600
H	3.70537400	-0.96526900	-1.58623200
C	2.02963500	-2.18594000	1.04581700
H	0.30094800	-3.15700500	0.02611400
H	3.95081100	-1.04589600	1.10113500
H	1.85406100	-2.41431200	2.08773400
C	0.15298200	-0.13349200	2.10796700
H	0.86193900	-0.13556300	2.94574700
H	-0.42593900	-1.06495000	2.17541800
H	-0.52605600	0.71394000	2.26464600
H	-1.82730700	1.39124300	-0.85449200
C	-2.93876500	-0.22103500	0.14916700
H	-2.84488900	-1.30763200	0.26054800
H	-2.83030300	0.22499600	1.14716300

C	-4.34566700	0.13645000	-0.39686600
H	-4.42536400	1.22578000	-0.51561600
H	-4.46591300	-0.29788300	-1.39776600
C	-5.46708800	-0.36402300	0.52528100
H	-5.37671000	-1.45202500	0.64686800
H	-5.33318500	0.07128200	1.52509400
C	-6.86178100	-0.01900900	-0.00633100
H	-7.63878600	-0.38944600	0.67006400
H	-6.99437500	1.06484300	-0.10425100
H	-7.03560900	-0.46827500	-0.99114200
Zr	1.11366900	-0.01088200	0.06458600

2b

C	-1.85977200	-0.85529000	0.40888100
C	-1.03691900	-0.58739800	1.45292600
H	-0.45159900	-1.38506300	1.91205100
H	-1.13603500	0.33938400	2.01582300
H	-0.20651200	2.74068800	1.27861200
C	0.44499100	2.45500300	0.46183900
C	1.86134100	2.48415800	0.48356700
C	0.03036000	2.04286800	-0.83789000
C	2.32570300	2.05370700	-0.78925300
H	2.48014400	2.78420200	1.31751100
C	1.18834300	1.79767400	-1.61156700
H	-0.99212900	1.95178800	-1.18199000
H	3.36100300	2.00162900	-1.10078200
H	1.20856700	1.49569900	-2.65051900
H	1.63898100	-3.07853300	1.16011600
C	1.87068700	-2.47703100	0.28966900
C	1.05320500	-2.32215500	-0.86455500
C	3.06580500	-1.74420300	0.08354700
C	1.72917300	-1.47417100	-1.77579100
H	0.09745000	-2.80113500	-1.03563000
C	2.97616900	-1.11090300	-1.18680100
H	3.89973500	-1.68130400	0.76926300
H	1.38307000	-1.19294600	-2.76191500
H	3.74863900	-0.51544200	-1.65524300
C	2.17755000	0.13216800	2.25825400
H	3.23151200	0.43548000	2.27752000
H	2.11757900	-0.85033800	2.74483000
H	1.62406300	0.85923000	2.86868300
H	-1.81123700	-1.84728300	-0.04180800
C	-2.92356300	0.04423400	-0.13064600
H	-2.84001700	1.04746000	0.30318900
H	-2.81360200	0.13521900	-1.22071500
C	-4.33164500	-0.53776300	0.16499500
H	-4.40225100	-1.55160400	-0.25172400
H	-4.45806200	-0.63470400	1.25088100
C	-5.45266400	0.33712400	-0.41485300
H	-5.31618900	0.42580000	-1.50144600
H	-5.36636500	1.35368900	-0.00734800
C	-6.84697700	-0.22122400	-0.11284100
H	-7.62397600	0.42130600	-0.53923900
H	-6.97532900	-1.22461100	-0.53544300
H	-7.02437700	-0.28685400	0.96689800
Zr	1.22490500	0.02393600	0.20853800

1st TS

Zr/Et

3a

H	-2.75412900	0.38100300	1.74409000
C	-2.40102200	-0.20134000	0.90232500
C	-2.51679000	0.15305100	-0.46377300
C	-1.77144100	-1.47792000	0.97546500
C	-1.96507900	-0.89999700	-1.24410300
H	-2.97035400	1.05767900	-0.84865900
C	-1.52154800	-1.91506200	-0.35468600
H	-1.57599400	-2.04264900	1.87896800

H	-1.92699900	-0.94022700	-2.32592800
H	-1.08958100	-2.86555400	-0.63914100
C	-0.01167200	1.80722800	1.61802700
H	-0.84669900	2.36655400	2.03779100
H	0.93118200	2.26573100	1.91478200
H	-0.04817600	0.80063700	2.13755000
C	1.74365600	-1.68779700	0.60885300
C	2.28786200	-0.47360500	1.10421100
C	1.69957000	-1.59695100	-0.81435600
H	1.46559100	-2.55019100	1.20158900
C	2.55024300	0.37720900	-0.00081300
H	2.47301600	-0.24082400	2.14599900
C	2.20259800	-0.32521200	-1.18901500
H	1.38040500	-2.37724700	-1.49326600
H	2.98521300	1.36773800	0.04858400
H	2.33068800	0.03096500	-2.20267100
Zr	0.00521500	0.06598900	0.06549500
H	0.57388700	3.35618700	-0.02096100
C	-0.22636000	2.69131700	-0.32764700
H	-1.22244600	3.04414500	-0.08314000
C	-0.05264000	1.88422300	-1.47988800
H	-0.91539900	1.73755000	-2.12329000
H	0.89691500	1.95805300	-1.99969500

Zr/Pro

3a

C	-3.52424000	-1.13694700	-0.04797600
H	-3.74140400	-0.07063900	-0.16059100
H	-3.87586400	-1.47535000	0.92950300
C	-2.06491200	-1.44719200	-0.30178600
H	-1.78358700	-2.47200700	-0.07344600
C	-1.39794600	-0.86652000	-1.43473900
H	-1.95986400	-0.10829900	-1.97476000
H	-0.86351700	-1.55738100	-2.08187300
H	-2.37506000	2.08593500	0.13884700
C	-1.29890200	2.15842400	0.04605600
C	-0.38011400	2.32064800	1.11638800
C	-0.56379200	2.16814600	-1.17151400
C	0.92650100	2.40115700	0.56863400
H	-0.63076200	2.37980800	2.16886600
C	0.81076700	2.31081800	-0.85053500
H	-0.97790700	2.10963200	-2.16912700
H	1.84260200	2.55338000	1.12514700
H	1.62380300	2.38501500	-1.56158000
H	0.67657000	-3.07130700	-0.78956100
C	1.26577600	-2.23577800	-0.43345300
C	1.91771100	-1.26950300	-1.24694600
C	1.54775300	-1.93607200	0.92173400
C	2.61525500	-0.37734900	-0.38957300
H	1.91321300	-1.23910200	-2.32971300
C	2.37346100	-0.77545400	0.95461600
H	1.21711000	-2.50452400	1.78211800
H	3.24239000	0.44664700	-0.70346200
H	2.79425900	-0.31642900	1.84101000
C	-1.39604600	-0.79890500	1.60597700
H	-0.46569200	-0.41694700	2.12455300
H	-1.55431700	-1.78148600	2.04952400
H	-2.20418700	-0.12831400	1.89413500
H	-4.10217100	-1.67304600	-0.81179500
Zr	0.15591900	0.04404000	0.06452300

3b

C	0.63289600	2.40466500	0.67060700
C	0.85025900	1.99590800	-0.67599800
H	1.49677200	2.68727500	1.26697200
H	-0.27045300	2.95382000	0.91134700
C	2.25405100	2.09284000	-1.26013800
H	0.06966800	2.31699100	-1.36432900
H	3.01776300	1.66312200	-0.60418200
H	2.32395700	1.60381800	-2.23550500

H	3.06072400	-0.34141400	0.83937600
C	2.28553600	-0.96564600	0.41392700
C	1.46010400	-1.87067300	1.12930100
C	1.96199500	-1.07426400	-0.96819500
C	0.60271200	-2.51717900	0.20062400
H	1.47950800	-2.04285100	2.19875000
C	0.92192400	-2.02906500	-1.10026100
H	2.45228900	-0.55625300	-1.77953500
H	-0.12769500	-3.28170700	0.43395500
H	0.48056600	-2.36070400	-2.03137100
C	0.25564100	0.98214000	2.19464400
H	-0.28248800	-0.00576200	2.33793200
H	-0.33153100	1.69674400	2.76948400
H	1.24192200	0.86575600	2.64346400
C	-2.00187300	0.30030400	-1.53132700
C	-2.25156600	1.22468600	-0.48131200
C	-2.16232800	-1.00961800	-1.00482800
H	-1.77169100	0.54993000	-2.56012900
C	-2.54809300	0.49178700	0.69415100
H	-2.24355800	2.30346100	-0.57164600
C	-2.48291700	-0.89557600	0.37619400
H	-2.08115800	-1.93333600	-1.56233100
H	-2.81023300	0.91052800	1.65775100
H	-2.69835600	-1.71608800	1.04978700
H	2.51510900	3.14801100	-1.41457100
Zr	-0.10477900	-0.08108000	0.15176100

Zr/But

3a

C	1.48678900	-0.31008900	-1.22019400
C	2.18592500	-0.63347100	-0.00665400
H	1.81421200	0.59756500	-1.72193100
H	1.29288000	-1.13605200	-1.90048700
C	3.44409400	0.13058500	0.37030900
H	2.22809100	-1.69348200	0.23525000
C	4.61798000	-0.33894100	-0.51112900
H	3.28205900	1.20577800	0.22841300
H	3.70365200	-0.02932200	1.42124700
H	5.52843400	0.19607000	-0.22406100
H	4.80763600	-1.41075500	-0.38630900
H	4.42810000	-0.14675900	-1.57152900
H	0.22464400	-3.07752300	-0.75959600
C	-0.64057100	-2.50486500	-0.45104300
C	-1.09141600	-2.33301000	0.88077000
C	-1.53963400	-1.82301500	-1.31513500
C	-2.27501300	-1.53996700	0.84733700
H	-0.63645000	-2.75613300	1.76762800
C	-2.55892800	-1.24221700	-0.51347000
H	-1.48039100	-1.78473400	-2.39608800
H	-2.88279500	-1.26306700	1.70033100
H	-3.41475800	-0.68791300	-0.87576900
C	1.14468900	-0.20635900	1.79681400
H	0.09261700	-0.15575300	2.21125200
H	1.64275900	0.70890300	2.11286200
H	1.58324800	-1.06363600	2.30628300
C	-0.39084200	2.22727900	-1.20303700
C	0.19433800	2.50199600	0.06413400
C	-1.75216600	1.88928000	-0.99111700
H	0.10306200	2.29356200	-2.16320800
C	-0.81226200	2.35816500	1.05437800
H	1.21731600	2.81076600	0.23843500
C	-2.01343700	1.96357900	0.40952500
H	-2.47550800	1.65822300	-1.76256700
H	-0.68870700	2.52387800	2.11796900
H	-2.96953600	1.79807900	0.88971800
Zr	-0.43494600	0.01446500	0.08158100

3b

C	-1.73322200	-1.14994600	1.16472100
---	-------------	-------------	------------

C	-1.83676500	-0.80827700	-0.21615300
H	-2.42956200	-0.68597600	1.85890000
H	-1.44864800	-2.16102700	1.43456800
C	-3.00137300	0.06798700	-0.67689000
H	-1.63697700	-1.64127900	-0.89007600
C	-4.33099100	-0.70749800	-0.68624100
H	-3.10017600	0.94882500	-0.03067500
H	-2.80925400	0.43797500	-1.68973700
H	-5.14419600	-0.06958000	-1.04848900
H	-4.27423500	-1.58285300	-1.34299300
H	-4.59875300	-1.05738500	0.31721800
H	-1.53030800	2.50290400	1.03197300
C	-0.62274700	2.36924500	0.45749900
C	0.70054100	2.46376300	0.95946300
C	-0.54570400	2.13524200	-0.94445400
C	1.59943000	2.25676400	-0.11960200
H	0.98058700	2.66240100	1.98695600
C	0.82506600	2.06199200	-1.30064900
H	-1.38121700	2.06766800	-1.62592100
H	2.68016300	2.29188800	-0.06363200
H	1.21379700	1.92753500	-2.30196800
C	-0.21563000	-0.32748900	2.38005100
H	0.86738300	-0.00004800	2.30249700
H	-0.18767100	-1.20942300	3.01817600
H	-0.74647700	0.47974100	2.88415000
C	1.19240900	-1.67011300	-1.58116500
C	0.90229600	-2.43728000	-0.42079700
C	2.30098900	-0.83256100	-1.28301700
H	0.68584600	-1.74082000	-2.53615800
C	1.81500200	-2.06502300	0.59661500
H	0.13381900	-3.19524500	-0.33836600
C	2.67790700	-1.06178100	0.06898400
H	2.79119900	-0.15731900	-1.97175600
H	1.87007600	-2.49042200	1.59089600
H	3.51035800	-0.59972100	0.58552800
Zr	0.40477500	0.03755000	0.16096800

Zr/Hex

3a

C	1.53525100	-0.64357700	0.14230300
C	0.90593100	-0.31713000	-1.11054700
H	0.75387400	-1.14339100	-1.80118700
H	1.26797400	0.58808900	-1.59281100
H	-1.35132700	-2.75419300	1.75414200
C	-1.76918500	-2.33307400	0.84832300
C	-2.95279400	-1.54359800	0.76336700
C	-1.26252200	-2.50625800	-0.46313500
C	-3.17890200	-1.24770400	-0.60831500
H	-3.59645800	-1.26605800	1.58941500
C	-2.12485500	-1.82699600	-1.36529400
H	-0.38376700	-3.07724800	-0.73417600
H	-4.01946000	-0.69526500	-1.00737100
H	-2.01997600	-1.79047700	-2.44284300
H	-0.43814800	2.26762000	-2.16688300
C	-0.97682100	2.21315200	-1.23028700
C	-2.34672800	1.87774800	-1.07848600
C	-0.45129600	2.50210800	0.05962300
C	-2.67301600	1.96736800	0.30740700
H	-3.03324400	1.63788400	-1.88028700
C	-1.50300200	2.36951600	1.00308600
H	0.56309900	2.81114300	0.27832200
H	-3.65070500	1.80778000	0.74421400
H	-1.42934000	2.54723800	2.06935200
C	0.40184400	-0.19035500	1.87575700
H	-0.67187000	-0.13961900	2.23150700
H	0.87909400	0.73180500	2.20346400
H	0.81542000	-1.03735500	2.42177500
H	1.55010200	-1.70331800	0.38816700
C	2.78030000	0.10284600	0.58590100
H	2.64799800	1.18036100	0.42591600
H	2.97632400	-0.05140500	1.65214400
C	4.00388700	-0.39238200	-0.21787200

H	4.10267200	-1.48050500	-0.09818700
H	3.83820300	-0.21059300	-1.28760500
C	5.30630100	0.28845700	0.22919300
H	5.20393500	1.37657000	0.11573000
H	5.46278700	0.10330100	1.30067800
C	6.52573200	-0.19910500	-0.56007600
H	7.43716000	0.30355700	-0.22074000
H	6.67474500	-1.27817600	-0.43585800
H	6.41350100	0.00208400	-1.63197200
Zr	-1.08283300	0.01360200	0.07598500

3b

C	-0.92105500	-0.50689800	1.52713400
C	-0.05967600	0.00033400	2.53934600
H	0.36389700	-0.68023000	3.27022900
H	-0.25508300	0.99853000	2.92226400
H	-0.48953500	2.84894100	1.01867100
C	0.02177700	2.47327400	0.14187700
C	1.40839700	2.59468900	-0.12498500
C	-0.58646700	1.82799000	-0.96931400
C	1.66953900	2.00183900	-1.39002400
H	2.14105300	3.06798500	0.51686600
C	0.42959300	1.53876900	-1.91689300
H	-1.64182200	1.62840000	-1.09093000
H	2.62925900	1.96457400	-1.88989800
H	0.28238300	1.08589400	-2.88847300
H	1.45881900	-2.89805800	1.31623600
C	1.53437900	-2.42058100	0.34723600
C	0.50651800	-2.35291600	-0.63526300
C	2.69572000	-1.80757600	-0.18949100
C	1.02809500	-1.67509100	-1.76663900
H	-0.48881000	-2.76816100	-0.55028600
C	2.38317600	-1.32809700	-1.48866500
H	3.65656300	-1.72106900	0.30349200
H	0.50347800	-1.49463900	-2.69599200
H	3.06813800	-0.83792600	-2.16863400
C	2.00057500	0.40314700	2.11924100
H	2.69588000	0.64609700	1.25574700
H	2.44650100	-0.44464600	2.63795100
H	2.02644300	1.28759200	2.75458300
H	-0.94988200	-1.59551200	1.49556500
C	-2.30572800	0.11248000	1.30924500
H	-2.87993700	-0.03025200	2.23675100
H	-2.24047900	1.19732000	1.16929600
C	-3.09858000	-0.53454500	0.16428300
H	-2.54893300	-0.43165900	-0.78383900
H	-3.17494800	-1.61575300	0.35078700
C	-4.50961200	0.04801600	0.00309000
H	-4.43879900	1.12931900	-0.18415000
H	-5.05265100	-0.06033700	0.95164800
C	-5.30757700	-0.61666400	-1.12341300
H	-6.30777000	-0.17991600	-1.20797400
H	-4.80905100	-0.49425200	-2.09296500
H	-5.42834100	-1.69151200	-0.94380400
Zr	0.95248000	0.06350600	0.07540700

1st β -product

Zr/Et

4a

H	-2.80261600	1.39109300	-0.33675800
C	-1.78402400	1.71075100	-0.15657000
C	-1.16300700	1.84218600	1.11090400
C	-0.85124200	2.11801400	-1.15291500
C	0.16750200	2.29518700	0.89869800
H	-1.62035400	1.64056500	2.06978400
C	0.35059400	2.48863700	-0.50563100
H	-1.03614600	2.14990900	-2.22105400

H	0.88639700	2.53717700	1.67110900
H	1.24474900	2.86682800	-0.98397700
C	-3.30466600	-1.80831400	-0.39513700
H	-3.73384700	-0.82024000	-0.20234800
H	-3.74592700	-2.50879100	0.32000100
H	-3.59190700	-2.12155600	-1.40355000
C	2.48487600	-0.12647200	-0.82924700
C	1.91543300	-1.38864600	-1.14200900
C	2.49854900	0.00381000	0.59168100
H	2.87470400	0.59263700	-1.53847400
C	1.58620100	-2.03901200	0.07798300
H	1.77568400	-1.79608900	-2.13719600
C	1.94880800	-1.18335000	1.14781600
H	2.91674000	0.83283700	1.14744100
H	1.14246800	-3.02143900	0.17542800
H	1.83118900	-1.39935800	2.20196700
Zr	0.11515600	0.03310400	-0.09576200
H	-1.38904000	-1.18238700	-1.11074900
C	-1.78072300	-1.80421000	-0.21949600
H	-1.36807600	-2.79383100	-0.43519200
C	-1.26088400	-1.26077300	1.10923400
H	-2.03969900	-0.75043100	1.67579100
H	-0.79506900	-2.02793400	1.72638300

Zr/Pro

4a

C	3.20683800	1.26681000	0.34771700
H	4.07462200	1.28053200	-0.32044200
H	3.57463200	1.28040200	1.37896700
C	2.38415300	-0.00062200	0.06367600
H	1.58406400	-0.00066500	0.93399200
C	1.65912500	-0.00055600	-1.26777300
H	1.84200300	-0.89516300	-1.86448400
H	1.84244600	0.89388000	-1.86460500
H	0.69747400	-2.94507900	-1.01176800
C	-0.14100800	-2.51011000	-0.48618100
C	-0.24589900	-2.31529100	0.92148100
C	-1.36152900	-2.08957500	-1.07654400
C	-1.53276000	-1.77451200	1.19752100
H	0.50475600	-2.57530800	1.65818400
C	-2.22359900	-1.63776600	-0.03900100
H	-1.60204800	-2.12563400	-2.13327800
H	-1.93166000	-1.54623300	2.17846100
H	-3.24079700	-1.29098200	-0.16508400
H	0.69967100	2.94461000	-1.01112900
C	-0.13926700	2.51011900	-0.48587100
C	-1.35985500	2.09045100	-1.07669500
C	-0.24475200	2.31519900	0.92173800
C	-2.22255100	1.63902800	-0.03950300
H	-1.59998800	2.12678700	-2.13350600
C	-1.53204500	1.77520100	1.19727400
H	0.50582600	2.57465000	1.65871900
H	-3.23993200	1.29291800	-0.16597300
H	-1.93142200	1.54705000	2.17805000
Zr	-0.28569100	0.00002200	-0.09675300
C	3.20694700	-1.26804600	0.34756600
H	2.63795700	-2.18447800	0.17154800
H	3.57473800	-1.28174800	1.37881500
H	4.07474100	-1.28163600	-0.32058200
H	2.63777400	2.18322500	0.17181900

4b

C	-2.25805700	-0.31332900	-0.74597300
C	-1.91023900	-0.38987900	0.72629600
H	-1.33277900	-0.01402200	-1.39345100
H	-2.47975000	-1.30641900	-1.14992600
C	-2.33993900	-1.65919100	1.46524300
H	-2.29349300	0.48895700	1.25261700
H	-3.43339900	-1.69561600	1.56997100

H	-2.03570800	-2.57445400	0.94695400
H	-0.50425600	-2.98003400	-0.93140100
C	0.38193800	-2.43265800	-0.63778000
C	1.24045900	-1.70238300	-1.51457000
C	0.90664700	-2.34340000	0.67178800
C	2.30493700	-1.17475800	-0.74061700
H	1.12720100	-1.61540300	-2.58892500
C	2.08845600	-1.54429900	0.61986500
H	0.48534700	-2.80115800	1.55812200
H	3.13989400	-0.59771900	-1.11673500
H	2.75015400	-1.33004400	1.45059200
Zr	0.23250200	0.03113100	0.05532200
C	-3.33314400	0.70055000	-1.15822600
H	-4.29286200	0.39853900	-0.72695500
H	-3.44853800	0.74867400	-2.24562000
H	-3.10266000	1.70498500	-0.78886100
C	0.76981100	2.11216800	1.41425700
C	-0.37962200	2.42882000	0.64164900
C	1.86297600	1.91792800	0.52571100
H	0.81110700	2.04946600	2.49619700
C	0.00395800	2.43117000	-0.73056200
H	-1.35711200	2.67669300	1.03202800
C	1.38862800	2.11260700	-0.80256500
H	2.88282900	1.69438400	0.81192100
H	-0.63585600	2.67548100	-1.57015600
H	1.98498100	2.06632000	-1.70556100
H	-1.92603700	-1.69396200	2.47922600

Zr/But

4a

C	-1.17862400	-0.50190200	-1.53476700
C	-2.06425500	-0.66605800	-0.31432100
H	-1.03701300	-1.42481000	-2.09847100
H	-1.50031200	0.29770900	-2.20328800
C	-3.21862600	0.36009000	-0.23138700
H	-1.43108100	-0.42660100	0.65506200
C	-3.92814100	0.44547700	1.12344000
H	-2.84095200	1.35002600	-0.51099800
H	-3.93836700	0.08074500	-1.01162200
H	-4.69624500	1.22466200	1.10026200
H	-4.42442600	-0.49247500	1.39020700
H	-3.22847700	0.69529000	1.93244800
H	-0.97343800	2.58391200	-1.47495100
C	-0.17660400	2.41057200	-0.76547400
C	-0.31287300	2.31888100	0.64894300
C	1.20417800	2.29557500	-1.07820000
C	0.98518600	2.15062100	1.20873700
H	-1.23721300	2.40582000	1.20685600
C	1.92300100	2.14267400	0.14024700
H	1.63780100	2.34395400	-2.07081500
H	1.22136100	2.08182800	2.26393000
H	2.99805500	2.07058100	0.23815200
C	-2.54114500	-2.10933300	-0.07588400
H	-1.72873000	-2.83343900	-0.17785100
H	-3.30036300	-2.35630300	-0.82608300
H	-2.98871000	-2.23635400	0.91375200
C	2.24291200	-1.67190700	-0.82212700
C	1.09965300	-2.40690500	-0.41103800
C	2.77616300	-1.00822600	0.31771300
H	2.65335000	-1.64223700	-1.82530900
C	0.92065600	-2.19189100	0.98574500
H	0.50337400	-3.05197000	-1.04090000
C	1.95581500	-1.32489700	1.43554600
H	3.67132500	-0.40069200	0.33724700
H	0.15648900	-2.64343100	1.60683900
H	2.11512200	-0.99598200	2.45548100
Zr	0.50611600	0.04782900	-0.11557500

4b

C	-1.85584500	-0.50168600	1.13450100
C	-1.77391100	-0.29164000	-0.36210000
H	-0.79917000	-0.44229300	1.63547900
H	-2.35457200	0.34180300	1.62403200
C	-2.70082600	0.77074400	-0.97045000
H	-1.91151200	-1.24133500	-0.88871200
C	-4.17362200	0.32767600	-1.01424600
H	-2.62757000	1.70960200	-0.40759300
H	-2.37427100	0.99833500	-1.99422700
H	-4.79589100	1.09920400	-1.48062600
H	-4.29311000	-0.59454700	-1.59413600
H	-4.56847800	0.14637400	-0.00768400
H	-1.08405700	2.61573500	1.22698300
C	-0.12003600	2.40097900	0.78485400
C	1.05195900	1.99867000	1.49488700
C	0.20681900	2.50369500	-0.58656900
C	2.10448300	1.86268300	0.55498200
H	1.13290200	1.87134900	2.56818300
C	1.57978000	2.14732200	-0.74091500
H	-0.46792100	2.79823700	-1.38062300
H	3.12957700	1.59848700	0.78086400
H	2.14507600	2.17301700	-1.66469800
C	-2.41599400	-1.83954100	1.63521500
H	-3.47517600	-1.90749300	1.36937000
H	-2.32982700	-1.93171400	2.72262400
H	-1.90221300	-2.68918800	1.17461000
C	1.39361200	-1.72290500	-1.60331700
C	0.59438500	-2.42545400	-0.66380900
C	2.50563400	-1.16657700	-0.91236000
H	1.19972700	-1.63971100	-2.66707500
C	1.21195400	-2.30339100	0.61452900
H	-0.29765800	-2.99325800	-0.88961300
C	2.39315800	-1.52561800	0.46078400
H	3.31335100	-0.60056900	-1.35869100
H	0.86858500	-2.76243900	1.53397700
H	3.10100200	-1.28154900	1.24337500
Zr	0.45954800	0.03305500	-0.01254300

Zr/hex

4a

C	-1.39721500	-2.66715000	-0.37113700
H	-0.44117400	-3.18796800	-0.27723800
H	-1.94139600	-3.12260200	-1.20576500
C	-1.21199800	-1.16830700	-0.66392200
H	-0.83910300	-0.73103000	0.36968400
C	-0.17224000	-0.87241300	-1.72873100
H	-0.52946600	-0.20189200	-2.51127000
H	0.26478200	-1.76716100	-2.17359900
H	-0.64357100	2.17234500	-1.90709000
C	0.03066800	2.22111100	-1.06363500
C	-0.33630600	2.17226700	0.31125100
C	1.43774800	2.40205100	-1.13290400
C	0.84533000	2.32837200	1.09021400
H	-1.34334700	2.07707800	0.69857500
C	1.94049000	2.47692200	0.19616500
H	2.02359200	2.49488100	-2.04050700
H	0.89660700	2.36719900	2.17180400
H	2.97105200	2.65118400	0.47569600
H	1.89455800	-2.95612100	-0.74025800
C	2.22191200	-2.16200100	-0.08406100
C	3.23158700	-1.20793800	-0.37627000
C	1.76215800	-1.92076000	1.24240800
C	3.40507500	-0.38198300	0.76932000
H	3.79046500	-1.13649800	-1.30263700
C	2.49356000	-0.81931300	1.76964200
H	1.01877400	-2.50223800	1.77435600
H	4.13035600	0.41412600	0.87309600
H	2.40101400	-0.41085700	2.76883600
C	-2.55674800	-0.43496000	-0.87743500
H	-2.35909500	0.59705600	-1.19180400
H	-3.04256200	-0.92145900	-1.73403700

H	-1.97246300	-2.83985600	0.54250500
C	-3.51391900	-0.42428100	0.32171100
H	-3.00526900	0.01042100	1.19771400
H	-3.78014000	-1.45086700	0.60334600
C	-4.80314500	0.36367300	0.04313800
H	-4.54675900	1.39703900	-0.23139700
H	-5.30473000	-0.06852400	-0.83326600
C	-5.76736400	0.37188500	1.23356100
H	-5.30585100	0.82687600	2.11851800
H	-6.67362000	0.94069500	1.00205900
H	-6.07336300	-0.64574600	1.50345600
Zr	1.06882900	0.10827200	-0.10066700

4b

C	-0.92285100	1.16651000	-0.52764800
C	-0.13221500	1.61014000	-1.74978300
H	-0.49709000	1.10902900	-2.65220600
H	0.96967900	1.24704500	-1.70986200
H	-0.59836200	-1.39724300	-2.62466400
C	0.04833700	-1.73750000	-1.82689700
C	1.47463600	-1.77461400	-1.86628400
C	-0.37335100	-2.25843000	-0.58199500
C	1.93045900	-2.32522500	-0.64191800
H	2.09545800	-1.48035500	-2.70477600
C	0.78907700	-2.60354900	0.16879100
H	-1.39951000	-2.37221600	-0.25584400
H	2.96211400	-2.51688400	-0.37637900
H	0.80183400	-3.07190600	1.14530000
H	1.83790100	2.90897200	0.64766400
C	1.93223200	1.92892100	1.09804400
C	1.04206000	1.35535300	2.03874300
C	3.00026200	1.00926200	0.87390700
C	1.54546300	0.06632300	2.38658900
H	0.14933100	1.81818800	2.43800800
C	2.76992500	-0.13075600	1.68409100
H	3.85752800	1.17336400	0.23096500
H	1.11575400	-0.60985400	3.11633900
H	3.41330100	-0.99741100	1.76191800
Zr	0.89220200	-0.11115000	-0.02703900
C	-0.01579900	3.12325400	-1.98176500
H	0.37775300	3.63768800	-1.09947400
H	-1.01069900	3.53053000	-2.18851200
H	0.63019100	3.35288500	-2.83500800
H	-0.96594700	1.98818400	0.19539000
C	-2.34169900	0.64794400	-0.78386500
H	-2.92461900	1.43748200	-1.28498400
H	-2.33008300	-0.19904000	-1.48264300
C	-3.08016000	0.24766800	0.50153400
H	-2.51943300	-0.54907100	1.01879700
H	-3.09097400	1.10323900	1.19249100
C	-4.52037100	-0.22376600	0.25863500
H	-4.51185000	-1.08072900	-0.43008200
H	-5.07470300	0.57322600	-0.25544700
C	-5.25334400	-0.60779300	1.54797800
H	-6.27639300	-0.93552000	1.33721800
H	-4.74332200	-1.42746100	2.06930700
H	-5.31191200	0.24140800	2.23913000

π -complexes

Zr/Et

5a

H	2.65731600	-1.62002300	1.61675700
C	2.28041000	-1.53548300	0.60426900
C	1.27302500	-2.35220500	0.00865900
C	2.72949000	-0.61358300	-0.36714300
C	1.11780100	-1.94557100	-1.33871400

H	0.75637800	-3.17632000	0.48431300
C	1.99834100	-0.85479200	-1.57007200
H	3.51117500	0.12252100	-0.23330700
H	0.45056400	-2.38878900	-2.06496000
H	2.15200200	-0.35452800	-2.51723400
C	-4.14377200	-1.15586400	-0.82282400
H	-5.09763000	-0.75242900	-0.46466000
H	-4.05271800	-2.18333200	-0.45169700
H	-4.18496800	-1.19932800	-1.91700200
C	1.35209000	2.34425900	-0.05008600
C	0.32890700	2.47620800	0.91700500
C	0.73156400	2.08664200	-1.30849700
H	2.41311600	2.46347100	0.12572400
C	-0.92587500	2.29974700	0.26293200
H	0.47431700	2.71502300	1.96305700
C	-0.67816700	2.07565900	-1.11248200
H	1.23942300	1.99903400	-2.25978700
H	-1.90126200	2.36611600	0.72692000
H	-1.42485800	1.93773500	-1.88208200
Zr	0.30188300	0.03321700	0.06709400
H	-2.99238300	-0.23430400	0.74605700
C	-2.96497400	-0.28616200	-0.35427800
H	-3.12395000	0.74031900	-0.70640400
C	-1.60593000	-0.82190500	-0.84619900
H	-1.54316400	-1.89450900	-0.59830300
H	-1.57454500	-0.78607800	-1.94530700
H	0.10247400	0.64391800	3.33729000
C	-0.63568500	0.07154400	2.78088500
H	-1.57409700	0.56966900	2.55477100
C	-0.45136600	-1.23765800	2.51352400
H	0.43495600	-1.76560600	2.85103000
H	-1.23262700	-1.83624600	2.04917200

5f

H	1.61554000	2.21261900	1.63380900
C	1.06727700	2.18452000	0.70025800
C	1.61668700	1.87586300	-0.56547100
C	-0.31428300	2.48789100	0.52285600
C	0.58487100	1.98617500	-1.53673900
H	2.64695000	1.61035000	-0.76191700
C	-0.60071000	2.38622700	-0.86500800
H	-1.00575300	2.81260600	1.28934700
H	0.69388600	1.83131800	-2.60212400
H	-1.54792400	2.61651000	-1.33258000
C	3.50347000	-1.52730700	-0.15348600
H	3.87745200	-1.94171700	0.78857800
H	3.80803300	-0.47715900	-0.21123900
H	3.98758100	-2.06190500	-0.97627900
C	-2.61088900	-0.28012100	0.26196300
C	-2.05266100	-1.51890500	0.67442100
C	-2.39587800	-0.15920600	-1.14337100
H	-3.16519900	0.41384500	0.88093700
C	-1.46017200	-2.13808400	-0.45389500
H	-2.08545000	-1.93093900	1.67526500
C	-1.68400700	-1.30258200	-1.58291900
H	-2.76431300	0.63554400	-1.77710500
H	-0.95916600	-3.09806900	-0.46305200
H	-1.39344100	-1.51392700	-2.60234500
Zr	-0.12330000	0.03308600	-0.05489700
H	1.57199000	-1.22419900	0.69782700
C	1.97860400	-1.67789800	-0.27239700
H	1.68676500	-2.72813400	-0.16638500
C	1.33408700	-1.04795900	-1.48813000
H	2.01019800	-0.39568000	-2.03937800
H	0.89681100	-1.77556100	-2.16777400
H	0.25146300	-1.77602300	2.67539400
C	0.53636600	-0.73088000	2.76547100
H	1.59971700	-0.52465400	2.85800700
C	-0.37997500	0.24429300	2.92099900
H	-1.44398900	0.03330100	2.95467700
H	-0.08588500	1.26627100	3.13489400

Zr/Pro

5a

C	1.47988200	-0.12759300	-1.07848500
C	2.83084800	-0.50104700	-0.39588000
H	1.55529900	0.88627400	-1.50085100
H	1.32270100	-0.76928400	-1.96079000
C	3.52200200	-1.67784200	-1.10915700
H	2.66684200	-0.80222500	0.65174000
H	2.88750600	-2.57013600	-1.16311500
H	3.77714700	-1.40037800	-2.13919400
H	0.92913900	-1.66326700	2.47810000
C	0.14394700	-1.86684400	1.75994000
C	-1.25315700	-1.64323800	1.95471800
C	0.31868200	-2.47333100	0.49268000
C	-1.93298100	-2.09425700	0.80269700
H	-1.71923200	-1.22622300	2.83950400
C	-0.96018700	-2.58256300	-0.11905500
H	1.25449400	-2.80256800	0.06858200
H	-3.00392200	-2.07727500	0.64839900
H	-1.16575900	-3.03055900	-1.08332300
C	3.79245500	0.70191500	-0.37192500
H	3.36156600	1.57203300	0.13786700
H	4.04562200	1.01341000	-1.39243100
H	4.72751300	0.44882300	0.14060000
C	-2.31101000	-0.08280500	-1.74399600
C	-1.21921000	0.60611800	-2.33931400
C	-2.81009000	0.71936600	-0.67631800
H	-2.73016000	-1.02134700	-2.08202300
C	-1.03462000	1.82209700	-1.63654200
H	-0.63726700	0.26621700	-3.18565600
C	-2.02096300	1.89601700	-0.61604400
H	-3.66338100	0.49112600	-0.05042900
H	-0.28898400	2.57448500	-1.85781000
H	-2.16775800	2.72283600	0.06721800
C	0.91751000	2.06687400	1.71000100
C	-0.19606200	1.54475300	2.27509800
H	-0.12651800	0.68886500	2.93822100
H	-1.14154900	2.08381000	2.26397800
H	1.85656800	1.52682900	1.83746100
C	1.01000300	3.37881400	0.99937100
H	0.03580100	3.85711400	0.86828700
H	1.50772500	3.28069300	0.02818500
H	4.44925100	-1.96102400	-0.59844900
H	1.64138800	4.05073400	1.59747900
Zr	-0.52590800	-0.10643900	0.02504300

5e

C	1.86642900	-0.29684700	-0.86012700
C	2.94651900	0.59965300	-0.18301200
H	1.81326200	-0.04269400	-1.92624900
H	2.18198200	-1.35117200	-0.83780400
C	4.25512500	-0.17745400	0.05254500
H	2.60279200	0.94698700	0.80617300
H	4.10155600	-1.05721800	0.68933100
H	4.66740800	-0.53013900	-0.90035900
H	2.15050700	-1.31128300	1.80799500
C	1.07814000	-1.22283100	1.89980400
C	0.37411500	-0.11612400	2.43194400
C	0.12288200	-2.19999200	1.50881100
C	-1.02075400	-0.42697300	2.41146700
H	0.82245700	0.78205800	2.83953900
C	-1.17232600	-1.71492700	1.85406700
H	0.34652500	-3.17266200	1.08816400
H	-1.82225700	0.19296200	2.79366000
H	-2.10672200	-2.24360400	1.71892600
C	3.23227000	1.85287900	-1.03032000
H	2.32483800	2.43180000	-1.24449600
H	3.67198300	1.57057700	-1.99435300
H	3.93921700	2.51983300	-0.52438700
C	-0.54181600	-1.49060600	-2.27237300
C	-0.88108300	-0.14411700	-2.56120700

C	-1.51122200	-2.00235200	-1.36919300
H	0.30399500	-2.03314900	-2.67341700
C	-2.06872800	0.17240000	-1.85113100
H	-0.33784100	0.51768600	-3.22400400
C	-2.45741200	-0.96922200	-1.10378000
H	-1.55430200	-3.01531800	-0.99095000
H	-2.60067000	1.11449100	-1.88924900
H	-3.34183300	-1.05743400	-0.48576200
H	0.70795300	2.29661100	0.39421800
C	-0.32071300	2.40130800	0.04650000
C	-1.32468700	2.57039400	0.94011100
H	-0.46586400	2.61874200	-1.00955900
C	-2.72882400	2.96672400	0.62203600
H	-1.08964400	2.46975900	1.99921200
H	-2.91023400	3.05298600	-0.45209800
H	-3.45284200	2.26892500	1.06066700
H	5.01062800	0.45382100	0.53440400
H	-2.93109300	3.94293000	1.08387100
Zr	-0.27798300	-0.25442400	-0.04700800

5f

C	0.68755800	0.38764200	-2.00987200
C	2.01798600	0.32211200	-1.26358600
H	0.52339900	1.33828200	-2.51575400
H	0.59373100	-0.41423100	-2.74121100
C	2.90624000	-0.85076300	-1.72078800
H	1.82550500	0.11928800	-0.15372700
H	2.38569000	-1.81139100	-1.65763400
H	3.19717300	-0.69841100	-2.76566400
H	0.36408000	-2.89113000	-1.33476300
C	-0.52179200	-2.42016700	-0.92870700
C	-0.95739800	-2.48692500	0.41861800
C	-1.48980300	-1.68584600	-1.66813600
C	-2.16718100	-1.75666500	0.53264000
H	-0.46063400	-3.01798000	1.22085600
C	-2.50319000	-1.27371800	-0.76909400
H	-1.47114100	-1.49445800	-2.73169100
H	-2.76700600	-1.64750100	1.42733600
H	-3.40052300	-0.73046300	-1.03403600
C	2.80763200	1.64358300	-1.28025700
H	2.21355800	2.48887900	-0.92152100
H	3.11913500	1.86519500	-2.30687600
H	3.70983200	1.57798700	-0.66231800
C	-1.92166600	2.02421700	-0.58869000
C	-0.62562700	2.56386800	-0.39091900
C	-2.38545000	1.53219600	0.66601300
H	-2.48110800	2.03836700	-1.51557700
C	-0.25942700	2.35242400	0.96154100
H	-0.02688700	3.05550400	-1.14315900
C	-1.36136500	1.72430900	1.61911900
H	-3.35860700	1.10182900	0.86143800
H	0.66430700	2.67374700	1.42693400
H	-1.42430900	1.47592000	2.67018700
C	1.76049200	-1.12210800	2.11906800
C	0.65390800	-0.50652000	2.58899300
H	-0.28857500	-1.03585000	2.69938800
H	0.73005800	0.46548600	3.06749700
H	1.67559800	-2.13797300	1.73278700
C	3.14753200	-0.56162800	2.19057000
H	3.15542300	0.48726800	2.50036800
H	3.68312100	-0.66420800	1.24134700
H	3.71941000	-1.13900000	2.93018600
H	3.82451400	-0.91963600	-1.12704000
Zr	-0.46091100	0.01496000	-0.05066100

5g

C	-0.69651700	1.71461700	-0.87830400
C	-1.93699500	1.54680600	0.00803900
H	-1.89901800	2.23912100	0.85579600
H	-1.96641400	0.53118400	0.49113100
H	2.46931800	2.22349600	0.65087100

C	1.93502300	1.47931900	1.22786500
C	0.68720100	1.66603800	1.87233000
C	2.38466600	0.15998400	1.52176200
C	0.33966000	0.45608100	2.52325600
H	0.10786100	2.57714600	1.87802200
C	1.39839100	-0.47626300	2.31224000
H	3.32652800	-0.27342900	1.21392500
H	-0.54466500	0.29354900	3.12668200
H	1.46078900	-1.47820700	2.71774500
H	0.25107600	-3.06418000	-1.44675500
C	0.73856600	-2.10934500	-1.60018700
C	0.24485800	-1.03799200	-2.38946800
C	1.98906400	-1.72572200	-1.05975700
C	1.21832000	-0.00171600	-2.37960500
H	-0.68416000	-1.03157500	-2.94664200
C	2.29002300	-0.41921200	-1.55242100
H	2.62886500	-2.33609500	-0.43538500
H	1.16340000	0.93144500	-2.92276900
H	3.20175300	0.13447400	-1.37063500
C	-3.27226700	1.70808600	-0.74025400
H	-3.36882800	0.97671700	-1.55124000
H	-3.32988300	2.70545000	-1.18809400
H	-4.12870300	1.59386400	-0.06725200
H	-0.95868600	1.34607400	-1.87839300
C	-0.18901200	3.14535800	-1.02349900
H	-0.95572900	3.79887000	-1.46393000
H	0.09872300	3.59192500	-0.06578100
H	-1.18653200	-2.01946600	2.25079200
C	-1.05122100	-2.28846800	1.20692300
C	-2.08286200	-2.21838400	0.33669500
H	-0.12863800	-2.80315500	0.94777300
C	-3.47016000	-1.76959700	0.67410400
H	-1.93781800	-2.58724300	-0.67858600
H	-3.86229300	-1.06018400	-0.06210200
H	-3.53543200	-1.32984900	1.67337700
H	-4.13510100	-2.64398800	0.64287900
H	0.68523300	3.19431400	-1.68275700
Zr	0.35169800	-0.11219500	0.02382500

Zr/But

5a

C	1.21904700	-0.21443300	-1.12570400
C	2.60941700	-0.11789700	-0.42683600
H	1.06744400	0.67748000	-1.75271100
H	1.22234500	-1.04807500	-1.84650200
C	3.54909000	-1.25507800	-0.89598500
H	2.50591900	-0.21331000	0.66749000
C	4.87582900	-1.35727700	-0.13460800
H	3.02376200	-2.21741800	-0.82150200
H	3.74583800	-1.11297400	-1.96809700
H	5.45621600	-2.21740100	-0.48446900
H	5.49818000	-0.46725000	-0.27200000
H	4.70999000	-1.48628700	0.94269300
H	0.94274900	-1.02741400	2.72634400
C	0.24745100	-1.55079300	2.08127200
C	-1.16959900	-1.61476300	2.24654400
C	0.59611200	-2.35194200	0.96724000
C	-1.69080100	-2.44253800	1.22816700
H	-1.74648800	-1.13958400	3.03111200
C	-0.60344400	-2.87783900	0.41514500
H	1.59537100	-2.54010700	0.60682300
H	-2.73208700	-2.70321200	1.09182400
H	-0.67085100	-3.54983500	-0.43136000
C	3.25400400	1.25577100	-0.69683300
H	2.57360500	2.07966100	-0.45130400
H	3.51510800	1.35712200	-1.75729400
H	4.16763300	1.39913700	-0.11107700
C	-2.43890600	-1.12915300	-1.68335500
C	-1.53457900	-0.30872300	-2.41046400
C	-3.15133600	-0.29852700	-0.76878600
H	-2.60064200	-2.18790200	-1.83824800
C	-1.67513500	1.02014700	-1.93970400
H	-0.86315700	-0.63870900	-3.19179100

C	-2.67905800	1.02757100	-0.93366800
H	-3.93954900	-0.61621400	-0.09832600
H	-1.13088700	1.88200600	-2.30277200
H	-3.04456500	1.89950900	-0.40598200
C	0.14385100	2.39845700	1.15791900
C	-0.79631400	1.72638200	1.86426900
H	-0.50697800	1.07581600	2.68339400
H	-1.85132700	1.98556200	1.79032000
H	1.19143300	2.16251600	1.35259800
C	-0.09904200	3.52877200	0.20538300
H	-1.17046000	3.64003100	0.00535600
H	0.40285000	3.32176200	-0.74896400
C	0.46969800	4.84612700	0.78134400
H	1.54611800	4.76878200	0.96683000
H	0.30797200	5.65906900	0.06763000
H	-0.02331100	5.11110100	1.72152200
Zr	-0.74874800	-0.38898700	0.03101000

5e

C	1.83457600	-0.36606800	-0.88806900
C	2.70293000	0.87893700	-0.53251700
H	1.71789500	-0.41870600	-1.97805100
H	2.36908900	-1.28991100	-0.61746000
C	4.14403900	0.45589600	-0.15731400
H	2.29503700	1.40430200	0.34862000
C	5.04466500	1.58987400	0.34538800
H	4.09357800	-0.32450200	0.61576500
H	4.60116800	-0.02446300	-1.03375500
H	6.01589200	1.19695900	0.66390000
H	5.23574300	2.33991500	-0.42886400
H	4.59753000	2.10344800	1.20626400
H	2.33123300	-0.48102700	1.93924000
C	1.26735500	-0.61525400	2.06622800
C	0.31972000	0.40630500	2.31571900
C	0.57039800	-1.85267900	2.01297300
C	-0.96332200	-0.20589800	2.46203500
H	0.54198300	1.45972700	2.43660700
C	-0.80495800	-1.59764600	2.28701100
H	1.01892500	-2.82633500	1.85868100
H	-1.89073100	0.29702900	2.70629500
H	-1.58852300	-2.34076100	2.35522000
C	2.70581900	1.88353900	-1.69990900
H	1.68994500	2.15298000	-2.01538100
H	3.21190400	1.45355200	-2.57286300
H	3.22222900	2.81202800	-1.43711300
C	-0.23616300	-2.38467400	-1.78826700
C	-0.88998500	-1.28172400	-2.39373500
C	-1.04734900	-2.83948600	-0.71467600
H	0.71260800	-2.80670100	-2.09198600
C	-2.11462400	-1.06571000	-1.70858300
H	-0.52455900	-0.71694400	-3.24227300
C	-2.21347500	-2.02010500	-0.66394100
H	-0.84203700	-3.69243200	-0.08092100
H	-2.85614600	-0.31595000	-1.95215500
H	-3.04669900	-2.13694300	0.01714100
H	0.11942000	2.16252800	-0.32226000
C	-0.90216500	1.93157600	-0.62869300
C	-1.93205100	2.11670500	0.23269900
H	-1.08014200	1.80249500	-1.69447800
C	-3.38947500	2.09597100	-0.10902700
H	-1.69705400	2.37861300	1.26489000
C	-4.03371800	3.47493300	0.15773200
H	-3.53402700	1.81047400	-1.15669000
H	-3.89843300	1.34599400	0.51308700
H	-5.10124800	3.43341100	-0.07619500
H	-3.92916100	3.76903500	1.20742600
H	-3.57703000	4.25091900	-0.46396200
Zr	-0.26454200	-0.56064200	0.01152400

5f

C	0.14962900	-1.87118700	1.17055300
C	-1.31659900	-1.48118900	1.00307400
H	0.46511200	-1.89238900	2.21291100
H	0.37038100	-2.84029700	0.72590500
C	-2.14635500	-2.59965600	0.32179700
H	-1.40274300	-0.59164000	0.28431200
C	-3.54407800	-2.20194400	-0.16138600
H	-1.57276700	-3.00039200	-0.52224900
H	-2.22427000	-3.42023400	1.04703300
H	-4.04287400	-3.05846200	-0.62631500
H	-4.18578800	-1.86041200	0.65728300
H	-3.50000000	-1.40363000	-0.91397300
H	-0.54886700	-1.96604400	-2.27435300
C	0.39014800	-1.44914800	-2.12539500
C	0.70608900	-0.14738100	-2.59821800
C	1.54898100	-1.98174200	-1.49984800
C	2.03785900	0.14983600	-2.22598600
H	0.04318900	0.49813700	-3.16048100
C	2.56225100	-0.99264900	-1.54514700
H	1.65354400	-2.97364500	-1.08529400
H	2.58048400	1.05692900	-2.46023200
H	3.57612500	-1.11150200	-1.18697900
C	-1.95829400	-0.99810900	2.31809600
H	-1.38487800	-0.18864700	2.78043500
H	-1.99211600	-1.83053300	3.02973400
H	-2.98120400	-0.63892100	2.17386400
C	2.62832200	0.09746200	1.78660000
C	1.45589600	0.57626900	2.43060900
C	2.99325000	1.04502400	0.79128800
H	3.17313700	-0.80156400	2.04491800
C	1.06742500	1.78120600	1.80479100
H	0.94955500	0.09883900	3.25752600
C	2.01920300	2.07272000	0.77921900
H	3.87046900	0.99806800	0.16013800
H	0.22286000	2.39717700	2.08711400
H	2.03597200	2.95290900	0.14994200
C	-1.82243900	1.63832100	-0.96099300
C	-0.67248200	2.34608200	-0.90798500
H	0.04669200	2.33716400	-1.72122300
H	-0.52861800	3.10374500	-0.14335800
H	-1.98737000	0.96334600	-1.80243400
C	-2.98984300	1.82907700	-0.03433500
H	-2.68167100	2.40080800	0.84889700
H	-3.36056700	0.85840700	0.31293900
C	-4.13829400	2.56338500	-0.76096500
H	-4.47964500	2.00186200	-1.63737300
H	-4.99022900	2.68134700	-0.08466300
H	-3.82390500	3.55742000	-1.09363800
Zr	0.82190000	-0.01465300	-0.01437500

5g

Zr/Hex

5a

C	0.98387000	2.77976500	-0.65062200
H	-0.07196200	2.78622400	-0.35409700
H	1.02291600	3.02531600	-1.71887900
C	1.64524400	1.41332400	-0.38459900
H	1.65076700	1.26725500	0.70856100
C	0.84642100	0.27506000	-1.08830700
H	1.48249900	-0.20913600	-1.84589300
H	0.02532500	0.71554800	-1.67708200
H	2.92122200	-0.91009300	0.62641400
C	2.14528500	-1.55962100	1.00057900
C	1.29714700	-1.29870500	2.10364100
C	1.80102500	-2.83605200	0.47793800
C	0.45687600	-2.43715600	2.29493200
H	1.32295900	-0.41240400	2.72595800
C	0.77505600	-3.38756600	1.30056900

H	2.29003100	-3.33436100	-0.34963700
H	-0.28104300	-2.56486800	3.07798200
H	0.32505300	-4.36500700	1.18716600
H	-2.20397000	-0.33116900	-2.34393200
C	-1.86080200	-1.28590800	-1.96758900
C	-0.71189100	-1.98666100	-2.40942500
C	-2.50095900	-2.07120900	-0.97072300
C	-0.62842700	-3.19921200	-1.67280200
H	-0.02320400	-1.65890000	-3.17659200
C	-1.74156500	-3.25304200	-0.78313900
H	-3.42684200	-1.82709500	-0.46559100
H	0.11212800	-3.97618400	-1.80945900
H	-1.98750500	-4.06977900	-0.11665100
C	3.12118300	1.42670800	-0.85103500
H	3.52433200	0.40383700	-0.81842700
H	3.14184600	1.71125400	-1.91353300
H	1.48176400	3.58610700	-0.10289400
C	4.05950500	2.34379800	-0.05355200
H	4.00595200	2.08159500	1.01469000
H	3.72256300	3.38604200	-0.12819800
C	5.51994300	2.26045900	-0.52089400
H	5.86697500	1.21995300	-0.44422600
H	5.57240500	2.52062800	-1.58727100
C	6.45885500	3.17271300	0.27508400
H	6.45637500	2.91384300	1.34099500
H	7.49006300	3.09050800	-0.08449700
H	6.15920500	4.22400900	0.18798900
H	-4.22154800	2.39058400	1.65512300
C	-3.74756500	2.68272700	0.70922800
C	-4.81091100	3.20139800	-0.26912000
H	-3.04076700	3.48887400	0.94745500
C	-2.96952600	1.46860200	0.13460100
C	-5.58912000	4.39699900	0.29009900
H	-5.50833300	2.38754600	-0.51058400
H	-4.32588200	3.48463800	-1.21344900
H	-3.67181300	0.65908200	-0.09551900
H	-2.49364000	1.78247800	-0.80429600
C	-1.92744900	1.00998700	1.10343000
H	-4.92284200	5.24049300	0.50545200
H	-6.34168000	4.74179300	-0.42634500
H	-6.10879800	4.13474400	1.21905300
H	-1.12565500	1.72220200	1.30471400
C	-1.94245300	-0.13997600	1.82115200
H	-2.77201700	-0.84158100	1.74341300
H	-1.26453000	-0.27230400	2.65829000
Zr	-0.22152000	-1.40125700	0.04367800

5e

C	1.80292900	-0.71174700	-1.01693300
C	2.49677800	0.67893600	-0.88879400
H	1.62908000	-0.92710300	-2.07903300
H	2.48078600	-1.50807700	-0.67450200
C	3.99514200	0.51970200	-0.53404900
H	2.04539300	1.27000500	-0.07251900
C	4.74189700	1.82408900	-0.22087800
H	4.08684000	-0.15094700	0.33369400
H	4.49238300	-0.00285600	-1.36429900
H	4.74239500	2.48007100	-1.10129000
H	4.20471400	2.37218000	0.56897200
H	2.47145400	-0.43435900	1.76494400
C	1.43623900	-0.65170600	1.98154600
C	0.40241200	0.29869000	2.15758100
C	0.87093300	-1.94562200	2.14357200
C	-0.79923600	-0.40744200	2.47341700
H	0.51867800	1.37500400	2.11844900
C	-0.50620700	-1.78800600	2.47552100
H	1.41013900	-2.88336100	2.09188300
H	-1.75898800	0.03354500	2.71213900
H	-1.20308400	-2.58585700	2.69604300
C	2.31807600	1.48876900	-2.18731300
H	1.26575200	1.55614900	-2.49142100
H	2.86172900	1.01189100	-3.01192200

H	2.69470900	2.51129100	-2.08535400
C	-0.01898300	-3.09253900	-1.47187400
C	-0.83491200	-2.18186200	-2.19033700
C	-0.71971300	-3.47556400	-0.29750400
H	0.96276100	-3.43721300	-1.76835900
C	-2.04682600	-2.01479300	-1.47100600
H	-0.58124500	-1.71192500	-3.13233600
C	-1.97766200	-2.80408700	-0.29447900
H	-0.38050800	-4.19251300	0.43868400
H	-2.88950200	-1.40763600	-1.77649300
H	-2.76083800	-2.91831100	0.44406900
H	-0.22117000	1.62756200	-0.77165100
C	-1.22550300	1.21730700	-0.88749100
C	-2.16128300	1.42171100	0.07297000
H	-1.50735700	0.87977400	-1.88253600
C	-3.62662600	1.14871200	-0.04147900
H	-1.84351900	1.89648600	1.00150100
C	-4.44721600	2.46121100	0.04311300
H	-3.85143100	0.63113900	-0.98095200
H	-3.94228600	0.49248400	0.78295300
H	-4.20573400	2.98273400	0.97942600
H	-4.14380900	3.12776100	-0.77437900
C	-5.95941900	2.20398400	-0.02802800
H	-6.25071700	1.53482100	0.79342100
H	-6.19241800	1.67022700	-0.95958000
C	-6.77949400	3.49603000	0.04298200
H	-6.53363800	4.16968300	-0.78607600
H	-7.85138400	3.28009400	-0.01022100
H	-6.59423500	4.03515700	0.97944300
C	6.19354000	1.59267400	0.22403600
H	6.20281500	0.94257100	1.11065600
H	6.72804700	1.04227600	-0.56261000
C	6.93998000	2.89376400	0.53599000
H	7.97028800	2.69419500	0.84916900
H	6.98036200	3.54885400	-0.34259600
H	6.44862300	3.45068100	1.34324800
Zr	-0.20135400	-1.03724300	0.04740200

5f

C	-1.20050800	1.62974800	1.41651800
C	0.29638100	1.34892100	1.32271800
H	-1.59515400	1.48719000	2.42169700
H	-1.45395600	2.63594500	1.08659800
C	1.09861300	2.59162300	0.85996700
H	0.49386600	0.56591700	0.50797700
C	2.54511000	2.34629200	0.41164700
H	0.55240800	3.08355400	0.04507800
H	1.08783000	3.30331200	1.69700000
H	3.11883500	1.86924000	1.21743700
H	2.55436300	1.64050300	-0.43463700
H	-0.16124100	2.15897400	-1.93963900
C	-1.08954000	1.60275600	-1.93768100
C	-1.31520800	0.35933400	-2.58709900
C	-2.31632600	2.02421900	-1.35907200
C	-2.66159500	-0.01595700	-2.37303900
H	-0.58413000	-0.19634600	-3.16068600
C	-3.28402400	1.02022900	-1.60936600
H	-2.49304800	2.95553400	-0.84156600
H	-3.14776400	-0.90232100	-2.76045500
H	-4.32822200	1.06692300	-1.33014300
C	0.86503000	0.73114100	2.61497600
H	0.31313200	-0.16493500	2.91628400
H	0.78484300	1.46063900	3.42861600
H	1.91825900	0.45441900	2.51460100
C	-3.60160900	-0.49507500	1.53546100
C	-2.47538700	-1.01766900	2.22660500
C	-3.82949000	-1.31591900	0.39718800
H	-4.20866700	0.34334400	1.85210300
C	-1.97698200	-2.11690600	1.49442500
H	-2.06960200	-0.63634600	3.15313000
C	-2.81322900	-2.30112100	0.35000500
H	-4.64486900	-1.21502800	-0.30624600
H	-1.13852900	-2.73880100	1.78094100

H	-2.73008800	-3.09126100	-0.38483500
C	1.16198200	-1.44737200	-0.93835700
C	0.05689700	-2.21898100	-1.04776600
H	-0.60327900	-2.15762500	-1.90739300
H	-0.08848700	-3.06660400	-0.38459400
H	1.33658400	-0.67262300	-1.68633900
C	2.27505500	-1.67984800	0.04075300
H	2.60298900	-0.73003300	0.47849600
H	1.93381100	-2.32374300	0.86057900
C	3.48837200	-2.33694700	-0.66454500
H	3.17445600	-3.29371100	-1.10186600
H	3.81108200	-1.70264800	-1.50172200
C	3.26331200	3.63797300	-0.00754900
H	3.25517700	4.34128200	0.83613000
H	2.69625500	4.12369400	-0.81432800
C	4.70666100	3.40250600	-0.46382000
H	5.18762500	4.34315200	-0.75108500
H	5.30790600	2.95304900	0.33562100
H	4.74789300	2.73101900	-1.33044500
C	4.66825800	-2.56317600	0.29164800
H	4.33819500	-3.18942400	1.13189100
H	4.97225900	-1.60019100	0.72499000
C	5.86826900	-3.21921200	-0.39895400
H	6.69305500	-3.36612300	0.30592200
H	5.60321100	-4.20007500	-0.81064400
H	6.24056400	-2.59986000	-1.22346800
Zr	-1.64644500	-0.08673400	-0.05182400

5g

C	1.10212100	1.38204100	-0.04189300
C	-0.16983000	1.84530600	0.68007300
H	0.03950700	2.02710200	1.73951100
H	-0.96460200	1.04594400	0.70039600
H	3.24466400	-0.88481300	1.51599100
C	2.23750100	-1.20955200	1.74272900
C	1.26289700	-0.46460900	2.45242600
C	1.67230600	-2.47785600	1.42979800
C	0.08595500	-1.24704700	2.54365900
H	1.39829400	0.52472900	2.86408500
C	0.33987000	-2.49928300	1.91046600
H	2.17968000	-3.29434900	0.93420200
H	-0.82388800	-0.96079800	3.05576300
H	-0.34395200	-3.33634600	1.84777700
H	-1.33854600	-2.22801800	-2.38716600
C	-0.32003300	-1.90455900	-2.21377800
C	0.21892100	-0.63046200	-2.53882200
C	0.70605300	-2.68894000	-1.63923400
C	1.60272000	-0.64661600	-2.21647600
H	-0.31403200	0.18615200	-3.01095800
C	1.90207500	-1.90665800	-1.64311100
H	0.61444600	-3.71471500	-1.30597500
H	2.30769700	0.15391000	-2.38453200
H	2.88101800	-2.23794500	-1.32221200
C	-0.83499200	3.08444900	0.05565100
H	-1.12683300	2.90079000	-0.98468500
H	-0.13110300	3.92296400	0.05854500
H	-1.72425500	3.39170600	0.61595000
H	0.99167000	1.64072100	-1.10256300
C	2.38714500	2.03765400	0.47110500
H	2.24348600	3.13105600	0.48164100
H	2.57162100	1.76131900	1.51782900
C	3.64497400	1.73928000	-0.35624600
H	3.83522000	0.65541200	-0.36996400
H	3.47037600	2.03337900	-1.40241900
C	4.89562100	2.46355700	0.16190900
H	5.06860600	2.18196300	1.21043600
H	4.70871600	3.54606500	0.16472000
C	6.15080300	2.16237600	-0.66332100
H	7.02212600	2.69309300	-0.26588700
H	6.38454600	1.09040300	-0.65770700
H	6.02331200	2.46978900	-1.70829100
H	-2.53171300	-1.58340000	1.43660500
C	-2.36922900	-1.56991200	0.36262000

C	-2.86176000	-0.56287300	-0.39398500
H	-1.99813500	-2.48713400	-0.08749100
C	-3.65328500	0.60207800	0.11636100
H	-2.77229700	-0.63152000	-1.47872700
H	-3.26478000	1.53671400	-0.30792400
H	-3.57253300	0.67278400	1.20800000
C	-5.14318400	0.46636600	-0.28958800
H	-5.54771800	-0.46104700	0.13615800
H	-5.21550100	0.36639400	-1.38140900
C	-5.98650900	1.66333400	0.17234600
H	-5.90343400	1.76574500	1.26302700
H	-5.57146600	2.58551300	-0.25757100
C	-7.46118000	1.52906800	-0.22098000
H	-8.03730300	2.39525100	0.12021300
H	-7.57837300	1.45826100	-1.30877700
H	-7.91139200	0.63349200	0.22299100
Zr	0.38082800	-0.79883500	0.03350400

2nd TS

Zr/Pro

6a

C	-1.63023400	-0.28591400	-0.55947000
C	-2.88515000	0.60628300	-0.50976000
H	-1.85534100	-1.24748000	-1.02466400
H	-0.93031000	0.21891600	-1.31100100
C	-3.13604000	1.21977000	-1.90489900
H	-2.70342000	1.43218300	0.19188900
H	-2.28168900	1.81006600	-2.25770400
H	-3.33295500	0.43781800	-2.64797600
H	-0.78838800	2.23390300	1.98783600
C	0.05699400	2.20487400	1.31158600
C	1.39600300	1.87457800	1.66122900
C	0.03118900	2.53268200	-0.06678600
C	2.19211000	1.98597300	0.49307900
H	1.75277200	1.61089100	2.64853800
C	1.34583900	2.37793100	-0.58410400
H	-0.83480400	2.85823300	-0.62834800
H	3.26176100	1.83153100	0.43600400
H	1.65921400	2.58494500	-1.59959300
C	-4.15278800	-0.13899400	-0.05543300
H	-4.08907500	-0.51981300	0.96777400
H	-4.37257100	-0.98257400	-0.72125800
H	-5.01086800	0.53968100	-0.09296800
C	2.48911600	-0.62118000	-1.56511300
C	1.32768500	-1.28749200	-2.02716300
C	2.84486900	-1.18097300	-0.30295100
H	3.02873000	0.15568800	-2.09121300
C	0.95809600	-2.25633900	-1.05200700
H	0.82212200	-1.10347800	-2.96765400
C	1.90990200	-2.20392600	0.00112600
H	3.70813500	-0.91141700	0.29272500
H	0.13504300	-2.95409600	-1.13465400
H	1.94055300	-2.85019700	0.86734400
C	-1.36784000	-1.05144800	1.48424000
C	-0.07139400	-0.92431700	2.08232300
H	0.03105100	-0.16955200	2.85652600
H	0.44380200	-1.85385900	2.30801600
H	-2.09165200	-0.29617700	1.77426100
C	-1.93306100	-2.43948200	1.27249400
H	-1.17301900	-3.13397200	0.90412100
H	-2.79730000	-2.47085600	0.60778600
H	-4.00911800	1.88027200	-1.87799300
H	-2.26005100	-2.80711600	2.25424000
Zr	0.63739000	0.03085800	0.05469000

6b

C	1.60120200	-0.61905500	-0.26583700
---	------------	-------------	-------------

C	3.02279800	-0.26208600	-0.72360300
H	0.95954400	-0.43302100	-1.19245300
H	1.54993400	-1.69382200	-0.06779200
C	4.10123200	-0.95903700	0.12387900
H	3.15883400	0.82545400	-0.66462800
H	4.05825900	-0.69365300	1.18415700
H	4.00668600	-2.04915300	0.04511300
H	-0.50099300	-2.96376900	1.40542600
C	-1.17644900	-2.42880300	0.74923300
C	-2.28921500	-1.63891100	1.15966500
C	-1.14096400	-2.43428900	-0.66606100
C	-2.92852400	-1.14839000	-0.00536700
H	-2.61084100	-1.46889500	2.17890800
C	-2.20731700	-1.62330200	-1.13966900
H	-0.42716500	-2.96295400	-1.28600700
H	-3.82274700	-0.53892300	-0.03046700
H	-2.46427200	-1.45471100	-2.17765900
C	3.20157900	-0.65757200	-2.20693600
H	2.49342700	-0.13023100	-2.85720000
H	3.06101700	-1.73545400	-2.35041300
H	4.21265800	-0.40580400	-2.54369100
C	-1.91483800	1.64498000	-1.42945900
C	-0.55037700	1.77463300	-1.78401500
C	-2.06744900	2.10295300	-0.08877400
H	-2.70631700	1.28032300	-2.07081400
C	0.14512000	2.32235100	-0.66623900
H	-0.11791900	1.52849600	-2.74655800
C	-0.79853300	2.54351400	0.36994800
H	-2.99762900	2.15908800	0.46302200
H	1.19591900	2.57853500	-0.64120900
H	-0.59986500	2.99521000	1.33191400
C	1.38897300	0.10140200	1.80703500
C	0.03274800	0.17315200	2.28108500
H	-0.33297400	-0.69788800	2.81683100
H	-0.26246300	1.11530600	2.73688800
H	1.90764000	-0.83372100	1.99857600
C	2.24894600	1.33673700	1.94089000
H	1.67854100	2.25510900	1.78727500
H	3.12881100	1.35480700	1.29845700
H	5.09751400	-0.68819800	-0.23999900
H	2.61059100	1.35099500	2.97825900
Zr	-0.65724500	-0.00157000	0.04773500

6c

C	3.13441700	1.22096500	-1.90482400
H	2.27914500	1.80954500	-2.25826300
H	3.33334100	0.43935000	-2.64771800
C	2.88388700	0.60704300	-0.50981000
H	2.70151000	1.43270600	0.19194000
C	1.62975400	-0.28622100	-0.55966400
H	1.85569000	-1.24762300	-1.02475700
H	0.92934800	0.21754900	-1.31144200
H	-0.81931800	-1.10386200	-2.96735900
C	-1.32554700	-1.28798400	-2.02725200
C	-0.95642000	-2.25660000	-1.05170400
C	-2.48756100	-0.62199500	-1.56620900
C	-1.90904800	-2.20440300	0.00066700
H	-0.13301500	-2.95403000	-1.13352600
C	-2.84415000	-1.18180600	-0.30427600
H	-3.02707800	0.15456200	-2.09285700
H	-1.94012100	-2.85048300	0.86701200
H	-3.70803800	-0.91251000	0.29061100
H	0.83063300	2.85819300	-0.63449400
C	-0.03351900	2.53279900	-0.06999100
C	-1.34958200	2.37710500	-0.58325300
C	-0.05508200	2.20590500	1.30875100
C	-2.19250200	1.98536300	0.49666900
H	-1.66615400	2.58309900	-1.59795100
C	-1.39293900	1.87540900	1.66259300
H	0.79231200	2.23595300	1.98243700
H	-3.26224600	1.83030000	0.44294700

H	-1.74666600	1.61243000	2.65117900
C	4.15208200	-0.13735500	-0.05557300
H	4.08880800	-0.51804500	0.96771400
H	4.37223800	-0.98093000	-0.72127900
H	4.00618400	1.88318100	-1.87742200
C	1.93352900	-2.43988400	1.27232600
H	2.79685400	-2.47130900	0.60642000
H	1.17329700	-3.13503400	0.90559100
C	1.36792800	-1.05200600	1.48403000
H	2.09163400	-0.29659400	1.77394300
C	0.07153800	-0.92505800	2.08234200
H	-0.03064000	-0.17031500	2.85661400
H	-0.44366400	-1.85457300	2.30810500
Zr	-0.63766700	0.03089100	0.05532900
H	5.00976100	0.54181200	-0.09340600
H	2.26215400	-2.80667300	2.25385200

6d

C	-1.60075400	-0.61984500	-0.26618600
C	-3.02212500	-0.26199800	-0.72383700
H	-1.54990900	-1.69477600	-0.06905000
H	-0.95887200	-0.43341500	-1.19257900
C	-3.20092300	-0.65661300	-2.20740500
H	-3.15771600	0.82556200	-0.66422000
H	-2.49251800	-0.12920500	-2.85733800
H	-3.06076100	-1.73446900	-2.35146500
H	-1.19722100	2.57917400	-0.63538500
C	-0.14643500	2.32316900	-0.66250700
C	0.79913900	2.54353700	0.37212000
C	0.54713900	1.77689000	-1.78214400
C	2.06725400	2.10352900	-0.08934000
H	0.60218100	2.99437600	1.33483800
C	1.91225700	1.64686700	-1.43019900
H	0.11295900	1.53171100	-2.74415100
H	2.99845500	2.15932700	0.46077200
H	2.70264800	1.28304300	-2.07336800
C	-4.10085800	-0.95906200	0.12317300
H	-4.05890800	-0.69303100	1.18332400
H	-4.00564700	-2.04917200	0.04511700
H	-5.09697500	-0.68898800	-0.24170900
C	2.20888800	-1.62167400	-1.14026300
C	1.14204700	-2.43311300	-0.66863300
C	2.92909500	-1.14822800	-0.00469900
H	2.46684800	-1.45195100	-2.17781900
C	1.17616600	-2.42927900	0.74674300
H	0.42873400	-2.96096600	-1.28982900
C	2.28864600	-1.64005600	1.15915000
H	3.82352300	-0.53899500	-0.02830300
H	0.50007400	-2.96494400	1.40169800
H	2.60944600	-1.47129800	2.17885800
C	-1.38900400	0.09907200	1.80651900
C	-0.03281200	0.17068000	2.28098700
H	0.26165700	1.11244600	2.73810800
H	0.33297400	-0.70073000	2.81605300
H	-1.90754200	-0.83630800	1.99716100
C	-2.24916500	1.33408000	1.94237000
H	-1.67830900	2.25282600	1.79269500
H	-3.12776900	1.35431600	1.29828300
H	-4.21187600	-0.40427900	-2.54410100
H	-2.61285200	1.34527100	2.97907000
Zr	0.65765100	-0.00133100	0.04770600

6e

C	-1.70409800	-0.41449900	-0.54725200
C	-3.12964000	0.08447100	-0.26650000
H	-1.73090600	-1.31943400	-1.15997900
H	-1.20797300	0.38134800	-1.20637200
C	-3.65382000	0.87616000	-1.48417000
H	-3.10640400	0.77243100	0.59104600
H	-3.01966800	1.74044600	-1.71657900
H	-3.70102800	0.24168100	-2.37709000

H	-1.52917700	2.65840200	0.22877800
C	-0.51744700	2.42310700	0.53335400
C	-0.12951700	1.86084700	1.77333500
C	0.65757900	2.65010800	-0.23690900
C	1.28895700	1.75463600	1.78754500
H	-0.79461100	1.59122000	2.58403400
C	1.77480100	2.25437100	0.55123500
H	0.69875900	3.10700100	-1.21778600
H	1.89541700	1.39510500	2.60947300
H	2.81489900	2.34915600	0.26935200
C	-4.10113500	-1.06518400	0.05578700
H	-3.83275800	-1.61340600	0.96338200
H	-4.14419300	-1.78078100	-0.77452600
H	-5.11105600	-0.66944400	0.20300600
C	0.98080700	-0.90766400	-2.34605200
C	1.17887600	-1.93949800	-1.39457300
C	1.96338100	0.09375000	-2.12565100
H	0.21311000	-0.88186900	-3.10973600
C	2.31244200	-1.59521100	-0.60328300
H	0.60434800	-2.85399300	-1.31951500
C	2.79636400	-0.34243800	-1.05504200
H	2.09082100	0.99882100	-2.70597500
H	2.75705100	-2.20283700	0.17136200
H	3.67028200	0.17194700	-0.67738200
H	-1.85335600	-0.59897200	1.87131200
C	-1.16066800	-1.29595500	1.41374100
C	0.17022000	-1.36609700	1.88404900
H	-1.61580500	-2.20212900	1.02491900
C	0.85844900	-2.71723800	2.00872700
H	0.39755300	-0.68062600	2.69846500
H	0.70683300	-3.35155600	1.12983600
H	1.93337800	-2.61701000	2.18173500
H	-4.66465500	1.24807600	-1.28641300
H	0.44706300	-3.25540900	2.87284400
Zr	0.51421900	0.13124600	-0.03845600

6f

C	2.78742200	0.87171500	-0.29853900
C	1.65540600	-0.07328500	-0.74611500
H	2.43051900	1.65076300	0.38164800
H	3.49871700	0.27119600	0.28516500
C	2.24453900	-1.32148000	-1.44163500
H	1.02864300	0.49521700	-1.52640300
H	3.33977700	-1.29506700	-1.43193800
H	1.95016300	-2.26285700	-0.96730500
H	-0.13502700	-3.13515800	-0.56449000
C	-0.87749500	-2.37391400	-0.76318600
C	-1.98678400	-2.04766400	0.07177200
C	-0.96254200	-1.57551800	-1.92805700
C	-2.73940000	-1.03691200	-0.57131500
H	-2.24523800	-2.52546100	1.00745500
C	-2.09464900	-0.72274700	-1.80177300
H	-0.28610400	-1.60426800	-2.77150900
H	-3.65893900	-0.60174600	-0.20375600
H	-2.44833900	-0.02199800	-2.54725400
C	3.54518900	1.54459400	-1.45763100
H	3.97324900	0.81050800	-2.14776500
H	4.36608000	2.16136500	-1.07638800
H	2.88050600	2.19624500	-2.03891100
C	-2.18521300	1.95930300	0.39918400
C	-1.32018600	2.36030400	-0.65831300
C	-1.42191200	1.88680200	1.58670000
H	-3.24437700	1.75898000	0.31057300
C	-0.03048200	2.59067800	-0.09972300
H	-1.61207100	2.55175500	-1.68329700
C	-0.08260400	2.27270900	1.27578900
H	-1.80677800	1.64464500	2.56954400
H	0.83458800	2.94694500	-0.64235300
H	0.73220100	2.36322200	1.98306100
H	-0.57764900	-0.23934900	2.87034700
C	-0.03153800	-1.05571900	2.40875600
C	1.30143600	-0.94858400	2.15694500
H	-0.50227300	-2.03319000	2.43550600

C	2.21216700	-2.11260000	1.92970400
H	1.78150600	0.02146200	2.27570800
H	1.66489600	-3.02508300	1.67608100
H	2.96699900	-1.91367100	1.16594200
H	2.75435700	-2.30058400	2.86781900
H	1.94957900	-1.39077700	-2.49399500
Zr	-0.49287800	0.05427000	-0.00272200

6g

C	3.06544700	0.18294400	-0.04705600
C	1.85519900	-0.76236000	0.00722100
H	2.75363900	1.22736200	0.03358900
H	3.68787300	-0.01968900	0.83332100
C	2.29896700	-2.21194500	0.19107200
H	1.32568600	-0.70040300	-1.01296000
H	2.96248000	-2.29549500	1.05867400
H	1.47244000	-2.91049700	0.33047900
H	-0.15417800	-2.97563800	-1.38001800
C	-0.93347300	-2.38994100	-0.90899100
C	-1.25043600	-2.37074500	0.47345900
C	-1.82781500	-1.51573500	-1.58013400
C	-2.36565200	-1.50664200	0.65729000
H	-0.76435300	-2.94966200	1.24846600
C	-2.72311400	-0.98109100	-0.60926600
H	-1.86281000	-1.33800800	-2.64724400
H	-2.88009600	-1.31445700	1.58967000
H	-3.55872500	-0.32418600	-0.80855700
C	3.93339600	0.01870100	-1.30931600
H	4.38099300	-0.97712700	-1.37611600
H	4.75112600	0.74628400	-1.29594000
H	3.35319900	0.18779100	-2.22509100
C	0.54973800	1.93938500	-1.48432900
C	0.35808700	2.44665200	-0.17561500
C	-0.72443200	1.62694700	-2.02994900
H	1.49821500	1.81864700	-1.99166600
C	-1.04122000	2.47627300	0.08477400
H	1.13360300	2.79908200	0.49116800
C	-1.70781400	1.97953600	-1.06301200
H	-0.91449600	1.25157900	-3.02736200
H	-1.51559500	2.85636800	0.97816400
H	-2.77939100	1.91555800	-1.19435900
H	1.16875000	-1.45150400	2.23226100
C	1.03620500	-0.38845800	2.06952100
C	-0.22314500	0.19722800	2.34534800
H	1.92696700	0.21069500	2.23258900
C	-0.29878400	1.53961700	3.05916200
H	-0.97880600	-0.51074000	2.67869300
H	0.41675400	2.26943700	2.66862400
H	-1.29975000	1.97746100	3.00974600
H	2.87482600	-2.55291600	-0.67797200
H	-0.06757100	1.39699900	4.12306100
Zr	-0.42344300	-0.00047800	-0.09880700

Zr/But

6a

C	1.33128400	0.10905600	-0.63543200
C	2.65413500	-0.55238700	-0.20408600
H	1.49116200	0.79687200	-1.46751300
H	0.71067700	-0.73414200	-1.09884600
C	3.00157500	-1.69417500	-1.20093900
H	2.51295300	-1.01267100	0.78492300
C	4.20991100	-2.55010100	-0.80097200
H	2.12739200	-2.35316600	-1.30404800
H	3.17005400	-1.25679700	-2.19490600
H	4.31895500	-3.39277300	-1.49124600
H	5.14630400	-1.98533100	-0.82834400
H	4.09267000	-2.96080500	0.20937200
H	0.78302900	-2.85035700	0.61163500

C	-0.12538500	-2.39531000	0.98451400
C	-0.22662300	-1.52319700	2.09709400
C	-1.42799000	-2.58439000	0.44933700
C	-1.59908300	-1.19319900	2.27486700
H	0.59224700	-1.19722600	2.72602600
C	-2.34093200	-1.85046000	1.26068300
H	-1.68622100	-3.22353300	-0.38545800
H	-2.01071400	-0.57223700	3.06001800
H	-3.41640800	-1.82473900	1.14232000
C	3.81876600	0.44873700	-0.10780200
H	3.64659000	1.23662100	0.63070200
H	4.00517600	0.92676800	-1.07756500
H	4.73692500	-0.06450100	0.18915000
C	-1.62532300	0.09112100	-2.41025800
C	-1.37544800	1.41498800	-1.94962900
C	-2.75255100	-0.40998500	-1.71359500
H	-1.06542000	-0.43581500	-3.17361300
C	-2.36725100	1.73825000	-0.98603200
H	-0.60662200	2.07957200	-2.32094600
C	-3.20616800	0.60590000	-0.82203700
H	-3.20670000	-1.38223200	-1.85403100
H	-2.48530300	2.68934400	-0.48551700
H	-4.07092700	0.54405300	-0.17308000
Zr	-0.92808800	-0.13700000	0.03963200
H	-0.47455000	1.28940100	2.49180900
C	-0.40580700	1.64955100	1.46962000
C	0.90100000	1.64665300	0.87855100
H	-1.01653900	2.52726600	1.27618600
C	1.35527300	2.87561100	0.10825300
H	1.67610200	1.16730000	1.47003500
C	1.79677100	3.97363400	1.09586200
H	2.18685700	2.64940200	-0.56313300
H	0.52997500	3.25045000	-0.50745700
H	2.12791100	4.85778200	0.54225300
H	0.97818700	4.27164100	1.75822600
H	2.63284300	3.63804700	1.71980100

6b

C	-1.16597000	-0.86842500	-0.09575800
C	-2.52479900	-1.04677000	0.60097300
H	-0.42120300	-1.31200600	0.64847400
H	-1.12888200	-1.51265000	-0.97906800
C	-3.68600200	-1.10463300	-0.41969000
H	-2.69298200	-0.20741100	1.28862700
C	-5.08364200	-1.05935300	0.21034900
H	-3.60247400	-0.27491300	-1.13132200
H	-3.57692100	-2.02373800	-1.01301100
H	-5.85164000	-1.05362000	-0.56962500
H	-5.27836000	-1.92415000	0.85196000
H	-5.21992000	-0.15480500	0.81557400
H	0.83217400	-1.21745100	-3.03885500
C	1.55262000	-1.22787000	-2.23021500
C	2.60225000	-0.28455300	-2.03467900
C	1.64919500	-2.20867800	-1.21364200
C	3.33478300	-0.67973000	-0.88828300
H	2.82165800	0.56645400	-2.66619900
C	2.73471200	-1.86234300	-0.36495600
H	1.00952600	-3.07506000	-1.09762300
H	4.21166000	-0.18341200	-0.49267700
H	3.08319200	-2.43299400	0.48651000
C	-2.48583200	-2.33119400	1.46033200
H	-1.69788600	-2.28193300	2.22137400
H	-2.30653000	-3.21762900	0.84000500
H	-3.43444300	-2.47588600	1.98457000
C	2.38594200	0.28808700	2.11644000
C	1.05877300	0.02319800	2.53244800
C	2.39715700	1.55070100	1.45597300
H	3.24440500	-0.34828800	2.28658400
C	0.24508200	1.12562900	2.13784700
H	0.72749300	-0.85081500	3.08046800
C	1.07886700	2.07529500	1.49317900
H	3.26814300	2.04827800	1.04767900

H	-0.81000900	1.23933600	2.34812000
H	0.77499000	3.04252300	1.11782700
C	-1.17218100	1.07109300	-1.12726800
C	0.13061200	1.58483300	-1.47077200
H	0.47880600	1.37269900	-2.47731800
H	0.33268000	2.60525300	-1.15343400
H	-1.65642800	0.47795500	-1.89917700
C	-2.11269700	1.98670200	-0.36689000
H	-1.55092000	2.58198000	0.35976700
H	-2.87504500	1.43651000	0.18551600
C	-2.81616200	2.93305800	-1.36250800
H	-3.41744900	2.37442400	-2.08850600
H	-3.48772000	3.60632500	-0.82059100
H	-2.09565500	3.54276000	-1.91654400
Zr	1.03958700	-0.00345000	-0.02041000

6c

C	2.47038500	-2.12458800	1.68200300
H	1.52516800	-2.67324100	1.77154100
H	2.66983800	-1.64491800	2.64799700
C	2.42404200	-1.07729500	0.54660200
H	2.26871400	-1.61424500	-0.40098300
C	1.22621800	-0.13529700	0.78783600
H	1.46620000	0.61080700	1.54759200
H	0.43103900	-0.78382600	1.29457700
H	-1.32847900	0.12524400	3.16707200
C	-1.76198900	0.61364900	2.30252500
C	-1.28343000	1.80237600	1.68353800
C	-2.91877300	0.18963400	1.60308700
C	-2.16497000	2.12785200	0.61806400
H	-0.43572300	2.38887900	2.01238500
C	-3.16476500	1.12342300	0.55387600
H	-3.52779900	-0.67213400	1.84332600
H	-2.10730600	3.00295000	-0.01428100
H	-3.99791800	1.09985400	-0.13739700
H	0.22151700	-3.08508900	-0.14913300
C	-0.55772800	-2.52912600	-0.65379100
C	-1.90871100	-2.42071800	-0.22799300
C	-0.41316900	-1.79682800	-1.85856100
C	-2.60838300	-1.64602400	-1.19827400
H	-2.34184900	-2.89581100	0.64309900
C	-1.68476400	-1.25867000	-2.20203400
H	0.49720500	-1.69583300	-2.43605200
H	-3.66665200	-1.41956100	-1.18681500
H	-1.91573300	-0.67783500	-3.08561300
C	3.77247900	-0.32457800	0.45021100
H	3.71474100	0.44623600	-0.32599000
H	3.94906900	0.20526800	1.39732800
H	3.25832700	-2.86179100	1.50591600
C	4.97545300	-1.22286500	0.13221800
H	4.80819600	-1.80475300	-0.78243200
H	5.19851900	-1.92372600	0.94190900
H	3.27274700	2.83233200	-1.81198900
C	2.47021100	3.37199200	-1.29661300
H	1.76051500	3.72498100	-2.05125500
C	1.78279300	2.48326900	-0.24122500
H	2.51790900	2.20581600	0.51775000
H	0.99438000	3.05583600	0.26026100
C	1.17708500	1.26193400	-0.91346000
H	1.89488900	0.59132500	-1.37751800
C	-0.06570400	1.41145100	-1.61398400
H	-0.12874300	0.94496800	-2.59271800
H	-0.51941000	2.39809900	-1.57269300
Zr	-0.99656000	-0.06528000	-0.04286900
H	2.91493300	4.24616500	-0.81080900
H	5.87040800	-0.61232600	-0.02448300

6d

C	1.26021400	-0.50042400	-0.57233100
C	2.71214300	-0.72110100	-0.12274500

H	1.16547600	-0.78051000	-1.62551600
H	0.67186500	-1.28361300	0.01598300
C	2.93111200	-2.23250000	0.17215100
H	2.88315200	-0.19172000	0.82441600
C	4.31626300	-2.57484100	0.73356300
H	2.17058600	-2.56085700	0.89541200
H	2.75217700	-2.80719800	-0.74747000
H	4.35891800	-3.63301200	1.01084600
H	5.11336200	-2.39681600	0.00565100
H	4.53940400	-1.98663200	1.63184500
H	1.01903500	0.55355600	2.48309500
C	-0.03697500	0.36463300	2.34391200
C	-1.04871500	1.34399400	2.16933900
C	-0.66549600	-0.91436700	2.38004600
C	-2.29539200	0.67422800	2.06125100
H	-0.90584900	2.41535300	2.14913000
C	-2.05784200	-0.72310100	2.20953600
H	-0.16933700	-1.86459000	2.53765400
H	-3.26291100	1.14694100	1.94552100
H	-2.81149300	-1.49959100	2.21112800
C	3.71193400	-0.21691900	-1.17762400
H	3.57479700	0.84009300	-1.42255600
H	3.61098000	-0.79202000	-2.10666700
H	4.74007700	-0.33340100	-0.82523400
C	-2.52730000	-1.86787700	-0.85598400
C	-1.52791000	-1.74296100	-1.85816600
C	-3.29968000	-0.66946500	-0.86129800
H	-2.71061400	-2.74402800	-0.24705200
C	-1.65382300	-0.46341800	-2.45086000
H	-0.79760600	-2.49938100	-2.11846500
C	-2.75730100	0.19936300	-1.84013400
H	-4.16490100	-0.46876600	-0.24250800
H	-1.04294300	-0.07075100	-3.25431500
H	-3.13572200	1.17994300	-2.09764800
C	0.94694900	1.65965200	-0.79396400
C	-0.43438800	2.06960800	-0.83981700
H	-0.71141900	2.87318600	-0.16130500
H	-0.87033400	2.17577900	-1.82890400
H	1.40631900	1.45857700	-1.75855200
C	1.85714300	2.36509900	0.19357600
H	1.30741600	2.58593900	1.11348500
H	2.72305000	1.76249500	0.47116900
C	2.35660200	3.68584500	-0.42902400
H	3.00619600	4.20683800	0.28123700
H	2.93640100	3.50425300	-1.34098000
H	1.52545400	4.35118700	-0.68288800
Zr	-0.99116900	-0.03884900	0.00287300

6e

C	-1.43569200	0.47842300	0.68377400
C	-2.85844200	0.70043000	0.14971300
H	-1.33003600	0.91069600	1.68212900
H	-1.32063500	-0.65238400	0.83262300
C	-3.80090200	-0.39240500	0.72576800
H	-2.85318600	0.57986800	-0.94425000
C	-5.22867700	-0.36298800	0.16634400
H	-3.36396400	-1.37973900	0.51635800
H	-3.82972200	-0.29692300	1.82011500
H	-5.79613300	-1.22237400	0.53757200
H	-5.77206900	0.53850800	0.46434200
H	-5.22986500	-0.41176000	-0.92940600
H	-1.98629100	-1.64006100	-1.61173000
C	-0.90922400	-1.66615200	-1.71408000
C	-0.12062500	-0.75530100	-2.45729500
C	-0.04196300	-2.64007100	-1.14388600
C	1.23734500	-1.16854400	-2.36740800
H	-0.49067800	0.09170300	-3.02111500
C	1.28302700	-2.34064700	-1.56817400
H	-0.34472000	-3.49548700	-0.55304600
H	2.08247800	-0.69788100	-2.85408100
H	2.16632000	-2.92480400	-1.34771500
C	-3.37795700	2.10996500	0.48436300
H	-2.74711800	2.90164600	0.07093500

H	-3.43423700	2.25404800	1.57067600
H	-4.38144400	2.25819300	0.07725500
C	0.84737400	-0.93767500	2.53750000
C	1.52529000	0.28017900	2.27928800
C	1.52680500	-1.97805500	1.84973700
H	-0.03665200	-1.05928000	3.15134400
C	2.65122400	-0.00999500	1.45641900
H	1.26317700	1.25140400	2.67907700
C	2.65213900	-1.40222500	1.19211400
H	1.26610900	-3.02871400	1.86767100
H	3.40063200	0.69594900	1.13004200
H	3.40070000	-1.93809300	0.62332600
Zr	0.59381800	-0.48265200	0.01742300
H	-1.03774500	1.87433900	-1.25746000
C	-0.27666400	1.94913900	-0.48907500
C	1.08539200	1.76399200	-0.83106600
H	-0.50979200	2.64222700	0.31420400
C	2.14890600	2.67636500	-0.22577800
H	1.25664600	1.54510500	-1.88456900
C	2.14353800	4.06609200	-0.88796500
H	1.99072200	2.78897500	0.85384800
H	3.14226000	2.23348100	-0.35770600
H	2.93357100	4.69558200	-0.46474700
H	2.31737200	3.99110900	-1.96735200
H	1.18622400	4.57757800	-0.73700500

6f

C	1.52002400	0.65272200	0.40122900
C	2.32541000	0.02718300	1.55728000
H	3.38121300	-0.00738000	1.26807300
H	2.02516400	-1.01199900	1.71762600
H	-0.14715200	1.69842700	-2.72290200
C	-0.94977300	1.63230600	-1.99943000
C	-2.09428100	0.79572200	-2.10468400
C	-1.07238800	2.39774300	-0.81221100
C	-2.91710800	1.03999200	-0.97569300
H	-2.31915000	0.11889300	-2.91859600
C	-2.27783100	2.01895200	-0.16319000
H	-0.37879900	3.15196000	-0.46299500
H	-3.88365700	0.59339200	-0.78706300
H	-2.67002100	2.44441700	0.75193400
H	0.34911900	-2.74756900	1.37495000
C	-0.55804600	-2.15860300	1.41026600
C	-0.82732000	-1.09187900	2.30504200
C	-1.71338200	-2.36135100	0.60684400
C	-2.13472800	-0.60796700	2.03842800
H	-0.16302400	-0.72320600	3.07399800
C	-2.68682800	-1.40732900	0.99551900
H	-1.84170900	-3.12600800	-0.14762500
H	-2.64486300	0.18079300	2.57653500
H	-3.69053400	-1.33259900	0.59992600
C	2.22428500	0.77003600	2.90629400
H	1.18504100	0.90679100	3.22602300
H	2.68511600	1.75878900	2.87488100
H	2.73685000	0.19165500	3.68225600
H	0.62083500	1.16685600	0.89019600
C	2.27532600	1.75504800	-0.35919200
H	3.18636100	1.30618800	-0.77552000
H	1.68083500	2.08221600	-1.21835400
C	2.67896300	3.00104600	0.44925200
H	1.82558300	3.44482900	0.97604500
H	3.45515200	2.78293400	1.18664900
H	2.30839700	-3.11781800	-2.58052500
C	3.09253000	-2.48255400	-2.15786800
H	3.43345400	-1.79688800	-2.94154800
C	2.59608200	-1.71283600	-0.91675800
H	2.26814300	-2.42733200	-0.15315800
H	3.43558000	-1.15206200	-0.50019700
C	1.45466900	-0.79138900	-1.30583400
H	1.76369200	0.03410300	-1.93942400
C	0.18764300	-1.38280100	-1.67100900

H	0.09543200	-2.44834900	-1.47350300
H	-0.19929900	-1.09761400	-2.64611800
Zr	-0.80640500	-0.05192000	-0.05114000
H	3.93783700	-3.12071500	-1.88155100
H	3.08111200	3.75985200	-0.23013800

6g

C	1.74790200	0.71387700	-0.20227600
C	2.66959300	0.47865300	-1.41258700
H	2.96793600	1.45859500	-1.80540300
H	2.11507400	-0.01135400	-2.21892700
H	-0.76003700	2.04925500	2.14422100
C	-0.87345600	0.97438000	2.18732000
C	-2.05914900	0.25011400	1.87944200
C	0.10699200	0.04772900	2.61854900
C	-1.80297900	-1.12383200	2.11545500
H	-3.00306300	0.67479700	1.56841100
C	-0.45522500	-1.25564700	2.55377700
H	1.10849900	0.28520800	2.95213200
H	-2.52112700	-1.92654900	2.01961600
H	0.03439500	-2.17552100	2.84736300
H	0.06810000	-0.99861400	-3.06333000
C	-0.18663100	-1.58906700	-2.19232500
C	0.72294400	-2.29656500	-1.36771500
C	-1.50240400	-1.83687500	-1.71106300
C	-0.01990900	-2.95876900	-0.35422200
H	1.79681900	-2.33899700	-1.49116000
C	-1.39965300	-2.68767300	-0.58247600
H	-2.42324700	-1.47449500	-2.14925200
H	0.38501500	-3.60976600	0.41004700
H	-2.22863500	-3.09521600	-0.02041900
C	3.93659500	-0.35729400	-1.14395000
H	3.69616400	-1.32586300	-0.68890600
H	4.64423600	0.14830500	-0.48492200
H	4.45141700	-0.55409000	-2.09016200
H	1.74595900	-0.25507200	0.41507300
C	2.20544600	1.85739300	0.72075500
H	2.43162600	2.72404200	0.08743400
H	1.38161400	2.16699300	1.36942700
C	3.43135500	1.57182300	1.61049300
H	3.31885200	0.64174200	2.18071300
H	4.35696400	1.49979500	1.03611100
H	-1.88531400	3.99041700	-1.88006900
C	-2.74904500	3.35922800	-1.64239000
H	-3.11637800	2.92663100	-2.57993100
C	-2.37856300	2.26089000	-0.62936400
H	-2.03178000	2.72948900	0.29890600
H	-3.28455300	1.69632300	-0.38165800
C	-1.31422200	1.31961900	-1.18966800
H	-1.65283600	0.78977100	-2.07843000
C	0.04179800	1.73584300	-1.25077900
H	0.31712800	2.63884800	-0.71428900
H	0.60890600	1.55704300	-2.15694000
Zr	-0.33172200	-0.48465200	0.13356900
H	3.55711600	2.38832000	2.32936500
H	-3.53831700	4.00308400	-1.23963600

Zr/Hex

6a

C	1.32943000	2.99482100	0.08152900
H	0.43318100	3.25672800	0.65060500
H	1.19625900	3.35577000	-0.94600800
C	1.63318000	1.48628900	0.09637900
H	1.78380600	1.17515200	1.14049100
C	0.49323100	0.64652200	-0.51163300
H	0.99083700	-0.32152500	-0.86679500
H	0.12473200	1.10005800	-1.43292700
H	2.53651000	-1.28884900	1.14241300
C	1.63865600	-1.84776100	1.37227600

C	0.66015500	-1.49399300	2.33380900
C	1.24506800	-3.07322000	0.76899700
C	-0.32967200	-2.51573700	2.35253300
H	0.68103500	-0.61685400	2.96842900
C	0.03353800	-3.49260500	1.39106900
H	1.80038100	-3.62069200	0.01792800
H	-1.19393000	-2.55670100	3.00290800
H	-0.50119000	-4.41101100	1.18612700
H	-1.70242700	-0.08765400	-2.67954700
C	-1.66360300	-1.06921000	-2.22597300
C	-0.64519200	-2.04359300	-2.43278200
C	-2.65758600	-1.64441600	-1.39222400
C	-1.00309900	-3.20939200	-1.71209800
H	0.23551300	-1.92502300	-3.05266500
C	-2.24195000	-2.95840100	-1.05393200
H	-3.58482700	-1.17768800	-1.09034000
H	-0.44361800	-4.13539500	-1.68354600
H	-2.79469400	-3.66396100	-0.44586600
C	2.95162200	1.18883200	-0.67092500
H	3.10402400	0.09943500	-0.70826300
H	2.83616500	1.51284700	-1.71540200
H	2.15854100	3.55333800	0.52312900
C	4.21489300	1.82696000	-0.07161400
H	4.27944000	1.57667100	0.99812400
H	4.15118700	2.92065300	-0.12854000
C	5.49989700	1.36936600	-0.77799900
H	5.58128100	0.27491100	-0.71112000
H	5.42738200	1.60560900	-1.84875200
C	6.76240300	2.01337800	-0.19588900
H	6.88001400	1.76990900	0.86690600
H	7.65951300	1.66507500	-0.71827400
H	6.72837200	3.10563200	-0.28533000
H	-3.60049600	2.42185600	1.18768500
C	-2.88732700	2.99736100	0.58341600
C	-3.64839100	3.98315800	-0.31600100
H	-2.26192000	3.55768100	1.29302200
C	-1.99864300	2.03018400	-0.23048300
C	-4.52877800	4.95190600	0.47993000
H	-4.27007100	3.41909800	-1.02543300
H	-2.92924100	4.55166000	-0.92172100
H	-2.62826600	1.46522900	-0.92815500
H	-1.30076700	2.62235400	-0.82881000
C	-1.27677100	1.07103000	0.70003700
H	-3.93041600	5.55862600	1.16973600
H	-5.06116500	5.63607800	-0.18879300
H	-5.27845300	4.41394800	1.07209500
H	-0.58500600	1.53962100	1.39387400
C	-2.00512100	-0.04958100	1.22919500
H	-3.03341500	-0.15239700	0.89279500
H	-1.87642400	-0.25006200	2.28880200
Zr	-0.52668700	-1.42303800	0.04063800

6b

-- not located

6c

C	-1.12705900	-2.94648000	-1.45959500
H	-0.10419200	-3.33747500	-1.40067600
H	-1.31307800	-2.65530200	-2.50056500
C	-1.34325900	-1.74922100	-0.50654400
H	-1.18355600	-2.10484800	0.52205100
C	-0.29539700	-0.66238600	-0.82434400
H	-0.59229400	-0.07931700	-1.69794800
H	0.62667800	-1.23633400	-1.18464500
H	2.41501100	-0.30916100	-3.10561200
C	2.64461000	0.39450000	-2.31436700
C	1.85524200	1.51749000	-1.93570600
C	3.79736200	0.37181100	-1.49154500
C	2.53654100	2.20117900	-0.89451400
H	0.93238100	1.82946100	-2.40603700
C	3.72569000	1.48425900	-0.60275500

H	4.60362900	-0.34806100	-1.54623300
H	2.22410600	3.12359100	-0.42523000
H	4.47096200	1.76113400	0.13257500
H	1.14662900	-3.22407900	0.58656500
C	1.80637800	-2.47698600	1.00816000
C	3.12762800	-2.19101200	0.56802800
C	1.51117600	-1.62714200	2.10229400
C	3.65994500	-1.18271000	1.42267900
H	3.65663800	-2.69588100	-0.23051200
C	2.66013900	-0.83008600	2.36470300
H	0.58384400	-1.60994600	2.66110500
H	4.66213800	-0.77651000	1.37812400
H	2.76465300	-0.10185200	3.15870400
C	-2.79582500	-1.22752700	-0.61228800
H	-2.92193400	-0.34148600	0.02074900
H	-2.97567000	-0.89359100	-1.64519000
H	-1.80480600	-3.76897600	-1.21653900
C	-3.87704200	-2.24291100	-0.20824900
H	-3.64557600	-2.64577400	0.78925500
H	-3.87387700	-3.09874400	-0.89457300
C	-5.28494200	-1.62927200	-0.19197500
H	-5.30311300	-0.77997300	0.50606500
H	-5.50906400	-1.21400000	-1.18458100
C	-6.37192400	-2.63572200	0.19849200
H	-6.19443300	-3.04486400	1.20038200
H	-7.36140300	-2.16666000	0.20129400
H	-6.40516000	-3.47742600	-0.50351900
H	-2.97734800	2.13556300	1.21925200
C	-2.26625200	2.79319100	0.69932300
C	-3.04103700	3.84538000	-0.10785700
H	-1.67440800	3.28795700	1.48038200
C	-1.33722400	1.93773300	-0.19199100
C	-3.97850700	4.68615300	0.76507000
H	-3.62148600	3.34413200	-0.89467800
H	-2.32776400	4.50366800	-0.62307400
H	-1.94428100	1.45870000	-0.96484200
H	-0.62023600	2.59399600	-0.69980900
C	-0.59150000	0.92265800	0.65717900
H	-3.42361100	5.22534700	1.54187700
H	-4.51387900	5.42769500	0.16326600
H	-4.72665300	4.05853400	1.26352200
H	-1.22303900	0.20324200	1.17028300
C	0.55854500	1.36530400	1.39723400
H	0.62850100	1.02734700	2.42702900
H	0.83517900	2.40820900	1.26652300
Zr	1.83127000	-0.07968800	0.05966700

6d

C	2.82632400	0.67457500	-1.64356200
H	2.37826300	1.66481000	-1.76585900
H	2.76986200	0.15873700	-2.61040000
C	2.14124800	-0.16027200	-0.54786400
H	2.28054800	0.33152900	0.42413300
C	0.63834200	-0.32350100	-0.81977200
H	0.36328700	-1.27423800	-0.24768900
H	0.48596800	-0.55405500	-1.87823800
H	-2.58475300	-2.60427800	2.28750000
C	-2.09178600	-1.64126200	2.27407400
C	-0.69316900	-1.42194500	2.27731100
C	-2.73690400	-0.37071000	2.27758800
C	-0.46778900	-0.01468100	2.28919700
H	0.07045400	-2.19040200	2.29366200
C	-1.73137200	0.63074800	2.30981800
H	-3.80589100	-0.19982900	2.30922000
H	0.49780600	0.47107700	2.32937800
H	-1.90536900	1.69608200	2.36852000
H	-0.98596900	-2.76898200	-2.27227000
C	-1.85254400	-2.24891000	-1.88245300
C	-2.65915400	-2.68336900	-0.79698800
C	-2.37753400	-1.02354400	-2.36019900
C	-3.71162400	-1.73597200	-0.63122000
H	-2.53401300	-3.60372600	-0.24094600
C	-3.53543400	-0.70986100	-1.59191400
H	-1.99060400	-0.44589900	-3.19067600

H	-4.51952800	-1.80331300	0.08599000
H	-4.18472500	0.14389800	-1.73485900
C	2.79188800	-1.56713200	-0.42777200
H	2.24046100	-2.14349700	0.33070000
H	2.66335100	-2.10624500	-1.37763200
H	3.88328100	0.82688000	-1.41032900
C	4.27782900	-1.56154000	-0.03696300
H	4.41632500	-0.94559100	0.86401300
H	4.87528500	-1.09147400	-0.82802000
C	4.82401400	-2.97319300	0.22423000
H	4.23968600	-3.44582800	1.02664800
H	4.67032800	-3.59142500	-0.67122400
C	6.30911600	-2.97750000	0.60128800
H	6.49001300	-2.39435700	1.51222400
H	6.66751000	-3.99633900	0.78173700
H	6.92293600	-2.54536600	-0.19794500
H	1.07894300	3.97044500	-1.37633500
C	0.59467200	3.97703900	-0.38948100
C	1.36237600	4.91866000	0.55003500
H	-0.42201600	4.36052500	-0.54651200
C	0.52479700	2.53152000	0.15771600
C	1.44143200	6.35217900	0.01477100
H	2.37707400	4.52725100	0.70700700
H	0.87723100	4.92060700	1.53613200
H	1.54461800	2.17119200	0.30543100
H	0.04160600	2.54761700	1.14020100
C	-0.26935700	1.66101700	-0.79633800
H	0.44204400	6.78208600	-0.12097900
H	1.99068600	6.99875200	0.70684300
H	1.95493000	6.38777300	-0.95323000
H	0.10586500	1.66130600	-1.81683100
C	-1.70804000	1.67030400	-0.67041600
H	-2.26944100	1.70641200	-1.59994100
H	-2.10715500	2.33159100	0.09528800
Zr	-1.56007200	-0.54924100	0.03621900

6e

C	1.91051100	3.03087100	-0.52162000
H	0.96384100	3.44644700	-0.16547200
H	1.93789100	3.13588300	-1.61353000
C	2.10581000	1.55987000	-0.11267800
H	2.10354800	1.49912000	0.98602600
C	0.98828500	0.66274400	-0.66523600
H	1.43208700	-0.39213600	-0.73411100
H	0.74878800	0.93940800	-1.69542400
H	1.83462900	-3.26675200	0.83355000
C	1.11992800	-2.63859900	1.35048600
C	1.37307000	-1.34306000	1.88340400
C	-0.21354200	-2.99540300	1.69603900
C	0.19424400	-0.89312600	2.52560400
H	2.31026800	-0.80513600	1.82281400
C	-0.79099100	-1.91192500	2.40866300
H	-0.69316200	-3.94031400	1.47877200
H	0.07272200	0.05147800	3.04058100
H	-1.79127300	-1.88463300	2.82269100
H	-1.55241800	-0.04704900	-2.82703100
C	-1.37994600	-1.00381200	-2.35088700
C	-0.20798000	-1.79347300	-2.46667800
C	-2.31625200	-1.72216100	-1.55353200
C	-0.39845000	-2.98228500	-1.71415600
H	0.68190300	-1.53761200	-3.02867800
C	-1.71043600	-2.94092300	-1.15932200
H	-3.32659600	-1.41545000	-1.32721100
H	0.30826100	-3.79727000	-1.62239600
H	-2.17971700	-3.72036200	-0.57320600
C	3.47919500	1.02116500	-0.60025600
H	3.55042000	-0.04666300	-0.34218800
H	3.51261100	1.07214200	-1.69820400
H	2.70759400	3.65389700	-0.10803700
C	4.70647900	1.73748800	-0.01544300
H	4.62486100	1.76769000	1.08151000
H	4.73212200	2.78131400	-0.35188800
C	6.02660200	1.05713800	-0.40818100

H	6.01415100	0.01384100	-0.06150200
H	6.09894100	1.01436900	-1.50391700
C	7.25810900	1.77076100	0.15881000
H	7.23020600	1.80295100	1.25460200
H	8.18048300	1.25937600	-0.13575300
H	7.32044500	2.80386900	-0.20310900
C	-1.93317500	0.67290900	0.66176800
C	-0.79527200	1.46260600	0.36804000
H	-0.13864800	1.77924800	1.17041500
H	-0.85586400	2.15292700	-0.46819000
H	-2.05439400	0.44101500	1.71930100
C	-3.25236400	0.94935500	-0.05128400
H	-3.09263500	1.06751400	-1.13092200
H	-3.93534600	0.10147100	0.07830400
C	-3.94513700	2.21553100	0.49519100
H	-4.08266400	2.11274000	1.58108700
H	-3.28380400	3.08196700	0.35106000
C	-5.30183800	2.48648200	-0.16893300
H	-5.16160100	2.58095700	-1.25512300
H	-5.95769000	1.61737500	-0.01901400
C	-5.98894800	3.74552100	0.37059100
H	-6.95258900	3.91033000	-0.12252200
H	-6.17555100	3.66561100	1.44811300
H	-5.37300700	4.63737700	0.20418300
Zr	-0.38315600	-1.11057400	0.00830200

6f

C	0.32090000	1.00830900	0.64049000
C	0.94067800	0.97094500	2.05073800
H	1.92708100	1.44479900	2.00988200
H	1.11710800	-0.06098500	2.36757100
H	-0.63406600	0.76272300	-2.93770900
C	-1.48936900	0.37735200	-2.39750700
C	-2.04720300	-0.92213000	-2.54348000
C	-2.27799600	1.09156100	-1.46094000
C	-3.17558700	-1.00970000	-1.68874300
H	-1.69616900	-1.69743800	-3.21202700
C	-3.31020600	0.22991000	-1.00166600
H	-2.13299700	2.11956600	-1.15479500
H	-3.84253700	-1.85669500	-1.60428800
H	-4.09531900	0.49102100	-0.30333500
H	0.62324400	-2.36946800	2.10432800
C	-0.41352100	-2.34674500	1.79467100
C	-1.42689600	-1.51048300	2.32958900
C	-1.01025300	-3.19421000	0.82196400
C	-2.64577700	-1.81286400	1.66945800
H	-1.30109500	-0.78373500	3.11999800
C	-2.38676800	-2.86519100	0.74375200
H	-0.51261900	-3.97329600	0.26045400
H	-3.61026500	-1.36642600	1.87510100
H	-3.11987500	-3.36139200	0.12233000
C	0.11766200	1.67886000	3.14750000
H	-0.90942900	1.30083600	3.20258100
H	0.05694800	2.75752500	2.99204100
H	0.58594800	1.51113000	4.12321000
H	-0.81382300	1.03107100	0.79687500
C	0.66507100	2.27322300	-0.16115500
H	1.75875500	2.32359100	-0.24674300
H	0.28819800	2.17423300	-1.18537900
C	0.16596500	3.62418500	0.39249100
H	-0.90553600	3.56211400	0.63522000
H	0.68175200	3.86355000	1.32900800
C	0.39599100	4.76899500	-0.60723100
H	-0.13149400	4.54349400	-1.54535600
H	1.46382100	4.81564300	-0.86177400
C	-0.06435200	6.12929800	-0.07398900
H	0.11016000	6.91915000	-0.81174300
H	-1.13550400	6.12416400	0.16101800
H	0.47661400	6.40225800	0.83958900
H	3.56803700	-2.04949300	-1.23757500
C	3.85063200	-1.09140300	-0.78319500
C	5.17291300	-1.25213600	-0.01871800
H	3.99223300	-0.38452300	-1.61287600

C	2.70483900	-0.58906400	0.12645300
C	6.31449900	-1.74700200	-0.91318600
H	5.02666200	-1.95367500	0.81444500
H	5.45067500	-0.29029300	0.43405000
H	2.54214800	-1.31495000	0.93262400
H	3.02540300	0.34737400	0.58977500
C	1.43736100	-0.40193600	-0.68455900
H	6.50589100	-1.04828000	-1.73606600
H	7.24290300	-1.85141700	-0.34230400
H	6.08150500	-2.72439900	-1.35206600
H	1.49476700	0.41404200	-1.39824200
C	0.76032900	-1.58020100	-1.18039000
H	1.12836800	-2.52618600	-0.78998600
H	0.58977400	-1.60487900	-2.25382800
Zr	-1.16226900	-0.81670500	-0.13345300

6g

C	1.35323400	0.48012600	-1.02454000
C	1.79089400	0.23171700	-2.47957600
H	1.62411500	1.15718900	-3.04448100
H	1.14860300	-0.52286800	-2.94406500
H	-0.35203700	1.62351400	2.05127200
C	-0.12203100	0.58119700	2.22654500
C	-1.07041700	-0.44375300	2.49857900
C	1.17251800	0.01019100	2.29156200
C	-0.35702500	-1.64745500	2.72397100
H	-2.14117800	-0.31686200	2.57105500
C	1.03228000	-1.37501000	2.57578600
H	2.11002600	0.53388500	2.15710700
H	-0.79231700	-2.59806200	2.99993400
H	1.84050900	-2.08124500	2.71748200
H	-0.69575800	-2.11439200	-2.75101500
C	-0.40522100	-2.56290100	-1.80946800
C	0.91959800	-2.84257400	-1.39121800
C	-1.29287500	-3.02476700	-0.79833100
C	0.86146900	-3.44952800	-0.10838400
H	1.82193400	-2.64448200	-1.95369500
C	-0.51166800	-3.57738000	0.24723500
H	-2.37420800	-2.99696500	-0.83364000
H	1.70576200	-3.81063200	0.46496500
H	-0.89557000	-4.05299400	1.13916600
C	3.25231300	-0.21697400	-2.67786400
H	3.48787100	-1.11031500	-2.08687400
H	3.97216800	0.55614400	-2.40388800
H	3.41837000	-0.46379400	-3.73178200
H	1.87256100	-0.31421500	-0.37699200
C	1.74523000	1.86316800	-0.47957800
H	1.43176200	2.61232100	-1.21803300
H	1.17586400	2.08137600	0.42874500
C	3.23987700	2.09363500	-0.16362800
H	3.63102700	1.26337500	0.44349600
H	3.82664700	2.09787900	-1.08777600
C	3.47094200	3.42020000	0.57729300
H	2.90583700	3.41339300	1.52056100
H	3.05631600	4.24343100	-0.02059700
C	4.95072900	3.69138900	0.86664900
H	5.07867100	4.63875300	1.40019000
H	5.38862900	2.89897700	1.48554600
H	5.53274600	3.75069500	-0.06041800
H	-3.39575800	2.35506200	-1.35885600
C	-3.91322900	1.65201200	-0.69055000
C	-4.95786700	2.40691100	0.14304700
H	-4.42102100	0.92730200	-1.34298500
C	-2.87137800	0.91363700	0.17537900
C	-5.99041100	3.14085200	-0.71934900
H	-4.44749100	3.12668700	0.79860300
H	-5.47152500	1.69791200	0.80744400
H	-2.34780400	1.64469400	0.80383900
H	-3.40428400	0.23622600	0.85346500
C	-1.88141900	0.12884000	-0.68088700
H	-6.54261500	2.44190300	-1.35871900
H	-6.71973600	3.66948800	-0.09683200
H	-5.51018800	3.88037500	-1.37114400

H	-2.36439100	-0.64589500	-1.27369000
C	-0.84011400	0.80997300	-1.36624400
H	-0.66403200	1.85031400	-1.11017900
H	-0.63682700	0.55716900	-2.40021200
Zr	0.01736900	-1.08215900	0.26411100

β-hydrogen TS to metal

Zr/Et

8a

H	-1.55226800	-2.86208200	-0.36565900
C	-1.82806800	-1.84653000	-0.11070000
C	-1.81651900	-1.28019400	1.19696300
C	-2.34405700	-0.87380300	-1.00857800
C	-2.30135900	0.05169400	1.09665000
H	-1.52776300	-1.78586800	2.10854900
C	-2.62930500	0.30342200	-0.26974200
H	-2.49787400	-1.00786500	-2.07386400
H	-2.44666900	0.73836700	1.92075500
H	-3.06832400	1.21108900	-0.66349600
C	1.88971300	1.54180900	-0.43902400
C	1.57383200	1.55820200	0.94936600
C	0.82507000	2.17469600	-1.14105100
H	2.80847900	1.17635200	-0.87875500
C	0.30225300	2.17813100	1.09807800
H	2.20275800	1.19894700	1.75252300
C	-0.15424300	2.56870200	-0.19438400
H	0.77843100	2.34156200	-2.21167700
H	-0.20299100	2.36917500	2.03625500
H	-1.07204500	3.09937200	-0.41219700
Zr	-0.12140500	0.03842200	-0.14918500
C	3.00872200	-1.87945800	0.67595800
H	3.51725900	-0.99241700	0.28926000
H	3.61564500	-2.75386400	0.40299800
H	1.04670000	-2.86121700	0.51176500
C	1.64821600	-2.07186100	0.06466000
H	0.77406900	-0.92422000	1.16732500
C	1.31015300	-1.64823600	-1.21770300
H	2.04940600	-1.11186400	-1.81006100
H	0.55438100	-2.19968800	-1.77601500
H	2.97058900	-1.83209800	1.76672700

Zr/Pro

8a

C	1.84065900	-0.00182100	-1.33583200
C	2.50649100	-0.00100500	-0.09315700
H	1.84097400	0.91783800	-1.91966600
H	1.84032400	-0.92244000	-1.91813000
C	3.14164500	-1.27109100	0.43226500
H	1.15823500	-0.00021300	1.02867600
H	2.62624100	-2.17365600	0.10049100
H	4.16506800	-1.31067000	0.03512800
H	0.50488600	-2.49292700	1.71363400
C	-0.24302200	-2.26569500	0.96620400
C	-1.52524000	-1.70392000	1.21518700
C	-0.14239200	-2.51838100	-0.43147300
C	-2.22553000	-1.63372500	-0.02358300
H	-1.91871300	-1.42794200	2.18538100
C	-1.37032100	-2.13294000	-1.03844300
H	0.68957500	-2.98836500	-0.93869000
H	-3.24200000	-1.28986200	-0.16266100
H	-1.61715400	-2.22388400	-2.09058700
Zr	-0.28645600	0.00008400	-0.16921900
C	3.14227100	1.26964100	0.43010900
H	2.62825300	2.17197100	0.09552300
H	4.16623700	1.30719400	0.03417200
H	3.21143400	1.27529800	1.52095900

C	-1.37285600	2.13164500	-1.03759400
C	-0.14231500	2.51766200	-0.43602900
C	-2.22447800	1.63506700	-0.01845700
H	-1.62372600	2.22084300	-2.08892800
C	-0.23783400	2.26774000	0.96245500
H	0.68797800	2.98629600	-0.94725400
C	-1.51935300	1.70702700	1.21740300
H	-3.24159700	1.29131700	-0.15294700
H	0.51299200	2.49586600	1.70667000
H	-1.90919400	1.43301700	2.18962300
H	3.21208200	-1.27427000	1.52304100

8b

C	-2.02399500	-1.35221800	-0.41115400
C	-2.02393400	-0.75330100	0.85688200
H	-0.90562300	-0.58095700	-1.33179400
H	-1.52700400	-2.31736500	-0.51018000
C	-1.23407600	-1.15892800	2.05882300
H	-2.73924700	0.04756700	1.01774400
H	-0.91916900	-2.20460100	2.06368800
H	-0.27034700	-0.55287000	2.21330100
H	0.69458300	-3.13742200	0.35571700
C	1.23200300	-2.24343900	0.06613200
C	1.36829100	-1.74530400	-1.25890300
C	2.04267000	-1.44277600	0.92368300
C	2.22176700	-0.61385400	-1.21355700
H	0.92126400	-2.16503300	-2.15017200
C	2.64759800	-0.43364400	0.13851500
H	2.19171500	-1.59366100	1.98618400
H	2.54260000	-0.02952300	-2.06606300
H	3.33953200	0.31964300	0.49262100
C	-3.17041400	-1.12508000	-1.37475600
H	-3.99543600	-1.79243800	-1.09762000
H	-2.88541700	-1.34741900	-2.40569200
H	-3.53986000	-0.09643600	-1.32724900
C	-0.38962100	2.33666400	1.10519900
C	-1.29534000	2.16993400	0.02130400
C	0.92376400	2.40456400	0.57155600
H	-0.65634900	2.43060300	2.15137800
C	-0.54366000	2.12939500	-1.18605600
H	-2.37392800	2.13965700	0.09341800
C	0.82955500	2.27629000	-0.84314400
H	1.83212500	2.56268000	1.13910300
H	-0.94818300	2.05672600	-2.18684400
H	1.65425900	2.33143400	-1.54102200
Zr	0.14631200	0.05433700	0.08485900
H	-1.77565100	-0.93390400	2.98196700

Zr/but

8a

C	-1.35997200	-0.48326300	-1.64791800
C	-2.19260600	-0.63583000	-0.51855100
H	-1.06275800	-1.38048700	-2.18993700
H	-1.49309200	0.40498000	-2.26451900
C	-3.18869200	0.46097900	-0.16936700
H	-1.05943700	-0.26335100	0.79423100
C	-3.70037100	0.50796100	1.27356600
H	-2.78331100	1.43320900	-0.46426900
H	-4.04044100	0.28022500	-0.84389300
H	-4.38017500	1.35608100	1.39841300
H	-4.25582400	-0.39542800	1.54226200
H	-2.87672800	0.62321700	1.98748200
H	-0.98965100	2.68586800	-1.30367500
C	-0.15478200	2.44445800	-0.65946500
C	-0.20301600	2.27835600	0.75359300
C	1.20181300	2.32766600	-1.07105600
C	1.12259600	2.03902100	1.20893200
H	-1.08276800	2.35725000	1.37748500
C	1.99140100	2.08116300	0.08097100

H	1.57114400	2.42933300	-2.08566900
H	1.42428900	1.90079100	2.23967000
H	3.06824700	1.97797600	0.10147100
C	-2.55880100	-2.02649600	-0.04507500
H	-1.82731000	-2.77810500	-0.34643700
H	-3.51497600	-2.28917600	-0.51853000
H	-2.70503000	-2.07984400	1.03555400
C	2.19878300	-1.77440200	-0.75830100
C	1.00490500	-2.44056600	-0.36009000
C	2.71657500	-1.08896600	0.36978200
H	2.64788400	-1.80572900	-1.74492400
C	0.79004500	-2.17058400	1.02064000
H	0.41118400	-3.09422400	-0.98499800
C	1.83873700	-1.32032900	1.46679200
H	3.63242200	-0.51356200	0.39783200
H	-0.00750900	-2.56649500	1.63424400
H	1.97288100	-0.95593000	2.47756200
Zr	0.50778200	0.03696000	-0.19765200

8b

C	1.84704700	-0.64742000	1.38214800
C	2.14338100	-0.20454600	0.08560800
H	0.33001900	-0.13235400	1.76023100
H	1.58564900	-1.69826300	1.50626200
C	1.93117600	-0.92394200	-1.20755300
H	2.66310400	0.74682300	0.00278900
C	2.99028700	-0.60875000	-2.27575400
H	1.82223100	-2.00327400	-1.06471400
H	0.93582100	-0.61569200	-1.71317200
H	2.74172100	-1.08876100	-3.22626500
H	3.07181300	0.46961100	-2.44634000
H	3.96658100	-0.97730200	-1.94763100
H	0.04686100	-3.19292300	0.21506500
C	-0.75051500	-2.46482100	0.13743000
C	-1.45657200	-1.88313400	1.22676200
C	-1.36684900	-2.02794600	-1.07126400
C	-2.47694500	-1.05610500	0.69222600
H	-1.26948300	-2.05807500	2.27781900
C	-2.42622400	-1.15359100	-0.73226100
H	-1.09068900	-2.32938800	-2.07457400
H	-3.20496600	-0.49891800	1.26709000
H	-3.10318600	-0.67434800	-1.42761000
C	2.50367800	-0.00943700	2.58910200
H	3.50746700	-0.43548500	2.70645800
H	1.94330200	-0.20342000	3.50665800
H	2.60973300	1.07228300	2.46559700
C	-0.00823200	2.25870400	-1.22569700
C	0.50952100	2.46408800	0.08326600
C	-1.40077000	2.01023500	-1.11120400
H	0.55294300	2.31705400	-2.15082600
C	-0.56158700	2.33898600	1.01123500
H	1.52800300	2.73244900	0.32856300
C	-1.74314600	2.05897600	0.26960300
H	-2.08627300	1.84899100	-1.93352000
H	-0.49883100	2.48660200	2.08113100
H	-2.73815700	1.95233300	0.68048700
Zr	-0.29297900	0.03435700	0.00161500

Zr/hex

8a

C	5.47494500	0.43923000	1.44055400
H	5.82881600	-0.56938900	1.68411500
H	6.35434400	1.07965600	1.31942600
H	4.90834100	0.81107400	2.30289000
C	4.61924100	0.43457500	0.16985700
H	4.31256000	1.46257000	-0.07173200
H	5.22520400	0.09066900	-0.67953100
C	3.37269000	-0.45417700	0.29700300

H	3.68953800	-1.47305900	0.55247600
H	2.75392300	-0.10423000	1.13587600
C	2.53045900	-0.47368600	-0.98631300
H	2.32508400	0.54838600	-1.32071100
H	3.12607800	-0.93116600	-1.79284500
C	1.24013500	-1.28012300	-0.96923600
H	0.57380500	-0.52625300	0.48374800
C	0.22656000	-0.99215800	-1.91016100
H	-0.40070700	-1.81495900	-2.25215300
H	0.42161200	-0.21999900	-2.65354700
H	-1.94397200	-2.98532900	-0.56981100
C	-2.18484700	-2.15450600	0.07986400
C	-1.57985400	-1.86280700	1.33427500
C	-3.23595000	-1.21714800	-0.13041500
C	-2.24401900	-0.73327400	1.88666500
H	-0.77975200	-2.41849500	1.80365200
C	-3.27754400	-0.34551000	0.98717000
H	-3.90571300	-1.19077400	-0.98296300
H	-2.03217300	-0.28016200	2.84711500
H	-3.98684900	0.45700900	1.14030400
H	0.75052900	2.17278700	-1.88887700
C	0.04534600	2.20973200	-1.06939000
C	-1.35510600	2.42611700	-1.18987900
C	0.36337400	2.13819900	0.31649400
C	-1.90609500	2.48042100	0.11587800
H	-1.90382600	2.54777100	-2.11737100
C	-0.84579500	2.29243900	1.04854000
H	1.35155500	2.02501100	0.74083500
H	-2.94393800	2.66612300	0.35895200
H	-0.93666400	2.31216700	2.12732800
Zr	-1.06440300	0.10323700	-0.18485700
C	1.35227100	-2.68125200	-0.40615200
H	0.40991000	-3.22854300	-0.45989100
H	1.72028000	-2.69496100	0.62148000
H	2.08327900	-3.22182700	-1.02302800

8b

C	-1.06915800	-1.16086300	1.03884000
C	-0.12346200	-1.23567400	2.07149600
H	-0.06905200	-0.39405400	2.76233900
H	1.35231900	-0.92234800	1.42943800
H	-0.06233200	2.10490400	2.33889700
C	0.64856600	2.05081100	1.52429300
C	1.98015600	1.55936700	1.61135000
C	0.46062100	2.58512100	0.21577000
C	2.59756500	1.74754900	0.34874100
H	2.45113800	1.13708600	2.48899800
C	1.65761700	2.39186600	-0.51279300
H	-0.43334100	3.07393300	-0.15211200
H	3.62225100	1.50108300	0.10322100
H	1.84114200	2.70867200	-1.53137500
H	2.73859900	-2.44713500	-0.41000800
C	2.07241500	-1.86264600	-1.03050200
C	0.71360600	-2.16803500	-1.32174800
C	2.41634100	-0.69135900	-1.76124800
C	0.22016000	-1.18715300	-2.22588600
H	0.17054800	-3.03156900	-0.96281400
C	1.27226400	-0.27467400	-2.49860400
H	3.39287900	-0.22689100	-1.78941000
H	-0.77338300	-1.15899000	-2.65746400
H	1.22157000	0.56744600	-3.17715300
Zr	0.74527100	0.05690600	-0.05172200
C	0.27303700	-2.57154700	2.66655500
H	0.33124400	-3.35225000	1.90234100
H	-0.49091800	-2.86969700	3.39481300
H	1.23316600	-2.51730200	3.18509900
H	-1.30980600	-2.09088800	0.53020900
C	-1.87459700	0.02210900	0.61029900
H	-1.91088900	0.79769200	1.38169300
H	-1.39547800	0.56186800	-0.29605500
C	-3.29147500	-0.32190300	0.10921700
H	-3.22085700	-1.09623800	-0.66654300
H	-3.83806100	-0.77040300	0.94838900

C	-4.06087200	0.89058400	-0.42869600
H	-3.50439700	1.33322200	-1.26812300
H	-4.11202300	1.66338000	0.35076500
C	-5.47827500	0.53160900	-0.88715400
H	-6.00087200	1.41439200	-1.26836900
H	-5.46016800	-0.21755200	-1.68730400
H	-6.07117800	0.12445500	-0.06017800

β -hydrogen transfer to monomer TS

Zr/Et

7a

H	1.86461200	2.07835900	1.65474300
C	1.24083900	2.12384600	0.77074300
C	1.65657000	1.83694200	-0.54745700
C	-0.12905000	2.51069900	0.73042800
C	0.54991000	2.04709800	-1.41967800
H	2.65340800	1.54005200	-0.84611600
C	-0.54071800	2.49210100	-0.62928700
H	-0.72971100	2.82976200	1.57242400
H	0.55768100	1.95170400	-2.49759800
H	-1.50857600	2.79697800	-1.00226000
C	3.24622400	-1.61549800	-0.29628100
H	3.45932700	-1.95717700	0.72081800
H	3.60672900	-0.58921400	-0.40779700
H	3.82494400	-2.24649900	-0.98155700
C	-2.55860100	-0.42101400	0.70029800
C	-1.94423000	-1.70240100	0.59983200
C	-2.61364700	0.13413600	-0.60351100
H	-2.96649600	0.02605500	1.59735300
C	-1.61100700	-1.92427700	-0.75544300
H	-1.78835500	-2.40028300	1.41319100
C	-2.00304300	-0.78015900	-1.50389900
H	-3.07610200	1.07405300	-0.87070800
H	-1.15225700	-2.81979900	-1.15551500
H	-1.91342700	-0.65457800	-2.57525300
H	1.23890100	-1.23023100	0.66830100
C	1.77838400	-1.74847100	-0.66414400
H	1.35757000	-2.73616000	-0.46437700
C	1.22335100	-1.04935300	-1.75572000
H	1.83282600	-0.30458400	-2.25614300
H	0.49138300	-1.54115800	-2.38410700
H	0.85950900	-2.11088600	2.29333600
C	1.02124500	-1.03858500	2.19118800
H	2.05732100	-0.72714300	2.31325300
C	-0.00257800	-0.15449600	2.55311700
H	-0.95356900	-0.54984400	2.88716500
H	0.24926800	0.83158300	2.92236200
Zr	-0.14617200	0.06189000	0.02943400

Zr/Pro

7a

C	0.91315500	-0.68179900	-2.00241700
C	2.05869500	-0.64146900	-1.17757800
H	0.78604700	0.08831700	-2.75443000
H	0.52329100	-1.65324600	-2.28373700
C	2.70194300	-1.95156300	-0.74432100
H	1.54509400	-0.28012800	0.32372400
H	3.35271900	-1.83116200	0.12672700
H	1.96578700	-2.72944100	-0.52949500
H	-1.99532800	-1.77335600	-2.16795200
C	-1.91438000	-1.73537200	-1.08950500
C	-1.01118300	-2.49053500	-0.28542000
C	-2.74649200	-0.99134100	-0.21775000
C	-1.26684700	-2.18743100	1.06742700
H	-0.28017200	-3.20088500	-0.64812200
C	-2.32625000	-1.23579000	1.11680700
H	-3.56754400	-0.35479900	-0.51873800

H	-0.75777300	-2.62087800	1.91926900
H	-2.77914500	-0.82745000	2.01112500
C	3.04483000	0.50110400	-1.37320600
H	2.55335700	1.44665400	-1.60831400
H	3.67970900	0.23700300	-2.22936100
H	3.70321900	0.64969900	-0.51587400
C	-1.53076500	1.85567800	-1.37946100
C	-0.15477100	2.18237100	-1.42016600
C	-1.98163100	2.04365500	-0.03844000
H	-2.14351900	1.57109600	-2.22552900
C	0.26464500	2.51848000	-0.10657200
H	0.46187300	2.19773900	-2.30733100
C	-0.87952300	2.45997700	0.74065100
H	-2.99741100	1.93101300	0.31624600
H	1.25371200	2.85165100	0.18057200
H	-0.91724000	2.73230100	1.78537000
H	-0.42072500	-0.54654000	2.88979400
C	0.26192400	0.16662900	2.44745800
C	1.50824600	-0.26505400	1.97956800
H	0.18080000	1.18054000	2.82182600
C	2.74798500	0.58556800	2.16534600
H	1.68685500	-1.34113000	1.97942200
H	3.59737500	0.23845800	1.57440500
H	2.56172400	1.63909900	1.93932000
Zr	-0.41238600	0.03458700	0.00440800
H	3.03647100	0.52095000	3.22226000
H	3.32878900	-2.30763800	-1.57203900

7b

C	2.19185300	-0.41987300	0.92251000
C	1.20781000	-0.83327700	1.84527200
H	1.62518000	0.08573200	-0.42899400
H	2.65221100	0.54830300	1.13561400
C	1.06939600	-0.20520700	3.21621800
H	0.99528200	-1.89970100	1.84441900
H	1.24687800	0.87305800	3.22091000
H	0.09424000	-0.40363900	3.66937600
H	0.79557700	2.47239400	1.73108400
C	-0.12587100	2.21148800	1.22795200
C	-0.48482400	2.59969700	-0.08157200
C	-1.21316200	1.47675400	1.78341700
C	-1.78478500	2.09600700	-0.35754600
H	0.11837900	3.19695000	-0.75136100
C	-2.24317000	1.43004200	0.80995100
H	-1.27765200	1.09011900	2.78989000
H	-2.34715300	2.24403200	-1.27049700
H	-3.22371600	0.99742800	0.94966500
C	3.13765300	-1.42345000	0.27907700
H	3.89104900	-1.70295700	1.02566300
H	3.67017400	-1.01557000	-0.58442500
H	2.62298700	-2.33795200	-0.02723300
C	-1.44333400	-2.19453000	0.59769800
C	-0.38021800	-2.59501500	-0.26215400
C	-2.39658500	-1.50455100	-0.19466400
H	-1.54437600	-2.43748400	1.64751900
C	-0.66137900	-2.12484700	-1.56231600
H	0.47820000	-3.18832900	0.02297700
C	-1.90188100	-1.42693000	-1.52307500
H	-3.35156900	-1.13095800	0.14650700
H	-0.04718900	-2.28544600	-2.43963500
H	-2.41117500	-0.97729300	-2.36554000
Zr	-0.33426500	0.00193600	-0.09912800
H	-0.16752200	-0.00205100	-3.06518200
C	0.30015700	0.72979200	-2.41886900
C	1.60591200	0.49190400	-1.94930400
H	-0.02086000	1.75305900	-2.57982000
C	2.62782200	1.60726800	-1.82140000
H	2.03262900	-0.47880100	-2.20738700
H	2.17850200	2.53935500	-1.46980500
H	3.45877100	1.34951400	-1.15852900
H	3.04777200	1.79745400	-2.81682300
H	1.82162700	-0.65628700	3.87954500

Zr/But

7a

C	-0.22490400	2.37384000	0.90016400
C	1.14188900	2.16573500	0.78963100
H	-0.69229100	2.36330400	1.87753700
H	-0.71400800	3.00044200	0.16367200
C	1.90168700	2.78168300	-0.37562300
H	1.14423300	0.33123300	-0.03926200
C	3.27959900	2.20548800	-0.71302000
H	1.26518400	2.78912700	-1.26565500
H	2.02668700	3.83941700	-0.09331900
H	3.70667800	2.74391100	-1.56456500
H	3.98254000	2.30556500	0.11972500
H	3.21902300	1.14594100	-0.98087400
H	-0.84167600	2.47204000	-2.10146300
C	-1.39587800	1.56101700	-1.92066000
C	-1.15306400	0.31908000	-2.53371500
C	-2.51940400	1.41775300	-1.04954500
C	-2.12722000	-0.61033900	-2.05163700
H	-0.37743800	0.11650800	-3.26137800
C	-2.99178400	0.08834700	-1.17259000
H	-2.97791500	2.20311500	-0.46285400
H	-2.24389300	-1.63862900	-2.36802000
H	-3.85571400	-0.32702900	-0.67083900
C	1.96210200	1.79262900	2.00054000
H	1.34960800	1.41409600	2.82053900
H	2.46391300	2.70410300	2.35533800
H	2.74445900	1.06580800	1.77215200
C	-1.06857900	-0.16384100	2.55545700
C	-0.06425000	-1.12661100	2.26359200
C	-2.27397400	-0.57353100	1.93769000
H	-0.94574800	0.71109600	3.17729000
C	-0.67503700	-2.16422800	1.50894300
H	0.95528400	-1.11703700	2.62370400
C	-2.02908200	-1.81880800	1.28617400
H	-3.22419400	-0.05825500	1.99499200
H	-0.19534400	-3.07825100	1.19068000
H	-2.76008700	-2.41837100	0.75903700
Zr	-0.70183200	-0.06250800	-0.00035600
H	0.28387100	-3.04409900	-0.89064000
C	0.57026000	-2.14099700	-1.41825500
C	1.71833500	-1.47697100	-1.10169400
H	0.08696400	-1.97576200	-2.37147200
H	2.06874800	-0.71033000	-1.79052200
C	2.71441100	-1.92672800	-0.06555800
H	3.12739200	-1.06256000	0.46478100
H	2.22693400	-2.56671500	0.67792400
C	3.86422300	-2.70449200	-0.74080100
H	4.59541900	-3.01610000	0.01154900
H	3.49302800	-3.60018700	-1.24868600
H	4.38562800	-2.08622200	-1.47970200

7b

C	0.28830800	2.13165200	-0.37837000
C	1.56728600	1.53565400	-0.32467300
H	-0.88795000	1.12649000	-0.28732300
H	-0.02691700	2.63956100	0.53688200
C	2.59532600	1.90717500	0.73070400
H	2.01976600	1.34004100	-1.29471300
C	3.32272100	3.20996500	0.33984400
H	2.12817300	2.04213000	1.71125700
H	3.34095000	1.11111000	0.83344000
H	4.08990500	3.45249300	1.08287200
H	3.81767300	3.11480900	-0.63310500
H	2.62673900	4.05436700	0.28427500
H	0.44402400	1.11635200	2.77409300
C	0.38549500	0.07685500	2.48075300
C	-0.79289100	-0.70007800	2.44118000
C	1.48020800	-0.76318100	2.12647300
C	-0.44463400	-2.02111200	2.04865500
H	-1.78703400	-0.35225500	2.68598100

C	0.96501100	-2.06234600	1.88474100
H	2.52386700	-0.48423500	2.11508500
H	-1.12354200	-2.85811400	1.94891000
H	1.55084800	-2.94167600	1.65756800
C	-0.22199500	2.78506100	-1.65481800
H	0.28101000	3.75374500	-1.76226100
H	-1.29838800	2.97640800	-1.63739300
H	0.01379000	2.19244500	-2.54287600
C	1.86039500	-1.36317400	-1.68041700
C	0.88733400	-0.69623100	-2.47961800
C	1.25870100	-2.54085600	-1.16876700
H	2.89246600	-1.06660300	-1.54703000
C	-0.30937000	-1.44128100	-2.43283700
H	1.04748100	0.20481900	-3.05632200
C	-0.09345900	-2.57627900	-1.60108400
H	1.75412100	-3.29914700	-0.57918100
H	-1.22561400	-1.19928500	-2.95649300
H	-0.80754600	-3.36233200	-1.39195000
Zr	0.08844000	-0.58667900	-0.00488200
H	-2.53902400	-1.50825200	-1.03408200
C	-2.40289300	-0.82851600	-0.20245900
C	-2.34366100	0.55719200	-0.44432100
H	-2.81212800	-1.17612800	0.74001500
C	-3.01143600	1.56425800	0.48404500
H	-2.34607500	0.85466700	-1.49539000
C	-4.50941200	1.68658300	0.15034900
H	-2.89082000	1.24892100	1.52601100
H	-2.54107500	2.55004800	0.39351100
H	-4.98101300	2.42134400	0.81045200
H	-4.66245900	2.01762800	-0.88285800
H	-5.02505400	0.72976200	0.27960600

Zr/Hex

7a

C	-4.29195900	3.47580700	-0.70401400
H	-4.87326900	3.40576200	0.22296300
H	-4.72766700	4.27738300	-1.30904900
H	-4.42536100	2.53547400	-1.25329500
C	-2.81244200	3.74651900	-0.41358000
H	-2.26478600	3.85248100	-1.36102000
H	-2.71097600	4.70927100	0.10579700
C	-2.15693700	2.64439000	0.43181000
H	-2.70833400	2.54496900	1.37558300
H	-2.25122000	1.68072600	-0.08600700
C	-0.67694300	2.93380900	0.71530800
H	-0.14788100	3.13333600	-0.22275700
H	-0.61442500	3.87171900	1.29198000
C	0.11017300	1.92986500	1.54116000
H	-0.28759200	0.38936400	0.27094200
C	1.49409400	1.92346200	1.47234200
H	2.07348400	1.57682500	2.31968000
H	1.98402600	2.66203200	0.84874200
H	0.00489800	-1.76557700	2.41755300
C	0.95992700	-1.78676200	1.91089100
C	1.31495800	-2.63990000	0.83143300
C	2.12207000	-1.05396100	2.27449600
C	2.66685000	-2.39588500	0.49306200
H	0.67142800	-3.37607200	0.37254500
C	3.16906900	-1.40692700	1.39017100
H	2.20702500	-0.37462300	3.11011000
H	3.23131100	-2.90420700	-0.27808900
H	4.18395100	-1.03204000	1.42466500
H	1.70910900	2.74862900	-1.47714300
C	2.14375100	1.76932100	-1.62449200
C	3.33372100	1.27501500	-1.00748400
C	1.64418600	0.77094400	-2.47955200
C	3.58432700	-0.01713800	-1.53019100
H	3.97335900	1.81926400	-0.32468000
C	2.52331200	-0.35471300	-2.40682800
H	0.76176600	0.85743700	-3.10059200
H	4.43312600	-0.64435200	-1.29192600
H	2.44477700	-1.26835300	-2.98123400

C	-0.60197200	1.32721200	2.72735100
H	0.03868100	0.65386700	3.29910900
H	-1.51611300	0.80012700	2.44656300
H	-0.89755400	2.15081800	3.39273300
H	-3.33627400	-2.72416600	-1.47984000
C	-3.52291800	-1.98818600	-0.68674500
C	-4.51196200	-2.56617600	0.33577800
H	-3.97285600	-1.11271100	-1.17557600
C	-2.17713100	-1.57955800	-0.04095900
C	-5.84977900	-2.96494200	-0.29557400
H	-4.68510100	-1.82608800	1.12964100
H	-4.05890800	-3.44062800	0.82318600
H	-2.37322000	-0.85221700	0.75446400
H	-1.71511900	-2.45894100	0.42303500
C	-1.26136200	-0.98899400	-1.07837600
H	-5.71254400	-3.72783900	-1.07082800
H	-6.53200600	-3.37404400	0.45678600
H	-6.34342700	-2.10272800	-0.75935500
H	-1.57551000	-0.03185000	-1.49060100
C	-0.27925800	-1.67394200	-1.73373900
H	-0.07315400	-2.71258900	-1.49993100
H	0.09360800	-1.32059300	-2.68570600
Zr	1.46125300	-0.22238600	-0.08430100

7b

C	-1.32437600	-1.26362300	-1.05110600
C	0.03837500	-1.60880400	-1.17658600
H	0.40545100	-2.34000800	-0.45176200
H	1.03880800	-0.53141100	-0.68184500
H	-2.59332000	-0.41094800	1.85614400
C	-1.61975900	0.01768700	2.03899400
C	-0.39183700	-0.69334300	2.16638800
C	-1.35313600	1.38733000	2.29133300
C	0.62018100	0.23829100	2.48721500
H	-0.25933200	-1.76374000	2.07772500
C	0.03769500	1.53313600	2.53800900
H	-2.09007300	2.17719300	2.32875300
H	1.65823900	0.00236700	2.67585600
H	0.55045700	2.45574500	2.77765400
H	1.05252700	2.57455200	-2.39591800
C	0.10196000	2.49791300	-1.88314400
C	-0.96890400	1.65921200	-2.25670800
C	-0.29428800	3.23919900	-0.73428500
C	-2.04393300	1.87444800	-1.34642700
H	-0.98351300	0.99639800	-3.11173600
C	-1.63258900	2.87485100	-0.42906600
H	0.29179500	3.99309200	-0.22479300
H	-3.01954800	1.40860100	-1.38675700
H	-2.24390000	3.31002900	0.34889400
C	0.68195500	-1.72512600	-2.55146400
H	0.37753400	-0.91232100	-3.21691100
H	0.34257500	-2.66526200	-3.00352600
H	1.77411100	-1.75732200	-2.51305900
H	-1.75889500	-0.81655900	-1.94353500
C	-2.32316400	-2.12330600	-0.28675200
H	-2.31165000	-3.11569800	-0.76626600
H	-2.01233400	-2.30517000	0.74750000
C	-3.76811500	-1.60451500	-0.33795600
H	-3.83004800	-0.59928300	0.10362300
H	-4.06509600	-1.48874100	-1.39054300
C	-4.76633200	-2.53399100	0.36654100
H	-4.48069200	-2.64216100	1.42286000
H	-4.69302400	-3.53864900	-0.07184400
C	-6.21335600	-2.03937500	0.27429000
H	-6.89692800	-2.72400800	0.78658400
H	-6.32815700	-1.05004500	0.73409300
H	-6.54057700	-1.96198300	-0.76935000
H	2.55853300	1.53479500	1.17805100
C	2.22561600	1.46066600	0.14850800
C	2.38395200	0.23551300	-0.53101600
H	2.27438900	2.38598500	-0.41199700
C	3.17362200	-0.91991100	0.06870300
H	2.46301200	0.30907100	-1.61797100

H	2.87842100	-1.87280200	-0.38709700
H	2.96333600	-1.00286500	1.14105000
C	4.68854000	-0.71298700	-0.14213900
H	4.99519000	0.22588100	0.33753900
H	4.89442500	-0.59383100	-1.21527900
C	5.52280400	-1.87672800	0.41239200
H	5.30455300	-2.00149500	1.48226300
H	5.21197400	-2.81078200	-0.07597800
C	7.02841100	-1.67053600	0.21611000
H	7.59544600	-2.51558900	0.61984300
H	7.28207200	-1.57608700	-0.84633800
H	7.37525100	-0.76315600	0.72438100
Zr	-0.20002400	0.82275500	0.08621700

H₂ π-complex

Zr/Et

9a

H	-1.59173700	-2.83175000	-0.22023500
C	-1.85432200	-1.80750800	0.00998800
C	-1.74231500	-1.17532400	1.28732200
C	-2.43732900	-0.87912400	-0.88455400
C	-2.25050500	0.14420400	1.16812100
H	-1.38583700	-1.64021300	2.19854300
C	-2.65705500	0.34116800	-0.18221900
H	-2.67642200	-1.06347900	-1.92494500
H	-2.33445900	0.86762300	1.96868300
H	-3.12191200	1.23189700	-0.58609800
C	1.89424900	1.54194800	-0.52921800
C	1.74432600	1.36882600	0.87421000
C	0.78408300	2.30926400	-0.99095500
H	2.73698700	1.22156400	-1.12713200
C	0.52907900	1.98929100	1.27232700
H	2.44348700	0.86860300	1.53259800
C	-0.06120000	2.57758000	0.11672600
H	0.63044500	2.65526100	-2.00596400
H	0.15188100	2.05401100	2.28504000
H	-0.97459600	3.15822800	0.09342500
Zr	-0.13966200	0.06112300	-0.22572200
C	2.96822000	-2.01764200	0.64316500
H	3.48664700	-1.10202200	0.34157300
H	3.45119200	-2.85604900	0.13229100
H	0.97222400	-2.89948100	0.55270500
C	1.48479200	-1.98034100	0.25299800
H	1.01286400	-1.22564300	1.00756000
C	1.17688300	-1.61653800	-1.17082600
H	2.04630500	-1.27962700	-1.73671100
H	0.63449800	-2.38281200	-1.72411900
H	0.00758800	-0.22531800	-2.33502000
H	-0.47524800	0.38312400	-2.34707900
H	3.09915800	-2.15366500	1.72125200

Zr/Pro

9a

C	3.16739400	1.26793700	0.42552400
H	2.63502100	2.18423600	0.15846600
H	4.10506800	1.25437000	-0.13987700
H	0.70064900	2.42201000	1.63388200
C	-0.12903700	2.23282000	0.96472400
C	-0.16617400	2.52324100	-0.42855600
C	-1.38343000	1.68060200	1.33687100
C	-1.46289600	2.18031600	-0.90677300
H	0.61690300	2.99464400	-1.00681700
C	-2.20967200	1.64847900	0.17713000
H	-1.67691900	1.38755900	2.33677600
H	-1.82623400	2.32654300	-1.91677100
H	-3.24159300	1.32489000	0.13841000
C	-0.12987200	-2.23237100	0.96549600

C	-0.16595600	-2.52330300	-0.42772700
C	-1.38460400	-1.68015500	1.33648800
H	0.69928200	-2.42134700	1.63537800
C	-1.46229900	-2.18060900	-0.90705200
H	0.61756200	-2.99489300	-1.00523200
C	-2.20992800	-1.64837200	0.17608000
H	-1.67888100	-1.38679900	2.33606700
H	-1.82482800	-2.32714600	-1.91729600
H	-3.24184000	-1.32485400	0.13643900
H	3.41671600	-1.30689000	1.49137900
C	3.16710700	-1.26830200	0.42584000
C	2.36577500	-0.00013100	0.08063500
H	2.63440800	-2.18453800	0.15922800
C	1.77571400	-0.00021500	-1.30215800
H	1.50280400	0.00003300	0.88045900
H	1.99981800	0.89537700	-1.88287300
H	1.99956200	-0.89599000	-1.88268800
H	-0.86731700	0.00015500	-2.32601800
H	-0.08950100	0.00007900	-2.35010900
H	3.41686400	1.30685100	1.49108400
H	4.10469400	-1.25520600	-0.13971200
Zr	-0.31587400	0.00003200	-0.23323300

9b

C	2.22664200	-0.05799800	0.78986100
C	2.04281800	-0.22614200	-0.69584900
H	1.22697600	0.15192300	1.34697600
H	2.52374300	-1.00405700	1.25372400
C	2.65267800	-1.48415900	-1.31417500
H	2.37798000	0.66479900	-1.23341500
H	2.29975600	-2.40313000	-0.83431300
H	2.42743000	-1.56114600	-2.38363700
H	0.78841000	-2.79408700	1.15433800
C	-0.14961800	-2.38365900	0.80392500
C	-1.07877600	-1.63457100	1.58915400
C	-0.67393200	-2.51123200	-0.49936300
C	-2.19606600	-1.33387900	0.76489800
H	-0.98462300	-1.41068200	2.64484400
C	-1.93784600	-1.84266200	-0.53605000
H	-0.20788600	-3.03188000	-1.32653800
H	-3.08992500	-0.80831800	1.07441300
H	-2.61276300	-1.80430100	-1.38258000
C	3.14542000	1.08696500	1.24018500
H	4.16941100	0.87232200	0.91882200
H	3.14703800	1.19893200	2.32906700
H	2.85010100	2.04129100	0.79294500
C	-1.02640300	2.11673500	-1.35631000
C	0.13014200	2.46571300	-0.60367100
C	-2.05710200	1.76012600	-0.44727100
H	-1.11361600	2.14308700	-2.43568600
C	-0.20329700	2.35853700	0.77702400
H	1.06533600	2.82733800	-1.00949900
C	-1.54772800	1.91218000	0.87478300
H	-3.06494900	1.46751200	-0.71322500
H	0.44440400	2.60267700	1.60992400
H	-2.09973300	1.75761800	1.79321600
H	-0.30632600	-0.28327900	-2.29436900
H	0.45253000	-0.32726200	-2.12013400
H	3.74736100	-1.46858000	-1.21979500
Zr	-0.25005600	-0.00466300	-0.15719800

Zr/But

9a

C	-2.49859200	-1.98182600	0.51269600
H	-1.73737200	-2.72697200	0.27120200

H	-3.39633700	-2.23957500	-0.05577300
H	0.20112000	-2.49686900	1.69910200
C	0.93021900	-2.14072900	0.98255700
C	0.95607600	-2.44131100	-0.40993000
C	2.05188300	-1.32295400	1.27988400
C	2.11653000	-1.83111800	-0.96218300
H	0.26726200	-3.08374500	-0.94118300
C	2.78518000	-1.12807000	0.07449500
H	2.32676100	-0.95410800	2.25959000
H	2.44621100	-1.90955500	-1.99107700
H	3.71592200	-0.58485300	-0.02531600
Zr	0.55100900	0.05460700	-0.23190600
C	-0.07828600	2.17591500	1.01293700
C	-0.17127000	2.48198700	-0.37517500
C	1.28410400	1.92013400	1.32004000
H	-0.89742500	2.16684500	1.72058900
C	1.14516900	2.44632100	-0.91463200
H	-1.06632100	2.76934800	-0.90980000
C	2.04183500	2.08589300	0.12525200
H	1.68188600	1.69059800	2.30023000
H	1.41889400	2.67835700	-1.93676100
H	3.11711800	2.00354000	0.03538000
H	-3.23899800	0.48945000	1.63331600
C	-3.10904300	0.51139600	0.54355400
C	-2.05381500	-0.55475100	0.14531800
C	-4.47244700	0.32385200	-0.13575500
H	-2.72504200	1.50564200	0.29282600
C	-1.51820100	-0.41502200	-1.25221600
H	-1.18864300	-0.34066900	0.91794700
H	-5.13023000	1.15917100	0.12441700
H	-4.38176600	0.29795500	-1.22716900
H	-4.97078300	-0.59500200	0.18644200
H	-1.54840900	-1.33261100	-1.84072700
H	-1.94662700	0.41358700	-1.81742300
H	1.02575600	0.18343300	-2.33908600
H	0.26758400	0.00595900	-2.34027700
H	-2.73698900	-2.06252200	1.57873700

9b

C	-1.80419500	-0.57124300	1.07880900
C	-1.85609900	-0.33733100	-0.40728700
H	-0.72431400	-0.47964500	1.50955400
H	-2.29884500	0.24321400	1.61878000
C	-2.85229100	0.71805400	-0.90594900
H	-1.99853500	-1.27847000	-0.94681000
C	-4.31748100	0.27333800	-0.75832800
H	-2.70894500	1.66340600	-0.36658000
H	-2.65959700	0.93956500	-1.96420400
H	-4.99435000	1.04087000	-1.14883700
H	-4.50725000	-0.65345100	-1.31162900
H	-4.58353200	0.10037100	0.29090400
H	-1.08469500	2.43752900	1.45467800
C	-0.13266800	2.30743200	0.95680100
C	1.06918000	1.83199400	1.56497600
C	0.13861300	2.59051600	-0.39825100
C	2.09198700	1.86124600	0.57924500
H	1.19565200	1.57629600	2.60996800
C	1.51722200	2.29773300	-0.64415200
H	-0.56824600	2.97277000	-1.12379600
H	3.12989200	1.59714100	0.73417000
H	2.04533100	2.45885700	-1.57623000
C	-2.28334500	-1.93886300	1.58671400
H	-3.36088300	-2.02665000	1.41873800
H	-2.09383500	-2.06078300	2.65806000
H	-1.79697800	-2.76084600	1.05232000
C	1.63490500	-1.74067000	-1.52007200
C	0.70652300	-2.40614700	-0.67053200
C	2.63119900	-1.14113900	-0.70573100
H	1.60186900	-1.71787700	-2.60254900
C	1.15518300	-2.24460800	0.67153700
H	-0.13956300	-2.99633100	-0.99580800
C	2.33503400	-1.45462400	0.65213000
H	3.48804500	-0.58180500	-1.05940100

H	0.69475100	-2.67216100	1.55341200
H	2.92840700	-1.17822700	1.51474200
Zr	0.46429900	0.06272700	-0.13871400
H	0.18924500	0.37687800	-2.25402600
H	-0.52817700	0.21615000	-1.99636300

Zr/Hex

9a

C	-1.52900900	-2.39763500	0.54953500
H	-0.65966800	-3.00950300	0.29870500
H	-2.37880800	-2.79703000	-0.01033700
H	1.23106900	-2.47018000	1.69579600
C	1.88419000	-2.00369600	0.96943600
C	1.93850900	-2.29848100	-0.42380200
C	2.86386200	-1.01586600	1.25145400
C	2.97956700	-1.51179500	-0.99120600
H	1.35389100	-3.04334800	-0.94610000
C	3.54018500	-0.70814600	0.03620800
H	3.08858400	-0.60509400	2.22733300
H	3.30357100	-1.53793600	-2.02456500
H	4.36946900	-0.02201100	-0.07628000
C	0.19369100	2.09922000	1.01274000
C	0.03741600	2.37879500	-0.37493200
C	1.58286900	2.06775200	1.30460800
H	-0.60615400	1.95963600	1.72872000
C	1.33651600	2.55368800	-0.92977700
H	-0.89827800	2.51347100	-0.90019600
C	2.29086500	2.34878800	0.10112200
H	2.02299000	1.90973500	2.28078000
H	1.55802200	2.82294100	-1.95538500
H	3.36449800	2.44078400	-0.00003100
H	-2.64013300	-0.07659100	1.69249700
C	-2.53295800	-0.03479800	0.60012700
C	-1.32706100	-0.91642200	0.18132900
C	-3.86686100	-0.43192300	-0.05455200
H	-2.31924000	1.00971200	0.34578500
C	-0.84203000	-0.69075500	-1.22288900
H	-0.49444900	-0.56665200	0.94191500
H	-3.74707000	-0.47344100	-1.14618000
H	-4.15769300	-1.44038900	0.26466300
H	-0.73732300	-1.60079600	-1.81498500
H	-1.40514400	0.06057300	-1.77760800
H	1.56317800	0.29988800	-2.34953300
H	0.84127800	0.00942300	-2.33937100
H	-1.74015400	-2.51676900	1.61774300
C	-4.99979400	0.54482300	0.29586700
H	-5.10868000	0.59718600	1.38802100
H	-4.72271900	1.55643400	-0.03360200
C	-6.33931100	0.14937200	-0.33408300
H	-6.66212200	-0.84125100	0.00732900
H	-7.12485400	0.86439200	-0.06885800
H	-6.27149300	0.11916200	-1.42815400
Zr	1.14283900	0.10100400	-0.23613000

9b

C	-1.66253300	0.54507200	0.28253200
C	-1.00773200	1.14552100	-0.93233500
H	-0.95491700	-0.17173100	0.87111800
H	-1.84426500	1.31105700	1.04518800
C	-1.05945800	2.67380300	-1.05745500
H	-1.38150800	0.67985800	-1.84959900
C	-2.47784400	3.20607000	-1.32382000
H	-0.66495900	3.14388800	-0.14757500
H	-0.40475500	3.00001000	-1.87663600
H	-2.46572900	4.29556100	-1.43623300
H	-2.89438500	2.77922700	-2.24332300
H	-3.16141300	2.96624400	-0.50101600
H	0.24636500	2.25569100	2.05155600
C	1.11197500	1.70351900	1.70962000

C	1.56147100	0.45090400	2.22834900
C	1.99762300	2.10226700	0.68686500
C	2.75338400	0.10127500	1.53894400
H	1.11822100	-0.09238600	3.05402400
C	3.01070100	1.10009200	0.56216200
H	1.93034600	3.01215200	0.10399300
H	3.36091500	-0.77436800	1.72629700
H	3.86591800	1.13983300	-0.10161800
C	-2.92255200	-0.31161400	0.05722400
H	-3.68847300	0.34794900	-0.36991000
H	-2.71674900	-1.07190800	-0.70794700
C	1.44945700	-1.73503200	-1.99399900
C	0.06595700	-1.89034000	-1.69668000
C	2.19535100	-2.11734500	-0.84837300
H	1.86310300	-1.40665800	-2.93973200
C	-0.03711200	-2.40396400	-0.37256700
H	-0.75318700	-1.72257100	-2.38298300
C	1.27467000	-2.53313400	0.15607800
H	3.27503400	-2.12852300	-0.76883600
H	-0.95301100	-2.67673700	0.13622500
H	1.52983800	-2.92006500	1.13464800
H	1.64736100	0.92079400	-1.92736000
H	0.90864000	1.16652600	-1.88775000
C	-3.46252900	-0.97433700	1.33049700
H	-2.68841300	-1.62566400	1.76494800
H	-3.66410900	-0.19975800	2.08315900
C	-4.73608700	-1.78948900	1.08108200
H	-4.56030600	-2.59571100	0.35876300
H	-5.09737000	-2.24573900	2.00802000
H	-5.53938400	-1.15737900	0.68586300
Zr	0.88396900	-0.04673000	-0.15830100

Hydrogenolysis TS

Zr/Et

10a

H	-1.45549600	-2.85187200	-0.60323100
C	-1.75227900	-1.88829000	-0.20940500
C	-1.65908500	-1.47253600	1.15104100
C	-2.40140800	-0.85304600	-0.94007900
C	-2.21793100	-0.17349500	1.25369300
H	-1.25609800	-2.05583800	1.97016600
C	-2.66904600	0.21526800	-0.04250600
H	-2.66253200	-0.88122200	-1.99004000
H	-2.31955800	0.40519300	2.16298600
H	-3.17850400	1.13810600	-0.28898400
C	1.81104200	1.63326400	-0.40885600
C	1.50789400	1.57873700	0.98187200
C	0.72384200	2.27365000	-1.06995100
H	2.73591100	1.31672000	-0.87323000
C	0.22442200	2.15123500	1.17595200
H	2.15346700	1.19065900	1.76050900
C	-0.26329700	2.57757000	-0.09489500
H	0.66992100	2.50933700	-2.12489500
H	-0.27481600	2.28437100	2.12708300
H	-1.19772600	3.09257200	-0.27770400
Zr	-0.15464800	0.06171700	-0.19350200
C	3.12220900	-1.80461900	0.69423500
H	3.57390800	-0.84056200	0.43971300
H	3.68229600	-2.58692500	0.17345400
H	1.19558000	-2.81885100	0.55315900
C	1.64700800	-1.86317300	0.27172100
H	1.12054800	-1.14555500	1.00558600
C	1.38364700	-1.56313000	-1.19210000
H	2.26457800	-1.17343400	-1.70495800
H	0.98778700	-2.42179300	-1.73500800
H	0.41588400	-0.60200400	-1.92450600
H	-0.24395800	0.06945200	-2.12531500
H	3.23263100	-1.96562700	1.77096700

Zr/Pro

10a

C	-3.17392700	-1.27213200	0.45721400
H	-2.63069700	-2.18703400	0.20686600
H	-4.11192400	-1.27568400	-0.10776800
H	-0.59509800	-2.43859000	1.69757800
C	0.19681900	-2.24263700	0.98536200
C	0.15610200	-2.51370600	-0.41171200
C	1.46753700	-1.69191600	1.29123300
C	1.42111900	-2.16013700	-0.96405100
H	-0.65909300	-2.97791100	-0.95085200
C	2.22543000	-1.63971200	0.08379700
H	1.81696200	-1.40859000	2.27588500
H	1.72450300	-2.29091600	-1.99468100
H	3.25247300	-1.31163100	-0.00885400
Zr	0.33032500	0.00031200	-0.20506800
C	0.18794900	2.24499600	0.98198900
C	0.15190400	2.51391800	-0.41554000
C	1.45834900	1.69661700	1.29339200
H	-0.60696300	2.44058600	1.69095200
C	1.41958700	2.16157200	-0.96275300
H	-0.66213800	2.97591100	-0.95833300
C	2.22097400	1.64441600	0.08891700
H	1.80461300	1.41533900	2.27975200
H	1.72654200	2.29149600	-1.99243900
H	3.24896400	1.31812900	0.00064500
H	-3.42380300	1.29329700	1.52101800
C	-3.17864700	1.26497700	0.45440200
C	-2.37823500	-0.00251900	0.10248400
H	-2.64060100	2.18125000	0.19787200
C	-1.86223700	-0.00299900	-1.32895900
H	-1.51342300	0.00024000	0.87605200
H	-2.15709500	-0.89567400	-1.88314600
H	-2.15927400	0.88827900	-1.88425300
H	0.49259400	0.00064200	-2.13368600
H	-0.45465400	-0.00093700	-1.98033100
H	-3.42262300	-1.29675000	1.52310500
H	-4.11862500	1.26162300	-0.10730300

10b

C	3.15193200	1.04548300	1.37628500
H	2.86319500	2.04390000	1.03225500
H	4.17660400	0.85815400	1.04049400
H	0.34664300	2.68200000	1.54707200
C	-0.31360400	2.38210800	0.74236600
C	-0.02829800	2.45869200	-0.64835600
C	-1.62735000	1.86654000	0.89633300
C	-1.18361800	2.01892000	-1.35923900
H	0.87595000	2.85219500	-1.09380700
C	-2.16652600	1.64531400	-0.40527300
H	-2.14577100	1.71919300	1.83519300
H	-1.30185400	2.00450900	-2.43505100
H	-3.16631800	1.29539700	-0.62775400
Zr	-0.28354200	-0.01064600	-0.13672600
C	-1.88936500	-1.47121200	1.17007200
C	-0.59142200	-1.97331200	1.43793200
C	-2.17015600	-1.68850400	-0.21116700
H	-2.56131500	-1.02764200	1.89356200
C	-0.06393000	-2.50294500	0.22263900
H	-0.10143000	-1.98388500	2.40404800
C	-1.05162200	-2.34816100	-0.78809300
H	-3.09543500	-1.44875800	-0.71920800
H	0.88558500	-3.00804900	0.10865500
H	-0.97408800	-2.68647800	-1.81335600
H	2.62914300	-2.17420000	-1.04630700
C	2.92122600	-1.17744100	-1.39079100
C	2.12448700	-0.06594100	-0.70611100
H	2.79643800	-1.14898100	-2.47831200
C	2.22009000	-0.03616700	0.80662000
H	2.40358700	0.90607400	-1.12110200
H	1.22140500	0.15867300	1.34780000

H	2.49058900	-1.02650100	1.18713000
H	0.86072400	-0.22523500	-1.68701600
H	0.00868000	-0.26732200	-2.05235500
H	3.14609600	1.03996400	2.47060100
H	3.99221000	-1.05740300	-1.18282000

Zr/But

10a

C	-2.52529300	-1.96065300	0.53735500
H	-1.75810500	-2.70857500	0.32453300
H	-3.41504100	-2.23064400	-0.03792900
H	0.27673300	-2.51096300	1.73610400
C	0.97630800	-2.15451800	0.99022600
C	0.93518300	-2.43848300	-0.40481400
C	2.11166300	-1.34285700	1.24145200
C	2.06929100	-1.82588500	-1.01054000
H	0.21799700	-3.07200900	-0.90945400
C	2.78668700	-1.13621300	0.00212200
H	2.43335400	-0.98182900	2.21007300
H	2.34942800	-1.89560800	-2.05360200
H	3.71322800	-0.59417900	-0.13520400
Zr	0.56931200	0.05309900	-0.20015900
C	-0.02780300	2.21585900	0.99949900
C	-0.14249000	2.47259800	-0.39585800
C	1.33485000	1.94927400	1.28907400
H	-0.83466000	2.23743300	1.72131900
C	1.16212500	2.39864700	-0.96399600
H	-1.04511400	2.75045700	-0.92380200
C	2.07168600	2.06238600	0.07270100
H	1.74904000	1.74617000	2.26851200
H	1.41812900	2.59237800	-1.99759400
H	3.14388000	1.96173500	-0.03342600
H	-3.23849200	0.52564000	1.63850100
C	-3.12127400	0.53632200	0.54737800
C	-2.07135000	-0.53927700	0.15689400
C	-4.49408500	0.34758400	-0.11197100
H	-2.73268000	1.52603100	0.28411300
C	-1.59480900	-0.42751400	-1.28328600
H	-1.21127300	-0.32574600	0.90898000
H	-5.14574100	1.18648600	0.15143100
H	-4.42317400	0.31417100	-1.20482400
H	-4.98988000	-0.56758600	0.22433200
H	-1.69540800	-1.36110700	-1.83936800
H	-2.08504200	0.37848200	-1.83181200
H	0.68623900	0.09462900	-2.13252100
H	-0.23148400	-0.11338600	-1.96057000
H	-2.77853500	-2.01958800	1.60116000

10b

C	-2.44236200	-1.67616900	1.67549700
H	-2.00948800	-2.57201800	1.21898600
H	-3.52111100	-1.69922100	1.49714100
H	0.60064400	-2.69397100	1.58483500
C	1.06491900	-2.29697100	0.69034800
C	0.57469100	-2.42977400	-0.63903500
C	2.28749700	-1.57855300	0.63969000
C	1.51515700	-1.81731600	-1.51723300
H	-0.31414900	-2.96797700	-0.94070900
C	2.56535800	-1.28038600	-0.72682900
H	2.91969800	-1.34160900	1.48579000
H	1.45454500	-1.79095600	-2.59757300
H	3.44584900	-0.77385100	-1.10075200
Zr	0.50646900	0.04853800	-0.12317700
C	2.03280900	1.71969100	1.01599300
C	0.72616600	1.98301900	1.49835300
C	2.06017700	2.02539700	-0.37605800
H	2.87059300	1.37365400	1.60753700
C	-0.05855800	2.45837800	0.40522900
H	0.39473200	1.88116700	2.52471100

C	0.77412600	2.50534900	-0.74495600
H	2.92358700	1.96176500	-1.02599200
H	-1.08251000	2.80181500	0.46090500
H	0.48675300	2.85794300	-1.72717400
H	-2.75588100	1.73193900	-0.54580700
C	-2.94691600	0.74434400	-0.98248600
C	-1.93704000	-0.27676200	-0.43691300
C	-4.40677300	0.34349200	-0.71835800
H	-2.80101500	0.85545800	-2.06471000
C	-1.84689200	-0.39457400	1.07076100
H	-2.11669300	-1.25814800	-0.88564200
H	-5.08757600	1.07598900	-1.16427400
H	-4.63503200	-0.63451900	-1.15688900
H	-4.63034000	0.29621200	0.35342000
H	-0.77008700	-0.38158400	1.49113700
H	-2.26846500	0.49793700	1.54524900
H	-0.82516900	0.09749000	-1.52929300
H	-0.03822200	0.28796900	-1.98382000
H	-2.27356200	-1.72198600	2.75598700

Zr/Hex

10a

C	-1.54345200	-2.41499800	0.51626300
H	-0.66750200	-3.02075700	0.27224200
H	-2.38708100	-2.81467400	-0.05289200
H	1.28534300	-2.49748400	1.70125100
C	1.92538100	-2.01652000	0.97218300
C	1.95823100	-2.28668700	-0.42542000
C	2.89626900	-1.02149300	1.25213800
C	2.97939200	-1.47883000	-1.00407800
H	1.36976700	-3.02824500	-0.94933300
C	3.54783400	-0.68717100	0.02789100
H	3.13338500	-0.62254300	2.23008600
H	3.28522200	-1.48664500	-2.04222900
H	4.36750500	0.00978600	-0.08718400
Zr	1.16246400	0.10322500	-0.20637500
C	0.22013400	2.13756600	0.99454500
C	0.04469300	2.36185900	-0.40037800
C	1.61190600	2.11235500	1.26550400
H	-0.56898900	2.02285500	1.72710100
C	1.33471900	2.51078500	-0.98649700
H	-0.89938900	2.47749700	-0.91604300
C	2.30222900	2.34179300	0.03863600
H	2.06744600	1.98793400	2.23966300
H	1.54018200	2.73869100	-2.02435600
H	3.37442500	2.42554000	-0.08181600
H	-2.64439000	-0.10835600	1.68281300
C	-2.54227100	-0.04874800	0.59096400
C	-1.33768100	-0.93000700	0.16418400
C	-3.88395400	-0.42156000	-0.06083000
H	-2.31865900	0.99840300	0.35596300
C	-0.90321000	-0.71623700	-1.27765700
H	-0.51408000	-0.59154300	0.91288100
H	-3.78250700	-0.42468900	-1.15529400
H	-4.17320800	-1.44003600	0.22659000
H	-0.87289400	-1.64317300	-1.85288900
H	-1.51612800	0.01879700	-1.80140300
H	1.26573900	0.14999300	-2.13896400
H	0.39324700	-0.20529600	-1.96188500
H	-1.76387600	-2.53960500	1.58169000
C	-5.00818500	0.54658700	0.33952100
H	-5.10666600	0.55368100	1.43383900
H	-4.72690900	1.56929500	0.05040300
C	-6.35595200	0.18733000	-0.29413900
H	-6.68219600	-0.81530000	0.00635100
H	-7.13374600	0.89499700	0.01051600
H	-6.29910200	0.20573700	-1.38906900

10b

C	-2.92259400	-0.43976300	0.09347600
H	-2.71531200	-1.20231100	-0.66939800
H	-3.72493900	0.18802100	-0.31305900
H	-0.72092500	-2.79110700	0.02424200
C	0.16994700	-2.42221500	-0.46901600
C	0.22797800	-1.82841800	-1.76064700
C	1.48864400	-2.47360600	0.05257600
C	1.59351500	-1.54128900	-2.05108200
H	-0.60629100	-1.68641500	-2.43500500
C	2.36967400	-1.92750800	-0.92675300
H	1.77830600	-2.89814600	1.00534100
H	1.97473900	-1.12813200	-2.97597100
H	3.44695900	-1.85917500	-0.84524800
Zr	0.92287300	-0.01483200	-0.13873900
C	2.46829300	0.14924400	1.86239500
C	1.26672200	0.80686300	2.22789900
C	3.08035900	0.89541500	0.81416200
H	2.86268400	-0.75165400	2.31457900
C	1.13970200	1.97251300	1.41314600
H	0.58997700	0.50410500	3.01770300
C	2.27067800	2.03619100	0.55812700
H	4.02597200	0.66941400	0.33779700
H	0.35913300	2.71721900	1.48912100
H	2.48753200	2.81888000	-0.15749600
H	-0.98317300	3.13858000	-0.26759500
C	-1.36860600	2.60336800	-1.14389000
C	-1.13040000	1.09328300	-0.98627600
C	-2.84908300	2.95963900	-1.34895100
H	-0.79404100	2.97158000	-2.00372200
C	-1.67856100	0.45429300	0.27197300
H	-1.49224600	0.56408200	-1.87307000
H	-2.96164300	4.03754800	-1.50524200
H	-3.26222700	2.45021400	-2.22690600
H	-3.45902000	2.68734300	-0.48032800
H	-0.94086900	-0.24974800	0.81969800
H	-1.85313700	1.21734000	1.03903600
H	0.36349600	1.17852500	-1.55759600
H	1.27211000	1.07473700	-1.72236200
C	-3.39341100	-1.10718300	1.39139500
H	-2.58169600	-1.72760300	1.80137600
H	-3.59534500	-0.33272200	2.14404900
C	-4.64561000	-1.96845000	1.19414200
H	-4.95613200	-2.42903900	2.13711800
H	-5.48490600	-1.36848200	0.82453400
H	-4.46739200	-2.77404100	0.47188200

2nd β -product

Zr/Et

11a

H	0.55280400	-3.18948300	0.50971200
C	1.26615800	-2.46977400	0.12959100
C	1.39307100	-2.05517700	-1.22769100
C	2.25609600	-1.80113500	0.89052000
C	2.46264700	-1.12364900	-1.30426100
H	0.80125800	-2.41710900	-2.06097000
C	2.99205600	-0.95677000	0.01072500
H	2.42324700	-1.91324000	1.95503200
H	2.83536300	-0.65273500	-2.20527500
H	3.84539200	-0.34687400	0.27914700
C	-5.40663900	-0.04438900	-0.58057800
H	-5.98176600	-0.25307700	-1.48807800
H	-5.38684500	1.04298800	-0.44086200
H	-5.94942500	-0.48035800	0.26572100
C	0.47544300	2.32319300	1.10373200
C	-0.43977100	2.31284100	0.02137600
C	1.78934000	2.20471200	0.56523500
H	0.22322400	2.41576000	2.15190000
C	0.30446200	2.21804000	-1.19205200
H	-1.51614900	2.40003200	0.09794000
C	1.67984500	2.16137500	-0.85817500
H	2.71305400	2.22681100	1.13061900

H	-0.10978600	2.21988600	-2.19417200
H	2.50468400	2.11234400	-1.55742200
Zr	0.68377700	0.02265600	0.04584800
H	-3.48561900	-0.19358900	-1.56644100
C	-3.98983900	-0.61901100	-0.68537200
H	-4.04386200	-1.70303600	-0.85532500
C	-3.14617600	-0.34343100	0.56525800
H	-3.07791200	0.73801900	0.74280100
H	-3.63989900	-0.76684700	1.44936000
H	-1.77911900	-2.02755200	0.35689000
C	-1.73120100	-0.94512900	0.51235400
H	-1.31975900	-0.58970000	-0.51781400
C	-0.78644400	-0.58206500	1.64603800
H	-1.16993000	0.22750300	2.26843200
H	-0.50433200	-1.43379600	2.26470200

Zr/Pro

11a

C	-2.77114200	-0.08566500	-0.73253300
C	-3.82897700	-0.25838000	0.37833600
H	-3.23028600	-0.34118100	-1.69681200
H	-2.49874700	0.97550600	-0.79944600
C	-3.30430800	0.10106200	1.77712700
H	-4.14294100	-1.31075000	0.39436600
H	-2.46459500	-0.53189900	2.09243400
H	-2.97806900	1.14946300	1.81911000
H	1.55447400	-2.89636700	-1.19791600
C	1.92197700	-2.24383200	-0.41838600
C	3.00136400	-1.32656100	-0.54151200
C	1.45080600	-2.18331900	0.92232200
C	3.21195200	-0.71825900	0.72904500
H	3.58870400	-1.15056200	-1.43561900
C	2.24838400	-1.23857600	1.63106900
H	0.65571600	-2.78389300	1.34659600
H	3.98448400	-0.00001800	0.96985700
H	2.15927600	-0.98899100	2.68198800
C	-5.06823100	0.58461500	0.03561200
H	-5.48004700	0.31192700	-0.94253000
H	-4.82495500	1.65470800	0.01118000
H	-5.85639200	0.44068400	0.78205800
C	1.35585300	2.25577700	1.08837400
C	0.00706700	2.31118500	0.63936300
C	2.19857600	2.27205300	-0.05967100
H	1.68617300	2.23864100	2.11997000
C	0.01913100	2.36961400	-0.78363700
H	-0.87309000	2.34704900	1.27011400
C	1.36875900	2.34245900	-1.21394900
H	3.28076700	2.28180100	-0.05594000
H	-0.84683400	2.44892400	-1.42570900
H	1.70977700	2.38258100	-2.24194900
C	-1.48155200	-0.93822400	-0.63805000
C	-0.46280500	-0.62287100	-1.72785200
H	-0.15183100	-1.50391200	-2.29030200
H	-0.79290500	0.15583700	-2.41678500
H	-1.03060500	-0.64358500	0.40396800
C	-1.78084000	-2.44120400	-0.50137700
H	-2.30036600	-2.67683700	0.43173600
H	-0.87239800	-3.04689000	-0.55002700
H	-2.42564500	-2.74765000	-1.33244500
H	-4.09290300	-0.02070800	2.52702800
Zr	0.94317900	0.07942200	-0.09926500

11b

C	-2.90901000	0.17366400	0.56158700
C	-3.81981700	0.16092000	-0.68146200
H	-2.69781300	1.21168700	0.84945300
H	-3.44097400	-0.27699100	1.41100200
C	-4.26518600	-1.25663200	-1.07405900
H	-3.24415900	0.58440800	-1.52169700

H	-3.42224000	-1.90827100	-1.33350700
H	-4.81879700	-1.73294100	-0.25507000
H	0.31723300	2.59802300	-1.97253900
C	0.79836800	2.43003400	-1.01546100
C	0.16747300	2.49839200	0.26220500
C	2.17176800	2.14906000	-0.81009400
C	1.15014600	2.26409100	1.25512300
H	-0.87667100	2.72189700	0.44055200
C	2.39016300	2.02210800	0.59479300
H	2.92711300	2.06317300	-1.58036700
H	0.99081200	2.27606600	2.32566500
H	3.34586700	1.85515700	1.07645900
C	-5.03867300	1.06677600	-0.44593100
H	-4.73925700	2.09283300	-0.20137500
H	-5.65355200	0.69109800	0.38127300
H	-5.67302200	1.10719000	-1.33765000
C	1.36765000	-1.80719500	-1.68902200
C	1.10380100	-2.44665800	-0.44282900
C	2.57587500	-1.07578000	-1.55812300
H	0.76965000	-1.89641400	-2.58898500
C	2.14520300	-2.11296500	0.45648600
H	0.26682300	-3.09890700	-0.23213300
C	3.05204800	-1.24900700	-0.22332900
H	3.06658700	-0.51143500	-2.34067300
H	2.23478700	-2.45450300	1.48003500
H	3.97810900	-0.85489100	0.17627400
H	-1.74272300	-1.63514400	0.17714600
C	-1.57405900	-0.58156100	0.41701200
C	-0.58612500	-0.45171800	1.57167000
H	-1.14119500	-0.17235000	-0.57869700
C	-0.52732600	-1.64280300	2.52844300
H	-0.80560800	0.45683200	2.14065200
H	-0.34433600	-2.59230300	2.01474800
H	0.25948900	-1.51031000	3.27908400
H	-4.92822100	-1.22428800	-1.94488600
H	-1.47367600	-1.74968400	3.07714900
Zr	0.94080000	0.07789300	-0.02959900

Zr/But

11a

C	2.36533500	-0.06358000	-0.99510300
C	3.52361400	-0.23863100	0.01370600
H	2.77447200	0.34067900	-1.92885600
H	1.97009100	-1.05424200	-1.25263800
C	3.07114300	-0.88391700	1.34077300
H	3.93056000	0.75517100	0.24936800
H	2.23176700	-0.31038900	1.76195000
H	2.68316800	-1.89315300	1.13029500
H	-1.68663100	3.10282900	-0.39685800
C	-2.06494100	2.30996400	0.23289600
C	-3.22503000	1.52894200	-0.01949500
C	-1.52382500	1.89484700	1.48158300
C	-3.41448200	0.64890800	1.08439000
H	-3.87583700	1.61550000	-0.88222300
C	-2.35936800	0.86714000	2.00731500
H	-0.65672800	2.31773700	1.97357700
H	-4.23290200	-0.04765600	1.20883900
H	-2.23250100	0.36682900	2.96028800
C	4.64500600	-1.04625000	-0.66283300
H	4.94982600	-0.58197600	-1.60749300
H	4.31620400	-2.06996400	-0.88484000
H	5.53387200	-1.11194100	-0.02947500
C	-1.77042400	-2.45086700	0.60771100
C	-0.47614400	-2.48518300	0.01727700
C	-2.70867500	-2.13855700	-0.41678700
H	-2.00647400	-2.66077700	1.64392400
C	-0.61816100	-2.20005300	-1.37057100
H	0.44980300	-2.72601300	0.52569500
C	-1.99281600	-1.98237900	-1.63694300
H	-3.78286900	-2.07792200	-0.30092900
H	0.17700200	-2.18084600	-2.10237500
H	-2.42490100	-1.75319300	-2.60409600

C	1.18728700	0.86383000	-0.60258400
C	0.06210100	0.88206200	-1.63097000
H	-0.22069900	1.88894500	-1.93993700
H	0.26586200	0.27152900	-2.51152300
H	0.78078000	0.38730300	0.39054500
C	1.63195700	2.27742900	-0.14729600
H	2.21728100	2.19723700	0.77611500
H	0.74117500	2.86414100	0.10106700
Zr	-1.27084000	-0.08604600	-0.07629500
C	4.16284400	-0.97627500	2.41511500
H	3.75173900	-1.36145000	3.35431500
H	4.97558200	-1.64440600	2.11585000
H	4.59745100	0.00897800	2.62205900
C	2.44517600	3.03772800	-1.20372200
H	2.65618700	4.05158800	-0.84926200
H	3.40573100	2.55516900	-1.40753800
H	1.90097800	3.12119000	-2.15080300

11b

C	-2.48145100	-0.10541900	-0.87297300
C	-3.43506500	-0.76018900	0.14862800
H	-2.13172600	-0.86985400	-1.57850400
H	-3.03431600	0.62970800	-1.47321600
C	-4.06337000	0.27339400	1.10801500
H	-2.84127900	-1.46488200	0.75719500
C	-4.94903100	-0.32675900	2.20697300
H	-3.26677200	0.85508100	1.59298600
H	-4.64827400	0.99297400	0.51684400
H	-5.28306300	0.45238300	2.90005100
H	-5.84429100	-0.80479000	1.79815600
H	-4.40463100	-1.07947300	2.79113800
H	-0.17239600	-3.04778300	0.07018600
C	0.69576400	-2.58630700	-0.38576300
C	0.73897100	-1.97740000	-1.67434700
C	2.00521600	-2.54012600	0.16432400
C	2.06781400	-1.55451400	-1.91732500
H	-0.09164600	-1.88394300	-2.36062600
C	2.85460400	-1.89045800	-0.77837200
H	2.31135100	-2.95623400	1.11576400
H	2.42422000	-1.06536100	-2.81667700
H	3.92131800	-1.73754300	-0.67425800
C	-4.50054600	-1.57392500	-0.60455300
H	-4.03905100	-2.28975500	-1.29508800
H	-5.15203600	-0.91555600	-1.19277800
H	-5.13433100	-2.14278900	0.08126800
C	1.42812900	0.65640400	2.46310500
C	1.22141500	1.83385900	1.68378100
C	2.68630200	0.11108200	2.10316100
H	0.76078700	0.27477700	3.22729600
C	2.34505900	2.01166000	0.84322100
H	0.36381100	2.49062800	1.74563200
C	3.24849400	0.93445000	1.08196900
H	3.14926000	-0.76503500	2.53862200
H	2.49049400	2.82191800	0.13990000
H	4.22521300	0.81026900	0.63064500
H	-1.55470800	1.45008400	0.36230500
C	-1.25717800	0.62426200	-0.29005900
C	-0.17900800	1.07240700	-1.25858800
H	-0.84404100	-0.13875600	0.49479300
C	-0.04754800	2.58310800	-1.49984700
H	-0.28879400	0.55836100	-2.21906200
C	-1.19990800	3.16554900	-2.33604300
H	0.00514900	3.11966600	-0.54424000
H	0.89799300	2.78623700	-2.02023700
H	-1.04591900	4.23571900	-2.51271200
H	-1.27139400	2.67240300	-3.31221100
H	-2.16444300	3.04875700	-1.82845500
Zr	1.23978900	-0.14359200	0.04883600

Zr/Hex

11a

C	1.48812900	0.27025500	-1.61156600
C	2.78234400	-0.40136300	-1.09682900
H	1.76491000	1.06582300	-2.31377800
H	0.92336700	-0.46180300	-2.20244700
C	2.50927600	-1.57962300	-0.13837600
H	3.36187000	0.35082100	-0.54284100
C	3.75967800	-2.20676300	0.49819100
H	1.85236600	-1.24556800	0.68037700
H	1.95363800	-2.36160200	-0.68135300
H	4.39027600	-2.65484000	-0.27976200
H	4.36333000	-1.41439500	0.96466500
H	-0.59956400	0.92275900	2.73762900
C	-1.58877200	0.83717600	2.30509300
C	-2.26844300	1.84384800	1.56386700
C	-2.46034200	-0.28251600	2.43431700
C	-3.55298200	1.34133700	1.22373400
H	-1.89216600	2.82995400	1.33094600
C	-3.67609300	0.03357000	1.77417200
H	-2.24693000	-1.19847100	2.97280400
H	-4.32071400	1.87512900	0.67508600
H	-4.55244800	-0.59856100	1.72067200
C	3.62518000	-0.83061200	-2.31065000
H	3.79071400	0.01110600	-2.99258500
H	3.12377900	-1.62603700	-2.87750700
H	4.60723800	-1.20523600	-2.00937100
C	-2.49905300	-2.50415800	-0.46198000
C	-1.37415600	-2.23388500	-1.29104700
C	-3.59257700	-1.73281700	-0.94648200
H	-2.52876400	-3.19903400	0.36861600
C	-1.77617500	-1.29956300	-2.28747600
H	-0.39476800	-2.68848800	-1.20335100
C	-3.14197100	-0.98773200	-2.07210700
H	-4.60225600	-1.74460800	-0.55766400
H	-1.16111400	-0.91672500	-3.08945700
H	-3.74302500	-0.31404300	-2.67179700
Zr	-1.88209900	-0.10507500	-0.02662900
H	-0.94292300	2.50575800	-0.90477000
C	-0.74231600	1.47169700	-1.18652700
C	0.53949600	0.92062900	-0.57297500
H	-0.78460000	1.37291900	-2.27173200
C	1.24695900	1.91132500	0.38552200
H	0.26178500	0.02744900	0.13782400
C	1.93878700	3.08754000	-0.32433600
H	0.50842700	2.31489800	1.08821700
H	1.98468400	1.37104500	0.99161900
H	2.74464400	2.71612000	-0.96991700
H	1.22286500	3.59499100	-0.98551900
C	2.52630300	4.10425700	0.66633800
H	1.72452100	4.48627800	1.31418700
H	3.23906400	3.59450400	1.32940700
C	3.22363600	5.27620300	-0.03224500
H	3.64148700	5.97776900	0.69710300
H	4.04648600	4.92699100	-0.66736700
H	2.52510600	5.83278700	-0.66833200
C	3.42800800	-3.27596400	1.54848300
H	2.80350200	-2.82867700	2.33646700
H	2.81708300	-4.06350100	1.08359800
C	4.67375700	-3.90472200	2.18148900
H	4.40222300	-4.66291600	2.92375600
H	5.30081600	-4.38974400	1.42422000
H	5.28703100	-3.14857200	2.68585300

11b

C	-1.54699900	0.20478600	-1.50331700
C	-2.66155600	-0.84006600	-1.28505300
H	-0.95540000	-0.07469600	-2.38498500
H	-1.99663600	1.17915300	-1.73719900
C	-3.63977000	-0.41646000	-0.16871400
H	-2.18018700	-1.78323200	-0.97144300
C	-4.70896600	-1.45715200	0.19794200
H	-3.07347600	-0.18048100	0.74441900
H	-4.13215300	0.52069100	-0.46946800
H	-5.36416300	-1.64318100	-0.66255400

H	-4.22217600	-2.41785800	0.42577100
H	0.44755200	-2.59152600	-1.99143900
C	1.43255500	-2.17876700	-1.80930200
C	1.96595700	-0.99533500	-2.39761800
C	2.44089400	-2.75461100	-0.98771600
C	3.29966700	-0.84231700	-1.93895300
H	1.46046100	-0.35166300	-3.10407800
C	3.59657400	-1.92645400	-1.06676800
H	2.35625900	-3.67845900	-0.42884300
H	3.98015400	-0.04490300	-2.21641500
H	4.54609700	-2.10962800	-0.58005600
C	-3.38166600	-1.10129200	-2.61837500
H	-2.67303000	-1.39164300	-3.40334800
H	-3.90814200	-0.20183600	-2.96147700
H	-4.11906400	-1.90364400	-2.52820400
C	1.36544100	-1.34492700	2.50084100
C	1.22886700	0.07582000	2.52719400
C	2.71970400	-1.64631500	2.20932200
H	0.58225700	-2.06337900	2.71320800
C	2.49067700	0.64762200	2.24537900
H	0.31959200	0.61936500	2.74791600
C	3.41643500	-0.41522300	2.02324700
H	3.15246600	-2.63656200	2.14667500
H	2.71379000	1.70619400	2.20348500
H	4.47737500	-0.30704600	1.83279900
H	-1.11645900	0.76471400	0.57551700
C	-0.58666700	0.42712300	-0.32005400
C	0.64418300	1.27146100	-0.56630600
H	-0.30308400	-0.66682600	-0.00340900
C	0.72293000	2.62865600	0.14576500
H	0.80635000	1.41236700	-1.63951400
C	-0.23466900	3.68366800	-0.44370200
H	0.50774500	2.51640200	1.21662400
H	1.74848500	3.01894900	0.07750000
H	-0.03249000	3.79520900	-1.51857900
H	-1.27073800	3.32388400	-0.36128300
Zr	1.80999300	-0.57154200	0.11259800
C	-5.57089800	-1.03028500	1.39439200
H	-6.04522500	-0.06444100	1.17089400
H	-4.92228600	-0.85636100	2.26542700
C	-6.64850400	-2.05781400	1.75558700
H	-7.24409500	-1.72442300	2.61214300
H	-7.33563700	-2.22321800	0.91718300
H	-6.20374900	-3.02624700	2.01557000
C	-0.11618600	5.05136600	0.24382100
H	0.91937100	5.40952400	0.15805800
H	-0.31215200	4.93488200	1.31926100
C	-1.07055500	6.09854800	-0.33973800
H	-2.11647700	5.78605800	-0.23499100
H	-0.95882600	7.06114600	0.17013700
H	-0.87672400	6.26221600	-1.40646000

β -hydrogen elimination products

Zr/Et

12a

H	-0.58598200	-3.15998600	-0.38671200
C	-1.17517200	-2.28080900	-0.15522500
C	-1.45590100	-1.78410100	1.14753300
C	-1.88393300	-1.47958800	-1.09839600
C	-2.30758200	-0.65460200	1.00433700
H	-1.10859900	-2.20277200	2.08153100
C	-2.58285500	-0.47664200	-0.38383300
H	-1.90212600	-1.62290000	-2.17315500
H	-2.72168800	-0.06919100	1.81520000
H	-3.23547900	0.27248300	-0.81304800
C	1.37094100	2.06976100	-0.05487600
C	0.61162400	2.12624400	1.14794500
C	0.47948300	2.22765500	-1.15130100
H	2.44724600	1.97174300	-0.11776700
C	-0.75396900	2.28991700	0.78753100
H	1.00624700	2.08465100	2.15336600

C	-0.83473000	2.35791500	-0.63572000
H	0.75522900	2.25310600	-2.19979100
H	-1.58151700	2.40391600	1.47580300
H	-1.73197500	2.52698500	-1.21703900
Zr	-0.12432000	0.01631000	-0.03887000
C	3.55012800	-1.14966000	0.69913500
H	3.96186700	-0.22107800	0.29517200
H	4.33540100	-1.91752100	0.65952600
H	1.88543300	-2.53311700	0.31609600
C	2.37189400	-1.63939400	-0.07503800
H	0.64659900	-0.40921700	1.56005200
C	1.91992000	-1.11544200	-1.24393600
H	2.44850900	-0.29827900	-1.72993100
H	1.19567900	-1.66589500	-1.84928300
H	3.29884100	-1.01283900	1.75583300

Zr/Pro

12a

C	1.99825400	-0.01143700	1.26288900
C	2.86177800	-0.02509000	0.20210500
H	1.78622700	-0.93632000	1.79934100
H	1.82023700	0.91971700	1.80042300
C	3.42662400	1.23844000	-0.38142900
H	0.52794300	-0.01334500	-1.59127900
H	3.06006500	2.13711500	0.11866000
H	4.52003400	1.21745500	-0.28581500
H	0.91715500	3.00253800	0.05699300
C	-0.05760200	2.53634900	0.00259400
C	-0.74270100	2.18263600	-1.19295300
C	-0.90462500	2.24098500	1.10554300
C	-2.00296800	1.64085200	-0.82201100
H	-0.38240000	2.32722600	-2.20162300
C	-2.10503400	1.68159100	0.60055700
H	-0.67949100	2.42031200	2.15100800
H	-2.77487600	1.30818400	-1.50370200
H	-2.96537300	1.38765800	1.18755100
C	3.37737200	-1.30307600	-0.39477600
H	2.94296200	-2.19302600	0.06444600
H	4.46577000	-1.34499000	-0.25609900
H	3.19999400	-1.32893200	-1.47598700
C	-1.13267900	-2.12868900	1.14948700
C	-0.13648200	-2.52289500	0.21020700
C	-2.23108900	-1.60291300	0.42632500
H	-1.07334700	-2.23539800	2.22689800
C	-0.62546300	-2.25289100	-1.09640500
H	0.80087800	-3.00792500	0.44882800
C	-1.91273300	-1.66380300	-0.96110000
H	-3.15944300	-1.24490800	0.85164100
H	-0.12503100	-2.47740000	-2.02772200
H	-2.55986200	-1.36661200	-1.77623700
Zr	-0.31017700	0.00159800	0.03001000
H	3.20974500	1.30438800	-1.45393600

12b

C	-2.69412500	-0.58770800	-0.24955300
C	-2.31231500	0.16457200	0.81510500
H	-0.54211400	-0.04803300	-1.68717400
H	-2.52789400	-1.66459400	-0.21482400
C	-1.69797000	-0.36713000	2.08445400
H	-2.57435800	1.22056800	0.81324600
H	-1.79968200	-1.44976200	2.18509200
H	-0.60968500	-0.12717100	2.21951400
H	-0.66333500	-3.09760400	0.30860500
C	0.22425000	-2.51603800	0.09376200
C	0.70770000	-2.18205800	-1.19978000
C	1.18199000	-2.06954500	1.05460600
C	1.93724100	-1.48969600	-1.03604400
H	0.23759800	-2.42421000	-2.14247400
C	2.23704600	-1.43747500	0.35769100

H	1.12814500	-2.21776600	2.12657000
H	2.56400800	-1.12006600	-1.83722100
H	3.12671700	-1.01045900	0.80203500
C	-3.48626200	-0.08165500	-1.41571400
H	-4.51188500	-0.46805100	-1.33913700
H	-3.07666900	-0.44113200	-2.36362900
H	-3.53438700	1.01056700	-1.43967100
C	0.43712100	2.33410300	1.03026300
C	-0.24775700	2.52824100	-0.19946300
C	1.73527900	1.84045500	0.73973600
H	0.04500300	2.54311600	2.01883100
C	0.63374200	2.17901100	-1.26013700
H	-1.24721200	2.92535600	-0.31909500
C	1.85717700	1.74841000	-0.67891500
H	2.51284700	1.62994000	1.46284900
H	0.42127000	2.26142200	-2.31673000
H	2.74659600	1.45420400	-1.22023900
Zr	0.18447400	0.01318300	-0.02071900
H	-2.15263200	0.11544500	2.95613000

Zr/But

12a

C	-1.58316400	-0.44632700	-1.52732500
C	-2.58837200	-0.59482800	-0.60975300
H	-1.13550000	-1.32936100	-1.98420300
H	-1.49666100	0.48899900	-2.08041000
C	-3.47338100	0.56387600	-0.22256300
H	-0.43062700	-0.04600600	1.50407400
C	-3.72078200	0.74590400	1.28517500
H	-3.08889900	1.48868900	-0.66510300
H	-4.43999400	0.37439400	-0.71572500
H	-4.35480000	1.62218500	1.44826600
H	-4.23405300	-0.11643900	1.72083400
H	-2.78126000	0.89402600	1.82770600
H	-1.19163500	2.76204600	-0.27130500
C	-0.15391400	2.47485100	-0.16321300
C	0.53239300	2.29656600	1.07027900
C	0.77341900	2.27616300	-1.22105100
C	1.87890500	1.95880100	0.76855000
H	0.11233800	2.42406500	2.05794800
C	2.02912900	1.94699900	-0.65056500
H	0.56407100	2.36825500	-2.28092000
H	2.66806200	1.79492800	1.49063600
H	2.94830700	1.77249400	-1.19452300
C	-2.93508700	-1.93614300	-0.02813300
H	-2.36831800	-2.74986100	-0.48551000
H	-4.00402100	-2.13389600	-0.17783400
H	-2.76668600	-1.94853600	1.05472600
C	1.74085200	-2.02725700	-0.94770800
C	0.76714400	-2.50539300	-0.02480600
C	2.69498200	-1.27055900	-0.22428200
H	1.76222700	-2.22231300	-2.01406700
C	1.12908400	-2.05817600	1.27493400
H	-0.06878100	-3.14996300	-0.26169600
C	2.31075900	-1.27771500	1.14815900
H	3.57691500	-0.79820700	-0.63678400
H	0.61729900	-2.29039800	2.19805800
H	2.85342300	-0.81709300	1.96343600
Zr	0.52117000	0.01828600	-0.05159500

12b

C	2.26725700	-0.83237300	1.15316100
C	2.28249400	-0.00444000	0.07664700
H	-0.18221400	-0.17734400	1.89817700
H	2.05352800	-1.88968600	0.99547700
C	2.06902000	-0.41908400	-1.35841100
H	2.59393000	1.02776000	0.23094300
C	3.10322200	0.20048900	-2.31575900
H	2.06496200	-1.50977400	-1.44806400

H	1.06824500	-0.08484700	-1.75716100
H	2.89960600	-0.09524300	-3.34867500
H	3.08987400	1.29408000	-2.26239400
H	4.10839300	-0.14106700	-2.05146600
H	0.34965900	-3.13595700	-0.18577100
C	-0.52478500	-2.49779400	-0.20065600
C	-1.34866600	-2.18797600	0.91439200
C	-1.12155600	-1.92761400	-1.36607100
C	-2.42799700	-1.39186700	0.44604200
H	-1.19659300	-2.51196400	1.93427900
C	-2.29517400	-1.24765300	-0.96676700
H	-0.75889400	-2.02540800	-2.38230800
H	-3.23929800	-1.01054700	1.05241200
H	-2.98305200	-0.72826200	-1.62123100
C	2.68621600	-0.44709500	2.53902300
H	3.66136500	-0.90591900	2.75281200
H	1.98317100	-0.82134400	3.28815000
H	2.78611900	0.63571200	2.65421000
C	-0.15211400	2.38830300	-0.83423200
C	0.15680900	2.47691500	0.55009700
C	-1.50680600	1.98656800	-0.95940300
H	0.52261100	2.60583400	-1.65402500
C	-1.01506400	2.15402800	1.28936400
H	1.10100700	2.79081400	0.97548000
C	-2.04116800	1.84487500	0.35597600
H	-2.05134200	1.86603700	-1.88706300
H	-1.11421900	2.17603200	2.36542900
H	-3.06584000	1.59784900	0.60023300
Zr	-0.36202800	0.01178900	0.09775400

Zr/Hex

12a

C	-0.46536500	-1.18087800	-1.76780900
C	-1.58409200	-1.52396400	-1.05619300
H	0.30254300	-1.93158300	-1.95683400
H	-0.50799800	-0.33968800	-2.45963200
C	-2.81541200	-0.65570700	-1.06056000
H	-0.16825900	-0.04764600	1.31838200
C	-3.43678600	-0.35142100	0.31922300
H	-2.61160900	0.27704500	-1.59833700
H	-3.56259100	-1.19545900	-1.66461000
H	-3.72977500	-1.28842200	0.80902600
H	-2.67957000	0.11396900	0.96459300
H	-1.20218400	2.08725200	-1.26284700
C	-0.20973100	2.16279200	-0.83819800
C	0.09168400	2.37312000	0.53556300
C	1.01344400	2.14236900	-1.56437600
C	1.50547200	2.45038900	0.65881200
H	-0.62439800	2.48262200	1.33747600
C	2.07477100	2.31581000	-0.64190000
H	1.11860600	2.02570500	-2.63716000
H	2.05063300	2.63882700	1.57436900
H	3.12689000	2.37765000	-0.88727500
C	-1.67585700	-2.83151700	-0.32136200
H	-0.81209900	-3.47429100	-0.50464200
H	-2.57846600	-3.36759800	-0.64071900
H	-1.77909300	-2.66922300	0.75777100
C	2.82736100	-1.70677500	-0.31335900
C	1.89014500	-2.20795700	0.63108500
C	3.45197500	-0.56591300	0.24957200
H	3.03757300	-2.12658900	-1.29070900
C	1.95099800	-1.39228700	1.79488400
H	1.27337700	-3.08865500	0.51014100
C	2.90621100	-0.36837300	1.55293400
H	4.23769200	0.02024400	-0.20875700
H	1.39340900	-1.54137000	2.70861100
H	3.20866200	0.39423300	2.25853300
Zr	1.03138600	0.08988000	-0.04861500
C	-4.66378500	0.56514700	0.21055200
H	-4.37521700	1.50403500	-0.28324000
H	-5.41077600	0.09401600	-0.44280400
C	-5.29309100	0.87435400	1.57277100

H	-6.16221000	1.53064400	1.46251600
H	-5.62887000	-0.04146100	2.07299900
H	-4.57936900	1.37539600	2.23791000

12b

C	-0.52742200	2.55359000	-0.41628900
C	-1.22802400	1.58094200	0.22277100
H	1.83494300	1.51417000	0.13471700
H	-0.41843300	2.49372300	-1.49933600
C	-1.92405700	0.41630200	-0.43508000
H	-1.41360200	1.70454100	1.28895100
C	-3.35259100	0.18544500	0.10461300
H	-1.94182000	0.53875200	-1.52298900
H	-1.39341900	-0.56501300	-0.25666300
H	-3.31209200	0.07478700	1.19689500
H	-3.93706500	1.09276600	-0.09411200
H	0.28829800	0.78914700	-3.06385000
C	0.92442900	0.11268700	-2.50716100
C	2.24914900	0.38449100	-2.07100200
C	0.62581400	-1.24881000	-2.19851100
C	2.75028800	-0.79244600	-1.45345000
H	2.78935900	1.31161200	-2.20043200
C	1.75067600	-1.80602900	-1.54851000
H	-0.29031700	-1.77274700	-2.44309700
H	3.74163700	-0.91189900	-1.03616100
H	1.84578800	-2.82828000	-1.20571400
C	-0.02163000	3.81009000	0.22421300
H	-0.64175700	4.65251800	-0.11179300
H	1.00663100	4.02668400	-0.07812400
H	-0.06951300	3.76535800	1.31578900
C	0.02829800	-0.97581100	2.24849000
C	0.68613000	0.24266900	2.56423700
C	0.99017700	-1.87201700	1.71402100
H	-1.02272200	-1.19132300	2.40123300
C	2.06615500	0.09779500	2.25063100
H	0.23272700	1.11664700	3.01335800
C	2.25262200	-1.20754600	1.72117400
H	0.80820500	-2.89584600	1.41337300
H	2.83670600	0.83717500	2.41786500
H	3.19803800	-1.64107700	1.42338700
Zr	0.85897300	-0.01716600	0.02237300
C	-4.04610500	-1.03239600	-0.51836600
H	-3.44752500	-1.93377100	-0.31952800
H	-4.07528000	-0.91456000	-1.61031200
C	-5.46882700	-1.23453900	0.01369500
H	-5.93564000	-2.11215000	-0.44424900
H	-5.47106600	-1.38384100	1.09978300
H	-6.10149300	-0.36725400	-0.20678900

β -hydrogen transfer products

ZrEt

13a

H	-0.81152400	2.70995900	-1.64663300
C	-0.29722400	2.50299200	-0.71530500
C	-0.90453100	2.32219000	0.56126600
C	1.10423800	2.40056500	-0.55421000
C	0.12373400	2.12783800	1.51434600
H	-1.96402500	2.37234700	0.77818500
C	1.36708900	2.15655700	0.82753200
H	1.84582000	2.52457100	-1.33247600
H	-0.01297000	1.98756700	2.57788200
H	2.34554000	2.08834000	1.28425100
C	1.42952800	-1.55700700	-1.61701500
C	1.08306200	-2.31428800	-0.46325300
C	2.36725500	-0.56888500	-1.23197300
H	1.05995100	-1.72273000	-2.62182400
C	1.82452200	-1.80815700	0.63450000
H	0.40222500	-3.15512000	-0.43369200

C	2.60891600	-0.71955900	0.16561400
H	2.84786400	0.14418100	-1.88898300
H	1.81209800	-2.19116500	1.64534000
H	3.32065700	-0.15373400	0.75176300
Zr	0.23111000	0.07213500	-0.01988300
C	-3.80112800	-0.52643300	-0.39362800
H	-3.64455600	-1.59032100	-0.20126800
H	-4.75109200	-0.40505200	-0.93264900
H	-2.80122200	1.14562300	-1.41099600
C	-2.71027200	0.07819000	-1.21249600
H	-1.77016200	-2.48786600	1.02322400
C	-1.67239900	-0.59110000	-1.77007100
H	-1.61066800	-1.67558400	-1.71506400
H	-1.03551400	-0.09605700	-2.50783800
C	-1.20909500	-2.19390500	1.92023200
H	-1.87780700	-2.36658500	2.77416600
H	-0.37662600	-2.89683000	2.02428000
C	-0.74102100	-0.72972700	1.88489800
H	-0.11833900	-0.52303900	2.76657400
H	-1.61669100	-0.06938700	1.99782900
H	-3.92342500	-0.00014800	0.56063900

Zr/Pro

13a

C	1.52231200	-0.58066200	-1.97905400
C	2.67265500	-0.41291900	-1.27497800
H	1.13143300	0.21342000	-2.60733400
H	1.14008600	-1.57888600	-2.16328400
C	3.37342400	-1.57445600	-0.62116900
H	1.56417100	-0.11924700	0.98654200
H	3.63859300	-1.35598600	0.41991400
H	2.78440900	-2.49461500	-0.65451300
H	-1.28914100	-2.04740000	-2.30923500
C	-1.43934300	-1.98033900	-1.23927100
C	-0.59628900	-2.53028100	-0.22792900
C	-2.55699300	-1.39377900	-0.59544700
C	-1.19209100	-2.27134100	1.02875600
H	0.31748600	-3.08757900	-0.39080300
C	-2.39259000	-1.54644700	0.80904100
H	-3.39928100	-0.93088200	-1.09142000
H	-0.80064400	-2.57182500	1.99123200
H	-3.07961200	-1.20681800	1.57352200
C	3.38785900	0.90914900	-1.19337400
H	2.84987100	1.71515600	-1.69744800
H	4.37399000	0.81451000	-1.66687800
H	3.57549100	1.20031000	-0.15268400
C	-1.47568000	1.63853600	-1.66355500
C	-0.22435700	2.20739100	-1.31846800
C	-2.31356500	1.71296800	-0.50855300
H	-1.76798400	1.27728100	-2.64145800
C	-0.26550400	2.58620500	0.04705600
H	0.61663700	2.34276600	-1.98462100
C	-1.56752100	2.29938400	0.54271900
H	-3.35526800	1.42676000	-0.45733000
H	0.53730000	3.05573900	0.60199600
H	-1.93400300	2.51093200	1.53728600
H	-0.73413200	-0.36779600	2.95977100
C	-0.18112600	0.27575200	2.27735100
C	1.26649200	-0.15339200	2.08268200
H	-0.24586000	1.30441900	2.63216100
C	2.31058800	0.71779100	2.80169900
H	1.40563300	-1.20810500	2.34255900
H	3.33344400	0.38913000	2.58720700
H	2.21792700	1.76932600	2.50904300
Zr	-0.53317300	0.01579600	0.02833500
H	4.31983100	-1.76157800	-1.14605000
H	2.15692500	0.65775300	3.88341200

13b

C	2.87091200	0.00540200	0.35139000
C	2.61074300	-1.29564100	0.08628900
H	0.93337400	1.74023000	-0.12943900
H	2.87922100	0.33083600	1.39317500
C	2.47830100	-2.39735000	1.09968800
H	2.69486000	-1.62427900	-0.95025800
H	2.40568300	-2.02331200	2.12444800
H	1.62678300	-3.05644000	0.89922500
H	0.95556100	-0.39799000	2.84558400
C	-0.05188100	-0.36842300	2.45350600
C	-0.86414900	0.78927400	2.35405600
C	-0.79170300	-1.47499700	1.96197700
C	-2.12696600	0.39900600	1.83195000
H	-0.58138400	1.79041400	2.65394100
C	-2.08405100	-0.99653900	1.58843100
H	-0.46364600	-2.50529900	1.93489000
H	-2.97776800	1.04554800	1.66802400
H	-2.90967100	-1.60017100	1.23662400
C	3.43666800	0.97696600	-0.65151000
H	4.52213800	1.04414100	-0.49741100
H	3.04651000	1.99210600	-0.53577400
H	3.27354600	0.65039900	-1.68380500
C	-0.19310200	-2.00836400	-1.59395400
C	0.26755600	-0.88942300	-2.35020000
C	-1.58906900	-1.85037400	-1.39845400
H	0.39713500	-2.85937800	-1.28098200
C	-0.83962900	-0.04728800	-2.60643300
H	1.27831200	-0.72756700	-2.70230900
C	-1.98678900	-0.62516300	-2.00061900
H	-2.24192500	-2.55574700	-0.90254200
H	-0.81602900	0.87901300	-3.16493400
H	-2.99109400	-0.22235200	-2.02786000
H	-1.75118700	2.24898200	-1.43315100
C	-1.21302200	2.09607400	-0.49944800
C	0.23918800	2.53840600	-0.55982300
H	-1.75432800	2.58488300	0.30984600
C	0.58457300	3.81165000	0.22966200
H	0.58855200	2.62337100	-1.59447300
H	0.28234300	3.72268400	1.27833000
H	1.65720500	4.03103900	0.19908600
Zr	-0.44916500	-0.01814900	-0.05656300
H	0.05136500	4.66418900	-0.20171400
H	3.37558300	-3.02865400	1.04494300

Zr/But

13a

C	-1.21634200	-2.07902100	0.53471400
C	-2.34688800	-1.32965800	0.63575500
H	-0.67630400	-2.40262900	1.41936600
H	-1.00416600	-2.61302800	-0.38524200
C	-3.25790000	-1.12666300	-0.55562700
H	-1.26012000	0.78216700	-0.25637500
C	-4.49305700	-2.05393800	-0.50648800
H	-3.60056600	-0.08452700	-0.58916000
H	-2.70740800	-1.31892400	-1.48336700
H	-5.10982200	-1.88986100	-1.39509000
H	-4.19514600	-3.10700700	-0.48747400
H	-5.11630900	-1.85746000	0.37103000
H	1.31351000	-3.08579000	-1.08074300
C	1.46137700	-2.08440100	-1.46452500
C	0.53533300	-1.33053000	-2.24564100
C	2.64394000	-1.31480200	-1.33772900
C	1.14803300	-0.10212300	-2.58794600
H	-0.44756500	-1.65547200	-2.56276500
C	2.44225500	-0.07529800	-2.00635500
H	3.54951400	-1.62794700	-0.83604400
H	0.70452500	0.68352900	-3.18460100
H	3.16256200	0.72796800	-2.09427400
C	-2.81818300	-0.75469300	1.94454700
H	-2.15451200	-0.99747800	2.77747200
H	-3.81321600	-1.14900500	2.18395700
H	-2.92790800	0.33518800	1.88134200

C	2.07748200	-1.01598700	1.97925500
C	0.91049700	-0.44313400	2.54266800
C	2.87246000	0.05218400	1.46093600
H	2.35040300	-2.06350200	1.99843700
C	0.95280000	0.95838100	2.33314700
H	0.12354400	-0.98120100	3.05317100
C	2.18037700	1.26700900	1.68314500
H	3.85730400	-0.04045100	1.02335900
H	0.20662000	1.67364200	2.65658600
H	2.53642300	2.25397900	1.42418800
H	0.91628700	2.44069500	-1.56666400
C	0.47397400	2.09041100	-0.63575100
C	-1.01153700	1.78341800	-0.73809100
H	0.67950000	2.81790100	0.14977000
C	-1.95771200	2.79134200	-0.04954100
H	-1.31713000	1.63171500	-1.78000500
C	-1.96428600	4.15619800	-0.74477200
H	-2.97705300	2.38337400	-0.03702100
H	-1.65213700	2.90799100	0.99909000
H	-2.64795700	4.84368900	-0.23661600
H	-0.96816100	4.61121800	-0.74465000
H	-2.29413900	4.06735300	-1.78651700
Zr	0.84184200	-0.09045700	-0.02203400

13b

C	-1.30034300	2.38462800	-0.09562500
C	-2.29038300	1.55003700	0.29932600
H	1.15265800	1.42636100	-0.05122500
H	-1.17286900	2.56849100	-1.16417200
C	-3.37153300	0.97381700	-0.57861300
H	-2.46725100	1.45397200	1.37203900
C	-4.70769200	1.70805400	-0.33906200
H	-3.09637100	1.05883600	-1.63550000
H	-3.51866400	-0.09240000	-0.36427800
H	-5.49545200	1.27037700	-0.96023800
H	-5.02342900	1.63163500	0.70726200
H	-4.62338700	2.76993900	-0.59083200
H	-1.16145000	0.55294300	-2.69097000
C	-0.62709400	-0.33780000	-2.38943100
C	0.77537500	-0.52799200	-2.47752800
C	-1.20291300	-1.51588100	-1.84825300
C	1.07207100	-1.84116800	-2.02282300
H	1.49136700	0.19173900	-2.85405700
C	-0.14604400	-2.45145600	-1.63197600
H	-2.25679900	-1.69950000	-1.68826500
H	2.04893600	-2.30345800	-1.99744600
H	-0.25832900	-3.47052000	-1.28741500
C	-0.54448700	3.30222900	0.82987300
H	-1.00339200	4.29926100	0.78444100
H	0.50342800	3.43250500	0.54567700
H	-0.59061700	2.96937000	1.87200400
C	-1.47888800	-1.27689500	1.81085000
C	-0.54986700	-0.41660300	2.47103700
C	-0.79013300	-2.46315000	1.45575000
H	-2.53363600	-1.08929700	1.66175300
C	0.70116200	-1.07445500	2.51455700
H	-0.77069200	0.54997100	2.90575600
C	0.56604400	-2.32922800	1.86348800
H	-1.22853100	-3.32902800	0.97817800
H	1.60580000	-0.68636900	2.96267600
H	1.34679800	-3.06892700	1.74034200
H	2.95905800	-0.75838100	1.05162600
C	2.46047800	-0.32831600	0.18564500
C	2.20545300	1.16297200	0.30248500
H	3.02493200	-0.57667800	-0.71277100
C	3.11895900	2.08237400	-0.53868000
H	2.20504200	1.48854200	1.34934000
C	4.56644100	2.07849400	-0.03844200
H	3.08339400	1.75559200	-1.58606100
H	2.72483300	3.10660800	-0.51608400
H	5.18485500	2.74255100	-0.65064100
H	4.62796500	2.42842500	0.99870500
H	5.00398400	1.07548200	-0.08293600

Zr	0.18745500	-0.59440000	0.03169100
----	------------	-------------	------------

Zr/Hex

13a

C	4.76792200	-3.12685900	-1.03750500
H	5.42774900	-2.79599600	-0.22674700
H	5.29838900	-3.89996200	-1.60252100
H	4.61037000	-2.27394700	-1.70911200
C	3.43971200	-3.65938500	-0.49091800
H	2.81747200	-4.02143700	-1.32141600
H	3.62819500	-4.53054600	0.15125400
C	2.65799500	-2.60621900	0.30810700
H	3.28385800	-2.24742800	1.13515300
H	2.46151600	-1.73668300	-0.33472300
C	1.32947100	-3.16055300	0.85664000
H	0.73073800	-3.57660700	0.03741200
H	1.56358300	-4.01316600	1.51486300
C	0.47810800	-2.22332300	1.68270300
H	0.66858100	0.13935500	0.33439900
C	-0.86979400	-2.16454000	1.50875800
H	-1.49902600	-1.69844500	2.25951900
H	-1.35905800	-2.84409500	0.81836300
H	-0.89063000	2.65324600	1.87741200
C	-1.75491900	2.05434300	1.62112400
C	-2.69159100	2.33879100	0.59122400
C	-2.15566400	0.85957600	2.26340900
C	-3.67610900	1.31771900	0.60683400
H	-2.67424100	3.19659500	-0.06769400
C	-3.33499400	0.38310200	1.62576700
H	-1.65883900	0.40581100	3.11102500
H	-4.56017400	1.28472700	-0.01431700
H	-3.91078100	-0.48933100	1.90881600
H	-0.63158600	-2.56427800	-1.61000000
C	-1.34803700	-1.77519400	-1.79753000
C	-2.69824900	-1.73740700	-1.34086200
C	-1.11298400	-0.61456100	-2.57089100
C	-3.29232700	-0.55560000	-1.85545600
H	-3.20326000	-2.49934300	-0.76088300
C	-2.30675100	0.15392500	-2.59281300
H	-0.18284200	-0.35428600	-3.05836700
H	-4.32683800	-0.26561600	-1.73613000
H	-2.44926100	1.09416000	-3.10931500
C	1.16112200	-1.47398600	2.79526000
H	0.45468600	-0.91150800	3.41110400
H	1.91902000	-0.78156100	2.41214900
H	1.69270300	-2.18191600	3.44449000
H	2.24779400	3.39970300	-0.94883000
C	2.92168500	2.68146400	-0.46223900
C	3.99244700	3.44303900	0.33154500
H	3.40333300	2.11408800	-1.27211100
C	2.10358700	1.71941400	0.41012200
C	4.80591800	4.40717800	-0.53823100
H	4.66853800	2.72256800	0.81285000
H	3.51016800	4.00158900	1.14623100
H	2.78408200	1.00956600	0.89974600
H	1.60540300	2.27993600	1.21326600
C	1.04383100	0.93542400	-0.39345900
H	4.16112400	5.16158100	-1.00474600
H	5.55894500	4.93493900	0.05622900
H	5.32922400	3.87407800	-1.34097300
H	1.53138500	0.33698600	-1.17162100
C	-0.10412700	1.74787900	-0.96895900
H	-0.18678900	2.73099400	-0.50579200
H	-0.05073500	1.86871100	-2.04931100
Zr	-1.54775800	0.17030400	-0.15038600

13b

C	-1.10275000	1.38192300	0.04232900
C	0.16941900	1.84531000	-0.67912900

H	-0.03977300	2.02807100	-1.73842900
H	0.96393200	1.04563200	-0.70023100
H	-3.24452800	-0.88077400	-1.51639900
C	-2.23791100	-1.20741300	-1.74276300
C	-1.26194900	-0.46465900	-2.45289800
C	-1.67486700	-2.47638000	-1.42874100
C	-0.08634000	-1.24913900	-2.54343500
H	-1.39557400	0.52465300	-2.86522900
C	-0.34234900	-2.50040500	-1.90919000
H	-2.18372500	-3.29166500	-0.93268400
H	0.82399300	-0.96478800	-3.05571000
H	0.34004700	-3.33858200	-1.84578300
H	1.33979300	-2.22887000	2.38579700
C	0.32126100	-1.90507200	2.21317000
C	-0.21706200	-0.63080400	2.53867700
C	-0.70545700	-2.68910000	1.63933100
C	-1.60111200	-0.64654200	2.21735000
H	0.31647000	0.18562700	3.01047300
C	-1.90124400	-1.90644600	1.64410300
H	-0.61436200	-3.71484700	1.30584200
H	-2.30580300	0.15410400	2.38607600
H	-2.88053900	-2.23742400	1.32397100
C	0.83503200	3.08365200	-0.05361300
H	1.12677200	2.89898100	0.98657000
H	0.13141900	3.92240200	-0.05579200
H	1.72440700	3.39109700	-0.61362500
H	-0.99297900	1.64081600	1.10299000
C	-2.38768700	2.03710100	-0.47144300
H	-2.24398100	3.13049100	-0.48294800
H	-2.57210800	1.75983500	-1.51792600
C	-3.64550300	1.73951700	0.35621900
H	-3.83581600	0.65567300	0.37098900
H	-3.47082800	2.03455000	1.40211400
C	-4.89615600	2.46335400	-0.16254900
H	-5.06908800	2.18095300	-1.21086900
H	-4.70928600	3.54586500	-0.16618600
C	-6.15136800	2.16276700	0.66285200
H	-7.02268100	2.69317800	0.26499000
H	-6.38509600	1.09078800	0.65802200
H	-6.02392300	2.47095200	1.70760000
H	2.53201500	-1.58288700	-1.43806800
C	2.36984700	-1.57002900	-0.36403100
C	2.86243400	-0.56332600	0.39298000
H	1.99900500	-2.48757700	0.08562600
C	3.65357900	0.60207600	-0.11694000
H	2.77338900	-0.63262600	1.47771100
H	3.26494300	1.53638900	0.30792800
H	3.57254600	0.67334700	-1.20852200
C	5.14359400	0.46653600	0.28861000
H	5.54826700	-0.46057800	-0.13765500
H	5.21616400	0.36606200	1.38037000
C	5.98653600	1.66392800	-0.17292100
H	5.90337900	1.76671400	-1.26356000
H	5.57123300	2.58582400	0.25735200
C	7.46126600	1.52997200	0.22028700
H	8.03710700	2.39646200	-0.12060300
H	7.57853000	1.45878800	1.30805200
H	7.91173600	0.63470400	-0.22404200
Zr	-0.38080800	-0.79880700	-0.03344300

Hf Dichloride precursor

Hf	0.00002700	-0.07363300	-0.00091900
Cl	0.04645600	-1.64289700	1.85000700
Cl	-0.04877400	-1.67370700	-1.82454400
C	-2.27276500	0.38393900	1.09022800
C	-2.54486000	-0.18759900	-0.17567700
C	-2.11320700	0.73020700	-1.17472500
C	-1.55187600	1.85417100	-0.52494500
C	-1.63228800	1.63298300	0.88332400
C	2.04751500	0.86570100	1.17726300
C	2.53567200	-0.15653900	0.31272700

C	2.32869800	0.26267300	-1.02085000
C	1.67732700	1.52525200	-0.99276200
C	1.53112600	1.90876300	0.37288300
H	-2.46455600	-0.07821000	2.04815300
H	-2.98272900	-1.16026400	-0.35529300
H	-2.17484000	0.57549200	-2.24346200
H	-1.14535400	2.73198900	-1.00939800
H	-1.31132700	2.31764000	1.65765700
H	2.05627800	0.83617200	2.25877500
H	2.96157800	-1.09994000	0.62603800
H	2.56772000	-0.30594100	-1.90815200
H	1.39564400	2.11409700	-1.85635900
H	1.10298600	2.83551200	0.73054100

Cation/Hf

1

Hf	-0.00021800	0.21256200	-0.07423600
C	-1.96828500	-0.97735600	-1.06366900
C	-2.42383400	0.32453000	-0.68781600
C	-2.35922000	0.42274400	0.72361800
C	-1.85046900	-0.81373000	1.22903100
C	-1.64237600	-1.68585300	0.12279400
C	1.91645200	-1.10472300	-1.00284100
C	2.39289300	0.22765200	-0.79970900
C	2.39246000	0.48948300	0.59253800
C	1.90090800	-0.67579000	1.25834900
C	1.64015300	-1.66773200	0.27129600
H	-1.93736400	-1.37610500	-2.07167600
H	-2.76995300	1.09889000	-1.36179200
H	-2.64321000	1.28541400	1.31305700
H	-1.72424500	-1.07158300	2.27429800
H	-1.29889900	-2.71053700	0.17635500
H	1.83963300	-1.61728500	-1.95517200
H	2.71344600	0.91570800	-1.57343200
H	2.70739100	1.41032200	1.06597600
H	1.81768000	-0.80885400	2.33109500
H	1.29424400	-2.67529900	0.46052300
C	0.00126400	2.41859800	0.06330600
H	-0.90151800	2.91467100	-0.31275000
H	0.87137100	2.91457900	-0.38502600
H	0.04742900	2.66867600	1.14214200

1st π -complex

Hf/Et

2a

Hf	0.00055000	0.06031100	0.09296700
C	-2.13393200	-0.18919600	-1.29481200
C	-2.54018700	0.25418500	0.00192200
C	-2.23624000	-0.76909700	0.93136400
C	-1.60983100	-1.83133200	0.22282700
C	-1.57076200	-1.47651300	-1.16024000
C	2.22324900	-0.00772600	-1.18658700
C	2.55170000	0.25172100	0.17736900
C	2.18862000	-0.88376700	0.94024800
C	1.60732500	-1.83680000	0.05788500
C	1.64156000	-1.29407600	-1.26227800
H	-2.26600400	0.34918300	-2.22595500
H	-3.05359000	1.17944200	0.22801600
H	-2.44354500	-0.74790100	1.99218500
H	-1.30030600	-2.77874300	0.64489500
H	-1.19587400	-2.09426100	-1.96512300
H	2.42456300	0.64338900	-2.02802300
H	3.03923200	1.13920500	0.55973700
H	2.32906900	-1.00474900	2.00570800
H	1.27590000	-2.83118300	0.32666000
H	1.32003000	-1.79299400	-2.16664300
C	-0.00358900	0.71897100	2.22757200

H	-0.89278800	1.32103700	2.46167600
H	0.88396200	1.32557500	2.45663600
H	0.00022200	-0.10705200	2.95260800
H	-1.21060800	2.89806500	0.39341700
C	-0.72722600	2.70361100	-0.56039000
H	-1.36843400	2.64398600	-1.43485800
C	0.61878800	2.69323500	-0.66956200
H	1.10799500	2.62671400	-1.63693400
H	1.25371100	2.88857900	0.19046700

Hf/Pro

2a

C	3.79193500	-0.87281400	0.26450800
H	3.57121100	-1.94072000	0.33777100
H	3.78733400	-0.42985100	1.26639600
C	2.85741800	-0.15656800	-0.65038900
H	2.98955700	0.92314200	-0.71912800
C	1.91298700	-0.74428000	-1.42679400
H	1.84002700	-1.82607500	-1.48418700
H	1.41480300	-0.17419800	-2.21547100
H	0.24978900	-3.19643100	0.02347900
C	-0.56714300	-2.49019100	-0.05785700
C	-1.34239200	-1.99688900	1.01950100
C	-1.08926400	-1.94057400	-1.26708500
C	-2.31950600	-1.11099500	0.48599000
H	-1.21210700	-2.24540700	2.06356100
C	-2.17395100	-1.09820900	-0.93318900
H	-0.73627800	-2.15104300	-2.26964900
H	-3.08805900	-0.60052000	1.05230300
H	-2.79351200	-0.55087300	-1.63139200
H	1.04135800	2.31466800	-1.90796500
C	0.34615800	2.24097300	-1.07978200
C	-1.04388700	1.97892200	-1.18778100
C	0.65635900	2.43425900	0.29380500
C	-1.59704400	2.02466400	0.12665400
H	-1.59421400	1.82794600	-2.10746900
C	-0.54462200	2.31254600	1.03701900
H	1.63055900	2.66435000	0.70540000
H	-2.64432300	1.92088900	0.37758000
H	-0.64098600	2.42156300	2.10913300
Hf	-0.13492600	0.00721400	0.06804400
C	0.80625700	-0.22985100	2.08263400
H	0.08913100	-0.09647400	2.90603400
H	1.60487900	0.50264200	2.25978300
H	1.23143900	-1.23506700	2.21288100
H	4.81423800	-0.75388300	-0.12161500

2b

C	-2.15258000	-0.17848900	1.30190300
C	-2.82221400	-0.78456900	0.28986600
H	-2.33618500	0.86538000	1.54577300
H	-1.63508200	-0.77738900	2.05250300
C	-3.77243100	-0.12635100	-0.65315300
H	-2.71058500	-1.86189100	0.17310500
H	-3.86194600	0.94916200	-0.48286000
H	-3.49444600	-0.31081400	-1.69846500
H	-0.48377700	2.96541000	1.33518900
C	-0.06459500	2.54664000	0.42895600
C	1.31173100	2.30403700	0.18924500
C	-0.78687700	2.17451000	-0.73726100
C	1.44024000	1.75650000	-1.11605800
H	2.12026200	2.49846900	0.88106900
C	0.13719100	1.68138100	-1.69244200
H	-1.85510100	2.27215200	-0.88353000
H	2.36874500	1.50198300	-1.61020500
H	-0.09906500	1.35192800	-2.69595800
Hf	0.22045900	0.02365200	0.18896300
C	1.03244900	0.12410100	2.27142500
H	2.12671100	0.22837400	2.30276500

H	0.79776400	-0.77790600	2.85366200
H	0.62797200	0.98806100	2.81655800
C	-0.14844200	-2.08461000	-1.20034700
C	0.13628800	-2.51561500	0.13303800
C	1.00889700	-1.45916500	-1.71356900
H	-1.06985400	-2.24881600	-1.74548500
C	1.47279600	-2.16111700	0.43210500
H	-0.53024500	-3.06858300	0.78407100
C	2.00596100	-1.47466200	-0.69539000
H	1.12083900	-1.04432900	-2.70646100
H	1.99735800	-2.36918800	1.35389800
H	3.01811700	-1.10113300	-0.78890500
H	-4.76503700	-0.57936900	-0.52194200

Hf/But

2a

C	8.91632600	0.09757500	2.67286400
C	8.27057600	1.27173600	2.88800400
H	10.00147500	0.05754300	2.67792800
H	8.38945600	-0.85475000	2.77939600
C	8.92614800	2.60515200	3.05142300
H	7.18740000	1.25688700	3.01437100
C	8.73095000	3.12949300	4.49331700
H	9.99340700	2.53736200	2.81371800
H	8.47436400	3.31924900	2.35147100
H	9.19567000	4.11498000	4.58749800
H	7.66960900	3.23206900	4.74309000
H	9.19427300	2.46105100	5.22529700
H	5.47552600	1.42378700	1.01747800
C	5.75359000	0.48852200	0.54929600
C	5.90848400	0.27792500	-0.84392900
C	5.99097800	-0.74642700	1.21090700
C	6.25904500	-1.08410300	-1.04581300
H	5.78019300	1.02492800	-1.61615200
C	6.31259500	-1.72015700	0.23021700
H	5.90812400	-0.92639400	2.27639000
H	6.40248700	-1.56872700	-2.00249500
H	6.50685200	-2.76908500	0.41327700
Hf	8.21661300	-0.09048400	0.13711400
C	8.36619900	2.06236600	-0.44615300
H	8.26112100	2.21800000	-1.52997000
H	9.34588300	2.48039400	-0.17405100
H	7.59061200	2.68133900	0.02353500
C	10.21773200	-1.66205800	0.28522600
C	10.73222700	-0.37638600	-0.06084600
C	9.41528200	-2.11541300	-0.78606800
H	10.42575600	-2.20964800	1.19674600
C	10.25786400	-0.04685200	-1.35347200
H	11.40526300	0.22523100	0.53727500
C	9.41665400	-1.10608700	-1.79414100
H	8.90126700	-3.06614700	-0.83870900
H	10.48936000	0.85286700	-1.90625800
H	8.92950200	-1.16831600	-2.75897200

2b

C	8.09659800	0.97294200	2.61486200
C	8.57148600	-0.15240300	3.20661100
H	7.04645200	1.24499500	2.69562800
H	8.78524700	1.75627600	2.29430700
C	7.76571300	-1.18139900	3.93420900
H	9.65058000	-0.30790300	3.22252200
C	8.18229900	-1.24631700	5.42160200
H	6.69597200	-0.96116800	3.85242400
H	7.94015100	-2.16718900	3.47975600
H	7.59986100	-2.01898600	5.93115800
H	9.24299000	-1.49618500	5.52965500
H	7.99996700	-0.29226300	5.92516600
H	5.18792900	1.36121500	0.59185700
C	5.64085200	0.50801400	0.10276600
C	6.05518900	0.45443900	-1.25222000

C	5.89581300	-0.76010900	0.69134800
C	6.59091100	-0.83909800	-1.49667600
H	5.98049100	1.25960900	-1.97082300
C	6.48663300	-1.59423400	-0.29067900
H	5.65771300	-1.05043000	1.70663500
H	6.95575600	-1.20670700	-2.44695300
H	6.76423100	-2.63224700	-0.16106000
Hf	8.17609800	0.21660900	0.10602600
C	8.22033900	2.39472200	-0.40445600
H	8.26381400	2.58354300	-1.48691000
H	9.09437400	2.90310200	0.02636300
H	7.32144800	2.91093300	-0.04033200
C	10.18952900	-1.28858500	0.53069400
C	10.68090300	0.05372900	0.49824800
C	9.71025400	-1.60934900	-0.75833400
H	10.21894900	-1.96236500	1.37818500
C	10.50968700	0.55148800	-0.81503500
H	11.15350100	0.58286000	1.31708500
C	9.87585800	-0.46237400	-1.58762000
H	9.29268700	-2.55949200	-1.06385700
H	10.80214800	1.52936200	-1.17047700
H	9.63354800	-0.39732700	-2.64107500

Hf/Hex

2a

C	-2.03113200	0.33097200	-0.72981200
C	-1.17349900	-0.48608400	-1.39575400
H	-0.58437300	-0.10280600	-2.23367900
H	-1.28122600	-1.56474600	-1.32682600
H	-0.50539300	2.83765500	0.66258800
C	0.44943900	2.49130300	0.28874100
C	1.59397000	2.21878300	1.07836100
C	0.79027200	2.26954900	-1.07417900
C	2.63890300	1.80575700	0.20849400
H	1.65822900	2.30892300	2.15454100
C	2.13974800	1.83903000	-1.12826600
H	0.14414700	2.42878600	-1.92951100
H	3.65403300	1.57088400	0.49988700
H	2.70454300	1.62527600	-2.02628700
H	1.24693100	-2.22724700	-2.27894500
C	1.63336400	-2.06406100	-1.28000000
C	2.81673900	-1.36192400	-0.95549100
C	1.06005300	-2.54867600	-0.06705600
C	2.97454900	-1.39852400	0.46186900
H	3.49329800	-0.89493600	-1.65899000
C	1.90046400	-2.15740900	1.00346300
H	0.16294700	-3.14845600	0.02234600
H	3.80647800	-0.99016000	1.02104300
H	1.75007200	-2.39104300	2.04822200
Hf	0.93963200	-0.01280100	0.07069900
C	-0.03001300	-0.16157300	2.07851400
H	0.68731900	-0.15441800	2.91175100
H	-0.59165600	-1.10250800	2.16834800
H	-0.72534200	0.66657000	2.26738600
H	-1.99567700	1.40051700	-0.93822000
C	-3.09795300	-0.11347800	0.21269800
H	-2.96623400	-1.16905100	0.47608400
H	-3.03980600	0.47208800	1.13948000
C	-4.50058000	0.10324500	-0.41844100
H	-4.62018000	1.16006700	-0.69305800
H	-4.56921000	-0.47347300	-1.34973500
C	-5.62992000	-0.31248700	0.53600200
H	-5.49307200	-1.36427100	0.82160800
H	-5.55341400	0.27270800	1.46242800
C	-7.01825900	-0.12316600	-0.08359500
H	-7.80163100	-0.42671500	0.61827900
H	-7.19716200	0.92518000	-0.34963500
H	-7.13398900	-0.72471100	-0.99271800

2b

C	-2.01879700	-0.66867400	0.56394300
C	-1.18144700	-0.18299600	1.51688000
H	-0.61627300	-0.86888500	2.14977000
H	-1.27302900	0.84404300	1.86441700
H	0.43665500	2.93719600	1.41297700
C	0.79553800	2.53262300	0.47489400
C	2.15230800	2.28668100	0.14572900
C	-0.00084500	2.18625900	-0.65063400
C	2.19516500	1.76111100	-1.17427500
H	3.00357100	2.46365600	0.78913000
C	0.85831600	1.70716400	-1.67020700
H	-1.07552300	2.29039700	-0.72755600
H	3.08933900	1.50868700	-1.72937800
H	0.55764200	1.39826200	-2.66281700
H	0.27101200	-3.06677400	0.78368400
C	0.88851100	-2.51989100	0.08123300
C	0.48851000	-2.05390600	-1.20951200
C	2.25667800	-2.20413400	0.25693300
C	1.60806600	-1.44785700	-1.82098100
H	-0.48669100	-2.17980000	-1.66360900
C	2.69749800	-1.50966000	-0.90486100
H	2.86188100	-2.44408900	1.11958700
H	1.63536500	-1.01645400	-2.81260400
H	3.70536800	-1.15886400	-1.08876600
Hf	1.04566100	0.01332300	0.17546400
C	2.06516100	0.05578800	2.17073400
H	3.15991100	0.13126200	2.09869600
H	1.86259500	-0.85065200	2.75819100
H	1.73714300	0.91877700	2.76632300
H	-1.98746500	-1.73757500	0.35068500
C	-3.06896300	0.10269200	-0.16410500
H	-2.98033100	1.17418500	0.04746600
H	-2.95259500	-0.03995700	-1.24801100
C	-4.48352700	-0.39222800	0.24276200
H	-4.56754800	-1.46769400	0.03645600
H	-4.60745900	-0.26882000	1.32623300
C	-5.59563100	0.36482900	-0.49802200
H	-5.46245100	0.23478800	-1.58074800
H	-5.49533500	1.44059200	-0.29976500
C	-6.99517900	-0.10553300	-0.08878600
H	-7.76613600	0.45068800	-0.63151900
H	-7.13724200	-1.17060400	-0.30576200
H	-7.16814500	0.04482100	0.98316700

1st TS

Hf/Et

3a

Hf	-0.00144900	0.05181900	0.03978800
C	-2.17059400	-0.37273600	-1.19267100
C	-2.52399800	0.32986500	-0.00644200
C	-2.24392500	-0.51262100	1.10122500
C	-1.68163300	-1.71963700	0.60928700
C	-1.64452400	-1.63449200	-0.81473600
C	2.52834200	0.27021600	-0.17270800
C	2.29206400	-0.40541600	1.05015500
C	1.67995200	-1.65464000	0.75623500
C	1.57450700	-1.76318400	-0.66215400
C	2.09230900	-0.57281500	-1.23417500
H	-2.30814600	-0.02388800	-2.20753900
H	-2.97505400	1.31311600	0.04046000
H	-2.42987000	-0.27855800	2.14236700
H	-1.39028300	-2.57582000	1.20401700
H	-1.32208600	-2.41477000	-1.49143700
H	2.99546300	1.24097400	-0.28268400
H	2.53904300	-0.03855600	2.03871800
H	1.41041100	-2.41708600	1.47590000
H	1.20220900	-2.62018000	-1.20741100
H	2.17312500	-0.36073100	-2.29264300
C	0.00424200	1.71156400	1.62786600
H	-0.89845200	2.19805700	1.99662400

H	0.88697600	2.20778400	2.02985000
H	0.00282400	0.68500500	2.11479000
H	-0.89028300	1.88399900	-2.04859100
C	0.02846000	1.86568500	-1.47110900
H	0.93665400	1.82091600	-2.06460200
C	0.06470600	2.67291600	-0.30546300
H	0.99741100	3.14276600	-0.01429600
H	-0.82506200	3.21775300	-0.01008900

Hf/Pro

3a

C	-3.56767800	-1.03065200	-0.03106700
H	-3.75791100	0.04046700	-0.14459100
H	-3.92205200	-1.36015200	0.94837300
C	-2.12135700	-1.38139500	-0.29738000
H	-1.86541000	-2.41097400	-0.06108700
C	-1.43958600	-0.82050400	-1.43697200
H	-1.99924900	-0.06027100	-1.97772300
H	-0.95760500	-1.54223900	-2.09294100
H	-2.32898700	2.12727600	0.15291200
C	-1.25183700	2.16355400	0.05208200
C	-0.31889900	2.28935900	1.11589000
C	-0.52660800	2.15654000	-1.17111900
C	0.98457900	2.32963300	0.55794500
H	-0.55866700	2.35169900	2.17053400
C	0.85512100	2.24877800	-0.86089100
H	-0.95026700	2.11584000	-2.16543300
H	1.90954100	2.44559800	1.10822000
H	1.66388700	2.29989700	-1.57858700
H	0.54264200	-3.07739800	-0.81248800
C	1.15165200	-2.26168000	-0.44434700
C	1.84359700	-1.31129000	-1.24571100
C	1.42391300	-1.97544900	0.91479000
C	2.55706900	-0.44561400	-0.37584100
H	1.85411200	-1.27691900	-2.32829200
C	2.28024300	-0.83734000	0.96396000
H	1.06394800	-2.53566100	1.76855300
H	3.21201100	0.36078100	-0.67778100
H	2.70304600	-0.39440800	1.85744200
Hf	0.12464800	0.03113300	0.03568900
C	-1.40425200	-0.73350000	1.59345900
H	-0.46154300	-0.35301700	2.09492400
H	-1.55745000	-1.70969100	2.05290700
H	-2.19750600	-0.05281800	1.89878300
H	-4.16296300	-1.55222600	-0.79209700

3b

C	-2.15258000	-0.17848900	1.30190300
C	-2.82221400	-0.78456900	0.28986600
H	-2.33618500	0.86538000	1.54577300
H	-1.63508200	-0.77738900	2.05250300
C	-3.77243100	-0.12635100	-0.65315300
H	-2.71058500	-1.86189100	0.17310500
H	-3.86194600	0.94916200	-0.48286000
H	-3.49444600	-0.31081400	-1.69846500
H	-0.48377700	2.96541000	1.33518900
C	-0.06459500	2.54664000	0.42895600
C	1.31173100	2.30403700	0.18924500
C	-0.78687700	2.17451000	-0.73726100
C	1.44024000	1.75650000	-1.11605800
H	2.12026200	2.49846900	0.88106900
C	0.13719100	1.68138100	-1.69244200
H	-1.85510100	2.27215200	-0.88353000
H	2.36874500	1.50198300	-1.61020500
H	-0.09906500	1.35192800	-2.69595800
Hf	0.22045900	0.02365200	0.18896300
C	1.03244900	0.12410100	2.27142500
H	2.12671100	0.22837400	2.30276500
H	0.79776400	-0.77790600	2.85366200

H	0.62797200	0.98806100	2.81655800
C	-0.14844200	-2.08461000	-1.20034700
C	0.13628800	-2.51561500	0.13303800
C	1.00889700	-1.45916500	-1.71356900
H	-1.06985400	-2.24881600	-1.74548500
C	1.47279600	-2.16111700	0.43210500
H	-0.53024500	-3.06858300	0.78407100
C	2.00596100	-1.47466200	-0.69539000
H	1.12083900	-1.04432900	-2.70646100
H	1.99735800	-2.36918800	1.35389800
H	3.01811700	-1.10113300	-0.78890500
H	-4.76503700	-0.57936900	-0.52194200

Hf/But

3a

C	8.43950400	0.07028500	2.44916900
C	8.20843200	1.49082700	2.34516000
H	9.44353500	-0.20717400	2.76339100
H	7.66362800	-0.49419300	2.96239000
C	9.24841200	2.47488400	2.85059500
H	7.18305700	1.80886600	2.52288400
C	9.22124300	2.50479200	4.39163000
H	10.24468500	2.17611100	2.50373200
H	9.05380100	3.48297500	2.47241600
H	9.95320800	3.23228900	4.75555600
H	8.23724400	2.80455200	4.76863100
H	9.46823500	1.52811400	4.81865600
H	5.27150900	1.45428700	-0.20914300
C	5.62798400	0.43335500	-0.15680600
C	6.06726600	-0.35526900	-1.26011100
C	5.70634000	-0.36309900	1.01075100
C	6.39087400	-1.64902500	-0.76596700
H	6.08858700	-0.04627400	-2.29812600
C	6.18877400	-1.64878700	0.63966900
H	5.42488500	-0.05570700	2.00966100
H	6.71935200	-2.49096900	-1.36076500
H	6.33924800	-2.48986600	1.30548900
Hf	8.09974400	-0.05955300	0.16953700
C	8.15733000	2.24415000	0.36177300
H	7.89730800	1.92396700	-0.69440300
H	9.13101500	2.72682000	0.29228900
H	7.39224300	2.98311500	0.59767000
C	10.35450600	-1.19489800	0.34225900
C	10.61530900	0.13419300	-0.09117500
C	9.62332100	-1.85334900	-0.68030800
H	10.67757900	-1.63805600	1.27443600
C	10.07218000	0.28577600	-1.39530300
H	11.16978700	0.88442900	0.45781100
C	9.44755000	-0.93467100	-1.75798100
H	9.29948800	-2.88616400	-0.66384400
H	10.12967800	1.17569800	-2.01042600
H	8.96202000	-1.14500700	-2.70239200

3b

C	-1.79306700	-1.11567000	1.14933400
C	-1.89966900	-0.77352300	-0.23391800
H	-2.46453500	-0.62965400	1.85264600
H	-1.52387000	-2.12934200	1.42547800
C	-3.07245100	0.10602300	-0.67658200
H	-1.74069700	-1.62252500	-0.89935100
C	-4.40725700	-0.65826400	-0.65115100
H	-3.15076900	0.99400900	-0.03707300
H	-2.89880900	0.46585200	-1.69669800
H	-5.22368200	-0.01789600	-1.00164200
H	-4.37134000	-1.53989800	-1.30110500
H	-4.65716700	-0.99778800	0.36063800
H	-1.50626900	2.49652300	1.08653000
C	-0.62553200	2.34549300	0.47579100
C	0.72002500	2.41120600	0.92306800

C	-0.60993000	2.11621500	-0.92910700
C	1.56895000	2.18972600	-0.19193600
H	1.04607300	2.60024500	1.93862000
C	0.74356000	2.01219100	-1.34105200
H	-1.47318500	2.07129400	-1.57638400
H	2.65139300	2.19815200	-0.17858000
H	1.08751200	1.87088400	-2.35765800
Hf	0.32615600	0.02542900	0.11904000
C	-0.22509600	-0.31997600	2.32597100
H	0.85555300	0.01511900	2.21938000
H	-0.16708700	-1.20909800	2.95213900
H	-0.73355600	0.48045700	2.86326200
C	1.09342500	-1.64792100	-1.61629100
C	0.77366800	-2.42749500	-0.47030000
C	2.21540100	-0.83911200	-1.29263900
H	0.59852700	-1.69562800	-2.57879300
C	1.67871900	-2.08698100	0.56321800
H	-0.01010800	-3.17143300	-0.40898100
C	2.56620600	-1.09038300	0.06255500
H	2.72641400	-0.16287300	-1.96475900
H	1.71076400	-2.52493900	1.55276100
H	3.39990400	-0.65154800	0.59695000

Hf/Hex

3a

C	1.69466700	-0.62802100	0.13044400
C	1.06417300	-0.29482400	-1.12491200
H	0.95031100	-1.12003100	-1.82496900
H	1.44144900	0.61030200	-1.59690800
H	-1.01781900	-2.77327300	1.67959000
C	-1.49449000	-2.33871600	0.81017100
C	-2.69190300	-1.56388600	0.81428500
C	-1.06386700	-2.47306900	-0.53156900
C	-3.00476800	-1.24285400	-0.53413100
H	-3.29038100	-1.31698700	1.68289800
C	-1.98681500	-1.78288300	-1.36510600
H	-0.19578500	-3.02442800	-0.86849900
H	-3.87337900	-0.69185900	-0.86946200
H	-1.94454200	-1.71823800	-2.44567300
H	-0.29657900	2.24920500	-2.17861200
C	-0.82937400	2.18649500	-1.23931900
C	-2.19355300	1.83062200	-1.08034500
C	-0.29931600	2.47767500	0.04831900
C	-2.51221800	1.91211000	0.30824800
H	-2.88154400	1.58408100	-1.87875300
C	-1.34374900	2.32780200	0.99778600
H	0.71254100	2.79821700	0.26162000
H	-3.48434900	1.73702800	0.75113800
H	-1.26610700	2.50310500	2.06398700
Hf	-0.90077900	0.00971500	0.04628400
C	0.53807800	-0.16920400	1.84708900
H	-0.54125400	-0.10576600	2.19016000
H	1.01481100	0.74891900	2.18685300
H	0.92980000	-1.01923400	2.40452800
H	1.70230500	-1.68762400	0.37740200
C	2.93592100	0.11339100	0.58725400
H	2.80668600	1.19209700	0.43432300
H	3.12759100	-0.05045200	1.65275900
C	4.16089100	-0.37910100	-0.21733300
H	4.25686300	-1.46832800	-0.10609400
H	3.99910500	-0.18784700	-1.28589400
C	5.46328300	0.29519700	0.24009400
H	5.36350800	1.38439400	0.13565700
H	5.61580900	0.10030600	1.31037700
C	6.68399700	-0.18839800	-0.54959900
H	7.59546300	0.30875300	-0.20236600
H	6.82982100	-1.26893900	-0.43483500
H	6.57607000	0.02309700	-1.61993200

3b

C	-1.12427200	-1.11559000	0.93569800
C	-0.29255800	-1.25083700	2.08504800
H	0.26608700	-2.16848700	2.23184700
H	-0.60403000	-0.76878200	3.00807100
H	-0.70332700	2.31455300	1.83350500
C	-0.23844200	2.23805800	0.85889800
C	1.11298200	2.54760900	0.55259000
C	-0.89075800	1.87878000	-0.35382900
C	1.30999600	2.34454700	-0.83751900
H	1.86618500	2.88073500	1.25617100
C	0.06582300	1.93400900	-1.40005600
H	-1.93827600	1.64546900	-0.46919700
H	2.23059800	2.51468600	-1.38096400
H	-0.12988800	1.74679900	-2.44803000
H	0.95390900	-3.18887500	-0.02652800
C	1.39712300	-2.34752400	-0.54373200
C	0.87913000	-1.71886000	-1.71028800
C	2.61100900	-1.70659800	-0.19830600
C	1.78469500	-0.69415200	-2.09108900
H	-0.02461800	-1.99910000	-2.23738200
C	2.84696600	-0.66761400	-1.14370300
H	3.25893100	-1.97057000	0.62789100
H	1.69532200	-0.05857100	-2.96194100
H	3.71388300	-0.01939800	-1.17700700
Hf	0.79634300	0.05994900	0.08884000
C	1.50849300	-0.11555200	2.26837600
H	2.30383000	0.37462700	1.62282100
H	2.03273800	-0.92500200	2.77414400
H	1.20540000	0.64207300	2.99086000
H	-1.13244000	-2.00908300	0.31066400
C	-2.52195400	-0.50307700	1.10232400
H	-3.02274600	-1.02107600	1.93317200
H	-2.46899700	0.54915200	1.40652700
C	-3.40405900	-0.65862200	-0.14522500
H	-2.90887000	-0.21350400	-1.02148700
H	-3.50637100	-1.72901500	-0.37491600
C	-4.79985900	-0.04226500	0.02274000
H	-4.70031100	1.02974200	0.24722300
H	-5.28740100	-0.49092900	0.89884000
C	-5.68984600	-0.22698200	-1.21060500
H	-6.67415500	0.22679500	-1.05685200
H	-5.24433200	0.23869600	-2.09830500
H	-5.84462600	-1.28920700	-1.43353800

1st β -product

Hf/Et

4a

Hf	-0.09362400	0.02869100	-0.05843300
C	1.56165100	1.73739300	-0.82323900
C	1.76524600	1.58600500	0.57399100
C	0.59854500	2.05853300	1.24799800
C	-0.31838400	2.51227900	0.26575100
C	0.26050000	2.28931800	-1.01658800
C	-1.77606200	-1.32264800	1.22102800
C	-2.34422400	-0.03982500	0.99719800
C	-2.54785300	0.11112400	-0.40800000
C	-2.12159700	-1.09068700	-1.04307200
C	-1.63924900	-1.96998600	-0.04204400
H	2.27432500	1.50467900	-1.60219500
H	2.66463800	1.21588800	1.05023500
H	0.45859300	2.10623100	2.32171400
H	-1.28999200	2.94931500	0.45626600
H	-0.18283000	2.55559900	-1.96926800
H	-1.53095800	-1.75174900	2.18583500
H	-2.60539900	0.68301100	1.75962700
H	-3.00565100	0.96193000	-0.89708100
H	-2.15802000	-1.29819300	-2.10594300
H	-1.25443600	-2.96759000	-0.20781900
C	3.18959800	-1.85902400	0.50950800
H	3.66294200	-2.61483700	-0.12491300
H	3.41134100	-2.10196800	1.55348500

H	3.64394200	-0.89270700	0.26958300
H	2.07652100	-0.94906000	-1.71182300
C	1.24263400	-1.37203400	-1.14948100
H	0.77526700	-2.16430700	-1.73590400
C	1.68287400	-1.85616900	0.23305100
H	1.24107200	-1.18528500	1.08292900
H	1.23747500	-2.82239700	0.48586900

Hf/pro

4a

C	-3.23086600	-1.26608100	0.35789600
H	-4.09064900	-1.27843300	-0.32068300
H	-3.61160400	-1.27773400	1.38464100
C	-2.40554600	-0.00075900	0.07897100
H	-1.61058900	-0.00054200	0.95841700
C	-1.66691200	-0.00066300	-1.26034300
H	-1.88631300	0.88801200	-1.85458800
H	-1.88574100	-0.88964200	-1.85435100
H	-0.74590800	2.90642600	-1.01932600
C	0.08482300	2.47682500	-0.47786600
C	0.16608600	2.28343200	0.93074100
C	1.31428100	2.05064400	-1.04921200
C	1.44967000	1.74209400	1.22839200
H	-0.59497500	2.54671900	1.65531700
C	2.16171800	1.60797900	0.00384700
H	1.57071600	2.08527100	-2.10211000
H	1.83336800	1.51707300	2.21596800
H	3.18026500	1.26025000	-0.10514000
H	-0.74412100	-2.90745500	-1.01818000
C	0.08654100	-2.47701400	-0.47727400
C	1.31532300	-2.04991700	-1.04939900
C	0.16844100	-2.28328700	0.93127700
C	2.16296500	-1.60632300	0.00311400
H	1.57123300	-2.08459000	-2.10242300
C	1.45172300	-1.74082200	1.22809000
H	-0.59195200	-2.54719700	1.65633200
H	3.18113600	-1.25768900	-0.10649600
H	1.83579300	-1.51532300	2.21541200
Hf	0.23138400	0.00004300	-0.08165300
C	-3.23152400	1.26417100	0.35771000
H	-2.66416700	2.18244300	0.18806100
H	-3.61208100	1.27589800	1.38452200
H	-4.09145000	1.27581600	-0.32070200
H	-2.66291000	-2.18406500	0.18864000

4b

C	-2.27864600	-0.24732100	-0.75020400
C	-1.89809200	-0.34178700	0.73428600
H	-1.37272500	0.05110300	-1.42214500
H	-2.51806200	-1.23644600	-1.15263400
C	-2.42312200	-1.59572100	1.44505400
H	-2.28641500	0.53829200	1.25487200
H	-3.52063600	-1.59651400	1.49113500
H	-2.12134000	-2.52320200	0.94681700
H	-0.63293000	-2.94850500	-0.92057600
C	0.26494000	-2.42267400	-0.62362300
C	1.16264800	-1.74368300	-1.50002900
C	0.76831200	-2.31738700	0.69608200
C	2.22704000	-1.22617300	-0.71849500
H	1.07064300	-1.67580300	-2.57802200
C	1.97534800	-1.55870200	0.64660500
H	0.31737700	-2.74225400	1.58368500
H	3.08548300	-0.68305300	-1.09185100
H	2.62700000	-1.34319700	1.48463600
Hf	0.19104500	0.02433500	0.01078000
C	-3.36085200	0.77137100	-1.12469800
H	-4.30340400	0.47731200	-0.65172300
H	-3.52262300	0.81367500	-2.20657500
H	-3.10923600	1.77631700	-0.77124700
C	0.72204400	2.02856900	1.43040400
C	-0.37604500	2.40494800	0.61198800

C	1.84872600	1.81373400	0.58822800
H	0.70945200	1.94653900	2.51143000
C	0.06638500	2.41115500	-0.74154700
H	-1.36314600	2.67276800	0.96215000
C	1.44280900	2.04460500	-0.75647900
H	2.84580700	1.54832500	0.91529600
H	-0.52564500	2.69522700	-1.60350300
H	2.07853300	1.99277400	-1.63179900
H	-2.06232600	-1.64107000	2.47844400

Hf/but

4a

C	8.69650600	0.29941500	2.45742100
C	8.40876300	1.73135100	2.00132100
H	9.73600900	0.16063800	2.75866100
H	8.04447700	-0.01351900	3.27481300
C	7.21683700	2.39494400	2.72664900
H	8.04746000	1.71408500	0.87117500
C	6.69635600	3.69074700	2.09652700
H	6.39847600	1.67161700	2.80954600
H	7.55162800	2.58818900	3.75406600
H	5.82617500	4.05735200	2.64967900
H	7.44680200	4.48699100	2.10650100
H	6.38490300	3.53840100	1.05424500
H	5.30214600	1.13272700	0.56517100
C	5.66991900	0.12001900	0.45500500
C	5.92847400	-0.54376900	-0.77908800
C	5.92118300	-0.79940200	1.51206400
C	6.32918800	-1.87538400	-0.48205400
H	5.79487900	-0.12499400	-1.76916000
C	6.33930900	-2.02819600	0.93196900
H	5.78258700	-0.61584200	2.56785000
H	6.55880000	-2.64686500	-1.20461100
H	6.58800600	-2.93417300	1.47316200
Hf	8.12627800	-0.34628700	0.39555400
C	9.64941400	2.63780200	1.96367800
H	10.50456700	2.14850700	1.49126500
H	9.93517000	2.87752200	2.99380900
H	9.45917600	3.57768100	1.43772800
C	10.18203300	-1.62683300	-0.26423200
C	10.61431600	-0.31208200	0.06156600
C	9.37336700	-1.54964900	-1.43187200
H	10.45119800	-2.53382900	0.26532600
C	10.05590300	0.58140500	-0.89572000
H	11.27986000	-0.05004400	0.87156200
C	9.28389100	-0.18375700	-1.81692000
H	8.92751200	-2.38747700	-1.95088400
H	10.22448300	1.65017100	-0.94467500
H	8.76107600	0.20034000	-2.68440500

4b

C	1.76719800	-0.81871200	-1.33582000
C	1.85596500	-0.48812100	0.16223300
H	0.67942700	-0.73893900	-1.74781000
H	2.26898500	-0.04999300	-1.93194100
C	3.01245400	0.45097800	0.54188900
H	1.98263700	-1.42154000	0.71984500
C	3.11803100	0.67725100	2.05363700
H	3.96090500	0.01703600	0.19024900
H	2.91936000	1.41517700	0.02581500
H	3.97171000	1.31717300	2.29844800
H	2.21523200	1.15442400	2.45795700
H	3.25309300	-0.27167600	2.58582200
H	1.33776400	2.27996500	-1.65334800
C	0.41432000	2.21285400	-1.09326600
C	-0.86935800	1.90116000	-1.63357300
C	0.26545600	2.45007200	0.29439100
C	-1.81252600	1.95674500	-0.57600000
H	-1.09060600	1.70470600	-2.67646300
C	-1.11074000	2.27002100	0.62631900

H	1.05578700	2.72463900	0.98074500
H	-2.87897600	1.79554300	-0.66556100
H	-1.55689600	2.42738700	1.60085900
Hf	-0.31433300	0.02869700	-0.03966400
C	2.21843600	-2.22082700	-1.75907500
H	3.28545500	-2.33085800	-1.54017400
H	2.07247700	-2.38918600	-2.83091100
H	1.68259200	-3.00037000	-1.20827500
C	-1.23228200	-1.43935900	1.78341200
C	-0.61128400	-2.31136000	0.84983500
C	-2.34993100	-0.83158200	1.14619500
H	-0.92349400	-1.28591200	2.81131200
C	-1.33627700	-2.23344100	-0.37325000
H	0.24017500	-2.94721800	1.04788200
C	-2.41175800	-1.31721100	-0.19021600
H	-3.04560200	-0.14120700	1.60562200
H	-1.13769400	-2.80953400	-1.26922900
H	-3.16659800	-1.06657700	-0.92531100

Hf/hex

4a

C	-1.55981400	-2.66305700	-0.34136700
H	-0.60985000	-3.19244900	-0.23895900
H	-2.09973800	-3.11474500	-1.18087000
C	-1.36234500	-1.16780100	-0.63798800
H	-0.99372700	-0.72800200	0.40079400
C	-0.30610800	-0.87909700	-1.70763300
H	-0.68671000	-0.23350200	-2.50079200
H	0.09411600	-1.79140900	-2.15272700
H	-0.77577000	2.12442800	-1.90500900
C	-0.11656300	2.17080300	-1.04996200
C	-0.50546200	2.11294100	0.31784400
C	1.29368700	2.34761000	-1.09598800
C	0.66519300	2.26209900	1.11705800
H	-1.51844200	2.01846900	0.68889100
C	1.77358000	2.42040800	0.24118400
H	1.89296700	2.44616700	-1.99405300
H	0.69902500	2.29687800	2.19928800
H	2.79932900	2.59216200	0.53828600
H	1.69848500	-2.95825100	-0.71331400
C	2.01984500	-2.16549500	-0.05298500
C	3.03621400	-1.21323300	-0.33527600
C	1.53940200	-1.91642600	1.26396300
C	3.19888900	-0.38756700	0.81155400
H	3.60951700	-1.14912900	-1.25322900
C	2.26673000	-0.81355000	1.79771300
H	0.78718800	-2.49370500	1.78771400
H	3.92561500	0.40573800	0.92352700
H	2.16193100	-0.40241200	2.79432700
Hf	0.89698500	0.08365600	-0.09041200
C	-2.70183900	-0.43120900	-0.86233500
H	-2.50068600	0.59899300	-1.17902600
H	-3.17923100	-0.91953800	-1.72273400
H	-2.14571700	-2.83053800	0.56666700
C	-3.67232400	-0.41499800	0.32644600
H	-3.17244100	0.02048700	1.20720200
H	-3.94503000	-1.43980400	0.60805700
C	-4.95542900	0.37649400	0.03029800
H	-4.69218200	1.40786400	-0.24521800
H	-5.44813400	-0.05724400	-0.85036700
C	-5.93370800	0.39289000	1.20909800
H	-5.48143300	0.85011800	2.09763800
H	-6.83508900	0.96383500	0.96421700
H	-6.24661200	-0.62248100	1.47955700

4b

C	-1.07284300	1.10756600	-0.46580900
C	-0.29607600	1.59458100	-1.70302500
H	-0.64250700	1.07953300	-2.60433100

H	0.82387200	1.28697300	-1.67451800
H	-0.72314700	-1.36667800	-2.58672400
C	-0.06672400	-1.69737800	-1.79322400
C	1.35787400	-1.72294100	-1.84379300
C	-0.47528900	-2.20974200	-0.53784700
C	1.82883800	-2.25957300	-0.61777500
H	1.97016200	-1.42874700	-2.68866900
C	0.69603100	-2.54416900	0.20337300
H	-1.49787200	-2.32713700	-0.20260700
H	2.86408100	-2.44207600	-0.36085200
H	0.72114400	-3.00493000	1.18317000
H	1.67827900	2.92738800	0.58266000
C	1.78088000	1.95354500	1.04420900
C	0.89949400	1.38610400	1.99913100
C	2.85582500	1.03841400	0.82974200
C	1.41462300	0.10628200	2.36275100
H	0.00504300	1.84704100	2.39563500
C	2.63909300	-0.08989000	1.65959600
H	3.70908400	1.19851200	0.18042000
H	0.99293000	-0.56249800	3.10377600
H	3.28837200	-0.95109600	1.74559700
Hf	0.76442300	-0.08333000	-0.02306800
C	-0.25818900	3.11038000	-1.93200400
H	0.12408800	3.64231200	-1.05532900
H	-1.27696000	3.46571200	-2.11805700
H	0.35727500	3.37596000	-2.79752200
H	-1.14645300	1.94396200	0.23808800
C	-2.49299700	0.60372600	-0.76116400
H	-3.05840100	1.39076800	-1.28482900
H	-2.46989400	-0.25177400	-1.44972200
C	-3.26806800	0.21907700	0.50704500
H	-2.72578100	-0.57607200	1.04481600
H	-3.29198600	1.08009400	1.19089200
C	-4.70449500	-0.24495000	0.22901700
H	-4.68313600	-1.10460900	-0.45605700
H	-5.24193100	0.55274400	-0.30160500
C	-5.47166300	-0.62108500	1.50080000
H	-6.49107600	-0.94375100	1.26570400
H	-4.97909200	-1.44191700	2.03673700
H	-5.54246000	0.23035000	2.18807400

2nd π -complexes

Hf/Et

5a

Hf	0.24887900	0.02282200	0.03804500
C	1.00798900	-1.97330400	-1.32026900
C	1.18092300	-2.35249500	0.03212500
C	2.20826800	-1.53401700	0.59312600
C	2.65418900	-0.64306800	-0.40729900
C	1.89632400	-0.89681000	-1.59100100
C	-0.91092000	2.29037300	0.29599400
C	0.35940000	2.42950000	0.93004900
C	1.36200900	2.28915700	-0.05714500
C	0.71501100	2.06080100	-1.30778700
C	-0.69100900	2.08009600	-1.08599400
H	0.31914700	-2.42116200	-2.02326500
H	0.66358600	-3.16132200	0.53179800
H	2.60302500	-1.60098200	1.60005200
H	3.44534100	0.08711800	-0.30223400
H	2.03968000	-0.41992300	-2.55177000
H	-1.87730100	2.37372000	0.77531000
H	0.52973000	2.65501400	1.97505700
H	2.42811500	2.38130300	0.10232600
H	1.20383100	1.97364800	-2.26898400
H	-1.45486200	1.96195100	-1.84224400
C	-4.23970200	-1.05613600	-0.83322200
H	-4.25459000	-1.05895600	-1.92922300
H	-5.19147100	-0.63956800	-0.48459900
H	-4.18725700	-2.09899100	-0.49896900
H	-1.66581100	-1.87648900	-0.55221500
C	-1.68678600	-0.79628600	-0.77509000
H	-1.65714000	-0.75584800	-1.87746300

C	-3.04929300	-0.24134600	-0.30440500
H	-3.10179600	-0.22669300	0.79567300
H	-3.17005300	0.80203500	-0.62206200
C	-0.48589600	-1.24994700	2.45014400
H	-1.26036100	-1.85777400	1.98784100
H	0.39732900	-1.76872700	2.80840600
C	-0.67942800	0.06295200	2.69899200
H	-1.62127400	0.54949600	2.46420000
H	0.04634700	0.64211600	3.26379700

5f

Hf	-0.10574400	0.02859600	-0.06314100
C	1.57380700	1.89299300	-0.55918400
C	1.06274000	2.14802700	0.73314600
C	-0.33048500	2.42993400	0.61221900
C	-0.66108600	2.37269300	-0.76863800
C	0.50665500	2.01522300	-1.49185500
C	-1.96035200	-1.55354300	0.71458300
C	-2.55371000	-0.32565300	0.32016000
C	-2.37257500	-0.19509800	-1.09029400
C	-1.64662800	-1.32104600	-1.54925800
C	-1.37624300	-2.15427800	-0.42779000
H	2.60046300	1.65226000	-0.79978100
H	1.64260900	2.15551600	1.64767800
H	-1.00112900	2.71818100	1.41096700
H	-1.62844500	2.59844500	-1.19509200
H	0.58251900	1.89269400	-2.56427800
H	-1.96223600	-1.97035100	1.71385800
H	-3.11076600	0.35277200	0.95361500
H	-2.77215700	0.59321500	-1.71292800
H	-1.36990700	-1.52067000	-2.57462500
H	-0.85269500	-3.10169200	-0.45189200
C	3.52657400	-1.43476500	-0.18997600
H	4.01839400	-1.94312000	-1.02496000
H	3.91676700	-1.85682700	0.74228400
H	3.80619000	-0.37701000	-0.23149000
H	2.00635400	-0.33043800	-2.06380700
C	1.33265500	-0.98564100	-1.51161100
H	0.92760500	-1.72745500	-2.19715400
C	2.00685200	-1.62091400	-0.30677700
H	1.59244700	-1.19116100	0.67288000
H	1.74065700	-2.67873400	-0.21058400
H	0.35527500	-1.83283200	2.61761500
C	0.63522300	-0.78870500	2.72905400
H	1.69838000	-0.57763100	2.81081300
C	-0.28363000	0.17635600	2.92897000
H	-1.34561500	-0.04014100	2.97838900
H	0.01007300	1.19259800	3.16817500

Hf/Pro

5a

C	1.58089900	-0.06579700	-0.97513300
C	2.93793200	-0.53877700	-0.36531900
H	1.73115400	0.91084600	-1.45804400
H	1.33518300	-0.72306500	-1.83608200
C	3.57318900	-1.66852500	-1.19655800
H	2.78556800	-0.92746800	0.65377400
H	2.91198400	-2.53860600	-1.29259500
H	3.79655400	-1.31753900	-2.21155000
H	0.90382100	-1.62141200	2.50632200
C	0.14248000	-1.82274200	1.76250000
C	-1.26004100	-1.58967100	1.90517600
C	0.35991800	-2.42715100	0.50273300
C	-1.89988000	-2.04167200	0.73059500
H	-1.75661900	-1.17191400	2.77268300
C	-0.89751600	-2.52859000	-0.15842500
H	1.31093800	-2.75360600	0.11013900

H	-2.96418000	-2.01647000	0.53729200
H	-1.06969900	-2.97746000	-1.12893200
Hf	-0.44705100	-0.08622100	0.00545200
C	3.93865500	0.62571500	-0.25822200
H	3.54995500	1.46059600	0.33675800
H	4.18298900	1.01832000	-1.25287800
H	4.87433100	0.29808600	0.20868900
C	-2.23104800	0.01095500	-1.73767600
C	-1.11435100	0.67097200	-2.31848400
C	-2.70194100	0.81174100	-0.65664300
H	-2.68007900	-0.90780600	-2.09118300
C	-0.88539900	1.86795300	-1.59428800
H	-0.54148100	0.32399300	-3.16865000
C	-1.87185800	1.95915100	-0.57509100
H	-3.56236500	0.60169300	-0.03413000
H	-0.11413300	2.59667600	-1.80439100
H	-1.99664000	2.78207600	0.11648200
C	1.01649900	1.97603600	1.69565100
C	-0.13340900	1.50375100	2.23729500
H	-0.10821100	0.66211400	2.92019900
H	-1.05015900	2.08877000	2.21412700
H	1.92671400	1.39539600	1.84568400
C	1.18540600	3.28161900	0.99017600
H	0.23731100	3.79880800	0.82247700
H	1.71874800	3.16332600	0.04117400
H	4.51132900	-2.01363300	-0.74707500
H	1.81743900	3.92638200	1.61743200

5e

C	1.86847400	-0.17206600	-0.86432900
C	3.03110000	0.58697000	-0.14982100
H	1.83271000	0.16495300	-1.90967300
H	2.13178800	-1.24263700	-0.94485500
C	4.29785600	-0.28123600	-0.05113300
H	2.74408800	0.85298700	0.88111700
H	4.12241100	-1.19893600	0.52417800
H	4.63603200	-0.58133900	-1.05035900
H	2.17081000	-1.33998400	1.73726400
C	1.10032900	-1.24378600	1.84281300
C	0.41273600	-0.14606600	2.41042200
C	0.13032800	-2.20217500	1.43177600
C	-0.98621400	-0.44139500	2.39027700
H	0.87429200	0.73597800	2.83778200
C	-1.15465600	-1.71552800	1.80632300
H	0.34048000	-3.16746400	0.98778100
H	-1.77876800	0.17474100	2.79657800
H	-2.09546100	-2.23035900	1.66377300
C	3.36094500	1.90125700	-0.88015200
H	2.49354600	2.56877700	-0.95890900
H	3.70795000	1.69694000	-1.90020000
H	4.15448400	2.45142600	-0.36228100
C	-0.55425500	-1.27955100	-2.32858000
C	-0.91267100	0.08312200	-2.49257200
C	-1.49046100	-1.87731000	-1.44263400
H	0.28779600	-1.77470700	-2.79396500
C	-2.08459200	0.32330500	-1.72718400
H	-0.39296800	0.80456400	-3.11013200
C	-2.44112000	-0.88169700	-1.07001300
H	-1.51072700	-2.91841100	-1.14806300
H	-2.62730200	1.25780900	-1.67124600
H	-3.30550000	-1.03068800	-0.43580800
H	0.81365000	2.19060800	0.54978900
C	-0.19185000	2.36381700	0.16308500
C	-1.21547000	2.58637600	1.02485100
H	-0.27919500	2.62868100	-0.88853400
C	-2.57342400	3.09086700	0.67039800
H	-1.03267600	2.43266000	2.08786100
H	-2.70052900	3.25002300	-0.40286800
H	-3.35931100	2.41942800	1.03873900
Hf	-0.23880500	-0.23092300	-0.04921900
H	5.11790300	0.26211500	0.43227400
H	-2.73389500	4.04985400	1.18235400

5f

C	0.73798800	0.41838600	-1.97465100
C	2.08194100	0.35016100	-1.23310300
H	0.59192300	1.37500100	-2.47713900
H	0.67309900	-0.36454400	-2.73092700
C	2.97834300	-0.80118000	-1.72515100
H	1.89845400	0.12215400	-0.12833700
H	2.46633400	-1.76768400	-1.68922500
H	3.26259700	-0.61549100	-2.76657500
H	0.48576000	-2.86042100	-1.30301000
C	-0.40878100	-2.39847600	-0.90608400
C	-0.85783400	-2.46723800	0.43724500
C	-1.38215700	-1.68287000	-1.65769300
C	-2.07723900	-1.75280100	0.53747400
H	-0.36350600	-2.99045800	1.24582300
C	-2.40771800	-1.27786300	-0.76971700
H	-1.35405800	-1.49244900	-2.72098100
H	-2.68501300	-1.64610500	1.42688500
H	-3.30989000	-0.74826600	-1.04539100
C	2.85994700	1.67784200	-1.22594300
H	2.26473600	2.50921900	-0.83801800
H	3.15494300	1.92799000	-2.25097500
H	3.77154600	1.60512500	-0.62249100
C	-1.86060100	2.00660600	-0.53345800
C	-0.56277400	2.54177200	-0.32406900
C	-2.32144900	1.48318400	0.70814500
H	-2.42045800	2.04505800	-1.45935900
C	-0.19199200	2.29106600	1.01959600
H	0.03402100	3.05214700	-1.06489100
C	-1.29232700	1.64248600	1.66214800
H	-3.29295000	1.04471200	0.89286900
H	0.73316300	2.59894400	1.49086900
H	-1.35348200	1.36412800	2.70563700
C	1.87159200	-1.13919100	2.06807300
C	0.76900900	-0.53280100	2.56080500
H	-0.16819900	-1.06742900	2.68467700
H	0.85234300	0.43001200	3.05619900
H	1.78464200	-2.14767600	1.66397800
C	3.25729500	-0.57657000	2.13608800
H	3.26530500	0.47008800	2.45307300
H	3.78992000	-0.67319500	1.18492100
H	3.83154300	-1.15833700	2.87065800
H	3.90080300	-0.88037200	-1.13907000
Hf	-0.40240300	0.01628900	-0.05718600

5g

C	-0.54295100	1.94355000	-0.61045100
C	-1.89440500	1.54626300	-0.00005200
H	-2.00268500	1.96125400	1.00790200
H	-1.96339200	0.42728900	0.16485800
H	2.27316500	2.14527100	1.14782600
C	1.78834500	1.25564600	1.52780300
C	0.53179800	1.20924100	2.18794100
C	2.31195300	-0.06598900	1.50137500
C	0.26130400	-0.13518900	2.53302300
H	-0.10478700	2.05565400	2.40100200
C	1.36148300	-0.93277600	2.09995200
H	3.27800400	-0.35971100	1.11482300
H	-0.61066700	-0.48361200	3.07127600
H	1.48278400	-1.99738800	2.25363000
H	-0.18583700	-2.66959400	-1.95788100
C	0.44668600	-1.79163800	-1.92821500
C	0.14848600	-0.53510300	-2.51486000
C	1.71954100	-1.70712400	-1.31310500
C	1.26903100	0.31911000	-2.31226400
H	-0.74873500	-0.28644400	-3.06835200
C	2.23440700	-0.39856500	-1.56618500
H	2.23837100	-2.50765300	-0.80114600
H	1.37433700	1.33206200	-2.67453300
H	3.21548800	-0.03552600	-1.29170500
C	-3.12078700	1.90588100	-0.85704100
H	-3.07829000	1.41890800	-1.83754700

H	-3.14541900	2.98760900	-1.02328600
H	-4.05974000	1.62270300	-0.36930000
H	-0.66019800	1.90438900	-1.69830700
C	-0.07398600	3.35495200	-0.26077000
H	-0.77907800	4.11444800	-0.62733600
H	0.03503600	3.51901700	0.81642800
H	-1.21076100	-2.45039200	1.89971100
C	-1.19953100	-2.44463000	0.81411700
C	-2.29463300	-2.06531300	0.11822000
H	-0.36558500	-2.94866800	0.33613000
C	-3.59047100	-1.62797700	0.73024900
H	-2.29120900	-2.16746900	-0.96721800
H	-4.00501200	-0.74277000	0.23754200
H	-3.50031800	-1.43663100	1.80341400
H	-4.32731500	-2.43112700	0.59038200
H	0.89408100	3.57409800	-0.72629700
Hf	0.30708500	-0.07677400	-0.00972800

Hf/But

5a

C	1.31811500	-0.20931300	-1.02952700
C	2.72601500	-0.33998800	-0.36668600
H	1.32991300	0.64701900	-1.71998800
H	1.17005800	-1.07023700	-1.71419700
C	3.49258000	-1.56745500	-0.91622700
H	2.62757600	-0.48352000	0.72220200
C	4.81086300	-1.88603800	-0.20137300
H	2.84120400	-2.45197600	-0.86442200
H	3.67953600	-1.40457700	-1.98727100
H	5.25413300	-2.80432700	-0.60056200
H	5.55013300	-1.08822800	-0.32486300
H	4.65638200	-2.03425300	0.87514400
H	0.82940000	-0.96741400	2.76908000
C	0.11435600	-1.43869700	2.10594600
C	-1.30887500	-1.37425700	2.21429300
C	0.43285300	-2.28322000	1.01762700
C	-1.86164400	-2.17106300	1.18818000
H	-1.87155700	-0.83896700	2.96963600
C	-0.78799800	-2.70770300	0.41958600
H	1.42543100	-2.55815800	0.69516200
H	-2.91594000	-2.33882800	1.01226400
H	-0.88093200	-3.38673800	-0.41903100
Hf	-0.68341600	-0.25331000	0.00606900
C	3.54810300	0.94416900	-0.58181100
H	3.01508600	1.83709200	-0.23538000
H	3.76496900	1.08852900	-1.64756600
H	4.50300400	0.91038400	-0.04809600
C	-2.45289200	-0.78642300	-1.66980600
C	-1.44156800	-0.11263300	-2.40700900
C	-3.04251300	0.15225100	-0.77319100
H	-2.76134300	-1.81431400	-1.80820000
C	-1.39247700	1.23129600	-1.95895700
H	-0.81773700	-0.54795000	-3.17688500
C	-2.38858600	1.39664900	-0.95857700
H	-3.86825200	-0.03984500	-0.10009600
H	-0.73351200	2.00096800	-2.33784700
H	-2.63641600	2.32191200	-0.45508700
C	0.50183400	2.29182800	1.15198400
C	-0.58296500	1.82907000	1.82173800
H	-0.46281000	1.17421400	2.67754900
H	-1.56195900	2.28425100	1.68790400
H	1.47677700	1.87204000	1.40388100
C	0.51438000	3.43086300	0.17974600
H	-0.50754900	3.71993200	-0.08779600
H	1.03507800	3.13205500	-0.73784000
C	1.25702200	4.64033500	0.79561900
H	2.29208000	4.38760600	1.04813700
H	1.27679100	5.46260900	0.07457800
H	0.75675300	4.99104300	1.70332700

5e

C	1.82015700	-0.19224800	-0.89497400
C	2.76970300	0.97063200	-0.46387900
H	1.72262100	-0.16484100	-1.98907500
H	2.32186600	-1.15823500	-0.70215000
C	4.19737200	0.44746200	-0.17888700
H	2.41771300	1.43774300	0.47220600
C	5.17920700	1.49453900	0.35964000
H	4.13190400	-0.38023300	0.54289200
H	4.59433700	0.00446100	-1.10326300
H	6.13725700	1.02958400	0.61477500
H	5.38432400	2.28151400	-0.37313900
H	4.79262900	1.97492900	1.26766400
H	2.32263300	-0.52944600	1.91463200
C	1.25719200	-0.66212900	2.03219800
C	0.31800100	0.35073000	2.33476200
C	0.54917100	-1.89154600	1.90699000
C	-0.97194300	-0.25723300	2.43674600
H	0.54929600	1.39388200	2.51329400
C	-0.82278900	-1.63984200	2.19388400
H	0.99116700	-2.85955800	1.70541800
H	-1.89672400	0.23847800	2.70445600
H	-1.61420500	-2.37734300	2.21327800
C	2.78752700	2.07053800	-1.54147100
H	1.77691200	2.40772800	-1.80362100
H	3.25240100	1.69642400	-2.46199500
H	3.34953100	2.95171100	-1.21690100
C	-0.25883000	-2.16144900	-1.90514000
C	-0.89685100	-1.00408700	-2.42054000
C	-1.06968500	-2.68266000	-0.86166500
H	0.68190800	-2.57315800	-2.24624300
C	-2.11200700	-0.82009800	-1.70980400
H	-0.52696400	-0.38407100	-3.22720200
C	-2.22013300	-1.84920500	-0.73975400
H	-0.87492400	-3.58457500	-0.29627400
H	-2.84357600	-0.04374900	-1.89206200
H	-3.04903200	-2.00024000	-0.06038100
H	0.24179100	2.16995700	-0.05126900
C	-0.76149000	2.00673400	-0.44839000
C	-1.84513600	2.19381400	0.34695500
H	-0.86402900	1.97624600	-1.53111700
C	-3.26939700	2.28842600	-0.09837000
H	-1.67742700	2.35992000	1.41149700
C	-3.85713700	3.67620900	0.24628300
H	-3.34921600	2.10390900	-1.17483600
H	-3.86278700	1.52033300	0.41814800
H	-4.90393700	3.71801200	-0.06735400
H	-3.81895600	3.87125200	1.32315200
H	-3.31366800	4.47438600	-0.26814300
Hf	-0.23375600	-0.49425800	-0.00283200

5f

C	8.56158700	0.04827900	2.51007200
C	8.45934800	1.55701400	2.23996000
H	9.54192500	-0.22686300	2.89971900
H	7.81970300	-0.27352200	3.24065500
C	7.39397200	2.23760900	3.13535800
H	8.08404300	1.73521600	1.17344000
C	7.00038000	3.66750000	2.75307900
H	6.49548300	1.60893600	3.15420700
H	7.78945500	2.22282800	4.15957700
H	6.24713300	4.05294600	3.44784100
H	7.85076900	4.35668500	2.78490600
H	6.56521200	3.71143600	1.74587000
H	5.32714600	0.88023600	1.20846400
C	5.69079100	-0.04270800	0.77573000
C	5.78979900	-0.33048600	-0.61415700
C	6.05828300	-1.21368900	1.48986400
C	6.26566400	-1.65211800	-0.76221600
H	5.52465500	0.34195300	-1.41998000
C	6.44086800	-2.20047000	0.54685700
H	6.03452700	-1.34201200	2.56158900
H	6.43134000	-2.16956300	-1.69837800
H	6.73993700	-3.21403700	0.77938600

Hf	8.17890600	-0.43546700	0.33040700
C	9.82519700	2.26531400	2.31151600
H	10.56269900	1.79986000	1.64926700
H	10.21179700	2.20213500	3.33486500
H	9.76047000	3.32347500	2.04229500
C	9.91261800	-2.23065000	0.71431700
C	10.66189400	-1.02455500	0.63152800
C	9.35353200	-2.48142000	-0.56751300
H	9.82929700	-2.86727100	1.58582300
C	10.52036900	-0.50440800	-0.67214100
H	11.23709800	-0.58194800	1.43212200
C	9.69669500	-1.40332700	-1.41991000
H	8.76904800	-3.34757500	-0.84701200
H	10.99782200	0.39129300	-1.04763300
H	9.44215700	-1.31936100	-2.46835000
C	7.77119300	2.41426300	-1.27082100
C	8.25170400	1.35145700	-1.95483100
H	7.59427300	0.59313100	-2.36790400
H	9.27736000	1.34888400	-2.31035000
H	6.70897300	2.44585200	-1.02421300
C	8.55449200	3.65374900	-0.95090700
H	9.62604100	3.47236200	-1.09299200
H	8.40110800	3.93853700	0.09579300
C	8.09460200	4.82236400	-1.85175400
H	7.02960300	5.03843100	-1.71420600
H	8.65626300	5.72669000	-1.59944700
H	8.26394900	4.59708300	-2.90916800

5g

C	0.58107600	1.86317100	-0.26551800
C	-0.63750000	2.26103100	0.60305900
H	-0.30303800	2.55937900	1.60292200
H	-1.32129200	1.39733000	0.79722800
H	1.38740400	1.37982000	2.55575500
C	1.33951700	0.34003200	2.26991200
C	0.28429300	-0.55591600	2.56540300
C	2.33385200	-0.36922200	1.54790400
C	0.63975700	-1.83931300	2.05094000
H	-0.60354200	-0.31790100	3.13691000
C	1.91237900	-1.72357000	1.44138900
H	3.26730900	0.04137700	1.18483800
H	0.06580600	-2.75191200	2.15203100
H	2.47170400	-2.52785200	0.98333500
H	-0.89733800	0.11920100	-2.93528900
C	-0.15897100	-0.51982100	-2.46640000
C	1.22223500	-0.22471300	-2.31973000
C	-0.37857600	-1.83438400	-1.96920500
C	1.84025700	-1.32754800	-1.67890800
H	1.71819200	0.67906700	-2.63951600
C	0.84401900	-2.33015200	-1.46570800
H	-1.31690400	-2.37447900	-1.98345600
H	2.89488100	-1.42036800	-1.45475200
H	1.00411100	-3.31068900	-1.03693100
Hf	0.31389200	-0.36600300	0.03790100
C	-1.49922000	3.37960600	-0.00721000
H	-1.89778900	3.08973000	-0.98645100
H	-0.89509700	4.28089400	-0.15338600
H	-2.34022700	3.64341200	0.64328300
H	0.27819400	2.01471700	-1.31214500
C	1.79718200	2.76950700	-0.01581000
H	1.47535500	3.82145500	-0.06477900
H	2.17357300	2.62980200	1.00581500
C	2.95669800	2.58715800	-1.00057800
H	3.37349900	1.57315300	-0.96080100
H	2.63942000	2.78098800	-2.03289900
H	-5.48272800	-0.08738000	-1.19708500
C	-5.33552900	0.15910100	-0.14017800
H	-5.64212900	-0.70330900	0.45946900
C	-3.86792800	0.54837800	0.15096200
H	-3.61676700	1.43545300	-0.44372900
H	-3.75381700	0.81351400	1.20809400
C	-2.94982000	-0.57896600	-0.20783500
H	-2.92284200	-0.84266900	-1.26533600
C	-2.25413800	-1.33867700	0.67077900

H	-1.79611600	-2.27550000	0.36064900
H	-2.35354500	-1.17350700	1.73972400
H	-5.99318700	0.99818700	0.10451500
H	3.76920800	3.28606600	-0.77651700

Hf/Hex

5a

C	1.17508600	2.92582200	-0.54253200
H	0.13200400	3.02206100	-0.21839400
H	1.20784100	3.18007900	-1.60923500
C	1.72673300	1.50645500	-0.30848100
H	1.75281400	1.34601900	0.78204000
C	0.81347100	0.44122700	-0.99578200
H	1.42335900	-0.12633200	-1.72585500
H	0.08827500	0.95929800	-1.64154600
H	2.79126600	-0.87062300	0.71725600
C	1.98567300	-1.51179900	1.04010900
C	1.10948800	-1.26707000	2.12276400
C	1.61633200	-2.75322600	0.44900400
C	0.22184400	-2.38106800	2.23422600
H	1.14348900	-0.40689800	2.78023800
C	0.54788300	-3.30271500	1.21550200
H	2.11792600	-3.23403600	-0.38162400
H	-0.54693100	-2.51660500	2.98543000
H	0.06647900	-4.25625200	1.04341600
H	-2.15652000	0.03191700	-2.34117800
C	-1.90794300	-0.95237200	-1.96797500
C	-0.82679100	-1.75687300	-2.40750300
C	-2.62397100	-1.68057900	-0.97984300
C	-0.86197700	-2.97709600	-1.67981200
H	-0.10436200	-1.48919800	-3.16743900
C	-1.97919800	-2.93005400	-0.79545500
H	-3.52816000	-1.35594000	-0.48153500
H	-0.19228800	-3.81630400	-1.81414300
H	-2.30202500	-3.72183000	-0.13165200
Hf	-0.30891100	-1.23171900	0.01849400
C	3.18518800	1.40751000	-0.81751200
H	3.51156800	0.35695500	-0.78601000
H	3.19720000	1.68253700	-1.88267600
H	1.75305400	3.68098100	-0.00070700
C	4.21276600	2.25581900	-0.05427300
H	4.15720100	2.01863700	1.01971500
H	3.96424700	3.32140200	-0.14354700
C	5.65234500	2.04157900	-0.54390600
H	5.91497900	0.97830500	-0.44622600
H	5.70628600	2.27071400	-1.61735200
C	6.67674100	2.89336300	0.21275900
H	6.67161700	2.66315900	1.28521300
H	7.69140400	2.71754500	-0.16009400
H	6.46240700	3.96314500	0.10192000
H	-3.83609300	2.90674900	1.63324400
C	-3.28893600	3.15181600	0.71390700
C	-4.22657900	3.85003300	-0.28207000
H	-2.48086400	3.83765900	1.00195900
C	-2.67546300	1.85344100	0.12418200
C	-4.83827400	5.13300200	0.28965300
H	-5.02781000	3.15693800	-0.57316300
H	-3.66912800	4.08283500	-1.19977600
H	-3.47782300	1.15868200	-0.14826700
H	-2.12865200	2.11864500	-0.78985100
C	-1.74385800	1.22819700	1.11149500
H	-4.06184800	5.85845700	0.55912600
H	-5.49902900	5.60874900	-0.44218200
H	-5.43069600	4.92617100	1.18850500
H	-0.85840900	1.81349900	1.36302300
C	-1.95017900	0.07157300	1.79225500
H	-2.86918500	-0.49776500	1.66628200
H	-1.34425300	-0.16749200	2.65922200

5e

C	1.75895400	-0.40567100	-1.02346000
C	2.49843400	0.94752400	-0.77353900

H	1.61244200	-0.51889300	-2.10620400
H	2.43364600	-1.24108000	-0.76215200
C	4.00974300	0.72167700	-0.53270600
H	2.10989300	1.44328400	0.13281800
C	4.81678100	1.97614200	-0.16916500
H	4.13229400	-0.01801700	0.27379600
H	4.43871000	0.25356900	-1.43098000
H	4.79294300	2.69287400	-1.00042500
H	4.34183800	2.48285300	0.68549300
H	2.45036200	-0.38194100	1.76133400
C	1.42759400	-0.66576900	1.96144700
C	0.35447400	0.21460700	2.23032200
C	0.92121700	-1.99629500	1.99783100
C	-0.81415700	-0.57263200	2.47368800
H	0.42332200	1.29390600	2.29299700
C	-0.45724500	-1.93277900	2.34965800
H	1.50269700	-2.89958700	1.86050500
H	-1.79303500	-0.20182100	2.75069600
H	-1.11782500	-2.77816000	2.48957000
C	2.26084300	1.90737200	-1.95455500
H	1.19419200	2.02238100	-2.18481000
H	2.74681100	1.52536300	-2.86079200
H	2.66041900	2.90665400	-1.75639300
C	-0.01378000	-2.77302900	-1.71023100
C	-0.85423000	-1.78780600	-2.29014200
C	-0.68197700	-3.30836500	-0.57695800
H	0.96526400	-3.06319000	-2.06811600
C	-2.04979600	-1.72666600	-1.52714300
H	-0.62615000	-1.19993900	-3.17007500
C	-1.94493800	-2.65670600	-0.46130200
H	-0.31810000	-4.10698500	0.05615200
H	-2.90425100	-1.09594000	-1.73364600
H	-2.70610600	-2.86690300	0.27895500
H	-0.16091700	1.75034000	-0.34040800
C	-1.14865100	1.37642800	-0.61516700
C	-2.17909900	1.47759400	0.26402700
H	-1.33527700	1.21010400	-1.67421400
C	-3.62878200	1.29211800	-0.03853500
H	-1.95060400	1.79075600	1.28290500
C	-4.41191100	2.61311500	0.18500400
H	-3.77020700	0.94914600	-1.06930500
H	-4.04895700	0.52745900	0.63137700
H	-4.26161600	2.95539000	1.21787100
H	-3.99761800	3.39180900	-0.46807900
Hf	-0.17306600	-0.93910900	0.02260800
C	-5.91329200	2.44662500	-0.09093100
H	-6.31565100	1.66093600	0.56332800
H	-6.05538600	2.09464500	-1.12179000
C	-6.69588500	3.74660500	0.12074600
H	-6.33820700	4.54004300	-0.54571400
H	-7.76102400	3.59654600	-0.08254200
H	-6.60070500	4.10612000	1.15199000
C	6.28142700	1.66989100	0.17668900
H	6.31623400	0.96435300	1.01917200
H	6.75195800	1.15402400	-0.67189800
C	7.08982300	2.92395400	0.52525900
H	8.12800100	2.67247600	0.76707500
H	7.10532400	3.63137900	-0.31259800
H	6.66276500	3.44431900	1.39130000

5f

C	-0.96876300	1.64875800	1.37249400
C	0.53527900	1.34854100	1.28204200
H	-1.33725700	1.56124400	2.39472400
H	-1.18892000	2.66062500	1.03217000
C	1.35196700	2.58530000	0.83093100
H	0.72653400	0.57051600	0.46517000
C	2.80113500	2.33292900	0.39492000
H	0.81720700	3.08401200	0.01247700
H	1.33681200	3.29470400	1.66998800
H	3.36441400	1.84752500	1.20318200
H	2.81342700	1.63211800	-0.45548100

H	0.04647500	2.13499000	-1.92674600
C	-0.87997600	1.57596100	-1.92695200
C	-1.09419100	0.31936200	-2.55455700
C	-2.11576200	2.00411200	-1.37255500
C	-2.44213600	-0.05655000	-2.34988400
H	-0.35574100	-0.24385200	-3.11070300
C	-3.07731500	0.99180300	-1.61383500
H	-2.30020900	2.94175900	-0.86957800
H	-2.91979700	-0.95323100	-2.72362400
H	-4.12477400	1.04063100	-1.34794400
Hf	-1.46099600	-0.05632200	-0.03754900
C	1.08722600	0.72134800	2.57631100
H	0.53008600	-0.17581000	2.86541800
H	0.99742800	1.44558200	3.39373800
H	2.14129600	0.44325100	2.48875900
C	-3.41019400	-0.44243800	1.51531100
C	-2.28139200	-0.92032700	2.23578000
C	-3.61140000	-1.30593200	0.40437800
H	-4.03504300	0.39546500	1.79688200
C	-1.75127900	-2.02976500	1.54312500
H	-1.89377300	-0.49986200	3.15259200
C	-2.57384700	-2.26877200	0.39747200
H	-4.41901700	-1.24286000	-0.31219500
H	-0.90373100	-2.62419100	1.85932200
H	-2.46856900	-3.08029200	-0.31046000
C	1.37790200	-1.43723000	-0.90957600
C	0.25784000	-2.19372700	-0.97103900
H	-0.40878300	-2.16136300	-1.82704000
H	0.11924100	-3.02040000	-0.28100800
H	1.54828900	-0.68755500	-1.68336200
C	2.50445100	-1.65388500	0.05561800
H	2.85267000	-0.69554300	0.45713100
H	2.17112500	-2.26868700	0.90047700
C	3.69625500	-2.34700000	-0.65338400
H	3.36257500	-3.31121100	-1.05835800
H	4.01211100	-1.74000600	-1.51302300
C	3.53212300	3.62162000	-0.01118600
H	3.52213900	4.32041200	0.83620700
H	2.97522100	4.11570900	-0.81990400
C	4.97738100	3.37813800	-0.45715900
H	5.46739200	4.31675700	-0.73567200
H	5.56908800	2.92016200	0.34458400
H	5.02070800	2.71095800	-1.32702100
C	4.88944400	-2.56213900	0.28890900
H	4.56649900	-3.16249600	1.15049300
H	5.21153800	-1.59188600	0.69175800
C	6.06995100	-3.24998400	-0.40439100
H	6.90391700	-3.39008400	0.29098800
H	5.78631200	-4.23714500	-0.78764000
H	6.43660600	-2.65550600	-1.24943800

5g

C	-0.97693000	1.47035000	-0.02069300
C	0.27268700	1.91177600	-0.81670700
H	0.01676700	2.05076100	-1.87262700
H	1.06330600	1.11586500	-0.83946400
H	-1.41339400	0.56256600	-2.83639500
C	-1.27007400	-0.41965400	-2.41196600
C	-0.09548300	-1.20322800	-2.50914700
C	-2.23304700	-1.15336700	-1.67225700
C	-0.33998600	-2.44594400	-1.85089500
H	0.80456300	-0.92599600	-3.04259100
C	-1.66555200	-2.41789400	-1.35339700
H	-3.23499900	-0.82198200	-1.43155800
H	0.34429400	-3.28252100	-1.78608000
H	-2.16397300	-3.22381300	-0.83220800
H	0.48940600	0.30610200	2.93332300
C	-0.09640100	-0.49506500	2.49917000
C	-1.48900000	-0.45084200	2.22142300
C	0.36770400	-1.80287600	2.19008400
C	-1.86857500	-1.70630500	1.68544400
H	-2.14648700	0.38949600	2.38632800
C	-0.71305000	-2.54776000	1.66817100

H	1.37295500	-2.17513600	2.34121100
H	-2.87204000	-1.99606200	1.40240000
H	-0.68046700	-3.58366100	1.35668000
Hf	-0.36404100	-0.70956400	-0.03313200
C	0.94764100	3.18251200	-0.27405300
H	1.27578100	3.04988900	0.76340100
H	0.23793500	4.01598700	-0.29038100
H	1.81575300	3.47054100	-0.87672700
H	-0.81058100	1.78414700	1.01959000
C	-2.26269900	2.16152200	-0.49727000
H	-2.09154700	3.24965300	-0.53605000
H	-2.49614200	1.86978700	-1.53035100
C	-3.49896600	1.91328300	0.37770000
H	-3.71702000	0.83492100	0.41850300
H	-3.28209400	2.22222100	1.41172200
C	-4.74706400	2.66136300	-0.11212200
H	-4.96547500	2.36191600	-1.14711400
H	-4.52971200	3.73761200	-0.14687800
C	-5.97990900	2.41585100	0.76368600
H	-6.84963300	2.96258800	0.38479000
H	-6.24417000	1.35131700	0.79202900
H	-5.80610600	2.74316900	1.79588000
H	5.25228300	0.40216200	1.40962300
C	5.17214400	0.52423300	0.32076300
C	6.03709600	1.71087900	-0.12828700
H	5.55148400	-0.40340300	-0.12696500
C	3.68144300	0.70349500	-0.06949100
C	7.51219700	1.53619400	0.24701000
H	5.64695200	2.63381500	0.32247200
H	5.94513200	1.83457800	-1.21597200
H	3.31496200	1.63232600	0.38578100
H	3.59496200	0.80756000	-1.15771800
C	2.87320600	-0.45897400	0.41313700
H	7.93772900	0.63902400	-0.21761000
H	8.10380100	2.39537600	-0.08521800
H	7.63904900	1.44366600	1.33203900
H	2.79189100	-0.55898100	1.49572600
C	2.34435600	-1.42840200	-0.37111300
H	1.97859300	-2.35922300	0.05570100
H	2.50676900	-1.41455100	-1.44491000

2nd TS

Hf/Et

6

Hf	0.28953800	0.02811300	0.06478200
C	1.85415100	-0.98525900	-1.61873400
C	0.94806900	-2.02451400	-1.28085200
C	1.14435400	-2.35743100	0.08474000
C	2.20500200	-1.54869100	0.58452300
C	2.63955400	-0.69872400	-0.46321000
C	-0.71587200	2.32265800	0.53220000
C	0.68754700	2.43238100	0.74781900
C	1.33742300	2.23674800	-0.49712200
C	0.33867300	1.99458700	-1.48478500
C	-0.92923300	2.07480300	-0.84613000
H	1.96915000	-0.53356300	-2.59556300
H	0.23206200	-2.48200500	-1.95250900
H	0.61982500	-3.12898700	0.63421300
H	2.63505800	-1.59866900	1.57569200
H	3.45522900	0.00997800	-0.40685300
H	-1.48576600	2.45204300	1.28215500
H	1.17397000	2.66469100	1.68643600
H	2.40289700	2.29829300	-0.67370800
H	0.51031300	1.85029500	-2.54386100
H	-1.89007100	1.97141100	-1.33423200
C	-4.07767100	-0.88013700	-1.21786600
H	-3.68548300	-0.43122300	-2.13842600
H	-5.12014300	-0.56361800	-1.11127000
H	-4.06875900	-1.96849600	-1.34358800
H	-1.75151700	-1.99995500	-0.10132300
C	-1.80478400	-0.90918300	-0.05511100

H	-1.39070700	-0.55623300	-1.06634300
C	-3.25909600	-0.45391300	0.01186000
H	-3.71645800	-0.89447400	0.90658100
H	-3.31761400	0.63461700	0.13690600
C	-1.23515400	-0.63454000	2.11178400
H	-2.05930100	0.06344100	2.20451200
H	-1.51027100	-1.68121600	2.18998400
C	0.06757700	-0.22215700	2.44135100
H	0.18787000	0.76377400	2.88003400
H	0.75971300	-0.97400100	2.80404400

Hf/Pro

6a

C	1.70288600	-0.26516100	0.56124300
C	2.95810800	0.62778500	0.48990300
H	1.93484700	-1.20973700	1.05719900
H	1.00582200	0.25496200	1.31021400
C	3.21796400	1.27256300	1.86878300
H	2.77697700	1.43659900	-0.23112300
H	2.36542700	1.86861700	2.21643600
H	3.42201000	0.50718700	2.62709100
H	0.87854500	2.16960800	-2.01813000
C	0.04008700	2.15053700	-1.33307200
C	-1.30313300	1.81455500	-1.66429400
C	0.07834900	2.50012100	0.03937200
C	-2.08733300	1.94157000	-0.49045300
H	-1.66935800	1.53591200	-2.64387200
C	-1.22992200	2.34856900	0.57296000
H	0.94878900	2.83532700	0.58755400
H	-3.15588600	1.78593600	-0.42061500
H	-1.53284300	2.57104200	1.58816600
Hf	-0.53115700	0.02071000	-0.05421000
C	4.22283400	-0.13110000	0.04909200
H	4.15494800	-0.53725300	-0.96411200
H	4.44372300	-0.95820000	0.73495000
H	5.08232700	0.54658800	0.06639200
C	-2.35191200	-0.56968300	1.58901700
C	-1.17948200	-1.20359300	2.06805900
C	-2.70524400	-1.17571200	0.34832700
H	-2.89558100	0.22203700	2.08754400
C	-0.80579700	-2.20695000	1.12833700
H	-0.67330200	-0.98147900	2.99975400
C	-1.76188500	-2.20244800	0.07928500
H	-3.57331100	-0.93735900	-0.25346400
H	0.02352600	-2.89373300	1.23356000
H	-1.79001400	-2.88042700	-0.76215300
C	1.43722600	-1.09163600	-1.47358000
C	0.13138900	-0.96553500	-2.05368700
H	0.03782800	-0.23344500	-2.85099000
H	-0.38105700	-1.90000100	-2.26638000
H	2.16398600	-0.34477900	-1.77700400
C	1.99724700	-2.47282400	-1.22160700
H	1.23991300	-3.15068900	-0.81849100
H	2.87235600	-2.48460300	-0.57072100
H	4.08928300	1.93432500	1.82170000
H	2.30604300	-2.87388400	-2.19648900

6b

C	1.66600700	-0.64410400	-0.25673300
C	3.07938900	-0.25668700	-0.72276100
H	1.01659900	-0.47133500	-1.18549300
H	1.63722700	-1.72277800	-0.07780500
C	4.16718500	-1.00122000	0.07133500
H	3.21694700	0.82516200	-0.60174100
H	4.11816200	-0.81973600	1.14908800
H	4.08584800	-2.08314300	-0.09020000
H	-0.43768300	-2.95309100	1.36003000
C	-1.09266100	-2.40257200	0.69608600
C	-2.20858000	-1.60897800	1.09152100

C	-1.02438900	-2.38755900	-0.71827500
C	-2.81427400	-1.09345100	-0.08041700
H	-2.55231300	-1.45009500	2.10517900
C	-2.06999400	-1.55823300	-1.20444600
H	-0.30126500	-2.91361000	-1.32917300
H	-3.70142500	-0.47455500	-0.11705200
H	-2.29989800	-1.37188700	-2.24559000
C	3.24256400	-0.56683600	-2.22714000
H	2.52971200	-0.00144900	-2.83940200
H	3.09717900	-1.63440200	-2.43085800
H	4.25071600	-0.29907400	-2.56030700
C	-1.73720600	1.65325900	-1.44465200
C	-0.36311000	1.74791400	-1.77215200
C	-1.90436200	2.10857600	-0.10574100
H	-2.52403400	1.30608300	-2.10087100
C	0.32361500	2.28176400	-0.64143600
H	0.08103400	1.49437600	-2.72720300
C	-0.63325800	2.52156800	0.37703700
H	-2.84332900	2.18720000	0.42805700
H	1.37896600	2.51447900	-0.59637100
H	-0.44285700	2.96736400	1.34326700
C	1.44758700	0.02971200	1.83571800
C	0.07879500	0.14468300	2.27452900
H	-0.31164800	-0.71449600	2.81298800
H	-0.17861000	1.09112900	2.74539200
H	1.92960000	-0.92660100	2.01733000
C	2.34763100	1.22965100	2.00547500
H	1.82319000	2.17043500	1.82608100
H	3.25794400	1.20851300	1.40765800
H	5.16062400	-0.69114300	-0.26830300
H	2.65751100	1.22945400	3.05984500
Hf	-0.55108100	0.00483700	0.05344100

6c

C	-3.21778200	1.27156000	1.86964500
H	-2.36517700	1.86706700	2.21805200
H	-3.42231000	0.50567200	2.62730400
C	-2.95769200	0.62773000	0.49032600
H	-2.77648400	1.43701400	-0.23013100
C	-1.70251100	-0.26532500	0.56122900
H	-1.93452500	-1.20995700	1.05704300
H	-1.00530000	0.25446700	1.31029600
H	0.67044600	-0.98369700	2.99920700
C	1.17769200	-1.20499500	2.06789700
C	0.80528100	-2.20771400	1.12707600
C	2.35043900	-0.57038300	1.59054900
C	1.76240400	-2.20212000	0.07891900
H	-0.02393800	-2.89483700	1.23083500
C	2.70528100	-1.17542200	0.34977400
H	2.89341900	0.22106100	2.09026300
H	1.79151300	-2.87949100	-0.76298200
H	3.57396400	-0.93646800	-0.25088500
H	-0.94656500	2.83534200	0.59248000
C	-0.07742600	2.50034200	0.04210900
C	1.23196900	2.34828000	0.57264700
C	-0.04236600	2.15130700	-1.33058000
C	2.08695000	1.94166100	-0.49288800
H	1.53724300	2.57009800	1.58728400
C	1.30012600	1.81571100	-1.66508900
H	-0.88233500	2.17087000	-2.01377400
H	3.15566000	1.78592000	-0.42559400
H	1.66412800	1.53780100	-2.64569200
C	-4.22239700	-0.13078500	0.04880100
H	-4.15456500	-0.53585200	-0.96484400
H	-4.44316100	-0.95862200	0.73380600
H	-4.08887200	1.93364300	1.82281300
C	-1.99737200	-2.47243300	-1.22251500
H	-2.87259000	-2.48412100	-0.57177900
H	-1.24033600	-3.15069200	-0.81951800
C	-1.43690200	-1.09133600	-1.47397600
H	-2.16347200	-0.34419000	-1.77714800
C	-0.13108000	-0.96539300	-2.05401400
H	-0.03741300	-0.23314100	-2.85115000

H	0.38126000	-1.89988900	-2.26683800
Hf	0.53152500	0.02075200	-0.05441400
H	-5.08194900	0.54681000	0.06689600
H	-2.30613300	-2.87307900	-2.19757600

6d

C	-1.66580700	-0.64467700	-0.25631800
C	-3.07898800	-0.25706900	-0.72279900
H	-1.63749600	-1.72322900	-0.07665700
H	-1.01605200	-0.47300400	-1.18503400
C	-3.24218800	-0.56856800	-2.22688800
H	-3.21618900	0.82494100	-0.60285800
H	-2.52836300	-0.00487500	-2.83958500
H	-3.09827200	-1.63655900	-2.42939500
H	-1.37982300	2.51217500	-0.60179900
C	-0.32418500	2.28038300	-0.64481300
C	0.63062300	2.52215400	0.37509400
C	0.36507200	1.74602100	-1.77378800
C	1.90300800	2.11003600	-0.10506100
H	0.43807600	2.96872900	1.34053900
C	1.73868900	1.65314200	-1.44376300
H	-0.07707500	1.49113900	-2.72941000
H	2.84095300	2.19015200	0.43031400
H	2.52705700	1.30618100	-2.09824500
Hf	0.55131200	0.00501900	0.05366100
C	-4.16719600	-1.00048400	0.07184300
H	-4.11801000	-0.81842700	1.14948400
H	-4.08649800	-2.08254300	-0.08907600
H	-5.16048500	-0.69004400	-0.26790900
C	2.07193000	-1.55761000	-1.20310700
C	1.02483600	-2.38675400	-0.72001400
C	2.81411800	-1.09425300	-0.07707900
H	2.30398200	-1.37019600	-2.24357100
C	1.09025100	-2.40333600	0.69452500
H	0.30264100	-2.91172700	-1.33294300
C	2.20594100	-1.61100400	1.09303300
H	3.70173300	-0.47585300	-0.11125000
H	0.43370800	-2.95426800	1.35657500
H	2.54790300	-1.45360100	2.10750900
C	-1.44742100	0.03070300	1.83574200
C	-0.07864600	0.14603800	2.27458900
H	0.17865900	1.09279900	2.74487800
H	0.31175800	-0.71279500	2.81363700
H	-1.92938400	-0.92549600	2.01805000
C	-2.34752000	1.23077000	2.00446500
H	-1.82284000	2.17145000	1.82527900
H	-3.25735500	1.20964000	1.40592900
H	-4.24986900	-0.29972300	-2.56061300
H	-2.65829200	1.23085500	3.05857000

6e

C	1.75582400	0.41309100	-0.55068000
C	3.18013300	-0.07389300	-0.23591800
H	1.79616400	1.27921000	-1.21678100
H	1.26635200	-0.41476400	-1.18210700
C	3.71659700	-0.92441100	-1.40675000
H	3.15192200	-0.71514200	0.65687300
H	3.08508400	-1.79975800	-1.60234000
H	3.77062800	-0.33457000	-2.32944000
H	1.64859600	-2.57260900	0.36463600
C	0.63032100	-2.33747200	0.64534200
C	0.21856900	-1.72435300	1.85221000
C	-0.53032200	-2.61072900	-0.13194900
C	-1.20222200	-1.63426300	1.84112200
H	0.86860700	-1.40932000	2.65858500
C	-1.66399000	-2.19709800	0.62352000
H	-0.55155900	-3.11279500	-1.09096500
H	-1.82480100	-1.24477500	2.63682200
H	-2.69838500	-2.31828900	0.33194400
C	4.14697900	1.09318800	0.03498100
H	3.86938100	1.68762900	0.91018400
H	4.19725700	1.76507400	-0.83072600

H	5.15599200	0.70752200	0.21224800
C	-0.85701000	0.77697500	-2.37575100
C	-1.05911700	1.85944900	-1.48211200
C	-1.84189300	-0.20983200	-2.10793100
H	-0.08422800	0.70862700	-3.13138700
C	-2.19898600	1.55910300	-0.68166100
H	-0.48320300	2.77549700	-1.45170300
C	-2.68057800	0.28324400	-1.06686000
H	-1.96459900	-1.14595800	-2.63746600
H	-2.65014700	2.20807800	0.05398500
H	-3.55777200	-0.20804400	-0.66737800
H	1.89765800	0.74342800	1.85357200
C	1.19257400	1.40381200	1.36235400
C	-0.14664400	1.46763600	1.81192100
H	1.63434900	2.29309400	0.92251400
C	-0.84885500	2.81825800	1.87924200
H	-0.35950100	0.82627000	2.66543600
H	-0.69439600	3.42037600	0.97832500
H	-1.92503600	2.71447800	2.04402500
Hf	-0.42626100	-0.10746300	-0.02442100
H	4.72604100	-1.28516800	-1.18293900
H	-0.45188000	3.39304100	2.72592200

6f

C	2.85541500	0.84666900	-0.24670900
C	1.71028600	-0.06307500	-0.75134200
H	2.50114000	1.60947000	0.45351900
H	3.53987700	0.21289100	0.33435500
C	2.31151200	-1.29912100	-1.47072700
H	1.14846600	0.53908000	-1.54879800
H	3.40625200	-1.28010900	-1.43178200
H	2.00174800	-2.25433300	-1.03526900
H	-0.05742000	-3.11404000	-0.57703300
C	-0.79217100	-2.34655900	-0.77981100
C	-1.91602600	-2.02480100	0.03605800
C	-0.84757700	-1.52937300	-1.93504100
C	-2.64693000	-0.99773400	-0.60550600
H	-2.19735700	-2.51335200	0.95938800
C	-1.97600700	-0.67094400	-1.81907600
H	-0.15420000	-1.55152200	-2.76411300
H	-3.57015300	-0.56195300	-0.24889000
H	-2.30992700	0.04294500	-2.56094000
Hf	-0.40863900	0.04474800	-0.00241800
C	3.65688100	1.54379700	-1.35926600
H	4.08463500	0.82661900	-2.06745700
H	4.48288900	2.12674200	-0.93756500
H	3.02229600	2.23242500	-1.93191300
C	-2.09361100	1.93677600	0.38123600
C	-1.19921400	2.33631000	-0.65262000
C	-1.35928700	1.84174900	1.58445000
H	-3.15262100	1.75091900	0.26687000
C	0.07954400	2.54468900	-0.06214200
H	-1.46521700	2.54444800	-1.68127500
C	-0.00762900	2.21077100	1.30869600
H	-1.77041200	1.59252600	2.55477100
H	0.96048800	2.89719100	-0.58032100
H	0.79194600	2.28487400	2.03494300
H	-0.54407600	-0.27145100	2.85877000
C	-0.00879900	-1.08686500	2.38321600
C	1.32846300	-0.99530100	2.14544100
H	-0.48860700	-2.05980100	2.40172700
C	2.22355500	-2.16522800	1.89880500
H	1.82037000	-0.03222500	2.27163000
H	1.66496900	-3.07166100	1.64899900
H	2.96868600	-1.96644400	1.12552300
H	2.77787400	-2.36054700	2.82855700
H	2.04991400	-1.33514600	-2.53354800

6g

C	-3.10777000	-0.22138400	-0.00085800
C	-1.89412000	0.72148300	0.07845400

H	-2.79951800	-1.26917600	0.02194200
H	-3.70829300	-0.06241800	0.90345800
C	-2.35539700	2.15684100	0.33844700
H	-1.38856800	0.71381600	-0.96215600
H	-3.02850800	2.17900200	1.20258900
H	-1.54252000	2.85808000	0.53149200
H	-0.02591600	3.00309300	-1.23106900
C	0.77667400	2.41280200	-0.80817000
C	1.13531100	2.34114700	0.56236900
C	1.66502200	1.58442100	-1.54234000
C	2.27194700	1.49175200	0.67484300
H	0.66552500	2.87911400	1.37564300
C	2.59988600	1.02741500	-0.62267000
H	1.67004200	1.45269600	-2.61647700
H	2.81888000	1.27076700	1.58189700
H	3.44142700	0.39695100	-0.87435700
Hf	0.34959100	0.00758000	-0.07941100
C	-4.00770700	0.00599000	-1.23022300
H	-4.45553600	1.00388600	-1.23595100
H	-4.82597500	-0.72116400	-1.23355700
H	-3.45139200	-0.11644700	-2.16813500
C	-0.64438400	-1.84160700	-1.52777700
C	-0.41712500	-2.40829800	-0.24920400
C	0.61337600	-1.49348100	-2.08883000
H	-1.60503600	-1.70422300	-2.00627800
C	0.98941800	-2.44006700	-0.02648300
H	-1.17291500	-2.79590100	0.42049300
C	1.62350800	-1.88464000	-1.16520100
H	0.77491400	-1.06897900	-3.07123300
H	1.48871600	-2.86284500	0.83323300
H	2.69085000	-1.80679500	-1.31952300
H	-1.20127800	1.30065900	2.33833700
C	-1.03411300	0.24975700	2.13479800
C	0.24777000	-0.30698300	2.34308900
H	-1.90503700	-0.38567800	2.26447600
C	0.38364800	-1.67629500	2.99808200
H	0.98771100	0.40919600	2.69401400
H	-0.32001000	-2.41183500	2.59678000
H	1.39578000	-2.07932200	2.90173300
H	-2.92878400	2.54393800	-0.51245700
H	0.17924800	-1.58526400	4.07272400

Hf/but

6a

C	-1.44035200	0.10231900	0.63074800
C	-2.76177900	-0.55837700	0.18823600
H	-1.60928200	0.76532400	1.48128200
H	-0.81808000	-0.74941800	1.08563500
C	-3.11305500	-1.71275300	1.16840700
H	-2.62104000	-1.00284300	-0.80800900
C	-4.31408800	-2.56946900	0.74859100
H	-2.23741500	-2.36959500	1.27356600
H	-3.29207500	-1.28670700	2.16546700
H	-4.42908900	-3.41715200	1.43169000
H	-5.25237000	-2.00746100	0.76853100
H	-4.18396000	-2.97299900	-0.26308000
H	-0.71971500	-1.10642100	-2.72598500
C	0.09166000	-1.44475300	-2.09411100
C	1.46838900	-1.12051900	-2.25635700
C	-0.02245500	-2.33137500	-0.99479600
C	2.19804300	-1.79288000	-1.24405200
H	1.88978100	-0.49162700	-3.02975200
C	1.27377100	-2.53125200	-0.44883500
H	-0.93536900	-2.78697200	-0.63504100
H	3.27236900	-1.77327700	-1.11602500
H	1.52078700	-3.18252000	0.37976300
Hf	0.78629000	-0.10474300	-0.04024200
C	-3.92689300	0.44392000	0.10541700
H	-3.75373700	1.24433300	-0.61927900
H	-4.11675900	0.90555300	1.08246900
H	-4.84383900	-0.06482200	-0.20283700
C	2.57675600	-0.43252800	1.70781000

C	1.43707500	0.03927900	2.40426200
C	3.03085800	0.60960400	0.84823100
H	3.03441600	-1.40611200	1.82363600
C	1.18492400	1.37632100	1.98196300
H	0.87413800	-0.51248800	3.14733000
C	2.18349800	1.73293800	1.03875200
H	3.90293600	0.57296300	0.20733600
H	0.40887000	2.02535300	2.36501900
H	2.30051500	2.69873300	0.56738400
C	-1.01461400	1.68587000	-0.86016100
C	0.30066300	1.68844000	-1.43442700
H	0.36664900	1.35747900	-2.46717800
H	0.90146600	2.57074200	-1.22936700
H	-1.78753700	1.20968200	-1.45675900
C	-1.47554100	2.89370200	-0.06498600
H	-0.65471700	3.25969800	0.56161000
H	-2.31043300	2.65090000	0.59626500
C	-1.91485900	4.00899400	-1.03528400
H	-2.74780200	3.68362900	-1.66860200
H	-2.24976100	4.88166900	-0.46607800
H	-1.09382300	4.32094000	-1.68802300

6b

C	-1.28232800	-0.85837500	-0.24417300
C	-2.62419100	-1.12103500	0.46326200
H	-0.51959300	-1.42265800	0.40069600
H	-1.27636100	-1.38276300	-1.20404400
C	-3.80183100	-1.09353000	-0.54068500
H	-2.78748600	-0.34945500	1.22662600
C	-5.18914100	-1.08244500	0.11289500
H	-3.72044900	-0.21515400	-1.19201600
H	-3.71042800	-1.96714700	-1.20165800
H	-5.96966000	-1.02756500	-0.65261900
H	-5.37664100	-1.98376900	0.70444200
H	-5.31291800	-0.21595600	0.77404900
H	0.70674700	-0.86303200	-3.13039500
C	1.41550700	-0.95482700	-2.31677100
C	2.45419100	-0.03044300	-2.00433700
C	1.50683300	-2.03894900	-1.40990100
C	3.17156200	-0.53981300	-0.89380200
H	2.67669700	0.88477400	-2.53669200
C	2.57473300	-1.77721900	-0.51123700
H	0.87335200	-2.91727600	-1.39761700
H	4.03754300	-0.08255300	-0.43299200
H	2.91289500	-2.43268900	0.28095000
C	-2.56426200	-2.47772600	1.19970200
H	-1.76978000	-2.48967200	1.95554200
H	-2.38127700	-3.30165100	0.49942900
H	-3.50596000	-2.68172200	1.71677800
C	2.17577400	0.03161900	2.14273400
C	0.84985600	-0.33029200	2.48266100
C	2.15779700	1.37028600	1.65811500
H	3.05079900	-0.59671900	2.24203200
C	0.00804900	0.79298300	2.22854400
H	0.53788000	-1.28036700	2.89928800
C	0.82119300	1.84568900	1.73831100
H	3.01925600	1.94570900	1.34229300
H	-1.05360100	0.84488500	2.42863200
H	0.49398500	2.84596500	1.49198800
C	-1.30288600	1.19270900	-1.03252200
C	0.00993600	1.74777600	-1.27245400
H	0.36351500	1.67765900	-2.29765800
H	0.18043600	2.73077000	-0.83828300
H	-1.76502000	0.69510500	-1.88133700
C	-2.26854500	1.99430700	-0.18318400
H	-1.73722500	2.46541800	0.64927300
H	-3.06129700	1.37845400	0.24223100
C	-2.91770900	3.08762700	-1.05933900
H	-3.47810600	2.65015200	-1.89307000
H	-3.61840900	3.67393000	-0.45682000
H	-2.16963800	3.77012900	-1.47412500
Hf	0.87768800	0.01523800	-0.02238700

6c

C	2.60595000	-2.15261600	1.63681200
H	1.66153300	-2.70187900	1.73076500
H	2.81624000	-1.68602400	2.60695100
C	2.54872800	-1.08917500	0.51740600
H	2.39167700	-1.61034200	-0.43840100
C	1.35275700	-0.14753000	0.77821400
H	1.60332600	0.57345600	1.55819900
H	0.55749400	-0.80307500	1.28421900
H	-1.37212300	-0.17554300	3.11682700
C	-1.69563300	0.43448500	2.28201200
C	-1.07839900	1.63854700	1.83219500
C	-2.83569800	0.20070100	1.47435300
C	-1.84674100	2.14823800	0.75540200
H	-0.21270500	2.11019100	2.27761700
C	-2.91923800	1.24861200	0.51355200
H	-3.52867600	-0.62374300	1.57768100
H	-1.66813300	3.07361200	0.22601600
H	-3.69633600	1.37046200	-0.23099100
H	0.37548100	-3.05834400	-0.14827900
C	-0.40165300	-2.49522600	-0.64747300
C	-1.75010900	-2.38154000	-0.21621200
C	-0.25586600	-1.75518500	-1.84716600
C	-2.44957400	-1.59850600	-1.18098900
H	-2.18236500	-2.85979200	0.65351900
C	-1.52713400	-1.21041200	-2.18462100
H	0.65350500	-1.65343300	-2.42586700
H	-3.50624100	-1.36520200	-1.16556200
H	-1.75787600	-0.62290000	-3.06357500
C	3.89535900	-0.33126400	0.42819700
H	3.83235900	0.45641300	-0.33065200
H	4.07652100	0.17871600	1.38531500
H	3.39108500	-2.88830500	1.44271300
C	5.09821300	-1.22019600	0.08433200
H	4.92686900	-1.78278400	-0.84154200
H	5.32646900	-1.93778500	0.87770400
H	3.33246800	2.95670700	-1.76504100
C	2.52540700	3.45586500	-1.21719300
H	1.79419500	3.81797800	-1.94639100
C	1.87953400	2.51022100	-0.18424000
H	2.63485900	2.22318100	0.55111800
H	1.08405700	3.04028900	0.35198100
C	1.30124600	1.29977600	-0.89489600
H	2.03419200	0.64766700	-1.36048100
C	0.05334000	1.43088800	-1.59290300
H	0.01572500	0.97952700	-2.58046200
H	-0.40586500	2.41559200	-1.55606400
H	2.95562200	4.32232600	-0.70544500
H	5.99138000	-0.60499900	-0.06409700
Hf	-0.83510600	-0.05147300	-0.04220100

6d

C	1.37065100	-0.44926700	-0.62725100
C	2.81549800	-0.71325500	-0.17163000
H	1.29356100	-0.65954600	-1.69775000
H	0.77193900	-1.28199200	-0.11342500
C	3.01445500	-2.23718400	0.06177500
H	2.98747600	-0.22405600	0.79654000
C	4.39314500	-2.62201500	0.61088700
H	2.24765500	-2.58475900	0.76945700
H	2.82966100	-2.77127100	-0.88101300
H	4.42147100	-3.69172100	0.84184600
H	5.19419100	-2.42267600	-0.10710400
H	4.62185700	-2.07666900	1.53450100
H	1.23151500	0.38039900	2.44911900
C	0.17304100	0.20130300	2.31754300
C	-0.84078400	1.18921200	2.23459600
C	-0.45582200	-1.07798000	2.26902500
C	-2.09133500	0.52767100	2.10182200
H	-0.69879000	2.25930100	2.28951000
C	-1.85163300	-0.87534100	2.14750200
H	0.04219000	-2.03682800	2.34769900

H	-3.06069700	1.00692100	2.04269100
H	-2.60507800	-1.65058000	2.10617100
Hf	-0.83705300	-0.01707800	0.00135000
C	3.82796500	-0.17903900	-1.20001800
H	3.68996100	0.88359800	-1.41978900
H	3.73934400	-0.72925900	-2.14515400
H	4.85219600	-0.30223000	-0.83852600
C	-2.34425300	-1.81170600	-0.91669800
C	-1.36224600	-1.61709000	-1.92412400
C	-3.13103800	-0.62470200	-0.84130200
H	-2.50716200	-2.72382300	-0.35711200
C	-1.51043800	-0.30642300	-2.43916100
H	-0.62727900	-2.34815300	-2.23744700
C	-2.61353300	0.30550900	-1.77581000
H	-3.98875200	-0.47022900	-0.19953400
H	-0.91633000	0.13979400	-3.22702600
H	-3.00637100	1.29493800	-1.96938400
C	1.05898100	1.72560100	-0.71871500
C	-0.32924300	2.12456800	-0.69650800
H	-0.57814200	2.89123600	0.03433500
H	-0.77900700	2.30882900	-1.66833500
H	1.49320600	1.58196700	-1.70481400
C	1.99783200	2.36575300	0.28461500
H	1.48269500	2.51582900	1.23807400
H	2.87923100	1.75488200	0.48279700
C	2.46190600	3.73275400	-0.26288300
H	3.13206900	4.20978800	0.45898200
H	3.01005300	3.62122300	-1.20505400
H	1.61624400	4.40451500	-0.43946200

6e

C	1.50088100	0.52226400	-0.68357500
C	2.92365100	0.74941200	-0.14711000
H	1.40962500	0.93485600	-1.69184100
H	1.38765200	-0.61375800	-0.82458700
C	3.86870200	-0.35725200	-0.68985200
H	2.91363800	0.65961500	0.94979100
C	5.29370300	-0.31489400	-0.12440500
H	3.43035300	-1.33927400	-0.45889800
H	3.90288600	-0.28909500	-1.78615100
H	5.86311400	-1.18305200	-0.47143400
H	5.83868300	0.57903600	-0.44172700
H	5.28965400	-0.33655100	0.97222500
H	2.08241800	-1.49284700	1.62310500
C	1.00551500	-1.53394800	1.71746700
C	0.19818100	-0.62941100	2.44626200
C	0.15722500	-2.52341800	1.14463400
C	-1.15395700	-1.06358500	2.34759100
H	0.55066700	0.22741000	3.00629700
C	-1.17522000	-2.24290900	1.55933100
H	0.47746100	-3.37916500	0.56378200
H	-2.01006600	-0.60202500	2.82357500
H	-2.04769900	-2.84139500	1.33542500
C	3.44619400	2.14965300	-0.51594600
H	2.81195500	2.95228400	-0.12945900
H	3.51060000	2.26427500	-1.60531400
H	4.44642600	2.30944800	-0.10522400
C	-0.71170200	-0.94454500	-2.48971300
C	-1.36593400	0.29738600	-2.28488900
C	-1.42306700	-1.94394300	-1.77557600
H	0.17771800	-1.10758600	-3.08564800
C	-2.50963600	0.06024500	-1.46936700
H	-1.07802100	1.24759700	-2.71603800
C	-2.54305600	-1.32085700	-1.15257000
H	-1.18267000	-2.99905100	-1.74893100
H	-3.25090500	0.79109400	-1.18329600
H	-3.31086500	-1.81850900	-0.57504100
H	1.09588700	1.95888000	1.23443700
C	0.33175700	2.02700900	0.46858400
C	-1.02948500	1.82833900	0.80248100
H	0.56833000	2.70084000	-0.34971300
C	-2.09163800	2.73830300	0.18626300

H	-1.20099800	1.63048500	1.86035500
C	-2.08714300	4.13386400	0.83441100
H	-1.93133800	2.83991500	-0.89433000
H	-3.08543600	2.29672900	0.32025100
H	-2.87637200	4.75972300	0.40440400
H	-2.26224000	4.06958300	1.91431500
H	-1.12961600	4.64414500	0.67991200
Hf	-0.50278700	-0.39797100	-0.00922700

6f

C	-2.39637900	1.75522300	-0.46870100
C	-1.58822100	0.72474300	0.35395900
H	-2.22185200	1.62147200	-1.54156900
H	-3.46186000	1.54382000	-0.31789500
C	-2.35282300	0.25669700	1.60773100
H	-0.66835000	1.29804300	0.74356400
C	-2.53108100	1.32746000	2.70233400
H	-3.34958300	-0.06837200	1.29932800
H	-1.87787700	-0.62041800	2.05119000
H	-2.98866500	0.87375000	3.58780900
H	-1.57587300	1.77015900	3.01027300
H	-3.18632700	2.14007100	2.37858300
H	-0.42275600	-2.31173400	2.05758800
C	0.47729100	-1.72912000	1.91101900
C	1.60567400	-2.12984100	1.14232000
C	0.76351400	-0.46466400	2.48433500
C	2.58149600	-1.10741700	1.23496300
H	1.71290400	-3.06269500	0.60508900
C	2.05551500	-0.06457600	2.05164000
H	0.12131700	0.09774200	3.14904800
H	3.56357200	-1.12828200	0.78143000
H	2.57043100	0.84195800	2.34300100
Hf	0.65917500	-0.09025300	-0.03389300
C	-2.13517800	3.23501100	-0.13094900
H	-2.36225800	3.47168300	0.91103700
H	-2.76150100	3.87551700	-0.76073300
H	-1.09149200	3.51473000	-0.31444800
C	2.66599500	1.22800300	-0.83636300
C	1.57349900	2.12845500	-0.82533700
C	2.41377900	0.23517500	-1.82395800
H	3.54234200	1.28922400	-0.20548200
C	0.65729800	1.71337700	-1.83779100
H	1.47987800	3.00605300	-0.19739300
C	1.18408200	0.55679100	-2.45849900
H	3.06987400	-0.58639800	-2.08406000
H	-0.24475800	2.23202200	-2.12677000
H	0.73896400	0.02334800	-3.28768300
H	0.08517800	-1.85280100	-2.19013200
C	-0.37602800	-1.77993900	-1.20764500
C	-1.58606800	-1.00183800	-1.13921200
H	-0.41467600	-2.73847600	-0.69340400
C	-2.87371300	-1.66559100	-0.69654500
H	-1.72295300	-0.28200200	-1.94313500
C	-3.33964600	-2.65294400	-1.78753000
H	-2.72305400	-2.20625700	0.24452700
H	-3.66503800	-0.92907100	-0.53744600
H	-4.28987200	-3.10605900	-1.48803500
H	-3.49880900	-2.14462300	-2.74495800
H	-2.61151600	-3.45422000	-1.94362100

6g

C	-2.21550900	1.91899400	0.74354400
C	-1.75879600	0.79335300	-0.20553100
H	-1.39699500	2.20673200	1.40775300
H	-2.42226100	2.80235600	0.12671400
C	-2.68110800	0.61672100	-1.42798700
H	-1.78598100	-0.19754700	0.38579600
C	-3.97100200	-0.19635700	-1.19994900
H	-2.95617300	1.61693700	-1.78510500
H	-2.13494000	0.14741800	-2.25183200
H	-4.48129200	-0.34809000	-2.15691100

H	-3.76178000	-1.18574100	-0.77545800
H	-4.67241600	0.30434300	-0.53072700
H	-1.89409700	-2.14070000	-1.56933300
C	-0.82126200	-2.13074900	-1.43545700
C	0.11519400	-1.42601800	-2.23172700
C	-0.10718800	-2.84135000	-0.43437600
C	1.41926800	-1.72715800	-1.74724700
H	-0.11386200	-0.80580700	-3.08886700
C	1.28204100	-2.60613600	-0.64505900
H	-0.53806000	-3.50144400	0.30733800
H	2.35435000	-1.38093500	-2.16772000
H	2.09418700	-3.05353000	-0.08938500
Hf	0.27399100	-0.40929700	0.10017700
C	-3.45701200	1.63427700	1.61142300
H	-4.37698400	1.59536100	1.02502900
H	-3.57622300	2.43354200	2.35056600
H	-3.37039400	0.68736200	2.15807900
C	-0.19904300	0.04530200	2.57162600
C	0.80219600	0.96589400	2.17722300
C	0.33881800	-1.26589400	2.47231200
H	-1.19920700	0.29068900	2.90232900
C	1.97823200	0.22763700	1.86093100
H	0.71056600	2.04353500	2.16623800
C	1.69432400	-1.14686300	2.05462500
H	-0.17119900	-2.18401600	2.73440600
H	2.93390000	0.64284000	1.57524200
H	2.39920700	-1.95901800	1.94438800
H	-0.58368300	1.68291200	-2.13254900
C	-0.01426900	1.83599700	-1.22322400
C	1.32744100	1.38550500	-1.14896500
H	-0.29121400	2.72023700	-0.65711000
C	2.40292500	2.29348900	-0.55094400
H	1.66838500	0.87917700	-2.05060000
C	2.81789200	3.40067800	-1.53568400
H	2.04821600	2.75289100	0.37903500
H	3.29074500	1.70400900	-0.29465500
H	3.61399500	4.01840700	-1.10643900
H	3.19309300	2.97703800	-2.47422700
H	1.97390800	4.05648100	-1.77792900

Hf/Hex

6a

C	-1.53242300	3.07807100	-0.11675500
H	-0.64987800	3.37502000	-0.69001600
H	-1.41442000	3.45458400	0.90703900
C	-1.76906500	1.55708100	-0.11702600
H	-1.90362400	1.23084200	-1.15884100
C	-0.59079100	0.77751600	0.50326600
H	-1.04611600	-0.21131700	0.86981000
H	-0.26581500	1.25523500	1.42882500
H	-2.53152800	-1.16372900	-1.13687500
C	-1.61346900	-1.69060700	-1.36045500
C	-0.64020400	-1.30252400	-2.31356400
C	-1.18248400	-2.90073000	-0.75271900
C	0.38371400	-2.29137200	-2.32508200
H	-0.68501400	-0.42542000	-2.94680800
C	0.04684200	-3.28000900	-1.36692600
H	-1.72565600	-3.46668700	-0.00675500
H	1.25424000	-2.30218500	-2.96803100
H	0.61126100	-4.17935700	-1.15799900
H	1.57625100	0.17407500	2.68572200
C	1.57656600	-0.80840600	2.23280000
C	0.58141000	-1.81235300	2.41612700
C	2.60285000	-1.35298900	1.41957300
C	0.99128000	-2.96800200	1.70696700
H	-0.31436500	-1.72084400	3.01850100
C	2.23273800	-2.67929200	1.07113600
H	3.52172400	-0.85924300	1.13633400
H	0.45947600	-3.90944700	1.66585000
H	2.82004600	-3.36797600	0.47643800
Hf	0.51788500	-1.20506900	-0.03926200
C	-3.07347800	1.21265400	0.65427900

H	-3.18055300	0.11835100	0.70455700
H	-2.96908500	1.55215200	1.69509400
H	-2.38590500	3.59516200	-0.56233400
C	-4.36421600	1.79103100	0.05309600
H	-4.42350500	1.52542200	-1.01324300
H	-4.34470100	2.88700000	0.09634500
C	-5.62654500	1.29119800	0.77174900
H	-5.66637700	0.19385900	0.71597200
H	-5.55664300	1.54054800	1.83973000
C	-6.91634300	1.88071400	0.19182300
H	-7.03097200	1.62290600	-0.86789900
H	-7.79623000	1.50323700	0.72316000
H	-6.92374400	2.97427200	0.27100200
H	3.45062100	2.73574000	-1.14767000
C	2.70226300	3.28441300	-0.56131400
C	3.40294400	4.30879900	0.34391100
H	2.06590000	3.81161300	-1.28614700
C	1.84189100	2.28514300	0.24622700
C	4.25611800	5.30810600	-0.44400300
H	4.03418500	3.77744600	1.06982800
H	2.64835500	4.85060200	0.93072200
H	2.48353700	1.75416000	0.95903700
H	1.10637500	2.84973800	0.82564700
C	1.18466800	1.29196000	-0.69257200
H	3.64648700	5.87940900	-1.15382200
H	4.74141300	6.02301300	0.22839400
H	5.04293400	4.79893300	-1.01290300
H	0.47608900	1.72211400	-1.39391800
C	1.96094000	0.19050400	-1.19593700
H	2.98847400	0.14278700	-0.84434000
H	1.86778700	-0.00251300	-2.26116600

6b

C	-1.40622600	-1.98198900	2.65467100
H	-0.47659400	-1.76482500	3.19437000
H	-1.30744600	-2.97275600	2.19891300
C	-1.71426500	-0.88747900	1.60741600
H	-1.69962100	0.06650700	2.15012700
C	-0.60903100	-0.85968400	0.53692700
H	-0.80730500	-1.63123100	-0.21053700
H	0.31852300	-1.22153500	1.10546800
H	1.20760600	-3.24497100	-0.57592400
C	1.77864800	-2.43036000	-1.00389600
C	1.40051800	-1.63637200	-2.11317600
C	3.04171400	-1.97365600	-0.54127000
C	2.44782700	-0.70290400	-2.36508500
H	0.49168200	-1.74246400	-2.69241700
C	3.46294300	-0.91663600	-1.40054000
H	3.61090600	-2.39998500	0.27478300
H	2.47833200	0.02107900	-3.16865500
H	4.40337000	-0.38447500	-1.33928400
H	0.27560200	1.54414800	2.41665900
C	1.24410100	1.38508900	1.96224400
C	2.15653800	0.33863400	2.28904700
C	1.85631500	2.20775000	0.98357900
C	3.32389200	0.51643700	1.50788800
H	2.00107900	-0.43488600	3.03137800
C	3.13133500	1.65890200	0.68039600
H	1.44340000	3.11091300	0.55698500
H	4.21085000	-0.10200000	1.54101400
H	3.85378200	2.07472600	-0.01106300
Hf	1.47495600	-0.05033100	-0.11765800
C	-3.13663400	-1.06752500	1.01587900
H	-3.84367400	-0.95913400	1.84911200
H	-3.36348400	-0.24169800	0.32933000
H	-2.21207300	-2.03350100	3.39485700
C	-3.42749600	-2.39615700	0.29922200
H	-3.24657300	-3.23929500	0.97814300
H	-2.74280800	-2.53624400	-0.55132800
C	-4.87168800	-2.47837400	-0.21928400
H	-5.56333900	-2.35092200	0.62453500
H	-5.06242600	-1.63619300	-0.89963400

C	-5.17542200	-3.79738900	-0.93687500
H	-5.02917600	-4.65549200	-0.27005600
H	-6.21119100	-3.82496200	-1.29072700
H	-4.52299100	-3.93716300	-1.80763900
H	-2.05045300	3.21260200	-1.63891000
C	-2.60642100	2.76749800	-0.80367400
C	-3.34373600	3.86818200	-0.02700000
H	-3.34041000	2.08164400	-1.24976600
C	-1.63633100	1.96370700	0.09737700
C	-4.31553000	4.65997900	-0.90833900
H	-2.60857000	4.55260900	0.41857400
H	-3.89144700	3.41585600	0.81122400
H	-0.89979300	2.64863000	0.53050400
H	-2.21253700	1.54184700	0.92253400
C	-0.94633600	0.90467800	-0.73545900
H	-5.08259700	4.00662800	-1.34056500
H	-4.82697000	5.43514600	-0.32853300
H	-3.79207900	5.15347100	-1.73564900
H	-1.62642000	0.20976300	-1.22171300
C	0.21292700	1.29224800	-1.50584700
H	0.47345400	2.34712300	-1.44824000
H	0.24872500	0.90741400	-2.52171000

6c

C	-1.32254300	-2.95995000	-1.43419800
H	-0.29682700	-3.34417100	-1.37906900
H	-1.51531200	-2.67592100	-2.47595400
C	-1.54213800	-1.75799900	-0.48828400
H	-1.38367600	-2.10555300	0.54299800
C	-0.50094800	-0.66452800	-0.81220100
H	-0.80039800	-0.10301300	-1.69912200
H	0.42626100	-1.23881300	-1.17039200
H	2.12996400	-0.37394100	-3.09042600
C	2.36325800	0.34695000	-2.31617600
C	1.57473400	1.47836400	-1.95826200
C	3.52416900	0.34805000	-1.50485900
C	2.26193500	2.18608500	-0.93855300
H	0.64783800	1.77774300	-2.42831600
C	3.45529600	1.47728000	-0.63823200
H	4.32994400	-0.37287200	-1.54788000
H	1.95101500	3.11774300	-0.48730600
H	4.20568200	1.77341400	0.08412300
H	0.89357200	-3.17689900	0.59789900
C	1.55790100	-2.42638700	1.00500900
C	2.87313300	-2.14382100	0.54533100
C	1.27426800	-1.56510000	2.09270800
C	3.41661300	-1.12877700	1.38581400
H	3.39245600	-2.65758700	-0.25364200
C	2.42785900	-0.76673900	2.33494900
H	0.35268400	-1.54029800	2.66050400
H	4.41826900	-0.72366000	1.32659800
H	2.54138100	-0.03021000	3.11987900
C	-2.99714900	-1.24312000	-0.59813700
H	-3.12912700	-0.35684400	0.03346900
H	-3.17669600	-0.91157500	-1.63188300
H	-1.99321200	-3.78597900	-1.18358200
C	-4.07471600	-2.26279300	-0.19491600
H	-3.84245900	-2.66496800	0.80265200
H	-4.06758600	-3.11841700	-0.88141300
C	-5.48503000	-1.65469300	-0.17964100
H	-5.50729100	-0.80604700	0.51910300
H	-5.70976700	-1.23946300	-1.17213800
C	-6.56848100	-2.66572600	0.20882400
H	-6.39022200	-3.07529400	1.21039800
H	-7.55977000	-2.20050000	0.21133300
H	-6.59785900	-3.50675800	-0.49414600
H	-3.20447600	2.14832100	1.21106400
C	-2.50046000	2.80327000	0.67847300
C	-3.28632700	3.83923500	-0.13917600
H	-1.90743500	3.31270700	1.44905000
C	-1.57059700	1.94173400	-0.20751400
C	-4.22284600	4.68697000	0.72795700
H	-3.86892500	3.32327000	-0.91475400

H	-2.58012300	4.49397600	-0.66832800
H	-2.17875600	1.44650400	-0.96901400
H	-0.86101300	2.59615200	-0.72763000
C	-0.81641100	0.94766900	0.65535400
H	-3.66587300	5.24154800	1.49232800
H	-4.76731700	5.41574900	0.11879100
H	-4.96328200	4.06223800	1.24129900
H	-1.43976400	0.22556100	1.17437300
C	0.34495100	1.39825300	1.37560700
H	0.40778000	1.08360400	2.41371900
H	0.60458200	2.44436700	1.23336700
Hf	1.58315100	-0.05193700	0.05740000

6d

C	3.03914900	0.58851000	-1.64226000
H	2.64799800	1.60318700	-1.76044700
H	2.96550900	0.08623000	-2.61498200
C	2.29332300	-0.21697400	-0.56390400
H	2.45666800	0.25138600	0.41580800
C	0.78396900	-0.27002900	-0.85455300
H	0.44909800	-1.23769000	-0.33711700
H	0.63325400	-0.45016200	-1.92268000
H	-2.46317300	-2.45534800	2.21695100
C	-1.90429000	-1.52911600	2.22037200
C	-0.49461600	-1.40770100	2.17318100
C	-2.45806300	-0.21894500	2.28730600
C	-0.16965300	-0.02022600	2.22964400
H	0.21250900	-2.22752800	2.13521400
C	-1.38231400	0.70901600	2.31917300
H	-3.51032100	0.02486200	2.36573800
H	0.82869900	0.39492500	2.24792500
H	-1.47976500	1.78042700	2.42252400
H	-0.91755400	-2.53987000	-2.34575500
C	-1.75509000	-2.00611400	-1.91386300
C	-2.54121600	-2.44980500	-0.81738500
C	-2.25385700	-0.74986300	-2.33624000
C	-3.55835200	-1.47650600	-0.58947800
H	-2.42726900	-3.39056000	-0.29438000
C	-3.37820600	-0.42594300	-1.52257300
H	-1.87343600	-0.15696200	-3.15876800
H	-4.34607600	-1.54134600	0.14982500
H	-4.00215000	0.45303100	-1.61659600
C	2.85239000	-1.66329900	-0.46199700
H	2.25719600	-2.21758000	0.27988400
H	2.70124500	-2.17683900	-1.42280400
H	4.10003100	0.67876500	-1.39497300
C	4.33067100	-1.75877000	-0.05521000
H	4.49495900	-1.17534200	0.86297300
H	4.96552700	-1.30615300	-0.82716600
C	4.78661700	-3.20737500	0.17557300
H	4.16151800	-3.66447200	0.95600800
H	4.61066200	-3.79143300	-0.73860400
C	6.26215500	-3.31264200	0.57422800
H	6.46339600	-2.76767900	1.50433300
H	6.55490700	-4.35620400	0.73026000
H	6.91421400	-2.89686900	-0.20306700
H	1.44820700	3.99508100	-1.36060900
C	0.99417400	4.01630500	-0.35976100
C	1.84330000	4.89896900	0.56709500
H	-0.00271500	4.45961700	-0.48108500
C	0.85783100	2.56923500	0.17278000
C	1.99103100	6.33173500	0.04443000
H	2.83719100	4.44657400	0.68890100
H	1.38831400	4.91704100	1.56720600
H	1.85951000	2.15095700	0.28626300
H	0.40321300	2.59937800	1.16819400
C	-0.01097500	1.76458000	-0.77191900
H	1.01519200	6.82096200	-0.05720400
H	2.59737100	6.93651500	0.72653400
H	2.47749300	6.34863500	-0.93794600
H	0.33439600	1.76490300	-1.80271900
C	-1.44616500	1.83072800	-0.59458100
H	-2.02416800	1.94034800	-1.50861600

H	-1.77998800	2.50237500	0.19371500
Hf	-1.37559100	-0.38580200	0.03037400

6e

C	1.96734400	3.13468900	-0.58158300
H	1.01615300	3.56090900	-0.25064500
H	2.01279600	3.21599100	-1.67489600
C	2.14992100	1.67199400	-0.13728500
H	2.13391900	1.63908800	0.96238300
C	1.02701100	0.77450000	-0.68315800
H	1.47027600	-0.28496700	-0.75108000
H	0.80047000	1.04372700	-1.71837700
H	1.90899300	-3.06239200	0.80815700
C	1.18698700	-2.44150900	1.32344200
C	1.42570400	-1.14214900	1.85445400
C	-0.13995800	-2.81574000	1.67717600
C	0.24324400	-0.70413300	2.49612700
H	2.35538400	-0.59265800	1.78892200
C	-0.72999600	-1.73666300	2.38484100
H	-0.60773700	-3.76741800	1.46488300
H	0.11055500	0.24096500	3.00720600
H	-1.72923600	-1.72077400	2.80184900
H	-1.46406900	0.09534000	-2.81927800
C	-1.29929400	-0.85656100	-2.33105000
C	-0.13137100	-1.65536900	-2.43165400
C	-2.24382800	-1.56108300	-1.53061800
C	-0.33281200	-2.83395500	-1.66705400
H	0.76299800	-1.41145600	-2.99150800
C	-1.64666900	-2.77830100	-1.11794300
H	-3.25465000	-1.24866100	-1.31632500
H	0.36998700	-3.65029400	-1.56024000
H	-2.12472700	-3.54808200	-0.52649000
Hf	-0.33663600	-0.94859400	0.01019600
C	3.52556500	1.11654400	-0.59627800
H	3.58845900	0.05384400	-0.31530000
H	3.57154800	1.14341200	-1.69467200
H	2.75947900	3.76429700	-0.16841000
C	4.75017300	1.83871200	-0.01328900
H	4.65629800	1.89339500	1.08176800
H	4.78501600	2.87489600	-0.37183600
C	6.07135100	1.14387600	-0.37585700
H	6.05006700	0.10852900	-0.00649400
H	6.15576900	1.07660200	-1.46951000
C	7.29984400	1.86422600	0.18910400
H	7.26007500	1.92042800	1.28356800
H	8.22307500	1.34258100	-0.08400500
H	7.37089800	2.88893000	-0.19446200
C	-1.89300900	0.80148700	0.64812800
C	-0.76604900	1.60178400	0.34276600
H	-0.10125500	1.93110400	1.13316800
H	-0.82575700	2.27288400	-0.50891300
H	-2.00998500	0.59318500	1.71131900
C	-3.21974100	1.07621600	-0.05590500
H	-3.06875100	1.18712400	-1.13760500
H	-3.90200700	0.22930800	0.08447000
C	-3.90706300	2.34579800	0.48734800
H	-4.03430900	2.25132700	1.57529700
H	-3.24711800	3.21132100	0.33081000
C	-5.26994300	2.61245100	-0.16565400
H	-5.14028000	2.69852300	-1.25385500
H	-5.92460300	1.74475400	-0.00288900
C	-5.95159500	3.87577400	0.37076600
H	-6.91998800	4.03696300	-0.11415200
H	-6.12766200	3.80426600	1.45065100
H	-5.33720700	4.76620800	0.19144500

6f

C	0.47772400	1.08083800	0.65932200
C	1.11898200	1.05331000	2.06172400
H	2.11610700	1.50087600	1.99293600

H	1.27757500	0.02361900	2.39330900
H	-0.46079300	0.90155500	-2.88260900
C	-1.31850000	0.52949700	-2.33726600
C	-1.90636500	-0.75691200	-2.49173900
C	-2.08637100	1.25112000	-1.38954100
C	-3.02882200	-0.82922300	-1.62965200
H	-1.57707900	-1.53275300	-3.17044500
C	-3.13070300	0.40601300	-0.92815900
H	-1.91906700	2.27259700	-1.07452200
H	-3.71259800	-1.66266600	-1.54857800
H	-3.90468600	0.67740300	-0.22164000
H	0.74691200	-2.23928500	2.11071400
C	-0.29035400	-2.18971500	1.80676500
C	-1.27651000	-1.31775800	2.33666100
C	-0.91820600	-3.03323300	0.85017900
C	-2.50778700	-1.59494500	1.68894800
H	-1.12566200	-0.58530400	3.11682600
C	-2.28498200	-2.66637300	0.77571300
H	-0.44675100	-3.83266800	0.29502400
H	-3.45737600	-1.11821400	1.89484300
H	-3.03558900	-3.15068500	0.16638700
Hf	-1.00731700	-0.68617300	-0.11498300
C	0.34061900	1.80219500	3.16418100
H	-0.70000700	1.46711000	3.23943300
H	0.32043400	2.88105200	3.00056300
H	0.81690100	1.62440600	4.13423300
H	-0.65802300	1.12411300	0.84031300
C	0.83138600	2.34054200	-0.15112200
H	1.92612100	2.38158800	-0.22832100
H	0.46538400	2.23601000	-1.17798700
C	0.33953800	3.70234200	0.38254300
H	-0.72989200	3.64761900	0.63629300
H	0.86289600	3.95796200	1.31025800
C	0.56330300	4.82880500	-0.63923300
H	0.02578400	4.58892800	-1.56816400
H	1.62865100	4.86691000	-0.90541300
C	0.11336100	6.20010000	-0.12568700
H	0.28283500	6.97606100	-0.87918800
H	-0.95527500	6.20314300	0.12059100
H	0.66483500	6.48717300	0.77719400
H	3.66808300	-2.05532900	-1.23081900
C	3.97334000	-1.10475400	-0.77557500
C	5.29153600	-1.29688700	-0.01114400
H	4.13112000	-0.39999300	-1.60402500
C	2.83927200	-0.57758400	0.13687900
C	6.41987000	-1.82021600	-0.90625600
H	5.12868100	-1.99394900	0.82263200
H	5.59281100	-0.34166200	0.44040700
H	2.65797100	-1.30390300	0.93829200
H	3.18150900	0.34916700	0.60383400
C	1.58392100	-0.35842600	-0.67909400
H	6.62790300	-1.12696000	-1.72969900
H	7.34569700	-1.94688900	-0.33571500
H	6.16273200	-2.79193700	-1.34419400
H	1.65724200	0.46775800	-1.37936500
C	0.85829200	-1.50881100	-1.17119800
H	1.20965900	-2.46583400	-0.79140500
H	0.69652600	-1.52212100	-2.24670600

6g

C	-1.19156300	1.07385900	0.71369900
C	-0.97198000	1.68404400	2.11155400
H	-0.75130600	2.74957700	1.97156500
H	-0.07887600	1.25494000	2.57148500
H	-0.73786900	0.54538200	-2.87485300
C	-0.78545000	-0.44454100	-2.43985700
C	0.23221300	-1.43659400	-2.51542000
C	-1.89127200	-1.00400200	-1.75224800
C	-0.24277600	-2.59888400	-1.85986700
H	1.18629000	-1.33846900	-3.01652100
C	-1.55205900	-2.32811900	-1.36802000
H	-2.83722700	-0.51723900	-1.55961800
H	0.28280300	-3.54063200	-1.78572900

H	-2.19957600	-3.02782200	-0.85568300
H	1.70123500	-0.12028600	2.60866500
C	1.25072800	-0.99643100	2.16218600
C	-0.05010700	-1.49216500	2.42196400
C	1.89335800	-1.89513900	1.26409600
C	-0.23159800	-2.68051600	1.66468400
H	-0.78074700	-1.05293500	3.08778600
C	0.98230600	-2.93871900	0.96738500
H	2.91297500	-1.82426700	0.91376300
H	-1.11075200	-3.31200600	1.67274100
H	1.18935800	-3.80181300	0.35022000
Hf	-0.00112000	-0.84503900	-0.05093100
C	-2.13452700	1.55917300	3.11529000
H	-2.49018600	0.52600200	3.20904200
H	-2.99026200	2.18002800	2.84292800
H	-1.79764000	1.88464000	4.10523400
H	-1.66641200	0.03117300	0.85487800
C	-2.15134100	1.89516300	-0.16777800
H	-1.91973300	2.95700300	-0.01364100
H	-1.95693000	1.70101200	-1.22794400
C	-3.66493500	1.68650100	0.06480800
H	-3.90554900	0.61309300	0.03395200
H	-3.95119500	2.02756300	1.06396300
C	-4.51527400	2.42756200	-0.97908800
H	-4.25030400	2.07138000	-1.98518300
H	-4.26043100	3.49598000	-0.95759300
C	-6.02060900	2.25477700	-0.75283400
H	-6.59575900	2.79108700	-1.51445600
H	-6.31308900	1.19869900	-0.79757400
H	-6.32280300	2.64323700	0.22675200
H	4.02409000	1.82245700	-1.77247800
C	3.99313600	1.87493500	-0.67470500
C	5.42548600	1.87617700	-0.12325800
H	3.50202500	2.82730900	-0.42809300
C	3.14104700	0.70879300	-0.13412300
C	6.27163800	3.03380000	-0.66379000
H	5.90974000	0.92100000	-0.37065400
H	5.39151700	1.92696300	0.97432000
H	3.65235000	-0.23160500	-0.37335900
H	3.09814000	0.77612800	0.96017600
C	1.73472100	0.71055300	-0.73223900
H	5.83107500	4.00382800	-0.40415400
H	7.28510400	3.00738700	-0.25012500
H	6.35642200	2.98785800	-1.75601300
H	1.74239800	0.59197700	-1.81462200
C	0.77606800	1.64675800	-0.26965500
H	0.15489000	2.17818300	-0.98133000
H	0.99357700	2.19409900	0.64248000

β-hydrogen TS to metal

Hf/Et

8a

Hf	-0.09305800	0.02662900	-0.07667400
C	1.85203100	1.55855300	-0.44645400
C	1.55616500	1.60112200	0.94529000
C	0.26662000	2.18532500	1.09770900
C	-0.22010600	2.52627500	-0.19695200
C	0.75414000	2.13123200	-1.14992500
C	-1.77834800	-1.31382800	1.20871900
C	-2.28776400	0.00686700	1.07545700
C	-2.56866500	0.23601400	-0.30588700
C	-2.22506000	-0.94099300	-1.02089200
C	-1.72736300	-1.89351400	-0.09117800
H	2.77452200	1.20893700	-0.89060600
H	2.20800500	1.28262800	1.74740600
H	-0.23087100	2.38606500	2.03816100
H	-1.15809300	3.01997700	-0.41440100
H	0.68670700	2.26786700	-2.22357100

H	-1.50893300	-1.80277500	2.13531300
H	-2.48074700	0.69871400	1.88538100
H	-3.01331600	1.12833900	-0.72683000
H	-2.33393700	-1.08971700	-2.08956300
H	-1.41556700	-2.90375000	-0.32420100
C	3.06771000	-1.81480500	0.65530900
H	3.68744200	-2.66048100	0.32503100
H	3.05707200	-1.81886600	1.74768100
H	3.54375900	-0.89883600	0.29627600
H	2.05741400	-1.02735400	-1.79628400
C	1.32314000	-1.56599900	-1.20028200
H	0.59660500	-2.15156900	-1.76263000
C	1.69903600	-2.01673000	0.07003700
H	0.83622900	-0.92363200	1.21789700
H	1.12470500	-2.82995800	0.50980500

Hf/Pro

8a

C	-1.82067600	-0.00054600	-1.30968300
C	-2.52913600	-0.00108500	-0.07997700
H	-1.84720900	-0.91651000	-1.89869200
H	-1.84807500	0.91547600	-1.89853500
C	-3.18260100	1.26707800	0.42271700
H	-1.22712600	-0.00089400	1.08541800
H	-2.65357600	2.17025000	0.11603500
H	-4.18736600	1.30768600	-0.02013000
H	-0.55511000	2.52567000	1.70372000
C	0.18882900	2.27174500	0.96088600
C	1.47078900	1.71113500	1.22258000
C	0.08508900	2.48312700	-0.44275500
C	2.16538100	1.60142400	-0.01543200
H	1.86740500	1.46307700	2.19918000
C	1.30588100	2.06583800	-1.04422300
H	-0.74607700	2.94054800	-0.96191700
H	3.17904500	1.24796100	-0.14784800
H	1.54872400	2.12372700	-2.09945800
Hf	0.22531800	0.00005000	-0.09426700
C	-3.18124100	-1.27014600	0.42227500
H	-2.65080100	-2.17258400	0.11585000
H	-4.18569000	-1.31210300	-0.02116200
H	-3.30036200	-1.26939400	1.50879500
C	1.30954800	-2.06371800	-1.04400700
C	0.08853200	-2.48282200	-0.44417000
C	2.16737000	-1.59902600	-0.01394000
H	1.55368100	-2.12070500	-2.09899300
C	0.19050600	-2.27221500	0.95972200
H	-0.74153900	-2.94087900	-0.96453400
C	1.47152200	-1.71028300	1.22319800
H	3.18075400	-1.24423900	-0.14494900
H	-0.55393800	-2.52747300	1.70159100
H	1.86671400	-1.46231800	2.20039900
H	-3.30112100	1.26610900	1.50930300

8b

C	-2.36083400	-0.57988100	-0.65105200
C	-2.08767400	-0.58154000	0.72694700
H	-0.92952800	-0.07095600	-1.45645500
H	-2.30927500	-1.53812200	-1.16838700
C	-2.06025900	-1.84883000	1.57592600
H	-2.45004400	0.29617300	1.26420700
H	-1.84957400	-2.74473100	0.98633200
H	-1.33668500	-1.80233800	2.39937200
H	-0.26289200	-3.08116300	-0.74137700
C	0.55707200	-2.39999900	-0.55719200
C	1.22019400	-1.61272300	-1.54428600
C	1.19837300	-2.18165300	0.68713400
C	2.26540300	-0.90172700	-0.90006500
H	0.99057900	-1.59437800	-2.60144800
C	2.24522100	-1.24013400	0.48823600

H	0.94001100	-2.65186800	1.62834000
H	2.97771000	-0.24464400	-1.38134900
H	2.94915800	-0.90262800	1.23820500
C	-3.24179300	0.44699200	-1.31795400
H	-4.28085100	0.10813200	-1.20630900
H	-3.03375400	0.54406200	-2.38633200
H	-3.16559300	1.42941300	-0.84446400
C	0.45456500	2.08743100	1.45379000
C	-0.67467600	2.32489000	0.61807900
C	1.60347000	2.00535900	0.62607400
H	0.44334400	2.01501900	2.53574800
C	-0.22184800	2.38652600	-0.72961600
H	-1.68677800	2.49746900	0.95811100
C	1.18563100	2.17338900	-0.72508300
H	2.62064400	1.85500300	0.96366800
H	-0.82867400	2.59667800	-1.59988500
H	1.83008300	2.19005900	-1.59471900
Hf	0.16568600	0.03631700	0.03413600
H	-3.04437400	-1.98462000	2.04330800

Hf/but

8a

C	-1.37951200	-0.45508800	-1.60990100
C	-2.25263800	-0.61442700	-0.50022600
H	-1.11524200	-1.35477500	-2.16479100
H	-1.52784300	0.42650100	-2.23252800
C	-3.25304100	0.48244600	-0.17185700
H	-1.16858300	-0.26500600	0.84981200
C	-3.81456700	0.51915100	1.25249900
H	-2.83549100	1.45546200	-0.44467400
H	-4.08015900	0.30995100	-0.87908200
H	-4.49561100	1.36858400	1.35992000
H	-4.38144000	-0.38437200	1.49532900
H	-3.01513100	0.62759400	1.99434800
H	-1.12770500	2.38536600	1.40113400
C	-0.25539600	2.27472600	0.77148500
C	1.07133900	2.02075100	1.22078700
C	-0.21660100	2.40818000	-0.64470800
C	1.92914000	2.02130300	0.08446100
H	1.38100200	1.90167100	2.25163500
C	1.13240400	2.24843900	-1.06758800
H	-1.05218400	2.64936500	-1.28740500
H	3.00356700	1.89692700	0.09697100
H	1.49339200	2.31886400	-2.08761200
Hf	0.40603600	0.02729500	-0.11972100
C	-2.64283600	-2.00633500	-0.05470200
H	-1.90529400	-2.75999100	-0.33431400
H	-3.58025800	-2.25709700	-0.57082100
H	-2.83446000	-2.06867800	1.01830400
C	2.08640500	-1.72663900	-0.75232500
C	0.89819500	-2.41662000	-0.37583900
C	2.60539900	-1.08665300	0.40293100
H	2.53732700	-1.72374500	-1.73839900
C	0.68047800	-2.19447200	1.01226400
H	0.30795200	-3.05005600	-1.02382200
C	1.72781300	-1.35686700	1.48939500
H	3.51848900	-0.50895900	0.45208300
H	-0.11624500	-2.61340800	1.61144900
H	1.85981900	-1.02681300	2.51234700

8b

C	-1.97561300	-0.56631600	1.19582500
C	-2.03322900	-0.40891700	-0.19943300
H	-0.32797600	-0.41249000	1.65662300
H	-2.22745200	0.30313900	1.80381000
C	-2.74859000	0.75482500	-0.88808400
H	-2.09234400	-1.34382800	-0.76097700
C	-4.20459600	0.38557300	-1.23007400
H	-2.73813500	1.64200400	-0.24655300

H	-2.23900200	1.03530800	-1.82170900
H	-4.69740600	1.21611400	-1.74621700
H	-4.25028400	-0.49144800	-1.88498900
H	-4.77377300	0.16000700	-0.32195700
H	-1.19037600	2.61216000	1.19612200
C	-0.21836000	2.36768100	0.78969700
C	0.90896900	1.92588200	1.54325800
C	0.17678800	2.49276700	-0.56530100
C	1.99613000	1.77113700	0.64479400
H	0.93800700	1.77695500	2.61451400
C	1.54152200	2.10773900	-0.66733600
H	-0.44957500	2.82677800	-1.38371400
H	3.00489700	1.48468100	0.91131700
H	2.14695900	2.13986000	-1.56412800
Hf	0.35356700	0.02780000	-0.00994000
C	-2.16521600	-1.89187500	1.89120300
H	-3.24594900	-2.04611100	2.01365400
H	-1.70933700	-1.91039900	2.88420400
H	-1.78029200	-2.72841900	1.30211200
C	1.15594000	-1.65280200	-1.69760700
C	0.47057500	-2.38560100	-0.68694300
C	2.31483700	-1.07919200	-1.11434500
H	0.86113800	-1.57373800	-2.73821400
C	1.20612300	-2.26207400	0.52502100
H	-0.41790400	-2.98470300	-0.83342900
C	2.33971400	-1.44196100	0.26295900
H	3.05739200	-0.48372200	-1.62940200
H	0.97108400	-2.73823000	1.46728200
H	3.11351200	-1.18667900	0.97555100

Hf/hex

8a

C	-1.52617900	-2.66819300	-0.40830800
H	-0.58488600	-3.21801100	-0.44576200
H	-2.23886100	-3.19186400	-1.06062500
C	-1.39520200	-1.25762800	-0.93939300
H	-0.76999800	-0.53691900	0.53917100
C	-0.35246200	-0.95539600	-1.85825600
H	-0.55929200	-0.19385200	-2.60933600
H	0.24126800	-1.79334800	-2.22278200
H	-0.87241500	2.13408100	-1.86759600
C	-0.16694000	2.16977400	-1.04879600
C	-0.48648600	2.13591200	0.33741100
C	1.24029000	2.33501700	-1.17493700
C	0.72835400	2.27155900	1.06693200
H	-1.47756900	2.06111500	0.76365500
C	1.79185500	2.40952800	0.13033500
H	1.79143200	2.41996000	-2.10481700
H	0.82089400	2.31352000	2.14505000
H	2.83473800	2.56984800	0.36863500
H	1.75415200	-2.96421100	-0.63094400
C	1.99680000	-2.15741100	0.04731300
C	3.03461700	-1.20028400	-0.14339000
C	1.40165600	-1.91493000	1.31612000
C	3.08618900	-0.37488700	1.00982100
H	3.69714600	-1.13993300	-0.99964700
C	2.06476800	-0.80054200	1.90357300
H	0.60989200	-2.49201500	1.77357100
H	3.79072200	0.42678900	1.18539700
H	1.85961800	-0.38437100	2.88211800
Hf	0.87303900	0.07911500	-0.11124300
C	-2.68143000	-0.44829100	-0.97020500
H	-2.46751600	0.57834100	-1.28311500
H	-3.25658900	-0.89173900	-1.79961900
C	-3.55416100	-0.44757000	0.29265600
H	-3.88227400	-1.46868000	0.52356700
H	-2.95284100	-0.11443200	1.15079800
C	-4.79224500	0.45098100	0.15120700
H	-4.47375000	1.47983700	-0.07055400
H	-5.38295100	0.12224000	-0.71477500
C	-5.67362800	0.44534500	1.40416500
H	-5.12207700	0.80201300	2.28247900

H	-6.54573900	1.09376300	1.27329600
H	-6.03966500	-0.56362100	1.62739400
H	-1.92706700	-2.70266300	0.60643000

8b

C	-0.63858100	1.99773900	-0.28363400
C	0.40541600	2.25780900	-1.18505400
H	0.23498000	2.01902800	-2.23508000
H	1.51257200	1.02974700	-1.02893100
H	-0.63595400	-0.15088300	-3.06577300
C	-0.23002500	-0.85453800	-2.35106400
C	1.14899600	-1.19858500	-2.20998100
C	-0.97744600	-1.66093300	-1.45952000
C	1.24295400	-2.20430400	-1.21494200
H	1.96733500	-0.79974500	-2.79417200
C	-0.07257300	-2.47765200	-0.72939000
H	-2.05472900	-1.65831500	-1.35124100
H	2.14987000	-2.70311500	-0.90054800
H	-0.34110900	-3.23301400	-0.00211900
H	3.10285500	1.36813400	1.04517100
C	2.37828200	0.65722100	1.41844000
C	1.18018800	0.96569200	2.12179200
C	2.48560300	-0.76011300	1.34497900
C	0.55666500	-0.26056500	2.49148400
H	0.83903500	1.95521800	2.39264100
C	1.36598400	-1.32491700	2.01894500
H	3.30590200	-1.30732600	0.89959200
H	-0.36018000	-0.36189000	3.06027400
H	1.17456600	-2.38060100	2.16125500
Hf	0.49826400	-0.14943200	-0.02125900
C	1.42402900	3.34900200	-0.94561000
H	1.66066100	3.46040000	0.11650600
H	0.98582400	4.29587900	-1.28739800
H	2.34967300	3.18445900	-1.50309300
H	-0.56218800	2.52380700	0.66820200
C	-2.06848000	1.60608100	-0.63134100
H	-2.69147300	2.50955000	-0.69827200
H	-2.12759100	1.12472000	-1.61409900
C	-2.64819400	0.68491400	0.45861300
H	-1.97547600	-0.19476900	0.61980500
H	-2.64257800	1.21733400	1.41896500
C	-4.05572600	0.15477800	0.16640200
H	-4.05420300	-0.38799200	-0.78950600
H	-4.71631200	1.01990500	0.01776700
C	-4.61536000	-0.74039900	1.27566500
H	-5.62504800	-1.08332300	1.02977200
H	-3.99194200	-1.63113500	1.42606500
H	-4.66988200	-0.20432300	2.23015300

β -hydrogen transfer to monomer TS

Hf/Et

7a

H	1.94735000	2.00500800	1.59505800
C	1.29457000	2.06515900	0.73323600
C	1.66291600	1.79262000	-0.60125700
C	-0.07342800	2.46711400	0.74207800
C	0.52779100	2.01452700	-1.43290500
H	2.64584400	1.48996400	-0.93642100
C	-0.53132300	2.46331100	-0.60130900
H	-0.64339600	2.78383400	1.60553800
H	0.49755600	1.92496600	-2.51093200
H	-1.50873700	2.78027300	-0.93670100
C	3.26739200	-1.58625800	-0.26951600
H	3.48380700	-1.91702300	0.75059700
H	3.61924000	-0.55818500	-0.39042000
H	3.85128300	-2.21834100	-0.94948400
C	-2.52464900	-0.38686200	0.65717200
C	-1.91275400	-1.67336700	0.63527800

C	-2.54855200	0.10114000	-0.67517200
H	-2.95310100	0.10447200	1.52078100
C	-1.53975800	-1.96069700	-0.69576600
H	-1.77616000	-2.32895000	1.48618300
C	-1.91483100	-0.85506800	-1.51122000
H	-3.00386400	1.02502700	-1.00269300
H	-1.06877600	-2.87346900	-1.03841100
H	-1.79787800	-0.78193500	-2.58447600
Hf	-0.12458600	0.05259600	0.01989400
H	1.25645100	-1.21303700	0.68161200
C	1.80146800	-1.73742700	-0.63630900
H	1.39231000	-2.72715100	-0.42356900
C	1.23531500	-1.05773900	-1.73786800
H	1.84617200	-0.32829800	-2.25860900
H	0.52531400	-1.58172100	-2.36532400
H	0.83752900	-2.08681200	2.29565000
C	1.01166600	-1.01694200	2.18792900
H	2.04873600	-0.71628200	2.32731900
C	-0.00966600	-0.11758900	2.52695900
H	-0.96171700	-0.50262500	2.86959400
H	0.25526700	0.86182000	2.90436000

Hf/Pro

7a

C	0.96039000	-0.67362200	-1.98262500
C	2.11369800	-0.62118800	-1.16144300
H	0.84293700	0.08298500	-2.75000200
H	0.60132200	-1.65405800	-2.27434000
C	2.77315900	-1.92525900	-0.73426700
H	1.61006400	-0.26692900	0.32208000
H	3.43712100	-1.79775200	0.12579000
H	2.04694200	-2.70832500	-0.50592100
H	-1.89245200	-1.78657600	-2.16280000
C	-1.81266700	-1.74424200	-1.08462000
C	-0.90008200	-2.48562400	-0.27745100
C	-2.65290400	-1.00695300	-0.21584400
C	-1.15741300	-2.17868800	1.07340900
H	-0.16143100	-3.18892300	-0.63764100
C	-2.22736500	-1.23793600	1.11933300
H	-3.48147600	-0.38192000	-0.51950000
H	-0.64132300	-2.60078800	1.92655200
H	-2.68301300	-0.82924800	2.01189200
C	3.09188800	0.52629400	-1.36825000
H	2.59499300	1.47156900	-1.59125500
H	3.71127900	0.26668600	-2.23706200
H	3.76544000	0.67278700	-0.52239000
C	-1.47306000	1.80701400	-1.38231900
C	-0.09944000	2.14535300	-1.41811800
C	-1.93130100	1.99801000	-0.04460300
H	-2.07889900	1.51363100	-2.23024000
C	0.31260900	2.48752200	-0.10406500
H	0.51964800	2.16371900	-2.30304200
C	-0.83594700	2.42396300	0.73784700
H	-2.94709800	1.87827500	0.30713500
H	1.29714900	2.83110500	0.18585200
H	-0.88152300	2.70010500	1.78091200
H	-0.35244900	-0.53728700	2.88835800
C	0.31225500	0.17563900	2.41903600
C	1.56484600	-0.25429500	1.95592500
H	0.23990100	1.18756900	2.80040800
C	2.80020000	0.60096900	2.15011500
H	1.74878900	-1.32950800	1.96408700
H	3.65770300	0.25417600	1.57082600
H	2.61271100	1.65284000	1.91792400
Hf	-0.34810600	0.02667400	0.00278800
H	3.07537300	0.54189300	3.21092600
H	3.38871200	-2.27833600	-1.57165100

7b

C	2.21487400	-0.62648300	0.81776900
C	1.21516400	-1.26705200	1.58477600
H	1.66612000	0.16963600	-0.38479700
H	2.65264800	0.26707300	1.26986100
C	1.05980100	-1.03429800	3.07482700
H	1.03624300	-2.30326900	1.30859200
H	1.22954700	0.00160600	3.37750100
H	0.08007900	-1.35038400	3.44432600
H	0.86739300	1.87301000	2.33691300
C	-0.04151800	1.79104200	1.75685700
C	-0.33208700	2.51656400	0.58228900
C	-1.17158700	0.97971200	2.06654400
C	-1.63874200	2.16002500	0.14749500
H	0.31896100	3.23778100	0.10798000
C	-2.16520700	1.23622500	1.08561700
H	-1.28767200	0.34677100	2.93407000
H	-2.15856900	2.56209800	-0.71220500
H	-3.16507900	0.82663500	1.07560700
C	3.19367800	-1.43469000	-0.02117800
H	3.93921100	-1.86601400	0.65820900
H	3.73256900	-0.83034800	-0.75579000
H	2.70481600	-2.26365800	-0.53985400
C	-1.31922000	-2.28118100	0.07677400
C	-0.30915100	-2.40694000	-0.92313900
C	-2.32455300	-1.42518100	-0.43596900
H	-1.35043500	-2.80036100	1.02546800
C	-0.68462800	-1.61773700	-2.02944100
H	0.56952100	-3.03515800	-0.86405500
C	-1.91902800	-0.97889300	-1.72308000
H	-3.25539100	-1.18113700	0.05540700
H	-0.13009300	-1.52451900	-2.95441500
H	-2.48181900	-0.32706900	-2.37869600
Hf	-0.28057500	0.02470300	-0.07958600
H	-0.16100000	0.74880900	-2.94708900
C	0.32841100	1.27780300	-2.13926100
C	1.63658400	0.90285400	-1.76877900
H	0.04971400	2.32231700	-2.05251700
C	2.69176700	1.93498700	-1.41419900
H	2.03123600	0.00779500	-2.25262300
H	2.27379000	2.77464700	-0.85378200
H	3.52637900	1.51711500	-0.84434500
H	3.09946400	2.33431700	-2.35113500
H	1.80645100	-1.64686000	3.60011500

Hf/But

7a

C	-0.58763700	-1.88501500	1.05610800
C	-1.79177300	-1.17940000	0.80026200
H	-0.25205100	-1.97633100	2.08346000
H	-0.39131300	-2.76533800	0.45420700
C	-2.72329200	-1.68917600	-0.30385200
H	-1.38351500	0.14341400	-0.00894600
C	-3.55883900	-2.89727200	0.16162400
H	-3.40087700	-0.88904300	-0.62356000
H	-2.13561300	-1.97984800	-1.18009900
H	-4.17101400	-3.26051700	-0.66969700
H	-2.91924600	-3.72028600	0.49674300
H	-4.23639700	-2.63505200	0.97974400
H	1.98373800	-2.91785600	-0.26574300
C	1.80648900	-2.07111300	-0.91554400
C	0.68761500	-1.89166600	-1.78141600
C	2.68686500	-0.98193600	-1.12043700
C	0.86624900	-0.68520800	-2.48750300
H	-0.13728000	-2.58042400	-1.90287600
C	2.09265500	-0.09813700	-2.06034200
H	3.65051500	-0.85355300	-0.64721400
H	0.19410600	-0.28523800	-3.23610800
H	2.52998800	0.81713300	-2.43784300
C	-2.50080100	-0.52187200	1.97748100
H	-1.81498600	-0.00323800	2.64829400
H	-2.98514000	-1.31590000	2.55872700
H	-3.27911400	0.17692300	1.66540600

C	2.16769500	0.02415200	1.99085600
C	0.89909700	0.36837700	2.51726400
C	2.58942200	1.09285600	1.14612400
H	2.73837600	-0.86314500	2.23378300
C	0.50378400	1.61004600	1.95835300
H	0.33979000	-0.21077700	3.23753600
C	1.56901200	2.06818000	1.12794000
H	3.53958000	1.16801800	0.63543400
H	-0.40315000	2.15360800	2.18951500
H	1.61836800	3.01585000	0.61203200
H	0.24504000	1.81945300	-2.26980700
C	-0.23038600	1.94814700	-1.30624900
C	-1.49125400	1.37725800	-1.07460300
H	-0.01092000	2.88873400	-0.81300400
C	-2.57480200	2.14951600	-0.33907600
H	-1.86365300	0.68851800	-1.83519800
C	-3.19443000	3.20340800	-1.27720200
H	-3.36355400	1.47852900	0.01128700
H	-2.14968600	2.64389600	0.54173000
H	-3.98987800	3.74423100	-0.75486400
H	-2.44664300	3.93015000	-1.60925700
H	-3.63402100	2.73777900	-2.16623200
Hf	0.62270200	-0.01106300	-0.00480800

7b

C	0.31383700	2.19398500	-0.35423300
C	1.58042900	1.56554100	-0.31657100
H	-0.87700200	1.21864700	-0.27217900
H	0.01483300	2.69521000	0.56993700
C	2.63174400	1.92566900	0.72235800
H	2.02112100	1.38649600	-1.29499300
C	3.36446400	3.22254600	0.32432400
H	2.18515100	2.06067400	1.71235900
H	3.37111000	1.12144900	0.80813300
H	4.14727700	3.45507400	1.05415900
H	3.84098300	3.12711300	-0.65780800
H	2.67606700	4.07415500	0.28460200
H	0.44454200	1.21145900	2.73648800
C	0.37160800	0.17173000	2.44784500
C	-0.81580100	-0.58987000	2.41650300
C	1.45438300	-0.68445400	2.09141900
C	-0.48674200	-1.91712600	2.02643200
H	-1.80432100	-0.22811500	2.66254600
C	0.92110400	-1.97792400	1.85908200
H	2.50145800	-0.42045900	2.07693700
H	-1.17754300	-2.74447800	1.92942900
H	1.49463300	-2.86563700	1.63456600
C	-0.18709400	2.88067100	-1.61645700
H	0.34198200	3.83678400	-1.71084600
H	-1.25781900	3.10072600	-1.58927600
H	0.02780700	2.29681200	-2.51542100
C	1.81016200	-1.27468100	-1.66890200
C	0.83836800	-0.59539300	-2.46115800
C	1.20046300	-2.44871500	-1.15953100
H	2.84597600	-0.98956200	-1.54128500
C	-0.36402800	-1.32880500	-2.41023500
H	1.00397200	0.30563700	-3.03592700
C	-0.15495100	-2.46816000	-1.58158200
H	1.69223500	-3.21434900	-0.57695800
H	-1.28128500	-1.07458400	-2.92601800
H	-0.87604200	-3.24652400	-1.36866200
H	-2.56888100	-1.39316700	-1.02314400
C	-2.40359600	-0.72017500	-0.19146500
C	-2.33320200	0.66669800	-0.43620100
H	-2.82930800	-1.05664800	0.74777600
C	-2.99351100	1.68314600	0.48692600
H	-2.33033700	0.96287800	-1.48756700
C	-4.48955000	1.81583600	0.14795800
H	-2.87910900	1.37145900	1.53047300
H	-2.51482200	2.66465200	0.39371500
H	-4.95736400	2.55596800	0.80470200
H	-4.63693600	2.14530100	-0.88655100
H	-5.01294700	0.86345200	0.27843900

Hf	0.06730600	-0.49921600	-0.00412100
----	------------	-------------	-------------

Hf/hex

7a

C	-4.31631700	3.63367100	-0.73641000
H	-4.90713400	3.57997800	0.18565100
H	-4.72050500	4.45087500	-1.34239800
H	-4.47592000	2.69975500	-1.28957600
C	-2.83109900	3.85467700	-0.43285100
H	-2.27235000	3.94511000	-1.37537000
H	-2.70250500	4.81204700	0.09047000
C	-2.22076400	2.72792800	0.41385900
H	-2.78497700	2.64190900	1.35129200
H	-2.33887000	1.76994700	-0.10980100
C	-0.73489900	2.96523300	0.71343400
H	-0.19140400	3.15773900	-0.21709400
H	-0.64272700	3.89234400	1.30386400
C	0.00918100	1.92645400	1.53430500
H	-0.42539600	0.46677200	0.28509500
C	1.40302300	1.87770200	1.48914800
H	1.94412300	1.54511200	2.36797900
H	1.91472300	2.63486500	0.90533600
H	-0.29631700	-1.70527700	2.34244100
C	0.67048700	-1.75594100	1.86158700
C	1.01329800	-2.58991300	0.76207200
C	1.85527500	-1.08917000	2.27599000
C	2.38423600	-2.40339700	0.46839800
H	0.34742500	-3.27500300	0.25950200
C	2.90788600	-1.46354100	1.40487000
H	1.95100900	-0.43919200	3.13317200
H	2.94319400	-2.91324400	-0.30538800
H	3.93742700	-1.13604000	1.47386700
H	1.62105200	2.75428700	-1.42872000
C	2.00986800	1.75661900	-1.57857900
C	3.19538600	1.21969600	-0.99071500
C	1.44326000	0.77147600	-2.40867200
C	3.37609800	-0.08705300	-1.50387700
H	3.87182800	1.74136400	-0.32608400
C	2.27621000	-0.38968500	-2.34712900
H	0.54814700	0.89162500	-3.00490200
H	4.20389200	-0.74676400	-1.28048400
H	2.14615100	-1.30437100	-2.90958600
C	-0.73646400	1.35299800	2.71409600
H	-0.12954700	0.65737500	3.29499800
H	-1.66957800	0.86473100	2.42632000
H	-1.00099100	2.19224500	3.37319700
H	-3.78604400	-2.59672800	-1.52271800
C	-3.84735700	-1.90520000	-0.67217100
C	-4.78757500	-2.47913100	0.39701600
H	-4.26719000	-0.96822100	-1.06436500
C	-2.42322200	-1.64108900	-0.12831800
C	-6.19773700	-2.75002800	-0.13725800
H	-4.84201300	-1.77999900	1.24345200
H	-4.35943600	-3.41011500	0.79406100
H	-2.49399100	-0.95857000	0.72743900
H	-1.99516100	-2.58290700	0.23597800
C	-1.54922600	-1.04075800	-1.19253300
H	-6.17882800	-3.47363800	-0.96061600
H	-6.84357900	-3.15652600	0.64797800
H	-6.66520200	-1.83128700	-0.51095200
H	-1.83503800	-0.04495900	-1.52764500
C	-0.59344500	-1.69649500	-1.89309800
H	-0.36242800	-2.73977100	-1.70148800
H	-0.19290800	-1.28204300	-2.80913500
Hf	1.29325600	-0.18227400	-0.03937200

7b

C	1.30494200	1.37875200	-0.97784800
C	-0.05452600	1.75481900	-1.07489000

H	-0.40405800	2.45410600	-0.31123900
H	-1.06285000	0.67334100	-0.62428400
H	2.60292100	0.37071100	1.82858600
C	1.61517700	-0.02805900	2.00217100
C	0.41382700	0.72204400	2.16126600
C	1.30019600	-1.39507500	2.21540100
C	-0.62977900	-0.18201000	2.45251100
H	0.31852800	1.79839600	2.10785600
C	-0.09312000	-1.49879000	2.46127700
H	2.00740100	-2.21204900	2.22628800
H	-1.65861700	0.08470800	2.64918400
H	-0.63822000	-2.40986100	2.67086000
H	-1.14446300	-2.37321600	-2.42397500
C	-0.17960400	-2.30308200	-1.93827600
C	0.86764700	-1.43696200	-2.31263300
C	0.25935900	-3.07793700	-0.82740600
C	1.97404700	-1.67218200	-1.44407100
H	0.84947100	-0.74537200	-3.14413500
C	1.60335200	-2.70928100	-0.55201100
H	-0.30323500	-3.85463800	-0.32603600
H	2.94283800	-1.19449400	-1.49742000
H	2.24459200	-3.16311600	0.18994300
Hf	0.17166400	-0.71329900	0.06091700
C	-0.70868400	1.95331300	-2.43460200
H	-0.42295500	1.17335900	-3.14570300
H	-0.35727900	2.91096000	-2.83836000
H	-1.79984400	2.00063800	-2.38465300
H	1.71960700	0.98107900	-1.90227100
C	2.32613300	2.20874200	-0.20565500
H	2.30517700	3.21891600	-0.64552500
H	2.04468000	2.35101800	0.84257200
C	3.76846200	1.69135500	-0.31176700
H	3.84222400	0.67213800	0.09459600
H	4.03929300	1.61142500	-1.37472200
C	4.78383500	2.59749500	0.39896600
H	4.52381300	2.66953300	1.46485900
H	4.69943700	3.61628600	-0.00342400
C	6.22840500	2.10828000	0.25490800
H	6.92380600	2.77669600	0.77270600
H	6.35518400	1.10451300	0.67883500
H	6.52999000	2.06590500	-0.79842100
H	-2.57234400	-1.44838500	1.15841600
C	-2.22862200	-1.35102900	0.13425100
C	-2.39534500	-0.10712100	-0.51394900
H	-2.30160100	-2.26015300	-0.44958500
C	-3.20218400	1.02271700	0.11098100
H	-2.46798100	-0.15125700	-1.60294100
H	-2.90366700	1.99429200	-0.30096100
H	-3.01689400	1.06497800	1.19016200
C	-4.71022700	0.81306400	-0.14336500
H	-5.01928000	-0.14884700	0.28639400
H	-4.88994800	0.74074700	-1.22537400
C	-5.56881700	1.94327800	0.44246700
H	-5.38272500	2.01698200	1.52299700
H	-5.25150800	2.90204000	0.00931300
C	-7.06631700	1.73660400	0.19176600
H	-7.65216300	2.55597200	0.62074700
H	-7.28799500	1.69448400	-0.88116700
H	-7.42006600	0.80208100	0.64290400

H₂ π-complex

Hf/Et

9a

H	-1.43825000	-2.87943600	-0.19744000
C	-1.73505600	-1.86780300	0.04537000
C	-1.63246900	-1.24250300	1.32697800
C	-2.35761800	-0.95264800	-0.83657300
C	-2.18924900	0.05921700	1.22337200
H	-1.25457900	-1.70299300	2.23167100
C	-2.61392000	0.25340500	-0.12177200
H	-2.59941000	-1.13719000	-1.87617200
H	-2.29100200	0.77286200	2.03037800

H	-3.11389500	1.13051600	-0.51320200
C	1.84668700	1.57011600	-0.50283900
C	1.72198200	1.37891000	0.90089000
C	0.70523400	2.30505400	-0.94199600
H	2.68992300	1.28219300	-1.11598000
C	0.49250800	1.95562900	1.32174000
H	2.44741900	0.89871200	1.54525700
C	-0.13275500	2.53518900	0.18009100
H	0.52795300	2.65811800	-1.95054700
H	0.12904400	2.00019700	2.34035100
H	-1.06538900	3.08464100	0.17491700
Hf	-0.11674000	0.04874100	-0.18110700
C	3.04590400	-1.92247900	0.65737500
H	3.53994800	-0.99376900	0.35509800
H	3.54031600	-2.74580100	0.13284000
H	1.07250000	-2.85168200	0.58527800
C	1.55811600	-1.91839300	0.28548400
H	1.07655000	-1.18164800	1.05168800
C	1.22369800	-1.55330800	-1.14042300
H	2.09072700	-1.20692200	-1.70509500
H	0.72233300	-2.35189300	-1.68759200
H	0.02127500	-0.21122300	-2.23668500
H	-0.48398000	0.38760600	-2.24371400
H	3.19546900	-2.06395600	1.73247600

Hf/Pro

9a

C	-3.20631500	-1.26731000	0.43976600
H	-2.66859200	-2.18596800	0.19358700
H	-4.12887900	-1.25763100	-0.15013900
H	-0.76187900	-2.37246200	1.69894400
C	0.06217700	-2.18968200	1.02127400
C	0.08757800	-2.49273200	-0.37089700
C	1.32426200	-1.64530900	1.37911200
C	1.38240000	-2.16242300	-0.86156100
H	-0.70208900	-2.96336500	-0.94010900
C	2.14117800	-1.62592500	0.21248200
H	1.62777400	-1.34656700	2.37411100
H	1.73709600	-2.32017300	-1.87274500
H	3.17424200	-1.30808200	0.16264900
C	0.05231700	2.19580500	1.01103500
C	0.09188800	2.49223800	-0.38189200
C	1.30978000	1.65079700	1.38416200
H	-0.77836500	2.38222700	1.67949300
C	1.39161400	2.15798800	-0.85799800
H	-0.69148600	2.96126600	-0.96112400
C	2.13873000	1.62594000	0.22617200
H	1.60273900	1.35651500	2.38365700
H	1.75710200	2.31162200	-1.86596800
H	3.17172200	1.30624800	0.18845600
H	-3.48343000	1.30227600	1.49395000
C	-3.20858200	1.26468300	0.43442200
C	-2.39782300	-0.00117300	0.10663700
H	-2.67421100	2.18328800	0.18065200
C	-1.77967500	-0.00298900	-1.27392200
H	-1.55129300	0.00082000	0.92422800
H	-2.02236000	-0.89553900	-1.85276100
H	-2.02462800	0.88713000	-1.85556300
H	0.85846900	0.00179900	-2.21612100
H	0.07479700	0.00018300	-2.25068100
H	-3.48388600	-1.29880600	1.49876600
Hf	0.26059400	0.00009600	-0.18712900
H	-4.13281000	1.24889100	-0.15278100

9b

C	2.24377700	-0.02840200	0.80672100
C	2.04469800	-0.20357400	-0.68437100
H	1.24894200	0.17732200	1.37664800
H	2.54900000	-0.97162500	1.27011000

C	2.69321400	-1.45038400	-1.29339900
H	2.39105300	0.68703900	-1.21606200
H	2.35854600	-2.37620300	-0.81350700
H	2.47277400	-1.53623800	-2.36364800
H	0.88462400	-2.74461900	1.19366700
C	-0.05926000	-2.34906000	0.84258100
C	-0.99611900	-1.60520400	1.62368700
C	-0.58336700	-2.49248200	-0.45936100
C	-2.11951900	-1.32682200	0.79885000
H	-0.90476600	-1.37451800	2.67810400
C	-1.85641200	-1.84101800	-0.49892600
H	-0.11022200	-3.01066700	-1.28386900
H	-3.01980100	-0.81128400	1.10584600
H	-2.53354900	-1.81855700	-1.34417500
C	3.16225700	1.11995400	1.24518600
H	4.18202000	0.90820100	0.90865400
H	3.18000300	1.23247800	2.33398700
H	2.85840900	2.07313500	0.80166600
C	-1.00027800	2.07193400	-1.32990900
C	0.15556800	2.43581600	-0.58315400
C	-2.02340200	1.70666500	-0.41497900
H	-1.09286800	2.09622700	-2.40874500
C	-0.17060700	2.32856300	0.79977000
H	1.08511600	2.80523900	-0.99429400
C	-1.51041200	1.86892100	0.90434600
H	-3.02864100	1.40130000	-0.67594100
H	0.47648100	2.58581900	1.62899000
H	-2.05655400	1.71108900	1.82559500
H	-0.30933500	-0.29030600	-2.20875700
H	0.45920000	-0.32913200	-2.04109300
H	3.78654500	-1.41067600	-1.19644700
Hf	-0.20497000	-0.00574300	-0.12665200

Hf/But

9a

C	-2.59154700	-1.97172900	0.52339300
H	-1.83535000	-2.72358500	0.28838600
H	-3.48192300	-2.21571000	-0.06252700
H	0.05361600	-2.48365300	1.72788400
C	0.79065100	-2.12870000	1.01923100
C	0.82928500	-2.42626400	-0.37426700
C	1.91723300	-1.32246400	1.33075000
C	2.00124100	-1.82458000	-0.91226300
H	0.14143100	-3.06107300	-0.91533600
C	2.66494000	-1.13052400	0.13384800
H	2.18557200	-0.95996100	2.31440500
H	2.34227200	-1.90504700	-1.93714300
H	3.60079700	-0.59457800	0.04533400
C	-0.17561600	2.12898400	1.05353700
C	-0.25849900	2.44037200	-0.33476500
C	1.18473400	1.87070600	1.36878400
H	-0.99832400	2.12351800	1.75677500
C	1.06159900	2.40315400	-0.86557800
H	-1.14864600	2.73098900	-0.87522600
C	1.95061500	2.03787600	0.17952700
H	1.57559300	1.63860500	2.35092000
H	1.34265700	2.63986300	-1.88446900
H	3.02606800	1.95298400	0.09648500
H	-3.33005000	0.49320700	1.65074700
C	-3.18451200	0.52123900	0.56295600
C	-2.12942600	-0.54698900	0.17213400
C	-4.53950100	0.34430900	-0.13607700
H	-2.79469200	1.51558600	0.32359100
C	-1.57047500	-0.40231600	-1.22428400
H	-1.27360700	-0.34352700	0.95958100
H	-5.19462000	1.18393400	0.11675200
H	-4.43385000	0.32038900	-1.22611600
H	-5.04921000	-0.57146600	0.17687100
H	-1.62873700	-1.31867800	-1.81362100
H	-2.01219000	0.42193100	-1.78665400
H	0.97011000	0.17536100	-2.23327400
H	0.20376800	0.00221800	-2.24034300

H	-2.84953100	-2.05823700	1.58453800
Hf	0.45672900	0.04275700	-0.18609900

9b

C	-1.86253100	-0.56491100	1.09004300
C	-1.89926800	-0.32065800	-0.40268900
H	-0.78424300	-0.49351400	1.53279000
H	-2.34618400	0.25522000	1.63071600
C	-2.90577800	0.73395800	-0.89154300
H	-2.07059900	-1.26184300	-0.93439500
C	-4.36989100	0.28916500	-0.74608700
H	-2.76316300	1.67823200	-0.34989700
H	-2.71345600	0.96121200	-1.94925900
H	-5.04850800	1.05678400	-1.13337000
H	-4.55922000	-0.63612100	-1.30230900
H	-4.63653100	0.11209700	0.30246300
H	-1.16744900	2.39865500	1.46773800
C	-0.21098100	2.26313100	0.98047200
C	0.97941800	1.77181200	1.59895700
C	0.07788600	2.55199500	-0.36992600
C	2.01368700	1.79926300	0.62445900
H	1.09278500	1.51047200	2.64402000
C	1.45648400	2.24796400	-0.60267600
H	-0.61798400	2.94314000	-1.10117600
H	3.04731700	1.52516900	0.78900100
H	1.99660700	2.41081100	-1.52746100
C	-2.36835900	-1.92541100	1.58837700
H	-3.44537300	-1.99304200	1.40809800
H	-2.19311000	-2.05530200	2.66134000
H	-1.89195300	-2.75406900	1.05554400
C	1.52328000	-1.73206400	-1.49756900
C	0.58975900	-2.39224200	-0.64939800
C	2.52439500	-1.14179700	-0.68156100
H	1.49134800	-1.70845800	-2.57991800
C	1.03933600	-2.23663000	0.69360400
H	-0.26122700	-2.97403800	-0.97620800
C	2.22620700	-1.45654300	0.67549600
H	3.38450300	-0.58697600	-1.03405000
H	0.57808200	-2.66599500	1.57397800
H	2.82126600	-1.18649900	1.53874900
H	0.15753400	0.38257000	-2.17759700
H	-0.56970700	0.22501900	-1.92157800
Hf	0.38357500	0.04908700	-0.11218000

Hf/Hex

9a

C	-1.71088600	-2.39488900	0.57344100
H	-0.84448800	-3.01457900	0.33341800
H	-2.55484500	-2.78359000	-0.00252700
H	1.00311400	-2.47011100	1.73095200
C	1.65970300	-2.00499500	1.00714100
C	1.71772400	-2.29806600	-0.38703600
C	2.64857900	-1.02759300	1.29501400
C	2.76812800	-1.51936900	-0.94859100
H	1.12908000	-3.03594700	-0.91416300
C	3.33181500	-0.72277200	0.08302400
H	2.87385400	-0.62166400	2.27258000
H	3.09697200	-1.54764000	-1.98020400
H	4.16700400	-0.04338300	-0.02493300
C	0.01369900	2.04397000	1.05540100
C	-0.13268800	2.33120800	-0.33235800
C	1.40124200	2.00828500	1.35608100
H	-0.79084300	1.90755800	1.76641100
C	1.17082300	2.50457600	-0.87807400
H	-1.06389800	2.47141100	-0.86360400
C	2.11783900	2.29251300	0.15853200
H	1.83433900	1.84582500	2.33445400
H	1.39943300	2.78036500	-1.90022600
H	3.19227800	2.38051700	0.06460800

H	-2.81940100	-0.07315600	1.71460800
C	-2.70121500	-0.03110500	0.62324000
C	-1.49354500	-0.91428700	0.21474700
C	-4.02983300	-0.42626700	-0.04382300
H	-2.48568500	1.01312900	0.37085900
C	-0.98751500	-0.68289900	-1.18985600
H	-0.66852800	-0.57203800	0.98895200
H	-3.89947000	-0.47252400	-1.13397900
H	-4.32784000	-1.43220000	0.27657900
H	-0.90918000	-1.59695800	-1.78062400
H	-1.56518900	0.05984400	-1.74219700
H	1.41258500	0.29526000	-2.24280300
H	0.68425400	0.00183300	-2.23852500
H	-1.94097600	-2.51796100	1.63741900
Hf	0.95953100	0.08073100	-0.18955900
C	-5.16262600	0.55596700	0.29156900
H	-5.28125500	0.61402000	1.38242400
H	-4.87940700	1.56507300	-0.04026200
C	-6.49761000	0.16152600	-0.34849400
H	-6.82621200	-0.82672500	-0.00570000
H	-7.28346300	0.87981300	-0.09322100
H	-6.42028900	0.12640100	-1.44177900

9b

C	-1.78087700	0.52915600	0.30221100
C	-1.10564900	1.14713700	-0.90233600
H	-1.08195100	-0.19468200	0.89589500
H	-1.97138900	1.28568200	1.07162000
C	-1.18879700	2.67829700	-1.01063500
H	-1.49161700	0.69767500	-1.82295500
C	-2.60835800	3.19235500	-1.29912400
H	-0.81948000	3.14606100	-0.08883800
H	-0.52253400	3.02499900	-1.81270900
H	-2.61203500	4.28292800	-1.40132000
H	-3.00118800	2.76797700	-2.23028100
H	-3.30466100	2.93503100	-0.49217500
H	0.04927700	2.20981900	2.09118400
C	0.92300000	1.67099600	1.74939900
C	1.37849400	0.41408400	2.25220900
C	1.81330000	2.09316700	0.73982400
C	2.58060700	0.08660700	1.56844100
H	0.93439200	-0.14497200	3.06673700
C	2.83731400	1.10252000	0.60929700
H	1.74104900	3.00998800	0.16883300
H	3.19460800	-0.78591800	1.74793500
H	3.69832700	1.16029400	-0.04548700
C	-3.03868100	-0.32159500	0.05131800
H	-3.79406500	0.34530600	-0.38315300
H	-2.82492100	-1.07633300	-0.71701000
C	1.32658900	-1.66811200	-1.96680900
C	-0.05721000	-1.83459400	-1.67700200
C	2.07008400	-2.05981900	-0.82220900
H	1.74210600	-1.32826300	-2.90747800
C	-0.16304100	-2.36393000	-0.35862100
H	-0.87415200	-1.66257800	-2.36450300
C	1.14779400	-2.49324500	0.17317100
H	3.14932800	-2.06418400	-0.73799700
H	-1.07889500	-2.65204400	0.14132400
H	1.40091600	-2.89026200	1.14805100
H	1.52992100	0.92465400	-1.82142500
H	0.78187100	1.16960000	-1.78386800
Hf	0.74315100	-0.03602500	-0.12435500
C	-3.60289000	-0.99144400	1.31048200
H	-2.84030800	-1.65179800	1.75188000
H	-3.81111300	-0.22178400	2.06635900
C	-4.87782800	-1.79570900	1.03409300
H	-4.69624400	-2.59703700	0.30783700
H	-5.25697300	-2.25712900	1.95127200
H	-5.67021400	-1.15449900	0.63156400

Hydrogenolysis TS

Hf/Et**10a**

Hf	-0.12931500	0.05187300	-0.16323600
C	1.81375100	1.60459000	-0.40453400
C	1.55170200	1.51744000	0.99296400
C	0.27234700	2.08089400	1.23807100
C	-0.25377500	2.53510700	-0.00749100
C	0.70482800	2.25624200	-1.01821000
C	-1.56898400	-1.48771900	1.19141700
C	-2.13678400	-0.19348200	1.31119200
C	-2.61303400	0.19925600	0.02565400
C	-2.35373600	-0.86279000	-0.88264000
C	-1.68450000	-1.89752300	-0.16973400
H	2.72536500	1.30368100	-0.90372200
H	2.22204800	1.11717100	1.74366300
H	-0.19757200	2.19178000	2.20664000
H	-1.19472500	3.05036900	-0.15079700
H	0.61936200	2.51632200	-2.06521200
H	-1.15096800	-2.07364000	2.00085700
H	-2.22628500	0.37922300	2.22526200
H	-3.13320400	1.11954000	-0.20687800
H	-2.63316400	-0.88693200	-1.92789100
H	-1.38900100	-2.85675700	-0.57436800
C	3.13486000	-1.76944200	0.71094800
H	3.69213100	-2.55638700	0.19413800
H	3.25389400	-1.91881200	1.78851600
H	3.58337800	-0.80811400	0.44169400
H	2.25829800	-1.15872500	-1.68611200
C	1.37914200	-1.54089900	-1.16490800
H	0.98175200	-2.40406900	-1.69920800
C	1.65850900	-1.83765000	0.29710100
H	1.13256900	-1.11771900	1.03543700
H	1.20992200	-2.79140600	0.58798800
H	-0.26424400	0.10214100	-2.07712000
H	0.39518200	-0.56663000	-1.89888900

Hf/Pro**10a**

C	-3.20576300	-1.26980600	0.46913500
H	-2.66829000	-2.18670500	0.21568800
H	-4.14200100	-1.26533200	-0.09866500
H	-0.70320000	-2.40003700	1.71933900
C	0.09974700	-2.20653000	1.01929400
C	0.08243900	-2.48322600	-0.37782100
C	1.36842500	-1.66165600	1.34560600
C	1.35898500	-2.13743500	-0.90848500
H	-0.72378200	-2.94715600	-0.93001100
C	2.14749700	-1.61702600	0.15177900
H	1.70217200	-1.37795400	2.33540200
H	1.68019400	-2.27374400	-1.93287800
H	3.17733400	-1.29407800	0.07589000
Hf	0.27364300	0.00020700	-0.17031300
C	0.09012600	2.21107400	1.01199400
C	0.08332400	2.48337500	-0.38583500
C	1.35599300	1.66642000	1.34963600
H	-0.71811700	2.40667700	1.70529600
C	1.36391100	2.13551600	-0.90589400
H	-0.71879200	2.94543700	-0.94560600
C	2.14428100	1.61854300	0.16196100
H	1.68211800	1.38594500	2.34289400
H	1.69297100	2.26897100	-1.92816800
H	3.17458600	1.29514200	0.09507900
H	-3.46226700	1.29362500	1.53155200
C	-3.20990400	1.26413600	0.46654100
C	-2.40569600	-0.00190800	0.11992900
H	-2.67543200	2.18216900	0.21069800
C	-1.87035600	-0.00186900	-1.30521000
H	-1.54563900	0.00054800	0.90560100
H	-2.16571900	-0.89269700	-1.86194400

H	-2.16700100	0.88854900	-1.86191600
H	0.50511900	0.00070800	-2.07608900
H	-0.44021400	-0.00030700	-1.94842200
H	-3.45817100	-1.29762700	1.53417400
H	-4.14618800	1.25529900	-0.10113800

10b

C	3.16214100	1.06197400	1.37574800
H	2.87848400	2.05270800	1.00664400
H	4.18806000	0.86492600	1.04948200
H	0.45050800	2.65351200	1.55267100
C	-0.21930600	2.35446500	0.75592100
C	0.05158200	2.42539600	-0.63831700
C	-1.53663500	1.85167200	0.92553700
C	-1.11586600	1.99392900	-1.33504400
H	0.95359600	2.81042800	-1.09493700
C	-2.09210400	1.63211500	-0.36918300
H	-2.04599900	1.71341900	1.87051600
H	-1.24686700	1.97925600	-2.40931000
H	-3.09704400	1.29013400	-0.57988500
Hf	-0.23035700	-0.00963400	-0.11755900
C	-1.83138900	-1.41541500	1.20281400
C	-0.53274000	-1.90833600	1.48715100
C	-2.10545700	-1.66038900	-0.17444300
H	-2.50657600	-0.95692700	1.91349400
C	-0.00144800	-2.46759600	0.28583000
H	-0.04874100	-1.90241700	2.45618100
C	-0.98398900	-2.33363700	-0.73186700
H	-3.02786600	-1.43086700	-0.69211200
H	0.94722100	-2.97653500	0.18708600
H	-0.90177900	-2.69331900	-1.74942700
H	2.63667600	-2.20436500	-0.99104400
C	2.92102400	-1.21423800	-1.35971800
C	2.13008600	-0.08760400	-0.68979800
H	2.77938800	-1.21068000	-2.44598600
C	2.23530400	-0.03085400	0.82246900
H	2.427772600	0.87289600	-1.11841500
H	1.23284500	0.16960500	1.36561000
H	2.50284800	-1.01452600	1.22112300
H	0.84059000	-0.24401100	-1.68859900
H	-0.01074800	-0.28048500	-2.02794600
H	3.15090000	1.08161400	2.46998000
H	3.99523900	-1.08959000	-1.17350900

Hf/But

10a

C	-2.60678200	-1.95442700	0.54465800
H	-1.84901700	-2.70983500	0.32732300
H	-3.49844900	-2.21052300	-0.03384500
H	0.11143700	-2.48953500	1.76087500
C	0.82423300	-2.13672800	1.02627600
C	0.80719900	-2.42370800	-0.36938000
C	1.96299800	-1.33536600	1.29732400
C	1.95785700	-1.82161800	-0.95416400
H	0.09583400	-3.05284700	-0.88702200
C	2.66254000	-1.13640800	0.07079800
H	2.27026700	-0.97698700	2.27132900
H	2.25680900	-1.89552800	-1.99160600
H	3.59542600	-0.60188500	-0.05067100
Hf	0.47250900	0.04290300	-0.16769700
C	-0.14447000	2.16055800	1.03789100
C	-0.24379000	2.43161400	-0.35675700
C	1.21614800	1.89575100	1.34032400
H	-0.95790600	2.17775300	1.75202200
C	1.06760700	2.36577700	-0.91006900
H	-1.13976100	2.71456200	-0.89268500
C	1.96639500	2.02153700	0.13376700
H	1.61955700	1.68599900	2.32262300
H	1.33503500	2.56995600	-1.93865900

H	3.03967700	1.92361700	0.03839800
H	-3.31038500	0.53076700	1.65158800
C	-3.18899300	0.54216100	0.56081700
C	-2.14115800	-0.53549000	0.17151900
C	-4.55989400	0.35642000	-0.10370500
H	-2.79989700	1.53140800	0.29927000
C	-1.64656400	-0.41898600	-1.26322800
H	-1.28295400	-0.32903600	0.93490500
H	-5.20770700	1.20061700	0.15208700
H	-4.48384500	0.31660600	-1.19593600
H	-5.06263400	-0.55377200	0.23554400
H	-1.75118200	-1.35033300	-1.82229000
H	-2.13466000	0.38788100	-1.81238000
H	0.65754100	0.09869600	-2.07880000
H	-0.26096000	-0.10564400	-1.93196300
H	-2.86279700	-2.01743700	1.60766300

10b

C	-2.47535300	-1.75039900	1.65069700
H	-2.04440000	-2.63233100	1.16673800
H	-3.55529500	-1.77152500	1.47895400
H	0.48086200	-2.70621700	1.55713400
C	0.96258500	-2.28354000	0.68421600
C	0.51297900	-2.39851900	-0.66107300
C	2.17595600	-1.54676500	0.68291800
C	1.47029600	-1.75582800	-1.49972000
H	-0.35863300	-2.94304200	-0.99877400
C	2.48982000	-1.22003100	-0.66907500
H	2.77920500	-1.31782200	1.55204600
H	1.44153800	-1.71157500	-2.58069700
H	3.37163700	-0.69105000	-1.00720200
Hf	0.41316100	0.04243700	-0.10572400
C	1.98876700	1.70044500	0.90978500
C	0.74523900	1.85406600	1.57662800
C	1.81455400	2.08472600	-0.44935700
H	2.91259700	1.36029700	1.35896700
C	-0.19539500	2.36723000	0.63117600
H	0.56086800	1.68073000	2.62987200
C	0.46838200	2.52164700	-0.61086800
H	2.58282300	2.10266100	-1.21208500
H	-1.21829100	2.64712000	0.84308700
H	0.03393800	2.90891400	-1.52360500
H	-2.79325600	1.71801700	-0.50237500
C	-2.98792500	0.73790300	-0.95463700
C	-1.97736000	-0.29665100	-0.43178000
C	-4.44917200	0.33879400	-0.69940000
H	-2.84181400	0.86880200	-2.03516600
C	-1.89307600	-0.45095500	1.07437100
H	-2.17004200	-1.26768600	-0.89703900
H	-5.12861000	1.08185700	-1.12966700
H	-4.68084600	-0.62977100	-1.15689700
H	-4.67264100	0.27011800	0.37141400
H	-0.81276600	-0.43740100	1.49932300
H	-2.31932900	0.42619100	1.57160900
H	-0.85336900	0.09890000	-1.53800800
H	-0.06418200	0.30132600	-1.96736200
H	-2.29934300	-1.82473800	2.72856600

Hf/Hex

10a

C	-1.71788600	-2.40930400	0.54724200
H	-0.84939800	-3.02686900	0.30857100
H	-2.56350600	-2.80123300	-0.02412400
H	1.03722500	-2.49095700	1.73358200
C	1.68574200	-2.01482200	1.00926800
C	1.73077400	-2.28783100	-0.38825600
C	2.66573900	-1.03072600	1.29816100
C	2.76682100	-1.49153000	-0.95645100
H	1.14201900	-3.02464300	-0.91789900

C	3.33304600	-0.70436400	0.08064900
H	2.89766100	-0.63432500	2.27819500
H	3.08339800	-1.50361100	-1.99124300
H	4.16078500	-0.01604900	-0.02694400
Hf	0.97663800	0.08463000	-0.17234800
C	0.02328600	2.07167600	1.03475800
C	-0.13706000	2.31230300	-0.35996700
C	1.41244200	2.04602100	1.32094900
H	-0.77322700	1.95164800	1.75805600
C	1.15973700	2.46973200	-0.92919800
H	-1.07457200	2.43526900	-0.88529700
C	2.11615300	2.29033800	0.10489200
H	1.85677300	1.91245100	2.29884500
H	1.37664400	2.71035800	-1.96173500
H	3.18941600	2.37581700	-0.00269500
H	-2.81049900	-0.09021000	1.69599600
C	-2.70421600	-0.04183100	0.60389000
C	-1.49968700	-0.92806900	0.18859800
C	-4.04381000	-0.42180000	-0.04880500
H	-2.48262900	1.00252900	0.35790200
C	-1.04677200	-0.71960000	-1.24926800
H	-0.67707300	-0.58946700	0.94642400
H	-3.93612400	-0.44495100	-1.14237300
H	-4.33930100	-1.43348300	0.25540900
H	-1.01184500	-1.65070300	-1.81733100
H	-1.66272900	0.00603000	-1.78259800
H	1.13784600	0.15802100	-2.08462700
H	0.26583200	-0.19552900	-1.92996900
H	-1.94460100	-2.52772300	1.61214800
C	-5.16608200	0.55804500	0.32812500
H	-5.26864700	0.58710900	1.42170900
H	-4.88036100	1.57389000	0.01990200
C	-6.51266900	0.19072000	-0.30336400
H	-6.84346100	-0.80467800	0.01562400
H	-7.28914100	0.90684100	-0.01559000
H	-6.45176700	0.18733400	-1.39821400

10b

C	-3.03856400	-0.40613000	0.06326400
H	-2.82184000	-1.16003400	-0.70507900
H	-3.82299300	0.23698400	-0.35456100
H	-0.93376700	-2.73622400	0.11933300
C	-0.04232600	-2.38954400	-0.38810800
C	0.01320400	-1.81646100	-1.69049300
C	1.28150200	-2.46373300	0.11800400
C	1.38117700	-1.56538300	-2.00071100
H	-0.82505600	-1.66613400	-2.35773800
C	2.16242000	-1.95071200	-0.87904000
H	1.57249500	-2.87702100	1.07533900
H	1.76073100	-1.17471900	-2.93588400
H	3.24167100	-1.90038500	-0.81033700
Hf	0.76605900	-0.02645600	-0.11459700
C	2.50977700	0.13556200	1.66455800
C	1.28193600	0.54526600	2.25241300
C	2.86370700	1.08429700	0.66721500
H	3.07974800	-0.74394000	1.93381200
C	0.90112300	1.77956600	1.64215100
H	0.77029400	0.05456100	3.07132000
C	1.87530900	2.11292300	0.67320400
H	3.75510100	1.06506500	0.05272600
H	0.03705900	2.37524000	1.90461500
H	1.87656600	2.99419700	0.04450900
H	-0.98147100	3.14146700	-0.16217000
C	-1.38202500	2.65253600	-1.05889200
C	-1.20517500	1.12822800	-0.95257400
C	-2.84297100	3.08041300	-1.26274500
H	-0.78420800	3.02617100	-1.90101200
C	-1.79374200	0.47489700	0.28295200
H	-1.59711900	0.64728800	-1.85386400
H	-2.91022600	4.16746400	-1.37597100
H	-3.26777500	2.62407000	-2.16406100
H	-3.47377600	2.79920200	-0.41166600
H	-1.07086100	-0.23843700	0.84724300

H	-1.98168200	1.22585600	1.05778100
H	0.29950700	1.15528800	-1.54013100
H	1.20154400	1.00680400	-1.69273600
C	-3.55042600	-1.08413800	1.34022500
H	-2.75790100	-1.72019800	1.76375800
H	-3.76139000	-0.31659800	2.09745700
C	-4.80825100	-1.92619100	1.10022000
H	-5.14854200	-2.39478700	2.02884900
H	-5.62984600	-1.31007600	0.71762600
H	-4.62251100	-2.72463000	0.37196300

2nd β -product

Hf/et

11a

Hf	0.57599900	0.02228500	-0.10893900
C	0.56744600	2.07342900	1.31947000
C	-0.64794200	2.09166500	0.57363500
C	-0.32066600	2.25565100	-0.80107300
C	1.09701700	2.33250800	-0.90541000
C	1.64300900	2.23772000	0.40496100
C	1.28293800	-1.90527600	1.33640900
C	1.23061100	-2.41757300	0.00630100
C	2.22811400	-1.76435900	-0.75809600
C	2.89442800	-0.83218400	0.08906500
C	2.31673700	-0.93314200	1.39106800
H	0.65326500	1.99663700	2.39675500
H	-1.64713400	2.03765600	0.98833800
H	-1.02173100	2.34489900	-1.61883800
H	1.65939400	2.47791200	-1.82088100
H	2.69316400	2.29134900	0.66126000
H	0.67053300	-2.23299400	2.16861400
H	0.55975100	-3.18671400	-0.35333500
H	2.44321600	-1.94135400	-1.80509400
H	3.73814100	-0.21187600	-0.18640100
H	2.62862700	-0.38271900	2.26960400
C	-5.41068300	-0.07685000	0.62158400
H	-5.38102400	1.00854700	0.46876000
H	-5.97415700	-0.26864200	1.54003900
H	-5.97125400	-0.51622500	-0.21119500
H	-3.68041200	-0.84561900	-1.42583500
C	-3.16961100	-0.41607700	-0.55423100
H	-3.09176900	0.66218000	-0.74770200
C	-3.99927700	-0.66701700	0.71138600
H	-4.06323700	-1.74836200	0.89416700
H	-3.47765300	-0.23951500	1.58164800
C	-1.76406600	-1.03321800	-0.51691000
H	-1.33238300	-0.66255900	0.50926700
H	-1.81562400	-2.10997400	-0.32791300
C	-0.82588100	-0.69896300	-1.67524600
H	-0.52972300	-1.58568500	-2.23784700
H	-1.26493500	0.03065300	-2.35725000

Hf/Pro

11a

C	-2.88730600	-0.06945200	-0.71972500
C	-3.96146800	-0.25039700	0.37459100
H	-3.33475000	-0.31307200	-1.69266600
H	-2.61056200	0.99095100	-0.77329000
C	-3.45681800	0.09086300	1.78523100
H	-4.27921000	-1.30165700	0.37402500
H	-2.61635100	-0.54056700	2.10160900
H	-3.13964500	1.14084500	1.84854000
H	1.38388300	-2.90742500	-1.14059700
C	1.73860900	-2.24768600	-0.36150300
C	2.83367500	-1.34418700	-0.47181900
C	1.23343800	-2.15857100	0.96467200
C	3.02040700	-0.72045900	0.79370300

H	3.44764500	-1.19378900	-1.35264600
C	2.02183800	-1.20797600	1.67715400
H	0.42067500	-2.74215000	1.37834300
H	3.79451400	-0.00721200	1.04298600
H	1.90984000	-0.94150900	2.72137500
Hf	0.79992200	0.06184000	-0.11033000
C	-5.19288900	0.60063200	0.02370000
H	-5.59256200	0.33941300	-0.96258300
H	-4.94565700	1.67003700	0.01347100
H	-5.99154000	0.45198900	0.75797900
C	1.14212800	2.18084400	1.15077800
C	-0.18549900	2.23369200	0.63862900
C	2.03875700	2.23310500	0.04540800
H	1.42256800	2.14777500	2.19637000
C	-0.10593700	2.32246500	-0.78028400
H	-1.09429400	2.24947700	1.22772100
C	1.26487700	2.31357000	-1.14575100
H	3.11917400	2.25146100	0.10105500
H	-0.93945200	2.40592900	-1.46300800
H	1.65322500	2.37680200	-2.15571300
C	-1.60424800	-0.92915600	-0.62349300
C	-0.57431900	-0.62470800	-1.72326900
H	-0.30300100	-1.52045100	-2.28460400
H	-0.92967000	0.13340900	-2.42368800
H	-1.14984800	-0.63371900	0.42298800
C	-1.91630300	-2.42783200	-0.48172100
H	-2.43434600	-2.65949500	0.45337400
H	-1.01577000	-3.04397800	-0.53796600
H	-2.56887600	-2.72575800	-1.30994600
H	-4.25405800	-0.04827500	2.52284900

11b

C	-2.99696000	0.12626500	0.56395900
C	-3.91112500	0.15004100	-0.67738600
H	-2.77775000	1.15570800	0.87406900
H	-3.53056000	-0.33983800	1.40401500
C	-4.38229500	-1.25255000	-1.09243800
H	-3.32986500	0.57721700	-1.51213400
H	-3.55187600	-1.91622800	-1.36175400
H	-4.94531300	-1.73108800	-0.28127200
H	-0.62259800	2.56685800	-1.42152300
C	0.17462200	2.39391600	-0.70782400
C	0.03850200	2.38074700	0.71050000
C	1.54927700	2.20534500	-1.01758000
C	1.32158100	2.17827400	1.27618400
H	-0.88098100	2.52199800	1.26184900
C	2.26014200	2.06272100	0.21055200
H	1.98373500	2.20565300	-2.00901200
H	1.54862500	2.12933000	2.33466200
H	3.33162300	1.94910200	0.31458200
C	-5.11339200	1.07332200	-0.42502200
H	-4.79577500	2.09010700	-0.16516300
H	-5.73324400	0.69544800	0.39739200
H	-5.74836900	1.13844000	-1.31478500
C	1.28732900	-1.63393900	-1.78628900
C	0.97276000	-2.37950400	-0.61221400
C	2.48636600	-0.91719400	-1.54021500
H	0.72987600	-1.64528600	-2.71608600
C	1.97312300	-2.12266500	0.35800100
H	0.12896300	-3.04618600	-0.49282200
C	2.90419200	-1.20144400	-0.20506300
H	3.00509100	-0.28209900	-2.24633700
H	2.02092200	-2.55221100	1.35035000
H	3.81092700	-0.84414000	0.26708700
H	-1.85305300	-1.67768800	0.11240000
C	-1.67262200	-0.63847800	0.40025500
C	-0.67500400	-0.57463100	1.57061500
H	-1.23278800	-0.19968300	-0.58685300
C	-0.64889000	-1.83820000	2.43782200
H	-0.93158800	0.27712300	2.20785200
H	-0.44271900	-2.74533000	1.85952300
H	0.11439200	-1.76153200	3.21992000
H	-5.04401500	-1.19403800	-1.96289300

H	-1.61057800	-1.99181800	2.94615400
Hf	0.79099000	0.06316700	0.01024500

Hf/But

11a

C	2.51757300	-0.07396600	-0.99249000
C	3.68787000	-0.24913400	0.00338300
H	2.91721900	0.33069100	-1.93042500
H	2.11911300	-1.06365100	-1.24798900
C	3.25416100	-0.89401300	1.33695600
H	4.09699500	0.74481700	0.23367600
H	2.40476400	-0.33612300	1.75902200
H	2.88767700	-1.91297400	1.13634000
H	-1.45729200	3.11376900	-0.30298900
C	-1.83131400	2.30595400	0.30988900
C	-3.00989700	1.54819900	0.05890300
C	-1.26730100	1.84118100	1.53077500
C	-3.18670500	0.63600700	1.13682200
H	-3.68044000	1.67611800	-0.78338800
C	-2.10216700	0.80279800	2.03820200
H	-0.38365200	2.23550500	2.01660900
H	-4.01096800	-0.05403500	1.25672700
H	-1.95981800	0.26863700	2.96999300
Hf	-1.09340800	-0.05658400	-0.09306800
C	4.80180900	-1.05623900	-0.68588900
H	5.09936700	-0.58921300	-1.63150400
H	4.46928200	-2.07856500	-0.90847700
H	5.69604900	-1.12578600	-0.06049800
C	-1.49977100	-2.39326400	0.66240200
C	-0.23548500	-2.40059100	0.00592100
C	-2.49820400	-2.12252700	-0.31602000
H	-1.67611000	-2.59857500	1.71110800
C	-0.45654100	-2.13629700	-1.37560400
H	0.72025700	-2.61247800	0.46929000
C	-1.85039100	-1.95615300	-1.57152600
H	-3.56592200	-2.08811700	-0.14523200
H	0.29770300	-2.10257900	-2.14851400
H	-2.33702300	-1.74882400	-2.51757500
C	1.34720300	0.85768600	-0.59293000
C	0.21162600	0.89917100	-1.62690900
H	-0.02975400	1.92013600	-1.92795300
H	0.43834000	0.31466200	-2.52015300
H	0.93564600	0.37257100	0.40128200
C	1.80581700	2.26075500	-0.12286400
H	2.39010000	2.16745100	0.80010700
H	0.92193900	2.85583300	0.12781400
C	2.62760700	3.02141000	-1.17314700
H	2.84374500	4.03162200	-0.81156100
H	3.58547300	2.53377300	-1.37702800
H	2.08634600	3.11418400	-2.12084900
C	4.35320400	-0.95520600	2.40614000
H	3.95713900	-1.34890100	3.34822900
H	5.18189300	-1.60228200	2.10430900
H	4.76271700	0.04173200	2.60843000

11b

C	-2.63755500	-0.10283000	-0.87778600
C	-3.59487300	-0.77795900	0.12763300
H	-2.28758600	-0.85165600	-1.59937400
H	-3.18745300	0.64629500	-1.46309700
C	-4.23109600	0.23723100	1.10141300
H	-3.00195800	-1.49173700	0.72664500
C	-5.11376700	-0.38442400	2.19081800
H	-3.43940000	0.81753200	1.59602500
H	-4.82012100	0.96140800	0.52009400
H	-5.45425100	0.38265100	2.89409500
H	-6.00521200	-0.86310400	1.77451600
H	-4.56472000	-1.14117100	2.76533800
H	-0.29914700	-3.02666700	0.03605300

C	0.55315000	-2.53490700	-0.41821400
C	0.56961700	-1.89896800	-1.69295200
C	1.86747800	-2.46839600	0.12135500
C	1.88589500	-1.43482100	-1.93848600
H	-0.27054500	-1.80612500	-2.36717900
C	2.69243200	-1.78105500	-0.81673100
H	2.19263000	-2.89818800	1.06007100
H	2.22004100	-0.91706300	-2.83001000
H	3.75593200	-1.60486800	-0.71858100
C	-4.65461700	-1.58153300	-0.64446300
H	-4.18818800	-2.28599900	-1.34330900
H	-5.30350900	-0.91474900	-1.22601700
H	-5.29144700	-2.16143400	0.02911100
C	1.22495500	0.63792100	2.44343300
C	0.99758700	1.81784500	1.67579400
C	2.48942200	0.11284800	2.07269700
H	0.56639800	0.23843500	3.20622900
C	2.11557100	2.01891600	0.82949300
H	0.13075800	2.46103400	1.74626300
C	3.03646100	0.95480100	1.05768500
H	2.96644900	-0.76002200	2.49881900
H	2.24516900	2.83633200	0.13186200
H	4.01298200	0.84868500	0.60180300
Hf	1.05234000	-0.11598700	0.04171100
H	-1.71670700	1.41946800	0.39702100
C	-1.41583400	0.61299400	-0.27705600
C	-0.32617500	1.09958900	-1.24059200
H	-1.00721200	-0.17129000	0.49250100
C	-0.26941200	2.62215000	-1.45963600
H	-0.46253600	0.61426200	-2.21298000
C	-1.46956800	3.18514600	-2.23710800
H	-0.19377400	3.14415100	-0.49720000
H	0.64871400	2.86511200	-2.01091400
H	-1.35466100	4.26221900	-2.40117400
H	-1.56674600	2.70675900	-3.21861500
H	-2.41041400	3.03355200	-1.69499300

Hf/Hex

11a

C	1.69522100	0.28037200	-1.61023800
C	2.99140000	-0.40142700	-1.11265300
H	1.97057700	1.08402600	-2.30399900
H	1.12576100	-0.44098100	-2.20861500
C	2.72388800	-1.58835400	-0.16337700
H	3.57846600	0.34302200	-0.55642400
C	3.97798900	-2.21465500	0.46692400
H	2.06614700	-1.26426700	0.65868300
H	2.17210600	-2.36892600	-0.71199600
H	4.60943200	-2.65459500	-0.31494100
H	4.57889900	-1.42297300	0.93807800
H	-0.25673700	0.81611300	2.70047700
C	-1.25996700	0.76092900	2.29686100
C	-1.95063700	1.80615000	1.62273400
C	-2.14031000	-0.35518100	2.40268400
C	-3.25371800	1.33254200	1.30339200
H	-1.57053300	2.79666600	1.41722300
C	-3.37621100	0.00619900	1.80360300
H	-1.92202800	-1.29520000	2.89518000
H	-4.03153300	1.89965100	0.80461000
H	-4.26115500	-0.61358800	1.75086200
C	3.82240400	-0.82146100	-2.33783700
H	3.98900100	0.02736400	-3.01066500
H	3.31149600	-1.60639800	-2.91075800
H	4.80393000	-1.20655300	-2.04828300
C	-2.24818100	-2.43837000	-0.42676000
C	-1.12695600	-2.16639500	-1.26139100
C	-3.34932000	-1.67828800	-0.91388700
H	-2.27163800	-3.13048300	0.40586100
C	-1.53820500	-1.24052900	-2.26183600
H	-0.14555700	-2.61630400	-1.17463500
C	-2.90615000	-0.93460400	-2.04256500
H	-4.35754300	-1.69312000	-0.52182700

H	-0.92927200	-0.85605000	-3.06731700
H	-3.51144600	-0.26638400	-2.64413500
H	-0.68523000	2.54939800	-0.87680800
C	-0.53102500	1.50851200	-1.16596700
C	0.75652900	0.92708600	-0.56260500
H	-0.54820800	1.44133000	-2.25512600
C	1.48383800	1.89355700	0.40375300
H	0.46708800	0.02409900	0.14226100
C	2.19419500	3.06372300	-0.29961300
H	0.75673600	2.30694900	1.11153900
H	2.21479700	1.33599700	1.00254800
H	2.99934100	2.68451200	-0.94138600
H	1.48821400	3.58148200	-0.96312900
C	2.78737500	4.07070000	0.69763800
H	1.98421800	4.46937500	1.33354200
H	3.48137400	3.54916900	1.37137400
C	3.51645800	5.22750700	0.00618300
H	3.92620900	5.92960900	0.73958600
H	4.34932000	4.86214600	-0.60634300
H	2.84056000	5.78784200	-0.65073600
C	3.65237200	-3.29257600	1.51024400
H	3.03112800	-2.85219900	2.30460900
H	3.04000600	-4.07702500	1.04210100
C	4.90184600	-3.92492600	2.13218400
H	4.63469700	-4.68556200	2.87353000
H	5.52309700	-4.40775800	1.36876200
H	5.51945500	-3.17129100	2.63505200
Hf	-1.65150300	-0.05253000	-0.03685500

11b

C	-1.76885600	0.24513200	-1.48950700
C	-2.84436800	-0.84435200	-1.29218700
H	-1.17568000	0.01153900	-2.38324100
H	-2.25337100	1.20955300	-1.69280000
C	-3.82935100	-0.49057900	-0.15717400
H	-2.32620200	-1.77793900	-1.00879500
C	-4.84333500	-1.58933100	0.19547300
H	-3.26565800	-0.24798300	0.75592300
H	-4.36804000	0.42860000	-0.43252200
H	-5.49449700	-1.79162100	-0.66440300
H	-4.30744700	-2.52861800	0.40139100
H	0.22309900	-2.32201800	-2.10634200
C	1.21281000	-1.94628000	-1.87673100
C	1.79974900	-0.76011800	-2.40077800
C	2.17743500	-2.58524300	-1.04486600
C	3.12198400	-0.66280400	-1.88797100
H	1.33771400	-0.07307100	-3.09558100
C	3.36042100	-1.79551300	-1.06098800
H	2.04765500	-3.52742500	-0.52645500
H	3.83524900	0.12167300	-2.11464500
H	4.28584900	-2.02440900	-0.54850300
C	-3.56504400	-1.09450700	-2.62730300
H	-2.85315600	-1.33932500	-3.42472500
H	-4.12426000	-0.20463600	-2.94227200
H	-4.27395600	-1.92374800	-2.55409600
C	1.20511700	-1.22100900	2.45272800
C	1.03079100	0.19464300	2.47563700
C	2.56021400	-1.48838900	2.13144000
H	0.44588700	-1.95950400	2.68304400
C	2.27218500	0.79969300	2.16325500
H	0.11269900	0.71486500	2.71405900
C	3.22073300	-0.23938500	1.92751200
H	3.01639800	-2.46743500	2.06206800
H	2.46480800	1.86366300	2.11216600
H	4.27395400	-0.10424500	1.71326000
H	-1.34119200	0.77755600	0.59421300
C	-0.80810000	0.47054400	-0.31002200
C	0.41100200	1.36449900	-0.54969700
H	-0.50048700	-0.62409900	-0.01145900
C	0.39085700	2.72902200	0.16155300
H	0.52351600	1.53769600	-1.62457100
C	-0.64296400	3.71594400	-0.41094600
H	0.20045600	2.60140000	1.23573800

H	1.38681400	3.18720600	0.08163000
H	-0.46380800	3.84133200	-1.48865400
H	-1.65244200	3.28902300	-0.31613600
C	-5.71762700	-1.22965300	1.40524200
H	-6.24363700	-0.28625800	1.20246200
H	-5.07263300	-1.03736400	2.27514100
C	-6.73735000	-2.31828400	1.75496600
H	-7.34297900	-2.03109900	2.62117900
H	-7.42145900	-2.50468100	0.91848800
H	-6.24107400	-3.26659400	1.99499600
C	-0.61026600	5.08924500	0.27454800
H	0.39824000	5.51569000	0.17911600
H	-0.78745800	4.96143600	1.35200200
C	-1.63748500	6.07030200	-0.30007700
H	-2.65937700	5.68908000	-0.18531300
H	-1.58540800	7.03903400	0.20776800
H	-1.46519600	6.24496000	-1.36880800
Hf	1.58494100	-0.43713500	0.08583400

β-hydrogen elimination products

Hf/et

12a

H	0.42605600	-3.15713100	0.38111200
C	1.05084600	-2.29744800	0.17140200
C	1.41109900	-1.82410300	-1.11912700
C	1.73228500	-1.50553300	1.14277800
C	2.28849400	-0.71808800	-0.94430300
H	1.09063200	-2.23713500	-2.06508200
C	2.50101300	-0.53560900	0.45366200
H	1.69712700	-1.64030000	2.21808000
H	2.75849800	-0.15203200	-1.73847400
H	3.15350100	0.19848000	0.90772500
C	-1.34312000	2.07937100	0.02930600
C	-0.53245300	2.17087300	-1.13557500
C	-0.49523000	2.15936700	1.16901600
H	-2.42306300	2.00502600	0.04116200
C	0.82134800	2.27713700	-0.71262500
H	-0.88483700	2.17502100	-2.15744000
C	0.84208500	2.28016100	0.71466100
H	-0.81373700	2.14742100	2.20530500
H	1.68066400	2.39707500	-1.35983700
H	1.71742100	2.39750300	1.34004100
Hf	0.09996600	0.01554400	-0.02243400
C	-3.57463600	-1.10467700	-0.67074000
H	-3.98782700	-0.16882000	-0.28569100
H	-4.35826300	-1.87391000	-0.62202700
H	-1.92169100	-2.48862200	-0.25296800
C	-2.39843500	-1.57905900	0.11260100
H	-0.65769600	-0.37853700	-1.62342100
C	-1.92248900	-1.00869700	1.25096000
H	-2.44333500	-0.17372800	1.71277500
H	-1.19881700	-1.54356400	1.87098800
H	-3.31704400	-0.98806900	-1.72912100

Hf/Pro

12a

H	0.42605600	-3.15713100	0.38111200
C	1.05084600	-2.29744800	0.17140200
C	1.41109900	-1.82410300	-1.11912700
C	1.73228500	-1.50553300	1.14277800
C	2.28849400	-0.71808800	-0.94430300
H	1.09063200	-2.23713500	-2.06508200
C	2.50101300	-0.53560900	0.45366200
H	1.69712700	-1.64030000	2.21808000
H	2.75849800	-0.15203200	-1.73847400
H	3.15350100	0.19848000	0.90772500
C	-1.34312000	2.07937100	0.02930600

C	-0.53245300	2.17087300	-1.13557500
C	-0.49523000	2.15936700	1.16901600
H	-2.42306300	2.00502600	0.04116200
C	0.82134800	2.27713700	-0.71262500
H	-0.88483700	2.17502100	-2.15744000
C	0.84208500	2.28016100	0.71466100
H	-0.81373700	2.14742100	2.20530500
H	1.68066400	2.39707500	-1.35983700
H	1.71742100	2.39750300	1.34004100
Hf	0.09996600	0.01554400	-0.02243400
C	-3.57463600	-1.10467700	-0.67074000
H	-3.98782700	-0.16882000	-0.28569100
H	-4.35826300	-1.87391000	-0.62202700
H	-1.92169100	-2.48862200	-0.25296800
C	-2.39843500	-1.57905900	0.11260100
H	-0.65769600	-0.37853700	-1.62342100
C	-1.92248900	-1.00869700	1.25096000
H	-2.44333500	-0.17372800	1.71277500
H	-1.19881700	-1.54356400	1.87098800
H	-3.31704400	-0.98806900	-1.72912100

12b

C	-2.74621500	-0.44411600	-0.21577800
C	-2.28797500	0.30942900	0.81735700
H	-0.55546000	-0.00287800	-1.70818800
H	-2.66101400	-1.52841400	-0.14825500
C	-1.71390100	-0.23217100	2.10424100
H	-2.47191500	1.38126700	0.78548300
H	-1.89554900	-1.30122700	2.23178500
H	-0.61329100	-0.07038500	2.23232100
H	-0.90577400	-2.99840600	0.44453700
C	0.01084700	-2.48644500	0.18107200
C	0.48166600	-2.24562100	-1.13685900
C	1.02121100	-2.05881100	1.09773000
C	1.75873500	-1.63179700	-1.03595300
H	-0.03266000	-2.48755000	-2.05618100
C	2.09947400	-1.53907600	0.34473100
H	0.98972600	-2.15826100	2.17598500
H	2.38191300	-1.33187100	-1.86864300
H	3.02564600	-1.15029300	0.74745000
C	-3.50099200	0.08265400	-1.39541000
H	-4.55100000	-0.22908800	-1.30750500
H	-3.11883800	-0.33505100	-2.33113000
H	-3.47110800	1.17402900	-1.45313500
C	0.44821800	2.29953100	0.99821500
C	-0.09919800	2.52283400	-0.29253300
C	1.73001800	1.70872100	0.83933100
H	-0.02012100	2.55155400	1.94243100
C	0.85305800	2.09552600	-1.25928400
H	-1.05695600	2.97620900	-0.51303500
C	1.98175900	1.59110600	-0.56099400
H	2.41881600	1.45807000	1.63587600
H	0.74179300	2.16552400	-2.33221500
H	2.89449800	1.22484300	-1.01187800
Hf	0.15024400	0.00727700	-0.04638300
H	-2.13652500	0.30740600	2.95865900

Hf/But

12a

C	-1.60587700	-0.43650100	-1.51567600
C	-2.62591200	-0.60604800	-0.61240300
H	-1.15535100	-1.31270200	-1.98194700
H	-1.54738000	0.49600400	-2.07591200
C	-3.54016600	0.53462800	-0.24515500
H	-0.56183300	-0.06777300	1.51221100
C	-3.84516300	0.70345100	1.25346400
H	-3.15937000	1.46824400	-0.67119800
H	-4.48455300	0.32851900	-0.77452800
H	-4.50143700	1.56675800	1.39593400

H	-4.35776800	-0.17030300	1.66638200
H	-2.92930600	0.86760500	1.83009300
H	0.04320800	2.42437400	2.06831800
C	0.44257500	2.29274700	1.07256100
C	1.78189300	1.95192500	0.74389900
C	-0.27522500	2.44808000	-0.14468100
C	1.89616600	1.91895700	-0.67883600
H	2.58875200	1.79759300	1.44861600
C	0.62507400	2.23288700	-1.22277400
H	-1.31663300	2.72866500	-0.22955700
H	2.80133800	1.73906500	-1.24383500
H	0.39051300	2.30897200	-2.27842300
Hf	0.42298800	0.01833500	-0.00893100
C	-2.94983000	-1.94849200	-0.02495500
H	-2.36842300	-2.75612100	-0.47351900
H	-4.01548000	-2.16446700	-0.17237300
H	-2.78178800	-1.94594000	1.05838400
C	1.74715300	-1.88214600	-0.98062600
C	0.71991900	-2.46927900	-0.18366900
C	2.62852200	-1.19144900	-0.11205700
H	1.86108900	-1.98149700	-2.05412000
C	0.96664100	-2.13761000	1.17412000
H	-0.07230800	-3.11064500	-0.54557300
C	2.13544200	-1.32687000	1.21544900
H	3.52563100	-0.66293100	-0.40618600
H	0.38517300	-2.45464700	2.02823800
H	2.59351400	-0.92454500	2.11005200

12b

C	-2.30804800	-0.91436300	-1.08803300
C	-2.30768200	-0.02519400	-0.06105800
H	0.14536800	-0.24432400	-1.88822600
H	-2.09940100	-1.96228800	-0.87350700
C	-2.09571400	-0.35984800	1.39693200
H	-2.62001000	0.99612500	-0.27312300
C	-3.10842200	0.34414700	2.31720700
H	-2.12005200	-1.44279700	1.55083000
H	-1.08292600	-0.03293800	1.76965800
H	-2.90962500	0.10511600	3.36560200
H	-3.06659900	1.43195600	2.19887800
H	-4.12355800	0.01543600	2.07540500
H	-0.43075200	-3.09401300	0.37995400
C	0.44329900	-2.45615500	0.35098000
C	1.26925200	-2.22586200	-0.78083900
C	1.04161400	-1.80907500	1.47619300
C	2.35139300	-1.40358900	-0.36761900
H	1.11122200	-2.60931900	-1.77887600
C	2.22004800	-1.16577700	1.03155600
H	0.68283300	-1.84174700	2.49773200
H	3.15970200	-1.06006900	-1.00016800
H	2.90843800	-0.60386600	1.64910600
Hf	0.30241800	0.00543900	-0.10646000
C	-2.72089800	-0.60401400	-2.49304900
H	-3.69331600	-1.07758300	-2.68668600
H	-2.01222900	-1.01682700	-3.21648000
H	-2.82215800	0.47061800	-2.66699400
C	-0.01535100	2.37900400	0.73099700
C	-0.22239300	2.42316300	-0.67346300
C	1.33215600	2.00090000	0.96764000
H	-0.75024600	2.61166500	1.49246100
C	1.00523300	2.09723500	-1.31399600
H	-1.13808500	2.70151700	-1.17837800
C	1.96424800	1.83125200	-0.30088700
H	1.80928200	1.91979200	1.93580900
H	1.17874300	2.07925800	-2.38069800
H	3.00685900	1.59175800	-0.46254800

Hf/Hex

12a

C	0.59142800	1.10176900	-1.77618500
C	1.71169800	1.47020200	-1.07133600
H	-0.16625600	1.85264300	-2.00261300
H	0.65659500	0.25753400	-2.46130500
C	2.94883400	0.61250200	-1.06794500
H	0.39658700	0.10103000	1.28074900
C	3.60156900	0.35464300	0.30697400
H	2.74579300	-0.33573500	-1.57748600
H	3.67718600	1.14423000	-1.70227900
H	3.89479600	1.30808600	0.76359900
H	2.86306800	-0.10052600	0.97970300
H	0.58505700	-2.49984400	1.48882600
C	-0.05319500	-2.37060300	0.62621200
C	-1.47361500	-2.38811100	0.62357500
C	0.37937800	-2.17144100	-0.71331800
C	-1.91805700	-2.22074700	-0.72274100
H	-2.10823300	-2.55332900	1.48453500
C	-0.77002200	-2.09443500	-1.54524400
H	1.40901000	-2.12986000	-1.04327200
H	-2.94456800	-2.23892600	-1.06470700
H	-0.77428600	-1.97335600	-2.62249500
Hf	-0.85561000	-0.07293200	-0.01852500
C	1.79473500	2.78473300	-0.35192700
H	0.93004500	3.42317200	-0.54168100
H	2.69808900	3.31927900	-0.67157100
H	1.89472700	2.62913400	0.72865100
C	-2.80553400	1.47589000	-0.35616700
C	-1.80115400	2.23059400	0.31954500
C	-3.25422400	0.46212200	0.52658500
H	-3.19092700	1.66828400	-1.35099000
C	-1.62896800	1.67976900	1.61621700
H	-1.30448300	3.11061400	-0.06653900
C	-2.51284100	0.57094100	1.73585600
H	-4.03274600	-0.26040900	0.32061500
H	-0.96159200	2.04270300	2.38496100
H	-2.62974000	-0.05115400	2.61403600
C	4.83636100	-0.55158200	0.19787500
H	4.54831100	-1.50730500	-0.26279200
H	5.56495000	-0.09151900	-0.48362800
C	5.49554600	-0.81501100	1.55560400
H	6.36976200	-1.46468100	1.44658800
H	5.83055700	0.11829700	2.02303600
H	4.80056800	-1.30464300	2.24839700

12b

C	0.60580200	2.59425700	-0.15541400
C	1.31421500	1.50379200	-0.54892800
H	-1.74291000	1.39763400	-0.53373300
H	0.49269700	2.78891600	0.91102700
C	2.02922200	0.53737600	0.36398400
H	1.50560000	1.38139200	-1.61363500
C	3.45083200	0.18930600	-0.12662500
H	2.05943500	0.92141000	1.38865700
H	1.50209800	-0.45725700	0.44031700
H	3.39489700	-0.19325600	-1.15504800
H	4.02832200	1.12129900	-0.17462200
H	-0.12823300	1.44854700	2.77702400
C	-0.77414400	0.67398900	2.38389100
C	-2.10024400	0.85603700	1.90985600
C	-0.48862000	-0.72642000	2.37637900
C	-2.61793300	-0.42201700	1.56874300
H	-2.62841900	1.79525300	1.82627400
C	-1.62829700	-1.39974900	1.87901500
H	0.42229300	-1.19450000	2.72893800
H	-3.61097200	-0.61834700	1.18550200
H	-1.73439300	-2.47080600	1.76681500
Hf	-0.73702700	-0.01446900	-0.02739200
C	0.08091400	3.65471500	-1.07243300
H	0.67906900	4.56623900	-0.93566200
H	-0.95498300	3.91089600	-0.83295500
H	0.14084000	3.36016400	-2.12371700
C	0.23069600	-1.42809200	-1.89891600
C	-0.48652200	-0.37665900	-2.52871700

C	-0.69550800	-2.22267100	-1.17360700
H	1.29701100	-1.60599900	-1.97150800
C	-1.86587600	-0.53021700	-2.21671100
H	-0.07022200	0.38818800	-3.17112300
C	-1.99480400	-1.66812900	-1.37707200
H	-0.46481300	-3.12506700	-0.62225200
H	-2.67065900	0.09566300	-2.57578900
H	-2.92313400	-2.07407000	-0.99779700
C	4.16759500	-0.82739300	0.77081800
H	3.57255400	-1.75132600	0.82224800
H	4.21826400	-0.43468300	1.79558900
C	5.58039700	-1.15564000	0.27663300
H	6.06590800	-1.88048400	0.93742100
H	5.56028000	-1.58451800	-0.73207100
H	6.20906900	-0.25841800	0.24696000

β-hydrogen transfer products

Hf/et

13a

H	-0.73667200	2.70070300	-1.65668400
C	-0.25810500	2.47593200	-0.71061700
C	-0.91038700	2.29715900	0.54456600
C	1.13501400	2.34958000	-0.50397100
C	0.08300300	2.07820300	1.52824100
H	-1.97442700	2.36627100	0.73050500
C	1.34918100	2.08743500	0.88293500
H	1.90303200	2.46479700	-1.25725200
H	-0.09172700	1.92802000	2.58494300
H	2.31044300	1.99838700	1.37128400
C	1.36046200	-1.54062700	-1.62884100
C	0.97424100	-2.31710000	-0.50070000
C	2.32235900	-0.59254600	-1.20482500
H	1.00239300	-1.66898900	-2.64309100
C	1.71622000	-1.86228600	0.61935200
H	0.26723200	-3.13644400	-0.50035800
C	2.53933200	-0.78570400	0.19138400
H	2.83292700	0.12228900	-1.83652000
H	1.67217600	-2.26736100	1.62082800
H	3.25833100	-0.25677700	0.80244200
C	-3.82686100	-0.41886100	-0.44257400
H	-3.69307000	-1.48112300	-0.22782800
H	-4.75309800	-0.29120400	-1.02094600
H	-2.76841800	1.22593100	-1.43879700
C	-2.70133300	0.15901100	-1.22945200
H	-1.92455500	-2.51459600	0.96521900
C	-1.65381100	-0.53097800	-1.74830400
H	-1.62306400	-1.61667400	-1.69629500
H	-1.00565800	-0.05216200	-2.48720200
C	-1.35263000	-2.22616700	1.85687900
H	-2.01003700	-2.39790400	2.71885400
H	-0.52428800	-2.93651300	1.94694700
C	-0.86920500	-0.76354600	1.81188600
H	-0.25954800	-0.57078900	2.70938500
H	-1.74201500	-0.10170900	1.94252500
H	-3.97829900	0.12642000	0.49660600
Hf	0.19990900	0.05420000	0.00110700

Hf/Pro

13a

C	1.60451300	-0.48113500	-1.98448900
C	2.76785200	-0.32073100	-1.29781400
H	1.19835600	0.32241900	-2.59043500
H	1.24216700	-1.48039700	-2.19824500
C	3.49088300	-1.49556500	-0.69517200
H	1.65677400	-0.23133000	0.94196200
H	3.80006500	-1.29772400	0.33761200
H	2.89891100	-2.41400500	-0.72250400

H	-1.13865900	-1.85859300	-2.46007400
C	-1.33651200	-1.85438700	-1.39581400
C	-0.54697400	-2.47887400	-0.38236000
C	-2.47331900	-1.28856500	-0.76859700
C	-1.19644400	-2.28660400	0.85908500
H	0.36290800	-3.04475700	-0.53752500
C	-2.37346300	-1.52485100	0.63006200
H	-3.28075500	-0.77424000	-1.27193200
H	-0.85555100	-2.65170000	1.81786800
H	-3.08487200	-1.21312500	1.38409200
C	3.46930000	1.00495900	-1.17967900
H	2.93472200	1.81683600	-1.67732200
H	4.46480600	0.92745800	-1.63607600
H	3.63601300	1.27610300	-0.12972600
C	-1.36351100	1.75189800	-1.53188900
C	-0.08615100	2.24690500	-1.17165400
C	-2.18080300	1.77814300	-0.35891500
H	-1.68359700	1.46879600	-2.52649400
C	-0.08976500	2.53032900	0.21785700
H	0.74698300	2.39770100	-1.84323300
C	-1.39651000	2.26426600	0.71476100
H	-3.23126600	1.52541900	-0.30789600
H	0.73894700	2.92946700	0.78937800
H	-1.73768300	2.41691100	1.72861000
H	-0.63325100	-0.58230700	2.92374300
C	-0.08841700	0.08938100	2.26055500
C	1.35350100	-0.36918000	2.02625800
H	-0.10134000	1.08514600	2.70706200
C	2.41934700	0.38556900	2.83728300
H	1.45293600	-1.44986500	2.17625300
H	3.43341000	0.04239700	2.60377100
H	2.36815700	1.46370200	2.64971000
Hf	-0.46791600	0.01478100	0.03502800
H	4.41393400	-1.67321900	-1.26350700
H	2.24667700	0.22535100	3.90598400

13b

C	3.03612800	-0.00434300	0.30478100
C	2.75872000	-1.30550500	0.06661600
H	1.01554700	1.66212400	-0.08655300
H	3.07441000	0.33729400	1.34082300
C	2.63706700	-2.38785900	1.10185300
H	2.80602000	-1.65101200	-0.96688300
H	2.60989100	-1.99446400	2.12180800
H	1.76228700	-3.02866100	0.94432100
H	1.09008500	-0.42136600	2.75983200
C	0.06853400	-0.38359900	2.40764400
C	-0.74224900	0.77895500	2.35163500
C	-0.69404800	-1.48183900	1.93249000
C	-2.02578600	0.39935300	1.87334700
H	-0.44448200	1.77569500	2.65060700
C	-1.99804400	-0.99357900	1.60999000
H	-0.37050200	-2.51259200	1.88083500
H	-2.87671000	1.05310900	1.74159700
H	-2.83809900	-1.59024900	1.28120400
C	3.55984500	0.95733900	-0.72821600
H	4.64419800	1.06560600	-0.59082100
H	3.13776200	1.96239800	-0.63350200
H	3.39571500	0.59913000	-1.74985000
C	-0.12611800	-1.97120100	-1.55059400
C	0.32715300	-0.84521500	-2.30177000
C	-1.52852900	-1.83532400	-1.37514200
H	0.47345600	-2.81251200	-1.22937100
C	-0.78935300	-0.01952700	-2.57140500
H	1.33941800	-0.66839500	-2.64165400
C	-1.93614900	-0.61580300	-1.98056100
H	-2.17624200	-2.54933600	-0.88489600
H	-0.77327900	0.90838300	-3.12702200
H	-2.94478100	-0.22432100	-2.01579500
H	-1.64778300	2.30968500	-1.39492700
C	-1.13002200	2.09614900	-0.46062800
C	0.34670400	2.49063300	-0.51147100
H	-1.64722400	2.61377200	0.34797400

C	0.73620800	3.74144500	0.29010000
H	0.70225000	2.57183700	-1.54389900
H	0.42857100	3.65470200	1.33708900
H	1.81539700	3.92631900	0.26308400
Hf	-0.43503200	-0.00385600	-0.04790700
H	3.51466100	-3.04409500	1.02872600
H	0.23141200	4.61409500	-0.13544400

Hf/But

13a

C	-1.30224200	-2.09462200	0.42825200
C	-2.44190800	-1.36711100	0.58719100
H	-0.75103600	-2.46786600	1.28585300
H	-1.11050700	-2.58635600	-0.51896200
C	-3.37479600	-1.11890300	-0.57779600
H	-1.41877100	0.76494800	-0.17000500
C	-4.58763800	-2.07687100	-0.56089900
H	-3.74157800	-0.08513800	-0.54841700
H	-2.83503800	-1.24719200	-1.52260200
H	-5.22178000	-1.87879000	-1.43007500
H	-4.26590400	-3.12213500	-0.60404300
H	-5.20103200	-1.94288800	0.33511200
H	1.20764000	-2.99467700	-1.17790600
C	1.35009600	-1.97706100	-1.51822500
C	0.41950000	-1.19398000	-2.26680000
C	2.53160700	-1.21089400	-1.36430400
C	1.02730300	0.04901400	-2.55740000
H	-0.56209600	-1.50901600	-2.59721200
C	2.32346300	0.05542200	-1.97622900
H	3.43718600	-1.54038100	-0.87332400
H	0.58069000	0.85890900	-3.11757400
H	3.03770700	0.86727300	-2.02570100
C	-2.89920700	-0.86085100	1.92830400
H	-2.23010700	-1.14721000	2.74247100
H	-3.89338100	-1.26494800	2.15437500
H	-3.00768000	0.23112200	1.92190400
C	1.97731500	-1.06158100	1.90535600
C	0.78743100	-0.56498800	2.49182600
C	2.73602900	0.06323500	1.45461100
H	2.28727200	-2.09808600	1.86544700
C	0.77823900	0.84715600	2.36261300
H	0.02035700	-1.16009000	2.96723300
C	1.99977100	1.23664700	1.74420000
H	3.72522200	0.03187500	1.01820900
H	0.00511700	1.51608500	2.71976600
H	2.31863600	2.24887800	1.54140200
H	0.71048600	2.53662100	-1.43885800
C	0.29962900	2.10593500	-0.52630100
C	-1.18708700	1.76994900	-0.64624600
H	0.46651800	2.81411800	0.28712400
C	-2.15809600	2.75763700	0.03648800
H	-1.47866300	1.62015600	-1.69258400
C	-2.16817500	4.13083100	-0.64214200
H	-3.17309600	2.33854700	0.02603200
H	-1.87231500	2.86524900	1.09168200
H	-2.86976000	4.80347200	-0.13852700
H	-1.17813600	4.59799300	-0.61724000
H	-2.47741100	4.05102700	-1.69095900
Hf	0.73366700	-0.05604600	-0.02232800

13b

C	1.46613100	2.43860400	0.05246600
C	2.42965700	1.55817000	-0.30330700
H	-0.99776600	1.54141400	0.09000400
H	1.32424700	2.65126000	1.11389900
C	3.46404400	0.95318000	0.60965600
H	2.62077200	1.42457800	-1.36961600
C	4.84039400	1.61222400	0.37977300
H	3.17348600	1.07947000	1.65836700

H	3.56084000	-0.12480800	0.42528100
H	5.59275000	1.15180000	1.02779700
H	5.17183200	1.49294800	-0.65762100
H	4.80502500	2.68314200	0.60310000
H	1.20718200	0.62402700	2.62494600
C	0.63800700	-0.25164300	2.34491400
C	-0.76919700	-0.39100900	2.45541200
C	1.16522800	-1.45924000	1.81870400
C	-1.11783900	-1.70086900	2.02877100
H	-1.45459100	0.36066600	2.82563300
C	0.07239200	-2.36083200	1.63154500
H	2.20979800	-1.68274100	1.64975200
H	-2.11227600	-2.12474300	2.01640700
H	0.14417800	-3.38931600	1.30481300
C	0.75862800	3.35849700	-0.90723800
H	1.22958900	4.34947100	-0.85559000
H	-0.29696500	3.50731100	-0.66215800
H	0.83637100	3.01475100	-1.94386500
C	1.43892900	-1.24606100	-1.75598100
C	0.56191600	-0.33448500	-2.41957600
C	0.69168500	-2.40967400	-1.44045200
H	2.49799000	-1.10968300	-1.58467900
C	-0.71576700	-0.93476900	-2.49787800
H	0.83223000	0.62925000	-2.83131300
C	-0.64834200	-2.20761800	-1.86902700
H	1.08154000	-3.30223500	-0.97014100
H	-1.59483900	-0.49851200	-2.95220900
H	-1.46508000	-2.91123800	-1.77045100
H	-2.97529400	-0.48252600	-1.05111000
C	-2.42982700	-0.12763000	-0.17804900
C	-2.06735900	1.35317900	-0.27216800
H	-3.02940600	-0.33049000	0.71011500
C	-2.91686100	2.32498900	0.57530400
H	-2.03821700	1.69097700	-1.31444100
C	-4.36063900	2.42092400	0.07261600
H	-2.90608200	1.98865200	1.62002800
H	-2.45580600	3.32110200	0.56155200
H	-4.93393900	3.12008900	0.68955200
H	-4.39684200	2.78237900	-0.96171800
H	-4.86419800	1.44923700	0.10921500
Hf	-0.21907800	-0.53447000	-0.02859000

Hf/Hex

13a

C	5.19841500	-2.77851000	-1.01321000
H	5.80384300	-2.48761100	-0.14662000
H	5.79217100	-3.47481300	-1.61400800
H	5.02775300	-1.87983200	-1.61860100
C	3.87599000	-3.41787700	-0.57869400
H	3.30937700	-3.73301200	-1.46611200
H	4.07979700	-4.33298100	-0.00601300
C	3.00796500	-2.47767700	0.27049600
H	3.57472400	-2.17264000	1.15940500
H	2.80358900	-1.56052900	-0.29894800
C	1.68104400	-3.13622900	0.69244900
H	1.14190700	-3.49306300	-0.19371700
H	1.92166400	-4.04060900	1.27528200
C	0.74796500	-2.32592300	1.56344100
H	0.81048300	0.10568900	0.38314700
C	-0.59480300	-2.33387100	1.34272900
H	-1.28019600	-1.98468400	2.10758800
H	-1.01204100	-2.98287000	0.58034900
H	-0.63313500	2.33315100	2.13549000
C	-1.51651600	1.79466500	1.81748800
C	-2.44917200	2.22539700	0.83439400
C	-1.95870100	0.55036900	2.32683400
C	-3.45992000	1.23751600	0.73197000
H	-2.40512900	3.15078100	0.27673800
C	-3.14749300	0.18237700	1.64066400
H	-1.47729100	-0.00944500	3.11710300
H	-4.34224500	1.30179700	0.11080600
H	-3.74814200	-0.69947400	1.82381200

H	-0.43049300	-2.47305100	-1.72280400
C	-1.17639500	-1.69921900	-1.84842000
C	-2.51210400	-1.72481000	-1.34616500
C	-1.00164600	-0.49742100	-2.57120800
C	-3.15880000	-0.54069800	-1.78798800
H	-2.97527300	-2.52800000	-0.78776000
C	-2.21919500	0.23390400	-2.51851200
H	-0.09627300	-0.18432900	-3.07343700
H	-4.19569200	-0.28704100	-1.61721700
H	-2.40383800	1.19453800	-2.98153400
C	1.34847300	-1.63611500	2.75873700
H	0.59013700	-1.18158400	3.40102400
H	2.06534800	-0.86200400	2.46150600
H	1.91286400	-2.36184900	3.35867700
H	2.38005100	3.37907000	-0.86482100
C	3.06159900	2.64758400	-0.41008000
C	4.15386000	3.38698700	0.37544300
H	3.52204700	2.09617200	-1.24303400
C	2.25969800	1.66948000	0.45966900
C	4.95515700	4.36251000	-0.49292400
H	4.83527700	2.65339500	0.82864700
H	3.69229800	3.93269400	1.21049500
H	2.94786700	0.94345100	0.91378900
H	1.78595800	2.21352800	1.28839600
C	1.17376900	0.91516800	-0.33621100
H	4.30541200	5.12848800	-0.93293700
H	5.72273600	4.87559300	0.09574700
H	5.45949700	3.84128700	-1.31539000
H	1.63776500	0.33368900	-1.14119000
C	0.01094300	1.75384000	-0.86508800
H	-0.04829300	2.71425800	-0.35106300
H	0.08670000	1.94308600	-1.93511300
Hf	-1.38669500	0.14222300	-0.13184100

13b

C	1.10228400	2.22658700	-0.53636000
C	2.16887900	1.42808200	-0.77401300
H	-1.19012300	1.03256200	-0.25671800
H	0.95756900	2.61235900	0.47464200
C	3.29995500	1.14534400	0.17763900
H	2.34907000	1.12705100	-1.80749400
C	4.56548100	1.94124300	-0.22128500
H	3.02034200	1.41111300	1.20362400
H	3.55361300	0.07637200	0.17468600
H	4.83324900	1.70380400	-1.26039400
H	4.33406900	3.01431800	-0.19929900
H	1.14291200	0.93492700	2.33478900
C	0.70298700	-0.04895300	2.24848800
C	-0.66551700	-0.36071200	2.44955500
C	1.39109500	-1.24837100	1.92966700
C	-0.82719900	-1.76332500	2.28789200
H	-1.44616000	0.34400300	2.70552600
C	0.43897700	-2.31302600	1.96487800
H	2.45339100	-1.34999000	1.75446500
H	-1.74902600	-2.31684000	2.40006600
H	0.65384300	-3.36440100	1.83022500
C	0.25601100	2.85556600	-1.61177400
H	0.59575800	3.88860800	-1.76677000
H	-0.80300000	2.91754000	-1.34531500
H	0.34994900	2.33466500	-2.57024900
C	1.54611300	-1.70660000	-1.63354000
C	0.53877100	-1.06040100	-2.41301300
C	0.97038500	-2.87284000	-1.06754800
H	2.58061800	-1.40430400	-1.54204300
C	-0.64828900	-1.82212700	-2.31250800
H	0.66728600	-0.16907900	-3.01341000
C	-0.39476800	-2.93015400	-1.45938700
H	1.48832200	-3.60078700	-0.45802400
H	-1.58955400	-1.59634100	-2.79485700
H	-1.10701200	-3.69868200	-1.18745400
H	-2.91615800	-1.40051600	-0.85836500
C	-2.40132500	-0.81449000	-0.09864800
C	-2.24679500	0.65310700	-0.48988100

H	-2.94116600	-0.91789900	0.84322700
C	-3.16782900	1.66107700	0.22918100
H	-2.31651300	0.78606200	-1.57549500
C	-4.64049000	1.50320400	-0.17377200
H	-3.06533500	1.52890700	1.31478100
H	-2.83796000	2.68507000	0.00671800
H	-4.73338300	1.63385700	-1.26182800
H	-4.97184800	0.47874500	0.04307300
C	-5.56430900	2.50068600	0.53954500
H	-5.23153300	3.52481800	0.32039900
H	-5.46490100	2.37229700	1.62663500
C	-7.03437100	2.34208500	0.13755000
H	-7.66680400	3.06504600	0.66315000
H	-7.17141900	2.50021000	-0.93880000
H	-7.40574000	1.33844700	0.37692000
C	5.76154500	1.64825500	0.69536100
H	5.98451400	0.57217700	0.66690300
H	5.48708300	1.87851100	1.73432600
C	7.01307300	2.44242600	0.30748600
H	7.84768700	2.21168200	0.97753500
H	7.33193400	2.20838700	-0.71507700
H	6.83110900	3.52217300	0.36164600
Hf	-0.15059300	-0.89340100	0.00951600