

C-H and C-O Bond Activation with a Rhodium(I) β -Diiminate Complex

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Reaction of 1a with epoxides - spectra of crude products.

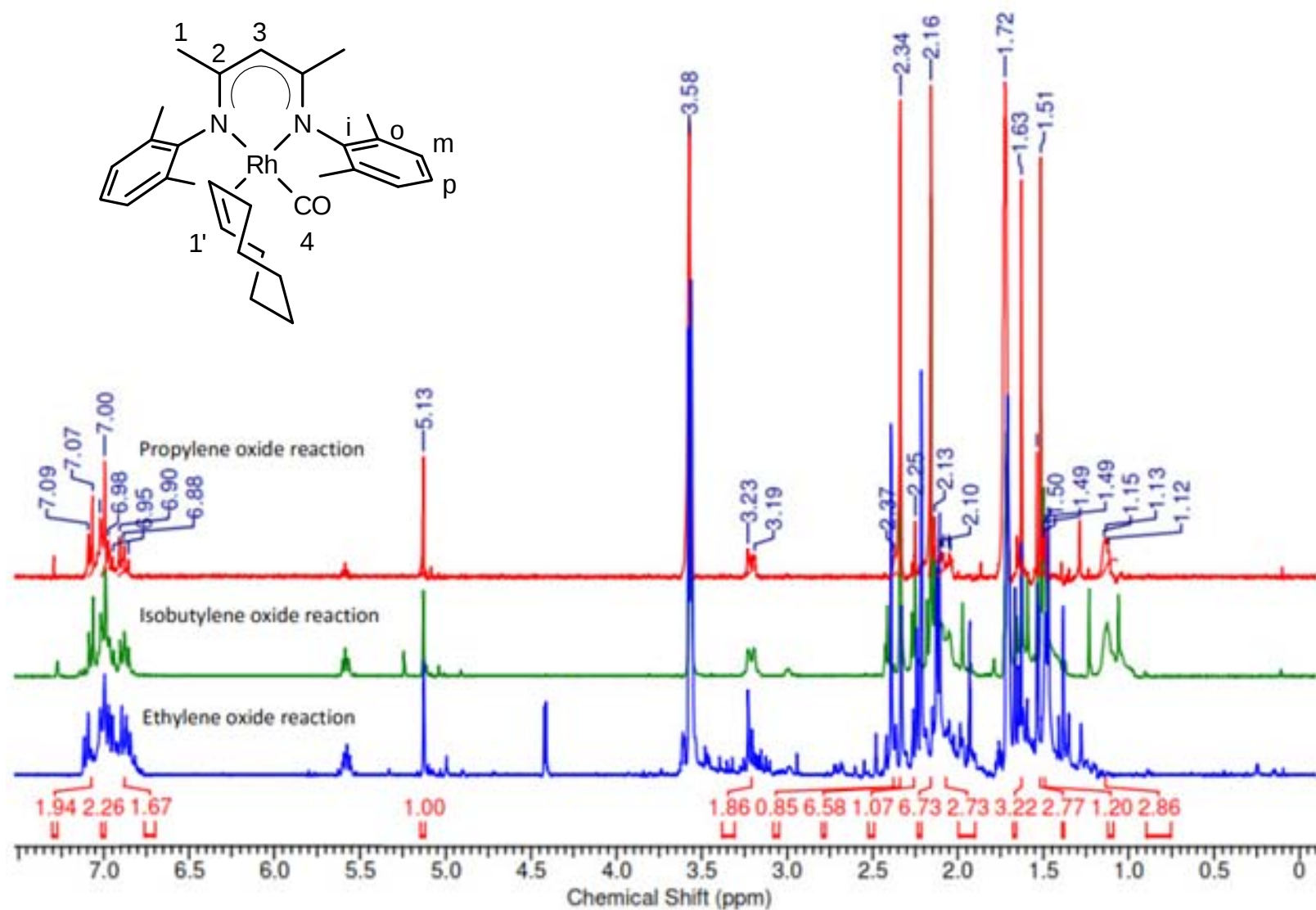


Figure S1. ^1H NMR of crude products from reaction of 1a with epoxides.

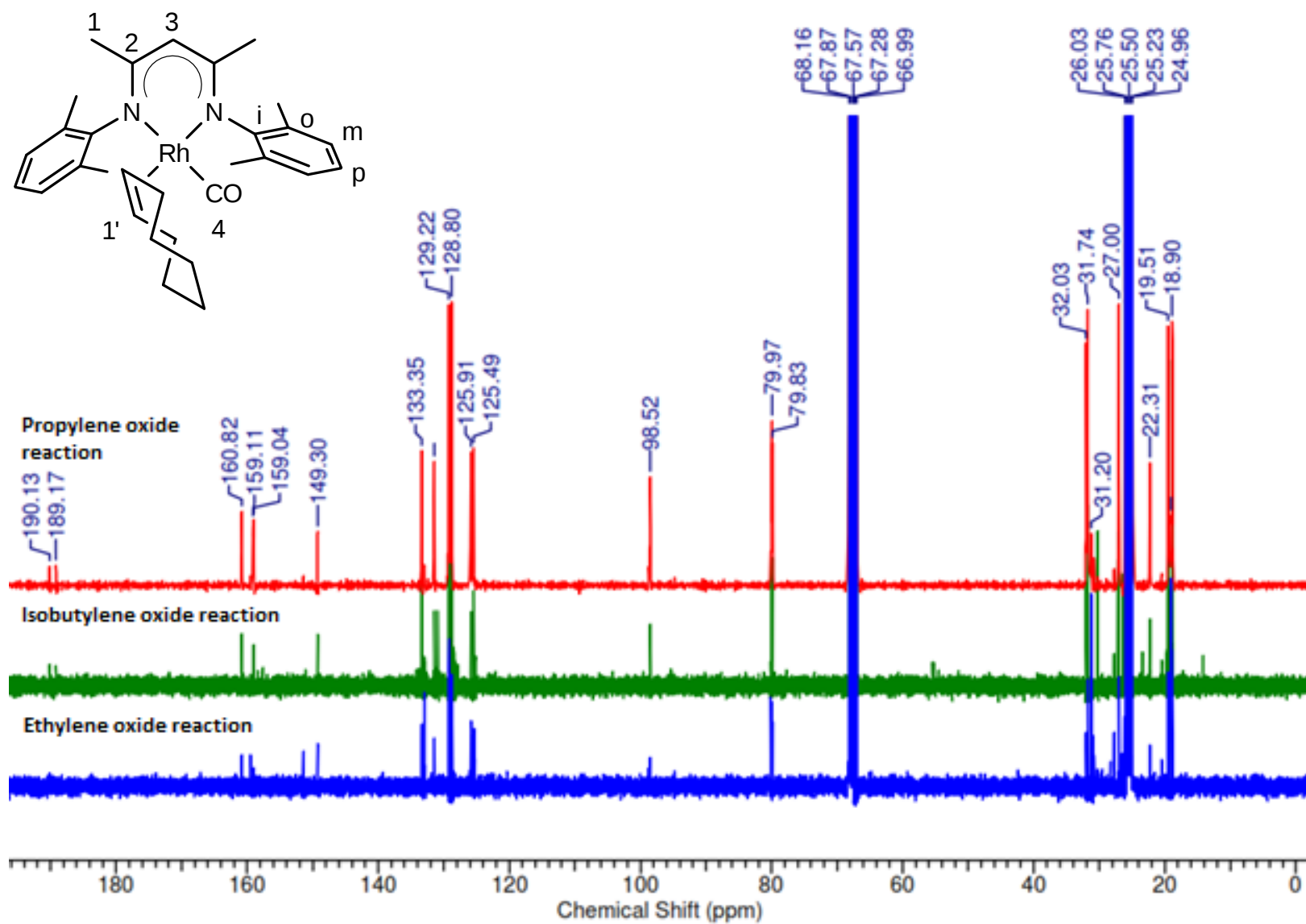


Figure S2. ^{13}C NMR of crude products from reaction of 1a with epoxides.

Epoxide opening

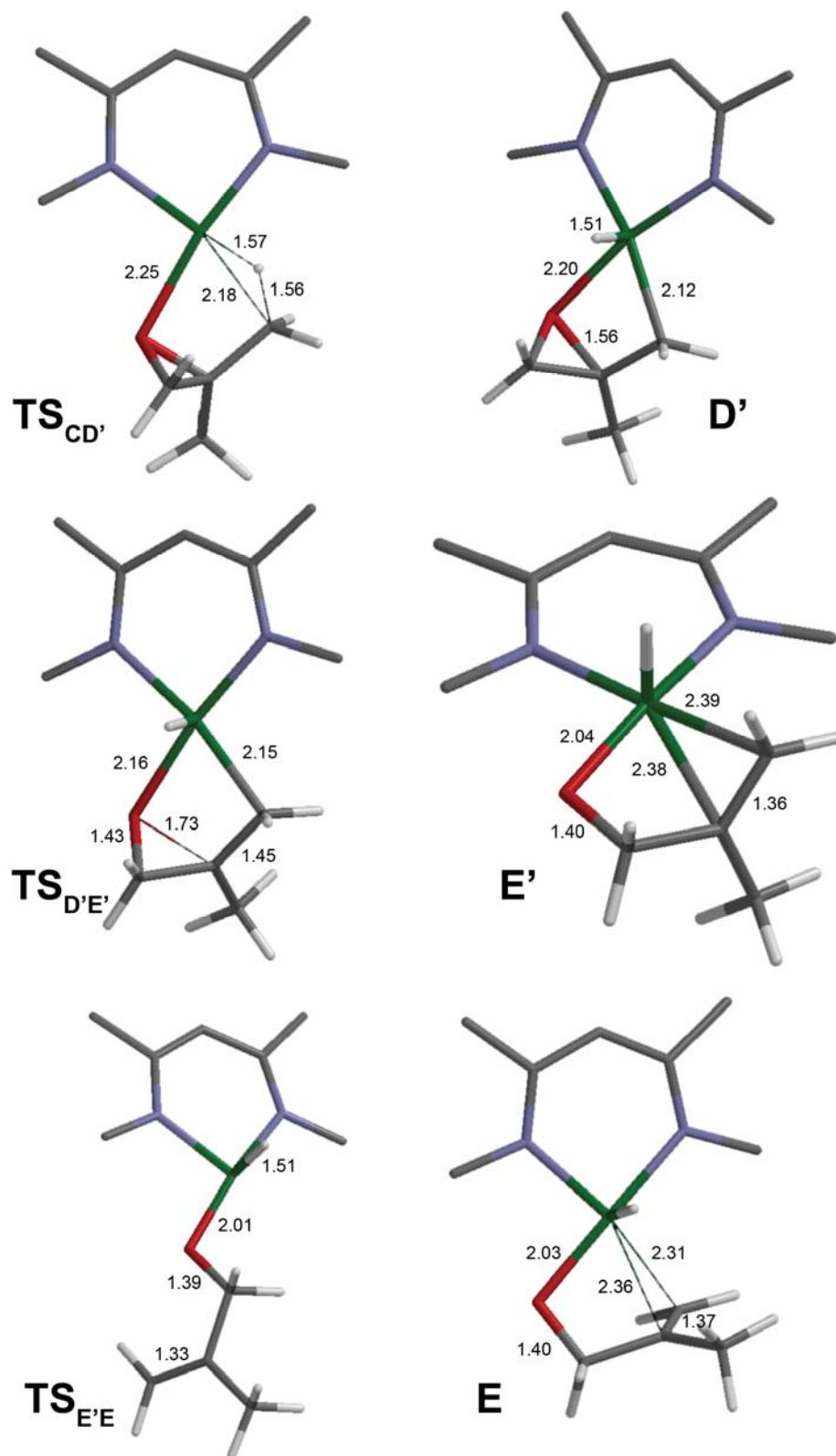
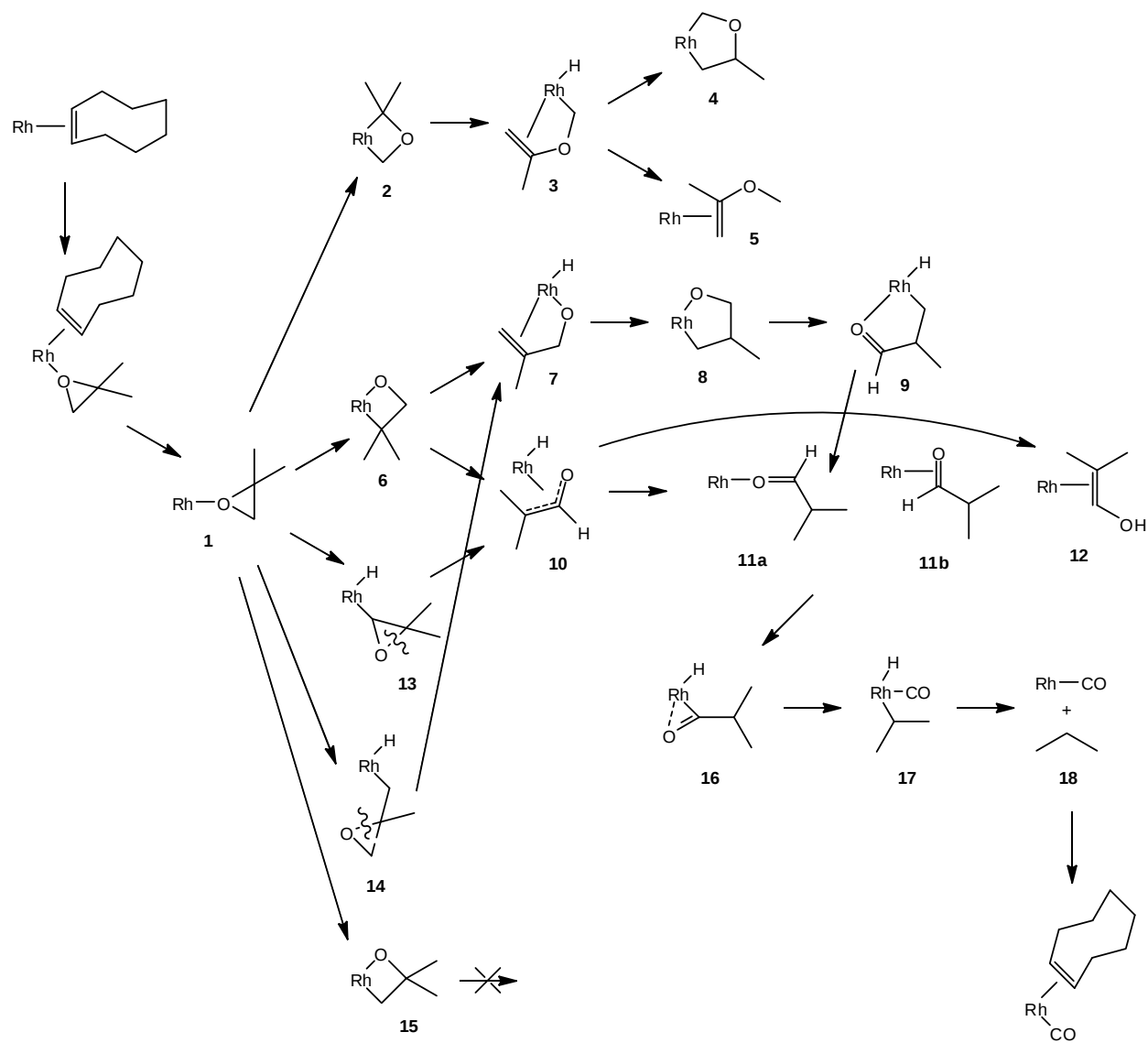


Figure S3. Diastereomeric path for opening of 2,2-dimethyloxirane.



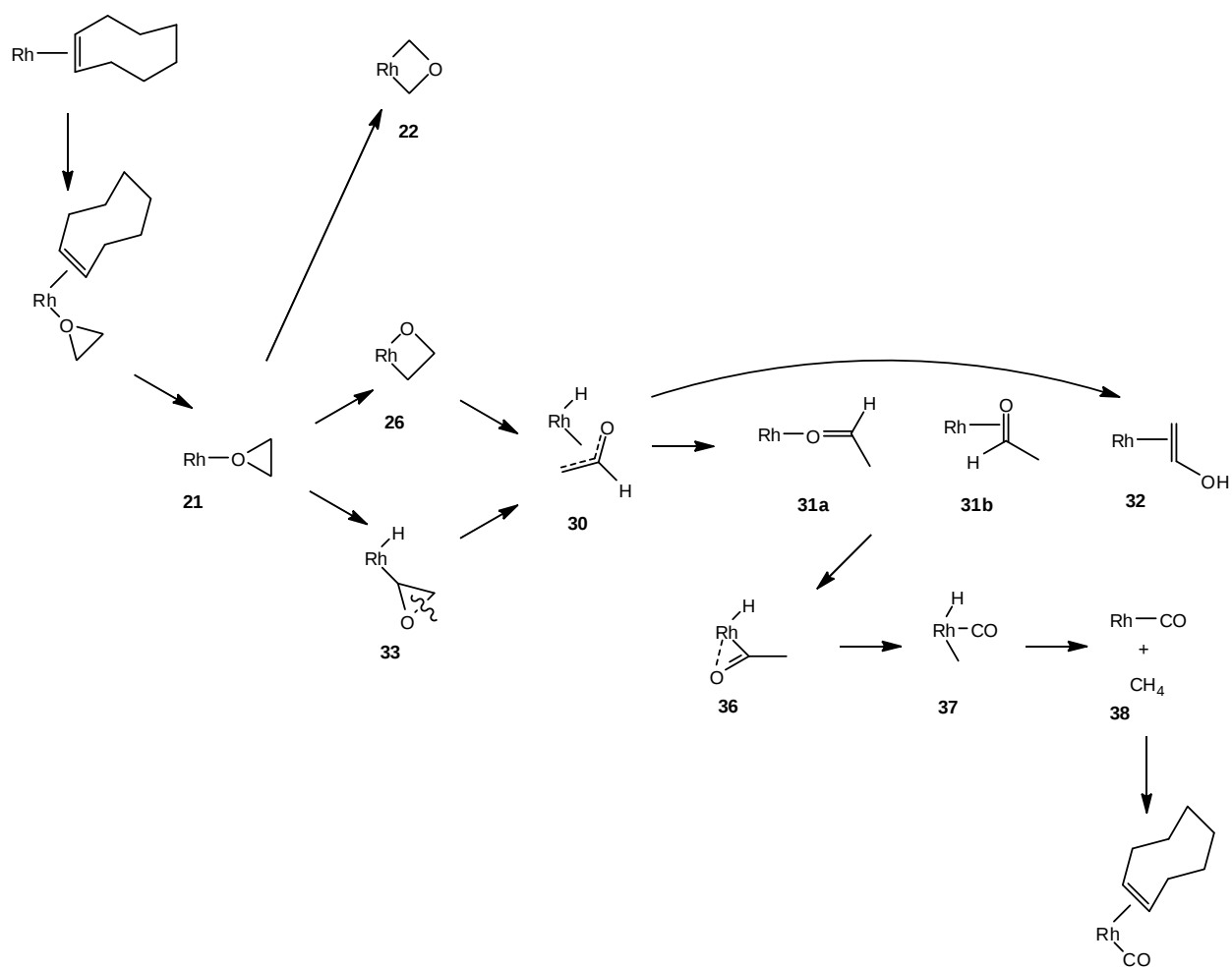


Figure S5. Compound numbering for opening of oxirane.

Table S1. Total and relative energies for epoxide opening with 1a.

Table S1. Total and relative energies for epoxide opening with Ru.								
b3-lyp/TZVP opt					b3-lyp/TZVPP/b3-lyp/TZVP			Grel
Name	E _{tot} (h)	ZPE (h)	Hcorr (h)	TScorr (h)	E _{tot} (h)	G	on scale	(kcal/mol)
COE	-313.13574	0.20329	0.21100	0.03666	-313.15034	-312.96390		
Me2Oxir	-232.36733	0.11276	0.11859	0.03121	-232.38048	-232.28280		
PrH	-119.09516	0.10309	0.10791	0.02728	-119.10090	-119.01127		
Oxir	-153.75704	0.05711	0.06079	0.02480	-153.76694	-153.72277		
MeH	-40.50108	0.04461	0.04809	0.01903	-40.50315	-40.46781		
LRh_COE	-1348.19533	0.61256	0.64284	0.08835	-1348.26115	-1347.67751	-1034.71360	0.00
LRh_COE_Oxir	-1580.54968	0.72850	0.76455	0.10010	-1580.62640	-1579.92891	-1034.68221	19.70
LRh_1	-1267.40195	0.52123	0.55035	0.08715	-1267.46500	-1266.97304	-1034.69024	14.66
LRh_TS_1_2	-1267.37977	0.52048	0.54812	0.08144	-1267.44481	-1266.95125	-1034.66845	28.33
LRh_2a	-1267.40423	0.52098	0.54883	0.08220	-1267.46862	-1266.97486	-1034.69207	13.51
LRh_2b	-1267.40426	0.52117	0.54893	0.08177	-1267.46865	-1266.97450	-1034.69170	13.74
LRh_3	-1267.40524	0.51758	0.54588	0.08327	-1267.46888	-1266.97879	-1034.69599	11.05
LRh_3a	-1267.40558	0.51877	0.54687	0.08240	-1267.46913	-1266.97748	-1034.69468	11.88
LRh_3b	-1267.40614	0.51807	0.54632	0.08307	-1267.46970	-1266.97904	-1034.69624	10.89
LRh_4	-1267.40861	0.52183	0.54967	0.08290	-1267.47105	-1266.97692	-1034.69412	12.22
LRh_TS_3_5a	-1267.39887	0.51846	0.54597	0.08081	-1267.46348	-1266.97165	-1034.68886	15.53
LRh_5	-1267.42583	0.52180	0.55003	0.08264	-1267.49113	-1266.99647	-1034.71367	-0.05
LRh_TS_1_6	-1267.36707	0.51939	0.54825	0.08593	-1267.43010	-1266.93942	-1034.65662	35.76
LRh_6	-1267.42171	0.52165	0.54941	0.08164	-1267.48591	-1266.99120	-1034.70840	3.26
LRh_6beta	-1267.42172	0.52181	0.54951	0.08124	-1267.48592	-1266.99085	-1034.70805	3.48
LRh_7	-1267.42156	0.51928	0.54737	0.08248	-1267.48493	-1266.99282	-1034.71002	2.25
LRh_TS_7_7a	-1267.40389	0.516616	0.545272	0.086779	-1267.4674	-1266.98028	-1034.69748	10.12
LRh_7a	-1267.42307	0.519068	0.547143	0.082728	-1267.4867	-1266.99494	-1034.71214	0.92
LRh_8	-1267.43194	0.52308	0.55088	0.08301	-1267.49415	-1266.99888	-1034.71609	-1.56
LRh_TS_8_9	-1267.40918	0.51814	0.54556	0.08159	-1267.47364	-1266.98274	-1034.69995	8.57
LRh_9b	-1267.43535	0.51838	0.54650	0.08294	-1267.49764	-1267.00672	-1034.72392	-6.47
LRh_TS_9_11a	-1267.42550	0.51780	0.54570	0.08280	-1267.48881	-1266.99858	-1034.71579	-1.37
LRh_TS_9_11b	-1267.42448	0.51804	0.54587	0.08258	-1267.48786	-1266.99731	-1034.71451	-0.57
LRh_TS_6_10	-1267.40167	0.52000	0.54755	0.08128	-1267.46613	-1266.97304	-1034.69024	14.66
LRh_10a	-1267.44010	0.51842	0.54703	0.08380	-1267.50421	-1267.01333	-1034.73053	-10.62
LRh_10b	-1267.43649	0.51847	0.54693	0.08320	-1267.50055	-1267.00937	-1034.72657	-8.14
LRh_TS_10_11	-1267.40750	0.51660	0.54504	0.08352	-1267.47103	-1266.98195	-1034.69915	9.07
LRh_11a	-1267.43949	0.52058	0.55021	0.08981	-1267.50184	-1267.01180	-1034.72900	-9.66
LRh_11b	-1267.45393	0.52193	0.55070	0.08513	-1267.51757	-1267.02391	-1034.74111	-17.26
LRh_TS_11_16	-1267.44402	0.51801	0.54648	0.08486	-1267.50960	-1267.01998	-1034.73718	-14.80
LRh_16	-1267.44887	0.51899	0.54793	0.08684	-1267.51379	-1267.02404	-1034.74124	-17.35
LRh_TS_16_17a	-1267.43267	0.51748	0.54599	0.08403	-1267.49874	-1267.00905	-1034.72625	-7.94
LRh_TS_16_17b	-1267.43266	0.51727	0.54589	0.08464	-1267.49873	-1267.00955	-1034.72675	-8.25
LRh_17	-1267.45587	0.51825	0.54713	0.08476	-1267.52098	-1267.03064	-1034.74784	-21.48

LRh_TS_17_18	-1267.45310	0.51746	0.54609	0.08435	-1267.51880	-1267.02922	-1034.74643	-20.60
LRh_CO	-1148.38993	0.41585	0.44053	0.07674	-1148.44925	-1148.06014	-1034.78861	-47.07
LRh_COE_CO	-1461.55104	0.62284	0.65466	0.09129	-1461.62488	-1461.03139	-1034.79596	-51.68
LRh_TS_10_12	-1267.39574	0.51558	0.54482	0.08815	-1267.45964	-1266.97389	-1034.69109	14.13
LRh_12	-1267.43703	0.52122	0.54995	0.08373	-1267.50144	-1267.00759	-1034.72479	-7.02
LRh_TS_1_13a	-1267.37599	0.51649	0.54498	0.08484	-1267.44063	-1266.95249	-1034.66969	27.55
LRh_TS_1_13b	-1267.38104	0.51634	0.54497	0.08552	-1267.44615	-1266.95848	-1034.67568	23.80
LRh_TS_1_13c	-1267.37503	0.51568	0.54411	0.08417	-1267.44102	-1266.95330	-1034.67050	27.05
LRh_TS_1_13d	-1267.36363	0.51689	0.54522	0.08408	-1267.42860	-1266.93971	-1034.65692	35.57
LRh_13	-1267.38405	0.51825	0.54692	0.08562	-1267.44815	-1266.95860	-1034.67580	23.72
LRh_TS_13_10	-1267.35918	0.51491	0.54352	0.08451	-1267.42361	-1266.93672	-1034.65392	37.45
LRh_TS_1_14a	-1267.38451	0.51789	0.54556	0.08192	-1267.44897	-1266.95829	-1034.67549	23.91
LRh_TS_1_14b	-1267.38483	0.51799	0.54566	0.08200	-1267.44931	-1266.95858	-1034.67579	23.73
LRh_14a	-1267.39754	0.51805	0.54618	0.08313	-1267.46087	-1266.97039	-1034.68759	16.32
LRh_14b	-1267.39824	0.51830	0.54633	0.08267	-1267.46143	-1266.97049	-1034.68769	16.26
LRh_14c	-1267.37718	0.51749	0.54576	0.08404	-1267.44100	-1266.95155	-1034.66875	28.15
LRh_TS_14_7a	-1267.39638	0.51751	0.54525	0.08216	-1267.45971	-1266.96951	-1034.68672	16.87
LRh_TS_14_7b	-1267.39732	0.51765	0.54535	0.08196	-1267.46048	-1266.97005	-1034.68725	16.54
LRh_TS_1_15	-1267.37659	0.51921	0.54791	0.08523	-1267.44011	-1266.94931	-1034.66651	29.55
LRh_15	-1267.43493	0.52150	0.54963	0.08337	-1267.49826	-1267.00449	-1034.72169	-5.08
LRh_COE	-1348.19533	0.61256	0.64284	0.08835	-1348.26115	-1347.67751	-1034.71360	0.00
LRh_COE_Oxir	-1501.95042	0.67329	0.70682	0.09436	-1502.02376	-1501.38016	-1034.69349	12.62
LRh_21	-1188.79349	0.46616	0.49271	0.08110	-1188.85278	-1188.41440	-1034.69163	13.79
LRh_TS_21_22	-1188.77744	0.46471	0.49060	0.07914	-1188.83793	-1188.40036	-1034.67759	22.60
LRh_22a	-1188.79624	0.46468	0.49046	0.07836	-1188.85611	-1188.41815	-1034.69538	11.44
LRh_22b	-1188.79623	0.46459	0.49044	0.07873	-1188.85611	-1188.41842	-1034.69566	11.26
LRh_TS_21_26	-1188.76683	0.46394	0.49025	0.08016	-1188.82690	-1188.39035	-1034.66759	28.88
LRh_TS_21_26a	-1188.76683	0.46407	0.49026	0.07964	-1188.82690	-1188.39000	-1034.66723	29.10
LRh_26	-1188.82816	0.46625	0.49198	0.07855	-1188.88779	-1188.44843	-1034.72567	-7.57
LRh_26b	-1188.82814	0.46629	0.49196	0.07822	-1188.88777	-1188.44822	-1034.72545	-7.43
LRh_35	-1188.82819	0.46653	0.49209	0.07760	-1188.88784	-1188.44774	-1034.72497	-7.14
LRh_TS_26_30	-1188.80639	0.46372	0.48882	0.07660	-1188.86824	-1188.43074	-1034.70798	3.53
LRh_30a	-1188.84496	0.46245	0.48844	0.07873	-1188.90569	-1188.46999	-1034.74722	-21.10
LRh_30b	-1188.84202	0.46249	0.48842	0.07821	-1188.90270	-1188.46668	-1034.74391	-19.02
LRh_TS_30_31	-1188.82075	0.45990	0.48598	0.07900	-1188.88106	-1188.44801	-1034.72525	-7.31
LRh_31a	-1188.84355	0.46381	0.49120	0.08360	-1188.90242	-1188.46723	-1034.74446	-19.36
LRh_31b	-1188.85879	0.46536	0.49180	0.07977	-1188.91915	-1188.48080	-1034.75803	-27.88
LRh_TS_31_36	-1188.84790	0.46120	0.48742	0.07965	-1188.90998	-1188.47592	-1034.75316	-24.82
LRh_36	-1188.85313	0.46220	0.48884	0.08091	-1188.91444	-1188.47981	-1034.75705	-27.26
LRh_TS_36_37a	-1188.84348	0.46091	0.48695	0.07872	-1188.90654	-1188.47232	-1034.74956	-22.56
LRh_TS_36_37b	-1188.84347	0.46077	0.48686	0.07896	-1188.90652	-1188.47256	-1034.74980	-22.71
LRh_37	-1188.86964	0.46105	0.48767	0.07979	-1188.93114	-1188.49692	-1034.77416	-38.00
LRh_TS_37_38	-1188.86587	0.46049	0.48685	0.07948	-1188.92819	-1188.49459	-1034.77182	-36.53

LRh_CO	-1148.38993	0.41585	0.44053	0.07674	-1148.44925	-1148.06014	-1034.80518	-57.47
LRh_COE_CO	-1461.55104	0.62284	0.65466	0.09129	-1461.62488	-1461.03139	-1034.81253	-62.08
LRh_TS_30_32	-1188.80904	0.46093	0.48656	0.07755	-1188.87094	-1188.43635	-1034.71358	0.01
LRh_32	-1188.84471	0.46559	0.49191	0.07969	-1188.90545	-1188.46693	-1034.74416	-19.18
LRh_TS_21_33a	-1188.76696	0.46113	0.48717	0.08001	-1188.82847	-1188.39491	-1034.67215	26.02
LRh_TS_21_33b	-1188.77093	0.46134	0.48734	0.07973	-1188.83265	-1188.39873	-1034.67596	23.62
LRh_TS_21_33c	-1188.76813	0.46135	0.48712	0.07862	-1188.83000	-1188.39556	-1034.67280	25.61
LRh_TS_21_33d	-1188.76419	0.46098	0.48678	0.07878	-1188.82635	-1188.39235	-1034.66958	27.62
LRh_33	-1188.77561	0.46332	0.48924	0.07926	-1188.83623	-1188.40010	-1034.67734	22.76
LRh_TS_33_30	-1188.74146	0.45968	0.48562	0.07872	-1188.80190	-1188.36901	-1034.64625	42.27

Table S2. Solvent effects on ring opening vs C-H activation.^a

	Gas phase	rel (kcal/mol)	THF	rel (kcal/mol)
LRh_1	-1267.46500	0.00	-1267.47405	0.00
LRh_6	-1267.48591	-13.12	-1267.49893	-15.61
LRh_6beta	-1267.48592	-13.13	-1267.49895	-15.62
LRh_14a	-1267.46087	2.59	-1267.47039	2.30
LRh_14b	-1267.46143	2.24	-1267.47056	2.19
LRh_TS_1_6	-1267.43010	21.90	-1267.44067	20.95
LRh_TS_1_14a	-1267.44897	10.06	-1267.45869	9.64
LRh_TS_1_14b	-1267.44931	9.85	-1267.45840	9.82

^a Total energies, b3-lyp/TZVPP//b3-lyp/TZVP, for gas phase and COSMO solvent correction ($\epsilon = 7.6$).

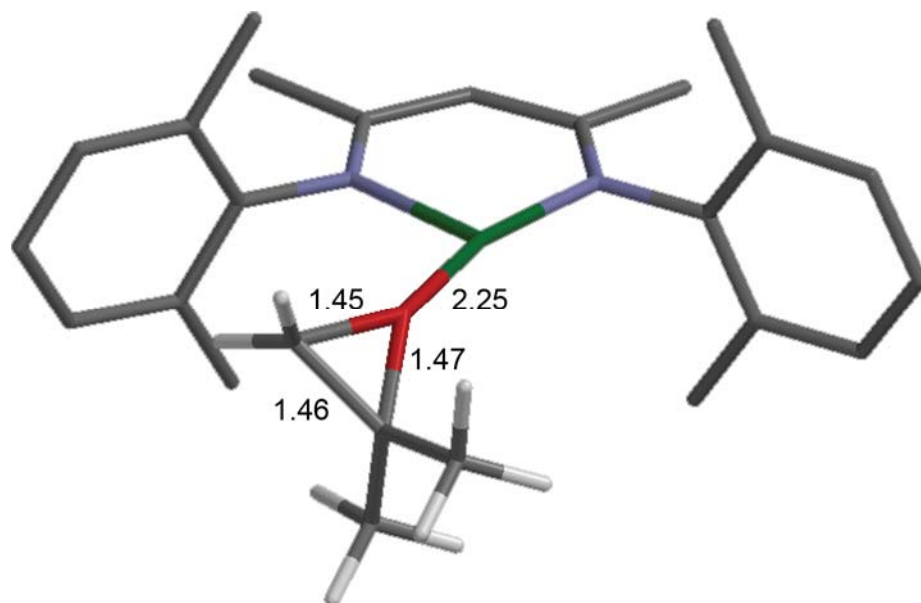


Figure S6. Structure of 1.

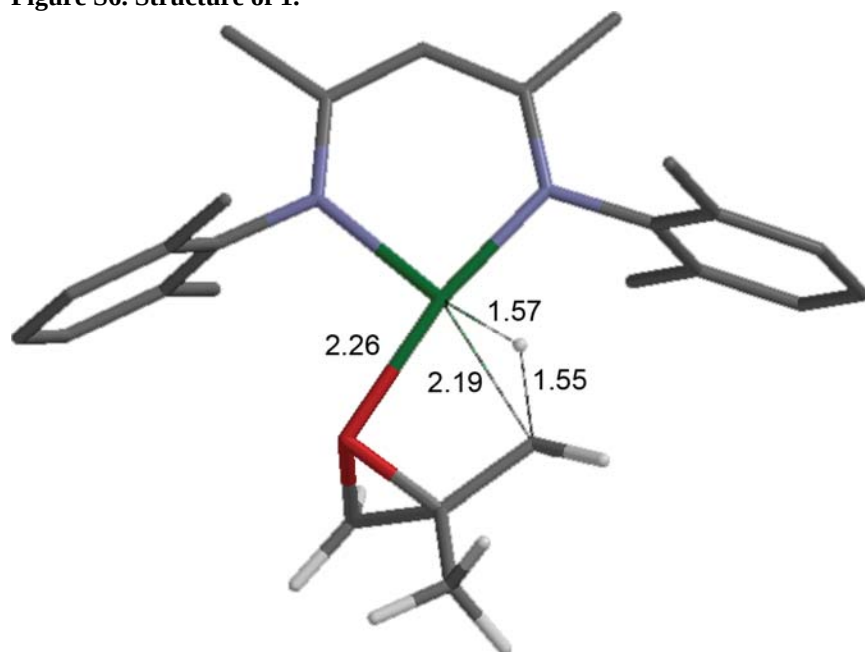


Figure S7. Structure of TS_1_14.

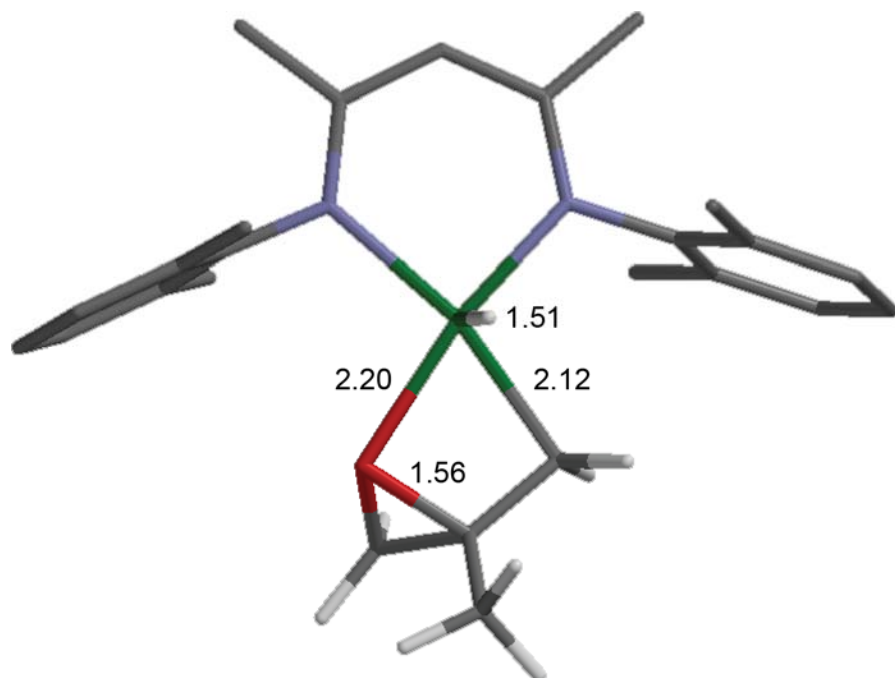


Figure S8. Structure of 14.

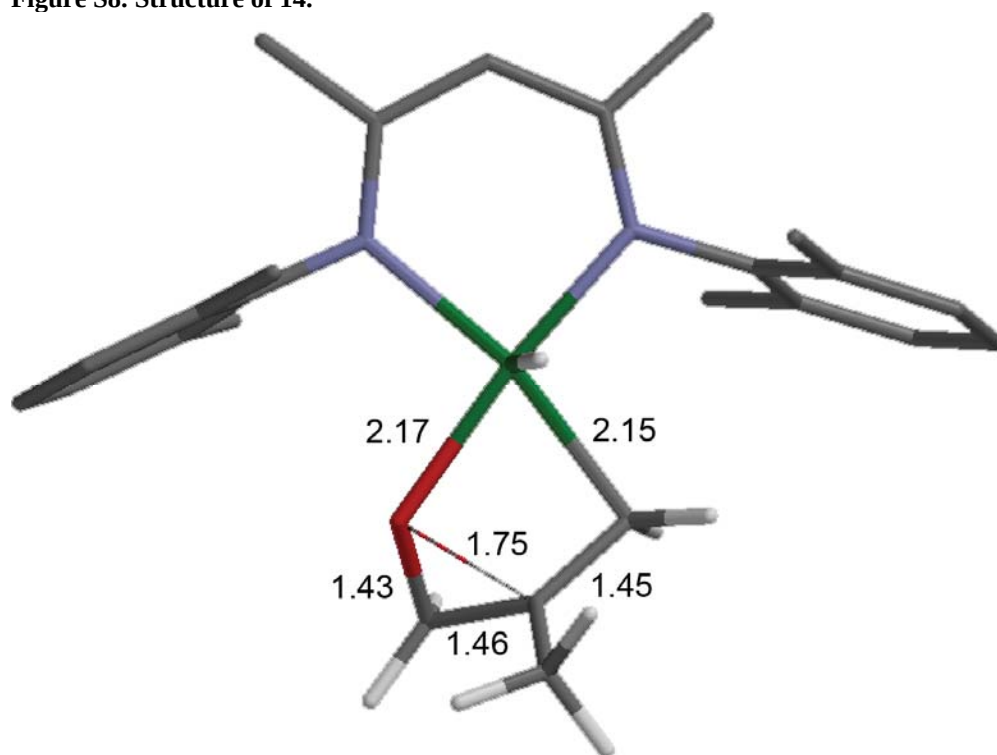


Figure S9. Structure of TS_14_7.

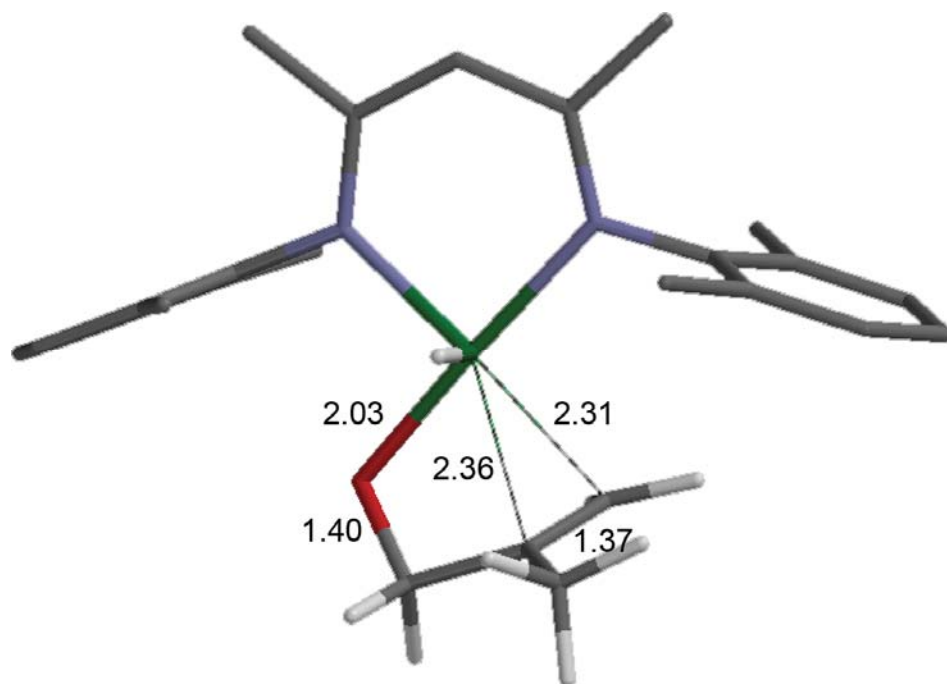


Figure S10. Structure of 7.

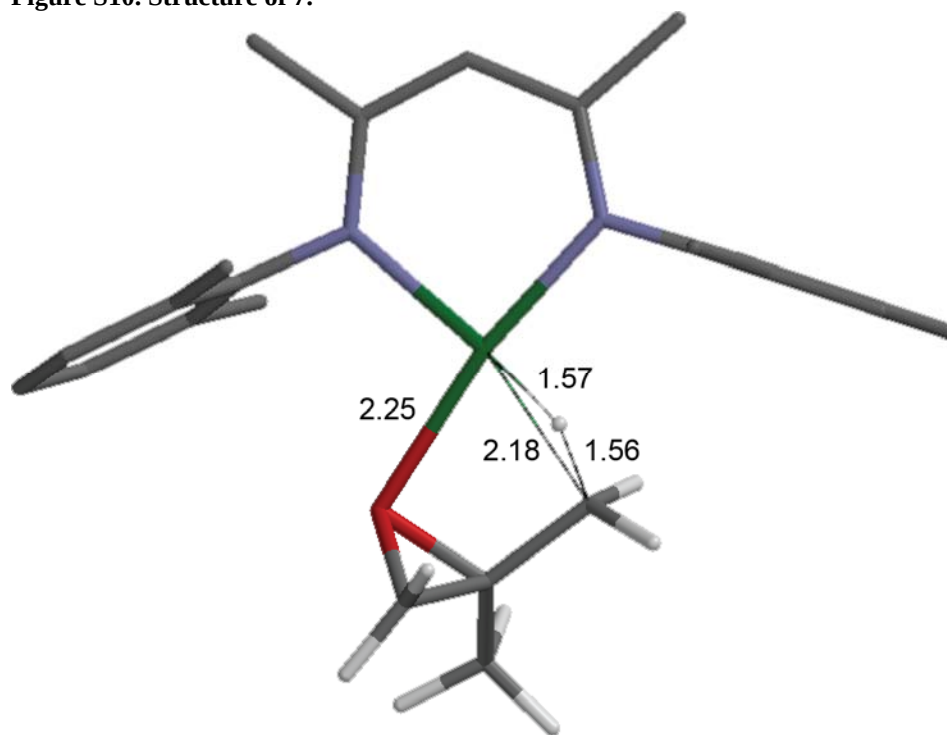


Figure S11. Structure of TS_1_14'.

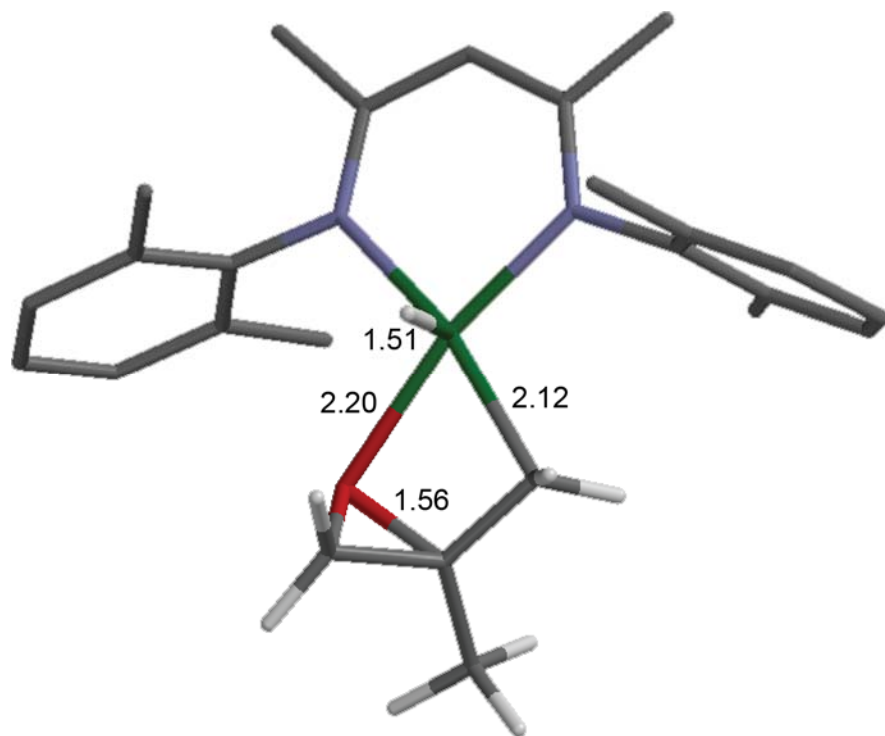


Figure S12. Structure of 14'.

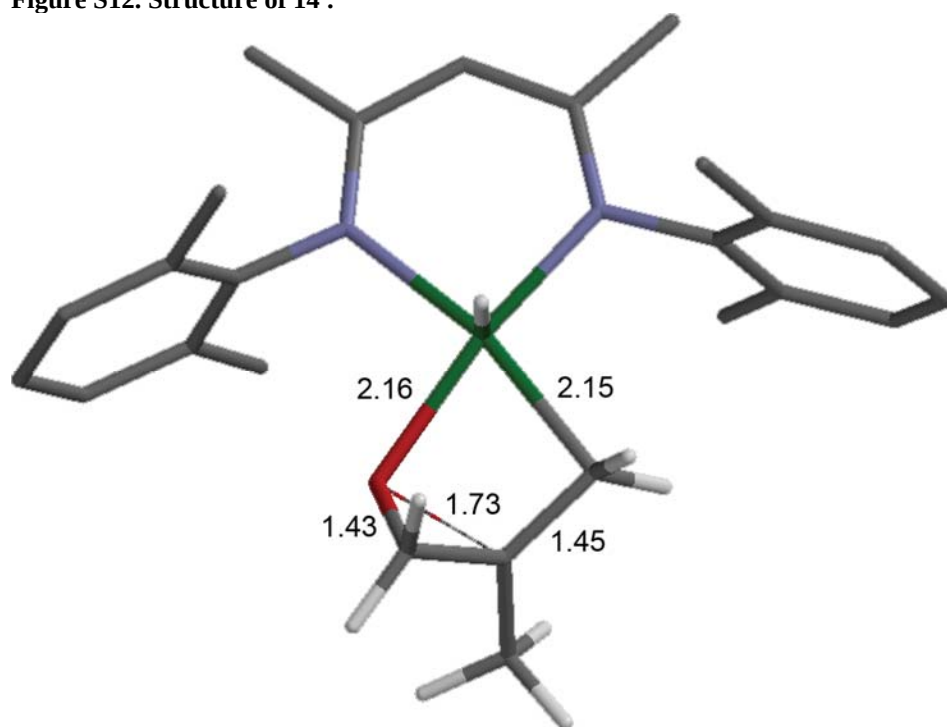


Figure S13. Structure of TS_14'_7'.

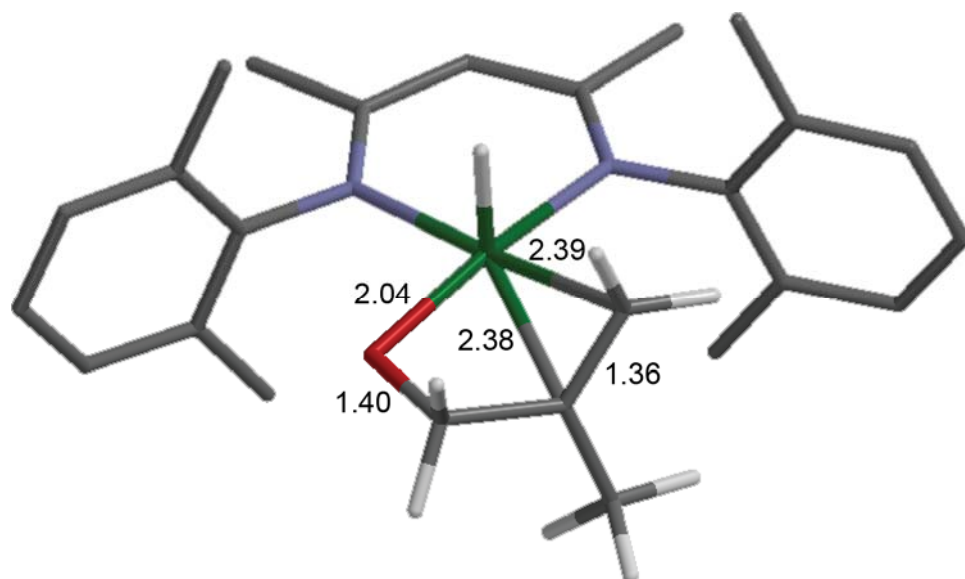


Figure S14. Structure of 7'.

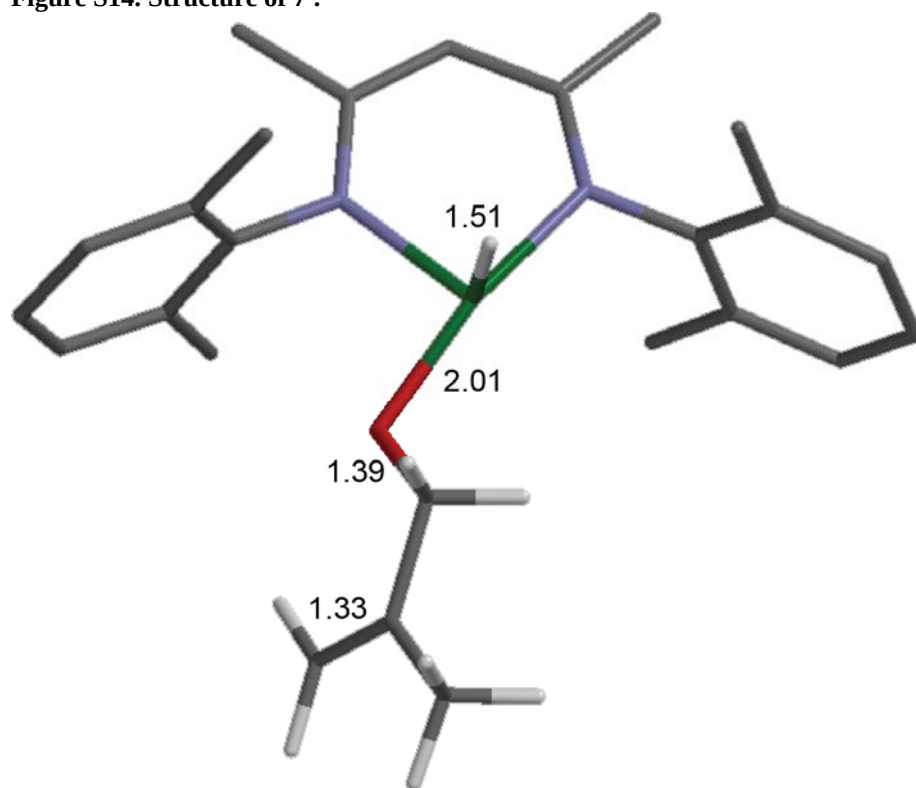


Figure S15. Structure of TS_{7'_7}.

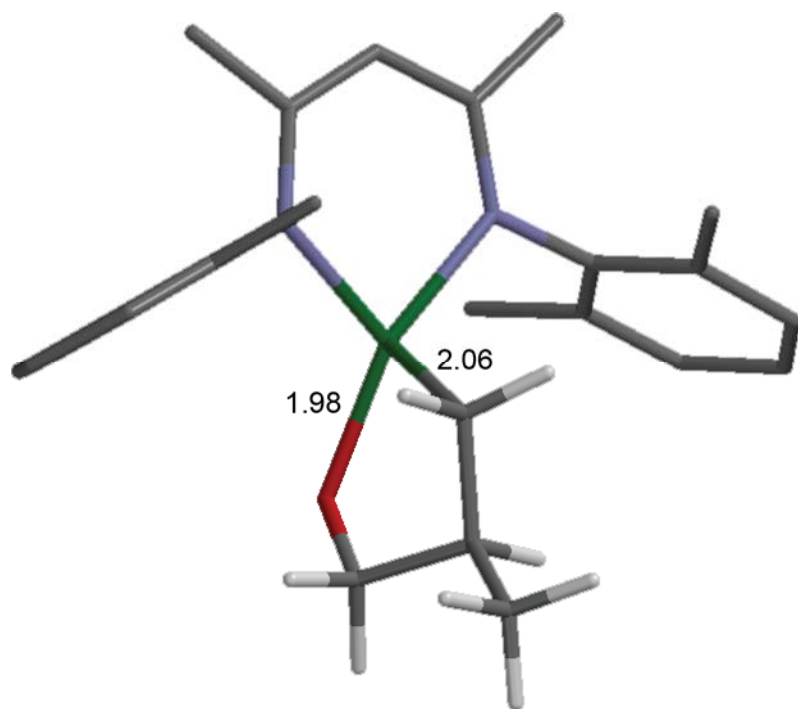


Figure S16. Structure of 8.

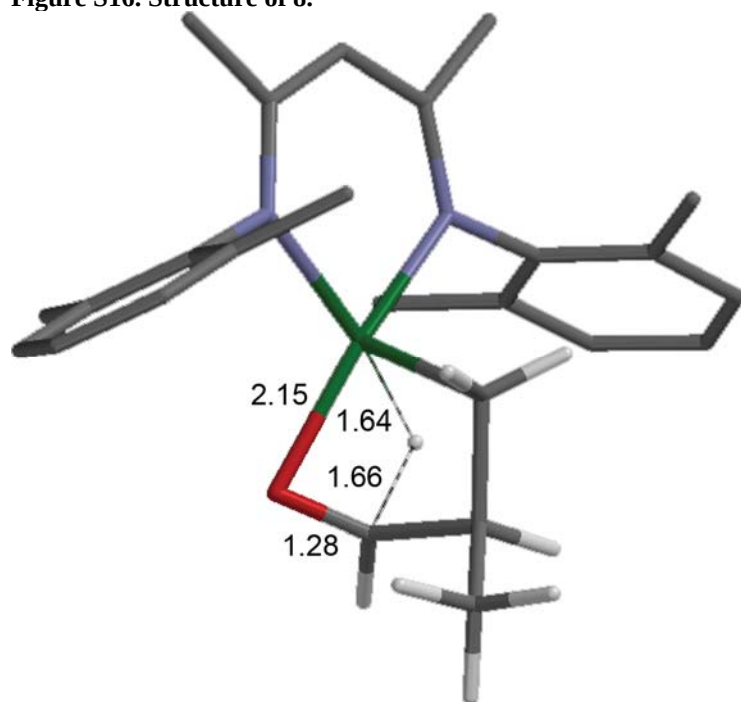


Figure S17. Structure of TS_8_9.

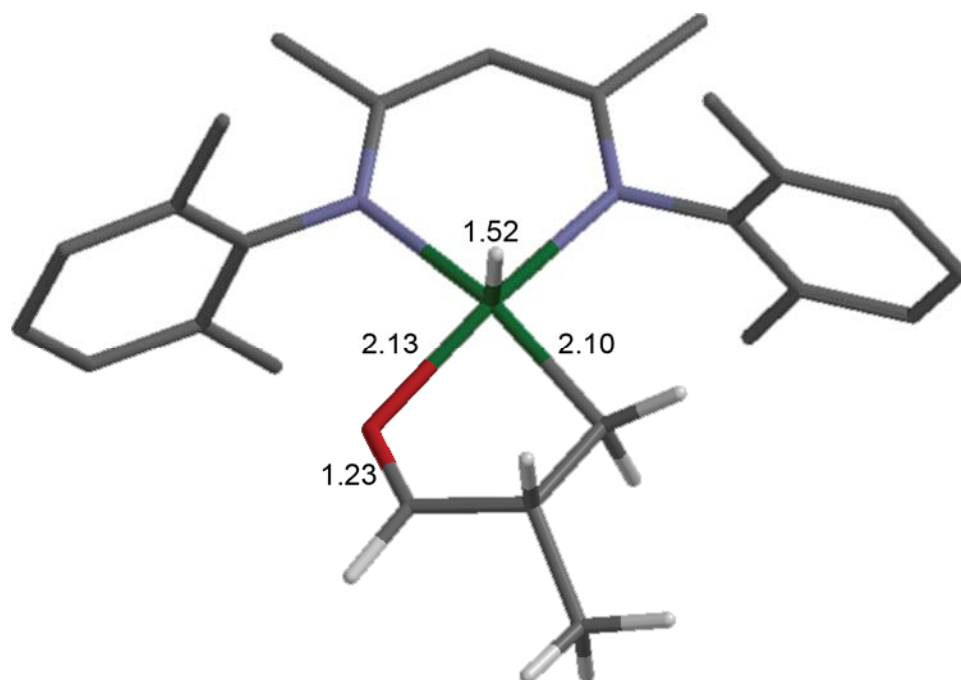


Figure S18. Structure of 9.

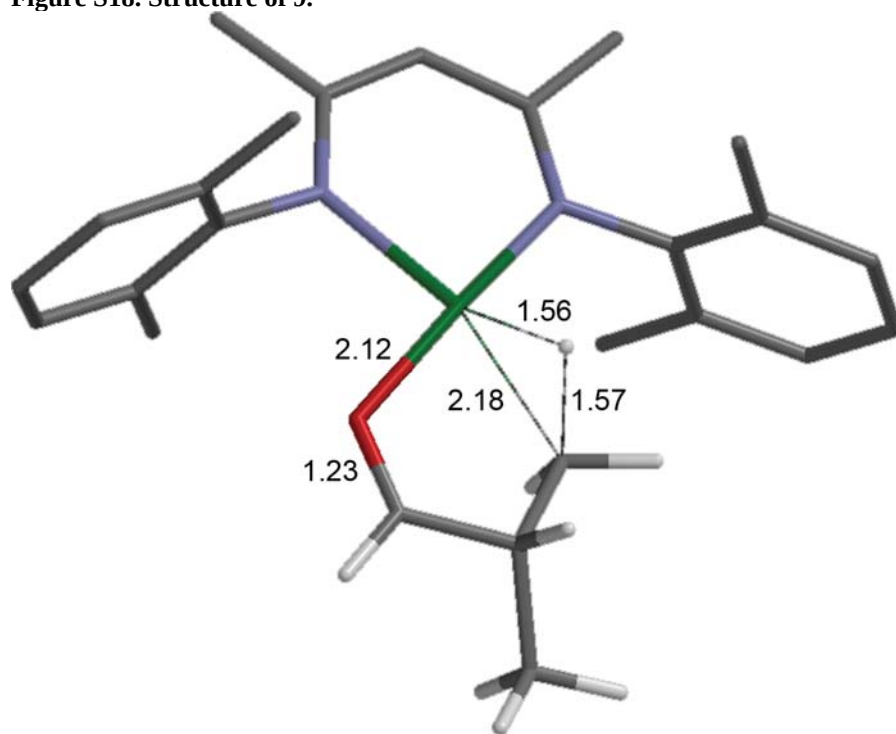


Figure S19. Structure of TS_9_11.

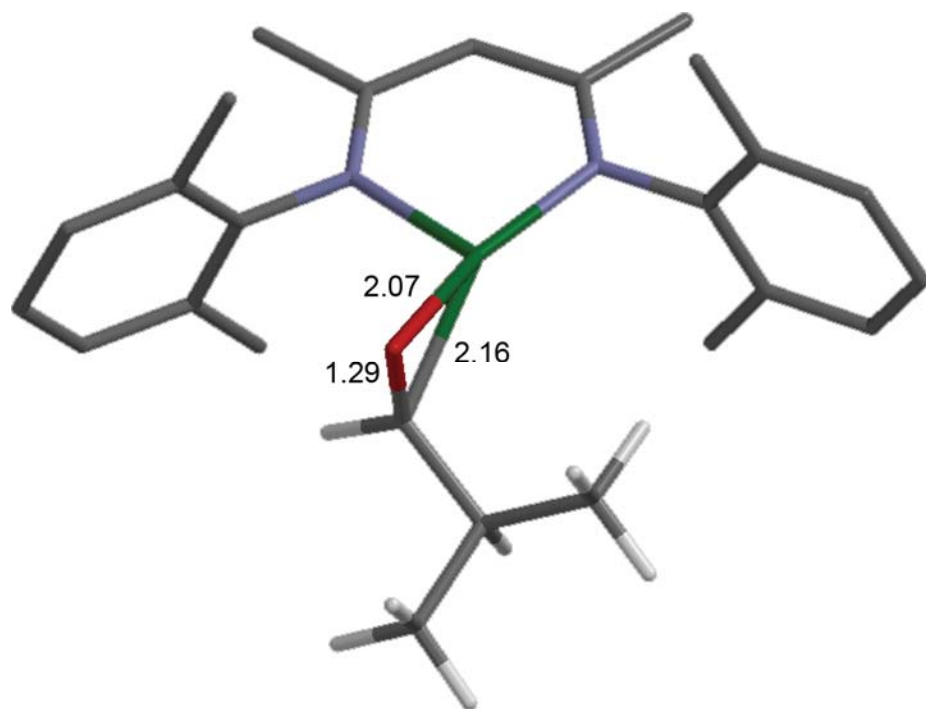


Figure S20. Structure of 11.

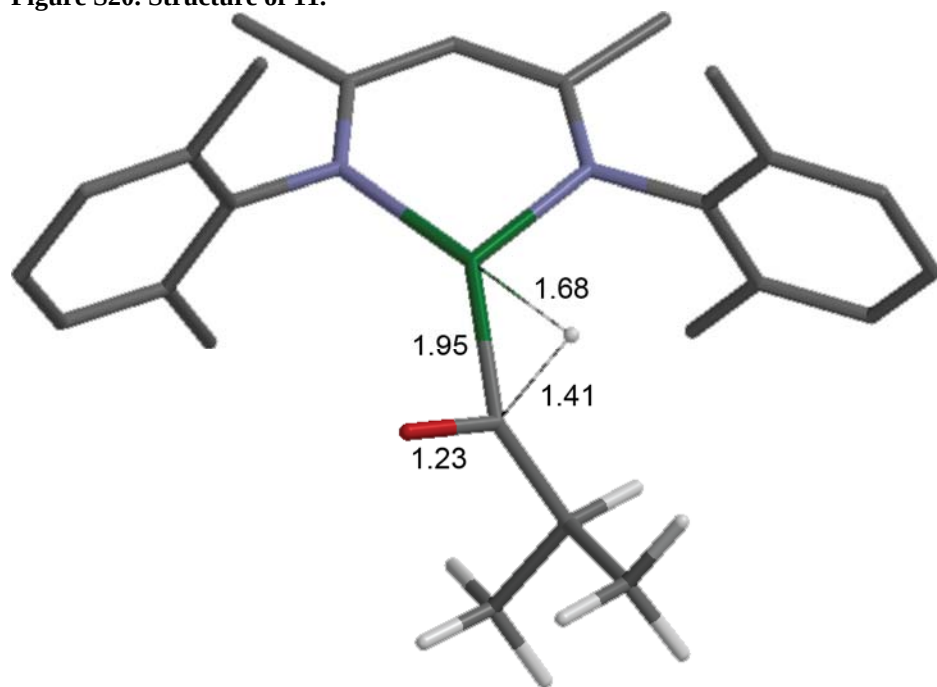


Figure S21. Structure of TS_11_16.

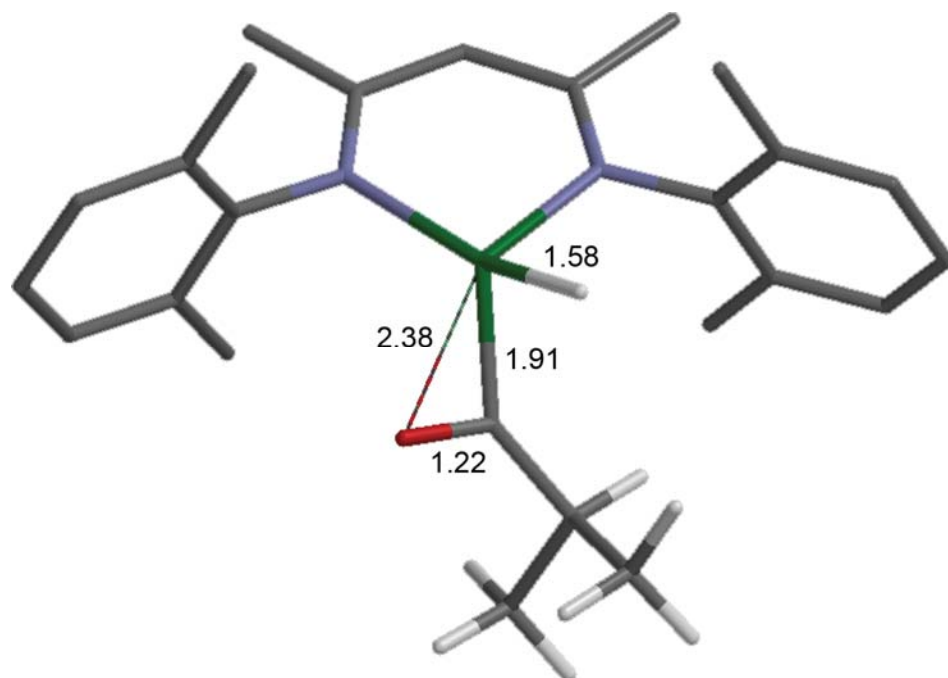


Figure S22. Structure of 16.

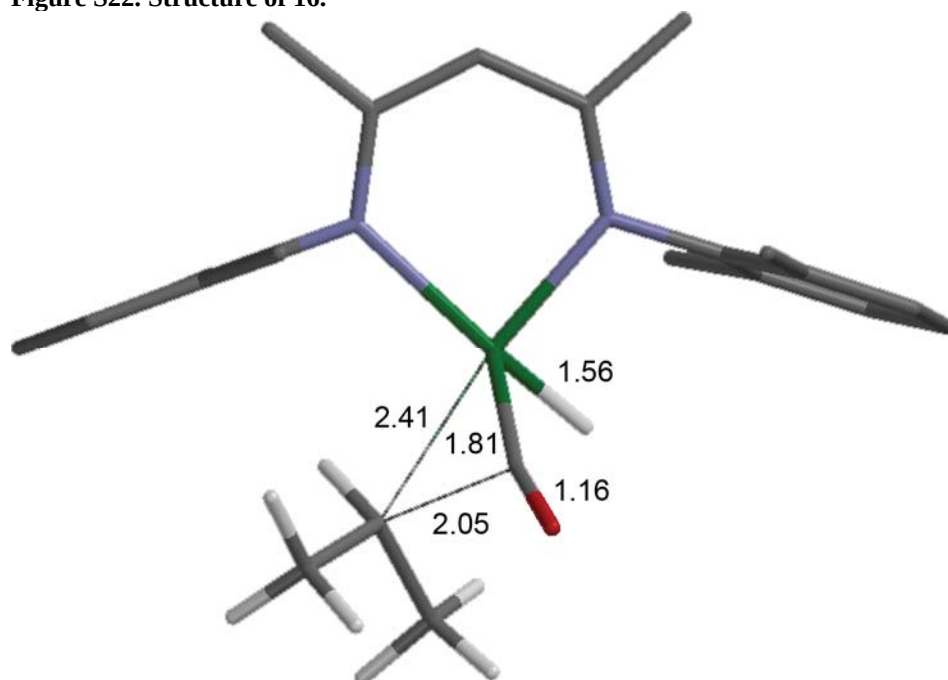


Figure S23. Structure of TS_16_17.

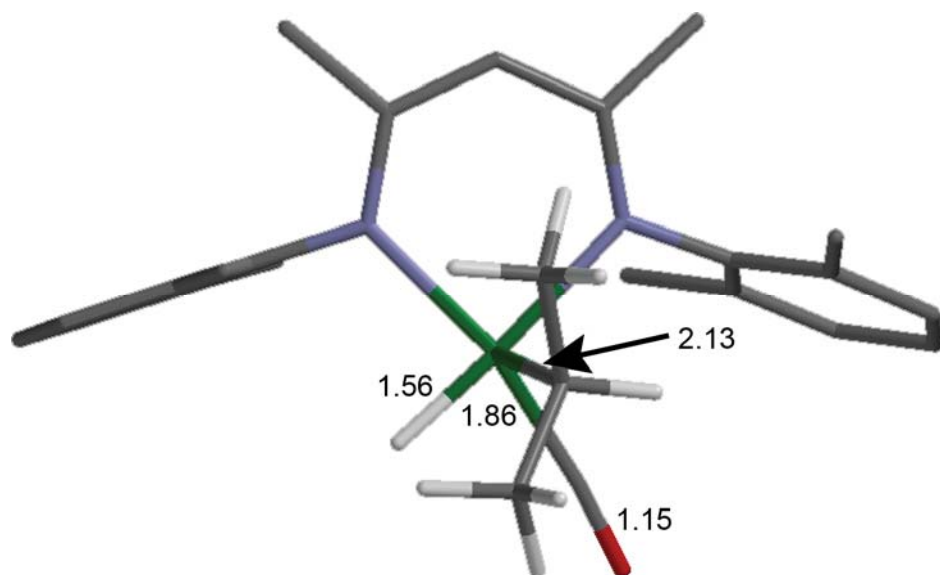


Figure S24. Structure of 17.

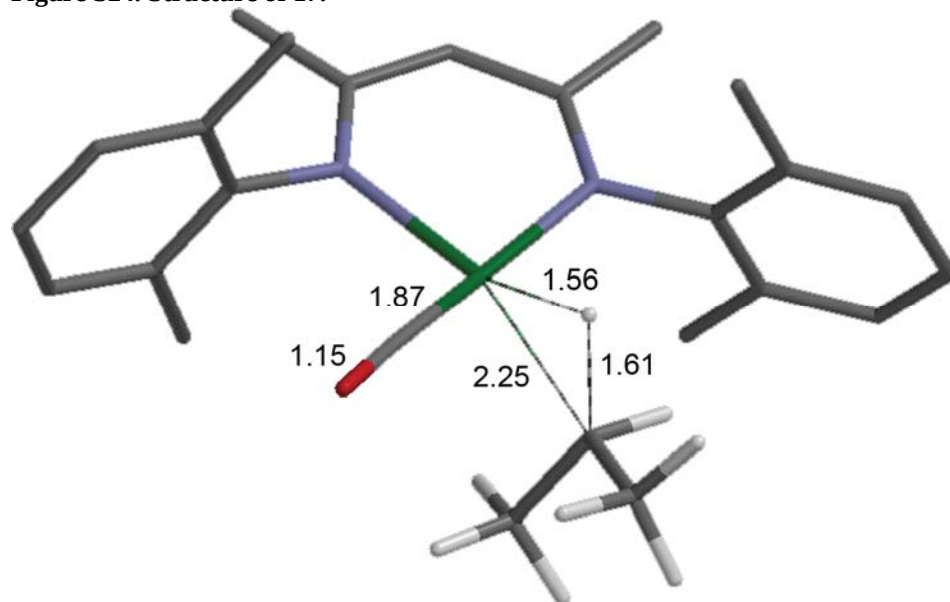


Figure S25. Structure of TS_{17_18}.

Olefin hydrogenation

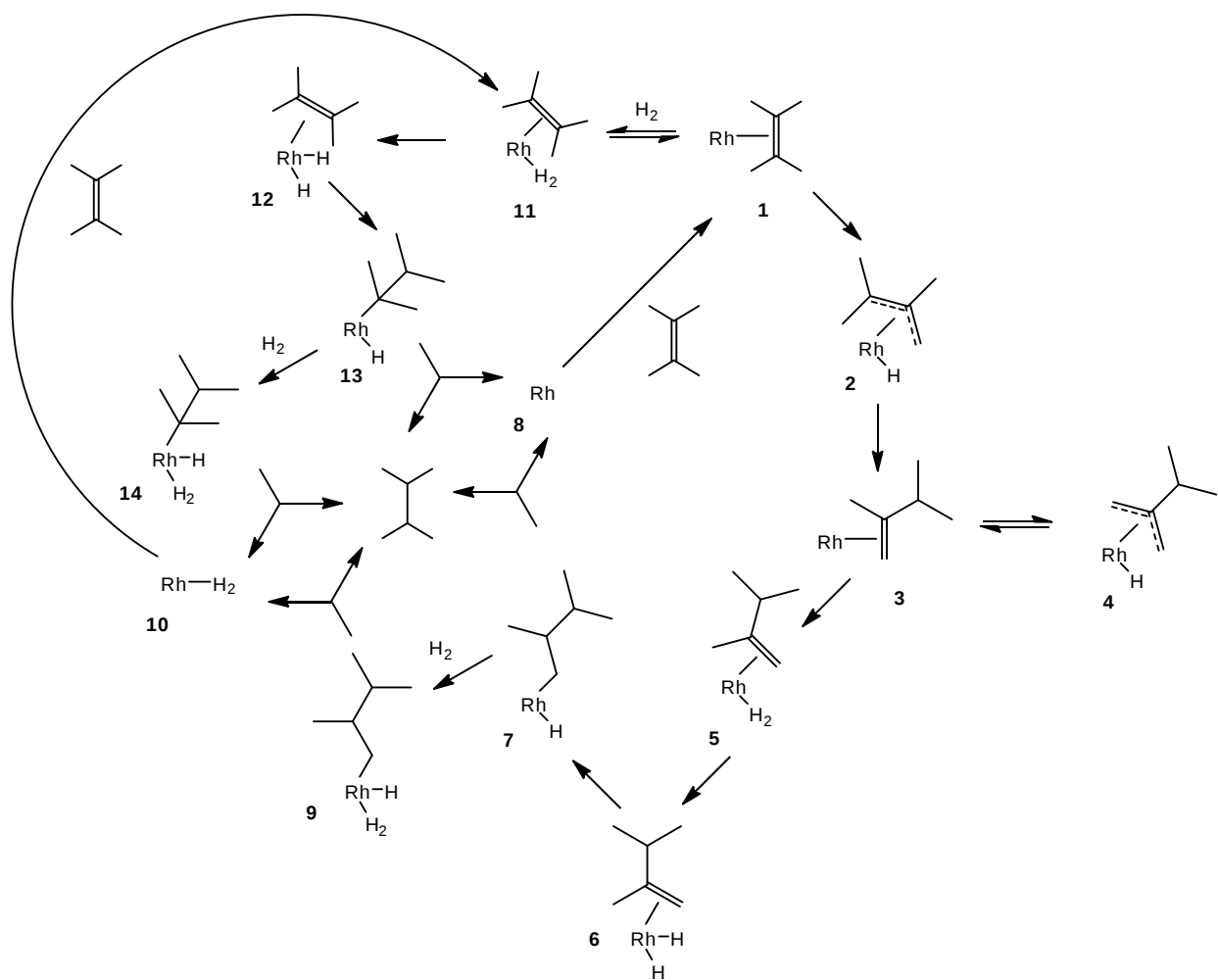


Figure S26. Compound numbering for hydrogenation of 2,3-dimethyl-2-butene.

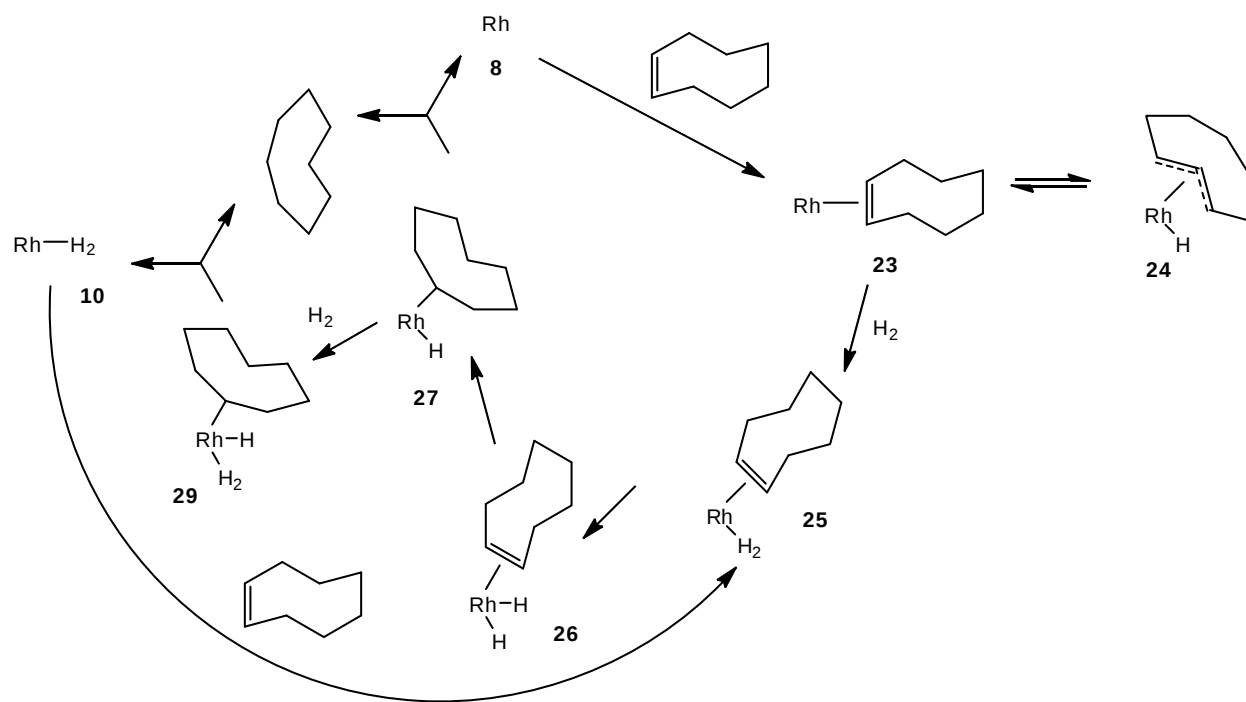


Figure S27. Compound numbering for hydrogenation of cyclooctene.

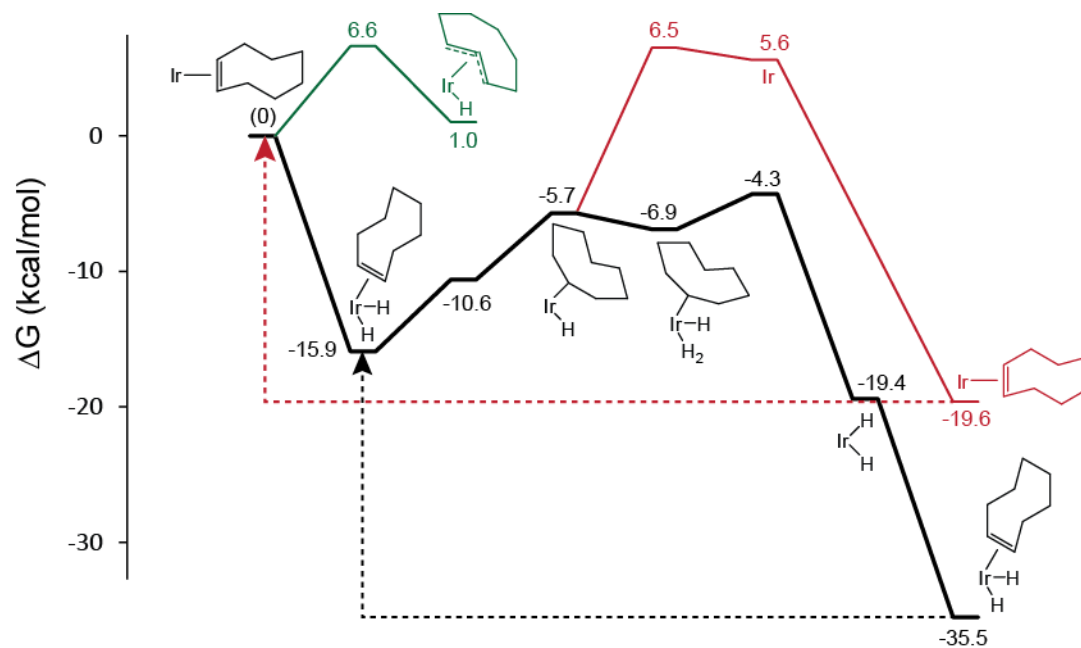


Figure S28. Calculated free-energy profile for potential catalytic COE hydrogenation using 1b.

The solid black line represents the preferred path involving H₂ coordination prior to C-H reductive elimination; the red line is the alternative path involving "naked" LIr. The green step corresponds to "ring walking" via the allyl-hydride mechanism.

Table S3. Total and relative energies for olefin hydrogenation with 1a.

Name	b3-lyp/TZVP opt				b3-lyp/TZVPP//b3-lyp/TZVP			Grel on scale (kcal/mol)
	E _{tot} (h)	ZPE (h)	Hcorr (h)	TScorr (h)	E _{tot} (h)	G		
H2	-1.17289	0.01006	0.01300	0.01337	-1.17325	-1.16921		
COE	-313.13574	0.20329	0.21100	0.03666	-313.15034	-312.96390		
COA	-314.36088	0.22730	0.23512	0.03607	-314.37536	-314.16440		
DMBn2	-235.76501	0.16297	0.17144	0.03720	-235.77703	-235.63051		
DMBn1	-235.76204	0.16426	0.17189	0.03600	-235.77355	-235.62579		
DMBlH	-236.98545	0.18769	0.19566	0.03569	-236.99659	-236.82484		
LRh_COE_2	-1661.31578	0.82051	0.85750	0.10056	-1661.39449	-1660.60436	-1034.67656	23.25
LRh_23	-1348.19533	0.61256	0.64284	0.08835	-1348.26115	-1347.67750	-1034.71360	0.00
LRh_TS_23_24	-1348.16687	0.60857	0.63814	0.08603	-1348.23468	-1347.65418	-1034.69028	14.64
LRh_24	-1348.17496	0.60948	0.63931	0.08598	-1348.24154	-1347.65983	-1034.69593	11.09
LRh_25	-1349.38722	0.63092	0.66127	0.08757	-1349.45403	-1348.85143	-1034.71832	-2.96
LRh_TS_26_27	-1349.37478	0.62879	0.65885	0.08738	-1349.44187	-1348.84157	-1034.70846	3.23
LRh_27	-1349.37639	0.63234	0.66283	0.09008	-1349.44326	-1348.84078	-1034.70767	3.72
LRh_TS_27_8a	-1349.35690	0.63138	0.66183	0.08899	-1349.42315	-1348.82095	-1034.68783	16.17
LRh_TS_27_8b	-1349.36690	0.63047	0.66086	0.08896	-1349.43436	-1348.83310	-1034.69999	8.54
LRh_8	-1035.01616	0.40677	0.42968	0.07239	-1035.06737	-1034.68619	-1034.71748	-2.44
LRh_23	-1348.19533	0.61256	0.64284	0.08835	-1348.26115	-1347.67750	-1034.74489	-19.64
LRh_29	-1350.55744	0.64956	0.68100	0.09223	-1350.62397	-1350.00476	-1034.70244	7.00
LRh_TS_29_10	-1350.55146	0.64822	0.67940	0.09161	-1350.61867	-1350.00064	-1034.69832	9.59
LRh_10	-1036.22131	0.42359	0.44676	0.07252	-1036.27382	-1035.87565	-1034.73773	-15.14
LRh_25	-1349.38722	0.63092	0.66127	0.08757	-1349.45403	-1348.85143	-1034.74961	-22.59
LRh_23	-1348.19533	0.61256	0.64284	0.08835	-1348.26115	-1347.67750	-1034.71360	-11.85
LRh_1	-1270.80743	0.57292	0.60279	0.08530	-1270.87087	-1270.32523	-1034.69472	0.00
LRh_TS_1_2	-1270.79096	0.56935	0.59900	0.08552	-1270.85532	-1270.31362	-1034.68310	7.29
LRh_2	-1270.80443	0.57036	0.60011	0.08506	-1270.86754	-1270.32442	-1034.69390	0.51
LRh_TS_2_3	-1270.79429	0.56986	0.59903	0.08406	-1270.85855	-1270.31584	-1034.68533	5.89
LRh_3	-1270.81513	0.57346	0.60309	0.08533	-1270.87860	-1270.33268	-1034.70217	-4.68
LRh_TS_3_4	-1270.79510	0.56995	0.59916	0.08537	-1270.85969	-1270.31772	-1034.68721	4.71
LRh_4	-1270.80793	0.57057	0.60027	0.08687	-1270.87131	-1270.32924	-1034.69872	-2.51
LRh_5	-1271.99831	0.59169	0.62189	0.08680	-1272.06175	-1271.49801	-1034.69829	-2.24
LRh_TS_5_6	-1271.99643	0.58928	0.61954	0.08699	-1272.05999	-1271.49874	-1034.69902	-2.70
LRh_6	-1271.99541	0.59025	0.62099	0.08928	-1272.05833	-1271.49717	-1034.69744	-1.71
LRh_TS_6_7	-1271.98965	0.58856	0.61870	0.08725	-1272.05305	-1271.49281	-1034.69309	1.02
LRh_7	-1271.99751	0.59164	0.62203	0.08817	-1272.06041	-1271.49746	-1034.69773	-1.89
LRh_TS_7_8	-1271.98757	0.59165	0.62196	0.08833	-1272.05123	-1271.48845	-1034.68873	3.76
LRh_8	-1035.01616	0.40677	0.42968	0.07239	-1035.06737	-1034.68619	-1034.71131	-10.41
LRh_1	-1270.80743	0.57292	0.60279	0.08530	-1270.87087	-1270.32523	-1034.71983	-15.76
LRh_9	-1273.18113	0.61116	0.64227	0.09092	-1273.24446	-1272.66311	-1034.69417	0.34
LRh_TS_9_10	-1273.17918	0.60987	0.64070	0.08958	-1273.24298	-1272.66230	-1034.69337	0.85

LRh_10	-1036.22131	0.42359	0.44676	0.07252	-1036.27382	-1035.87565	-1034.73156	-23.12
LRh_11	-1271.98401	0.59157	0.62181	0.08631	-1272.04739	-1271.48341	-1034.70880	-8.84
LRh_11	-1271.98401	0.59157	0.62181	0.08631	-1272.04739	-1271.48341	-1034.68369	6.92
LRh_TS_11_12	-1271.98156	0.58922	0.61953	0.08645	-1272.04501	-1271.48341	-1034.68368	6.92
LRh_12	-1271.98348	0.59017	0.62106	0.08828	-1272.04616	-1271.48425	-1034.68453	6.39
LRh_TS_12_13	-1271.97554	0.58917	0.61929	0.08662	-1272.03882	-1271.47757	-1034.67785	10.59
LRh_13	-1271.98344	0.59359	0.62372	0.08621	-1272.04566	-1271.47970	-1034.67998	9.25
LRh_TS_13_8a	-1271.98200	0.59117	0.62142	0.08745	-1272.04635	-1271.48352	-1034.68379	6.85
LRh_TS_13_8b	-1271.97714	0.59148	0.62214	0.09011	-1272.04016	-1271.47839	-1034.67867	10.07
LRh_14	-1273.16363	0.61150	0.64230	0.08823	-1273.22661	-1272.64342	-1034.67448	12.70
LRh_TS_14_10	-1273.15966	0.60997	0.64055	0.08769	-1273.22311	-1272.64131	-1034.67238	14.02
Llr_COE_2	-1655.12141	0.82146	0.85807	0.09951	-1655.20351	-1654.41212	-1028.48431	17.46
Llr_23	-1341.99083	0.61288	0.64304	0.08819	-1342.05998	-1341.47604	-1028.51213	0.00
Llr_TS_23_24	-1341.97418	0.60891	0.63843	0.08625	-1342.04622	-1341.46557	-1028.50167	6.57
Llr_24	-1341.98639	0.60985	0.63966	0.08628	-1342.05624	-1341.47439	-1028.51049	1.03
Llr_26	-1343.20303	0.63076	0.66132	0.08846	-1343.27266	-1342.67060	-1028.53749	-15.91
Llr_TS_26_27	-1343.19261	0.62968	0.65961	0.08733	-1343.26321	-1342.66211	-1028.52899	-10.58
Llr_27	-1343.18697	0.63274	0.66311	0.08932	-1343.25765	-1342.65437	-1028.52126	-5.73
Llr_TS_27_8a	-1343.15474	0.63158	0.66170	0.08780	-1343.22541	-1342.62253	-1028.48942	14.26
Llr_TS_27_8b	-1343.16518	0.63078	0.66102	0.08854	-1343.23661	-1342.63491	-1028.50179	6.49
Llr_8	-1028.79923	0.40700	0.42988	0.07255	-1028.85324	-1028.47197	-1028.50326	5.57
Llr_29	-1344.37549	0.64969	0.68088	0.09102	-1344.44532	-1343.82542	-1028.52310	-6.88
Llr_TS_29_10	-1344.36865	0.64806	0.67952	0.09299	-1344.43856	-1343.82134	-1028.51902	-4.32
Llr_10	-1030.02431	0.42339	0.44664	0.07292	-1030.07874	-1029.68096	-1028.54304	-19.40
Llr_23	-1341.99083	0.61288	0.64304	0.08819	-1342.05998	-1341.47604	-1028.51213	-10.40
Llr_1	-1264.60448	0.57323	0.60279	0.08493	-1264.67195	-1264.12607	-1028.49555	0.00
Llr_TS_1_2	-1264.59670	0.57007	0.59940	0.08461	-1264.66508	-1264.12237	-1028.49185	2.32
Llr_2	-1264.61495	0.57067	0.60045	0.08570	-1264.68107	-1264.13804	-1028.50753	-7.51
Llr_TS_2_3	-1264.60254	0.57026	0.59943	0.08428	-1264.67093	-1264.12797	-1028.49746	-1.19
Llr_3	-1264.61348	0.57346	0.60294	0.08516	-1264.68127	-1264.13539	-1028.50488	-5.85
Llr_TS_3_4	-1264.60175	0.57034	0.59954	0.08584	-1264.67061	-1264.12858	-1028.49807	-1.58
Llr_4	-1264.61834	0.57112	0.60076	0.08697	-1264.68503	-1264.14254	-1028.51203	-10.34
Llr_6	-1265.81453	0.59169	0.62211	0.08811	-1265.88012	-1265.31704	-1028.51732	-13.66
Llr_TS_6_7	-1265.80030	0.58909	0.61925	0.08774	-1265.86669	-1265.30623	-1028.50651	-6.87
Llr_7	-1265.80294	0.59169	0.62211	0.08840	-1265.86894	-1265.30606	-1028.50633	-6.76
Llr_TS_7_8	-1265.78498	0.59215	0.62225	0.08771	-1265.85241	-1265.28893	-1028.48920	3.98
Llr_8	-1028.79923	0.40700	0.42988	0.07255	-1028.85324	-1028.47197	-1028.49708	9.44
Llr_9	-1266.99967	0.61082	0.64199	0.09214	-1267.06641	-1266.48615	-1028.51722	-13.59
Llr_TS_9_10	-1266.99593	0.60983	0.64079	0.09058	-1267.06285	-1266.48275	-1028.51381	-11.46
Llr_10	-1030.02431	0.42339	0.44664	0.07292	-1030.07874	-1029.68096	-1028.53687	-25.92
Llr_12	-1265.80237	0.59142	0.62196	0.08715	-1265.86747	-1265.30389	-1028.50417	-5.41
Llr_13	-1265.79211	0.59387	0.62396	0.08645	-1265.85725	-1265.29120	-1028.49148	2.56
Llr_TS_13_8a	-1265.78114	0.59114	0.62132	0.08740	-1265.84949	-1265.28673	-1028.48700	5.36

Llr_14	-1266.98119	0.61109	0.64184	0.08810	-1267.04726	-1266.46445	-1028.49551	0.03
Llr_TS_14_10	-1266.97940	0.60945	0.64064	0.09017	-1267.04520	-1266.46497	-1028.49604	-0.30

Benzene/H₂ reactivity

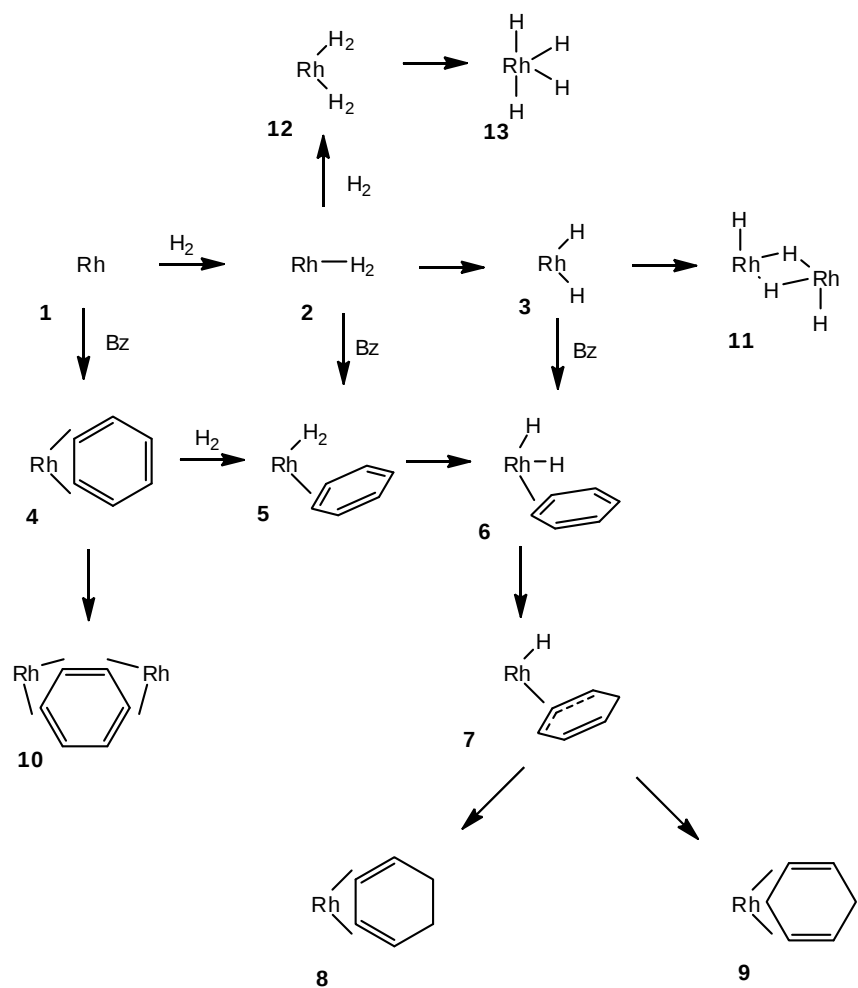


Figure S29. Compound numbering for benzene/H₂ reactivity.

Polyhydride complexes (**3**, **6**, **13**) do not exist for Rh, dihydrogen complexes (**2**, **5**, **12**) do not exist for Ir.

Table S4. Total and relative energies for benzene/H₂ reactivity.

Name	b3-lyp/TZVP opt				b3-lyp/TZVPP//b3-lyp/TZVP			Grel (kcal/mol)
	E _{tot} (h)	ZPE (h)	Hcorr (h)	TScorr (h)	E _{tot} (h)	G	on scale	
H2	-1.17289	0.01006	0.01300	0.01337	-1.17325	-1.16921		
Bz	-232.17411	0.10009	0.10472	0.02721	-232.18570	-232.09921	-232.09921	
13CHD	-233.33923	0.12202	0.12729	0.03004	-233.35051	-233.24334	-232.07413	
14CHD	-233.33898	0.12178	0.12715	0.02980	-233.35065	-233.24347	-232.07426	
LRh_1	-1035.01616	0.40678	0.42968	0.07234	-1035.06737	-1034.68616	-1034.68616	0.00
LRh_2	-1036.22131	0.42357	0.44676	0.07264	-1036.27382	-1035.87573	-1034.70652	-12.77
LRh_11	-2072.48954	0.84795	0.89422	0.12266	-2072.59204	-2071.78000	-1034.72079	-21.73
LRh_12	-1037.42315	0.44140	0.46475	0.07187	-1037.47707	-1037.06046	-1034.72204	-22.52
LRh_4	-1267.21350	0.50878	0.53603	0.08116	-1267.27694	-1266.79529	-1034.69607	-6.22
LRh_5	-1268.40206	0.52668	0.55438	0.08222	-1268.46560	-1267.96631	-1034.69789	-7.36
LRh_TS_6_7	-1268.36450	0.52447	0.55168	0.08129	-1268.42853	-1267.93132	-1034.66289	14.60
LRh_7	-1268.38364	0.52787	0.55547	0.08176	-1268.44673	-1267.94604	-1034.67761	5.36
LRh_TS_7_8	-1268.37532	0.52718	0.55441	0.08127	-1268.43952	-1267.93956	-1034.67114	9.43
LRh_8	-1268.42157	0.53267	0.55995	0.08166	-1268.48539	-1267.98015	-1034.71173	-16.04
LRh_1	-1035.01616	0.40678	0.42968	0.07234	-1035.06737	-1034.68616	-1034.66108	15.74
LRh_TS_7_9	-1268.36963	0.52669	0.55404	0.08171	-1268.43407	-1267.93478	-1034.66635	12.43
LRh_9	-1268.41628	0.53257	0.55941	0.07851	-1268.47888	-1267.97207	-1034.70364	-10.97
LRh_1	-1035.01616	0.40678	0.42968	0.07234	-1035.06737	-1034.68616	-1034.66120	15.66
LRh_10	-2302.27179	0.91778	0.96782	0.13292	-2302.38632	-2301.50755	-1034.70417	-11.30
Llr_1	-1028.79923	0.40700	0.42988	0.07255	-1028.85324	-1028.47197	-1028.47197	0.00
Llr_3	-1030.02430	0.42329	0.44658	0.07303	-1030.07873	-1029.68109	-1028.51188	-25.04
Llr_11	-2060.11814	0.84847	0.89496	0.12380	-2060.22621	-2059.41420	-1028.53789	-41.36
Llr_13	-1031.23891	0.43969	0.46345	0.07293	-1031.29577	-1030.88118	-1028.54276	-44.42

Cartesian coordinates for epoxide opening.

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22

COE.xyz

C	-0.6228470	0.1078317	-0.0549629
C	-0.8363605	-0.3262423	1.4222626
H	-0.0645313	0.1224426	2.0550087
C	-0.8424124	-1.8249933	1.5842287
H	-1.7873564	0.0685017	1.7854571
C	0.2110498	-2.6416376	1.5544946
H	-1.8230629	-2.2846102	1.6790126
C	1.6733036	-2.2785499	1.4271283
H	0.0068855	-3.7058655	1.6396088
H	2.2413796	-3.2119169	1.4441337
H	1.9963896	-1.7260521	2.3184490
C	2.1205897	-1.4754995	0.1772905
H	3.1785204	-1.7057088	0.0215242
C	1.9846785	0.0588072	0.2798113
H	1.5996979	-1.8519885	-0.7084216
H	-0.7896946	-0.7615690	-0.6950569
C	0.7554528	0.7176866	-0.3675937
H	-1.3853519	0.8382446	-0.3403274
H	0.7551752	1.7711371	-0.0655838
H	0.8834015	0.7214904	-1.4556345
H	2.8653967	0.5189749	-0.1789999
H	2.0364077	0.3413999	1.3361976

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7

Epox2.xyz

C	0.6343796	0.0248314	-0.3695823
C	-0.6415012	0.0727111	0.3504720
O	0.0843066	-1.1537150	0.2260697
H	-1.5716191	0.1198328	-0.2090614
H	-0.6764017	0.4911824	1.3525036
H	0.6377873	0.0368884	-1.4559721
H	1.5330485	0.4082689	0.1055704

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13

Epox.xyz

C	-0.0517266	-0.1400090	0.0629509
C	-1.3302546	-0.0950040	0.7854689
O	-0.6076037	-1.3286405	0.6641080
H	-2.2629965	-0.0473157	0.2286965
H	-1.3684682	0.3232532	1.7883906
C	-0.0451763	-0.1450813	-1.4478116
H	0.7835744	-0.7518190	-1.8223237
H	0.0754498	0.8689127	-1.8384981
H	-0.9749528	-0.5601362	-1.8380543
C	1.2034497	0.3725220	0.7295286
H	2.0684373	-0.2183624	0.4168058
H	1.1203929	0.3071824	1.8148369
H	1.3898748	1.4144977	0.4559016

=====

5

MeH.xyz

C	0.0000000	0.0000000	-0.0000001
H	-0.0008482	0.8899494	0.6292982
H	0.0008482	-0.8899494	0.6292982
H	0.8899496	0.0008481	-0.6292981
H	-0.8899496	-0.0008480	-0.6292981

11

PrH.xyz

C	1.2758479	0.0000946	-0.2291457
H	1.3219874	0.8824180	-0.8739554
H	1.3216093	-0.8816947	-0.8747046
H	2.1711791	-0.0003546	0.3972880
C	0.0000000	0.0000006	0.6146636
H	-0.0000584	0.8747957	1.2731851
H	0.0000585	-0.8747933	1.2731868
C	-1.2758479	-0.0000950	-0.2291457
H	-1.3216114	0.8816949	-0.8747034
H	-2.1711790	0.0003512	0.3972879
H	-1.3219855	-0.8824176	-0.8739565

62

XyNacnacRh_1.xyz

C	-0.7397898	-1.9513357	-1.5758680
H	-0.6544469	-3.9740701	-0.9740898
C	-0.4142914	-2.9667097	-0.6664679
C	0.1886716	-2.8323955	0.5939513
N	-0.5202933	-0.6520516	-1.3703929
N	0.5441385	-1.6567372	1.0819408
C	-1.3758524	-2.3869733	-2.8830642
H	-1.4793385	-3.4701577	-2.9103785
H	-0.7735522	-2.0791965	-3.7410251
H	-2.3658184	-1.9457920	-3.0177306
C	0.4384519	-4.0840188	1.4071056
H	0.1050876	-4.9664401	0.8632277
H	-0.0916906	-4.0505972	2.3621801
H	1.4999749	-4.2036243	1.6372405
Rh	0.3511201	0.1141045	0.2514913
O	0.6004861	2.3228943	-0.1099857
C	-0.0557833	3.5321059	0.3909072
C	0.2671962	3.3827996	-1.0355201
H	1.1336108	3.8892302	-1.4499835
H	-0.5164717	3.1345976	-1.7412082
C	-1.4743116	3.3460048	0.8628577
H	-1.4883674	2.8794678	1.8504691
H	-2.0379415	2.7158451	0.1777158
H	-1.9712441	4.3169228	0.9372414
C	0.8372376	4.3643314	1.2776522
H	1.8533953	4.4016554	0.8845902
H	0.8716031	3.9447542	2.2860593
H	0.4527368	5.3848652	1.3502168
C	1.1571093	-1.4844469	2.3553302
C	2.3608546	-1.0079346	4.8254633

C	0.3517904	-1.2547305	3.4917373	H	2.6768331	0.6673879	1.8544258
C	2.5651829	-1.4653211	2.4533480	C	-0.0118965	2.9720678	0.3869086
C	3.1448796	-1.2266106	3.6996731	H	0.6787229	3.8121714	0.4677420
C	0.9756543	-1.0211011	4.7172323	H	-1.0160731	3.2935470	0.1279356
H	4.2259673	-1.2109264	3.7838885	H	0.3787519	2.4436755	-0.5551338
H	0.3642609	-0.8446657	5.5955047	C	-1.1248847	2.0436593	2.5462894
H	2.8288028	-0.8222772	5.7853184	H	-1.0733367	1.1657305	3.1896119
C	-0.9096599	0.3006789	-2.3550208	H	-2.0687005	2.0332770	2.0049004
C	-1.6630144	2.1885410	-4.2695833	H	-1.1019475	2.9304002	3.1917024
C	0.0205497	0.7162239	-3.3293318	C	1.9558696	-1.6447408	1.3815155
C	-2.2113204	0.8406955	-2.3285619	C	4.2979009	-2.3953301	2.6980781
C	-2.5676437	1.7837537	-3.2947104	C	1.9740931	-1.7033605	2.7847780
C	-0.3786530	1.6569234	-4.2801554	C	3.1096486	-1.9445114	0.6346864
H	-3.5695672	2.1994351	-3.2824445	C	4.2707455	-2.3187102	1.3114146
H	0.3298092	1.9741583	-5.0378120	C	3.1549901	-2.0875147	3.4231815
H	-1.9571733	2.9167506	-5.0165046	H	5.1625550	-2.5518786	0.7399812
C	-3.2080879	0.3972607	-1.2896582	H	3.1731565	-2.1391902	4.5063240
H	-3.5841543	-0.6088651	-1.4978241	H	5.2058728	-2.6908949	3.2104876
H	-4.0664754	1.0707671	-1.2629481	C	-1.7170864	1.2138591	-1.9396220
H	-2.7479552	0.3556787	-0.2999733	C	-2.5992643	3.3490005	-3.5185018
C	1.4171149	0.1542571	-3.3478157	C	-1.0040593	1.5700064	-3.1047853
H	1.8872090	0.2538385	-2.3657909	C	-2.8774711	1.9221829	-1.5753038
H	2.0291304	0.6635053	-4.0938633	C	-3.2975166	2.9877655	-2.3767313
H	1.4187061	-0.9139176	-3.5815423	C	-1.4615145	2.6352948	-3.8780332
C	3.4296247	-1.7073185	1.2432194	H	-4.1890538	3.5375921	-2.0932822
H	3.3440746	-2.7384107	0.8884952	H	-0.9157871	2.9076961	-4.7747571
H	4.4787127	-1.5199129	1.4764048	H	-2.9385725	4.1783464	-4.1278183
H	3.1277158	-1.0654458	0.4125178	C	-3.6976573	1.5499483	-0.3635863
C	-1.1513600	-1.2667007	3.3901218	H	-4.6004136	1.0029315	-0.6543020
H	-1.4901821	-0.6342612	2.5664336	H	-3.1412272	0.9169548	0.3245092
H	-1.6028011	-0.9173491	4.3198383	H	-4.0302004	2.4427209	0.1712678
H	-1.5336187	-2.2717514	3.1898803	C	0.2272704	0.8076459	-3.5243656
=====				H	0.6224145	1.2033555	-4.4609025
62	XyNacnacRh_2a.xyz			H	0.0169873	-0.2553793	-3.6663797
C	-1.6953898	-1.0439428	-1.2073283	H	1.0148211	0.8680579	-2.7681948
H	-1.7503736	-3.0647053	-0.6265765	C	3.1079066	-1.8461006	-0.8687205
C	-1.2126581	-2.1413821	-0.4708063	H	2.3425714	-2.4800247	-1.3230665
C	-0.0818608	-2.2536421	0.3411713	H	4.0769208	-2.1400349	-1.2741247
N	-1.1998576	0.1752876	-1.1044255	H	2.8970363	-0.8227834	-1.1929081
N	0.7587945	-1.2640176	0.6797091	C	0.7704118	-1.3226421	3.6072908
C	-2.8221669	-1.3346751	-2.1818843	H	-0.1614131	-1.6962711	3.1809856
H	-3.0399661	-2.4005035	-2.2152747	H	0.6840172	-0.2346600	3.6669631
H	-2.5608752	-1.0021427	-3.1888423	H	0.8634952	-1.7068052	4.6243950
H	-3.7361418	-0.8072678	-1.9020891	=====			
C	0.2198999	-3.6600425	0.8335243	62	XyNacnacRh_2b.xyz		
H	-0.5584873	-4.3480291	0.5105851	C	-1.5874613	-1.0689739	-1.3279170
H	0.2880350	-3.6986814	1.9215378	H	-1.6529629	-3.0910586	-0.7531553
H	1.1765451	-4.0170373	0.4470058	C	-1.1421261	-2.1598230	-0.5588955
Rh	0.4703943	0.6939483	0.1927952	C	-0.0716752	-2.2556123	0.3330421
C	0.0509349	2.0844095	1.6152946	N	-1.1191973	0.1575489	-1.1895743
O	1.2618295	2.1341080	2.2867646	N	0.7271138	-1.2536921	0.7314280
C	2.0765719	1.3867983	1.3093881	C	-2.6371757	-1.3756593	-2.3805767
H	2.7198557	2.0870754	0.7645959	H	-2.8356864	-2.4445522	-2.4295210

H	-2.3098300	-1.0381218	-3.3662101	=====			
H	-3.5766096	-0.8626030	-2.1669269	62			
C	0.2143891	-3.6575948	0.8468743	XyNacnacRh_3a.xyz			
H	-0.5264388	-4.3574254	0.4662850	C	-1.6814405	-0.8733270	-1.3902421
H	0.2007928	-3.6962598	1.9369375	H	-2.5238044	-2.6309862	-0.5986856
H	1.2030144	-3.9989512	0.5338237	C	-1.8060942	-1.8518538	-0.3894334
Rh	0.4467566	0.6999312	0.2228953	C	-1.1247491	-1.9882476	0.8229984
C	-0.0896694	2.0850909	1.6112660	N	-0.8596073	0.1628182	-1.3192108
O	1.0711348	2.1527336	2.3647116	N	-0.2019214	-1.1461380	1.2937732
C	1.9615621	1.4152535	1.4478954	C	-2.5675052	-1.0597784	-2.6100453
H	2.6321207	2.1233224	0.9479018	H	-3.1953705	-1.9417797	-2.4997058
H	2.5316255	0.7042434	2.0347714	H	-1.9742413	-1.1718878	-3.5193644
C	-0.0801349	2.9707177	0.3799035	H	-3.2132268	-0.1927905	-2.7628295
H	0.5903646	3.8212467	0.5072026	C	-1.4802817	-3.2168735	1.6422988
H	-1.0684817	3.2766863	0.0507954	H	-2.2462657	-3.8019057	1.1374808
H	0.3836127	2.4477789	-0.5315051	H	-1.8493386	-2.9427222	2.6320790
C	-1.3260625	2.0286069	2.4591579	H	-0.6076182	-3.8537821	1.7992063
H	-1.3074844	1.1510613	3.1047432	Rh	0.3888933	0.6162474	0.4053818
H	-2.2303207	2.0065279	1.8543493	H	-0.4813217	1.4349744	1.3266707
H	-1.3588058	2.9152159	3.1043265	C	2.1248932	2.1222444	-0.2248367
C	1.8746015	-1.6167186	1.5200563	C	2.8968852	1.9447170	-1.4937193
C	4.1240734	-2.3322554	3.0065071	H	3.7504666	2.6305894	-1.4633635
C	1.7898019	-1.6763995	2.9207488	H	2.2945183	2.1781995	-2.3689648
C	3.0849986	-1.8979617	0.8607561	H	3.3016578	0.9344656	-1.5728557
C	4.1984390	-2.2548222	1.6215925	C	0.9169595	2.7788704	-0.1278962
C	2.9260240	-2.0428676	3.6449152	H	0.4423285	3.1237637	-1.0347087
H	5.1336064	-2.4736295	1.1178284	H	0.6488221	3.2857507	0.7874428
H	2.8647083	-2.0953248	4.7264194	O	2.8261497	1.7569156	0.8835812
H	4.9960766	-2.6142005	3.5848132	C	1.8650010	1.0997292	1.7921130
C	-1.5928220	1.1893250	-2.0583951	H	1.6046375	1.7948238	2.5936498
C	-2.3972361	3.3129555	-3.6933841	H	2.3864062	0.2418184	2.2100157
C	-0.8066618	1.5582819	-3.1713446	C	0.3891425	-1.4466883	2.5660921
C	-2.7864306	1.8791240	-1.7746071	C	1.5766651	-2.0252371	5.0239616
C	-3.1668913	2.9392752	-2.6025537	C	1.5724563	-2.2067146	2.6071571
C	-1.2263026	2.6176250	-3.9738368	C	-0.1959641	-0.9647871	3.7509371
H	-4.0842138	3.4748610	-2.3809278	C	0.4152905	-1.2668330	4.9695360
H	-0.6243051	2.8999121	-4.8305627	C	2.1478892	-2.4894908	3.8463321
H	-2.7066210	4.1378562	-4.3242540	H	-0.0334314	-0.9017910	5.8868866
C	-3.6816412	1.4919239	-0.6222662	H	3.0583262	-3.0775004	3.8830056
H	-4.0715868	2.3784302	-0.1167269	H	2.0356111	-2.2521094	5.9790097
H	-4.5487492	0.9229756	-0.9732046	C	-0.8182803	1.0602249	-2.4303756
H	-3.1608116	0.8740692	0.1062354	C	-0.6793871	2.8559333	-4.5664526
C	0.4624837	0.8157748	-3.5053968	C	0.0731066	0.8158855	-3.4921636
H	0.2788124	-0.2498961	-3.6635264	C	-1.6438718	2.2012401	-2.4385915
H	1.1944088	0.8859418	-2.6961388	C	-1.5585920	3.0850131	-3.5152477
H	0.9158187	1.2198599	-4.4115287	C	0.1274933	1.7259513	-4.5498842
C	3.1929359	-1.7978991	-0.6385759	H	-2.1927548	3.9648991	-3.5253342
H	2.9907478	-0.7775790	-0.9773681	H	0.8130601	1.5408778	-5.3699744
H	2.4731705	-2.4430206	-1.1482652	H	-0.6247916	3.5534275	-5.3939421
H	4.1936867	-2.0763667	-0.9712240	C	-2.6083451	2.4669914	-1.3122484
C	0.5231093	-1.3150993	3.6523021	H	-3.1234391	3.4167084	-1.4624261
H	-0.3695438	-1.6917970	3.1518935	H	-2.0940544	2.4948349	-0.3495952
H	0.4223762	-0.2286611	3.7164413	H	-3.3661410	1.6828544	-1.2330224
H	0.5415728	-1.7093305	4.6695495	C	2.2279348	-2.6961550	1.3411839

H	2.5716590	-1.8590354	0.7265006	C	-1.1826672	2.7578954	-2.0028551
H	1.5451735	-3.2796657	0.7196346	C	-0.9844556	3.7367708	-2.9787227
H	3.0925045	-3.3191750	1.5733914	C	0.0365114	2.1299664	-4.4404053
C	-1.4518119	-0.1338269	3.7272331	H	-1.3128405	4.7514692	-2.7805089
H	-1.2697184	0.8399373	3.2644113	H	0.5115721	1.8870337	-5.3847080
H	-1.8197272	0.0337380	4.7401811	H	-0.2352567	4.2032422	-4.9386028
H	-2.2485734	-0.6038925	3.1472456	C	-1.8491003	3.1115876	-0.6983018
C	0.9429617	-0.4158782	-3.5116308	H	-2.0030003	4.1891039	-0.6241977
H	1.6986841	-0.3416829	-4.2947855	H	-1.2525822	2.7818974	0.1542802
H	0.3586386	-1.3211692	-3.7012425	H	-2.8250469	2.6280326	-0.5966906
H	1.4474542	-0.5707401	-2.5566123	C	1.5503710	-3.4904489	0.4590660
=====				H	0.6356664	-3.7991641	-0.0528966
62	XyNacnacRh_3b.xyz			H	2.2453674	-4.3310981	0.4474521
C	-2.0222896	-0.2751453	-1.2511044	H	1.9860005	-2.6851412	-0.1392194
H	-3.2428656	-1.7951642	-0.4561378	C	-0.7735445	-0.4249775	3.7713346
C	-2.2901682	-1.3032933	-0.3282974	H	-0.3913088	0.5122517	3.3569615
C	-1.4997856	-1.8101730	0.7056217	H	-0.8893380	-0.3003275	4.8486943
N	-0.9061827	0.4329531	-1.2668837	H	-1.7642602	-0.5711275	3.3357463
N	-0.2944723	-1.3552342	1.0583667	C	0.3386911	-0.2781405	-3.7741297
C	-3.1045287	-0.0141640	-2.2845632	H	0.8005751	-0.3349097	-4.7604716
H	-3.9601350	-0.6667359	-2.1214691	H	-0.4751228	-1.0064092	-3.7399843
H	-2.7311811	-0.1825351	-3.2969851	H	1.0748378	-0.6039243	-3.0346318
H	-3.4474010	1.0214695	-2.2460268	=====			
C	-2.0802362	-2.9936038	1.4603984	62	XyNacnacRh_3.xyz		
H	-3.0536337	-3.2621165	1.0552531	C	-1.0897653	-1.4878553	-1.7003712
H	-2.1961741	-2.7729430	2.5229046	H	-0.9003679	-3.5268057	-1.2130395
H	-1.4254385	-3.8645706	1.3912021	C	-0.6172496	-2.5362007	-0.8901410
Rh	0.6893084	0.2256052	0.1958060	C	0.1351708	-2.4934732	0.2872154
H	0.1491823	1.1941693	1.2238661	N	-0.8333243	-0.2109796	-1.4775578
C	2.3372991	2.0854845	0.2394062	N	0.5937737	-1.3912289	0.8849801
C	1.9824222	3.5244169	0.4397943	C	-1.9536319	-1.8948898	-2.8806203
H	1.3954518	3.6593297	1.3488937	H	-2.0445984	-2.9777908	-2.9380249
H	1.4464946	3.9294109	-0.4170894	H	-1.5371618	-1.5310109	-3.8214751
H	2.9138205	4.0863085	0.5673264	H	-2.9558299	-1.4689308	-2.7967344
C	2.2411745	1.4242479	-0.9634371	C	0.4247626	-3.8403264	0.9283440
H	2.8936499	0.5817660	-1.1640844	H	-0.0102825	-4.6432338	0.3370473
H	1.8487425	1.9536649	-1.8186717	H	0.0158240	-3.8960666	1.9388669
O	2.9194656	1.5124383	1.3159641	H	1.4983196	-4.0167842	1.0147616
C	2.3471829	0.1534301	1.4509008	Rh	0.3952300	0.5198158	0.1464589
H	2.1386542	0.0330338	2.5114251	H	1.7965139	0.4248893	-0.4144382
H	3.1080895	-0.5756295	1.1494057	C	1.3461554	1.4006510	1.7637661
C	0.3812608	-1.9979616	2.1465498	H	2.3928228	1.1596973	1.9381428
C	1.7232138	-3.2491454	4.2479780	H	0.7742945	1.1272690	2.6563008
C	1.2863807	-3.0397138	1.8731999	O	1.2976345	2.8756542	1.7365556
C	0.1595275	-1.5671318	3.4672661	C	0.4133703	3.4018885	0.8970493
C	0.8394933	-2.2094710	4.5038478	C	0.0097003	2.7459388	-0.2232616
C	1.9434928	-3.6560712	2.9384258	H	-0.7508527	3.1579880	-0.8688791
H	0.6704199	-1.8843735	5.5246307	H	0.7735903	2.1189926	-0.7552176
H	2.6369430	-4.4644995	2.7340293	C	-0.0767778	4.7505857	1.3201629
H	2.2411141	-3.7377485	5.0649007	H	-0.5857082	4.6862238	2.2853362
C	-0.7584220	1.4419024	-2.2671152	H	-0.7523187	5.1772118	0.5806512
C	-0.3807675	3.4315553	-4.1918433	H	0.7769184	5.4211188	1.4506259
C	-0.1401708	1.1226555	-3.4908633	C	1.3233909	-1.5413426	2.1093170

C	2.7130476	-1.7977572	4.5156057	C	0.8944201	2.4743461	2.2030988
C	0.6218169	-1.4962071	3.3288778	C	1.5519204	1.6727011	0.1520607
C	2.7205474	-1.7053889	2.0910966	O	2.0176275	2.0410907	1.4029608
C	3.3949134	-1.8339943	3.3070048	H	2.3647238	1.2150468	-0.4108158
C	1.3346297	-1.6293836	4.5208169	H	1.1262366	2.5495082	-0.3955455
H	4.4711814	-1.9673928	3.2994891	C	1.3966185	2.7053500	3.6182031
H	0.7980194	-1.5996659	5.4627328	H	2.2018442	3.4432508	3.6397315
H	3.2531719	-1.9004533	5.4493751	H	1.7669757	1.7704887	4.0439882
C	-1.3738915	0.7634081	-2.3722416	H	0.5797047	3.0671964	4.2464056
C	-2.3944254	2.7315908	-4.0697376	H	0.5556502	3.4338959	1.7788726
C	-0.6334261	1.1634313	-3.5001160	C	0.5665068	-1.5819328	1.9635795
C	-2.6168359	1.3574485	-2.0843038	C	1.0437216	-2.2029482	4.6373557
C	-3.1119004	2.3352958	-2.9480213	C	-0.5118777	-1.9176996	2.8039733
C	-1.1626986	2.1481732	-4.3361895	C	1.8824609	-1.5526204	2.4537617
H	-4.0722781	2.7914364	-2.7330601	C	2.0964263	-1.8689647	3.7977327
H	-0.5963635	2.4587064	-5.2075319	C	-0.2526386	-2.2273106	4.1378683
H	-2.7918765	3.4928243	-4.7306870	H	3.1097471	-1.8543929	4.1837454
C	-3.3956825	0.9663022	-0.8548231	H	-1.0789886	-2.4869116	4.7901915
H	-4.3521240	1.4897553	-0.8230576	H	1.2317297	-2.4458511	5.6766067
H	-2.8427461	1.2158321	0.0556196	C	-1.0975293	1.1671962	-2.6612683
H	-3.5945656	-0.1069853	-0.8145933	C	-2.1560381	3.3632291	-4.0222992
C	0.7052881	0.5445516	-3.8110341	C	-2.4716068	1.4639974	-2.5494260
H	1.1713739	1.0445542	-4.6609093	C	-0.2519245	1.9739190	-3.4499409
H	0.6168743	-0.5178186	-4.0553516	C	-0.8035242	3.0639744	-4.1235033
H	1.3818343	0.6066978	-2.9562518	C	-2.9795564	2.5650307	-3.2395069
C	3.4932322	-1.7394529	0.7988402	H	-0.1586348	3.6853351	-4.7350122
H	4.5294405	-2.0277632	0.9798710	H	-4.0359829	2.7958966	-3.1587776
H	3.4930121	-0.7589443	0.3143163	H	-2.5662268	4.2154954	-4.5509888
H	3.0640044	-2.4377242	0.0778871	C	1.2201125	1.6756755	-3.5778075
C	-0.8745838	-1.3136263	3.3602903	H	1.4049842	0.6696628	-3.9613927
H	-1.2385806	-1.3109292	4.3884165	H	1.7279482	1.7379681	-2.6138235
H	-1.3971952	-2.1059495	2.8189722	H	1.6954519	2.3856485	-4.2557565
H	-1.1728164	-0.3715769	2.8928759	C	-3.3869314	0.6109921	-1.7073271
=====				H	-3.0808396	0.6075491	-0.6573422
62	XyNacnacRh_4.xyz			H	-3.3897150	-0.4316777	-2.0343149
C	-0.4263804	-1.1205240	-2.4231231	H	-4.4106868	0.9833509	-1.7579823
H	0.1580425	-3.1347176	-2.2066718	C	-1.9265313	-1.9249281	2.2868151
C	0.0564723	-2.2040027	-1.6689419	H	-2.6177626	-2.2512197	3.0647530
C	0.3578713	-2.2718957	-0.3051954	H	-2.0478366	-2.5859203	1.4252256
N	-0.5532371	0.0855295	-1.9088732	H	-2.2272994	-0.9251739	1.9612755
N	0.2887186	-1.2720688	0.5879707	C	3.0579105	-1.1766296	1.5884279
C	-0.8385119	-1.3942611	-3.8546168	H	3.9753134	-1.6205344	1.9787305
H	-0.6122397	-2.4214239	-4.1350303	H	3.1855038	-0.0917502	1.5800781
H	-0.3347280	-0.7232119	-4.5521877	H	2.9335769	-1.4979057	0.5544287
H	-1.9120769	-1.2328226	-3.9822279	=====			
C	0.7666651	-3.6467123	0.1982483	62	XyNacnacRh_5.xyz		
H	0.7597864	-4.3627424	-0.6205341	C	-0.9211000	-1.0475346	-2.1772802
H	0.0874333	-4.0024654	0.9748440	H	-1.0424106	-3.1354547	-1.9160400
H	1.7654716	-3.6309798	0.6364328	C	-0.8047474	-2.2119899	-1.4094533
Rh	-0.1551460	0.6221667	0.1013755	C	-0.4373308	-2.3350540	-0.0653613
C	-0.2159794	1.4324389	2.0543311	N	-0.6762266	0.1631128	-1.6992813
H	-0.1294722	0.6709722	2.8284718	N	-0.1073108	-1.3257707	0.7426630
H	-1.1976738	1.9132968	2.1686887	C	-1.3624903	-1.2154571	-3.6176152

H	-1.5086820	-2.2680841	-3.8530562	H	3.6627433	-2.0948134	1.6311502
H	-0.6227157	-0.8065975	-4.3089284	=====			
H	-2.2985627	-0.6864769	-3.8094833	62			
C	-0.4431911	-3.7496524	0.4899616	XyNacnacRh_6beta.xyz			
H	-0.7557816	-4.4540996	-0.2783011	C	-0.8057189	-1.3073642	-1.8481523
H	-1.1257400	-3.8397091	1.3372157	H	-0.2170543	-3.3146308	-1.6185168
H	0.5432405	-4.0486936	0.8482147	C	-0.1089437	-2.3297902	-1.1895279
Rh	-0.0886032	0.6425527	0.2277196	C	0.7475680	-2.2503997	-0.0868577
C	1.1076134	2.0254980	1.2949827	N	-0.7860930	-0.0381181	-1.4622505
C	0.2239448	1.4965079	2.2419622	N	1.0448957	-1.1336492	0.5818901
H	-0.6951883	2.0270544	2.4625126	C	-1.5834294	-1.7076012	-3.0868693
H	0.5906217	0.8615331	3.0346206	H	-1.4262078	-2.7601701	-3.3140403
O	2.4747057	1.9917813	1.3281659	H	-1.2746716	-1.1164904	-3.9513768
C	3.1028836	1.5059984	2.5144386	H	-2.6541929	-1.5420209	-2.9564017
H	4.1707413	1.6565570	2.3663430	C	1.4124288	-3.5494389	0.3301518
H	2.9042438	0.4461633	2.6745421	H	1.1461142	-4.3474745	-0.3598990
H	2.7675693	2.0727726	3.3876252	H	1.1136074	-3.8489823	1.3353929
C	0.5716884	2.9829617	0.2716486	H	2.4986695	-3.4453093	0.3420417
H	0.0890827	3.8512636	0.7289667	Rh	0.3653237	0.6988096	0.1128539
H	-0.2738920	2.5281179	-0.3271312	C	-0.6218630	1.8180096	1.5415512
H	1.3388444	3.2965456	-0.4308160	C	0.6337516	1.9150319	2.3825562
C	0.2892093	-1.6540339	2.0788575	H	0.5917409	1.1857497	3.2085473
C	1.0785090	-2.2806231	4.6781033	H	0.7802867	2.9125267	2.8361910
C	1.6348752	-1.9710885	2.3380933	O	1.6306710	1.5997266	1.4440745
C	-0.6630532	-1.6480583	3.1132542	C	-0.6669206	2.8309783	0.4296792
C	-0.2472338	-1.9644896	4.4072895	H	-0.0351093	2.5147330	-0.4662561
C	2.0093825	-2.2822527	3.6466544	H	-0.1697506	3.7670838	0.6962223
H	-0.9756896	-1.9605086	5.2108678	H	-1.6626404	3.0018242	0.0277082
H	3.0448097	-2.5302657	3.8546381	C	-1.9076231	1.4033476	2.1933815
H	1.3847450	-2.5247990	5.6885861	H	-1.7801745	0.4898442	2.7749051
C	-0.8511824	1.3009045	-2.5489413	H	-2.7139195	1.2528265	1.4760999
C	-1.1559926	3.5794089	-4.1276770	H	-2.2303760	2.1866109	2.8942284
C	-2.0940426	1.9617381	-2.5836785	C	1.9181542	-1.2320687	1.7230379
C	0.2423613	1.7824785	-3.2938160	C	3.6188358	-1.4467619	3.9181836
C	0.0672132	2.9222369	-4.0796717	C	1.3965147	-1.6198397	2.9671254
C	-2.2249811	3.0996106	-3.3814750	C	3.2851137	-0.9364018	1.5719909
H	0.9047917	3.2984955	-4.6570149	C	4.1191377	-1.0597244	2.6799322
H	-3.1793123	3.6141068	-3.4137122	C	2.2668744	-1.7190265	4.0564156
H	-1.2745962	4.4647059	-4.7414689	H	5.1743200	-0.8348839	2.5711059
C	1.5793503	1.0894766	-3.2394142	H	1.8699049	-2.0153671	5.0216653
H	1.9158495	0.9614162	-2.2077358	H	4.2817834	-1.5292037	4.7716388
H	2.3311503	1.6593917	-3.7872501	C	-1.5103354	0.9338279	-2.2275153
H	1.5357055	0.0872966	-3.6750658	C	-2.8625966	2.9343184	-3.6311353
C	-3.2624749	1.4588798	-1.7753245	C	-0.8188766	1.7081359	-3.1824108
H	-2.9896411	1.3277428	-0.7252682	C	-2.8796114	1.1493944	-1.9884018
H	-3.6101027	0.4834119	-2.1272306	C	-3.5350226	2.1594953	-2.6979193
H	-4.1006409	2.1545509	-1.8367741	C	-1.5135606	2.7007467	-3.8721395
C	-2.1000362	-1.2967730	2.8351401	H	-4.5894954	2.3334522	-2.5111517
H	-2.6817402	-1.2885254	3.7580581	H	-0.9864543	3.2977581	-4.6080344
H	-2.5662359	-2.0075700	2.1475478	H	-3.3855805	3.7142295	-4.1719709
H	-2.1736418	-0.3156942	2.3595092	C	-3.6639648	0.3010697	-1.0176843
C	2.6551028	-1.9816010	1.2280939	H	-3.0198610	-0.1727091	-0.2795527
H	2.6090606	-1.0636114	0.6381776	H	-4.2020676	-0.4965758	-1.5405954
H	2.4845315	-2.8049913	0.5286622	H	-4.4148090	0.8994557	-0.4976612

C	0.6423858	1.4718277	-3.4713448
H	0.9810831	2.1186204	-4.2815303
H	0.8367321	0.4359512	-3.7597197
H	1.2664757	1.6701897	-2.5956188
C	-0.0597835	-1.9698135	3.1534192
H	-0.6930676	-1.4782055	2.4171084
H	-0.2275371	-3.0479640	3.0547691
H	-0.3979958	-1.6863815	4.1519964
C	3.8398765	-0.4656495	0.2554587
H	3.5531442	-1.1182492	-0.5724864
H	4.9292314	-0.4201603	0.2920704
H	3.4606828	0.5348504	0.0336278

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XyNacnacRh_6.xyz

C	-1.0468448	-1.3538396	-1.6860636
H	-0.5234124	-3.3736013	-1.4123891
C	-0.3300712	-2.3757087	-1.0484319
C	0.6382476	-2.2846685	-0.0434961
N	-0.9335955	-0.0700532	-1.3709344
N	1.0495797	-1.1527664	0.5330583
C	-1.9640679	-1.7750829	-2.8177768
H	-1.8777603	-2.8440274	-3.0026298
H	-1.7192105	-1.2430731	-3.7393333
H	-3.0075148	-1.5502642	-2.5903196
C	1.2878107	-3.5923741	0.3705519
H	0.9179686	-4.4087021	-0.2465499
H	1.0830337	-3.8298382	1.4151595
H	2.3727861	-3.5388188	0.2663033
Rh	0.4036474	0.6855496	0.0398661
C	-0.3837626	1.9166180	1.5002322
C	0.9545242	1.9940643	2.2047991
H	0.9671218	1.3071473	3.0673067
H	1.1884057	3.0038044	2.5894644
O	1.8357803	1.5886028	1.1884993
C	-0.5001789	2.8766463	0.3473154
H	0.0221578	2.4887165	-0.5900260
H	0.0607381	3.7999289	0.5132490
H	-1.5239417	3.0750428	0.0392622
C	-1.6122316	1.5939902	2.2983032
H	-1.4639724	0.7044038	2.9111361
H	-2.4932227	1.4470274	1.6741440
H	-1.8289335	2.4240859	2.9859671
C	2.0304158	-1.2384010	1.5842942
C	3.9365879	-1.4301911	3.6059163
C	1.6232150	-1.5429851	2.8926169
C	3.3858066	-1.0139852	1.2821381
C	4.3230737	-1.1246832	2.3056944
C	2.5956764	-1.6321378	3.8927439
H	5.3700068	-0.9547873	2.0802042
H	2.2876384	-1.8644103	4.9067612
H	4.6794586	-1.5040280	4.3916424
C	-1.6891278	0.8978046	-2.1107185
C	-3.0892821	2.8905676	-3.4778720

C	-1.0654161	1.5903368	-3.1694283
C	-3.0163589	1.1908097	-1.7485947
C	-3.6962231	2.1956610	-2.4424509
C	-1.7830634	2.5805333	-3.8388151
H	-4.7177234	2.4294131	-2.1614377
H	-1.3082155	3.1146575	-4.6543201
H	-3.6303369	3.6675056	-4.0050413
C	-3.7340135	0.4296908	-0.6610210
H	-4.3582882	-0.3638523	-1.0849336
H	-4.3998131	1.0887446	-0.1001504
H	-3.0393367	-0.0400812	0.0323716
C	0.3472884	1.2697719	-3.5890642
H	0.4661510	0.2128939	-3.8400263
H	1.0651685	1.4798717	-2.7913004
H	0.6297146	1.8594383	-4.4620497
C	0.1802013	-1.8153842	3.2413868
H	-0.0409654	-1.4741788	4.2545609
H	-0.0428292	-2.8875944	3.2110098
H	-0.5039723	-1.3260995	2.5504536
C	3.8219847	-0.6309124	-0.1055337
H	4.9102823	-0.6346575	-0.1807208
H	3.4640731	0.3747892	-0.3384618
H	3.4251420	-1.3069302	-0.8665209

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XyNacnacRh_7.xyz

C	-1.8581857	-0.8078105	-1.2655514
H	-2.8343301	-2.4476887	-0.3792482
C	-2.0415749	-1.7309308	-0.2267358
C	-1.3100318	-1.8913193	0.9551810
N	-0.9536844	0.1640446	-1.2595917
N	-0.2970151	-1.1185823	1.3321601
C	-2.7625549	-0.9833163	-2.4729356
H	-3.4613770	-1.8011907	-2.3093819
H	-2.1824561	-1.2035105	-3.3715272
H	-3.3333784	-0.0773575	-2.6825719
C	-1.7131554	-3.0573567	1.8374755
H	-2.5579137	-3.5886835	1.4034335
H	-1.9881377	-2.7196752	2.8379763
H	-0.8864242	-3.7596193	1.9606218
Rh	0.3511021	0.5487048	0.3495589
H	-0.6861367	1.3931573	1.0403582
O	1.8063397	0.7681756	1.7642556
C	2.5091958	1.9021078	1.3432343
H	3.5941248	1.7507111	1.4398908
H	2.2458865	2.8011022	1.9245346
C	2.1094594	2.0872771	-0.1159770
C	3.0438934	1.5681385	-1.1707831
H	3.9271712	2.2170185	-1.2024103
H	2.5937412	1.5621889	-2.1631000
H	3.4043974	0.5653747	-0.9275199
C	0.9483533	2.7429763	-0.3959351
H	0.6297794	2.9106923	-1.4150471
H	0.4576336	3.3284583	0.3711535

C	0.3815002	-1.4215798	2.5612981	C	2.1381004	2.1187630	1.6409103
C	1.6962220	-2.0541943	4.9318662	H	3.2275429	2.2855986	1.6093476
C	-0.0728240	-0.8720487	3.7705089	H	1.7451440	2.7100242	2.4835635
C	1.5109685	-2.2549127	2.5256542	C	1.4781570	2.5885952	0.3458857
C	2.1503773	-2.5678215	3.7242824	C	0.6601814	3.8460317	0.3686026
C	0.5962149	-1.2078924	4.9481103	H	-0.0525447	3.8489387	1.1955340
H	3.0184282	-3.2177490	3.7055189	H	0.1276502	4.0119606	-0.5678520
H	0.2469396	-0.7945347	5.8880590	H	1.3339108	4.6965166	0.5287324
H	2.2031392	-2.3064661	5.8561057	C	1.7775648	1.9194045	-0.8094917
C	-0.8567723	0.9892960	-2.4256939	H	1.3954537	2.2576527	-1.7621998
C	-0.6015373	2.6167933	-4.6777915	H	2.6140443	1.2281117	-0.8364214
C	-1.6345122	2.1574404	-2.5314898	C	0.4041311	-1.4912594	2.5610282
C	0.0405317	0.6287406	-3.4476665	C	1.7501141	-2.1710383	4.9004582
C	0.1555245	1.4580127	-4.5649756	C	-0.0212805	-0.9504982	3.7847230
C	-1.4916344	2.9568068	-3.6666206	C	1.5217687	-2.3379973	2.4950011
H	0.8460178	1.1856119	-5.3558158	C	2.1765678	-2.6750937	3.6790973
H	-2.0867581	3.8593242	-3.7538297	C	0.6626124	-1.3093892	4.9463358
H	-0.5007280	3.2507540	-5.5508103	H	3.0351576	-3.3363442	3.6376159
C	-1.2374812	0.0809636	3.8133524	H	0.3362664	-0.9018739	5.8969218
H	-1.5306251	0.2832261	4.8444759	H	2.2691446	-2.4420175	5.8125176
H	-0.9688750	1.0303493	3.3423799	C	-0.8526168	0.9934330	-2.3901480
H	-2.1102291	-0.3000791	3.2788324	C	-0.6125833	2.6769250	-4.6026579
C	2.0459133	-2.7886849	1.2226351	C	-1.5984916	2.1851173	-2.4410600
H	2.8652681	-3.4866360	1.4006219	C	0.0078444	0.6389994	-3.4457534
H	2.4286425	-1.9720787	0.6039326	C	0.1116787	1.4927064	-4.5442254
H	1.2817739	-3.3044648	0.6364123	C	-1.4601942	3.0147216	-3.5560554
C	0.8489843	-0.6414252	-3.3607542	H	0.7734892	1.2244382	-5.3603657
H	0.2128106	-1.5294764	-3.4128097	H	-2.0315483	3.9355371	-3.6013234
H	1.3965728	-0.7115379	-2.4191857	H	-0.5181721	3.3318579	-5.4607498
H	1.5665701	-0.6979438	-4.1803752	C	-1.1714649	0.0179856	3.8558445
C	-2.5989788	2.5520799	-1.4434232	H	-1.4203214	0.2434898	4.8936630
H	-3.3834939	1.8043362	-1.3014093	H	-0.9123445	0.9544108	3.3545004
H	-3.0796705	3.5015581	-1.6821419	H	-2.0701064	-0.3623690	3.3652027
H	-2.0930013	2.6511464	-0.4807707	C	2.0302848	-2.8594637	1.1759387
=====				H	2.8277955	-3.5869250	1.3326766
62	XyNacnacRh_7a.xyz			H	2.4375635	-2.0435773	0.5721722
C	-1.8789715	-0.7930734	-1.2293820	H	1.2459676	-3.3369815	0.5844745
H	-2.8867492	-2.4089888	-0.3348223	C	0.8161996	-0.6320765	-3.3945689
C	-2.0726651	-1.7150191	-0.1897576	H	0.1837076	-1.5173855	-3.2944418
C	-1.3276721	-1.9061473	0.9790258	H	1.4942964	-0.6393219	-2.5374613
N	-0.9389751	0.1430204	-1.2411826	H	1.4135944	-0.7441734	-4.3000291
N	-0.2937149	-1.1582817	1.3509655	C	-2.5470878	2.5637205	-1.3325524
C	-2.8102511	-0.9347920	-2.4205157	H	-3.4057115	1.8876983	-1.2861704
H	-3.5400633	-1.7218840	-2.2423180	H	-2.9295040	3.5742111	-1.4827375
H	-2.2529743	-1.1833940	-3.3262984	H	-2.0642134	2.5149472	-0.3556842
H	-3.3454670	-0.0068153	-2.6264385	=====			
C	-1.7368542	-3.0789729	1.8493065	62	XyNacnacRh_8.xyz		
H	-2.5998405	-3.5867394	1.4231410	C	-1.2336611	-1.3168006	-1.9858129
H	-1.9849994	-2.7543399	2.8609937	H	-1.1579163	-3.4154419	-1.7284806
H	-0.9214005	-3.7988315	1.9430406	C	-0.7969952	-2.4778175	-1.3330846
Rh	0.3923557	0.4888532	0.3564449	C	0.0560249	-2.5609892	-0.2294263
H	-0.6902244	1.3174989	0.9973375	N	-0.8347169	-0.1063083	-1.6300358
O	1.8244141	0.7601495	1.7689289	N	0.6215040	-1.5137425	0.3711249

C	-2.1804350	-1.4846526	-3.1544695	H	3.4584866	-0.3975037	-0.0477331
H	-2.2789967	-2.5357481	-3.4196231	H	3.1075214	-2.0439736	-0.5780341
H	-1.8291231	-0.9331208	-4.0280974	=====			
H	-3.1730767	-1.0995288	-2.9119087	62			
C	0.3729244	-3.9516379	0.2841646	XyNacnacRh_9b.xyz			
H	0.0074703	-4.7015272	-0.4150131	C	-0.9438518	-1.3690438	-2.0825623
H	-0.0924870	-4.1353626	1.2540022	H	-0.4376272	-3.4045925	-1.8841345
H	1.4476490	-4.0861594	0.4145523	C	-0.3368696	-2.4424478	-1.4043726
Rh	0.5722128	0.3952345	-0.2379257	C	0.3597195	-2.4568776	-0.1929249
C	-0.3723808	1.3387941	1.3257639	N	-0.9186865	-0.1235153	-1.6455864
H	-0.2136959	0.6942098	2.1922233	N	0.6026513	-1.3969099	0.5855512
H	-1.4405400	1.4265012	1.1219099	C	-1.6635986	-1.7098144	-3.3744781
C	0.3183201	2.6911604	1.5288516	H	-1.5947332	-2.7751506	-3.5869978
H	0.0698488	3.3417407	0.6815727	H	-1.2416971	-1.1600614	-4.2180475
O	2.0512710	1.5761227	0.3272886	H	-2.7191396	-1.4352248	-3.3189187
C	1.8125320	2.4037464	1.4489395	C	0.8588129	-3.8188954	0.2595776
H	2.1447362	1.8945754	2.3697695	H	0.5769797	-4.5835586	-0.4611517
H	2.4068323	3.3220918	1.3535207	H	0.4450334	-4.0924427	1.2318322
C	-0.1315906	3.3830336	2.8209253	H	1.9448235	-3.8299839	0.3674792
H	0.3567749	4.3541273	2.9417186	Rh	0.0536024	0.5127602	0.1620081
H	0.1098494	2.7741783	3.6969823	H	1.4489236	0.9118150	-0.2738090
H	-1.2115098	3.5537438	2.8196379	C	0.6879892	1.3717996	1.9675879
C	1.3685165	-1.6939900	1.5822544	H	1.6234555	0.9967601	2.3799761
C	2.8309130	-2.0075796	3.9336682	H	-0.0984689	1.1543725	2.7040064
C	0.6907165	-1.8622237	2.8048108	C	0.7830667	2.9009734	1.7767359
C	2.7770005	-1.6732090	1.5318267	C	-0.1884788	3.3168869	0.7291273
C	3.4863289	-1.8403521	2.7200724	H	-0.5314331	4.3608485	0.6596563
C	1.4444268	-2.0134409	3.9705084	O	-0.6221130	2.5167876	-0.0963818
H	4.5700354	-1.8327104	2.6891643	C	0.6642479	3.7463349	3.0546624
H	0.9293211	-2.1370601	4.9170132	H	0.7622560	4.8177960	2.8546178
H	3.4007528	-2.1287481	4.8475215	H	1.4476388	3.4632725	3.7586042
C	-1.3050462	1.0640833	-2.3040170	H	-0.2971344	3.5764294	3.5454796
C	-2.1373708	3.4138657	-3.5545416	H	1.7594723	3.1251029	1.3139624
C	-0.4913364	1.6536533	-3.2953101	C	1.3323931	-1.6127792	1.8022765
C	-2.5337714	1.6474704	-1.9413581	C	2.7271748	-2.0116296	4.1856650
C	-2.9278062	2.8255976	-2.5781436	C	0.6240347	-1.8768589	2.9881249
C	-0.9299037	2.8250062	-3.9097620	C	2.7366785	-1.5403334	1.8058767
H	-3.8699690	3.2844279	-2.2980613	C	3.4146586	-1.7438123	3.0093604
H	-0.3117053	3.2815894	-4.6745277	C	1.3399738	-2.0765381	4.1690471
H	-2.4589466	4.3290417	-4.0375261	H	4.4981234	-1.6934680	3.0176367
C	-3.4435197	1.0253049	-0.9112039	H	0.7984503	-2.2851330	5.0852886
H	-4.2300088	0.4310994	-1.3884426	H	3.2696732	-2.1707120	5.1103097
H	-3.9418863	1.7970240	-0.3215114	C	-1.5479701	0.8983826	-2.4214551
H	-2.9033705	0.3671621	-0.2339900	C	-2.7548774	2.9491323	-3.8794922
C	0.8310454	1.0461264	-3.6919367	C	-0.8112650	1.5772298	-3.4086575
H	0.7436139	-0.0197047	-3.9128198	C	-2.8780770	1.2603908	-2.1452430
H	1.5718726	1.1479409	-2.8929342	C	-3.4659660	2.2835473	-2.8892735
H	1.2289800	1.5455532	-4.5758999	C	-1.4348044	2.5968343	-4.1290260
C	-0.8155942	-1.9098643	2.8938811	H	-4.4942540	2.5613226	-2.6840867
H	-1.1817209	-2.9418868	2.8807342	H	-0.8723647	3.1204274	-4.8946928
H	-1.1567923	-1.4639086	3.8298762	H	-3.2251187	3.7419213	-4.4495395
H	-1.2931174	-1.3850127	2.0690369	C	-3.6572042	0.5733855	-1.0530738
C	3.5194388	-1.4510591	0.2410441	H	-4.6795582	0.9520360	-1.0135693
H	4.5720704	-1.7131418	0.3572706	H	-3.1977610	0.7421061	-0.0746901

H	-3.7014186	-0.5091877	-1.1933735	C	-3.1428619	3.0152984	-3.6832536
C	0.6272171	1.2224321	-3.6835936	C	-1.1161590	1.7269326	-3.3560793
H	0.7325882	0.2062571	-4.0740109	C	-3.0632650	1.3482041	-1.9266962
H	1.2231251	1.2649775	-2.7693909	C	-3.7466864	2.3380113	-2.6325368
H	1.0585922	1.9070175	-4.4153557	C	-1.8348551	2.7108551	-4.0349883
C	3.5088264	-1.2356056	0.5494207	H	-4.7639462	2.5817185	-2.3469880
H	4.5814617	-1.3259553	0.7263211	H	-1.3555027	3.2460551	-4.8472526
H	3.3009836	-0.2206459	0.1999012	H	-3.6867041	3.7829985	-4.2209555
H	3.2405924	-1.9020504	-0.2730879	C	-3.7274100	0.6509919	-0.7679902
C	-0.8818360	-1.9455927	2.9970681	H	-3.6891566	-0.4367338	-0.8595294
H	-1.2633430	-2.7081948	2.3136000	H	-4.7735916	0.9489227	-0.6898830
H	-1.3242247	-0.9970730	2.6820106	H	-3.2368456	0.9116617	0.1737919
H	-1.2493447	-2.1752513	3.9982057	C	0.3139744	1.4432069	-3.7346333
=====				H	0.6010033	2.0258648	-4.6106620
62	XyNacnacRh_10a.xyz			H	0.4865616	0.3879631	-3.9581584
C	-0.9988712	-1.2149125	-2.0575033	H	0.9908187	1.7028607	-2.9163021
H	-0.3252679	-3.2078940	-1.9789058	C	3.5679797	-0.5894211	0.2642787
C	-0.2617035	-2.2556428	-1.4741312	H	3.2698428	0.4355209	0.0267499
C	0.5363524	-2.2377464	-0.3244673	H	3.2750871	-1.2010619	-0.5907376
N	-1.0258006	0.0241181	-1.5908132	H	4.6551101	-0.6145075	0.3482495
N	0.7215983	-1.1778881	0.4610369	C	-0.4942487	-2.1158841	2.9187442
C	-1.8104476	-1.5641892	-3.2894535	H	-1.1197951	-1.4197597	2.3608211
H	-1.7313125	-2.6267378	-3.5107950	H	-0.8252584	-2.1252917	3.9581961
H	-1.4699535	-1.0012905	-4.1605957	H	-0.6898101	-3.1108570	2.5059383
H	-2.8634351	-1.3145645	-3.1471436	=====			
C	1.2254644	-3.5444374	0.0249147	62	XyNacnacRh_10b.xyz		
H	0.9652292	-4.3153315	-0.6972775	C	-1.7882308	-0.7175493	-1.3835040
H	0.9463153	-3.8953573	1.0193328	H	-2.2151138	-2.7770060	-1.4324588
H	2.3110028	-3.4260440	0.0265812	C	-1.5389171	-2.0455046	-1.0163031
Rh	-0.0230342	0.7017684	0.0783058	C	-0.5319192	-2.5582960	-0.1877028
H	1.2158896	0.9770245	-0.7267100	N	-1.0626549	0.3256980	-0.9866470
C	0.3884455	1.9953275	2.0442224	N	0.3970031	-1.8150965	0.3994018
C	-0.8609442	1.6827781	2.8333760	C	-2.9632416	-0.4904728	-2.3163384
H	-1.7560388	1.7016118	2.2112507	H	-3.4445443	-1.4358547	-2.5577993
H	-0.9954578	2.4408754	3.6162153	H	-2.6431505	-0.0184101	-3.2473268
H	-0.7908062	0.7183338	3.3384538	H	-3.7065207	0.1713890	-1.8685164
C	1.6709153	2.0184319	2.8321847	C	-0.5177497	-4.0601352	0.0166350
H	2.5194001	2.3213959	2.2158113	H	-1.3089961	-4.5315556	-0.5630491
H	1.8991570	1.0420849	3.2604427	H	-0.6568072	-4.3170050	1.0683523
H	1.5898391	2.7250963	3.6676128	H	0.4397136	-4.4879297	-0.2865394
C	0.3174698	2.7326060	0.8528988	Rh	0.5683643	0.2162753	0.2483481
H	1.2122516	3.2630396	0.5043003	H	-0.2340837	0.4532458	1.4939908
O	-0.7272179	2.7144097	0.0852292	O	2.3964699	0.4986465	1.3036588
C	1.5485619	-1.3297325	1.6216342	C	2.2789829	1.5713698	0.5736356
C	3.1482266	-1.6461098	3.8879566	H	2.9344030	1.6760875	-0.3036890
C	2.9273736	-1.0559894	1.5450804	C	1.3050577	2.5480187	0.7849124
C	0.9693041	-1.7615102	2.8298117	C	0.7252815	2.8002592	2.1548029
C	1.7862484	-1.9082075	3.9524621	H	-0.3516880	2.9791229	2.1214188
C	3.7084839	-1.2247423	2.6892962	H	1.1823543	3.7080250	2.5698607
H	1.3444179	-2.2396067	4.8858163	H	0.9314366	1.9755292	2.8343647
H	4.7722126	-1.0216211	2.6337442	C	1.2047692	3.6932616	-0.1852513
H	3.7697784	-1.7688258	4.7669426	H	0.1660046	3.9288660	-0.4221088
C	-1.7479279	1.0359300	-2.3072413	H	1.7226497	3.4825374	-1.1225578

H	1.6467137	4.5973133	0.2513839	C	0.6852773	2.9010891	0.5631481
C	1.3562321	-2.4357640	1.2685917	H	1.2578645	2.8178384	1.5058952
C	3.2306169	-3.6369961	2.9408053	C	0.5052001	4.2833099	0.0039637
C	1.0498508	-2.6255845	2.6268915	H	-0.0753217	4.1779966	-0.9155378
C	2.6047442	-2.8168486	0.7488824	C	1.8787501	4.8962870	-0.3219605
C	3.5260203	-3.4242624	1.6008126	H	2.4155553	4.3007656	-1.0626049
C	2.0023724	-3.2333298	3.4458162	H	2.5025559	4.9713750	0.5734071
H	4.4895379	-3.7262467	1.2055785	H	1.7531530	5.9039710	-0.7242712
H	1.7729762	-3.3874253	4.4944452	C	-0.2724734	5.1539377	1.0069756
H	3.9582658	-4.1086568	3.5907452	H	0.2634437	5.2401386	1.9566494
C	-1.4516463	1.6330969	-1.4259290	H	-1.2622257	4.7410262	1.2101924
C	-2.2247454	4.1591972	-2.3192815	H	-0.4019939	6.1618063	0.6064257
C	-2.3894021	2.3746025	-0.6839160	C	1.0467890	-2.1211113	2.1990390
C	-0.8863691	2.1580248	-2.6022823	C	2.4707645	-2.0935839	4.5968232
C	-1.2921959	3.4206987	-3.0358897	C	2.4539296	-2.2336183	2.1766799
C	-2.7603596	3.6377639	-1.1485744	C	0.3534896	-1.9833301	3.4211477
H	-0.8669640	3.8271763	-3.9468259	C	1.0865608	-1.9746750	4.6080339
H	-3.4850468	4.2138862	-0.5839464	C	3.1448152	-2.2200618	3.3885539
H	-2.5291770	5.1386439	-2.6686234	H	0.5617037	-1.8709386	5.5513111
C	0.1383581	1.3808441	-3.3882816	H	4.2256808	-2.3078576	3.3804534
H	0.4313113	1.9285384	-4.2847253	H	3.0241248	-2.0828890	5.5286730
H	-0.2334519	0.4008148	-3.6960522	C	-1.1762348	0.4700168	-2.0837771
H	1.0390788	1.1991164	-2.7950044	C	-1.8512341	2.6531482	-3.6787549
C	-3.0037179	1.8216435	0.5758362	C	-2.3862362	1.1488367	-1.8543625
H	-2.2386711	1.5310724	1.2981508	C	-0.2905699	0.8936815	-3.0906170
H	-3.5981542	0.9249178	0.3806014	C	-0.6495151	1.9855378	-3.8817640
H	-3.6568696	2.5609388	1.0407617	C	-2.7082789	2.2360055	-2.6675745
C	2.9652059	-2.5543790	-0.6900397	H	0.0256084	2.3146745	-4.6644053
H	3.9105190	-3.0358854	-0.9430271	H	-3.6429154	2.7608945	-2.5011890
H	3.0806839	-1.4810469	-0.8655535	H	-2.1175951	3.4973383	-4.3044957
H	2.2028038	-2.9140248	-1.3842244	C	1.0267473	0.1962697	-3.3037838
C	-0.2622127	-2.1704909	3.2102755	H	0.8929141	-0.8360260	-3.6389460
H	-0.3509810	-2.4917469	4.2486722	H	1.5923311	0.1460884	-2.3697256
H	-0.3418637	-1.0803577	3.1840536	H	1.6227552	0.7182390	-4.0540605
H	-1.1223354	-2.5587605	2.6602832	C	-3.3112203	0.7251291	-0.7443593
=====				H	-2.7768540	0.6828736	0.2082656
62	XyNacnacRh_11a.xyz			H	-3.7206059	-0.2747532	-0.9127240
C	-1.1670028	-1.8674628	-1.5887629	H	-4.1478241	1.4195823	-0.6532969
H	-1.2279944	-3.9543472	-1.2685848	C	-1.1479635	-1.8590221	3.4506962
C	-0.8692385	-3.0248597	-0.8511955	H	-1.4905017	-1.0806250	2.7650995
C	-0.1652774	-3.1240391	0.3561846	H	-1.4945709	-1.6246137	4.4582895
N	-0.8149891	-0.6300440	-1.2450274	H	-1.6344813	-2.7871445	3.1367332
N	0.3270280	-2.0613643	0.9720415	C	3.1993582	-2.3767987	0.8749260
C	-1.9514115	-2.0702855	-2.8724631	H	2.9911414	-3.3377702	0.3959385
H	-2.1649400	-3.1269737	-3.0217819	H	4.2758663	-2.3118322	1.0392600
H	-1.3981695	-1.7049269	-3.7401541	H	2.8993316	-1.6034168	0.1643509
H	-2.8986937	-1.5274063	-2.8512768	=====			
C	0.0312020	-4.4956975	0.9633529	62	XyNacnacRh_11b.xyz		
H	-0.4305867	-5.2607788	0.3415218	C	-0.9081505	-1.4561308	-2.1323168
H	-0.4081992	-4.5538314	1.9621617	H	-0.8462780	-3.5457944	-1.8398988
H	1.0923922	-4.7338191	1.0693001	C	-0.6950975	-2.5945807	-1.3517557
Rh	0.2149201	-0.1771873	0.4043406	C	-0.3102189	-2.6471883	-0.0045644
O	0.2338649	1.8952342	0.0276222	N	-0.7823254	-0.2276044	-1.6465274

N	-0.0917249	-1.5838098	0.7652551	H	2.5705425	-1.0930636	0.4946327
C	-1.3103298	-1.6483494	-3.5774690	H	2.6693002	-2.8408826	0.5550160
H	-1.3943474	-2.7071767	-3.8150664	H	3.7741813	-1.8785440	1.5345132
H	-0.5793044	-1.1997958	-4.2537300	=====			
H	-2.2694755	-1.1692277	-3.7857495	62			
C	-0.1644674	-4.0289682	0.6042153	XyNacnacRh_12.xyz			
H	-0.4433039	-4.7908398	-0.1210449	C	-0.8494004	-0.9942571	-2.1968629
H	-0.8007582	-4.1376022	1.4844869	H	-0.7128287	-3.0942320	-2.1065608
H	0.8593906	-4.2217543	0.9285596	C	-0.5138175	-2.1889596	-1.5527303
Rh	-0.3588608	0.3160522	0.2280643	C	0.0637119	-2.3667742	-0.2884088
C	0.9175589	1.4111845	1.5866725	N	-0.6752927	0.1965105	-1.6418055
H	1.6168210	0.6858994	2.0227563	N	0.4006611	-1.3914720	0.5554509
O	-0.3049742	1.3900303	2.0022302	C	-1.4268437	-1.0983700	-3.5937046
C	1.5645050	2.6953241	1.0913380	H	-1.5324882	-2.1406607	-3.8890246
H	2.3788227	2.3994331	0.4195948	H	-0.7862097	-0.5975941	-4.3232045
C	2.1897697	3.4311452	2.2930423	H	-2.4065942	-0.6203113	-3.6547311
H	2.8946621	2.7922255	2.8305166	C	0.3251661	-3.8081708	0.1153126
H	1.4142976	3.7447422	2.9961015	H	-0.0053180	-4.4850614	-0.6698742
H	2.7292488	4.3215710	1.9602729	H	-0.1979175	-4.0689801	1.0366880
C	0.5888446	3.5960246	0.3326318	H	1.3872668	-3.9837750	0.2959407
H	1.0952180	4.4945900	-0.0269441	Rh	0.1271592	0.5955152	0.2233982
H	-0.2383850	3.9014397	0.9751828	C	1.5481706	1.3647301	1.6780297
H	0.1667671	3.0919652	-0.5419802	C	0.2467987	1.8339927	1.9262491
C	0.3927900	-1.7688127	2.1015643	C	-0.4742016	1.5747760	3.2208509
C	1.3460795	-2.1137513	4.6921646	H	-0.1007069	0.6707935	3.7019469
C	1.7734226	-1.9403726	2.3137492	H	-1.5512319	1.4686180	3.0716892
C	-0.5113577	-1.7419693	3.1779730	H	-0.3162997	2.4074395	3.9181943
C	-0.0114666	-1.9244025	4.4671444	C	-0.2540959	2.9270625	1.0173701
C	2.2296373	-2.1159886	3.6210235	H	-0.2534220	2.6038402	-0.0651869
H	-0.6999881	-1.9111422	5.3045998	H	0.3780995	3.8225653	1.0127406
H	3.2913853	-2.2510014	3.7957972	H	-1.2791240	3.2142291	1.2424128
H	1.7156283	-2.2508350	5.7016369	H	1.9848159	0.6576402	2.3697403
C	-0.9959646	0.9321724	-2.4496340	O	2.5801793	2.0817357	1.0636905
C	-1.3856401	3.2552961	-3.9357900	H	2.2293272	2.6089674	0.3369183
C	-2.2690443	1.5380018	-2.4703555	C	0.9644630	-1.7703029	1.8174169
C	0.0852233	1.4925642	-3.1603730	C	2.0527932	-2.4871064	4.2817394
C	-0.1335556	2.6535951	-3.9004368	C	0.1109455	-2.0162726	2.9081593
C	-2.4406270	2.6999782	-3.2235201	C	2.3605814	-1.8860371	1.9517505
H	0.6916665	3.0926558	-4.4499161	C	2.8837662	-2.2472348	3.1941303
H	-3.4155498	3.1736861	-3.2468274	C	0.6767311	-2.3717295	4.1342739
H	-1.5371404	4.1596812	-4.5131938	H	3.9586099	-2.3373148	3.3063200
C	1.4514158	0.8593870	-3.1191338	H	0.0251310	-2.5609983	4.9805433
H	2.1839989	1.4930218	-3.6200424	H	2.4766584	-2.7639602	5.2399386
H	1.4625886	-0.1172825	-3.6106793	C	-1.0050241	1.3815195	-2.3690489
H	1.7748643	0.6929282	-2.0894165	C	-1.6172226	3.7618475	-3.6893564
C	-3.4276476	0.9502827	-1.7051635	C	-0.0218759	2.0155031	-3.1541505
H	-3.2008512	0.8636099	-0.6396234	C	-2.2918084	1.9400877	-2.2385632
H	-3.6747187	-0.0561682	-2.0529031	C	-2.5773206	3.1300444	-2.9086222
H	-4.3156801	1.5730120	-1.8185582	C	-0.3500881	3.2049021	-3.8066065
C	-1.9806841	-1.5027909	2.9584737	H	-3.5659059	3.5655074	-2.8122848
H	-2.1460675	-0.4868652	2.5917671	H	0.4017979	3.6983687	-4.4127790
H	-2.5326832	-1.6283192	3.8906778	H	-1.8547707	4.6868005	-4.2015861
H	-2.4016167	-2.1843759	2.2160842	C	-3.3417560	1.2735229	-1.3874043
C	2.7496544	-1.9361094	1.1648753	H	-4.2268625	1.9054588	-1.3026429

H	-2.9622525	1.0608143	-0.3852129	C	-1.3471273	0.4250693	-2.6305459
H	-3.6555644	0.3134366	-1.8065707	C	-2.3902057	2.1760670	-4.5353082
C	1.3591651	1.4278806	-3.2909278	C	-0.5093769	0.9380918	-3.6409058
H	1.3444946	0.4806207	-3.8371531	C	-2.7031151	0.7979551	-2.5629251
H	1.7966480	1.2101675	-2.3136778	C	-3.2040506	1.6687484	-3.5311748
H	2.0176027	2.1117676	-3.8281418	C	-1.0511309	1.8116710	-4.5838894
C	3.2776170	-1.6228149	0.7859225	H	-4.2491916	1.9550616	-3.4887179
H	3.0679602	-2.2899637	-0.0540101	H	-2.7972295	2.8546343	-5.2757333
H	4.3188605	-1.7640137	1.0781805	C	0.0886810	-1.2624784	3.4890665
H	3.1580789	-0.6037474	0.4118292	H	-0.4796482	-1.8419405	2.7619929
C	-1.3857164	-1.9233491	2.7591696	H	0.0152587	-1.7566490	4.4594855
H	-1.7860252	-2.7683091	2.1903786	H	-0.4037949	-0.2904411	3.5774120
H	-1.6737318	-1.0205776	2.2184795	C	3.7089427	-0.6610728	-0.0305844
H	-1.8715434	-1.9243156	3.7359780	H	4.7947198	-0.5878098	-0.1035805
=====							
62							
XyNacnacRh_13.xyz							
C	-0.7952841	-1.7417485	-1.7851840	H	3.2745864	0.2390231	-0.4759863
H	-0.2899077	-3.6686147	-1.0945175	H	3.3817255	-1.5046647	-0.6425748
C	-0.1722568	-2.6179914	-0.8744224	C	0.9483746	0.5580912	-3.7124158
C	0.6578742	-2.3361729	0.2145104	H	1.4859139	0.8574550	-2.8080875
N	-0.7888026	-0.4315323	-1.6323474	H	1.4281177	1.0418805	-4.5639854
N	0.9663281	-1.1195539	0.6860490	H	1.0876871	-0.5211134	-3.8147413
C	-1.4637093	-2.3673742	-2.9925780	C	-3.6043215	0.2977002	-1.4631588
H	-1.4216983	-3.4539556	-2.9429120	H	-3.4868158	-0.7720889	-1.2828500
H	-0.9732608	-2.0453526	-3.9144675	H	-3.3822876	0.8126653	-0.5254804
H	-2.5082865	-2.0602541	-3.0696942	H	-4.6494347	0.4886783	-1.7116399
C	1.2940031	-3.5393924	0.8890458	H	-0.4110478	2.2085928	-5.3641928
H	0.9642221	-4.4578753	0.4082498	=====			
H	1.0351501	-3.5894111	1.9477693	62			
H	2.3833082	-3.4917848	0.8330908	XyNacnacRh_14a.xyz			
Rh	0.1713768	0.5645921	-0.0060650	C	-0.3873717	-1.1521144	-2.2929642
H	1.1562623	1.3401887	0.9270610	H	0.2347182	-3.1672835	-2.2755221
C	-1.1286409	1.2213375	1.3367915	C	0.1656692	-2.2815040	-1.6614618
H	-1.7706216	0.4262043	1.7211675	C	0.6017279	-2.4371834	-0.3415261
C	-1.2116172	2.5528760	1.9628144	N	-0.5391151	0.0129212	-1.6901403
O	-1.8268469	2.2748913	0.6545653	N	0.6136757	-1.4800126	0.5899494
C	-0.0849998	3.5503970	1.9377493	C	-0.8324674	-1.3262299	-3.7323764
H	0.5667878	3.3862070	1.0821540	H	-0.6121947	-2.3313316	-4.0877608
H	0.5183807	3.4589584	2.8449495	H	-0.3341081	-0.6085197	-4.3870667
H	-0.4839942	4.5676228	1.8944018	H	-1.9058335	-1.1514646	-3.8354740
C	-2.2343636	2.7713143	3.0556049	C	1.0763993	-3.8275327	0.0420087
H	-1.7616462	2.6922866	4.0384417	H	1.0017756	-4.5018797	-0.8087425
H	-3.0376900	2.0360204	2.9968297	H	0.4806213	-4.2376260	0.8599649
H	-2.6754511	3.7686844	2.9755205	H	2.1127428	-3.8162518	0.3843930
C	1.9311357	-1.0031021	1.7466140	Rh	0.0770144	0.4416256	0.2933285
C	3.8420419	-0.7810606	3.7632282	H	1.5005818	0.9039576	0.0757156
C	1.5318349	-1.0883745	3.0900887	C	0.3623815	1.2476719	2.2275574
C	3.2814134	-0.7978953	1.4064077	H	1.3714719	1.2052378	2.6346746
C	4.2217017	-0.6912173	2.4297621	H	-0.3324201	0.7918876	2.9374944
C	2.5066499	-0.9783681	4.0839003	C	-0.0356414	2.6291619	1.8337894
H	5.2636579	-0.5335693	2.1740829	C	0.8575230	3.8018685	2.1177648
H	2.2068641	-1.0508946	5.1238373	H	0.8524100	4.0068544	3.1922225
H	4.5848554	-0.6992115	4.5480221	H	0.5305948	4.6980847	1.5878630
				H	1.8850475	3.5753742	1.8257762
				C	-1.4151936	2.8593673	1.3990247
				H	-1.8012115	3.8739812	1.3515366

H	-2.1690552	2.0953860	1.5689388	H	1.4358349	0.9637596	-0.3111831
O	-0.4728380	2.5728494	0.3381599	C	0.6686697	1.5056763	1.9910073
C	1.0844906	-1.8011802	1.9059990	H	1.7372228	1.6994382	2.0898427
C	1.9688709	-2.4070165	4.4816674	H	0.3077360	1.0162567	2.8971323
C	0.1585341	-2.2104050	2.8826352	C	-0.1172092	2.7285278	1.6624443
C	2.4511736	-1.6831273	2.2166246	C	0.2723747	3.5294445	0.5013030
C	2.8716220	-1.9928941	3.5114596	H	-0.1242164	4.5357500	0.3970932
C	0.6208925	-2.5123280	4.1638139	H	1.2311225	3.3622352	0.0233712
H	3.9248555	-1.9083223	3.7562392	C	-1.1249433	3.2811143	2.6299633
H	-0.0884140	-2.8332481	4.9189370	H	-1.7660195	4.0315707	2.1645140
H	2.3138692	-2.6466341	5.4807006	H	-0.5991653	3.7415193	3.4713743
C	-1.1490782	1.1029426	-2.3810414	H	-1.7515160	2.4807384	3.0292604
C	-2.3458519	3.2812469	-3.6501186	O	-0.7259825	2.5120728	0.2383638
C	-0.3514757	2.0195382	-3.0899199	C	1.5577375	-1.5152679	1.8307099
C	-2.5408400	1.2882843	-2.2856040	C	2.9609461	-1.7829805	4.2271554
C	-3.1211532	2.3802202	-2.9315938	C	0.8658835	-1.8448308	3.0105415
C	-0.9710674	3.0983392	-3.7217327	C	2.9485634	-1.3078452	1.8479657
H	-4.1945889	2.5228634	-2.8668188	C	3.6307690	-1.4479537	3.0581264
H	-0.3614926	3.8047986	-4.2747465	C	1.5860513	-1.9784286	4.1978574
H	-2.8104011	4.1248620	-4.1471973	H	4.7042065	-1.2938347	3.0772702
C	-3.4000810	0.3303306	-1.4992196	H	1.0580294	-2.2380271	5.1089870
H	-3.3404007	-0.6908026	-1.8842309	H	3.5073767	-1.8915203	5.1567362
H	-4.4457561	0.6399492	-1.5279757	C	-1.5078900	0.8174065	-2.2956648
H	-3.0904523	0.2813677	-0.4514619	C	-2.8680687	2.8384401	-3.6570187
C	1.1434663	1.8516326	-3.1644887	C	-0.8371161	1.5681195	-3.2793438
H	1.4278015	0.9039604	-3.6296720	C	-2.8477740	1.0964352	-1.9719213
H	1.5860550	1.8526116	-2.1660530	C	-3.5128250	2.1048730	-2.6696698
H	1.5919599	2.6595655	-3.7441408	C	-1.5371352	2.5712621	-3.9508998
C	3.4522225	-1.2224153	1.1903350	H	-4.5489704	2.3173782	-2.4292729
H	4.4659975	-1.2853046	1.5880256	H	-1.0265451	3.1494112	-4.7136726
H	3.2607507	-0.1872889	0.8951901	H	-3.3980180	3.6193548	-4.1899241
H	3.4080852	-1.8145828	0.2736422	C	-3.5568586	0.3355887	-0.8810356
C	-1.3107746	-2.3186190	2.5644886	H	-3.5105179	-0.7452589	-1.0320919
H	-1.5039507	-2.9954895	1.7287715	H	-4.6066969	0.6275254	-0.8291652
H	-1.8654944	-2.6825691	3.4303648	H	-3.1055517	0.5373572	0.0949655
H	-1.7262787	-1.3475811	2.2799937	C	0.6104307	1.3047592	-3.6053567
=====							
62							
XyNacnacRh_14b.xyz							
C	-0.7276500	-1.4183178	-2.0418798	C	3.7010224	-0.9329754	0.5987372
H	-0.0469729	-3.4093557	-1.8980928	H	4.7746020	-0.9078055	0.7902818
C	-0.0259485	-2.4533504	-1.3961164	H	3.3919129	0.0512806	0.2368813
C	0.6740522	-2.4330243	-0.1852889	H	3.5168470	-1.6316751	-0.2203656
N	-0.8022431	-0.1881197	-1.5684769	C	-0.6281484	-2.0439119	3.0059256
N	0.8214079	-1.3695924	0.6088926	H	-0.9799746	-2.3354024	3.9964607
C	-1.4371271	-1.7794570	-3.3328780	H	-0.9410423	-2.8123012	2.2951652
H	-1.2839186	-2.8286673	-3.5792508	H	-1.1481315	-1.1254825	2.7186769
H	-1.0782679	-1.1715706	-4.1656586	=====			
H	-2.5108288	-1.5959109	-3.2509882	62			
C	1.2900380	-3.7514298	0.2482424	XyNacnacRh_14c.xyz			
H	1.0863341	-4.5257073	-0.4886511	C	-0.9787693	-1.3868873	-1.9606073
H	0.8918370	-4.0783672	1.2108428	H	-0.3538375	-3.3952552	-1.8160243
H	2.3714598	-3.6653980	0.3694149	C	-0.2822653	-2.4343371	-1.3288927
Rh	0.1082758	0.4798416	0.2250914	C	0.4598655	-2.4267693	-0.1460756

N	-0.9839906	-0.1513753	-1.4997729	C	-0.6957544	-1.9584852	3.1016454
N	0.6863192	-1.3687522	0.6438765	H	-1.0190322	-2.2231379	4.1089512
C	-1.7584705	-1.7408421	-3.2117788	H	-1.0804571	-2.7145782	2.4128590
H	-1.6316294	-2.7919031	-3.4642409	H	-1.1762239	-1.0146669	2.8307190
H	-1.4348952	-1.1380526	-4.0623757	=====			
H	-2.8244756	-1.5451515	-3.0756239	62			
C	1.0353042	-3.7668959	0.2783166	XyNacnacRh_15.xyz			
H	0.7617591	-4.5376631	-0.4388861	C	-1.0748909	-1.4013077	-2.0687276
H	0.6667527	-4.0634014	1.2618614	H	-0.8656469	-3.5008303	-1.8941614
H	2.1235369	-3.7295950	0.3486981	C	-0.6033469	-2.5583063	-1.4378912
Rh	0.0795900	0.4954875	0.2457102	C	0.1572526	-2.6198635	-0.2675348
H	1.4507055	0.9205428	-0.2415734	N	-0.7891089	-0.1799031	-1.6395818
C	0.7507352	1.3994925	2.0149945	N	0.5901144	-1.5482841	0.3925390
H	1.7520945	1.1666942	2.3717422	C	-1.9258584	-1.5764915	-3.3083735
H	0.0289356	1.1196429	2.7919975	H	-2.0181853	-2.6310341	-3.5612064
C	0.5850985	2.8416245	1.6410982	H	-1.4883550	-1.0506827	-4.1593928
C	-0.5823072	3.0503857	0.6986641	H	-2.9273085	-1.1669165	-3.1645769
H	-0.5157676	2.3936487	-0.2096008	C	0.5258689	-3.9960838	0.2475944
H	-0.6069745	4.0541888	0.2699902	H	0.1873462	-4.7618938	-0.4475777
H	-1.5338277	2.8588470	1.1964887	H	0.0770559	-4.1936360	1.2222523
C	1.7072112	3.7851363	1.6199100	H	1.6064657	-4.0892528	0.3712631
H	1.7147159	4.6139644	0.9146405	Rh	0.4910754	0.3806529	-0.1659645
H	2.6878995	3.4466214	1.9449935	C	-0.3715995	1.5493792	1.3108036
O	0.7150188	3.8714919	2.6545811	H	-0.5952571	0.9466906	2.1870631
C	1.4673194	-1.5542257	1.8343069	H	-1.2564520	2.0204675	0.8865331
C	2.9518305	-1.9170966	4.1637313	C	0.8562723	2.4504076	1.4170931
C	0.8058242	-1.8444645	3.0409044	O	1.6698056	1.8438879	0.3897589
C	2.8676901	-1.4371316	1.7876075	C	0.5843249	3.9064471	1.0470410
C	3.5910751	-1.6239641	2.9668585	H	1.5261098	4.4561256	0.9775976
C	1.5677227	-2.0257205	4.1950311	H	-0.0457564	4.3901749	1.7986928
H	4.6718042	-1.5386274	2.9397284	H	0.0810017	3.9664657	0.0799552
H	1.0650163	-2.2520721	5.1286441	C	1.5768816	2.3495312	2.7594742
H	3.5298302	-2.0596467	5.0691338	H	2.5266216	2.8879169	2.7153461
C	-1.7189724	0.8650199	-2.1825951	H	1.7845593	1.3071149	3.0069056
C	-3.1194251	2.9339988	-3.4249258	H	0.9699075	2.7824212	3.5600011
C	-1.0918075	1.6235098	-3.1899264	C	1.2357827	-1.6912800	1.6625721
C	-3.0400852	1.1490007	-1.7866834	C	2.4796339	-1.9185952	4.1425422
C	-3.7240609	2.1848938	-2.4236416	C	0.4506355	-1.8589845	2.8195510
C	-1.8121286	2.6518098	-3.7994588	C	2.6395001	-1.6236406	1.7405978
H	-4.7433001	2.4055600	-2.1259642	C	3.2403289	-1.7474884	2.9933646
H	-1.3359026	3.2385487	-4.5774542	C	1.0948200	-1.9692700	4.0516380
H	-3.6633675	3.7368980	-3.9081452	H	4.3211306	-1.7011177	3.0642173
C	-3.7095988	0.3606137	-0.6893801	H	0.4988576	-2.0938832	4.9489532
H	-3.7352505	-0.7096196	-0.9072041	H	2.9648417	-2.0064943	5.1074216
H	-4.7356259	0.7004639	-0.5441553	C	-1.3653411	0.9718351	-2.2609319
H	-3.1823316	0.4693255	0.2629103	C	-2.4610435	3.2603326	-3.4065370
C	0.3280114	1.3387957	-3.6076850	C	-0.6309130	1.6795796	-3.2311827
H	0.6823024	2.0985637	-4.3053473	C	-2.6404766	1.4092035	-1.8535121
H	0.4209940	0.3662796	-4.0996681	C	-3.1702990	2.5574799	-2.4407765
H	0.9980521	1.3146108	-2.7460597	C	-1.2024602	2.8205548	-3.7948591
C	3.5892608	-1.0987443	0.5104283	H	-4.1507164	2.9032259	-2.1325398
H	4.6673453	-1.1994399	0.6411199	H	-0.6466201	3.3712928	-4.5451993
H	3.3766947	-0.0707253	0.2031797	H	-2.8868359	4.1512314	-3.8527174
H	3.2842190	-1.7364328	-0.3215755	C	-3.4240047	0.6600554	-0.8067090

H	-3.7797632	-0.3062611	-1.1765474	H	1.1390736	-2.6852197	5.9988186
H	-4.2970958	1.2354980	-0.4964980	C	-1.0713221	1.1030950	-2.2283191
H	-2.8131456	0.4520249	0.0730816	C	-1.6041326	3.3517180	-3.7864335
C	0.7481693	1.2383727	-3.6500046	C	-2.3842662	1.6041379	-2.2966015
H	0.7751850	0.1835480	-3.9313980	C	-0.0262798	1.7156588	-2.9430978
H	1.4659115	1.3699318	-2.8350813	C	-0.3143660	2.8445832	-3.7128374
H	1.0952627	1.8263640	-4.5003162	C	-2.6286659	2.7282661	-3.0844726
C	3.4874927	-1.3921184	0.5178019	H	0.4877118	3.3266240	-4.2614727
H	4.5387440	-1.5782253	0.7411931	H	-3.6382050	3.1197790	-3.1433071
H	3.3908326	-0.3569255	0.1772778	H	-1.8119268	4.2277644	-4.3895850
H	3.1950186	-2.0349143	-0.3146773	C	2.7674492	-1.7383338	1.7314013
C	-1.0537479	-1.9261261	2.7473946	H	2.5921341	-0.8193319	1.1692311
H	-1.4914856	-1.7581354	3.7323050	H	2.8709313	-2.5396018	0.9940660
H	-1.4008363	-2.9042138	2.3992073	H	3.7181225	-1.6464256	2.2575969
H	-1.4562600	-1.1860533	2.0554429	C	-2.1810548	-2.2045019	2.7575479
=====				H	-2.4487595	-1.2293095	2.3418612
62	XyNacnacRh_16.xyz			H	-2.8416045	-2.4057030	3.6016998
C	-0.7311339	-1.2458834	-1.9722718	H	-2.3918695	-2.9439831	1.9806080
H	-0.4214975	-3.3212972	-1.9600176	C	1.3785522	1.1660352	-2.9166004
C	-0.3960868	-2.4433295	-1.3319774	H	1.6414534	0.7708501	-1.9354624
C	-0.0663604	-2.6757784	0.0140276	H	2.0991202	1.9380776	-3.1912560
N	-0.7854423	-0.0365293	-1.4033077	H	1.5015001	0.3436472	-3.6287902
N	-0.0038661	-1.7124490	0.9166400	C	-3.5059511	0.9590195	-1.5278448
C	-1.0993659	-1.3643349	-3.4412805	H	-4.4613554	1.4198898	-1.7817450
H	-1.0631125	-2.4050131	-3.7561363	H	-3.3464528	1.0631655	-0.4509021
H	-0.4241242	-0.7898260	-4.0763062	H	-3.5783687	-0.1121678	-1.7295033
H	-2.1057125	-0.9827326	-3.6241943	=====			
C	0.1939664	-4.1121569	0.4196001	62	XyNacnacRh_17.xyz		
H	0.1154657	-4.7784411	-0.4374693	C	-0.3858089	-0.8885161	-1.9499865
H	-0.5219018	-4.4366783	1.1780710	H	0.2798859	-2.8713634	-1.8370231
H	1.1872457	-4.2242028	0.8581503	C	0.1592586	-1.9724132	-1.2506171
Rh	-0.4415797	0.3225076	0.5500282	C	0.4004776	-2.1372452	0.1309835
C	0.7202533	1.7339149	1.0949524	N	-0.5718440	0.3364107	-1.4490477
O	0.6611048	1.5044056	2.2902083	N	0.3535245	-1.1596775	1.0187425
H	-1.2278267	1.6818931	0.3876647	C	-0.8354187	-1.1838946	-3.3701196
C	1.5067753	2.8473768	0.4415324	H	-0.5008682	-2.1722907	-3.6786380
H	1.4060976	2.7305715	-0.6362801	H	-0.4540826	-0.4472753	-4.0776879
C	2.9876501	2.7520713	0.8369767	H	-1.9252304	-1.1547867	-3.4438689
H	3.5481280	3.5610617	0.3632594	C	0.6902965	-3.5577543	0.5834579
H	3.4282600	1.8050683	0.5189754	H	0.6412469	-4.2498806	-0.2546053
H	3.1063154	2.8365644	1.9183928	H	-0.0292301	-3.8777703	1.3399953
C	0.8848033	4.1944086	0.8498962	H	1.6796248	-3.6347244	1.0374617
H	1.4133051	5.0072272	0.3471149	Rh	0.0029687	0.9421800	0.4794286
H	0.9607429	4.3446681	1.9283895	H	-0.3579824	2.3954965	0.0269664
H	-0.1673909	4.2465726	0.5663466	C	2.0500804	1.5172704	0.4106909
C	0.3054921	-2.0102028	2.2794885	H	2.4156044	1.1034868	1.3494632
C	0.9059578	-2.4963661	4.9575716	C	-0.0304513	1.6774996	2.1881273
C	1.6472463	-2.0055408	2.7030065	O	-0.1279773	2.1931955	3.2054208
C	-0.7387416	-2.2355243	3.1958769	C	2.2953598	3.0155757	0.3850445
C	-0.4154265	-2.4824046	4.5299960	H	3.3778204	3.2039434	0.3805514
C	1.9258555	-2.2551210	4.0467799	H	1.8780131	3.5211698	1.2560128
H	-1.2143840	-2.6596971	5.2415055	H	1.8763809	3.4842131	-0.5064240
H	2.9578204	-2.2525359	4.3801894	C	2.7023542	0.7892479	-0.7492344

H	3.7922058	0.8148600	-0.6121954	Rh	0.2645115	0.5557438	0.4438408
H	2.4828889	1.2629854	-1.7032436	O	0.3362215	2.7710840	0.2197831
H	2.4098039	-0.2589135	-0.8165370	C	-0.5679706	3.8472486	-0.1100735
C	0.4886380	-1.4756631	2.4128320	C	0.7387505	3.7447886	-0.7675650
C	0.6704941	-1.9623321	5.1636381	H	1.5572783	4.3787663	-0.4446939
C	1.7511301	-1.5940741	3.0207065	H	0.7870215	3.3636384	-1.7801872
C	-0.6851567	-1.6160012	3.1848782	C	1.1354759	-1.0682601	2.5139255
C	-0.5732029	-1.8591783	4.5516933	C	2.3654014	-0.6322299	4.9779457
C	1.8166505	-1.8325054	4.3971246	C	0.3421067	-0.8641503	3.6630413
H	-1.4757866	-1.9678808	5.1428593	C	2.5440853	-1.0430802	2.5955624
H	2.7913011	-1.9201527	4.8661019	C	3.1373896	-0.8256617	3.8392205
H	0.7417762	-2.1459497	6.2290871	C	0.9793132	-0.6503133	4.8854080
C	-1.4076710	1.2469978	-2.1948381	H	4.2193245	-0.8050092	3.9110372
C	-3.0977333	2.9966838	-3.5775276	H	0.3772611	-0.4926350	5.7735865
C	-0.8694106	2.1416425	-3.1352052	H	2.8434873	-0.4617646	5.9356262
C	-2.7944241	1.2307647	-1.9461299	C	-0.9832586	0.7590159	-2.1575393
C	-3.6202093	2.1102179	-2.6460126	C	-1.7488780	2.6631921	-4.0512585
C	-1.7313164	3.0049764	-3.8150201	C	-0.0742327	1.1495013	-3.1623393
H	-4.6872192	2.0967512	-2.4526415	C	-2.2703003	1.3312604	-2.0917256
H	-1.3153940	3.6917154	-4.5441772	C	-2.6335065	2.2792462	-3.0501402
H	-3.7507312	3.6737051	-4.1154288	C	-0.4787928	2.1005173	-4.1010300
C	3.0459860	-1.5040077	2.2481477	H	-3.6251680	2.7172474	-3.0098163
H	2.8859246	-1.2720327	1.1992317	H	0.2129305	2.3990100	-4.8816094
H	3.6990283	-0.7352333	2.6694237	H	-2.0485659	3.3969100	-4.7904552
H	3.5945398	-2.4492995	2.3036844	C	-3.2387952	0.9216563	-1.0133277
C	-2.0497189	-1.5123405	2.5529707	H	-3.5755003	-0.1104274	-1.1450471
H	-2.2385183	-0.5068327	2.1676023	H	-4.1211324	1.5638287	-1.0196710
H	-2.8272976	-1.7420195	3.2824551	H	-2.7654346	0.9650734	-0.0287261
H	-2.1629391	-2.1948903	1.7077641	C	1.3046394	0.5470495	-3.2272487
C	0.6070215	2.2125557	-3.4185915	H	1.7952285	0.5930030	-2.2513041
H	1.1295851	2.7452005	-2.6204701	H	1.9192780	1.0637548	-3.9660908
H	0.7926529	2.7483248	-4.3508283	H	1.2697517	-0.5108072	-3.5018388
H	1.0633381	1.2251272	-3.4956027	C	3.3952874	-1.2522060	1.3700949
C	-3.3963512	0.2991329	-0.9259292	H	3.3113992	-2.2747819	0.9909300
H	-3.0478152	0.5409966	0.0822787	H	4.4460916	-1.0641512	1.5952465
H	-4.4839949	0.3795254	-0.9299726	H	3.0798236	-0.5920463	0.5588542
H	-3.1320772	-0.7449530	-1.1072230	C	-1.1621513	-0.8815081	3.5795307
=====				H	-1.5165340	-0.2170439	2.7881094
56	XyNacnacRh_21.xyz			H	-1.6033516	-0.5733439	4.5285129
C	-0.8026702	-1.5023640	-1.4042327	H	-1.5410709	-1.8796883	3.3419772
H	-0.6886296	-3.5302421	-0.8268817	H	-1.4529505	3.5396877	-0.6534257
C	-0.4528604	-2.5240247	-0.5121995	H	-0.7128285	4.5567807	0.6972843
C	0.1665703	-2.3973142	0.7412988	=====			
N	-0.5893354	-0.2040135	-1.1855167	56	XyNacnacRh_22a.xyz		
N	0.5075727	-1.2235485	1.2445122	C	-1.7874424	-0.8259708	-1.1487929
C	-1.4683150	-1.9252140	-2.7004553	H	-1.8269016	-2.8484984	-0.5521396
H	-1.5749995	-3.0078954	-2.7349524	C	-1.2898147	-1.9214889	-0.4180350
H	-0.8876196	-1.6112117	-3.5708589	C	-0.1649356	-2.0058862	0.4075780
H	-2.4606001	-1.4805003	-2.8055586	N	-1.2488727	0.3724965	-1.0662742
C	0.4467163	-3.6570665	1.5317196	N	0.6738771	-1.0089252	0.7310066
H	0.1098223	-4.5355254	0.9836232	C	-2.9610312	-1.0787795	-2.0724659
H	-0.0615642	-3.6409142	2.4989313	H	-3.2917574	-2.1139067	-2.0096365
H	1.5142772	-3.7690609	1.7361669	H	-2.6886156	-0.8661396	-3.1091333

H	-3.8039723	-0.4295623	-1.8287538	N	-1.1749771	0.3542374	-1.1537080
C	0.1362767	-3.3884296	0.9613050	N	0.6358756	-1.0002308	0.7755428
H	-0.5993290	-4.1050331	0.6026392	C	-2.7881307	-1.1219005	-2.2802955
H	0.1209771	-3.3919537	2.0523004	H	-3.1117572	-2.1602966	-2.2363206
H	1.1280737	-3.7289287	0.6588446	H	-2.4423033	-0.9115380	-3.2954238
Rh	0.4151492	0.8850930	0.1493173	H	-3.6533091	-0.4804899	-2.1030162
C	-0.0171448	1.9407454	1.7924288	C	0.1176941	-3.3873897	0.9687738
O	1.2431883	2.1450734	2.3500716	H	-0.5786578	-4.1149483	0.5575883
C	1.9977876	1.7250979	1.1659497	H	0.0223585	-3.3917325	2.0557245
H	2.3255094	2.6194089	0.6109844	H	1.1340964	-3.7126982	0.7402863
H	2.8529829	1.1351534	1.4834659	Rh	0.3923639	0.8898900	0.1750220
C	1.8322036	-1.3166259	1.5245336	C	-0.1668368	1.9412602	1.7819072
C	4.1166682	-1.9110220	3.0062907	O	1.0486982	2.1628513	2.4255509
C	1.7676845	-1.3055906	2.9268023	C	1.8891633	1.7517184	1.2978040
C	3.0362534	-1.6198110	0.8582951	H	2.2430200	2.6496549	0.7652551
C	4.1665477	-1.9150312	1.6167726	H	2.7278025	1.1733559	1.6752548
C	2.9256227	-1.6093077	3.6480831	C	1.7373116	-1.2908688	1.6521159
H	5.0959588	-2.1499122	1.1100644	C	3.9152909	-1.8518135	3.2980611
H	2.8826260	-1.6058201	4.7316888	C	1.5700195	-1.2803623	3.0458466
H	5.0036937	-2.1433184	3.5838085	C	2.9912305	-1.5766239	1.0762576
C	-1.7418872	1.4744260	-1.8228409	C	4.0669648	-1.8553985	1.9159218
C	-2.6002996	3.7187145	-3.2432405	C	2.6762393	-1.5671443	3.8504696
C	-1.1323590	1.7988482	-3.0522497	H	5.0343525	-2.0768900	1.4790051
C	-2.7728182	2.2801493	-1.2987846	H	2.5539368	-1.5640204	4.9280645
C	-3.1866827	3.3962288	-2.0265554	H	4.7608692	-2.0711005	3.9393553
C	-1.5804271	2.9217912	-3.7475713	C	-1.6300977	1.4498138	-1.9424378
H	-3.9785055	4.0206159	-1.6273041	C	-2.4207323	3.6836154	-3.4174980
H	-1.1178483	3.1739950	-4.6953726	C	-0.9403882	1.7860930	-3.1253296
H	-2.9327253	4.5906898	-3.7939377	C	-2.7077818	2.2385340	-1.4915504
C	-3.4354960	1.9449842	0.0131095	C	-3.0865381	3.3495868	-2.2455531
H	-4.1365328	1.1107776	-0.0904518	C	-1.3556207	2.9035537	-3.8493574
H	-2.7067094	1.6473013	0.7672535	H	-3.9141626	3.9608903	-1.9026080
H	-3.9990129	2.8000689	0.3887256	H	-0.8312595	3.1647773	-4.7618879
C	-0.0166012	0.9540335	-3.6137481	H	-2.7269696	4.5515331	-3.9894170
H	0.3072096	1.3412415	-4.5804351	C	-3.4551408	1.8905800	-0.2294305
H	-0.3194292	-0.0869924	-3.7500874	H	-4.0679838	2.7310597	0.0984450
H	0.8509512	0.9407910	-2.9479356	H	-4.1228575	1.0361051	-0.3776317
C	3.1188667	-1.6033082	-0.6456007	H	-2.7753149	1.6172579	0.5777675
H	2.3822741	-2.2648310	-1.1077673	C	0.2253393	0.9598839	-3.6072691
H	4.1100061	-1.9133566	-0.9787399	H	-0.0503135	-0.0858086	-3.7642401
H	2.9267597	-0.5992013	-1.0355812	H	1.0442565	0.9600906	-2.8822710
C	0.5073663	-0.9607346	3.6792817	H	0.6098800	1.3531051	-4.5489820
H	-0.3924744	-1.1627017	3.1006274	C	3.1835718	-1.5587358	-0.4174935
H	0.5052130	0.1018060	3.9341635	H	3.0068114	-0.5572396	-0.8210881
H	0.4524950	-1.5251233	4.6120094	H	2.4918622	-2.2301152	-0.9319759
H	-0.4224563	2.8489465	1.2951108	H	4.2005593	-1.8551982	-0.6768861
H	-0.7301401	1.5177135	2.5009230	C	0.2530853	-0.9537217	3.7034470
=====				H	-0.5988060	-1.1628760	3.0581814
56	XyNacnacRh_22b.xyz			H	0.2196967	0.1075768	3.9619107
C	-1.6879390	-0.8522245	-1.2746955	H	0.1350899	-1.5234469	4.6272598
H	-1.7392065	-2.8758532	-0.6825553	H	-0.5480541	2.8432847	1.2548781
C	-1.2270719	-1.9409682	-0.5104480	H	-0.9221775	1.5105431	2.4400013
C	-0.1630518	-2.0092176	0.3936723	=====			
				56			

XyNacnacRh_26b.xyz				H	3.4849422	0.7588652	0.3058820
C	-0.8979311	-1.1532173	-1.8219230	H	-0.9819380	1.0356647	2.2856368
H	-0.2977464	-3.1744666	-1.6379603	H	-1.3011870	2.3862755	1.1230611
C	-0.1827373	-2.1913694	-1.2067646	=====			
C	0.6539026	-2.1020816	-0.0925377	56			
N	-0.8118243	0.1030082	-1.4184217	XyNacnacRh_26.xyz			
N	0.9479734	-0.9707572	0.5525728	C	-1.1301640	-1.1938613	-1.6588547
C	-1.7736712	-1.5078035	-3.0042132	H	-0.6019876	-3.2303400	-1.4284899
H	-1.7009449	-2.5697143	-3.2315786	C	-0.4014971	-2.2342282	-1.0634875
H	-1.4812649	-0.9411599	-3.8908101	C	0.5484248	-2.1317758	-0.0452733
H	-2.8201858	-1.2674465	-2.8070683	N	-0.9505707	0.0746716	-1.3320143
C	1.2916274	-3.3912415	0.3874532	N	0.9548066	-0.9863268	0.5073481
H	1.0892482	-4.1944782	-0.3184220	C	-2.1341262	-1.5625667	-2.7296881
H	0.9076690	-3.6894137	1.3642404	H	-2.1331944	-2.6369584	-2.9038239
H	2.3720962	-3.2787926	0.4906120	H	-1.9049141	-1.0574222	-3.6704612
Rh	0.4308016	0.8769708	0.0113407	H	-3.1438414	-1.2591061	-2.4464091
C	-0.5483913	1.7519504	1.5946330	C	1.1773497	-3.4253678	0.4342873
C	0.7093395	2.4782266	2.0283837	H	0.8712360	-4.2503921	-0.2060136
H	1.1550006	2.0331200	2.9275743	H	0.8821263	-3.6593647	1.4582192
H	0.5723523	3.5527542	2.2145624	H	2.2663701	-3.3585454	0.4240120
O	1.5474492	2.2549605	0.8985311	Rh	0.4589302	0.8557086	-0.0709369
C	1.6681960	-1.0173224	1.7929701	C	-0.3192336	1.8415733	1.5578567
C	3.0581341	-1.0807873	4.2057908	C	1.0046388	2.5273492	1.8312077
C	0.9884632	-1.3609152	2.9769301	H	1.5197017	2.1007972	2.7019451
C	3.0380956	-0.6914307	1.8116549	H	0.9315099	3.6139478	1.9797757
C	3.7140231	-0.7384239	3.0299773	O	1.7148860	2.2183867	0.6359231
C	1.7046490	-1.3838074	4.1750959	C	1.7994209	-1.0080702	1.6674911
H	4.7700614	-0.4944085	3.0530834	C	3.4340998	-1.0224860	3.9225173
H	1.1872504	-1.6426081	5.0924961	C	1.2359761	-1.2650173	2.9317182
H	3.6003600	-1.1048771	5.1438357	C	3.1756725	-0.7443023	1.5267889
C	-1.5810351	1.1368589	-2.0364772	C	3.9747102	-0.7653429	2.6688245
C	-3.0435951	3.2208908	-3.1663521	C	2.0739774	-1.2647260	4.0483999
C	-1.0032916	1.9157005	-3.0576747	H	5.0362029	-0.5686747	2.5694953
C	-2.8837847	1.4026981	-1.5718405	H	1.6469615	-1.4567217	5.0267594
C	-3.5982897	2.4500484	-2.1524374	H	4.0715072	-1.0274790	4.7990066
C	-1.7561122	2.9517155	-3.6113755	C	-1.7309676	1.1137610	-1.9267435
H	-4.6013457	2.6630674	-1.7996489	C	-3.2039194	3.2108828	-3.0184565
H	-1.3207395	3.5555837	-4.3995857	C	-1.2231690	1.8130254	-3.0387403
H	-3.6117089	4.0325461	-3.6052084	C	-2.9683287	1.4656308	-1.3533459
C	-3.5007625	0.5786754	-0.4713808	C	-3.6893289	2.5180099	-1.9165872
H	-2.8321931	0.5001736	0.3868866	C	-1.9801458	2.8571441	-3.5710526
H	-3.7139492	-0.4433955	-0.7978736	H	-4.6421377	2.7970605	-1.4803831
H	-4.4406509	1.0222017	-0.1411507	H	-1.5984145	3.4000195	-4.4284002
C	0.3985599	1.6530429	-3.5475202	H	-3.7759716	4.0276760	-3.4424317
H	0.6334933	2.2975117	-4.3951467	C	-3.5104010	0.7261692	-0.1575322
H	0.5365876	0.6158473	-3.8613190	H	-3.8062013	-0.2961689	-0.4104574
H	1.1377134	1.8475063	-2.7649851	H	-4.3887423	1.2343243	0.2417663
C	-0.4752819	-1.7271581	2.9836178	H	-2.7629570	0.6494266	0.6331357
H	-1.0272439	-1.2214626	2.1934398	C	0.1101927	1.4580104	-3.6472982
H	-0.6191922	-2.8028716	2.8371374	H	0.1701293	0.4013451	-3.9178173
H	-0.9279184	-1.4728660	3.9434564	H	0.9312819	1.6531008	-2.9513468
C	3.7659734	-0.2657777	0.5653642	H	0.2884030	2.0485159	-4.5464884
H	3.5260625	-0.8999195	-0.2901908	C	-0.2322304	-1.5635327	3.1105053
H	4.8448917	-0.2958906	0.7236471	H	-0.5723510	-1.2308677	4.0926123

H	-0.4317034	-2.6387394	3.0503519	H	0.5119040	2.3832690	-4.3149694
H	-0.8435751	-1.0825400	2.3491526	H	0.4962257	0.7241655	-3.7073672
C	3.7834574	-0.4102292	0.1915043	H	0.9772507	2.0325121	-2.6458309
H	4.8710099	-0.4822500	0.2376601	C	3.6840142	-0.5666902	0.6342169
H	3.5182737	0.6131978	-0.0886088	H	3.3860109	0.4249935	0.2825292
H	3.4281719	-1.0713908	-0.6011216	H	3.4558582	-1.2622595	-0.1759490
H	-1.0885717	2.4888308	1.1328805	H	4.7640289	-0.5628361	0.7854383
H	-0.7107830	1.1762292	2.3211191	C	-0.5665204	-1.6417283	3.1982926
=====							
56							
XyNacnacRh_30a.xyz							
C	-0.8818924	-1.0190573	-1.7858247	H	-1.1023436	-0.7350716	2.9039520
H	-0.2003754	-3.0121157	-1.7158088	H	-0.8860792	-1.9069217	4.2065491
C	-0.1436277	-2.0625695	-1.2050847	H	-0.8979629	-2.4311703	2.5198374
C	0.6177233	-2.0562927	-0.0310008	H	1.6188480	1.9055086	2.7201848
N	-0.9198697	0.2143292	-1.3058251	H	-0.2136271	1.7399362	2.8082652
N	0.8053504	-0.9922374	0.7467643	=====			
C	-1.6932138	-1.3634074	-3.0188427	56			
H	-1.5628952	-2.4109799	-3.2830002	XyNacnacRh_30b.xyz			
H	-1.3988829	-0.7490115	-3.8714242	C	-1.7034554	-0.3555646	-1.2689922
H	-2.7557291	-1.1769524	-2.8500913	H	-2.1370271	-2.4131451	-1.3125537
C	1.2407731	-3.3783480	0.3749689	C	-1.4588868	-1.6822783	-0.8980841
H	1.0038696	-4.1495871	-0.3549472	C	-0.4525753	-2.1943360	-0.0652775
H	0.8767403	-3.7035578	1.3515049	N	-0.9754629	0.6870937	-0.8725896
H	2.3262997	-3.2981955	0.4553128	N	0.4751914	-1.4467870	0.5165108
Rh	0.1097949	0.8792711	0.3485299	C	-2.8765182	-0.1199992	-2.2012047
H	1.3375188	1.1163776	-0.4871675	H	-3.3467784	-1.0649049	-2.4655018
C	0.6619850	2.0012057	2.2236035	H	-2.5584634	0.3775023	-3.1193992
C	0.5291636	2.9009760	1.1553894	H	-3.6281025	0.5232134	-1.7396973
H	1.3965027	3.4818647	0.8168757	C	-0.4426092	-3.6945041	0.1483811
O	-0.5496444	2.9441737	0.4522530	H	-1.2373571	-4.1681407	-0.4246680
C	1.5812117	-1.1284318	1.9458602	H	-0.5781123	-3.9432809	1.2026143
C	3.0587132	-1.3475736	4.2992972	H	0.5124562	-4.1274042	-0.1553566
C	2.9718560	-0.9233979	1.9125147	Rh	0.6358903	0.5931040	0.3566989
C	0.9263247	-1.4383796	3.1514624	H	-0.1506511	0.8913915	1.6023791
C	1.6841279	-1.5459512	4.3175773	O	2.4875824	0.9696317	1.4404068
C	3.6918216	-1.0382663	3.1029784	C	2.3456724	1.9819121	0.6558263
H	1.1859566	-1.7867886	5.2500888	H	3.0916887	2.1288598	-0.1399123
H	4.7650330	-0.8839377	3.0853487	C	1.1976860	2.7856938	0.6762877
H	3.6338356	-1.4344899	5.2134978	C	1.4425095	-2.0621333	1.3808117
C	-1.7062826	1.2156831	-1.9668605	C	3.3388919	-3.2390420	3.0455200
C	-3.2356950	3.1744371	-3.2226538	C	1.1525098	-2.2353436	2.7448549
C	-1.1430623	1.9693924	-3.0108721	C	2.6851616	-2.4487117	0.8508497
C	-3.0188962	1.4570349	-1.5278460	C	3.6182148	-3.0427448	1.6996245
C	-3.7708012	2.4370565	-2.1750606	C	2.1156452	-2.8317809	3.5597226
C	-1.9289585	2.9418644	-3.6294852	H	4.5775936	-3.3481229	1.2969782
H	-4.7865022	2.6256572	-1.8454905	H	1.8990435	-2.9730022	4.6128386
H	-1.5037775	3.5254166	-4.4385395	H	4.0751644	-3.7007795	3.6928286
H	-3.8320865	3.9337904	-3.7145245	C	-1.3516785	2.0045490	-1.3000547
C	-3.6063752	0.6976908	-0.3660622	C	-2.0306328	4.5785966	-2.1229343
H	-3.5147422	-0.3840234	-0.4857275	C	-2.2780736	2.7494608	-0.5493349
H	-4.6633806	0.9381220	-0.2463924	C	-0.7573278	2.5433437	-2.4549936
H	-3.0993931	0.9619421	0.5666834	C	-1.1131108	3.8325923	-2.8516606
C	0.2838747	1.7635593	-3.4471282	C	-2.6041175	4.0363177	-0.9806159
				H	-0.6621590	4.2534518	-3.7435001
				H	-3.3189029	4.6173259	-0.4084789
				H	-2.2970190	5.5786357	-2.4440315

C	0.2576697	1.7609415	-3.2484643	C	-0.5431707	2.5703108	-3.8189322
H	0.5560954	2.3131261	-4.1403035	C	-2.6026307	2.8184898	-2.6054443
H	-0.1244382	0.7875046	-3.5639200	H	0.1335850	2.9024984	-4.5987832
H	1.1578347	1.5658658	-2.6578733	H	-3.5360828	3.3446415	-2.4368642
C	-2.8965145	2.1962823	0.7075874	H	-2.0069183	4.0884094	-4.2338641
H	-2.1407470	2.0473719	1.4834041	C	1.1276236	0.7729314	-3.2510177
H	-3.3670667	1.2242081	0.5465625	H	0.9909634	-0.2582747	-3.5881101
H	-3.6525616	2.8794580	1.0957041	H	1.6948794	0.7196306	-2.3182143
C	3.0260119	-2.2085966	-0.5970629	H	1.7235040	1.2952202	-4.0010440
H	3.9783410	-2.6762673	-0.8496259	C	-3.2120211	1.2970982	-0.6927370
H	3.1172428	-1.1376137	-0.8003145	H	-2.6806122	1.2524695	0.2614100
H	2.2645715	-2.5989685	-1.2757541	H	-3.6196862	0.2973206	-0.8656380
C	-0.1523170	-1.7716674	3.3380373	H	-4.0496134	1.9903000	-0.6017680
H	-0.2351431	-2.0918866	4.3772977	C	-1.0559078	-1.3024424	3.4935553
H	-0.2238636	-0.6809230	3.3125104	H	-1.3964353	-0.5217906	2.8098675
H	-1.0189474	-2.1543761	2.7944779	H	-1.4025342	-1.0696256	4.5012456
H	0.6852962	2.9707416	1.6104448	H	-1.5441539	-2.2285137	3.1772802
H	1.0766556	3.5341298	-0.0969997	C	3.2919672	-1.8213893	0.9187768
=====				H	3.0822937	-2.7803689	0.4365622
56	XyNacnacRh_31a.xyz			H	4.3684393	-1.7589478	1.0840239
C	-1.0709084	-1.2944220	-1.5459659	H	2.9940312	-1.0450436	0.2105831
H	-1.1362029	-3.3825921	-1.2343222	H	1.5788618	5.2910861	-0.1264231
C	-0.7760907	-2.4555069	-0.8128272	H	0.0863351	5.4702291	0.7810697
C	-0.0735850	-2.5608113	0.3947202	=====			
N	-0.7168994	-0.0592417	-1.1967697	56	XyNacnacRh_31b.xyz		
N	0.4200566	-1.5013354	1.0151091	C	-0.7614787	-1.0585192	-1.9842059
C	-1.8542957	-1.4904649	-2.8313188	H	-0.7014265	-3.1505471	-1.7027267
H	-2.0705193	-2.5459922	-2.9847264	C	-0.5529316	-2.2017374	-1.2089576
H	-1.2988986	-1.1235144	-3.6969397	C	-0.1748080	-2.2596676	0.1405804
H	-2.8000418	-0.9450306	-2.8093121	N	-0.6384428	0.1652959	-1.4873319
C	0.1196639	-3.9349842	0.9969981	N	0.0403852	-1.1983020	0.9136847
H	-0.3425902	-4.6969337	0.3717369	C	-1.1538693	-1.2369943	-3.4334593
H	-0.3212483	-3.9959816	1.9949350	H	-1.2246003	-2.2934722	-3.6856086
H	1.1802572	-4.1753345	1.1035392	H	-0.4245532	-0.7707262	-4.0995807
Rh	0.3123080	0.3849429	0.4554152	H	-2.1176167	-0.7662986	-3.6403062
O	0.3375990	2.4564281	0.0879384	C	-0.0316481	-3.6425016	0.7470085
C	0.7849116	3.4625600	0.6270867	H	-0.3052056	-4.4034788	0.0187145
H	1.3485431	3.3783143	1.5720937	H	-0.6734337	-3.7532611	1.6231239
C	0.6025873	4.8295609	0.0578303	H	0.9904566	-3.8346924	1.0775083
H	0.0335843	4.7849512	-0.8696289	Rh	-0.2247309	0.7029815	0.3849052
C	1.1389904	-1.5658832	2.2423600	C	1.0670752	1.8312906	1.6797525
C	2.5617235	-1.5465999	4.6409010	H	1.7604680	1.1290630	2.1584587
C	2.5459775	-1.6807316	2.2204612	O	-0.1539070	1.8552345	2.1068982
C	0.4452873	-1.4297416	3.4644274	C	1.6956064	3.0611489	1.0745378
C	1.1777504	-1.4252362	4.6516975	H	2.5844701	2.8037048	0.4951491
C	3.2362132	-1.6713654	3.4327079	C	0.5238385	-1.3771016	2.2505887
H	0.6526057	-1.3227430	5.5949164	C	1.4779992	-1.6964108	4.8443778
H	4.3169093	-1.7609337	3.4249693	C	1.9053460	-1.5408118	2.4647319
H	3.1146050	-1.5390739	5.5730396	C	-0.3807813	-1.3463467	3.3267224
C	-1.0754285	1.0456070	-2.0305849	C	0.1196297	-1.5160818	4.6174903
C	-1.7434108	3.2396952	-3.6130982	C	2.3619433	-1.7026986	3.7734438
C	-2.2842914	1.7255129	-1.7986455	H	-0.5691686	-1.4989881	5.4546158
C	-0.1878791	1.4726429	-3.0342775	H	3.4243527	-1.8302518	3.9496276

H	1.8479968	-1.8230736	5.8550507	C	2.2285082	-1.6470035	2.1708910
C	-0.8429988	1.3412414	-2.2679873	C	2.7500667	-1.9367655	3.4336010
C	-1.2146694	3.7002711	-3.7019825	C	0.5441582	-1.9491549	4.3853959
C	-2.1154706	1.9494492	-2.2877468	H	3.8232906	-2.0432795	3.5483494
C	0.2467392	1.9183534	-2.9528333	H	-0.1066298	-2.0641308	5.2453110
C	0.0367620	3.0974427	-3.6666019	H	2.3401009	-2.3149491	5.5077708
C	-2.2779562	3.1288071	-3.0152467	C	-0.9768986	1.5896586	-2.1467681
H	0.8682231	3.5485562	-4.1965864	C	-1.5744878	4.0483958	-3.3178078
H	-3.2523015	3.6037195	-3.0382020	C	0.0065805	2.2569736	-2.9068795
H	-1.3593884	4.6181677	-4.2594889	C	-2.2537627	2.1600960	-1.9583266
C	1.6108069	1.2802999	-2.9173786	C	-2.5315153	3.3893526	-2.5564228
H	2.3479290	1.9218786	-3.4014626	C	-0.3164309	3.4837028	-3.4864524
H	1.6211856	0.3139970	-3.4292331	H	-3.5110784	3.8337115	-2.4185487
H	1.9284747	1.0911676	-1.8897996	H	0.4330382	4.0021086	-4.0740552
C	-3.2823428	1.3473493	-1.5466640	H	-1.8069147	5.0034135	-3.7744802
H	-3.0710458	1.2520617	-0.4786938	C	-3.3034550	1.4611188	-1.1326919
H	-3.5192851	0.3434103	-1.9077760	H	-4.1837514	2.0943691	-1.0155781
H	-4.1714264	1.9670913	-1.6666615	H	-2.9211642	1.2045535	-0.1420795
C	-1.8510566	-1.1131454	3.1058494	H	-3.6250650	0.5233636	-1.5940002
H	-2.0213678	-0.0978636	2.7386108	C	1.3813928	1.6677510	-3.0869662
H	-2.4032185	-1.2401737	4.0378351	H	1.3449795	0.6894891	-3.5728985
H	-2.2690780	-1.7965780	2.3633982	H	1.8732865	1.5214558	-2.1225425
C	2.8815432	-1.5395982	1.3160382	H	2.0027621	2.3251409	-3.6962486
H	2.7074498	-0.6930412	0.6487020	C	3.1471552	-1.5159470	0.9830447
H	2.7949538	-2.4413885	0.7027206	H	3.1054316	-2.4043237	0.3448672
H	3.9065488	-1.4897235	1.6854760	H	4.1816766	-1.3944153	1.3072916
H	0.9879549	3.5949358	0.4362431	H	2.8690343	-0.6699423	0.3527387
H	2.0020692	3.7465562	1.8746776	C	-1.5070570	-1.4791303	3.0009851
=====				H	-1.9434233	-2.2238111	2.3299366
56	XyNacnacRh_32.xyz			H	-1.7432750	-0.5016450	2.5725446
C	-0.8639880	-0.8202403	-2.0412487	H	-2.0002746	-1.5689417	3.9697063
H	-0.7773738	-2.9241692	-1.9048761	H	0.4616413	0.9479169	3.1211383
C	-0.5697820	-2.0106899	-1.3675503	H	-0.2723467	2.4809891	2.4404056
C	-0.0436646	-2.1683981	-0.0764197	=====			
N	-0.6510737	0.3657342	-1.4953589	56	XyNacnacRh_33.xyz		
N	0.2816686	-1.1791510	0.7564557	C	-0.9391395	-1.3799266	-1.4829770
C	-1.4433386	-0.9128845	-3.4355776	H	-0.4319605	-3.3056417	-0.7881272
H	-1.5440473	-1.9517832	-3.7446737	C	-0.3039256	-2.2543066	-0.5771483
H	-0.8082216	-0.3959862	-4.1587127	C	0.5430266	-1.9714173	0.4978727
H	-2.4272260	-0.4407442	-3.4850289	N	-0.9131851	-0.0695096	-1.3428869
C	0.1540417	-3.6008805	0.3881079	N	0.8666437	-0.7538098	0.9588989
H	-0.1527945	-4.2954664	-0.3912378	C	-1.6456898	-2.0094153	-2.6663840
H	-0.4301397	-3.8121022	1.2858985	H	-1.5996872	-3.0958576	-2.6165600
H	1.1976253	-3.8016058	0.6360870	H	-1.1889484	-1.6870612	-3.6052378
Rh	0.1076980	0.7807152	0.3353969	H	-2.6934299	-1.7051512	-2.7070121
C	1.5434762	1.8238489	1.4906814	C	1.1808612	-3.1743372	1.1712270
C	0.4257322	1.6563089	2.3065290	H	0.8428398	-4.0935525	0.6974908
H	2.4706184	1.2826153	1.6251996	H	0.9332525	-3.2192506	2.2328502
O	1.7450654	3.0052535	0.7665985	H	2.2697328	-3.1306877	1.1036526
H	1.1344639	3.6819828	1.0853469	Rh	0.0954099	0.9322021	0.2537507
C	0.8353422	-1.5083370	2.0344546	H	1.0564490	1.7303059	1.2043121
C	1.9188895	-2.0899149	4.5349537	C	-1.2722277	1.5588134	1.5359725
C	-0.0185439	-1.6542263	3.1437439	H	-2.0167356	0.8123000	1.8141659

C	-1.2278466	2.8441651	2.2372002	H	1.7860653	-3.6119022	0.6247484
O	-1.8001030	2.7320630	0.9033405	Rh	0.5661904	0.7945486	0.0199810
C	1.8193044	-0.6381202	2.0303258	C	-0.3209723	1.8487680	1.5475226
C	3.7007212	-0.4197703	4.0736637	H	-0.8906711	1.2260981	2.2303168
C	1.3987835	-0.7154292	3.3683801	H	-0.9428639	2.5852256	1.0355206
C	3.1745951	-0.4412557	1.7087406	C	1.0193532	2.3732600	2.0232291
C	4.1004985	-0.3366887	2.7459381	O	1.8544651	1.9933238	0.9336108
C	2.3590650	-0.6074152	4.3758319	C	1.4018722	-1.2406698	1.8784162
H	5.1470175	-0.1853599	2.5052947	C	2.6588058	-1.4826761	4.3520138
H	2.0434232	-0.6721746	5.4115209	C	0.6254673	-1.4481011	3.0344166
H	4.4322463	-0.3388093	4.8691454	C	2.8042491	-1.1395965	1.9551146
C	-1.4809527	0.7873690	-2.3357638	C	3.4109849	-1.2722755	3.2032777
C	-2.5303837	2.5416093	-4.2353687	C	1.2766229	-1.5640909	4.2637489
C	-0.6546721	1.2771955	-3.3678155	H	4.4906242	-1.2012702	3.2713031
C	-2.8278234	1.1863414	-2.2447169	H	0.6855949	-1.7191243	5.1598301
C	-3.3324191	2.0579983	-3.2109073	H	3.1494408	-1.5764683	5.3137592
C	-1.1991267	2.1522357	-4.3073187	C	-1.2869791	1.3383991	-2.1186030
H	-4.3714865	2.3630196	-3.1505173	C	-2.3382430	3.6111462	-3.3386065
H	-2.9399905	3.2207903	-4.9738343	C	-0.5461295	1.9927788	-3.1217342
C	-0.0524765	-0.8768821	3.7411936	C	-2.5470435	1.8224248	-1.7166857
H	-0.5858107	-1.5498720	3.0690572	C	-3.0547204	2.9607870	-2.3417964
H	-0.1464637	-1.2608874	4.7582132	C	-1.0943758	3.1270259	-3.7213972
H	-0.5681300	0.0859488	3.7011249	H	-4.0234875	3.3412803	-2.0376108
C	3.6240640	-0.3093062	0.2778344	H	-0.5323584	3.6366199	-4.4958942
H	4.7117221	-0.2505890	0.2202275	H	-2.7463887	4.4959889	-3.8124611
H	3.2099728	0.5981620	-0.1725047	C	-3.3369785	1.1318981	-0.6351536
H	3.2940778	-1.1476092	-0.3399251	H	-3.6982418	0.1509338	-0.9571314
C	0.7950191	0.8720918	-3.4642290	H	-4.2061045	1.7279551	-0.3549274
H	1.3591853	1.1851054	-2.5807220	H	-2.7282056	0.9646944	0.2543894
H	1.2618909	1.3285360	-4.3378848	C	0.8137173	1.4957338	-3.5438468
H	0.9158357	-0.2111680	-3.5437537	H	0.7936554	0.4438481	-3.8377420
C	-3.7205812	0.7190454	-1.1228261	H	1.5404484	1.5830615	-2.7309701
H	-3.5349161	-0.3193659	-0.8468381	H	1.1869688	2.0762880	-4.3880204
H	-3.5584194	1.3283254	-0.2300784	C	3.6441514	-0.8600539	0.7382896
H	-4.7702417	0.8166734	-1.4049670	H	4.6960437	-1.0614689	0.9454598
H	-0.5677873	2.5307247	-5.1037567	H	3.5446343	0.1916475	0.4549789
H	-0.2965087	3.3946820	2.2894089	H	3.3411676	-1.4624612	-0.1201823
H	-1.9645693	3.0749242	3.0034264	C	-0.8771069	-1.5723452	2.9785226
=====				H	-1.3221331	-1.2475625	3.9204811
56	XyNacnacRh_35.xyz			H	-1.1876056	-2.6103727	2.8187718
C	-0.9986578	-1.0278910	-1.8445959	H	-1.3061900	-0.9842383	2.1692130
H	-0.7453341	-3.1158164	-1.6089983	H	1.0501083	3.4596503	2.1866064
C	-0.4890441	-2.1563883	-1.1855333	H	1.3518193	1.8826128	2.9473460
C	0.3046460	-2.1827584	-0.0370821	=====			
N	-0.7247172	0.2051652	-1.4537572	56	XyNacnacRh_36.xyz		
N	0.7518662	-1.1019312	0.6065741	C	-0.5260756	-0.8260063	-1.8651092
C	-1.8701098	-1.2579911	-3.0602984	H	-0.1944448	-2.8970387	-1.8705791
H	-1.9694150	-2.3221024	-3.2662611	C	-0.1754365	-2.0240947	-1.2354008
H	-1.4469600	-0.7710717	-3.9415093	C	0.1614202	-2.2656542	0.1082199
H	-2.8678979	-0.8389331	-2.9168281	N	-0.5863178	0.3805712	-1.2887976
C	0.7055940	-3.5487528	0.4847502	N	0.2135884	-1.3101567	1.0185573
H	0.3980143	-4.3224430	-0.2161295	C	-0.9053769	-0.9376020	-3.3316912
H	0.2463641	-3.7604066	1.4515641	H	-0.8663830	-1.9761867	-3.6529790

H	-0.2378677	-0.3557979	-3.9683222	C	0.3442787	-2.1471765	0.1971390
H	-1.9149874	-0.5598165	-3.5040909	N	-0.4716995	0.4133715	-1.3219484
C	0.4414529	-3.7022417	0.4994928	N	0.4550390	-1.1534440	1.0635909
H	0.3658332	-4.3622089	-0.3626603	C	-0.8658046	-1.0463076	-3.2680538
H	-0.2654670	-4.0418746	1.2596841	H	-0.8158909	-2.1027254	-3.5227642
H	1.4389114	-3.8056610	0.9306462	H	-0.2109700	-0.4963179	-3.9462020
Rh	-0.2317357	0.7269881	0.6604019	H	-1.8801300	-0.6918721	-3.4583117
C	1.0130928	2.0727367	1.1858011	C	0.7259823	-3.5573340	0.6087630
O	0.9391454	1.9033182	2.3879979	H	0.5693224	-4.2540679	-0.2123402
H	-0.9820370	2.1063662	0.5030378	H	0.1393144	-3.8930527	1.4655942
C	1.9024717	3.0485353	0.4794153	H	1.7747196	-3.6072351	0.9088361
H	2.7604754	2.5101178	0.0702404	Rh	-0.0374017	0.9168621	0.6699678
C	0.5346207	-1.6107026	2.3776905	H	-1.4762844	1.1661121	1.0734244
C	1.1547989	-2.0952072	5.0513833	C	-0.1994233	2.9924109	0.2585840
C	1.8780633	-1.5860238	2.7951351	H	-0.2284487	3.6158687	1.1523946
C	-0.5018363	-1.8540652	3.2983363	C	0.3837771	1.5013994	2.3996088
C	-0.1686411	-2.1006316	4.6299636	O	0.5992770	1.9300890	3.4351147
C	2.1665307	-1.8349539	4.1369139	C	0.9213957	-1.4524375	2.3862677
H	-0.9614014	-2.2922511	5.3446283	C	1.8196016	-1.9461743	4.9793105
H	3.1996755	-1.8161738	4.4660312	C	2.2928629	-1.3445295	2.6791131
H	1.3956057	-2.2830782	6.0910000	C	-0.0050947	-1.7922087	3.3891201
C	-0.8959878	1.5238173	-2.1013465	C	0.4667161	-2.0365456	4.6794957
C	-1.4807309	3.7798069	-3.6303508	C	2.7218818	-1.6001935	3.9821640
C	-2.2156561	2.0105123	-2.1434883	H	-0.2416825	-2.2978251	5.4579688
C	0.1297067	2.1552255	-2.8271490	H	3.7782643	-1.5211257	4.2142663
C	-0.1843121	3.2874906	-3.5821278	H	2.1684070	-2.1383622	5.9869692
C	-2.4861493	3.1382344	-2.9171393	C	-0.8496375	1.4633492	-2.2271579
H	0.6029716	3.7838026	-4.1394018	C	-1.5556323	3.5206385	-3.9719906
H	-3.5006654	3.5190832	-2.9548361	C	0.1478720	2.1161697	-2.9717497
H	-1.7084837	4.6588416	-4.2217145	C	-2.1982818	1.8420771	-2.3435099
C	2.9904947	-1.3012003	1.8194139	C	-2.5299411	2.8730056	-3.2246783
H	2.7804468	-0.4078566	1.2283707	C	-0.2263618	3.1410094	-3.8414579
H	3.1301402	-2.1203185	1.1072258	H	-3.5689755	3.1682330	-3.3216971
H	3.9345215	-1.1548634	2.3455917	H	0.5384782	3.6466737	-4.4205747
C	-1.9465556	-1.8413802	2.8669206	H	-1.8305726	4.3185761	-4.6515654
H	-2.2325684	-0.8653291	2.4654985	C	3.2875648	-0.9459135	1.6184005
H	-2.5997148	-2.0639308	3.7114098	H	3.0902399	0.0632684	1.2445721
H	-2.1489691	-2.5739872	2.0814400	H	4.3017802	-0.9610346	2.0190842
C	1.5414963	1.6239457	-2.8306654	H	3.2559984	-1.6089893	0.7506220
H	1.8091863	1.1784302	-1.8733095	C	-1.4794376	-1.8822152	3.0897929
H	2.2519135	2.4197894	-3.0614801	H	-1.8551585	-0.9500890	2.6617653
H	1.6740728	0.8453935	-3.5893737	H	-2.0425263	-2.0967753	3.9987329
C	-3.3165768	1.3488937	-1.3589633	H	-1.7042618	-2.6675596	2.3630102
H	-4.2821915	1.7949243	-1.6001437	C	1.5982595	1.7248918	-2.8455613
H	-3.1441583	1.4587735	-0.2844773	H	2.2207790	2.3512015	-3.4855153
H	-3.3754536	0.2764271	-1.5577066	H	1.7696627	0.6822909	-3.1261010
H	1.3689480	3.5099022	-0.3494294	H	1.9533256	1.8321571	-1.8175506
H	2.2565974	3.8043659	1.1822852	C	-3.2748585	1.1729979	-1.5296661
=====				H	-3.1519892	1.3857130	-0.4637883
56				H	-4.2607255	1.5264981	-1.8338734
XyNacnacRh_37.xyz				H	-3.2564136	0.0856782	-1.6301491
C	-0.4669609	-0.8301594	-1.8177707	H	0.6974255	3.2447324	-0.3127317
H	-0.1554650	-2.8989974	-1.7003145	H	-1.0770515	3.2132779	-0.3433275
C	-0.1051441	-1.9878853	-1.1233221	=====			

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XyNacnacRh_COE_CO.xyz

C	-1.1372092	-2.0728378	-2.3448103
H	-1.0798219	-4.0805347	-1.7418385
C	-0.8563000	-3.0770090	-1.4136782
C	-0.3312968	-2.9773443	-0.1218694
N	-0.9324586	-0.7760390	-2.1463415
N	0.0111480	-1.8431331	0.4907275
C	-1.7193243	-2.5448937	-3.6660550
H	-1.8249112	-3.6277812	-3.6691442
H	-1.0849512	-2.2567355	-4.5058453
H	-2.6998648	-2.1015026	-3.8478769
C	-0.1573802	-4.3051694	0.5994882
H	-0.4846405	-5.1265843	-0.0341232
H	-0.7326606	-4.3362848	1.5258811
H	0.8848111	-4.4773878	0.8724513
Rh	-0.1536790	0.1163757	-0.3949976
C	1.2541776	1.0558950	1.0762078
H	1.8246561	0.1884430	1.3814896
C	-0.0304721	1.1507195	1.6021706
H	-0.3246263	0.3487844	2.2651584
C	2.1373389	2.2272722	0.7137530
H	2.9000134	1.8954059	0.0060121
H	1.5849392	3.0249744	0.2178677
C	-0.8134242	2.4260719	1.8296240
H	-0.9055472	3.0217981	0.9213583
H	-1.8327307	2.1415163	2.1027288
C	2.8117788	2.7703097	2.0059382
H	3.8868176	2.8817028	1.8389634
H	2.7160521	2.0117316	2.7877792
C	-0.2335394	3.3449220	2.9410031
H	-1.0783624	3.8708294	3.3943019
C	2.2783664	4.1164901	2.5376821
H	2.7890941	4.9293769	2.0098548
H	0.2054862	2.7406196	3.7415155
H	2.5893811	4.2045696	3.5843707
C	0.7697100	4.4086505	2.4410819
H	0.5145293	4.6604696	1.4068789
H	0.6021994	5.3317298	3.0050645
C	-0.2721458	1.7806722	-1.2051409
O	-0.3171237	2.8252212	-1.6788751
C	-1.2798854	0.1097252	-3.2244740
C	-1.9361977	1.8666951	-5.2839029
C	-2.5694413	0.6674811	-3.2746504
C	-0.3137869	0.4335408	-4.1932927
C	-0.6638807	1.3142702	-5.2171331
C	-2.8777079	1.5439467	-4.3155108
H	0.0763838	1.5719892	-5.9665982
H	-3.8691938	1.9810687	-4.3598811
H	-2.1910188	2.5515269	-6.0840735
C	0.5256186	-1.9931712	1.8218799
C	1.5276232	-2.2650787	4.4142425
C	-0.3582848	-1.9732914	2.9181270
C	1.9088228	-2.1624203	2.0213283

C	2.3891629	-2.2935588	3.3258232
C	0.1635597	-2.1085381	4.2056394
H	3.4544364	-2.4218283	3.4842339
H	-0.5134034	-2.0922742	5.0529145
H	1.9169976	-2.3667046	5.4203639
C	-3.5963411	0.3459148	-2.2201332
H	-3.8375751	-0.7199687	-2.1931381
H	-3.2301205	0.6033064	-1.2227876
H	-4.5201498	0.8959883	-2.4033980
C	2.8615923	-2.2435686	0.8545128
H	2.7798289	-3.2052318	0.3388561
H	3.8934843	-2.1390527	1.1925863
H	2.6560152	-1.4761927	0.1067219
C	-1.8472896	-1.8429101	2.7158766
H	-2.3478585	-1.6423689	3.6643095
H	-2.2773927	-2.7604869	2.3029208
H	-2.0935575	-1.0460445	2.0119774
C	1.0786640	-0.1375796	-4.1229788
H	1.5555592	0.1037969	-3.1694184
H	1.6969152	0.2577525	-4.9298307
H	1.0803926	-1.2280471	-4.1998688

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XyNacnacRh_COE_Epox2.xyz

C	-1.3682234	-2.1191924	-2.1696694
H	-1.2216932	-4.1653681	-1.7253300
C	-0.9399566	-3.1836808	-1.3759356
C	-0.2074721	-3.1628410	-0.1835460
N	-1.0754373	-0.8446648	-1.9243356
N	0.2111456	-2.0716970	0.4578336
C	-2.2235432	-2.4925715	-3.3688845
H	-2.3477766	-3.5722938	-3.4252316
H	-1.7830325	-2.1477617	-4.3058079
H	-3.2143196	-2.0374973	-3.3030341
C	0.1081355	-4.5356567	0.3927191
H	-0.2806532	-5.3136162	-0.2609877
H	-0.3294930	-4.6713740	1.3826273
H	1.1833516	-4.6865555	0.5013902
Rh	-0.0209934	-0.1408954	-0.2243375
C	1.3633691	0.7381180	1.2534210
H	1.9767016	-0.0861142	1.5927761
C	0.0553031	0.7642795	1.7535490
H	-0.2090445	-0.0380093	2.4302007
C	2.1993582	1.9699411	0.9834201
H	3.0120515	1.7153394	0.2973863
H	1.6162279	2.7519340	0.5014064
C	-0.7878553	2.0030807	1.9702163
H	-0.8580531	2.5989327	1.0596476
H	-1.8064947	1.6731940	2.1933920
C	2.7879683	2.5035192	2.3208931
H	3.8673148	2.6528382	2.2195213
H	2.6714076	1.7251983	3.0794084
C	-0.3093491	2.9356057	3.1186792
H	-1.1991994	3.4175113	3.5351606

C	2.1830104	3.8193319	2.8502221	C	-0.5744236	-3.3255116	0.0790388
H	2.6843622	4.6621369	2.3602980	N	-1.3381615	-1.0188135	-1.7280763
H	0.1161194	2.3404941	3.9334176	N	0.0288401	-2.2620480	0.6083138
H	2.4418187	3.9014870	3.9117343	C	-2.8876229	-2.5717308	-2.8737795
C	0.6689310	4.0522738	2.6916797	H	-3.2421436	-3.5937214	-2.7539129
H	0.4504921	4.3163800	1.6513481	H	-2.4821849	-2.4665925	-3.8818319
H	0.4369177	4.9551635	3.2662940	H	-3.7466192	-1.9008331	-2.8101884
O	0.0058448	1.9876152	-1.1114474	C	-0.2622636	-4.7115370	0.6239698
C	-0.6207047	3.1546026	-1.6727042	H	-0.7556399	-5.4694908	0.0190046
H	-1.4600701	2.9557743	-2.3259558	H	-0.5939806	-4.8303147	1.6561347
H	-0.7379840	3.9722121	-0.9682934	H	0.8113944	-4.9073417	0.6122692
C	0.7278102	2.7478860	-2.0864465	Rh	-0.1583799	-0.3235492	-0.0724247
C	-1.6042685	0.1124765	-2.8422687	C	1.0101589	0.5010784	1.6269877
C	-2.6826441	1.9119935	-4.6893109	H	1.5692372	-0.3270813	2.0386061
C	-2.8633712	0.6951975	-2.5972325	C	-0.3684286	0.5092223	1.8938678
C	-0.8770066	0.4455267	-4.0009464	H	-0.7563930	-0.3129809	2.4830906
C	-1.4317871	1.3480831	-4.9109049	C	1.8490681	1.7552513	1.5755991
C	-3.3881216	1.5849990	-3.5367990	H	2.7778167	1.5529678	1.0341182
H	-0.8778748	1.6012284	-5.8088600	H	1.3368831	2.5466540	1.0386720
H	-4.3635548	2.0253222	-3.3590074	C	-1.2319830	1.7491679	1.9814304
H	-3.1048481	2.6028570	-5.4095747	H	-1.1032531	2.3720910	1.0936331
C	0.9098829	-2.3157581	1.6897702	H	-2.2765531	1.4252339	1.9798209
C	2.2746156	-2.8106621	4.0731629	C	2.1783196	2.2273980	3.0218324
C	0.1897541	-2.4386452	2.8909594	H	3.2585290	2.3625778	3.1349118
C	2.3116144	-2.4531157	1.6757185	H	1.9128476	1.4232287	3.7130993
C	2.9745529	-2.7013280	2.8773948	C	-0.9968522	2.6345318	3.2390106
C	0.8932004	-2.6791977	4.0739913	H	-1.9570293	3.0941242	3.4930988
H	4.0539507	-2.8075644	2.8721207	C	1.4923751	3.5299806	3.4778928
H	0.3429154	-2.7690990	5.0045711	H	2.0734819	4.3858682	3.1148622
H	2.8050223	-2.9985376	4.9994770	H	-0.7311517	2.0080779	4.0972491
C	-3.6398802	0.3527782	-1.3528329	H	1.5568404	3.5754773	4.5710454
H	-3.0273794	0.4930314	-0.4587073	C	0.0302446	3.7734794	3.0580292
H	-3.9519883	-0.6951872	-1.3469274	H	0.0005308	4.0916399	2.0108473
H	-4.5356209	0.9708448	-1.2735344	H	-0.3126039	4.6433798	3.6283368
C	0.4640124	-0.1874639	-4.2750233	O	0.1622424	1.9903821	-1.0028134
H	1.0988580	-0.1788826	-3.3867000	C	-0.2192270	2.7670123	-2.1625915
H	0.9778009	0.3281287	-5.0885725	H	-0.5718917	2.1979957	-3.0090590
H	0.3615490	-1.2374128	-4.5647468	H	-0.7924896	3.6584686	-1.9233535
C	-1.3173682	-2.3691173	2.9148091	C	1.1917723	2.6959461	-1.7760607
H	-1.7605717	-3.3412117	2.6733390	C	2.1429890	1.8019741	-2.5291230
H	-1.7023871	-1.6584722	2.1839362	H	1.6162839	0.9855694	-3.0176571
H	-1.6746430	-2.0885650	3.9073058	H	2.8836439	1.3787135	-1.8467199
C	3.0848591	-2.3475111	0.3869872	H	2.6749465	2.3795936	-3.2900916
H	2.8276376	-1.4331988	-0.1523238	C	1.8201052	3.9008984	-1.1144722
H	2.8577120	-3.1772506	-0.2884811	H	1.1024290	4.4250593	-0.4828192
H	4.1584903	-2.3574959	0.5804645	H	2.1587285	4.5925225	-1.8913962
H	1.5953113	3.2679391	-1.6936314	H	2.6847704	3.6268610	-0.5095977
H	0.8552836	2.2602110	-3.0443170	C	-1.7285190	-0.1141300	-2.7595206
=====				C	-2.5319372	1.5915486	-4.8241056
84				C	-2.8257634	0.7482782	-2.5671885
XyNacnacRh_COE_Epox.xyz				C	-1.0291380	-0.1166135	-3.9830911
C	-1.8531215	-2.2427394	-1.8092605	C	-1.4442349	0.7445500	-5.0012443
H	-1.9543378	-4.2513100	-1.2036371	C	-3.2127570	1.5891083	-3.6123169
C	-1.4945183	-3.3020617	-0.9736206	H	-0.9095623	0.7433872	-5.9453532

H	-4.0629924	2.2479560	-3.4711241	H	-2.0247028	2.0401883	1.5912025
H	-2.8465254	2.2499712	-5.6254169	C	2.5001614	3.0508630	1.5549727
C	0.9418243	-2.5337515	1.6850989	H	3.5837938	3.1745780	1.4695706
C	2.7683401	-3.0317645	3.7398215	H	2.3281287	2.6494106	2.5571070
C	0.4782853	-2.7163915	2.9986945	C	-0.6070702	3.6323180	1.9852583
C	2.3200483	-2.6206073	1.3945481	H	-1.5331301	4.1925114	2.1442508
C	3.2144139	-2.8710524	2.4316396	C	1.8576777	4.4461049	1.4518668
C	1.4123381	-2.9545558	4.0127917	H	2.3642725	5.0142441	0.6634427
H	4.2741691	-2.9366367	2.2106374	H	-0.1989169	3.4385849	2.9823558
H	1.0586585	-3.0869288	5.0300822	H	2.0715616	4.9804867	2.3841623
H	3.4768094	-3.2191566	4.5384563	C	0.3469969	4.5287069	1.1665097
C	-3.5905848	0.7454645	-1.2696892	H	0.1655455	4.3389957	0.1034928
H	-2.9203422	0.8655121	-0.4165504	H	0.0593990	5.5737848	1.3194972
H	-4.1159041	-0.2013333	-1.1151683	C	0.4299141	-2.2080096	1.8834996
H	-4.3311405	1.5467164	-1.2563461	C	1.2940621	-2.4965847	4.5167146
C	0.1260011	-1.0585990	-4.2117264	C	1.8010310	-2.3804162	2.1486302
H	0.7655364	-1.1294676	-3.3311349	C	-0.5103409	-2.1740450	2.9295937
H	0.7254901	-0.7370921	-5.0651086	C	-0.0559791	-2.3213350	4.2409705
H	-0.2217071	-2.0753750	-4.4199182	C	2.2119954	-2.5244067	3.4743527
C	-0.9899453	-2.7109312	3.3560123	H	-0.7740774	-2.2971679	5.0534042
H	-1.3243470	-3.7178601	3.6268732	H	3.2669823	-2.6575005	3.6876511
H	-1.6131844	-2.3657548	2.5338312	H	1.6302401	-2.6087167	5.5408792
H	-1.1761996	-2.0734375	4.2235885	C	-0.9810951	0.3151917	-2.7978085
C	2.8209000	-2.4269241	-0.0113775	C	-1.3437778	2.6196084	-4.3267736
H	2.5308497	-1.4413959	-0.3877205	C	-2.2328072	0.9671735	-2.7920638
H	2.3904390	-3.1591890	-0.6996724	C	0.0923633	0.8232807	-3.5600615
H	3.9074559	-2.5183133	-0.0505873	C	-0.1128459	1.9757915	-4.3187040
=====							
71							
XyNacnacRh_COE.xyz							
C	-0.9916014	-2.0582991	-2.3492530	H	-2.0247028	2.0401883	1.5912025
H	-0.9945467	-4.1228340	-1.9127968	C	2.5001614	3.0508630	1.5549727
C	-0.7833339	-3.1482505	-1.4981957	H	3.5837938	3.1745780	1.4695706
C	-0.3348430	-3.1336308	-0.1684200	H	2.3281287	2.6494106	2.5571070
N	-0.7738127	-0.8141007	-1.9572113	C	-0.6070702	3.6323180	1.9852583
N	-0.0125058	-2.0452212	0.5319119	H	-1.5331301	4.1925114	2.1442508
C	-1.4802997	-2.3293041	-3.7547581	C	1.8576777	4.4461049	1.4518668
H	-1.6123365	-3.3971513	-3.9201167	H	2.3642725	5.0142441	0.6634427
H	-0.7730276	-1.9496919	-4.4958596	H	-0.1989169	3.4385849	2.9823558
H	-2.4335857	-1.8298968	-3.9424598	H	2.0715616	4.9804867	2.3841623
C	-0.2188792	-4.4905131	0.5045307	C	0.3469969	4.5287069	1.1665097
H	-0.5174691	-5.2786152	-0.1837073	H	0.1655455	4.3389957	0.1034928
H	-0.8517371	-4.5509577	1.3917658	H	0.0593990	5.5737848	1.3194972
H	0.8030654	-4.6894261	0.8321559	C	0.4299141	-2.2080096	1.8834996
Rh	-0.1114553	-0.1591503	-0.1579482	C	1.2940621	-2.4965847	4.5167146
C	1.1898984	0.9207492	1.2056821	C	1.8010310	-2.3804162	2.1486302
H	1.7902589	0.2223802	1.7791830	C	-0.5103409	-2.1740450	2.9295937
C	-0.1369847	1.0831177	1.6214220	C	-0.0559791	-2.3213350	4.2409705
H	-0.4574346	0.5131301	2.4865547	C	2.2119954	-2.5244067	3.4743527
C	2.0089641	1.9956144	0.5223455	H	-0.7740774	-2.2971679	5.0534042
H	2.8653369	1.5291943	0.0300852	H	3.2669823	-2.6575005	3.6876511
H	1.4404837	2.4888997	-0.2712599	H	1.6302401	-2.6087167	5.5408792
C	-0.9999143	2.2898894	1.3056497	C	-0.9810951	0.3151917	-2.7978085
H	-1.0396329	2.4713248	0.2223970	C	-1.3437778	2.6196084	-4.3267736
=====							
51							
XyNacnacRh_CO.xyz							
C	-0.9112179	-0.9374798	-1.4630876	C	-0.1128459	1.9757915	-4.3187040
H	-0.8658059	-3.0138249	-1.0879342	C	-2.3919887	2.1161696	-3.5663267
C	-0.5618294	-2.0571935	-0.6902398	H	0.7070189	2.3723223	-4.9073604
C	0.1290293	-2.0885218	0.5266890	H	-3.3509543	2.6224351	-3.5676026
=====							

N	-0.6419431	0.3351109	-1.1705249	N	0.3507935	-1.3728195	0.6836997
N	0.5505624	-0.9820946	1.1101091	C	-1.5725347	-1.2529923	-3.4094751
C	-1.6659316	-1.2311782	-2.7479910	H	-1.5515380	-2.2972864	-3.7154344
H	-1.8164617	-2.3027813	-2.8603876	H	-1.0619523	-0.6603984	-4.1708054
H	-1.1219242	-0.8650481	-3.6204246	H	-2.6128002	-0.9202789	-3.3962317
H	-2.6415188	-0.7421064	-2.7559017	C	0.4484036	-3.7966749	0.2763299
C	0.3925168	-3.4268724	1.1775152	H	0.2105783	-4.5002444	-0.5190169
H	-0.0168011	-4.2378614	0.5779325	H	-0.1094332	-4.0877086	1.1686343
H	-0.0549807	-3.4728262	2.1730901	H	1.5071830	-3.8983102	0.5198505
H	1.4644644	-3.5966119	1.3029004	Rh	-0.0169489	0.6083346	0.3097498
Rh	0.3473795	0.9201038	0.4843071	C	0.3652365	1.2975952	2.5046141
C	0.2991057	2.7749913	0.1359033	H	0.9970909	0.5706931	2.9955714
O	0.3229117	3.9169585	0.0153763	H	-0.5960567	-3.1682713	-1.9765093
C	-1.0672654	1.3665376	-2.0698947	C	1.1167263	2.2647475	1.3456342
C	-1.8725018	3.4015585	-3.7864021	H	-0.6995557	1.2084458	2.6985182
C	-2.3272948	1.9644919	-1.8883035	O	0.8358272	2.6359334	2.6800038
C	-0.2007537	1.7890497	-3.0941003	C	0.2515239	2.9727597	0.3312336
C	-0.6262513	2.8090760	-3.9449959	H	0.8059939	3.3048584	-0.5423402
C	-2.7117662	2.9810876	-2.7626126	H	-0.2679841	3.8143536	0.7936240
H	0.0345012	3.1450002	-4.7363712	H	-0.6352893	2.3534867	-0.0318313
H	-3.6799787	3.4511795	-2.6308836	C	2.6040482	2.1869431	1.0949641
H	-2.1856366	4.1954249	-4.4541812	H	3.0379358	3.1784810	1.2669074
C	1.2568866	-0.9231332	2.3415391	H	2.8270661	1.8707296	0.0772808
C	2.6460457	-0.6580340	4.7422071	H	3.0725615	1.4934117	1.7924215
C	2.6699505	-0.9353498	2.3347941	C	0.8970537	-1.6952397	1.9663005
C	0.5395612	-0.7622335	3.5483837	C	1.9545972	-2.2319196	4.4913689
C	1.2570383	-0.6352602	4.7372247	C	0.0289962	-1.9422290	3.0468593
C	3.3425155	-0.8048546	3.5492060	C	2.2926679	-1.7280472	2.1433161
H	0.7164098	-0.5125598	5.6688956	C	2.8010834	-1.9935776	3.4160309
H	4.4266044	-0.8142704	3.5553118	C	0.5786268	-2.2093875	4.3013382
H	3.1863180	-0.5532984	5.6756989	H	3.8758175	-2.0135874	3.5609008
C	1.1635119	1.1743610	-3.2606254	H	-0.0844799	-2.3950571	5.1391685
H	1.7420493	1.2555967	-2.3366609	H	2.3653645	-2.4329933	5.4737398
H	1.7125545	1.6692113	-4.0624293	C	-1.3499876	1.2438426	-2.2274824
H	1.1073649	0.1085497	-3.4982839	C	-2.3247172	3.4883953	-3.5656952
C	-3.2362627	1.5375143	-0.7664738	C	-2.6752779	1.6645170	-2.0061206
H	-2.7314119	1.6272822	0.1989144	C	-0.5093989	1.9469931	-3.1109588
H	-3.5413635	0.4917450	-0.8603924	C	-1.0173230	3.0666879	-3.7715699
H	-4.1379513	2.1505382	-0.7484354	C	-3.1429168	2.7894721	-2.6869336
C	-0.9674200	-0.7430800	3.5618279	H	-0.3750788	3.6132025	-4.4536676
H	-1.3620344	-0.0194880	2.8457826	H	-4.1628349	3.1193224	-2.5217999
H	-1.3381915	-0.4897371	4.5555092	H	-2.7037020	4.3606438	-4.0853027
H	-1.3846808	-1.7161498	3.2874276	C	0.9113400	1.5026667	-3.3469066
C	3.4411040	-1.1008394	1.0504705	H	0.9545919	0.5767405	-3.9279588
H	3.2973092	-2.0959178	0.6200239	H	1.4223153	1.2960224	-2.4041653
H	3.1146704	-0.3825900	0.2957389	H	1.4679198	2.2636016	-3.8958065
H	4.5088133	-0.9641726	1.2247586	C	-3.5753122	0.9214214	-1.0531925
=====				H	-3.8000683	-0.0873648	-1.4109564
62	XyNacnacRh_TS_1_2.xyz			H	-4.5209353	1.4499148	-0.9253651
C	-0.9261377	-1.0870442	-2.0477801	H	-3.1015432	0.8028399	-0.0757115
C	-0.4673413	-2.2510935	-1.4215407	C	-1.4660320	-1.9232794	2.8596794
C	0.1059205	-2.3806017	-0.1529185	H	-1.7888426	-1.0278767	2.3245325
N	-0.8322170	0.1191006	-1.5070845	H	-1.9760223	-1.9646372	3.8230566
				H	-1.8083777	-2.7749591	2.2642920

C	3.2289006	-1.5089761	0.9827501	H	-3.6044368	-0.8188805	-1.4567479
H	2.8711746	-0.7146967	0.3276619	H	-4.3553681	0.5004023	-0.5593115
H	3.3141829	-2.4093130	0.3658482	H	-2.7511820	-0.1170923	-0.0979974
H	4.2311182	-1.2592927	1.3346802	C	0.6257711	1.7671119	-3.5520690
=====				H	0.7491099	0.9041018	-4.2124084
62				H	1.2876004	1.6028696	-2.6988006
XyNacnacRh_TS_1_6.xyz				H	0.9602741	2.6529270	-4.0936217
C	-0.5828765	-1.2824962	-2.3238131	C	-0.4923683	-2.5076637	2.3966308
C	0.1710672	-2.3439100	-1.7978439	H	-0.9917428	-2.5981354	3.3629249
C	0.9020341	-2.3588569	-0.6040011	H	-0.5296435	-3.4910080	1.9179512
N	-0.6409335	-0.0993286	-1.7385811	H	-1.0639883	-1.8304507	1.7608167
N	1.0098255	-1.3228555	0.2271840	C	3.7581034	-0.4528399	0.5229134
C	-1.3382314	-1.5179548	-3.6144084	H	4.7904368	-0.2620201	0.8205270
H	-1.1564772	-2.5249931	-3.9864123	H	3.3065227	0.4868878	0.1952132
H	-1.0371343	-0.8061605	-4.3865703	H	3.7682327	-1.1149677	-0.3458829
H	-2.4147706	-1.3955222	-3.4725017	=====			
C	1.6347136	-3.6436692	-0.2658999	62			
H	1.5064467	-4.3727454	-1.0639730	XyNacnacRh_TS_1_13a.xyz			
H	1.2730723	-4.0873974	0.6635382	C	-0.6652042	-1.4124837	-2.1716162
H	2.7036417	-3.4611934	-0.1338997	C	-0.1038123	-2.4964008	-1.4890805
Rh	0.3208540	0.5185265	-0.1066733	C	0.5704108	-2.4971310	-0.2587518
C	-0.3354215	2.1815364	2.1155591	N	-0.6210504	-0.1766172	-1.6985005
H	0.1848793	-3.2552046	-2.3778267	N	0.8091974	-1.4284610	0.4997016
O	1.2701631	1.9155797	1.1606144	C	-1.3333660	-1.6850087	-3.5015376
C	1.0645425	2.4059145	2.4693344	H	-1.2784707	-2.7424384	-3.7535118
H	1.4011078	3.4399014	2.5870334	H	-0.8578791	-1.1129102	-4.3014264
H	1.4728004	1.7636603	3.2545284	H	-2.3840546	-1.3877222	-3.4827269
C	-1.0951673	1.0985982	2.8063621	C	1.0673224	-3.8489332	0.2228280
H	-0.4704146	0.2361258	3.0252646	H	0.8181698	-4.6214785	-0.5015927
H	-1.9792974	0.7821221	2.2571725	H	0.6229824	-4.1201894	1.1818640
H	-1.4203470	1.5141021	3.7769968	H	2.1493323	-3.8450831	0.3661836
C	-1.0907490	3.2804801	1.4445288	Rh	0.2886463	0.4540523	0.0267553
H	-0.4282947	3.9354129	0.8807899	H	1.5108655	1.0226452	0.8248242
H	-1.5795294	3.8829233	2.2245948	C	0.4407932	1.4048463	1.8992362
H	-1.8727235	2.9058747	0.7831956	H	0.4524980	0.7466949	2.7626747
C	1.6480486	-1.4760174	1.4943452	C	-0.3178555	2.6728587	1.9831491
C	2.8626769	-1.7141672	3.9966211	H	-0.1971373	-3.4583420	-1.9705134
C	0.9261232	-2.0270951	2.5728306	O	1.1024442	2.6756442	2.1839161
C	2.9786733	-1.0445463	1.6664261	C	-1.1338414	3.0003594	3.2121660
C	3.5651150	-1.1743934	2.9255067	H	-0.7119859	2.5171687	4.0937353
C	1.5520713	-2.1365683	3.8160349	H	-2.1689879	2.6691215	3.0931055
H	4.5908440	-0.8498680	3.0631995	H	-1.1438075	4.0810616	3.3859435
H	1.0009103	-2.5598100	4.6492070	C	-0.7688558	3.3418626	0.7028128
H	3.3366335	-1.8077996	4.9668894	H	-0.1442747	3.0397677	-0.1466563
C	-1.4132938	0.9788497	-2.2567234	H	-0.6809196	4.4290033	0.7863234
C	-2.8898997	3.1666354	-3.1615987	H	-1.8088026	3.1012390	0.4739473
C	-0.8066041	1.9248320	-3.1099252	C	1.4975184	-1.6046937	1.7448121
C	-2.7558529	1.1321294	-1.8512140	C	2.8161635	-1.9119067	4.1768420
C	-3.4762964	2.2318440	-2.3164425	C	0.7526539	-1.8771608	2.9064279
C	-1.5654730	3.0102890	-3.5502225	C	2.8970272	-1.4746046	1.7927846
H	-4.5095992	2.3544848	-2.0098982	C	3.5369036	-1.6348314	3.0221895
H	-1.1066937	3.7411896	-4.2070692	C	1.4340059	-2.0303965	4.1148971
H	-3.4630524	4.0165600	-3.5134869	H	4.6157107	-1.5371125	3.0704460
C	-3.4044326	0.1237386	-0.9389104	H	0.8687203	-2.2404839	5.0162013

H	3.3303984	-2.0301874	5.1233199	H	-0.2827669	3.2696153	4.1593743
C	-1.1939601	0.9239260	-2.4000933	H	-1.5973987	2.0812232	4.1766333
C	-2.2810409	3.1521451	-3.6748415	H	-1.9163831	3.7506172	3.6811158
C	-0.3912748	1.6873173	-3.2726326	C	1.8697236	-1.0390198	1.5964658
C	-2.5357088	1.2816865	-2.1549616	C	3.2373025	-0.7913063	4.0101301
C	-3.0604247	2.3971817	-2.8069802	C	1.3455334	-1.6415640	2.7548552
C	-0.9573336	2.7972418	-3.9006578	C	3.0708466	-0.3074994	1.6395983
H	-4.0920686	2.6779570	-2.6257260	C	3.7406021	-0.1986388	2.8584313
H	-0.3475162	3.3900336	-4.5733489	C	2.0478425	-1.5055220	3.9536982
H	-2.7031903	4.0186577	-4.1700481	H	4.6688540	0.3605303	2.9011419
C	-3.3914978	0.4812659	-1.2066487	H	1.6515353	-1.9666102	4.8518103
H	-4.3622318	0.9590966	-1.0688313	H	3.7703770	-0.6951837	4.9488451
H	-3.5681163	-0.5332847	-1.5741821	C	-1.7123570	0.2870332	-2.4088475
H	-2.9122669	0.3762983	-0.2304648	C	-3.5963657	1.9548739	-3.6066383
C	1.0456548	1.3147891	-3.5351107	C	-1.2849966	1.2944445	-3.2982443
H	1.5327043	2.0740307	-4.1481083	C	-3.0787667	0.1260409	-2.1025349
H	1.1252369	0.3586228	-4.0601437	C	-4.0042730	0.9685745	-2.7177970
H	1.6051313	1.2050547	-2.6034424	C	-2.2456828	2.1149157	-3.8890803
C	3.6967100	-1.1686558	0.5539880	H	-5.0575586	0.8507026	-2.4889348
H	3.5577551	-1.9282483	-0.2196859	H	-1.9261320	2.8918685	-4.5748415
H	4.7603932	-1.1143096	0.7878747	H	-4.3293171	2.6030684	-4.0725901
H	3.3877214	-0.2184164	0.1114035	C	-3.5383535	-0.9237650	-1.1237322
C	-0.7484314	-2.0027631	2.8579654	H	-4.6255836	-0.9163325	-1.0378496
H	-1.1587269	-2.0862876	3.8650480	H	-3.1156217	-0.7478448	-0.1313196
H	-1.0665565	-2.8845390	2.2942411	H	-3.2277211	-1.9274104	-1.4240954
H	-1.2024197	-1.1405485	2.3642145	C	0.1771870	1.4894053	-3.6081554
=====				H	0.7639948	1.5934720	-2.6928082
62	XyNacnacRh_TS_1_13b.xyz			H	0.3235839	2.3793537	-4.2215456
C	-0.2872907	-1.6531346	-2.2743394	H	0.5961440	0.6373078	-4.1509562
C	0.6980690	-2.4269185	-1.6493532	C	3.6254993	0.3496528	0.4036097
C	1.3582845	-2.1827190	-0.4355041	H	3.8492977	-0.3791562	-0.3798336
N	-0.7441156	-0.5270673	-1.7504921	H	4.5445869	0.8897599	0.6345072
N	1.1436137	-1.1415979	0.3662899	H	2.9032987	1.0495015	-0.0243664
C	-0.8348626	-2.1405884	-3.5979112	C	0.0611450	-2.4293215	2.7118270
H	-0.3765398	-3.0858413	-3.8828867	H	0.1880361	-3.3824133	2.1897438
H	-0.6504137	-1.4130883	-4.3915196	H	-0.7223745	-1.8879604	2.1782460
H	-1.9167620	-2.2806828	-3.5441316	H	-0.2875699	-2.6504437	3.7213819
C	2.4051685	-3.2043875	-0.0284067	=====			
H	2.4839693	-3.9849178	-0.7823685	62	XyNacnacRh_TS_1_13c.xyz		
H	2.1591520	-3.6722845	0.9263612	C	-1.0143120	-1.0825774	-2.6798455
H	3.3858692	-2.7397439	0.0907959	C	-0.4105643	-2.2113777	-2.1192006
Rh	-0.1781249	0.3287998	0.0133183	C	0.2779340	-2.3038585	-0.9003385
H	0.6378675	1.3147775	0.9432054	N	-1.0116167	0.0916877	-2.0696912
C	-0.6032079	1.1613692	1.8631807	N	0.4686851	-1.3049496	-0.0389325
H	-0.5854767	0.4480930	2.6846618	C	-1.6782359	-1.2251070	-4.0313182
C	-0.8715322	2.5769885	2.2084473	H	-1.6026686	-2.2488106	-4.3934987
H	0.9950197	-3.3250008	-2.1703479	H	-1.2156660	-0.5627514	-4.7666852
O	-1.8931112	1.7544130	1.5793304	H	-2.7345083	-0.9521596	-3.9804675
C	-0.3552379	3.7072826	1.3534962	C	0.8486162	-3.6703869	-0.5644777
H	0.5816691	4.0966182	1.7610739	H	0.6360040	-4.3744885	-1.3663636
H	-1.0797595	4.5254866	1.3274843	H	0.4239673	-4.0628748	0.3611436
H	-0.1721057	3.3746253	0.3310674	H	1.9297064	-3.6249943	-0.4214135
C	-1.1863096	2.9375501	3.6413036	Rh	-0.1949033	0.5810290	-0.2698363

H	0.8500462	1.1768116	0.7879748	N	-0.4416490	0.3697777	-1.9599153
C	-0.4801428	1.7020036	1.3989770	N	1.3047061	-0.8091383	0.0447551
H	-0.4696726	-3.1210933	-2.6977885	C	-1.0511395	-1.0844901	-3.8401026
H	-0.9726136	2.4513433	0.7288271	H	-0.8972004	-2.1121981	-4.1640603
C	-0.1160425	2.2002218	2.7381730	H	-0.6608124	-0.4165897	-4.6119654
O	-1.2449698	1.3011356	2.5225802	H	-2.1253498	-0.8993447	-3.7744735
C	1.0424101	1.6090627	3.4987712	C	1.9702072	-3.1011744	-0.5133020
H	1.9380520	2.2202286	3.3553794	H	1.7506889	-3.8586633	-1.2629060
H	1.2581691	0.5948859	3.1701174	H	1.7492813	-3.5142691	0.4718909
H	0.8209142	1.5857944	4.5695779	H	3.0417398	-2.8923578	-0.5359472
C	-0.5185252	3.5997011	3.1423962	Rh	0.3263058	0.9437249	-0.1678927
H	-0.7716986	3.6318621	4.2057991	H	1.3252842	1.5155891	0.9274940
H	-1.3859866	3.9375885	2.5738653	C	0.1420423	1.9141299	1.7085368
H	0.3037800	4.2998644	2.9710898	H	0.3305623	-2.8164819	-2.4608881
C	1.1979408	-1.5693752	1.1659502	O	0.2935952	1.3867206	3.0294280
C	2.6193214	-2.1224673	3.4936348	C	-1.0522579	1.6157934	2.5630670
C	0.5069020	-2.0223736	2.3047825	H	0.3867029	2.9808266	1.6664956
C	2.5908759	-1.3735180	1.1885796	C	-1.9126737	0.3927899	2.3766587
C	3.2839555	-1.6565479	2.3660089	H	-1.3978334	-0.3721811	1.8025591
C	1.2420855	-2.3000264	3.4583634	H	-2.8335258	0.6597136	1.8517968
H	4.3582752	-1.5110925	2.3935410	H	-2.1955891	-0.0188460	3.3508494
H	0.7210711	-2.6544866	4.3407339	C	-1.7405920	2.7744174	3.2521936
H	3.1728845	-2.3421863	4.3990575	H	-1.0522919	3.6077994	3.3973959
C	-1.6054802	1.2559022	-2.6368020	H	-2.1111691	2.4648076	4.2344205
C	-2.7364183	3.5969421	-3.6404782	H	-2.5948883	3.1239836	2.6662235
C	-2.9494972	1.5634634	-2.3382932	C	2.3356005	-0.8592644	1.0479109
C	-0.8224647	2.1250814	-3.4245364	C	4.3685858	-0.8921958	2.9583338
C	-1.4104627	3.2895782	-3.9183658	C	2.0908124	-1.4215486	2.3107064
C	-3.4952834	2.7386558	-2.8543779	C	3.6050703	-0.3292252	0.7293818
H	-0.8165474	3.9634728	-4.5258107	C	4.6042582	-0.3521853	1.6989758
H	-4.5282693	2.9823785	-2.6321075	C	3.1241825	-1.4248018	3.2516865
H	-3.1762533	4.5071121	-4.0310954	H	5.5798101	0.0568003	1.4602795
C	-0.9895572	-2.1926238	2.2968285	H	2.9382111	-1.8551275	4.2298802
H	-1.3269020	-2.8380740	1.4828341	H	5.1557961	-0.9013117	3.7031595
H	-1.4829438	-1.2268447	2.1684549	C	-1.0929246	1.4811573	-2.5657525
H	-1.3282942	-2.6275865	3.2380092	C	-2.3231401	3.7443423	-3.6393464
C	3.3243375	-0.8682577	-0.0254100	C	-2.4609805	1.7195004	-2.3131291
H	2.9180649	0.0915864	-0.3545186	C	-0.3397274	2.3806929	-3.3530138
H	3.2287042	-1.5512281	-0.8738937	C	-0.9760260	3.5030842	-3.8805957
H	4.3864297	-0.7452531	0.1904063	C	-3.0546589	2.8574128	-2.8612319
C	-3.7839074	0.6492664	-1.4780351	H	-0.4041993	4.1970005	-4.4865361
H	-3.3121520	0.4741644	-0.5083114	H	-4.1050406	3.0474826	-2.6698387
H	-3.9179431	-0.3329057	-1.9390450	H	-2.7999467	4.6248136	-4.0538240
H	-4.7722399	1.0783142	-1.3095581	C	0.7654995	-2.0269446	2.6954121
C	0.6186381	1.8088851	-3.7321680	H	0.2489313	-1.3756855	3.4027612
H	1.1870718	1.6292668	-2.8168171	H	0.9134928	-2.9946424	3.1816647
H	1.0839351	2.6309906	-4.2773583	H	0.1119499	-2.1702460	1.8377418
H	0.7145991	0.9056490	-4.3411341	C	3.8891455	0.2555264	-0.6286124
=====							
62							
XyNacnacRh_TS_1_13d.xyz							
C	-0.3703793	-0.8292414	-2.5139472	H	3.7119844	-0.4664151	-1.4301216
C	0.3470722	-1.8775832	-1.9276930	H	4.9262278	0.5872584	-0.6934314
C	1.1639369	-1.8429431	-0.7846018	H	3.2332308	1.1069724	-0.8299091
				C	-3.2856395	0.7594446	-1.4944025
				H	-2.7366886	0.4006919	-0.6236141
				H	-3.5664603	-0.1239229	-2.0768994

H	-4.2082002	1.2353318	-1.1586140	C	-3.4776771	-0.1860603	-1.2982153
C	1.1202989	2.1331291	-3.6299716	H	-3.4336691	-1.1802051	-1.7523761
H	1.6870999	2.0366201	-2.7014084	H	-4.5297021	0.0687158	-1.1607448
H	1.5438851	2.9502428	-4.2149926	H	-3.0066712	-0.2790393	-0.3167029
H	1.2742081	1.2043616	-4.1858664	C	0.7542526	1.8356150	-3.2246836
=====				H	1.0792600	2.7072282	-3.7946171
62				H	1.1189451	0.9411812	-3.7376802
XyNacnacRh_TS_1_14a.xyz				H	1.2408908	1.8519801	-2.2464801
C	-0.3934144	-1.3286464	-2.2023261	C	3.7074028	-0.7744314	0.8716721
C	0.3115052	-2.3699986	-1.5871902	H	4.7145547	-0.5336088	1.2147342
C	0.8861420	-2.4041479	-0.3077716	H	3.2722832	0.1123433	0.4048845
N	-0.6085818	-0.1502978	-1.6301604	H	3.7917072	-1.5252155	0.0812573
N	0.8916720	-1.3884567	0.5491554	C	-0.7482996	-2.3434889	2.7210456
C	-0.9211844	-1.5905969	-3.5990562	H	-1.2747070	-1.5250777	2.2246335
H	-0.6349370	-2.5844666	-3.9384619	H	-1.2274714	-2.5416964	3.6808493
H	-0.5331072	-0.8562997	-4.3083340	H	-0.8883218	-3.2252843	2.0893043
H	-2.0100317	-1.5147169	-3.6334209	=====			
C	1.5380726	-3.7131586	0.0990046	62			
H	1.4666859	-4.4391852	-0.7085303	XyNacnacRh_TS_1_14b.xyz			
H	1.0600045	-4.1370767	0.9845176	C	-0.2427810	-1.2567997	-2.2518777
H	2.5923437	-3.5752273	0.3463884	C	0.4013420	-2.3227657	-1.6122082
Rh	0.1121715	0.4430566	0.2114389	C	0.9136598	-2.3826441	-0.3077596
H	1.2589597	1.1280084	1.0356895	N	-0.4776370	-0.0867456	-1.6714193
C	0.2353821	1.4404027	2.1561202	N	0.8603254	-1.3915633	0.5761792
H	-0.4383607	0.7898007	2.7132972	C	-0.6818574	-1.4830398	-3.6849775
H	1.1064371	1.6339514	2.7836402	H	-0.4391246	-2.4941049	-4.0069551
C	-0.4002671	2.7140689	1.6666495	H	-0.1956620	-0.7778600	-4.3625847
H	0.4144096	-3.2746362	-2.1680748	H	-1.7578065	-1.3322434	-3.7951257
O	-0.6975928	2.5475961	0.2025720	C	1.5716590	-3.6906874	0.0929446
C	-1.7775806	2.6765062	1.1613011	H	1.5404387	-4.3991166	-0.7325389
H	-2.3300419	3.6057341	1.0575733	H	1.0734399	-4.1428399	0.9525705
H	-2.3801807	1.7851429	1.2928388	H	2.6149597	-3.5398296	0.3772946
C	0.2411860	4.0306285	2.0061152	Rh	0.0329518	0.4255690	0.2608335
H	0.1411648	4.2234593	3.0777665	H	1.0751332	1.0986524	1.2190056
H	-0.2225180	4.8517001	1.4580420	C	-0.0753499	1.3015328	2.2589858
H	1.3064875	4.0086551	1.7652680	H	-0.6966426	0.5635857	2.7660604
C	1.4978707	-1.5690843	1.8353228	H	0.7282598	1.5804024	2.9452327
C	2.6482922	-1.8594445	4.3588852	C	-0.8649294	2.4972182	1.7962037
C	0.7102677	-2.0164679	2.9115223	H	0.5238437	-3.2190126	-2.2021151
C	2.8582919	-1.2596784	2.0176511	C	-2.1254532	2.8723052	2.5255093
C	3.4139085	-1.4135968	3.2888471	H	-2.6565156	3.6766667	2.0139917
C	1.3054164	-2.1566707	4.1662543	H	-1.8812339	3.2024559	3.5386998
H	4.4627045	-1.1798940	3.4366445	C	-0.2129107	3.4689344	0.9096694
H	0.7036655	-2.5020688	5.0000320	H	-0.6515743	4.4555582	0.7942585
H	3.0964032	-1.9731798	5.3391392	H	0.8490252	3.4007745	0.7056112
C	-1.3863189	0.8394173	-2.3059046	H	-2.7893213	2.0088427	2.6036722
C	-2.9051043	2.8137059	-3.5624846	O	-1.0170294	2.4192879	0.3111620
C	-0.7443209	1.8258002	-3.0771206	C	1.4143596	-1.5976375	1.8819311
C	-2.7846049	0.8524959	-2.1434626	C	2.4623677	-1.9317530	4.4444627
C	-3.5267881	1.8457828	-2.7837473	C	0.5967215	-2.1080842	2.9065333
C	-1.5230336	2.8006972	-3.7011842	C	2.7543603	-1.2511117	2.1348303
H	-4.6053090	1.8574879	-2.6668254	C	3.2586758	-1.4268467	3.4241708
H	-1.0340423	3.5613567	-4.3001406	C	1.1410018	-2.2686041	4.1819056
H	-3.4949021	3.5785861	-4.0543614	H	4.2912878	-1.1635839	3.6261071

H	0.5156523	-2.6612388	4.9764004	C	0.4273846	3.9149373	2.4047167
H	2.8702886	-2.0614889	5.4401597	H	1.3898858	4.4201019	2.2941841
C	-1.0972116	0.9651685	-2.4149468	H	-0.0393675	4.2672064	3.3282709
C	-2.2977735	3.0582359	-3.8138541	H	-0.2053298	4.1971874	1.5621530
C	-0.2968762	1.8649432	-3.1433164	C	1.2526320	-1.7149453	1.3921992
C	-2.4932628	1.1270166	-2.3621330	C	2.5025487	-2.0891463	3.8567215
C	-3.0750001	2.1763601	-3.0739787	C	0.4909597	-2.1242475	2.5052423
C	-0.9175854	2.9024009	-3.8399810	C	2.6354640	-1.4750212	1.5135456
H	-4.1517994	2.3027321	-3.0413873	C	3.2407602	-1.6751823	2.7542417
H	-0.3065921	3.5962733	-4.4074917	C	1.1362004	-2.3059943	3.7295142
H	-2.7648819	3.8687344	-4.3613219	H	4.3062453	-1.4997054	2.8545683
C	-3.3488407	0.1959835	-1.5433334	H	0.5570673	-2.6230157	4.5901809
H	-3.2755306	-0.8392444	-1.8869285	H	2.9904061	-2.2384604	4.8129564
H	-4.3971321	0.4942694	-1.5919877	C	-1.4703529	1.0685397	-2.3755692
H	-3.0361200	0.1973425	-0.4960201	C	-2.6400367	3.4168557	-3.3190001
C	1.2026227	1.7193552	-3.1692914	C	-0.7240419	1.9351550	-3.2016705
H	1.5169736	0.8150641	-3.6984038	C	-2.7978845	1.3808973	-2.0141073
H	1.6039380	1.6391038	-2.1563399	C	-3.3638559	2.5593853	-2.4991800
H	1.6638626	2.5735978	-3.6670690	C	-1.3310181	3.1038514	-3.6624693
C	3.6360149	-0.7049659	1.0421307	H	-4.3842749	2.8062721	-2.2269587
H	3.7816405	-1.4304320	0.2371016	H	-0.7649788	3.7760025	-4.2978310
H	4.6179280	-0.4395970	1.4366320	H	-3.0940765	4.3301907	-3.6854476
H	3.1901849	0.1787816	0.5798998	C	-0.9901276	-2.3764235	2.3818127
C	-0.8381932	-2.4845232	2.6404787	H	-1.4540751	-2.4410999	3.3672131
H	-1.3582637	-2.7041776	3.5740841	H	-1.1988849	-3.3137437	1.8573331
H	-0.9137985	-3.3697470	2.0020108	H	-1.4799130	-1.5885518	1.8055659
H	-1.3682279	-1.6848605	2.1186232	C	3.4456195	-1.0066819	0.3347171
=====				H	4.4945185	-0.8898575	0.6108297
62	XyNacnacRh_TS_1_15.xyz			H	3.0694628	-0.0491130	-0.0348472
C	-0.9137909	-1.2794828	-2.4372335	H	3.3879404	-1.7072429	-0.5018846
C	-0.3129770	-2.4255048	-1.8968260	C	0.6959595	1.6106221	-3.5876829
C	0.3904349	-2.5256497	-0.6896523	H	0.7486172	0.7178215	-4.2171547
N	-0.8536884	-0.0995642	-1.8425842	H	1.3071559	1.4060460	-2.7054105
N	0.6066838	-1.5055967	0.1375474	H	1.1415580	2.4382577	-4.1412574
C	-1.6469469	-1.4123935	-3.7546767	C	-3.5927756	0.4608398	-1.1246999
H	-1.5950286	-2.4368003	-4.1196085	H	-3.0206070	0.1882825	-0.2350526
H	-1.2192525	-0.7542039	-4.5145830	H	-4.5274357	0.9327224	-0.8182568
H	-2.6994045	-1.1372950	-3.6529491	H	-3.8427240	-0.4757590	-1.6314159
C	0.9485113	-3.8892782	-0.3303600	=====			
H	0.7302000	-4.6067309	-1.1192921	62	XyNacnacRh_TS_3_5a.xyz		
H	0.5246964	-4.2670438	0.6022623	C	0.0687119	-0.8471948	-2.1434625
H	2.0312755	-3.8483457	-0.1920273	C	0.6944795	-1.9530033	-1.5557860
Rh	0.0828575	0.3906260	-0.1687175	C	1.0644370	-2.1658753	-0.2231501
C	-0.4641188	1.5497971	2.0083554	N	-0.2845303	0.2663261	-1.5025068
H	-0.5541222	0.5609010	2.4332017	N	0.8866408	-1.2893524	0.7588949
H	-0.4028930	-3.3331114	-2.4755161	C	-0.1980625	-0.9715623	-3.6346831
O	0.9918957	1.8773895	1.1659370	H	0.1558773	-1.9307175	-4.0070188
H	-1.3460742	1.9974442	1.5709417	H	0.3029439	-0.1790827	-4.1937287
C	0.6307837	2.4141153	2.4479137	H	-1.2625348	-0.8876011	-3.8590473
C	1.5219570	1.9344027	3.5743038	C	1.7169634	-3.5030381	0.0792883
H	2.5055056	2.4044574	3.4986292	H	1.8090565	-4.0966497	-0.8280766
H	1.6547988	0.8535516	3.5361295	H	1.1371965	-4.0739587	0.8066632
H	1.0900713	2.2013332	4.5427345	H	2.7122241	-3.3690817	0.5074124

Rh	0.1093898	0.6413893	0.5642060	C	-0.2947504	-2.4093144	-1.1448221
H	1.1082937	1.1129870	1.6513677	C	0.5985339	-2.3431715	-0.0730637
C	-0.1531286	0.9804461	2.6707056	N	-0.8205733	-0.0886465	-1.4694650
H	-0.7776901	0.1168836	2.9024430	N	0.9911431	-1.2220246	0.5380832
H	0.9189678	-2.7661941	-2.2294529	C	-1.8208329	-1.7471816	-2.9899528
H	0.6114866	1.0842588	3.4414745	H	-1.7281515	-2.8107256	-3.2008551
O	-0.9186227	2.1786455	2.6097135	H	-1.5306990	-1.1890157	-3.8822752
C	-1.1889942	2.3514992	1.2430008	H	-2.8734405	-1.5262763	-2.8064812
C	-0.1723003	2.8490521	0.4494190	C	1.2006180	-3.6614178	0.3770410
H	-0.4045134	3.1816505	-0.5510845	H	0.8835306	-4.4640994	-0.2855441
H	0.7101028	3.2733234	0.9098337	H	0.9015434	-3.9171368	1.3939331
C	-2.6517515	2.3838337	0.9342897	H	2.2907454	-3.6120923	0.3705977
H	-3.1513784	1.4751866	1.2745442	Rh	0.5224887	0.6276828	-0.0683548
H	-2.8354991	2.5305940	-0.1277525	C	-0.2639153	1.9857752	1.3814376
H	-3.0937266	3.2229917	1.4831836	C	0.9642651	2.6553893	0.8024708
C	1.2879475	-1.6731280	2.0811572	H	1.1893796	3.6864509	1.1329229
C	2.0278107	-2.3673640	4.6805723	H	0.7291930	2.8140409	-0.3157521
C	0.3673580	-2.3351050	2.9144002	O	1.9747146	1.7331594	0.9435199
C	2.5787994	-1.3565778	2.5449903	C	-1.6026589	2.5825571	1.0295784
C	2.9279494	-1.7141521	3.8479819	H	-1.6968752	2.8337793	-0.0266712
C	0.7575577	-2.6735206	4.2117038	H	-1.7341583	3.5123084	1.6016087
H	3.9221552	-1.4761317	4.2101645	H	-2.4269931	1.9234343	1.3044469
H	0.0511195	-3.1819136	4.8589247	C	-0.1451036	1.5680631	2.8219431
H	2.3154911	-2.6353171	5.6904142	H	0.8311467	1.1407572	3.0352222
C	-0.9320976	1.2771407	-2.2844172	H	-0.9259759	0.8580236	3.0986370
C	-2.2001310	3.2700926	-3.7736294	H	-0.2771138	2.4538474	3.4603360
C	-2.3314610	1.2564936	-2.4278490	C	1.8384364	-1.3180295	1.6931499
C	-0.1641454	2.2876590	-2.8943616	C	3.4714533	-1.5072248	3.9407015
C	-0.8177544	3.2751862	-3.6326163	C	1.2703071	-1.6436951	2.9383616
C	-2.9462868	2.2637031	-3.1751081	C	3.2204674	-1.0848812	1.5652338
H	-0.2308837	4.0578945	-4.1010177	C	4.0182173	-1.1910248	2.7036602
H	-4.0253240	2.2534066	-3.2863718	C	2.1067136	-1.7307478	4.0524007
H	-2.6923150	4.0457117	-4.3485561	H	5.0842783	-1.0153228	2.6145142
C	1.3365439	2.3041231	-2.7622861	H	1.6751840	-1.9749162	5.0171027
H	1.7952294	1.4412133	-3.2534130	H	4.1081469	-1.5775759	4.8149784
H	1.6431177	2.2590620	-1.7149635	C	-1.5402285	0.9116761	-2.1981121
H	1.7533411	3.2057527	-3.2132783	C	-2.9015714	2.9285072	-3.5652661
C	-3.1609635	0.1538695	-1.8196507	C	-0.8758236	1.6452398	-3.2028205
H	-2.8447341	-0.0729596	-0.8011145	C	-2.8858285	1.1813073	-1.8840391
H	-3.0689299	-0.7770366	-2.3880490	C	-3.5469510	2.1955104	-2.5797930
H	-4.2172266	0.4271876	-1.8076460	C	-1.5757588	2.6482628	-3.8727245
C	3.5767204	-0.6552665	1.6602199	H	-4.5817289	2.4115803	-2.3368346
H	3.7855860	-1.2243136	0.7506317	H	-1.0715937	3.2134309	-4.6485952
H	4.5191810	-0.5052159	2.1885852	H	-3.4285408	3.7139679	-4.0939294
H	3.2047038	0.3182318	1.3306792	C	-3.6284305	0.3931493	-0.8341547
C	-1.0119877	-2.6930381	2.4216611	H	-4.1289909	-0.4778016	-1.2695371
H	-1.6369346	-3.0390750	3.2460787	H	-4.4025232	1.0059862	-0.3693742
H	-1.5025500	-1.8428834	1.9433448	H	-2.9595852	0.0246020	-0.0579418
H	-0.9809256	-3.4894849	1.6721282	C	0.5556708	1.3503413	-3.5759722
=====				H	0.7001894	0.2969416	-3.8266378
62	XyNacnacRh_TS_6_10.xyz			H	1.2452282	1.5708811	-2.7562745
C	-0.9561549	-1.3639442	-1.8053889	H	0.8559050	1.9487806	-4.4368589
H	-0.4760844	-3.3985968	-1.5371534	C	3.8406821	-0.7188837	0.2441538
				H	4.9275920	-0.7947336	0.2993293

H	3.5771529	0.3092701	-0.0150173	H	-0.4105182	3.2960633	-5.4201744
H	3.4933742	-1.3648651	-0.5651856	C	-0.9830164	0.1957517	3.5863329
C	-0.2027994	-1.9300911	3.0950181	H	-1.1573888	0.5108842	4.6157968
H	-0.5375811	-1.6701823	4.1004762	H	-0.7110422	1.0790092	3.0015380
H	-0.4217900	-2.9932836	2.9498634	H	-1.9277226	-0.1694577	3.1775365
H	-0.8030942	-1.3778012	2.3741257	C	1.8857173	-3.0856369	0.9813586
=====							
62				H	2.6324486	-3.8610980	1.1570561
XyNacnacRh_TS_7_7a.xyz							
C	-2.1908977	-0.8632073	-1.2636620	H	2.3194335	-2.3477612	0.3014982
H	-3.1970234	-2.3779179	-0.1877186	H	1.0349025	-3.5427149	0.4711112
C	-2.3277411	-1.7376930	-0.1703156	C	0.4512712	-0.9035808	-3.5849975
C	-1.4734787	-1.9149458	0.9223606	H	-0.2724611	-1.7073755	-3.4349895
N	-1.1796517	-0.0264596	-1.3680877	H	1.2042894	-1.0085724	-2.7984599
N	-0.3332045	-1.2552686	1.1476162	H	0.9489517	-1.0683783	-4.5411118
C	-3.2338731	-0.9298284	-2.3576107	C	-2.4705562	2.5791647	-1.2992882
H	-4.0090941	-1.6522770	-2.1091718	H	-3.3516911	1.9437981	-1.1791989
H	-2.7809878	-1.2234051	-3.3078485	H	-2.8142140	3.6026968	-1.4517873
H	-3.7038139	0.0424536	-2.5182807	H	-1.9260862	2.5361721	-0.3537287
C	-1.8751274	-2.9847968	1.9202793	=====			
H	-2.7947148	-3.4707416	1.6010012	62			
H	-2.0297429	-2.5627805	2.9146023	XyNacnacRh_TS_8_9.xyz			
H	-1.0947775	-3.7417755	2.0170712	C	-1.1765997	-1.0813346	-1.9171688
Rh	0.3478024	0.1826126	-0.0293819	H	-1.1708125	-3.1763589	-1.7723881
H	-0.4010182	1.2341297	0.7569359	C	-0.7801313	-2.2797799	-1.3146213
O	2.1038845	0.3604129	0.9414517	C	0.0532799	-2.4878078	-0.2022924
C	2.6414816	1.6434116	0.9595710	N	-0.7877178	0.1359236	-1.5338602
H	2.2712418	2.2253420	1.8254918	N	0.6418562	-1.5124690	0.4724166
H	2.3513675	2.2415153	0.0668534	C	-2.1049241	-1.2116032	-3.1108488
C	4.1568755	1.6741008	1.0105332	H	-2.2214888	-2.2574382	-3.3873253
C	4.7616049	3.0532196	1.0211048	H	-1.7228159	-0.6627245	-3.9730144
H	4.4939620	3.6117807	0.1172731	H	-3.0935223	-0.8051207	-2.8892349
H	5.8499527	3.0097037	1.0820252	C	0.2813852	-3.9305796	0.2058316
H	4.3967297	3.6385085	1.8721805	H	-0.1064756	-4.6083980	-0.5523486
C	4.8849708	0.5621029	1.0538394	H	-0.2174643	-4.1556097	1.1505569
H	5.9681060	0.5973476	1.0989886	H	1.3431024	-4.1343884	0.3515417
H	4.4040590	-0.4068950	1.0541076	Rh	0.5769335	0.5204930	-0.0588952
C	0.4287319	-1.5102922	2.3362501	C	-0.5728881	1.3605825	1.4373915
C	1.8907633	-2.0522749	4.6359220	H	-0.5206179	0.6755671	2.2806941
C	0.1107354	-0.8375111	3.5280120	H	-1.5947146	1.5000444	1.0998006
C	1.4928642	-2.4248796	2.2762709	C	0.2115984	2.6571158	1.6523385
C	2.2053626	-2.6916587	3.4439866	H	-0.2890169	3.4790882	1.1318727
C	0.8545485	-1.1289163	4.6716063	O	2.1349001	1.2725201	1.2179002
H	3.0245659	-3.4012516	3.4115630	C	1.5004481	2.3398360	0.8926472
H	0.6162177	-0.6200095	5.5991263	H	2.0556059	3.1612513	0.4166929
H	2.4575863	-2.2677356	5.5342886	H	0.7487866	2.0720906	-0.5620216
C	-1.0160818	0.8556580	-2.4784592	C	0.4722375	3.0404804	3.1104526
C	-0.5794651	2.6125523	-4.5964557	H	1.0609814	3.9599692	3.1812390
C	-1.6064869	2.1358832	-2.4519288	H	1.0165117	2.2450998	3.6227059
C	-0.1984765	0.4576081	-3.5560406	H	-0.4710237	3.2067510	3.6365547
C	0.0027258	1.3517897	-4.6074762	C	1.4088566	-1.8250137	1.6428789
C	-1.3756755	2.9966930	-3.5252454	C	2.9289150	-2.3520149	3.9241382
H	0.6260415	1.0524747	-5.4426587	C	0.7655240	-2.0337764	2.8757265
H	-1.8269402	3.9826052	-3.5156576	C	2.8135879	-1.8760736	1.5499355
				C	3.5524006	-2.1488140	2.6989719
				C	1.5464228	-2.2911212	4.0053964

H	4.6336557	-2.1937027	2.6302745	O	1.0156512	3.3356430	-0.7725445
H	1.0539030	-2.4472370	4.9595116	C	0.1897485	4.6809521	2.4593588
H	3.5199339	-2.5546714	4.8096965	H	0.4707183	5.7320940	2.3498520
C	-1.3095948	1.2811623	-2.2296807	H	0.3160299	4.4075891	3.5077542
C	-2.2444842	3.5639430	-3.5402875	H	-0.8704049	4.5828921	2.2145625
C	-0.5298305	1.8763500	-3.2432698	C	0.7897960	1.7495774	-3.1847982
C	-2.5645974	1.8138014	-1.8904466	C	1.0616817	-0.8719060	1.8160494
C	-3.0081635	2.9623667	-2.5531017	C	1.2606591	-1.2150784	4.5772301
C	-1.0148864	3.0133384	-3.8849023	C	-0.1068312	-0.9200093	2.5969776
H	-3.9731233	3.3811261	-2.2869900	C	2.3306152	-0.9945062	2.4112649
H	-0.4187159	3.4721187	-4.6659444	C	2.4075279	-1.1651245	3.7943966
H	-2.6048892	4.4525654	-4.0451792	C	0.0143416	-1.0938358	3.9770339
C	-3.4694736	1.1751501	-0.8636683	C	-1.4695167	-0.7960587	1.9651140
H	-4.3429769	0.7240606	-1.3451591	C	3.5869415	-0.9466024	1.5810032
H	-3.8479092	1.9211510	-0.1607117	H	3.3825926	-1.2612565	4.2596595
H	-2.9653926	0.3951497	-0.2983836	H	-0.8834434	-1.1307448	4.5846183
C	0.8096894	1.3079195	-3.6339977	H	1.3385607	-1.3482272	5.6499931
H	0.7539523	0.2391953	-3.8518869	C	0.7798210	3.8436662	-5.0269096
H	1.5393997	1.4252310	-2.8273942	C	2.0044388	2.2023344	-3.7289170
H	1.1986109	1.8165338	-4.5170368	C	-0.4265977	2.3583588	-3.5390294
C	3.5201600	-1.6298787	0.2425978	C	-0.4114679	3.4006886	-4.4666006
H	4.5764852	-1.8897582	0.3245131	C	1.9775204	3.2476846	-4.6526963
H	3.4551140	-0.5738963	-0.0329047	C	3.3141010	1.5832412	-3.3154560
H	3.0878602	-2.2098415	-0.5754898	C	-1.7254944	1.9086720	-2.9214959
C	-0.7384029	-2.0243140	3.0150078	H	-1.3478431	3.8708213	-4.7477008
H	-1.1403632	-3.0430701	3.0262565	H	2.9111908	3.5985834	-5.0792744
H	-1.2239119	-1.4940508	2.1985123	H	0.7755958	4.6540671	-5.7466327
H	-1.0351696	-1.5571291	3.9564002	H	-2.5532896	2.5260833	-3.2736250
=====				H	-1.6845076	1.9712573	-1.8308405
62	XyNacnacRh_TS_9_11a.xyz			H	-1.9566297	0.8674068	-3.1612280
C	0.6961266	-0.5573908	-2.6332911	H	4.1519369	2.1156170	-3.7683247
C	0.7156457	-1.6715517	-1.7840082	H	3.3832154	0.5331617	-3.6132268
C	0.8379764	-1.7173105	-0.3891596	H	3.4285236	1.6036051	-2.2288898
N	0.7987472	0.6975961	-2.2141309	H	4.4710991	-1.0025124	2.2177355
N	0.9567511	-0.6546370	0.4020635	H	3.6352864	-0.0296369	0.9889340
C	0.5527977	-0.8445323	-4.1161229	H	3.6330708	-1.7736472	0.8671397
H	0.4747759	-1.9153684	-4.2943689	H	-1.7254699	-1.6824860	1.3769902
H	1.4082656	-0.4614386	-4.6761740	H	-2.2387820	-0.6725553	2.7289624
H	-0.3338026	-0.3589180	-4.5286799	H	-1.5139438	0.0509417	1.2780661
C	0.8335600	-3.1030786	0.2322342	=====			
H	0.7303987	-3.8639705	-0.5388404	62	XyNacnacRh_TS_9_11b.xyz		
H	0.0139026	-3.2212892	0.9432376	C	0.7420779	-0.5438712	-2.6140068
H	1.7569124	-3.2942288	0.7825448	C	0.7455553	-1.6971586	-1.8183030
Rh	1.0193522	1.2851784	-0.2196353	C	0.8617799	-1.8106020	-0.4267730
H	1.9650851	1.6471040	0.9700566	N	0.8603644	0.6884574	-2.1362856
C	0.7254450	2.2674660	1.7001702	N	0.9959378	-0.7887525	0.4141218
H	0.6258105	-2.6304212	-2.2723414	C	0.5967121	-0.7589192	-4.1088435
H	-0.3568217	2.1056152	1.6898242	H	0.5049566	-1.8190672	-4.3374086
H	1.0959025	1.8766762	2.6469661	H	1.4578088	-0.3611397	-4.6498246
C	1.0453456	3.7653706	1.5700832	H	-0.2830171	-0.2428631	-4.4985000
H	2.1015849	3.9239011	1.8449617	C	0.8299956	-3.2237785	0.1286318
C	0.9898600	4.1648098	0.1311085	H	0.7188384	-3.9456691	-0.6780285
H	0.9482279	5.2298643	-0.1413630	H	0.0036233	-3.3609406	0.8284495

H	1.7461921	-3.4568541	0.6748089	C	0.1769965	-2.1276814	-1.7939163
Rh	1.0935719	1.1771711	-0.1158144	C	0.8008286	-2.1831453	-0.5401383
H	2.0639423	1.4609240	1.0736960	N	-0.7650800	0.0813100	-1.7468487
C	0.8332347	2.0712828	1.8548080	N	0.7854069	-1.2047583	0.3617377
H	0.6435093	-2.6304707	-2.3516515	C	-1.1256439	-1.3074693	-3.7438189
H	-0.2476808	1.9111969	1.8457650	H	-0.8732582	-2.3036345	-4.1026610
H	1.2131179	1.6296488	2.7754302	H	-0.7393132	-0.5743666	-4.4549366
C	1.1686430	3.5693403	1.7911281	H	-2.2125828	-1.2032506	-3.7458015
C	1.1151036	4.0366244	0.3727694	C	1.5495358	-3.4666320	-0.2270303
H	1.1010472	5.1142726	0.1523075	H	1.4835223	-4.1570733	-1.0655399
O	1.1221243	3.2525813	-0.5704174	H	1.1491448	-3.9636349	0.6580260
H	0.4342553	4.1602599	2.3567112	H	2.6047077	-3.2693095	-0.0270719
C	2.5625932	3.9133600	2.3646594	Rh	-0.0694982	0.6225129	0.1092647
H	3.3435648	3.3552649	1.8444411	H	1.0556618	1.2866556	0.9772176
H	2.5967314	3.6439785	3.4213299	C	0.0150562	1.7523526	2.0805306
H	2.7863040	4.9795020	2.2801441	H	0.2804579	-3.0108011	-2.4067349
C	0.8609430	1.7855617	-3.0556457	C	1.1781592	2.2491435	2.9534683
C	1.0897229	-1.0737709	1.8166328	H	1.9143622	2.8188936	2.3820646
C	1.2683089	-1.5510121	4.5593697	H	1.6927643	1.4009252	3.4069430
C	-0.0833318	-1.1359925	2.5897667	H	0.8059843	2.8873970	3.7640147
C	2.3530315	-1.2490784	2.4106758	C	-1.0265045	1.0509507	2.9694836
C	2.4198416	-1.4862456	3.7844414	H	-0.5873578	0.1555038	3.4066796
C	0.0276041	-1.3771337	3.9605328	H	-1.9212674	0.7642554	2.4181847
C	-1.4402891	-0.9555778	1.9591183	H	-1.3235488	1.7098553	3.7983821
C	3.6140017	-1.1866933	1.5885636	C	-0.6313746	2.8702398	1.3446775
H	3.3906034	-1.6231751	4.2484919	H	-0.8267537	3.8583688	1.7975938
H	-0.8737496	-1.4250453	4.5620710	O	-0.9361640	2.6647456	0.1734558
H	1.3382345	-1.7363069	5.6249144	C	1.4402904	-1.4304253	1.6162254
C	0.8702962	3.9668782	-4.7939126	C	2.6890133	-1.8328204	4.0793712
C	2.0796373	2.2530782	-3.5777636	C	0.7320042	-2.0483422	2.6640859
C	-0.3498308	2.4221949	-3.3793471	C	2.7775264	-1.0263343	1.7926722
C	-0.3251081	3.5080294	-4.2553863	C	3.3818394	-1.2358185	3.0332995
C	2.0624142	3.3423880	-4.4496423	C	1.3744192	-2.2376211	3.8892911
C	3.3834523	1.6021474	-3.1959131	H	4.4122418	-0.9285136	3.1753834
C	-1.6527466	1.9557330	-2.7830074	H	0.8323383	-2.7102514	4.7013553
H	-1.2571468	3.9998040	-4.5129726	H	3.1737594	-1.9863726	5.0363588
H	2.9993807	3.7051720	-4.8587042	C	-1.5039055	1.1091886	-2.4157611
H	0.8735196	4.8114139	-5.4732906	C	-2.9385096	3.1406403	-3.6737349
H	-2.4751869	2.5956210	-3.1063841	C	-0.8241647	2.0481637	-3.2122510
H	-1.6115263	1.9685437	-1.6905770	C	-2.8940073	1.1988906	-2.2245869
H	-1.8926397	0.9283929	-3.0696239	C	-3.5947922	2.2196733	-2.8676944
H	4.2268188	2.1554385	-3.6120573	C	-1.5618483	3.0540298	-3.8368926
H	3.4477815	0.5715385	-3.5565612	H	-4.6678243	2.2926627	-2.7274485
H	3.4920412	1.5560083	-2.1095899	H	-1.0449501	3.7805641	-4.4544667
H	4.4937644	-1.2943020	2.2245168	H	-3.4965322	3.9290341	-4.1654395
H	3.6849590	-0.2424728	1.0438169	C	-3.6191655	0.2211014	-1.3363725
H	3.6454407	-1.9768320	0.8336902	H	-4.6762925	0.4801364	-1.2620147
H	-2.2092912	-0.8433611	2.7249555	H	-3.1919826	0.2130762	-0.3301744
H	-1.4619127	-0.0818968	1.3051712	H	-3.5488019	-0.8042481	-1.7095242
H	-1.7148144	-1.8125723	1.3365746	C	0.6712169	1.9819247	-3.3819087
=====				H	0.9847418	1.0724630	-3.9023317
62				H	1.1732531	1.9721038	-2.4114281
XyNacnacRh_TS_10_11.xyz				H	1.0312392	2.8371020	-3.9556565
C	-0.5573315	-1.0786668	-2.3575858	C	-0.6849960	-2.5271722	2.4721004

H	-1.2766703	-1.8071018	1.9063949	H	-0.1417732	3.4295871	-4.5180866
H	-0.7177744	-3.4676697	1.9132091	H	-2.5945494	3.7146801	-4.4211637
H	-1.1661797	-2.7041325	3.4353675	C	-3.1667196	-0.0234157	-1.6900253
C	3.5587026	-0.4017206	0.6661213	H	-3.0595350	-1.0544274	-2.0355073
H	4.5583831	-0.1211835	1.0008218	H	-2.8874450	-0.0195567	-0.6331803
H	3.0547964	0.4845208	0.2740654	H	-4.2194112	0.2511219	-1.7656276
H	3.6657218	-1.0882338	-0.1780775	C	1.3797994	1.5163220	-3.3566556
=====							
62							
XyNacnacRh_TS_10_12.xyz							
C	-0.0405929	-1.4750883	-2.3590481	C	-0.9322373	-2.2489602	2.5711933
C	0.5817861	-2.5043409	-1.6428569	H	-1.4259745	-1.3794738	2.1297190
C	1.0216813	-2.4939353	-0.3103582	H	-1.4684508	-2.5260492	3.4796042
N	-0.2916871	-0.2874692	-1.8287328	H	-1.0389733	-3.0659653	1.8528442
N	0.9260367	-1.4579250	0.5183866	C	3.7040672	-0.8132762	1.0810761
C	-0.4452836	-1.7496048	-3.7908697	H	4.6967640	-0.6442825	1.4998339
H	-0.1944948	-2.7706328	-4.0721373	H	3.7949466	-1.5519702	0.2807263
H	0.0573845	-1.0680307	-4.4806939	H	3.3691474	0.1132845	0.6078219
H	-1.5190662	-1.6060391	-3.9305516	=====			
C	1.6317781	-3.7814679	0.2101318	62			
H	1.6289823	-4.5427534	-0.5673799	XyNacnacRh_TS_11_16.xyz			
H	1.0759895	-4.1614114	1.0694406	C	-0.5434381	-0.4468281	-1.6821928
H	2.6601243	-3.6288669	0.5423211	C	0.1612182	-1.4987809	-1.0843718
Rh	0.1494652	0.3084297	0.0226428	C	0.8376397	-1.5077994	0.1424645
H	1.3683310	1.1438833	0.6145678	N	-0.6906142	0.7425334	-1.1146582
H	0.7309370	-3.4299479	-2.1784359	N	0.8902644	-0.4823355	0.9901506
O	0.6796936	1.4175814	1.7994337	C	-1.1312564	-0.6947935	-3.0552908
C	0.0010426	2.5692154	1.5455602	H	-0.9302735	-1.7136088	-3.3812375
H	0.4938874	3.2745122	0.8730983	H	-0.7097445	-0.0059042	-3.7906421
C	-1.1755421	2.9012288	2.1075990	H	-2.2111916	-0.5355479	-3.0580112
C	-1.8745729	2.0113892	3.0928236	C	1.5859114	-2.7814193	0.4894019
H	-1.9966649	2.5230440	4.0543481	H	1.4564754	-3.5223593	-0.2968480
H	-1.3169805	1.0922487	3.2631746	H	1.2386855	-3.2121567	1.4295657
H	-2.8822177	1.7560258	2.7456301	H	2.6541449	-2.5869242	0.6069403
C	-1.8212015	4.2218673	1.7982874	Rh	0.0295192	1.3161462	0.6960783
H	-1.9210743	4.8339896	2.7021311	H	0.7072485	2.0042166	2.0746074
H	-2.8331585	4.0825815	1.4017158	C	-0.6523180	2.3703206	2.1878220
H	-1.2480840	4.7937113	1.0659868	H	0.2166173	-2.4131484	-1.6561136
C	1.4060118	-1.5639029	1.8644334	O	-0.9737360	3.3278417	1.4823062
C	2.3101365	-1.7490202	4.4888313	C	-1.1071914	2.1603979	3.6173524
C	2.7457394	-1.2538267	2.1564148	H	-0.7650918	1.1710789	3.9244051
C	0.5112986	-1.9485175	2.8787389	C	-2.6370038	2.2264321	3.7020134
C	0.9861214	-2.0401217	4.1863491	H	-3.1033502	1.4588464	3.0813538
C	3.1779400	-1.3567053	3.4788931	H	-3.0011779	3.1994329	3.3686165
H	0.3048702	-2.3390514	4.9752223	H	-2.9597401	2.0703473	4.7337478
H	4.2096357	-1.1213600	3.7152403	C	-0.4350459	3.2121879	4.5180068
H	2.6631804	-1.8221483	5.5108804	H	0.6537898	3.1570435	4.4541676
C	-0.9140161	0.7687371	-2.5589948	H	-0.7192570	3.0436091	5.5589236
C	-2.1239799	2.8896549	-3.8994081	H	-0.7451328	4.2191125	4.2319989
C	-0.1170702	1.6748646	-3.2885254	C	-1.3960012	1.7957581	-1.7773014
C	-2.3129421	0.9299225	-2.4867330	C	-2.7580917	3.8893102	-3.0077685
C	-2.8976486	1.9963842	-3.1691589	C	-0.6817603	2.7221943	-2.5600530
C	-0.7454586	2.7275299	-3.9537590	C	-2.7848331	1.9245931	-1.5898688
H	-3.9730056	2.1268177	-3.1224999	C	-3.4477720	2.9784715	-2.2185658

C	-1.3849519	3.7595488	-3.1716781	H	1.6287779	3.8408748	1.2133189
H	-4.5176152	3.0866595	-2.0785322	H	0.2087296	4.6542874	0.5664983
H	-0.8438497	4.4773121	-3.7781354	C	-0.6073017	3.8088891	3.0117227
H	-3.2877806	4.7047387	-3.4861764	H	-0.0851852	4.7634775	3.0858503
C	1.5993146	-0.6278437	2.2269754	H	-0.5047711	3.2432877	3.9418805
C	2.9490103	-0.8500631	4.6532374	H	-1.6775847	4.0145460	2.8882455
C	2.9339995	-0.1925201	2.3191532	C	1.7050008	-1.1584976	1.8192062
C	0.9352663	-1.1711925	3.3421863	C	3.1550270	-0.8574958	4.1860486
C	1.6300297	-1.2718560	4.5486627	C	1.1353713	-1.5585879	3.0428516
C	3.5917325	-0.3161471	3.5430253	C	3.0000751	-0.6097646	1.7773615
H	1.1255110	-1.6868545	5.4145319	C	3.7064886	-0.4668549	2.9729084
H	4.6212206	0.0149893	3.6234096	C	1.8768177	-1.4017638	4.2137281
H	3.4746340	-0.9358375	5.5970372	H	4.7058797	-0.0456824	2.9459137
C	-3.5483714	0.9515228	-0.7292152	H	1.4433084	-1.7129863	5.1582002
H	-4.5779832	1.2853989	-0.5947886	H	3.7195547	-0.7432977	5.1042067
H	-3.0842317	0.8469918	0.2535825	C	-1.7788867	0.2498718	-2.3687183
H	-3.5773831	-0.0495076	-1.1698394	C	-3.4711243	1.8967049	-3.8563435
C	0.8112004	2.6103019	-2.7329213	C	-1.2433782	1.0635325	-3.3850823
H	1.1838599	3.4135554	-3.3696636	C	-3.1545292	0.2805788	-2.0768774
H	1.1022763	1.6581444	-3.1842557	C	-3.9841534	1.1048837	-2.8371997
H	1.3245608	2.6696472	-1.7696541	C	-2.1074043	1.8761868	-4.1195132
C	3.6392665	0.4076271	1.1318411	H	-5.0465769	1.1272179	-2.6194458
H	4.6698901	0.6603499	1.3837423	H	-1.6997986	2.5037577	-4.9049938
H	3.1304696	1.3147414	0.7943373	H	-4.1293155	2.5325436	-4.4370889
H	3.6550629	-0.2742265	0.2779937	C	-3.7261700	-0.5336689	-0.9453290
C	-0.4918722	-1.6479552	3.2473442	H	-3.4253682	-1.5823301	-0.9953263
H	-0.5641747	-2.6085611	2.7282721	H	-4.8161531	-0.4896182	-0.9523904
H	-1.1115798	-0.9460882	2.6870698	H	-3.3831152	-0.1462741	0.0191670
H	-0.9196074	-1.7821756	4.2419715	C	0.2365438	1.0772136	-3.6686758
=====				H	0.5954961	0.1147916	-4.0443992
62	XyNacnacRh_TS_13_10.xyz			H	0.4772768	1.8363006	-4.4144627
C	-0.5517742	-1.7642517	-2.0083405	H	0.8067462	1.2850359	-2.7604321
H	0.5458669	-3.5520938	-1.7978117	C	3.6179201	-0.1615920	0.4793771
C	0.3563675	-2.5970082	-1.3300575	H	4.6490150	0.1592836	0.6349148
C	1.0469848	-2.3720612	-0.1313218	H	3.0579339	0.6725267	0.0473126
N	-0.9055575	-0.5623881	-1.5825503	H	3.6173177	-0.9516625	-0.2746678
N	0.9341552	-1.2788446	0.6193647	C	-0.2538388	-2.1409196	3.0992237
C	-1.1527936	-2.3156538	-3.2877663	H	-0.3547005	-3.0273523	2.4683046
H	-0.7962337	-3.3264777	-3.4779166	H	-0.5114356	-2.4223659	4.1213560
H	-0.8988296	-1.6918359	-4.1471578	H	-0.9996135	-1.4236359	2.7457734
H	-2.2431770	-2.3364735	-3.2275254	=====			
C	1.9679778	-3.4862228	0.3327515	62	XyNacnacRh_TS_14_7a.xyz		
H	1.9331840	-4.3239540	-0.3611172	C	-0.2980201	-1.1310545	-2.2919991
H	1.6856288	-3.8464072	1.3242573	H	0.4049755	-3.1185285	-2.2910622
H	3.0018921	-3.1428940	0.4068530	C	0.2820789	-2.2477914	-1.6642172
Rh	-0.2761611	0.3196854	0.2249796	C	0.6878518	-2.4079696	-0.3347139
H	0.9370210	1.0860752	-0.2445479	N	-0.5189343	0.0186840	-1.6787308
C	-0.5981100	1.6192596	1.7850989	N	0.6300819	-1.4645824	0.6068204
H	-1.0263247	1.2111535	2.7067762	C	-0.6934485	-1.2989774	-3.7466286
C	-0.1697422	2.9871796	1.8476043	H	-0.4373658	-2.2945171	-4.1046746
O	-1.5140764	1.9590306	0.7680913	H	-0.1922481	-0.5624844	-4.3778079
C	0.6244204	3.6703351	0.7993956	H	-1.7667547	-1.1482156	-3.8815063
H	0.7164060	3.0724056	-0.1014837	C	1.2118436	-3.7824273	0.0408759

H	1.1900539	-4.4459143	-0.8213247	C	-0.2965279	-1.2402059	-2.2283650
H	0.6123405	-4.2307636	0.8357538	H	0.3857612	-3.2316078	-2.1202728
H	2.2369915	-3.7319411	0.4122707	C	0.2955709	-2.3197528	-1.5487981
Rh	0.0071027	0.4424985	0.3107376	C	0.7640457	-2.3932706	-0.2321562
H	1.4055445	0.9513851	0.0546344	N	-0.4856437	-0.0497275	-1.6864360
C	0.2246845	1.2393882	2.2958765	N	0.7383504	-1.3947353	0.6516033
H	1.2144507	1.1418102	2.7339208	C	-0.7482394	-1.5012873	-3.6526951
H	-0.5336725	0.7531905	2.9118264	H	-0.5400681	-2.5297674	-3.9419766
C	-0.1171821	2.5902831	1.8937447	H	-0.2460151	-0.8346311	-4.3563086
C	0.8584269	3.7173592	2.0118841	H	-1.8199596	-1.3204880	-3.7606863
H	0.8638571	4.0651460	3.0508303	C	1.3218004	-3.7370531	0.2017691
H	0.5926107	4.5539747	1.3659839	H	1.2732547	-4.4510915	-0.6178625
H	1.8691315	3.3850649	1.7697809	H	0.7641852	-4.1446121	1.0473650
C	-1.4574736	2.8609018	1.3789520	H	2.3611348	-3.6511698	0.5241493
H	-1.7943987	3.8960679	1.3344092	Rh	0.0537634	0.4791925	0.2760599
H	-2.2616477	2.1692955	1.6348709	H	1.4354818	1.0009275	-0.0347977
O	-0.6727756	2.4982828	0.2396313	C	0.3105960	1.3916921	2.2093372
C	1.0762523	-1.7834806	1.9315026	H	1.3619808	1.6243889	2.3721352
C	1.9137269	-2.3778878	4.5257453	H	-0.0905376	0.7919577	3.0242475
C	0.1426061	-2.2454767	2.8767130	C	-0.5078060	2.5447635	1.8723632
C	2.4266577	-1.6071507	2.2832510	C	-0.0608916	3.4609810	0.8262508
C	2.8241374	-1.9125973	3.5862284	H	-0.5356224	4.4392959	0.7640580
C	0.5816181	-2.5402722	4.1678494	H	0.9948141	3.4798179	0.5626295
H	3.8650051	-1.7833764	3.8622467	C	-1.7841266	2.8401861	2.5964416
H	-0.1334639	-2.9015302	4.8988397	H	-2.4349912	3.4996421	2.0222530
H	2.2405174	-2.6130656	5.5318779	H	-1.5399207	3.3298288	3.5455036
C	-1.1475451	1.0923027	-2.3799738	H	-2.3233792	1.9209240	2.8327332
C	-2.3897702	3.2195419	-3.6881784	O	-0.8313338	2.4438640	0.1736710
C	-2.5463878	1.2268520	-2.3193278	C	1.2440705	-1.6285372	1.9724091
C	-0.3655403	2.0371153	-3.0675306	C	2.1948321	-2.0589837	4.5600580
C	-1.0078160	3.0894227	-3.7209460	C	0.3584524	-2.0555837	2.9787062
C	-3.1497692	2.2932958	-2.9856664	C	2.6025171	-1.4049987	2.2595340
H	-0.4104768	3.8167447	-4.2599884	C	3.0568492	-1.6273994	3.5608944
H	-4.2289399	2.3963436	-2.9491770	C	0.8538347	-2.2695116	4.2651901
H	-2.8722302	4.0426082	-4.2023337	H	4.1042148	-1.4606129	3.7877367
C	1.1366864	1.9338296	-3.0921243	H	0.1760403	-2.6041679	5.0429329
H	1.5480948	2.0355751	-2.0850341	H	2.5657826	-2.2303666	5.5637690
H	1.4788957	0.9679969	-3.4714381	C	-1.0610126	1.0030470	-2.4611199
H	1.5649242	2.7162091	-3.7202132	C	-2.1807477	3.0988906	-3.9227586
C	-3.3884354	0.2442783	-1.5453662	C	-0.2318777	1.8239898	-3.2477076
H	-3.1290402	0.2488969	-0.4828202	C	-2.4426287	1.2494849	-2.3788061
H	-3.2517260	-0.7827661	-1.8923854	C	-2.9848134	2.2962540	-3.1244495
H	-4.4470131	0.4925703	-1.6335877	C	-0.8129796	2.8635160	-3.9747039
C	3.4332439	-1.0880272	1.2904812	H	-4.0518040	2.4837784	-3.0716647
H	3.4477973	-1.6756908	0.3699619	H	-0.1797046	3.4953523	-4.5881846
H	4.4364729	-1.1009798	1.7185633	H	-2.6166280	3.9087351	-4.4961442
H	3.1971027	-0.0625268	0.9942638	C	-3.3289769	0.4147354	-1.4908784
C	-1.3103593	-2.4186051	2.5144724	H	-3.2177405	-0.6550055	-1.6808735
H	-1.4466602	-3.0935206	1.6661834	H	-4.3771914	0.6795121	-1.6365357
H	-1.7648034	-1.4656728	2.2282610	H	-3.0869449	0.5773443	-0.4365761
H	-1.8718666	-2.8191218	3.3595114	C	1.2567804	1.5988689	-3.3063612
=====				H	1.5108044	0.6245377	-3.7325939
62				H	1.6965358	1.6218685	-2.3070179
XyNacnacRh_TS_14_7b.xyz				H	1.7368056	2.3653389	-3.9162772

C	-1.1043486	-2.2708535	2.6858449	H	-3.4200839	3.5266181	-3.4208932
H	-1.2632392	-2.9877208	1.8770692	H	0.5262776	3.1402878	-5.0315942
H	-1.5864398	-1.3400589	2.3733922	H	-1.6654611	4.2865618	-4.9890531
H	-1.6235316	-2.6389758	3.5716414	C	3.0101217	-1.7438025	0.8261960
C	3.5588385	-0.9275033	1.1985785	H	2.7876535	-2.4927103	0.0611401
H	4.5757516	-0.8822890	1.5905497	H	4.0542431	-1.8629670	1.1179556
H	3.2822085	0.0676483	0.8408212	H	2.8999220	-0.7701531	0.3417069
H	3.5606138	-1.5783955	0.3213103	C	-1.6142357	-1.6507595	2.9199123
=====				H	-2.0873068	-1.7385127	3.8986097
62	XyNacnacRh_TS_16_17a.xyz			H	-2.0783848	-2.3855236	2.2567998
C	-1.0538490	-1.0274164	-2.1383279	H	-1.8569365	-0.6689528	2.5066442
H	-1.1585620	-3.1079079	-1.8900180	C	1.3671715	1.0608615	-3.5209170
C	-0.8538813	-2.1966851	-1.3978568	H	1.2985817	-0.0136215	-3.7072754
C	-0.2777597	-2.3661436	-0.1313227	H	1.8719573	1.1780552	-2.5575461
N	-0.7352855	0.2006507	-1.7307508	H	2.0013800	1.4984393	-4.2928012
N	0.1451154	-1.3700881	0.6410414	C	-3.3175723	1.5103778	-1.6244505
C	-1.6587579	-1.2103694	-3.5184529	H	-3.6027818	0.4652148	-1.7693930
H	-1.8649521	-2.2620704	-3.7062755	H	-4.2110383	2.1231551	-1.7487331
H	-0.9847152	-0.8452417	-4.2955702	H	-2.9826240	1.6012008	-0.5888968
H	-2.5891567	-0.6500372	-3.6224166	=====			
C	-0.1278210	-3.8020404	0.3387632	62	XyNacnacRh_TS_16_17b.xyz		
H	-0.5180554	-4.4932671	-0.4054941	C	-0.9474816	-0.9220659	-2.2336655
H	-0.6550458	-3.9715280	1.2789302	H	-0.8096519	-3.0150727	-2.1962753
H	0.9206961	-4.0468108	0.5202452	C	-0.6069182	-2.1287213	-1.6143550
H	0.3691612	2.0888139	-0.5853662	C	-0.0035571	-2.3567558	-0.3699438
Rh	0.0488799	0.7266593	0.1018499	N	-0.7679783	0.2874792	-1.7040867
C	-0.6694979	1.9788824	1.1934626	N	0.3098502	-1.4011055	0.4996044
O	-1.3572913	2.7694196	1.6939517	C	-1.5421745	-1.0345520	-3.6257244
C	1.1937429	1.6687083	1.9966480	H	-1.6265069	-2.0788356	-3.9193372
H	1.8127998	0.8048808	1.7666849	H	-0.9240570	-0.5166155	-4.3613901
C	0.7616397	1.6023657	3.4532852	H	-2.5326510	-0.5793739	-3.6729552
H	1.6553260	1.6145216	4.0873232	C	0.3134204	-3.8059105	-0.0461325
H	0.2162276	0.6891243	3.6837182	H	-0.0016825	-4.4590556	-0.8573548
H	0.1446103	2.4583949	3.7317922	H	-0.1830208	-4.1280760	0.8705802
C	1.9205356	2.9572613	1.6455330	H	1.3844897	-3.9459886	0.1130093
H	2.7771682	3.0820938	2.3193211	H	0.1292175	2.1652682	-0.3743943
H	1.2807776	3.8339538	1.7715089	Rh	-0.0299496	0.7143364	0.1731344
H	2.2951224	2.9533544	0.6225261	C	-0.8765710	1.7630651	1.3810582
C	0.7132687	-1.7111742	1.9084206	O	-1.6448747	2.4167996	1.9560257
C	1.8234293	-2.3498821	4.3876327	C	1.0171065	1.5872171	2.1552664
C	2.1055499	-1.8795231	2.0253852	H	1.7285794	0.8270940	1.8418307
C	-0.1240493	-1.8494929	3.0316042	C	1.5895267	2.9788696	1.9375151
C	0.4511819	-2.1778694	4.2599834	H	2.4321439	3.1325245	2.6228709
C	2.6405713	-2.1961835	3.2752278	H	0.8553028	3.7597667	2.1490884
H	-0.1895426	-2.2924790	5.1275317	H	1.9533899	3.1203118	0.9204259
H	3.7126682	-2.3291161	3.3711568	C	0.6071951	1.3266427	3.5964903
H	2.2540895	-2.6011102	5.3496404	H	1.4985970	1.3775416	4.2317459
C	-0.9939592	1.2985378	-2.6254326	H	0.1715750	0.3385346	3.7323046
C	-1.4769280	3.4497317	-4.3269141	H	-0.1013792	2.0741076	3.9572533
C	0.0156752	1.7261295	-3.5043928	C	0.9233439	-1.8004998	1.7282660
C	-2.2409449	1.9450561	-2.5847586	C	2.1184691	-2.5536726	4.1348576
C	-2.4615127	3.0201972	-3.4469301	C	0.1161245	-2.1450966	2.8289314
C	-0.2475526	2.8039308	-4.3502992	C	2.3266239	-1.8205327	1.8326219

C	2.9040038	-2.1977100	3.0462843	H	0.4878539	-3.0966298	-1.7746546
C	0.7346012	-2.5270134	4.0202563	C	-0.1795967	2.7365615	-0.6149548
H	3.9849930	-2.2168851	3.1321311	O	-0.3858088	3.8173380	-0.9333552
H	0.1179039	-2.7997731	4.8697034	C	-1.4516124	1.8262006	2.2085493
H	2.5825034	-2.8490210	5.0683858	H	-1.9115521	0.8888284	1.8962408
C	-1.1622668	1.4322502	-2.4830485	H	-1.9117784	2.6369352	1.6409611
C	-1.9113159	3.6726127	-3.9579913	H	-1.7080356	1.9834865	3.2660897
C	-2.4749889	1.9222412	-2.3765234	C	-1.0014261	0.9837707	-2.7889260
C	-0.2196604	2.0601740	-3.3148036	C	-2.2290701	2.6992204	-4.6106334
C	-0.6160334	3.1794507	-4.0472706	C	-2.3892649	1.1966485	-2.7147487
C	-2.8288128	3.0456128	-3.1254066	C	-0.2228101	1.6337319	-3.7634997
H	0.1052653	3.6698300	-4.6917419	C	-0.8578019	2.4873729	-4.6663065
H	-3.8390023	3.4322117	-3.0477068	C	-2.9843313	2.0572997	-3.6380915
H	-2.2032594	4.5440716	-4.5320778	H	-0.2635849	2.9950030	-5.4181854
C	1.1993092	1.5615375	-3.3994807	H	-4.0542997	2.2266147	-3.5866316
H	1.7000707	1.6418660	-2.4301845	H	-2.7061769	3.3670185	-5.3181482
H	1.7683746	2.1434863	-4.1254411	C	1.8456721	-0.8691685	1.8327707
H	1.2530373	0.5098441	-3.6909795	C	3.2727198	-0.8793466	4.2321670
C	-3.4823637	1.2715745	-1.4643439	C	3.1851896	-0.4363918	1.8484604
H	-3.1488318	1.2994002	-0.4247487	C	1.2208211	-1.3095663	3.0139686
H	-3.6446661	0.2193356	-1.7117289	C	1.9524278	-1.3057158	4.2038260
H	-4.4428522	1.7840251	-1.5279942	C	3.8797766	-0.4499792	3.0586832
C	-1.3878286	-2.1078764	2.7322000	H	1.4725355	-1.6384737	5.1177777
H	-1.8400553	-2.3385550	3.6974687	H	4.9124744	-0.1193834	3.0759150
H	-1.7705342	-2.8270115	2.0031227	H	3.8263057	-0.8798908	5.1637076
H	-1.7438661	-1.1265163	2.4102692	C	-3.2240592	0.5231405	-1.6564617
C	3.2005943	-1.4642757	0.6560930	H	-3.1757522	-0.5666983	-1.7259457
H	4.2536212	-1.4905579	0.9387460	H	-4.2697484	0.8201357	-1.7457949
H	2.9757718	-0.4669237	0.2692120	H	-2.8758668	0.7844824	-0.6539067
H	3.0597873	-2.1550332	-0.1796662	C	3.8739300	0.0162352	0.5867946
=====				H	3.3334091	0.8368390	0.1098092
62	XyNacnacRh_TS_17_18.xyz			H	3.9292302	-0.7864532	-0.1537929
C	-0.2179845	-1.1557920	-2.1459173	H	4.8912029	0.3455188	0.8021947
C	0.4386335	-2.1038439	-1.3537640	C	1.2692680	1.4328311	-3.8276238
C	1.0811420	-1.9505727	-0.1184280	H	1.7430224	1.6778350	-2.8736697
N	-0.3618825	0.1269556	-1.8292951	H	1.7078734	2.0615048	-4.6034031
N	1.1049291	-0.8315582	0.6022709	H	1.5354476	0.3949785	-4.0456730
C	-0.7756625	-1.6655084	-3.4627735	C	-0.2079390	-1.7930744	3.0140672
H	-0.6084477	-2.7362759	-3.5592163	H	-0.2879858	-2.8169685	2.6358362
H	-0.3061250	-1.1643872	-4.3113211	H	-0.8429252	-1.1768653	2.3781413
H	-1.8471623	-1.4732051	-3.5398626	H	-0.6154718	-1.7874007	4.0257872
C	1.8161528	-3.1808289	0.3863859	=====			
H	1.7057127	-4.0049714	-0.3150836	56	XyNacnacRh_TS_21_22.xyz		
H	1.4470619	-3.5049659	1.3597767	C	-0.9857203	-1.2212029	-2.0968684
H	2.8813159	-2.9735192	0.5080393	C	-0.5385679	-2.3802897	-1.4508927
Rh	0.2854224	1.0264349	-0.0234146	C	0.0593452	-2.4762134	-0.1864096
H	1.2506552	1.7272766	0.9757571	N	-0.8815738	-0.0233006	-1.5464764
C	0.0719052	1.8189821	2.0751806	N	0.3037114	-1.4434243	0.6182815
H	0.4864613	1.0279972	2.6920909	C	-1.6069225	-1.3575354	-3.4694526
C	0.6552992	3.1600610	2.5300606	H	-1.6190955	-2.3997975	-3.7834001
H	1.7469536	3.1501679	2.5537674	H	-1.0526260	-0.7804953	-4.2133663
H	0.3025379	3.3856404	3.5425676	H	-2.6334007	-0.9835603	-3.4777364
H	0.3407292	3.9834214	1.8850601	C	0.4462688	-3.8684323	0.2765688

H	0.1889458	-4.6040475	-0.4830475
H	-0.0657345	-4.1380541	1.2024738
H	1.5174284	-3.9405111	0.4751007
Rh	-0.1215723	0.4694991	0.2130567
C	-0.2147437	1.6750342	2.2314563
H	-0.4811040	0.8135667	2.8300784
H	-0.6699451	-3.3083213	-1.9874459
C	1.2256768	1.8514308	1.5578927
H	-1.0444163	2.2970436	1.8985853
O	0.8459572	2.4354798	2.7990565
C	0.9175293	-1.6601763	1.8904692
C	2.1107999	-1.9902416	4.3884073
C	0.1102750	-1.8817869	3.0233924
C	2.3206978	-1.6108899	2.0031486
C	2.8966337	-1.7771928	3.2630697
C	0.7284080	-2.0430689	4.2638024
H	3.9761252	-1.7361382	3.3591166
H	0.1138089	-2.2099715	5.1416605
H	2.5742535	-2.1116440	5.3603211
C	-1.3281407	1.1757007	-2.1693408
C	-2.1612796	3.5937909	-3.2786406
C	-2.6400056	1.6388479	-1.9280008
C	-0.4314252	1.9258126	-2.9611027
C	-0.8709938	3.1319593	-3.5064303
C	-3.0347261	2.8507171	-2.4943482
H	-0.1891028	3.7151830	-4.1152607
H	-4.0400663	3.2146642	-2.3137881
H	-2.4844464	4.5349312	-3.7079554
C	0.9691537	1.4364794	-3.2243296
H	0.9716611	0.5426959	-3.8547785
H	1.4721822	1.1625774	-2.2944114
H	1.5551097	2.2037762	-3.7317710
C	-3.6021528	0.8426790	-1.0849842
H	-3.8921636	-0.0899870	-1.5768895
H	-4.5105826	1.4152083	-0.8941304
H	-3.1513772	0.5635114	-0.1302139
C	-1.3901498	-1.9609989	2.9056975
H	-1.7864803	-1.1475478	2.2941365
H	-1.8566248	-1.9264413	3.8910416
H	-1.7063759	-2.8901199	2.4221235
C	3.1915581	-1.4005518	0.7910927
H	2.8161314	-0.5882271	0.1648956
H	3.2164920	-2.2909750	0.1554884
H	4.2175238	-1.1779146	1.0873919
H	1.3654701	2.5924045	0.7720394
H	2.0159613	1.1194990	1.6624575

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XyNacnacRh_TS_21_26.xyz

C	-0.6161369	-1.2502135	-2.3124447
C	0.1248192	-2.3056548	-1.7570524
C	0.8641624	-2.3000877	-0.5676841
N	-0.6746681	-0.0559719	-1.7501251
N	0.9883918	-1.2480003	0.2406117

C	-1.3607269	-1.5037514	-3.6052659
H	-1.2141811	-2.5301151	-3.9375308
H	-1.0187390	-0.8339126	-4.3977880
H	-2.4329570	-1.3315303	-3.4852576
C	1.5805988	-3.5861409	-0.2010933
H	1.4373012	-4.3334514	-0.9793023
H	1.2146015	-3.9993299	0.7408836
H	2.6527507	-3.4181367	-0.0776417
Rh	0.2471011	0.5670290	-0.1104821
C	-0.2806209	1.5750780	2.1684310
H	0.1248782	-3.2321552	-2.3124485
O	1.1871736	1.9071415	1.3208794
C	0.9810804	2.0465491	2.7210315
H	1.0557469	3.0786855	3.0599582
H	1.5572258	1.3495909	3.3289772
C	1.6633242	-1.3703066	1.4925280
C	2.9554627	-1.5454899	3.9591233
C	0.9615255	-1.8521382	2.6154964
C	3.0084137	-0.9653594	1.6035123
C	3.6355125	-1.0656786	2.8454688
C	1.6269471	-1.9320220	3.8406559
H	4.6727624	-0.7625202	2.9370904
H	1.0926058	-2.3034361	4.7085805
H	3.4596444	-1.6159502	4.9159336
C	-1.4122860	1.0309172	-2.3010788
C	-2.8170150	3.2349254	-3.2724472
C	-0.7726451	1.9344974	-3.1762134
C	-2.7514184	1.2347075	-1.9057603
C	-3.4354986	2.3423193	-2.4054443
C	-1.4963245	3.0293013	-3.6501481
H	-4.4651916	2.5057735	-2.1066217
H	-1.0125185	3.7293725	-4.3222560
H	-3.3621969	4.0926424	-3.6489207
C	-3.4353123	0.2734354	-0.9689954
H	-3.6191678	-0.6932545	-1.4464742
H	-4.3970237	0.6713343	-0.6425329
H	-2.8147804	0.0746241	-0.0927235
C	0.6577534	1.7250386	-3.6022890
H	0.7629410	0.8421521	-4.2390702
H	1.3079489	1.5664591	-2.7391884
H	1.0206726	2.5867751	-4.1635975
C	-0.4756019	-2.2961996	2.5065849
H	-0.9471464	-2.3232603	3.4902351
H	-0.5552742	-3.3004795	2.0789375
H	-1.0501255	-1.6391779	1.8511120
C	3.7561968	-0.4298713	0.4123288
H	4.7844684	-0.1851095	0.6823334
H	3.2695462	0.4686230	0.0250214
H	3.7808741	-1.1508812	-0.4085367
H	-0.5864613	0.5528963	2.3270974
H	-1.0351694	2.2954883	1.8896778

=====

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XyNacnacRh_TS_21_33a.xyz

C	-0.6704854	-1.4414158	-2.1728546	H	-0.6243676	3.1839294	0.8838637
C	-0.1007186	-2.5253986	-1.4982201	H	-1.1270791	2.9220147	2.6252857
C	0.5848450	-2.5223627	-0.2724063	=====			
N	-0.6170059	-0.2092880	-1.6929432	56			
N	0.8180105	-1.4527600	0.4856009	XyNacnacRh_TS_21_33b.xyz			
C	-1.3582235	-1.7020577	-3.4940366	C	-0.2778265	-1.6459447	-2.2823451
H	-1.3191540	-2.7590842	-3.7506951	C	0.7109882	-2.4184302	-1.6612074
H	-0.8875126	-1.1324607	-4.2986171	C	1.3621740	-2.1821312	-0.4411210
H	-2.4051574	-1.3926012	-3.4581571	N	-0.7416396	-0.5271235	-1.7495563
C	1.1011333	-3.8689022	0.2028038	N	1.1377106	-1.1493220	0.3692130
H	0.8587227	-4.6429005	-0.5223706	C	-0.8199556	-2.1247139	-3.6110926
H	0.6657306	-4.1486264	1.1634864	H	-0.3502202	-3.0608739	-3.9071620
H	2.1838083	-3.8502995	0.3402565	H	-0.6446869	-1.3855531	-4.3959678
Rh	0.2759345	0.4243615	0.0193566	H	-1.9000017	-2.2790115	-3.5589768
H	1.4586097	1.0300229	0.8653361	C	2.4098407	-3.2033147	-0.0353394
C	0.3150868	1.4074316	1.8595654	H	2.4954104	-3.9780732	-0.7944692
H	0.1995713	0.7647775	2.7271674	H	2.1594614	-3.6787906	0.9145107
C	-0.4163936	2.6918810	1.8333294	H	3.3883776	-2.7366899	0.0930811
H	-0.1949834	-3.4872390	-1.9798087	Rh	-0.1766345	0.3235513	0.0124319
O	0.9565728	2.6639577	2.2148680	H	0.6492012	1.3246784	0.9144390
C	1.5050104	-1.6149996	1.7329074	C	-0.5372150	1.1752513	1.8788171
C	2.8180345	-1.8795520	4.1725725	H	-0.5318975	0.4609977	2.6984750
C	0.7602729	-1.8963428	2.8926522	C	-0.7203718	2.5974714	2.2305955
C	2.9014671	-1.4565502	1.7862075	H	1.0162377	-3.3096078	-2.1891580
C	3.5385547	-1.5961287	3.0193124	O	-1.7957639	1.8433051	1.6446776
C	1.4389960	-2.0268303	4.1051306	C	1.8554820	-1.0544755	1.6049280
H	4.6148305	-1.4757089	3.0719191	C	3.2074831	-0.8255381	4.0289121
H	0.8739052	-2.2420617	5.0053245	C	1.3251118	-1.6680796	2.7547613
H	3.3298991	-1.9801543	5.1223373	C	3.0550320	-0.3214234	1.6616621
C	-1.1707896	0.9190966	-2.3610474	C	3.7165627	-0.2215447	2.8858280
C	-2.2110794	3.2110281	-3.5595349	C	2.0198350	-1.5416097	3.9589347
C	-0.3626808	1.6760254	-3.2363062	H	4.6432038	0.3392590	2.9393522
C	-2.4938209	1.3174683	-2.0735527	H	1.6190599	-2.0114306	4.8504872
C	-2.9943825	2.4651729	-2.6875258	H	3.7342817	-0.7362332	4.9717910
C	-0.9062292	2.8170090	-3.8267372	C	-1.7220587	0.2830476	-2.3942026
H	-4.0105710	2.7773663	-2.4739666	C	-3.6314431	1.9399853	-3.5660044
H	-0.2931831	3.4043087	-4.5011146	C	-1.3099066	1.3113455	-3.2667595
H	-2.6150746	4.1023104	-4.0249925	C	-3.0860620	0.0959102	-2.0909627
C	-3.3563824	0.5228405	-1.1266541	C	-4.0244902	0.9334536	-2.6931911
H	-4.3096771	1.0264125	-0.9623296	C	-2.2834239	2.1258258	-3.8448176
H	-3.5684414	-0.4778219	-1.5130775	H	-5.0758782	0.7960041	-2.4666604
H	-2.8649237	0.3845202	-0.1609574	H	-1.9760173	2.9187515	-4.5176264
C	1.0553001	1.2640302	-3.5393424	H	-4.3741544	2.5844041	-4.0215695
H	1.5487608	2.0157193	-4.1563092	C	-3.5291785	-0.9783012	-1.1312308
H	1.0937665	0.3120080	-4.0761757	H	-4.6140458	-0.9682169	-1.0204292
H	1.6341277	1.1290650	-2.6231005	H	-3.0822512	-0.8342391	-0.1443882
C	3.6992201	-1.1379270	0.5495844	H	-3.2317523	-1.9749643	-1.4671290
H	3.5743847	-1.8992133	-0.2248296	C	0.1489196	1.5329408	-3.5744484
H	4.7613139	-1.0661847	0.7861313	H	0.7352218	1.6303415	-2.6581189
H	3.3754214	-0.1921452	0.1075006	H	0.2814307	2.4351870	-4.1726301
C	-0.7373222	-2.0584434	2.8385464	H	0.5790655	0.6962282	-4.1321565
H	-1.1530669	-2.1151026	3.8452559	C	3.6184900	0.3453138	0.4347624
H	-1.0300637	-2.9687052	2.3067965	H	3.8551230	-0.3784989	-0.3495961
H	-1.2089696	-1.2271143	2.3099992	H	4.5320534	0.8892707	0.6780213

H	2.8975983	1.0433170	0.0017719	H	3.2546110	-1.4875611	-0.7631608
C	0.0412431	-2.4555987	2.6971755	H	4.3498413	-0.6211684	0.3195933
H	0.1669214	-3.3966006	2.1534094	C	-3.7905309	0.6643320	-1.4899708
H	-0.7438733	-1.9025121	2.1777046	H	-3.2929750	0.4885143	-0.5333884
H	-0.3053764	-2.6990059	3.7022805	H	-3.9438768	-0.3176598	-1.9456576
H	-0.3022155	3.3719820	1.5936878	H	-4.7709998	1.1001635	-1.2952569
H	-0.8845700	2.8815822	3.2668018	C	0.5607173	1.7997712	-3.8576292
=====				H	1.1459818	1.5908594	-2.9596391
56				H	1.0227813	2.6306677	-4.3919973
XyNacnacRh_TS_21_33c.xyz				H	0.6346053	0.9119717	-4.4921837
C	-1.0270102	-1.0821373	-2.7109239	H	1.0950122	0.9577486	3.0894699
C	-0.4045941	-2.1900511	-2.1278543	H	0.2787279	2.5757144	3.4128204
C	0.2758938	-2.2545421	-0.9016687	=====			
N	-1.0268864	0.1065832	-2.1303946	56			
N	0.4444703	-1.2428734	-0.0514400	XyNacnacRh_TS_21_33d.xyz			
C	-1.7089278	-1.2639970	-4.0482197	C	-0.2776043	-0.8094612	-2.6279311
H	-1.6132745	-2.2909185	-4.3962774	C	0.5373635	-1.8143310	-2.0963630
H	-1.2780026	-0.6008041	-4.8016815	C	1.3279881	-1.7660372	-0.9383538
H	-2.7713420	-1.0188580	-3.9813494	N	-0.3841246	0.3799796	-2.0592664
C	0.8669855	-3.6059739	-0.5412377	N	1.4383258	-0.7252201	-0.1124432
H	0.6766015	-4.3244088	-1.3358782	C	-1.0430302	-1.1068643	-3.8978602
H	0.4409311	-3.9951818	0.3847623	H	-0.8464332	-2.1210460	-4.2410934
H	1.9456286	-3.5370231	-0.3886102	H	-0.7668221	-0.4115505	-4.6938792
Rh	-0.1846380	0.6364933	-0.3617414	H	-2.1185673	-0.9966485	-3.7412107
H	0.9335658	1.2381815	0.5944830	C	2.1277646	-3.0196084	-0.6296365
C	-0.2371495	1.6486926	1.4554909	H	1.9725741	-3.7658320	-1.4061782
H	-0.4493804	-3.1113041	-2.6892678	H	1.8413860	-3.4556517	0.3288308
H	-0.6538171	2.6044678	1.1010098	H	3.1952697	-2.7993043	-0.5694298
C	0.3142254	1.6637094	2.8214440	Rh	0.5467147	1.0527247	-0.3773605
O	-0.9643167	1.0727616	2.5456259	H	1.6733690	1.8319924	0.4036225
C	1.1344565	-1.4749683	1.1826882	C	0.5068963	2.1733145	1.3519562
C	2.4640098	-1.9091022	3.5889921	H	0.5667868	-2.7431526	-2.6464376
C	0.4079041	-1.9229380	2.3015369	O	1.3805659	2.7127472	2.3664839
C	2.5206102	-1.2424039	1.2587807	C	0.3257878	1.8298358	2.7685618
C	3.1665382	-1.4648537	2.4754325	H	-0.1492997	2.9622534	0.9399004
C	1.0969026	-2.1354646	3.4968177	C	2.2396701	-0.8576797	1.0676223
H	4.2344957	-1.2897950	2.5447403	C	3.7767220	-1.1287446	3.3729414
H	0.5469151	-2.4791568	4.3656858	C	1.6590439	-1.4045792	2.2273763
H	2.9812740	-2.0778369	4.5263166	C	3.5825250	-0.4396918	1.0557782
C	-1.6365499	1.2595285	-2.7003418	C	4.3332735	-0.5848933	2.2228382
C	-2.7905539	3.5898750	-3.7039236	C	2.4483731	-1.5344897	3.3707002
C	-2.9744227	1.5708413	-2.3753736	H	5.3690583	-0.2641587	2.2248328
C	-0.8713387	2.1213218	-3.5149241	H	2.0103708	-1.9553411	4.2692907
C	-1.4710158	3.2801616	-4.0078848	H	4.3754716	-1.2321118	4.2703111
C	-3.5317114	2.7400564	-2.8922803	C	-1.1773534	1.4320607	-2.6002166
H	-0.8911232	3.9477964	-4.6353546	C	-2.6911300	3.5691234	-3.5548898
H	-4.5592749	2.9864733	-2.6492991	C	-2.5133551	1.5857484	-2.1732253
H	-3.2390439	4.4960890	-4.0937358	C	-0.5935334	2.3549660	-3.4938948
C	-1.0743241	-2.1766191	2.2226833	C	-1.3714635	3.4147354	-3.9603407
H	-1.3129582	-2.9871921	1.5284105	C	-3.2529205	2.6601896	-2.6668855
H	-1.5993688	-1.2852561	1.8795022	H	-0.9315249	4.1288379	-4.6476890
H	-1.4659113	-2.4492912	3.2032072	H	-4.2810625	2.7852453	-2.3454029
C	3.3006633	-0.7696664	0.0604475	H	-3.2792928	4.4005718	-3.9254677
H	2.8974073	0.1692614	-0.3273121	C	0.2174341	-1.8446878	2.2437700

H	-0.0994175	-2.0829408	3.2601902	C	-1.3719878	3.0840516	-3.7700943
H	0.0538960	-2.7349510	1.6294408	H	-4.4160596	2.8367669	-2.3057747
H	-0.4373326	-1.0675636	1.8435994	H	-0.8067589	3.7384713	-4.4245004
C	4.2083318	0.1473038	-0.1812120	H	-3.1283406	4.3195392	-3.8081662
H	4.1449007	-0.5350093	-1.0329066	C	-0.9806462	-2.3597452	2.3826256
H	5.2601568	0.3770833	-0.0069859	H	-1.4677565	-2.3453140	3.3590857
H	3.6966653	1.0648399	-0.4829575	H	-1.1420658	-3.3534353	1.9525635
C	-3.1364103	0.6137908	-1.2040216	H	-1.4849466	-1.6545711	1.7193325
H	-2.5507119	0.5382335	-0.2845569	C	3.4295364	-0.8631842	0.3599610
H	-3.1920282	-0.3960584	-1.6192986	H	4.4726229	-0.7169041	0.6443009
H	-4.1489395	0.9261398	-0.9455004	H	3.0328468	0.0799525	-0.0241244
C	0.8368887	2.2037088	-3.9440464	H	3.3974921	-1.5759294	-0.4678289
H	1.5131726	2.1141051	-3.0909315	C	0.6469937	1.5810749	-3.6774926
H	1.1426111	3.0613270	-4.5444746	H	0.6843710	0.6952544	-4.3182270
H	0.9777488	1.3038056	-4.5495571	H	1.2566645	1.3570677	-2.7991177
H	0.6527083	0.8619000	3.1300538	H	1.1044575	2.4075304	-4.2230708
H	-0.4788023	2.2965445	3.3344803	C	-3.6313677	0.5111258	-1.1585382
=====				H	-3.0554772	0.2519841	-0.2673434
56	XyNacnacRh_TS_21_35.xyz			H	-4.5603789	0.9959954	-0.8548919
C	-0.9363377	-1.2665228	-2.4438492	H	-3.8915993	-0.4327547	-1.6466219
C	-0.3114293	-2.3903415	-1.8798024	H	1.3276095	1.0735811	3.2714487
C	0.4000932	-2.4607023	-0.6755117	H	0.9943304	2.8444102	3.0122361
N	-0.8955805	-0.0752624	-1.8735966	=====			
N	0.6038434	-1.4297306	0.1438856	56	XyNacnacRh_TS_26_30.xyz		
C	-1.6702917	-1.4415073	-3.7557551	C	-0.9069335	-1.3786991	-1.8467084
H	-1.6105131	-2.4746756	-4.0939559	H	-0.4702320	-3.4217097	-1.5487245
H	-1.2497852	-0.8002775	-4.5341100	C	-0.2507198	-2.4287410	-1.1857031
H	-2.7249061	-1.1725610	-3.6588786	C	0.6525963	-2.3608632	-0.1204605
C	0.9878353	-3.8096138	-0.3057517	N	-0.7107793	-0.1027415	-1.5508562
H	0.7889482	-4.5365598	-1.0910955	N	1.0772557	-1.2328103	0.4522132
H	0.5696039	-4.1917720	0.6275146	C	-1.8525161	-1.7514938	-2.9698564
H	2.0688657	-3.7424249	-0.1641030	H	-1.8433331	-2.8267971	-3.1375112
Rh	0.0386500	0.4478443	-0.2063711	H	-1.5723607	-1.2521730	-3.8998012
C	-0.4517664	1.4797202	2.0697145	H	-2.8765548	-1.4482990	-2.7438046
H	-0.8546286	0.4885815	2.2082550	C	1.2114236	-3.6776879	0.3820024
H	-0.3864669	-3.3097861	-2.4418868	H	0.8510403	-4.5002207	-0.2326134
O	1.0612326	1.6837015	1.2622143	H	0.9242068	-3.8677818	1.4170802
H	-1.1294989	2.2695544	1.7815892	H	2.3026139	-3.6708783	0.3535945
C	0.8336195	1.8270672	2.6585670	Rh	0.6293262	0.6035759	-0.1760915
C	1.2461755	-1.6200875	1.4045449	C	-0.3081734	1.7486025	1.2580910
C	2.4824406	-1.9248858	3.8872333	C	0.8501677	2.5835009	0.7989858
C	0.4883553	-2.0445196	2.5141963	H	0.9466903	3.6380741	1.1065143
C	2.6203937	-1.3374744	1.5368496	H	0.6588855	2.7051625	-0.3535252
C	3.2183664	-1.5009017	2.7864207	O	1.9406531	1.7695792	0.9805181
C	1.1266323	-2.1908802	3.7477665	C	1.8835282	-1.2865275	1.6379477
H	4.2771496	-1.2918935	2.8944833	C	3.4286683	-1.3799789	3.9491959
H	0.5491037	-2.5188082	4.6055919	C	1.2570583	-1.4874751	2.8813175
H	2.9647419	-2.0457249	4.8503562	C	3.2733799	-1.1028162	1.5456407
C	-1.5124152	1.0798099	-2.4342224	C	4.0290590	-1.1649418	2.7159693
C	-2.6766490	3.4121426	-3.4242818	C	2.0509539	-1.5324383	4.0274334
C	-0.7677274	1.9231235	-3.2861981	H	5.1030600	-1.0296411	2.6550585
C	-2.8358847	1.4079373	-2.0710048	H	1.5775802	-1.6853143	4.9911674
C	-3.3990118	2.5779383	-2.5796200	H	4.0320569	-1.4178957	4.8486910

C	-1.4431901	0.9265644	-2.2233011	C	3.3967494	-1.1773079	2.9870005
C	-2.8075541	3.0182199	-3.4618165	C	1.3688672	-2.0735596	3.9105428
C	-0.8448243	1.6039586	-3.3040635	H	4.4341817	-0.8848719	3.1069699
C	-2.7213209	1.2928897	-1.7600859	H	0.8194748	-2.4803858	4.7525630
C	-3.3848466	2.3449777	-2.3939989	H	3.1851187	-1.8137274	5.0282580
C	-1.5473995	2.6441394	-3.9117269	C	-1.5023849	1.0980037	-2.4167704
H	-4.3676520	2.6369058	-2.0400498	C	-2.9184478	3.1503271	-3.6582998
H	-1.0954844	3.1682369	-4.7465047	C	-0.8107694	2.0502631	-3.1868573
H	-3.3365476	3.8331003	-3.9418158	C	-2.8946027	1.1846083	-2.2414588
C	-3.3867674	0.5630612	-0.6202821	C	-3.5859277	2.2161888	-2.8771430
H	-3.8717988	-0.3569309	-0.9625483	C	-1.5397213	3.0667788	-3.8042633
H	-4.1597604	1.1843018	-0.1655235	H	-4.6605644	2.2878629	-2.7499182
H	-2.6706216	0.2751327	0.1483555	H	-1.0145030	3.8040597	-4.4016719
C	0.5264692	1.2242188	-3.8034489	H	-3.4697083	3.9471645	-4.1438984
H	0.5910575	0.1630643	-4.0547516	C	-3.6310241	0.1970761	-1.3737796
H	1.2953830	1.4134675	-3.0488014	H	-4.6980671	0.4230094	-1.3557590
H	0.7819629	1.7999953	-4.6937036	H	-3.2567850	0.2234680	-0.3467049
C	3.9416567	-0.8071313	0.2302352	H	-3.5080894	-0.8313570	-1.7228985
H	5.0251681	-0.8939025	0.3222990	C	0.6872861	1.9891787	-3.3336279
H	3.7057611	0.2142070	-0.0818020	H	1.0138896	1.0777461	-3.8421206
H	3.6104541	-1.4797528	-0.5639742	H	1.1742702	1.9896967	-2.3552988
C	-0.2368438	-1.6592296	2.9944802	H	1.0522326	2.8424064	-3.9069308
H	-0.5569103	-1.5375281	4.0301818	C	-0.7186203	-2.3506526	2.5312925
H	-0.5618886	-2.6520057	2.6672902	H	-1.3210113	-1.5535040	2.0894102
H	-0.7718147	-0.9365840	2.3776397	H	-0.8248516	-3.2151341	1.8694802
H	-1.3205656	2.0273802	0.9736581	H	-1.1447780	-2.6180447	3.4992038
H	-0.2007449	1.3405397	2.2573164	C	3.5659103	-0.4474623	0.5844214
=====				H	4.5812611	-0.1942140	0.8924034
56	XyNacnacRh_TS_30_31.xyz			H	3.0849641	0.4513122	0.1907168
C	-0.5402021	-1.0902837	-2.3815034	H	3.6317902	-1.1494214	-0.2509855
C	0.1919518	-2.1417063	-1.8187704	H	-0.7257767	0.8280796	2.4547903
C	0.8052483	-2.2007325	-0.5594310	H	0.7557200	1.7532963	2.8388598
N	-0.7720323	0.0585535	-1.7561581	=====			
N	0.7817999	-1.2197227	0.3370377	56	XyNacnacRh_TS_30_32.xyz		
C	-1.0854676	-1.3019915	-3.7790105	C	-0.1480569	-1.3391925	-2.1758941
H	-0.8273315	-2.2936963	-4.1459403	C	0.4592859	-2.4138077	-1.5252126
H	-0.6864102	-0.5602036	-4.4739949	C	0.9653701	-2.4693391	-0.2163537
H	-2.1720884	-1.1962704	-3.7975771	N	-0.3645526	-0.1401393	-1.6269496
C	1.5364383	-3.4871967	-0.2242803	N	0.9169191	-1.4519588	0.6276462
H	1.4565330	-4.1941580	-1.0477072	C	-0.5859037	-1.5758952	-3.6085892
H	1.1280488	-3.9561249	0.6730164	H	-0.3604502	-2.5969686	-3.9098905
H	2.5950561	-3.3038103	-0.0297476	H	-0.0817821	-0.8933957	-4.2957140
Rh	-0.1257046	0.5660109	0.1119943	H	-1.6578556	-1.4079989	-3.7295031
H	1.0233552	1.3141950	0.8888826	C	1.5838211	-3.7806295	0.2247583
C	-0.0053023	1.5635708	2.0863822	H	1.5226338	-4.5195200	-0.5721184
H	0.3007299	-3.0223836	-2.4341721	H	1.0762574	-4.1778142	1.1061762
C	-0.6825940	2.7299757	1.5238088	H	2.6331189	-3.6521881	0.4975557
H	-0.7629834	3.7085807	2.0197061	Rh	0.1097139	0.3896792	0.2571658
O	-1.1240981	2.5857179	0.3778368	H	1.2765578	1.3032702	0.9280211
C	1.4432290	-1.4059253	1.5953644	H	0.5579061	-3.3190522	-2.1055550
C	2.6970291	-1.6995088	4.0674422	O	0.5729129	1.5816609	2.0556644
C	0.7220262	-1.9341901	2.6814589	C	-0.5472265	2.0587879	1.4942984
C	2.7885293	-1.0205188	1.7406848	H	-1.4532358	1.9265259	2.0806368

C	-0.5200540	2.6374829	0.2393691	H	0.7626620	2.0149566	2.0443259
C	1.4753298	-1.5882544	1.9412743	C	-0.6036383	2.3730896	2.1804737
C	2.5304535	-1.8023698	4.5095774	H	0.2285520	-2.4088956	-1.6638089
C	2.8303291	-1.2830667	2.1604873	O	-0.9369928	3.3408543	1.4964509
C	0.6413055	-1.9829310	3.0025995	C	-1.0551721	2.1356787	3.5923642
C	1.1909939	-2.0885930	4.2799477	H	-0.6343074	1.2202777	3.9999989
C	3.3386597	-1.3998381	3.4547783	C	-1.3932367	1.7989748	-1.7693436
H	0.5551302	-2.3939267	5.1036758	C	-2.7804005	3.8914288	-2.9724651
H	4.3826800	-1.1669931	3.6334511	C	-0.6955149	2.7237756	-2.5686781
H	2.9413407	-1.8857157	5.5089771	C	-2.7774045	1.9295312	-1.5506110
C	-0.9801933	0.8837033	-2.4199862	C	-3.4532224	2.9826249	-2.1665240
C	-2.1804896	2.8976204	-3.9244654	C	-1.4113262	3.7606155	-3.1664084
C	-0.1775271	1.7493121	-3.1835331	H	-4.5195430	3.0922869	-2.0029414
C	-2.3790545	1.0267798	-2.3955886	H	-0.8832849	4.4772558	-3.7855476
C	-2.9605120	2.0402096	-3.1584558	H	-3.3199608	4.7064081	-3.4404838
C	-0.7992224	2.7501008	-3.9314834	C	1.5992928	-0.6304985	2.2277040
H	-4.0387828	2.1564169	-3.1473570	C	2.9097605	-0.8619443	4.6743630
H	-0.1878917	3.4224865	-4.5234155	C	2.9340449	-0.2011607	2.3411699
H	-2.6474265	3.6800785	-4.5111243	C	0.9153455	-1.1727507	3.3317149
C	-3.2379560	0.1223499	-1.5502288	C	1.5910554	-1.2789810	4.5485045
H	-3.1244166	-0.9292561	-1.8251601	C	3.5716389	-0.3286990	3.5753011
H	-2.9651264	0.1946118	-0.4935435	H	1.0718820	-1.6940455	5.4056169
H	-4.2913663	0.3862731	-1.6525911	H	4.6008478	-0.0013781	3.6724859
C	1.3227748	1.6168321	-3.1843699	H	3.4201759	-0.9510989	5.6261178
H	1.7201031	1.6673910	-2.1676201	C	-3.5215000	0.9604679	-0.6686195
H	1.7790360	2.4092978	-3.7789920	H	-4.5509674	1.2891401	-0.5220318
H	1.6500477	0.6577726	-3.5950186	H	-3.0426407	0.8696161	0.3085266
C	-0.8187184	-2.2793856	2.7766437	H	-3.5499201	-0.0452995	-1.0977970
H	-1.3332277	-1.4149828	2.3491114	C	0.7934130	2.6111021	-2.7731502
H	-1.3067603	-2.5418541	3.7161329	H	1.1527457	3.4136792	-3.4182231
H	-0.9672606	-3.1061782	2.0769058	H	1.0745960	1.6586410	-3.2299394
C	3.7251582	-0.8356253	1.0333420	H	1.3273474	2.6711464	-1.8212016
H	4.7180261	-0.5855515	1.4090698	C	3.6611372	0.3962456	1.1657868
H	3.8408733	-1.6088315	0.2687251	H	4.6906230	0.6378149	1.4326103
H	3.3169011	0.0408858	0.5244152	H	3.1662900	1.3096733	0.8246682
H	0.3774856	3.1105664	-0.1358170	H	3.6815746	-0.2828464	0.3098931
H	-1.4532573	2.9305264	-0.2220268	C	-0.5136345	-1.6390833	3.2146814
=====				H	-0.5886239	-2.5842511	2.6685970
56	XyNacnacRh_TS_31_36.xyz			H	-1.1262581	-0.9184100	2.6703656
C	-0.5348536	-0.4435270	-1.6856535	H	-0.9482883	-1.7978192	4.2026636
C	0.1752624	-1.4943492	-1.0921890	H	-2.1458798	2.0866894	3.6070336
C	0.8520268	-1.5044798	0.1345007	H	-0.7480560	2.9848240	4.2097611
N	-0.6748455	0.7470407	-1.1191950	=====			
N	0.9083347	-0.4786538	0.9816532	56	XyNacnacRh_TS_33_30.xyz		
C	-1.1406572	-0.6945259	-3.0500892	C	-0.5397424	-1.7516992	-2.0035163
H	-0.9388798	-1.7120856	-3.3793888	H	0.5664266	-3.5346187	-1.8078151
H	-0.7348626	-0.0027872	-3.7914605	C	0.3691620	-2.5860451	-1.3306091
H	-2.2215520	-0.5417451	-3.0356890	C	1.0497264	-2.3709191	-0.1246553
C	1.5936692	-2.7811537	0.4843501	N	-0.9019691	-0.5539893	-1.5690580
H	1.4728576	-3.5178101	-0.3072517	N	0.9251927	-1.2835886	0.6329072
H	1.2329529	-3.2161561	1.4175672	C	-1.1328611	-2.2914080	-3.2909656
H	2.6605281	-2.5894474	0.6171938	H	-0.7610838	-3.2935567	-3.4961043
Rh	0.0643611	1.3260289	0.6810617	H	-0.8876262	-1.6501185	-4.1397442

H	-2.2226657	-2.3297431	-3.2320552	N	-0.7252609	0.2040535	-1.7380118
C	1.9730062	-3.4835483	0.3361630	N	0.1376633	-1.3882647	0.6255915
H	1.9443175	-4.3172278	-0.3626646	C	-1.6447869	-1.1985629	-3.5334681
H	1.6888285	-3.8502446	1.3245193	H	-1.8569049	-2.2480480	-3.7265396
H	3.0048270	-3.1354597	0.4157727	H	-0.9581638	-0.8367358	-4.3010557
Rh	-0.2792873	0.3092141	0.2292884	H	-2.5692258	-0.6303714	-3.6477330
H	0.9121891	1.0937574	-0.2720324	C	-0.1862606	-3.8122687	0.3443615
C	-0.5878886	1.6542510	1.7806582	H	-0.6178020	-4.5001785	-0.3800013
H	-1.0360808	1.3281018	2.7185266	H	-0.6907135	-3.9540780	1.3015619
C	-0.0651963	2.9578683	1.6609710	H	0.8598519	-4.0855693	0.4982295
O	-1.4691977	1.9846495	0.7193715	H	0.2828428	2.1259299	-0.5023512
C	1.6883287	-1.1687667	1.8398362	Rh	0.0357462	0.6989258	0.0996898
C	3.1256530	-0.8899738	4.2146413	C	-0.7459405	1.7695913	1.3284166
C	1.1136351	-1.5846837	3.0552575	O	-1.4992663	2.4228513	1.9263522
C	2.9795243	-0.6115042	1.8091583	C	1.0162643	1.5020419	2.0301428
C	3.6803765	-0.4811485	3.0092327	H	1.8925663	1.0185367	1.6028575
C	1.8495422	-1.4389792	4.2309451	C	0.7251476	-1.7043453	1.8907234
H	4.6771841	-0.0539417	2.9921533	C	1.8900427	-2.2192235	4.3733520
H	1.4129145	-1.7616042	5.1698669	C	2.1168736	-1.8900185	1.9820564
H	3.6855927	-0.7842113	5.1364294	C	-0.0849365	-1.7635777	3.0401534
C	-1.7882078	0.2546318	-2.3477200	C	0.5186434	-2.0252619	4.2714402
C	-3.5051903	1.8854278	-3.8202952	C	2.6791443	-2.1495174	3.2327344
C	-1.2628086	1.0941969	-3.3474014	H	-0.1005672	-2.0754908	5.1603266
C	-3.1657124	0.2479848	-2.0656269	H	3.7509682	-2.2965553	3.3084757
C	-4.0081178	1.0662538	-2.8182469	H	2.3418415	-2.4203479	5.3374381
C	-2.1400300	1.8985568	-4.0750803	C	-0.9662553	1.3050741	-2.6342412
H	-5.0721003	1.0618315	-2.6082315	C	-1.4152940	3.4575998	-4.3423707
H	-1.7417323	2.5464832	-4.8483560	C	0.0585755	1.7295302	-3.4962945
H	-4.1730298	2.5162576	-4.3951079	C	-2.2105298	1.9573093	-2.6105615
C	-3.7288074	-0.5985415	-0.9534361	C	-2.4142989	3.0327081	-3.4763928
H	-3.3986634	-1.6377325	-1.0139530	C	-0.1879106	2.8078402	-4.3466497
H	-4.8193438	-0.5844704	-0.9745991	H	-3.3710627	3.5430837	-3.4644810
H	-3.4107065	-0.2179929	0.0225452	H	0.5974431	3.1415864	-5.0159317
C	0.2179511	1.1465640	-3.6202124	H	-1.5910480	4.2944004	-5.0080632
H	0.6125982	0.1834454	-3.9547149	C	2.9945316	-1.8107696	0.7585954
H	0.4395682	1.8852079	-4.3915867	H	2.7331181	-2.5688212	0.0156946
H	0.7724776	1.4105112	-2.7166425	H	4.0418715	-1.9519418	1.0277981
C	3.5982161	-0.1369509	0.5209638	H	2.8996588	-0.8443966	0.2558545
H	4.6381459	0.1523301	0.6779849	C	-1.5760157	-1.5576735	2.9565837
H	3.0581983	0.7272382	0.1236987	H	-2.0245804	-1.5989784	3.9497702
H	3.5700040	-0.8997616	-0.2596546	H	-2.0594931	-2.3190225	2.3385170
C	-0.2751876	-2.1688273	3.0996090	H	-1.8273580	-0.5941522	2.5082390
H	-0.3755281	-3.0448682	2.4544747	C	1.4091662	1.0623219	-3.4887911
H	-0.5342492	-2.4665052	4.1164729	H	1.3418813	-0.0142854	-3.6621515
H	-1.0209110	-1.4454918	2.7580251	H	1.9030965	1.1932919	-2.5213418
H	0.4223388	3.2442316	0.7420094	H	2.0531387	1.4897569	-4.2582573
H	-0.1820441	3.7292219	2.4236577	C	-3.2999247	1.5320353	-1.6607207
=====				H	-3.5714853	0.4809546	-1.7857705
56				H	-4.1973536	2.1323053	-1.8143937
XyNacnacRh_TS_36_37a.xyz				H	-2.9844624	1.6507923	-0.6215982
C	-1.0544702	-1.0239275	-2.1462290	H	1.2101738	2.5644200	2.1364281
H	-1.2026008	-3.1012948	-1.8970331	H	0.7519559	1.0310279	2.9715386
C	-0.8806443	-2.1961970	-1.4042980	=====			
C	-0.3071184	-2.3782646	-0.1361974	56			

XyNacnacRh_TS_36_37b.xyz				H	2.9962315	-2.2206903	-0.2573277
C	-0.9559423	-0.9189751	-2.2382242	H	0.6456617	0.8098525	3.0650602
H	-0.8692708	-3.0143213	-2.1960981	H	0.9232029	2.4599461	2.3877858
C	-0.6448648	-2.1318611	-1.6159647	=====			
C	-0.0394126	-2.3725004	-0.3727434	56			
N	-0.7620693	0.2917562	-1.7096367	XyNacnacRh_TS_37_38.xyz			
N	0.3001423	-1.4188699	0.4838048	C	-0.1306204	-1.1482819	-2.1925040
C	-1.5365930	-1.0207199	-3.6367331	C	0.5654583	-2.0850670	-1.4214505
H	-1.6308519	-2.0630624	-3.9339560	C	1.1749260	-1.9373448	-0.1690785
H	-0.9028145	-0.5090758	-4.3634645	N	-0.3073931	0.1249025	-1.8537807
H	-2.5203247	-0.5522675	-3.6949338	N	1.1883705	-0.8185112	0.5527722
C	0.2483593	-3.8241004	-0.0379881	C	-0.7064983	-1.6595995	-3.5002663
H	-0.1116673	-4.4812094	-0.8271274	H	-0.4835170	-2.7167671	-3.6286842
H	-0.2252415	-4.1165007	0.9006796	H	-0.3006517	-1.1134445	-4.3535730
H	1.3203850	-3.9908305	0.0870323	H	-1.7897628	-1.5280121	-3.5311458
H	0.0322604	2.1829998	-0.2854302	C	1.8634884	-3.1793120	0.3701373
Rh	-0.0461090	0.6845945	0.1704079	H	1.7832277	-3.9985544	-0.3411671
C	-0.9358003	1.5332667	1.4950032	H	1.4263906	-3.5006116	1.3167299
O	-1.7540721	2.0349585	2.1511102	H	2.9212478	-2.9905090	0.5618690
C	0.8499456	1.3980924	2.1761325	Rh	0.4017429	1.0361439	-0.0776604
H	1.7729711	1.0608477	1.7085173	H	1.5287659	1.7775884	0.6851957
C	0.9394285	-1.7900696	1.7082170	C	0.4143006	1.8575733	1.9365682
C	2.1954064	-2.4134189	4.1206133	H	1.1908850	1.5097382	2.6116178
C	0.1601124	-2.0558537	2.8495768	H	0.6391557	-3.0715939	-1.8534257
C	2.3445343	-1.8232918	1.7738872	C	-0.1874424	2.7347792	-0.6046390
C	2.9528998	-2.1405344	2.9891158	O	-0.4896543	3.8094662	-0.8515851
C	0.8094256	-2.3682405	4.0452953	C	-1.0264766	0.9681816	-2.7683826
H	4.0355704	-2.1710020	3.0444591	C	-2.4103145	2.6594415	-4.4976617
H	0.2144154	-2.5772916	4.9275321	C	-2.4156039	1.1268290	-2.6192258
H	2.6827024	-2.6568497	5.0572601	C	-0.3236328	1.6621460	-3.7697561
C	-1.1314977	1.4422910	-2.4928486	C	-1.0365593	2.5021300	-4.6261291
C	-1.8310675	3.6900089	-3.9797721	C	-3.0897233	1.9762091	-3.4976557
C	-2.4400148	1.9470025	-2.4069991	H	-0.5015829	3.0427957	-5.3991760
C	-0.1676091	2.0609686	-3.3063170	H	-4.1610358	2.1045197	-3.3884441
C	-0.5394236	3.1840155	-4.0459465	H	-2.9482648	3.3177039	-5.1695363
C	-2.7691873	3.0734705	-3.1623055	C	1.8317909	-0.8795486	1.8355562
H	0.1982422	3.6672913	-4.6771222	C	3.0534250	-0.9354446	4.3416639
H	-3.7763523	3.4709416	-3.1017499	C	3.1867009	-0.5222682	1.9550697
H	-2.1041461	4.5638740	-4.5594640	C	1.0857923	-1.2632683	2.9639792
C	1.2486197	1.5505187	-3.3618800	C	1.7166453	-1.2860483	4.2090694
H	1.7337867	1.6402369	-2.3852286	C	3.7783554	-0.5571064	3.2189019
H	1.8342988	2.1203635	-4.0842172	H	1.1457078	-1.5774501	5.0838853
H	1.2996862	0.4952435	-3.6405284	H	4.8230166	-0.2835370	3.3185872
C	-3.4669833	1.3123731	-1.5056014	H	3.5281004	-0.9549155	5.3155491
H	-3.1583409	1.3658492	-0.4590560	C	-3.1676750	0.4096824	-1.5277601
H	-3.6198636	0.2541885	-1.7318357	H	-3.0917286	-0.6768698	-1.6209908
H	-4.4273500	1.8197592	-1.6032801	H	-4.2249185	0.6763499	-1.5511365
C	-1.3458492	-2.0150782	2.7942972	H	-2.7711125	0.6633372	-0.5409082
H	-1.7704747	-2.1995721	3.7817623	C	3.9968744	-0.1123961	0.7523208
H	-1.7500151	-2.7663009	2.1102138	H	3.5626749	0.7578363	0.2538662
H	-1.7120920	-1.0494241	2.4397976	H	4.0394423	-0.9048322	0.0004015
C	3.1875632	-1.5213630	0.5606775	H	5.0193395	0.1309764	1.0438188
H	4.2484095	-1.5754193	0.8075421	C	1.1699018	1.5208269	-3.9119030
H	2.9811179	-0.5232866	0.1642423	H	1.6808969	1.7555855	-2.9748230

H	1.5460011	2.1877815	-4.6884960
H	1.4629915	0.5007186	-4.1749940
C	-0.3664952	-1.6498375	2.8458703
H	-0.4931200	-2.6027149	2.3233015
H	-0.9343978	-0.9102740	2.2789240
H	-0.8178122	-1.7523695	3.8335590
H	-0.5431358	1.4264832	2.2320482
H	0.3523898	2.9423698	1.9802215

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Cartesian coordinates for hydrogenation.

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COA.xyz

C	-0.5831753	0.0626998	-0.0121300
C	-0.8562879	-0.3017023	1.4628021
H	-0.0864074	0.1441539	2.0975909
C	-0.9349242	-1.8128731	1.7449113
H	-1.7961111	0.1494443	1.7929879
C	0.1206379	-2.7134431	1.0810151
C	1.6042470	-2.3578471	1.2912512
H	2.1699127	-3.2941652	1.2496319
H	1.7569369	-1.9682673	2.3053138
C	2.2618725	-1.4000377	0.2748683
H	3.3426764	-1.5555508	0.3529102
C	2.0063676	0.1089040	0.4463704
H	1.9935187	-1.7130541	-0.7416816
H	-0.6766977	-0.8321641	-0.6324790
C	0.7867691	0.7168028	-0.2671386
H	-1.3536709	0.7467317	-0.3785610
H	0.7328909	1.7717390	0.0257083
H	0.9738969	0.7173306	-1.3468983
H	2.8838866	0.6491960	0.0766045
H	1.9636536	0.3350296	1.5169854
H	-0.8962066	-1.9644721	2.8295246
H	-1.9184469	-2.1791542	1.4284772
H	-0.0472129	-3.7246787	1.4656235
H	-0.0713110	-2.7829932	0.0051757

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22

COE.xyz

C	-0.6228470	0.1078317	-0.0549629
C	-0.8363605	-0.3262423	1.4222626
H	-0.0645313	0.1224426	2.0550087
C	-0.8424124	-1.8249933	1.5842287
H	-1.7873564	0.0685017	1.7854571
C	0.2110498	-2.6416376	1.5544946
H	-1.8230629	-2.2846102	1.6790126
C	1.6733036	-2.2785499	1.4271283
H	0.0068855	-3.7058655	1.6396088
H	2.2413796	-3.2119169	1.4441337
H	1.9963896	-1.7260521	2.3184490
C	2.1205897	-1.4754995	0.1772905
H	3.1785204	-1.7057088	0.0215242
C	1.9846785	0.0588072	0.2798113
H	1.5996979	-1.8519885	-0.7084216
H	-0.7896946	-0.7615690	-0.6950569
C	0.7554528	0.7176866	-0.3675937
H	-1.3853519	0.8382446	-0.3403274
H	0.7551752	1.7711371	-0.0655838
H	0.8834015	0.7214904	-1.4556345
H	2.8653967	0.5189749	-0.1789999
H	2.0364077	0.3413999	1.3361976

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DMBlH.xyz

C	0.3443475	0.6398241	-0.2701141
H	1.3783977	0.6300269	0.1014205
C	-0.3443530	-0.6398340	0.2701069
H	-1.3783990	-0.6300560	-0.1014392
C	0.3989623	0.6715276	-1.8046883
H	0.9871747	-0.1480413	-2.2188961
H	0.8488595	1.6043102	-2.1536116
H	-0.6074615	0.6117746	-2.2319313
C	-0.3241754	1.9244456	0.2413043
H	0.1563113	2.8055572	-0.1910882
H	-0.2666775	2.0220946	1.3259476
H	-1.3813092	1.9535575	-0.0427218
C	0.3241950	-1.9244505	-0.2412932
H	1.3813464	-1.9535131	0.0426856
H	0.2666512	-2.0221440	-1.3259333
H	-0.1562410	-2.8055624	0.1911563
C	-0.3989826	-0.6715191	1.8046813
H	0.6074268	-0.6116317	2.2319371
H	-0.8487695	-1.6043511	2.1536142
H	-0.9873039	0.1479848	2.2188633

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18

DMBn1.xyz

C	0.2427703	0.7218165	-0.4360044
C	0.1086219	0.7306838	-1.7619006
C	0.1971445	-0.5463639	0.4052744
H	1.0259276	-0.4710676	1.1218255
C	0.4582575	2.0041683	0.3291270
H	1.3985488	1.9676643	0.8894611
H	-0.3363639	2.1795566	1.0601188
H	0.4942077	2.8653625	-0.3389222
H	-0.0321941	-0.1732594	-2.3398705
H	0.1372129	1.6587221	-2.3214496
C	0.3946430	-1.8412651	-0.3880792
H	1.3173322	-1.8186615	-0.9711711
H	-0.4359193	-2.0214919	-1.0754053
H	0.4451618	-2.6947323	0.2920165
C	-1.1047804	-0.6208339	1.2284300
H	-1.0959539	-1.4982709	1.8797170
H	-1.9708051	-0.6995109	0.5660866
H	-1.2438115	0.2574834	1.8607462

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18

DMBn2.xyz

C	-0.0000000	-0.0000000	0.6720684
C	-0.0000000	-0.0000000	-0.6720684
C	1.2478773	0.0000000	-1.5241442
H	1.2597601	0.8766529	-2.1813799
H	1.2597601	-0.8766529	-2.1813799
H	2.1757577	0.0000000	-0.9584128
C	1.2478773	0.0000000	1.5241443

H	1.2597601	0.8766529	2.1813799	H	0.7188833	2.2763832	3.8755721
H	2.1757576	0.0000000	0.9584127	C	0.1237232	-1.6092413	2.1271048
H	1.2597601	-0.8766529	2.1813799	C	0.4764229	-2.1475117	4.8358567
C	-1.2478773	0.0000000	1.5241443	C	1.4103589	-1.9005306	2.6117885
H	-1.2597601	0.8766529	2.1813800	C	-0.9863449	-1.5810289	2.9874158
H	-1.2597601	-0.8766529	2.1813800	C	-0.7889308	-1.8580226	4.3406083
H	-2.1757577	0.0000000	0.9584128	C	1.5657555	-2.1638022	3.9740051
C	-1.2478773	0.0000000	-1.5241443	H	-1.6401874	-1.8393854	5.0125085
H	-1.2597601	0.8766529	-2.1813800	H	2.5552576	-2.3872540	4.3582227
H	-2.1757577	0.0000000	-0.9584128	H	0.6134215	-2.3575972	5.8902912
H	-1.2597601	-0.8766529	-2.1813800	C	-0.4821601	0.8245496	-2.9036748
=====				C	-0.6792452	2.8797393	-4.7760733
2				C	-1.7139900	1.4798771	-3.0871610
H2.xyz				C	0.6516848	1.1941378	-3.6508168
H	0.0000000	0.0000000	-0.3721230	C	0.5311219	2.2258199	-4.5830107
H	0.0000000	0.0000000	0.3721230	C	-1.7902046	2.5061975	-4.0305668
=====				H	1.4011807	2.5189240	-5.1605034
67				H	-2.7353217	3.0176643	-4.1773235
XyNacnacIr_1.xyz				H	-0.7554194	3.6803949	-5.5025831
C	-0.5861076	-1.4633362	-2.2798917	C	-2.9282597	1.0899257	-2.2847645
H	-0.7143262	-3.5093201	-1.8050757	H	-3.7580990	1.7684056	-2.4872508
C	-0.5296633	-2.5319719	-1.3851239	H	-2.7112043	1.1046233	-1.2137846
C	-0.3020180	-2.4971609	-0.0073769	H	-3.2597942	0.0742920	-2.5189308
N	-0.3639473	-0.2068290	-1.9104714	C	1.9732798	0.4980211	-3.4508200
N	-0.0674253	-1.3948636	0.7181149	H	2.2238947	0.4254884	-2.3900351
C	-0.9373232	-1.7824038	-3.7183823	H	2.7717950	1.0294560	-3.9708391
H	-1.0615814	-2.8560110	-3.8488346	H	1.9532219	-0.5271078	-3.8328244
H	-0.1633385	-1.4382952	-4.4068785	C	2.5974164	-1.9651620	1.6850744
H	-1.8659884	-1.2910537	-4.0176625	H	2.5734404	-1.1564701	0.9539242
C	-0.3583039	-3.8450663	0.6922823	H	3.5302834	-1.9123089	2.2488765
H	-0.5564904	-4.6307586	-0.0338244	H	2.6103652	-2.9012463	1.1170631
H	-1.1441113	-3.8730075	1.4492217	C	-2.3633282	-1.2691077	2.4626507
H	0.5773530	-4.0786502	1.2022272	H	-2.3528386	-0.3609348	1.8564142
Ir	0.1010776	0.4992666	-0.0042196	H	-3.0698803	-1.1416826	3.2841480
C	1.2386168	1.9911708	0.9663673	H	-2.7412109	-2.0677830	1.8172103
C	0.1395578	1.8348232	1.8593412	=====			
C	0.9510119	2.7456421	-0.3077319	67			
H	1.8028028	2.7907435	-0.9806923	XyNacnacIr_2.xyz			
H	0.0889558	2.2637143	-0.8874615	C	-1.8292300	-0.9161948	-1.7792765
C	-1.0820591	2.7430316	1.8139420	H	-2.4532320	-2.8545126	-1.2687636
H	-1.3313425	3.1148493	0.8223412	C	-1.8064783	-2.0480027	-0.9574280
H	-1.9610948	2.2127952	2.1877595	C	-1.0782180	-2.2875071	0.2137551
H	0.5376461	3.7463350	-0.1502940	N	-1.1074404	0.1810612	-1.5626931
H	-0.9321029	3.6118502	2.4722385	N	-0.2188953	-1.4296383	0.7657273
C	2.6875889	1.8530457	1.3552886	C	-2.7545869	-0.9799020	-2.9801463
H	3.0702746	2.8050914	1.7464490	H	-3.2420798	-1.9514266	-3.0332500
H	3.2987725	1.5806361	0.4920561	H	-2.2114606	-0.8135142	-3.9119153
H	2.8372736	1.1003895	2.1264695	H	-3.5260999	-0.2091670	-2.9263387
C	0.4098267	1.4024880	3.2856205	C	-1.3207511	-3.6339551	0.8729513
H	1.1832673	0.6465856	3.3825881	H	-2.0450750	-4.2107463	0.3014514
H	-0.4918889	1.0085474	3.7538410	H	-1.6997363	-3.5144333	1.8896005
				H	-0.4006208	-4.2156069	0.9496399
				Ir	0.2123920	0.5385798	0.0653358
				H	-0.7658613	1.2921801	0.9759276

C	1.8894995	1.8859165	0.2161065	C	-1.0372320	-1.4648623	-2.0220451
C	1.7029127	1.4118624	1.5611396	H	-1.4911853	-3.4677204	-1.5599779
C	0.8226779	2.5916709	-0.4176716	C	-1.1317466	-2.5413854	-1.1373000
H	0.9501263	2.8569919	-1.4606879	C	-0.8587554	-2.5688806	0.2336384
C	1.0296563	2.2968513	2.6014521	N	-0.5951406	-0.2643316	-1.6579944
H	0.5328043	1.6917754	3.3627882	N	-0.4319868	-1.5277962	0.9556059
H	1.7865120	2.9013225	3.1194463	C	-1.4930939	-1.7042356	-3.4470393
H	0.2156994	3.2970839	0.1348390	H	-1.8132359	-2.7367314	-3.5754576
H	0.2936846	2.9810656	2.1833964	H	-0.6979851	-1.4981283	-4.1656894
C	2.7993544	0.5859624	2.2050940	H	-2.3294011	-1.0509897	-3.7070798
H	3.6155131	1.2364526	2.5485048	C	-1.1094968	-3.8934306	0.9320929
H	3.2306646	-0.1641219	1.5457495	H	-1.4398011	-4.6380842	0.2105738
H	2.4171208	0.0636262	3.0822156	H	-1.8768576	-3.7993256	1.7031143
C	3.1175836	1.5422089	-0.5961304	H	-0.2116979	-4.2684519	1.4255104
H	3.9265078	2.2312221	-0.3274998	Ir	-0.0139715	0.3293706	0.2566830
H	2.9274722	1.6607868	-1.6636383	C	1.2998379	1.5560877	1.3770023
H	3.4874271	0.5322706	-0.4180216	C	0.1540567	1.3485043	2.1837576
C	0.4289615	-1.8541136	1.9741770	C	1.1209622	2.5328601	0.2212647
C	1.6880033	-2.7202739	4.3089553	H	0.2573975	2.1168060	-0.4391190
C	1.6352876	-2.5716229	1.8902969	C	2.6792274	1.1581708	1.8311216
C	-0.1499462	-1.5658693	3.2231445	H	3.1926429	2.0139254	2.2879416
C	0.4988777	-2.0051504	4.3783849	H	3.3058388	0.7936094	1.0162393
C	2.2473272	-2.9992186	3.0691479	H	2.6119124	0.3777876	2.5888328
H	0.0569143	-1.7873681	5.3446389	H	0.2687236	0.7441735	3.0744226
H	3.1769044	-3.5548905	3.0091865	H	-0.6382598	2.0851304	2.2522408
H	2.1756801	-3.0570396	5.2161390	C	2.3348508	2.6757735	-0.6979249
C	-1.2668996	1.2746218	-2.4799990	H	3.1338677	3.2143294	-0.1810616
C	-1.5316595	3.4155319	-4.2492113	H	2.0724837	3.2448508	-1.5913210
C	-2.2395142	2.2600299	-2.2366380	H	2.7223821	1.7096967	-1.0153280
C	-0.4258911	1.3570027	-3.6039134	C	0.5793135	3.9191559	0.6156125
C	-0.5747872	2.4352297	-4.4773093	H	1.3214516	4.4380749	1.2285492
C	-2.3545220	3.3223348	-3.1344736	H	-0.3454763	3.8559709	1.1863531
H	0.0711538	2.5031711	-5.3459808	H	0.3907801	4.5238190	-0.2742968
H	-3.1028603	4.0858389	-2.9518685	C	-0.2256456	-1.7487314	2.3628326
H	-1.6353081	4.2473725	-4.9359199	C	0.1862163	-2.1557343	5.0859708
C	0.6245984	0.3090688	-3.8686762	C	1.0241639	-2.2084169	2.8108889
H	1.3178443	0.2182634	-3.0282665	C	-1.2723872	-1.4940119	3.2653477
H	1.2013535	0.5600382	-4.7598348	C	-1.0456623	-1.7065048	4.6254470
H	0.1897117	-0.6826958	-4.0183754	C	1.2106451	-2.4021723	4.1814599
C	-3.1359917	2.1923809	-1.0281371	H	-1.8460812	-1.5094438	5.3302427
H	-2.5548923	2.2688713	-0.1059890	H	2.1735782	-2.7519800	4.5378246
H	-3.6811705	1.2473475	-0.9703271	H	0.3471332	-2.3110485	6.1465457
H	-3.8645657	3.0036896	-1.0450467	C	-0.5432142	0.7750367	-2.6468180
C	2.2649195	-2.8818725	0.5564378	C	-0.3953062	2.8424084	-4.5125202
H	2.4254186	-1.9732001	-0.0292610	C	-1.6248251	1.6663320	-2.7833574
H	1.6362234	-3.5341457	-0.0556296	C	0.6091899	0.9119225	-3.4431779
H	3.2277451	-3.3763092	0.6917665	C	0.6624622	1.9537426	-4.3710113
C	-1.4543160	-0.8189161	3.3257351	C	-1.5286640	2.6945753	-3.7221335
H	-1.7396817	-0.6861193	4.3700210	H	1.5492933	2.0674997	-4.9852561
H	-2.2668916	-1.3461522	2.8188167	H	-2.3569269	3.3861319	-3.8322078
H	-1.3858705	0.1640024	2.8563493	H	-0.3370653	3.6479953	-5.2353589
=====				C	-2.8665044	1.5170177	-1.9426673
67	XyNacnacIr_3.xyz			H	-2.6193896	1.4827863	-0.8787015
				H	-3.3959199	0.5866151	-2.1668805

H	-3.5540694	2.3451121	-2.1208887	C	-0.7858033	2.3763938	-4.1928861
C	1.7650430	-0.0468056	-3.3117386	H	-3.0108843	4.2884291	-2.5111657
H	2.6613538	0.3632324	-3.7797334	H	-0.1964819	2.3741406	-5.1036597
H	1.5511217	-1.0048923	-3.7960541	H	-1.6538510	4.3037114	-4.5789651
H	1.9781814	-0.2685104	-2.2648663	C	0.2371040	-1.9353457	2.2111620
C	2.1388865	-2.5113607	1.8423693	C	1.6307102	-2.7472702	4.4872251
H	2.2094970	-1.7460750	1.0685014	C	1.4640561	-2.6078858	2.0728557
H	3.0947907	-2.5808318	2.3640174	C	-0.2937102	-1.6623079	3.4839441
H	1.9753538	-3.4646168	1.3293138	C	0.4199856	-2.0777152	4.6090649
C	-2.6047109	-0.9852943	2.7825596	C	2.1451362	-3.0072966	3.2237549
H	-2.4807818	-0.0697743	2.1992633	H	0.0159236	-1.8698984	5.5938672
H	-3.2677559	-0.7824602	3.6247177	H	3.0913659	-3.5277167	3.1225845
H	-3.1024056	-1.7054859	2.1271467	H	2.1710204	-3.0628751	5.3719413
=====				C	-3.1397153	2.4044015	-0.5916325
67	XyNacnacIr_4.xyz			H	-3.8477275	3.2335632	-0.6202320
C	-2.1499451	-0.8606760	-1.4182801	H	-2.5098440	2.5233193	0.2933863
H	-2.8368565	-2.7833779	-0.9213270	H	-3.7012715	1.4791492	-0.4481502
C	-2.1384058	-2.0151376	-0.6247077	C	2.0479488	-2.8902394	0.7122123
C	-1.3591608	-2.3202680	0.4975068	H	1.3933965	-3.5197435	0.1038062
N	-1.3530747	0.1898631	-1.2309223	H	3.0098907	-3.3961522	0.8044915
N	-0.4593326	-1.4969917	1.0337361	H	2.2028357	-1.9676208	0.1460780
C	-3.1599864	-0.8408206	-2.5505587	C	-1.5952712	-0.9213561	3.6445803
H	-3.7237473	-1.7713425	-2.5734635	H	-1.5251479	0.0851810	3.2250384
H	-2.6776393	-0.7055582	-3.5195791	H	-1.8622963	-0.8386030	4.6989268
H	-3.8639059	-0.0141284	-2.4328295	H	-2.4192462	-1.4159001	3.1241615
C	-1.5884649	-3.6836335	1.1221806	C	0.1516511	0.0981433	-3.7076549
H	-2.3320742	-4.2417020	0.5565399	H	0.9170806	0.3906458	-4.4278707
H	-1.9342320	-3.5944378	2.1539218	H	-0.4412174	-0.6990511	-4.1684693
H	-0.6666488	-4.2676538	1.1511810	H	0.6398293	-0.3420428	-2.8386516
Ir	0.0129945	0.4534663	0.3692048	=====			
H	-0.9309372	1.2672761	1.2649280	69	XyNacnacIr_6.xyz		
C	1.7832954	1.6744498	0.6600759	C	-0.6842926	-1.7553454	-2.1358633
C	1.4269516	1.1179374	1.9252289	H	-1.1291370	-3.7188760	-1.5677285
C	0.8046103	2.4880634	0.0102116	C	-0.8543430	-2.7527344	-1.1724326
H	0.9894729	2.8161918	-1.0051530	C	-0.7750961	-2.6907924	0.2277148
H	2.1065929	0.4001233	2.3723902	N	-0.3595904	-0.4875099	-1.8808126
H	0.8863696	1.7195665	2.6475329	N	-0.4047477	-1.6218936	0.9257635
H	0.2305081	3.1950145	0.5990057	C	-0.9114295	-2.1816196	-3.5750263
C	3.1147032	1.2845360	0.0306578	H	-1.1093531	-3.2503257	-3.6264204
H	3.3354283	0.2609823	0.3540364	H	-0.0437210	-1.9592194	-4.1982600
C	4.2077061	2.1961807	0.6245583	H	-1.7580196	-1.6530260	-4.0173947
H	5.1907985	1.9095976	0.2425069	C	-1.1771828	-3.9652642	0.9524211
H	4.2319473	2.1306639	1.7135887	H	-1.4054361	-4.7553341	0.2400228
H	4.0302123	3.2400129	0.3520509	H	-2.0617529	-3.7955984	1.5702269
C	3.1615004	1.3244102	-1.4985397	H	-0.3924975	-4.3186096	1.6217456
H	4.1299735	0.9614122	-1.8509308	Ir	0.0784421	0.3616364	-0.0089359
H	3.0339788	2.3407645	-1.8779564	C	1.4206955	1.7666013	1.1476751
H	2.3885424	0.7009785	-1.9486994	C	0.5119101	1.1478394	2.0163896
C	-1.4647697	1.2915062	-2.1475633	H	0.8441213	0.3276040	2.6365585
C	-1.6037286	3.4591057	-3.9017914	C	1.3510395	3.2690624	0.8332473
C	-0.7078897	1.2792525	-3.3330373	H	1.7402959	3.4014710	-0.1816501
C	-2.3081783	2.3769204	-1.8473073	C	2.2831011	4.0450188	1.7903713
C	-2.3620754	3.4493947	-2.7381397	H	2.2231340	5.1151537	1.5796771

H	3.3277964	3.7496250	1.6880187	N	-0.5002393	-0.1066785	-1.7806105
H	0.4036191	1.6203312	-0.8991491	N	0.7610574	-1.9296909	0.1652667
H	-1.2002081	1.2027573	0.1270635	C	-0.7152578	-1.0389663	-4.0491125
H	-0.3156406	1.7118035	2.4269140	H	-0.4606699	-1.9535361	-4.5816263
H	1.9869369	3.8925156	2.8321284	H	-0.2391531	-0.1986312	-4.5581750
C	-0.0449903	3.8961991	0.8836700	H	-1.7933181	-0.8826841	-4.1276342
H	0.0165414	4.9493904	0.5996453	C	1.4037904	-4.0834372	-0.8232735
H	-0.4682705	3.8573420	1.8907861	H	1.3582051	-4.5895496	-1.7854090
H	-0.7359030	3.4038816	0.2012875	H	0.8675811	-4.6879386	-0.0892483
C	2.8115022	1.1769062	0.9991827	H	2.4457927	-4.0489332	-0.4996809
H	3.4714159	1.5347383	1.7962344	Ir	0.0384666	-0.0284369	0.3091693
H	3.2630072	1.4578603	0.0450264	H	1.4101881	0.6692657	0.2650092
H	2.7984932	0.0883128	1.0681857	C	0.0952679	0.4706725	2.3497494
C	-0.4243531	-1.7514411	2.3532248	H	1.0622618	0.6744964	2.8025353
C	-0.4347890	-1.9249686	5.1414978	C	-0.6616016	1.6684639	1.8409702
C	0.7130385	-2.2320049	3.0275838	H	-0.6595094	1.6413717	0.6216221
C	-1.5689853	-1.3603398	3.0723258	C	-0.0293052	3.0691347	2.0812517
C	-1.5539390	-1.4569976	4.4640097	H	-0.0963892	3.2134014	3.1675444
C	0.6885016	-2.3080331	4.4218925	C	1.4483443	3.1652212	1.6882332
H	-2.4349005	-1.1577522	5.0215825	H	1.8450677	4.1418760	1.9762060
H	1.5661397	-2.6727543	4.9447140	H	1.5720691	3.0637469	0.6069247
H	-0.4384809	-1.9890360	6.2232486	H	-0.4907632	-0.1737904	3.0058442
C	-0.3393546	0.4296847	-2.9925068	H	2.0613826	2.4043167	2.1706127
C	-0.2854655	2.2324038	-5.1179850	C	-2.1535592	1.6253505	2.1932034
C	-1.5186240	1.0972473	-3.3644654	H	-2.5351664	0.6065123	2.1104612
C	0.8669758	0.6619389	-3.6748280	H	-2.7606819	2.2651029	1.5523720
C	0.8723744	1.5664712	-4.7370859	H	-2.2915439	1.9474588	3.2295639
C	-1.4689581	1.9963134	-4.4312615	C	-0.8145487	4.1984965	1.3983345
H	1.8000963	1.7495033	-5.2682437	H	-0.8677776	4.0389072	0.3165578
H	-2.3749295	2.5161942	-4.7232548	H	-0.3188462	5.1576615	1.5642212
H	-0.2649791	2.9326332	-5.9448443	H	-1.8339146	4.2891270	1.7754448
C	2.1405862	-0.0290749	-3.2628160	C	1.2950414	-2.4543876	1.3940358
H	2.0451225	-1.1175145	-3.2779587	C	2.3024334	-3.4560570	3.7916598
H	2.4205002	0.2460148	-2.2421913	C	0.4374281	-3.1315152	2.2784021
H	2.9603919	0.2473885	-3.9271710	C	2.6529418	-2.2689634	1.7052382
C	-2.8119285	0.8723444	-2.6253282	C	3.1361943	-2.7798089	2.9110302
H	-2.7250962	1.1807287	-1.5805810	C	0.9614994	-3.6267976	3.4725644
H	-3.1033428	-0.1807044	-2.6119618	H	4.1836127	-2.6434361	3.1572165
H	-3.6206792	1.4413815	-3.0855215	H	0.3058291	-4.1518058	4.1586186
C	1.9400786	-2.6780631	2.2733377	H	2.6954460	-3.8477416	4.7225462
H	2.1949381	-1.9858318	1.4699776	C	-1.1297407	1.0755828	-2.2868054
H	1.7933982	-3.6545844	1.8009360	C	-2.3509604	3.4267298	-3.1644787
H	2.7959982	-2.7640596	2.9444135	C	-0.3407353	2.1142175	-2.8151521
C	-2.7932744	-0.8451594	2.3614833	C	-2.5273068	1.2116500	-2.1942168
H	-2.5573424	0.0334409	1.7577217	C	-3.1183706	2.3945659	-2.6399069
H	-3.5701630	-0.5776102	3.0787954	C	-0.9721276	3.2812625	-3.2480863
H	-3.2089956	-1.5876608	1.6749775	H	-4.1954241	2.5038688	-2.5722267
=====				H	-0.3687751	4.0858039	-3.6544522
69	XyNacnacIr_7.xyz			H	-2.8248122	4.3399092	-3.5051070
C	-0.2794507	-1.1228062	-2.5991933	C	-1.0248826	-3.3103053	1.9619318
H	0.4586520	-3.0626637	-2.9677538	H	-1.5160203	-3.9009309	2.7363244
C	0.3426672	-2.3170847	-2.1952027	H	-1.5336841	-2.3439631	1.8995805
C	0.8106863	-2.6913914	-0.9333357	H	-1.1837039	-3.8087281	1.0028013
				C	3.5756647	-1.5201725	0.7800974

H	4.6086077	-1.5982244	1.1218374	H	1.8491186	1.3446566	-4.1719049
H	3.3068702	-0.4614356	0.7371959	C	-0.9852067	-0.1541208	3.5917842
H	3.5254397	-1.8913488	-0.2455152	H	-1.3186892	0.5255479	2.8042112
C	1.1567919	1.9795555	-2.9101218	H	-1.3465926	0.2091502	4.5546496
H	1.6068624	2.9155360	-3.2440533	H	-1.4622822	-1.1189834	3.3965774
H	1.4522278	1.1968564	-3.6149022	C	3.4030854	-0.9869067	1.1670405
H	1.5886376	1.7050758	-1.9456508	H	3.1090094	-0.3159057	0.3566258
C	-3.3790123	0.1106752	-1.6151622	H	3.2050027	-2.0050171	0.8191634
H	-3.2670237	-0.8284535	-2.1624201	H	4.4765744	-0.8942400	1.3366154
H	-3.1052824	-0.1009428	-0.5778172				
H	-4.4334502	0.3893640	-1.6358477				
=====							
49				71			
XyNacnacIr_8.xyz				XyNacnacIr_9.xyz			
C	-0.9748614	-0.9888963	-1.4321860	C	-0.3695388	-2.2132318	-2.3060123
H	-0.9675261	-2.9778327	-0.7423200	H	0.0866590	-4.1366568	-1.6072190
C	-0.6422197	-1.9780785	-0.4931178	C	0.1327118	-3.0919239	-1.3389906
C	0.0506154	-1.8593135	0.7221029	C	0.7079171	-2.8331461	-0.0879993
N	-0.6537526	0.2965456	-1.2871164	N	-0.3837263	-0.8893270	-2.1732242
N	0.5239980	-0.7026833	1.1853114	N	0.8589701	-1.6262827	0.4647890
C	-1.7360713	-1.4027867	-2.6717848	C	-0.9115302	-2.8462509	-3.5724850
H	-1.9275557	-2.4741476	-2.6566308	H	-0.8406131	-3.9307611	-3.5227577
H	-1.1778365	-1.1682818	-3.5811986	H	-0.3620159	-2.5025684	-4.4507432
H	-2.6954908	-0.8851695	-2.7441645	H	-1.9564009	-2.5735564	-3.7315251
C	0.2707093	-3.1069725	1.5482402	C	1.2105926	-4.0540551	0.6611867
H	-0.1650749	-3.9710553	1.0500033	H	1.0586617	-4.9531195	0.0677865
H	-0.1844782	-3.0174872	2.5374460	H	0.6986977	-4.1815874	1.6154722
H	1.3344139	-3.3023382	1.7032074	H	2.2749901	-3.9632467	0.8854999
Ir	0.3209190	0.9813496	0.2440386	Ir	0.3637166	0.1899956	-0.4577469
C	1.2330884	-0.5666131	2.4217165	H	1.5117249	0.8932948	0.3483958
C	2.6185991	-0.2013227	4.8036676	C	-0.3847527	1.1431143	1.3182510
C	2.6390760	-0.6743878	2.4268374	H	0.1317420	0.6965403	2.1653184
C	0.5164238	-0.2713563	3.5996945	C	-0.3478075	2.6768202	1.4520880
C	1.2337346	-0.0937025	4.7827504	H	0.6057315	3.0295330	1.0452814
C	3.3118124	-0.4882972	3.6344932	H	0.5922058	1.5558943	-1.3373862
H	0.6961899	0.1360035	5.6957760	H	-0.3608450	1.5255376	-1.0947148
H	4.3930044	-0.5659501	3.6530657	C	-0.3297330	3.0941244	2.9547959
H	3.1590353	-0.0557040	5.7317419	H	0.4892718	2.5225551	3.4071756
C	-0.9888675	1.3156406	-2.2352642	C	-1.6113861	2.7322950	3.7175887
C	-1.5943251	3.3624142	-4.0158965	H	-1.4965319	2.9517311	4.7824751
C	-0.0758295	1.6302019	-3.2627871	H	-2.4693417	3.3070874	3.3587933
C	-2.2000932	2.0227821	-2.0892621	H	-1.4214825	0.7900476	1.3286072
C	-2.4823455	3.0445046	-2.9959162	H	-1.8554528	1.6721006	3.6241383
C	-0.4025187	2.6603422	-4.1447151	C	-1.4712788	3.3625732	0.6621150
H	-3.4089411	3.5980871	-2.8946367	H	-1.4107768	3.1314278	-0.4034075
H	0.2909271	2.9147235	-4.9382889	H	-1.4286496	4.4497839	0.7534339
H	-1.8290065	4.1624458	-4.7083339	H	-2.4563070	3.0352473	1.0050998
C	-3.1723940	1.6875148	-0.9888875	C	0.0076550	4.5791627	3.1430800
H	-3.9783668	2.4215409	-0.9522336	H	0.9210076	4.8512175	2.6068887
H	-2.6689927	1.6594689	-0.0197731	H	0.1628698	4.8080482	4.2010221
H	-3.6227646	0.7017758	-1.1372633	H	-0.7960647	5.2286295	2.7862577
C	1.2187208	0.8755243	-3.4155921	C	1.4670385	-1.5728895	1.7715619
H	1.0458326	-0.1611297	-3.7187602	C	2.6399385	-1.4106978	4.2951170
H	1.7621932	0.8384604	-2.4687265	C	0.6702091	-1.7329710	2.9180149
				C	2.8508917	-1.3429584	1.8797597
				C	3.4167664	-1.2664616	3.1523677

C	1.2780885	-1.6435286	4.1727886	C	1.3818000	-0.8568065	4.6921336
H	4.4829165	-1.0907103	3.2438347	H	4.4915251	-1.2176263	3.4022897
H	0.6670963	-1.7562118	5.0617899	H	0.8709391	-0.7949088	5.6464042
H	3.0958130	-1.3423487	5.2758840	H	3.3237957	-1.0943533	5.5776235
C	-0.9005721	-0.1007076	-3.2568134	C	-1.1611240	1.4562075	-2.1552099
C	-1.8857593	1.5135513	-5.3051212	C	-1.8986823	3.6086541	-3.7646627
C	-0.0285651	0.3526937	-4.2629717	C	-2.3806975	2.1211985	-1.9121468
C	-2.2601717	0.2579718	-3.2644961	C	-0.3022367	1.8766961	-3.1916750
C	-2.7333494	1.0646039	-4.3006709	C	-0.6939550	2.9539031	-3.9866696
C	-0.5432976	1.1585444	-5.2798852	C	-2.7307817	3.1934582	-2.7329073
H	-3.7806785	1.3460326	-4.3124770	H	-0.0398063	3.2838812	-4.7859515
H	0.1233583	1.5132700	-6.0582670	H	-3.6669014	3.7104151	-2.5535890
H	-2.2684851	2.1418266	-6.1008339	H	-2.1851060	4.4460439	-4.3899584
C	-3.1934199	-0.2085034	-2.1768884	C	1.0124409	1.1838386	-3.4422172
H	-3.3134138	-1.2955811	-2.1784013	H	0.8723664	0.1461588	-3.7578994
H	-4.1814987	0.2361742	-2.3015703	H	1.5737310	1.6978013	-4.2233288
H	-2.8143818	0.0602728	-1.1881925	H	1.6222485	1.1538996	-2.5360581
C	1.4348031	-0.0081228	-4.2473240	C	-3.2923603	1.6904200	-0.7920429
H	1.5932574	-1.0852539	-4.3498963	H	-2.7624502	1.6711144	0.1634120
H	1.9063948	0.2843778	-3.3057775	H	-3.6849904	0.6820580	-0.9510216
H	1.9601371	0.4856583	-5.0656542	H	-4.1411460	2.3698517	-0.7063479
C	3.7204673	-1.1905760	0.6588143	C	3.4402706	-1.0550984	0.9156809
H	4.7664794	-1.0771614	0.9461694	H	3.0824348	-1.8677049	0.2781317
H	3.4253050	-0.3190186	0.0701302	H	4.5092830	-1.1983843	1.0766806
H	3.6437185	-2.0539794	-0.0070550	H	3.2920266	-0.1295507	0.3545127
C	-0.8072628	-2.0239315	2.8258119	C	-0.8544342	-0.5548369	3.5773396
H	-0.9964558	-3.0922992	2.6774896	H	-1.1958178	-0.5298349	4.6127695
H	-1.2735018	-1.4992529	1.9935934	H	-1.4008193	-1.3480418	3.0603441
H	-1.3127556	-1.7328596	3.7478401	H	-1.1348396	0.3838331	3.0938191
=====				=====			
51				69			
XyNacnacIr_10.xyz				XyNacnacIr_12.xyz			
C	-1.0563972	-0.8756770	-1.5403689	C	-0.3561915	-1.5523566	-2.2641661
C	-0.6556402	-1.9134847	-0.6938272	H	-0.2606076	-3.5766845	-1.7662351
C	0.0868310	-1.8502697	0.4956893	C	-0.2075909	-2.5851332	-1.3430487
N	-0.7545023	0.3937974	-1.2917881	C	-0.0343299	-2.5491530	0.0513130
N	0.5677031	-0.7405702	1.0638405	N	-0.3402429	-0.2502972	-1.9632264
C	-1.8575901	-1.2321305	-2.7715653	N	0.1068695	-1.4481173	0.7834529
H	-2.0193114	-2.3066696	-2.8340397	C	-0.5575058	-1.9734049	-3.7083065
H	-1.3453072	-0.9047567	-3.6789803	H	-0.5000893	-3.0563892	-3.7975119
H	-2.8298955	-0.7346009	-2.7621858	H	0.1973553	-1.5312439	-4.3606200
C	0.3592086	-3.1738298	1.1854145	H	-1.5278697	-1.6467428	-4.0869804
H	-0.0878004	-3.9884930	0.6196465	C	-0.0295420	-3.9180529	0.7176763
H	-0.0516993	-3.1889734	2.1962239	H	-0.1844356	-4.7025025	-0.0201710
H	1.4300938	-3.3631455	1.2761285	H	-0.8177450	-3.9926656	1.4688077
Ir	0.3402397	1.0935863	0.3506196	H	0.9118337	-4.1137704	1.2320750
H	1.7180941	1.6350122	0.9137057	Ir	-0.0315868	0.6619259	-0.1175062
H	0.3298268	1.7969218	1.7697526	C	1.2288343	2.0948765	1.1162169
H	-0.9572144	-2.9059822	-0.9935598	C	-0.0351970	2.0907650	1.7408947
C	1.3156463	-0.8422514	2.2903097	C	1.7103931	3.2760313	0.2884753
C	2.7600882	-1.0234779	4.6548139	H	2.4248835	2.9549377	-0.4723572
C	0.6360277	-0.7605918	3.5171092	H	0.9139656	3.8189744	-0.2106892
C	2.7100889	-1.0025728	2.2315737	C	-1.0171085	3.2295959	1.5070877
C	3.4147967	-1.0941268	3.4320323	H	-1.0091802	3.6150543	0.4916837

H	-2.0357548	2.9037501	1.7300394	N	-0.6869089	0.0758630	-1.6049993
H	-0.0620726	1.9901534	-0.9466664	N	0.9548746	-1.5734932	0.3380571
H	-1.4762445	1.1758772	0.0126823	C	-1.5584912	-1.2546582	-3.4893715
H	2.2373983	3.9768570	0.9500624	H	-1.5599370	-2.2909540	-3.8218912
H	-0.7892165	4.0581883	2.1904278	H	-1.0674014	-0.6472273	-4.2529450
C	-0.2388589	1.5078068	3.1216163	H	-2.5929419	-0.9111879	-3.4310031
H	0.4207677	0.6848071	3.3679599	C	1.0143088	-3.9346091	-0.3419287
H	-1.2663280	1.1696668	3.2594609	H	0.6037849	-4.5726852	-1.1214527
H	-0.0671549	2.3033903	3.8594893	H	0.7397229	-4.3553413	0.6261039
C	2.4130210	1.3781815	1.7341003	H	2.1036547	-3.9707613	-0.4051261
H	2.9449067	2.0690031	2.4013503	Ir	0.4480428	0.3719131	0.2737524
H	3.1278499	1.0747948	0.9646832	H	1.5470639	0.6260908	1.3827561
H	2.1402813	0.5039988	2.3132682	C	-0.8308747	0.9151196	1.8877554
C	0.2219110	-1.6717463	2.1947839	C	-1.2812448	2.2759265	1.3091372
C	0.4068193	-2.0786208	4.9540379	H	-2.0338582	2.0605267	0.5478776
C	1.4765079	-1.9187433	2.7815846	C	-2.0023480	-0.0548969	1.9994306
C	-0.9457101	-1.6667025	2.9847249	H	-1.6953854	-1.0057965	2.4304523
C	-0.8322690	-1.8743627	4.3577064	H	-2.4649842	-0.2544032	1.0334673
C	1.5478473	-2.1021788	4.1655730	C	-1.9141671	3.2572412	2.3070338
H	-1.7290519	-1.8665132	4.9677468	H	-2.7699266	2.8096302	2.8178302
H	2.5159659	-2.2779896	4.6228100	H	-2.2714745	4.1489093	1.7836396
H	0.4798265	-2.2260165	6.0251546	H	-2.7764212	0.3614914	2.6592408
C	-0.5900977	0.6759410	-3.0414536	H	-1.2001079	3.5806989	3.0672580
C	-1.0624259	2.4872923	-5.1073845	C	-0.1311999	1.0403004	3.2418373
C	0.4940445	1.2018424	-3.7650151	H	0.6495159	1.8015792	3.2379450
C	-1.9096239	1.0512933	-3.3454782	H	0.3380753	0.0978131	3.5235129
C	-2.1232283	1.9605189	-4.3832571	H	-0.8539462	1.2989540	4.0272230
C	0.2362926	2.1062908	-4.7953834	C	-0.0873728	2.9236498	0.5886728
H	-3.1390846	2.2554429	-4.6228506	H	0.6624104	3.2983113	1.2844334
H	1.0688257	2.5164378	-5.3565079	H	-0.4106418	3.7348208	-0.0687364
H	-1.2463829	3.1905901	-5.9111867	H	0.4814743	2.2654646	-0.1381979
C	-3.0803976	0.5122993	-2.5656919	C	1.9718298	-1.9489075	1.2964364
H	-4.0207732	0.8266526	-3.0203009	C	3.9798834	-2.6133933	3.1199916
H	-3.0631949	0.8730411	-1.5336932	C	1.6315040	-2.5642801	2.5107783
H	-3.0764202	-0.5784130	-2.5103871	C	3.3214128	-1.6921750	0.9769369
C	1.9130864	0.8206607	-3.4324613	C	4.3066770	-2.0292110	1.9012891
H	2.0768757	-0.2583401	-3.4904029	C	2.6530578	-2.8813262	3.4120010
H	2.1684972	1.1221404	-2.4130835	H	5.3449504	-1.8299538	1.6599989
H	2.6111703	1.3049212	-4.1165839	H	2.3915203	-3.3535038	4.3532163
C	-2.2996711	-1.4536409	2.3592099	H	4.7585185	-2.8668218	3.8300386
H	-2.3132005	-0.5535929	1.7421376	C	-1.1062902	1.2381174	-2.3313921
H	-3.0696050	-1.3679052	3.1271490	C	-1.8319604	3.6023876	-3.6439437
H	-2.5757670	-2.2819911	1.7001100	C	-0.1466242	1.9510181	-3.0844662
C	2.7327517	-2.0562572	1.9549882	C	-2.4343890	1.6972365	-2.2654293
H	2.6696495	-1.5063567	1.0182006	C	-2.7719881	2.8849172	-2.9216881
H	2.9191013	-3.1049865	1.7003680	C	-0.5284204	3.1262014	-3.7285701
H	3.6042235	-1.7031297	2.5094983	H	-3.7951306	3.2418395	-2.8637831
=====				H	0.2086958	3.6730777	-4.3063094
69	XyNacnacIr_13.xyz			H	-2.1116412	4.5210395	-4.1462958
C	-0.8528555	-1.1173206	-2.1530880	C	-3.5209932	0.9334386	-1.5472520
H	-0.6120496	-3.2050351	-2.1334936	H	-4.2341423	0.5124893	-2.2632578
C	-0.3656859	-2.3090894	-1.5830731	H	-4.0899854	1.5887470	-0.8834060
C	0.5032111	-2.5141612	-0.5082634	H	-3.1210264	0.1132744	-0.9569124
				C	1.2705455	1.4525465	-3.2145004

H	1.8452470	2.1030425	-3.8751584	C	-2.3516976	1.0084956	-2.9440607
H	1.3082354	0.4385334	-3.6202433	C	-2.6181134	1.8418224	-4.0330123
H	1.7768790	1.4175123	-2.2458725	C	-0.4555027	1.3876306	-4.9640148
C	3.7110476	-1.0514625	-0.3289576	H	-3.5792080	2.3416818	-4.0877690
H	4.7959106	-1.0447262	-0.4431411	H	0.2811598	1.5345639	-5.7463344
H	3.3538091	-0.0186303	-0.3724853	H	-1.9037285	2.6902191	-5.8729445
H	3.2806795	-1.5730825	-1.1871164	C	1.7916428	-1.5898993	1.6932289
C	0.2140287	-2.9256909	2.8815788	C	3.7689541	-1.7421324	3.6664979
H	-0.1221494	-2.3509925	3.7486466	C	1.4333402	-1.8791197	3.0213558
H	0.1485304	-3.9823866	3.1560716	C	3.1486082	-1.4185351	1.3444177
H	-0.4841369	-2.7415581	2.0693502	C	4.1161774	-1.4929157	2.3438192
=====							
71							
XyNacnacIr_14.xyz							
C	-1.0285935	-1.7780414	-1.8482782	C	-2.3516976	1.0084956	-2.9440607
H	-0.8735667	-3.7478485	-1.1544071	C	-2.6181134	1.8418224	-4.0330123
C	-0.5752752	-2.7348252	-0.9293018	C	-0.4555027	1.3876306	-4.9640148
C	0.3242615	-2.6202579	0.1398416	H	-3.5792080	2.3416818	-4.0877690
N	-0.7714800	-0.4778636	-1.7588631	H	0.2811598	1.5345639	-5.7463344
N	0.7920282	-1.4767149	0.6551773	H	-1.9037285	2.6902191	-5.8729445
C	-1.8172214	-2.3110107	-3.0298256	C	1.7916428	-1.5898993	1.6932289
H	-2.0165996	-3.3743160	-2.9117037	C	3.7689541	-1.7421324	3.6664979
H	-1.2677210	-2.1664481	-3.9628606	C	1.4333402	-1.8791197	3.0213558
H	-2.7677788	-1.7876215	-3.1424376	C	3.1486082	-1.4185351	1.3444177
C	0.8192402	-3.9443853	0.6982736	C	4.1161774	-1.4929157	2.3438192
H	0.4352048	-4.7714120	0.1054154	C	2.4384444	-1.9420260	3.9922758
H	0.5098834	-4.0936808	1.7328903	H	5.1587239	-1.3593689	2.0766550
H	1.9097298	-3.9870230	0.6857825	H	2.1599952	-2.1571009	5.0186801
Ir	0.3305914	0.4506905	-0.1127303	H	4.5343138	-1.7934750	4.4320458
H	1.5263198	1.0037615	0.7498147	C	-3.3917856	0.8451027	-1.8654165
C	-0.5778793	1.5230035	1.5965795	H	-4.3766298	1.1318431	-2.2377338
C	0.2799645	1.4680012	2.8617305	H	-3.1664017	1.4813125	-1.0055096
H	0.5797024	0.4525893	3.1004393	H	-3.4493695	-0.1775614	-1.4920288
H	1.1908063	2.0572797	2.7671192	C	1.1869329	-0.1514328	-3.8446939
H	0.7477252	1.7650242	-0.9753176	H	1.0861470	-1.2400631	-3.8474655
H	-0.2207756	1.8424434	-0.7890556	H	1.7334414	0.1065910	-2.9340382
C	-0.9357766	3.0011333	1.2388782	H	1.7980625	0.1307774	-4.7028663
H	-1.4665697	2.9753011	0.2810764	C	3.5729772	-1.1821944	-0.0818235
C	-1.8536534	0.6980856	1.7913140	H	3.1797711	-1.9489526	-0.7538850
H	-1.6399592	-0.3678106	1.8517391	H	4.6609709	-1.1870201	-0.1609935
H	-2.5665076	0.8492416	0.9803595	H	3.2024819	-0.2223755	-0.4490683
H	-2.3529741	0.9728909	2.7288966	C	0.0121592	-2.1515530	3.4586591
H	-0.2831694	1.8528758	3.7217682	H	-0.0602775	-3.1388317	3.9239956
C	-1.9166028	3.6451723	2.2443633	H	-0.6931075	-2.1172141	2.6326940
H	-1.4931141	3.6941331	3.2502206	H	-0.3144583	-1.4235293	4.2055450
H	-2.8659180	3.1117796	2.3007562	=====			
H	-2.1349826	4.6702553	1.9341925	71			
C	0.2748013	3.9335050	1.0828325	XyNacnacIr_23.xyz			
H	1.0484720	3.5122624	0.4415595	C	-1.0025736	-2.0749981	-2.3615259
H	0.7329299	4.1521994	2.0502546	H	-0.9957417	-4.1343499	-1.9062870
H	-0.0397470	4.8878712	0.6526293	C	-0.7874493	-3.1549927	-1.5016596
C	-1.1083535	0.3559458	-2.8807074	C	-0.3351546	-3.1295641	-0.1760740
C	-1.6805305	2.0378992	-5.0369042	N	-0.7875962	-0.8240748	-1.9756063
C	-0.1509348	0.5411754	-3.8977225	N	-0.0133092	-2.0304834	0.5170661
				C	-1.4929508	-2.3579701	-3.7628689
				H	-1.6214753	-3.4278244	-3.9180335
				H	-0.7890670	-1.9829849	-4.5094571
				H	-2.4485248	-1.8641199	-3.9535427
				C	-0.2081352	-4.4756880	0.5128695
				H	-0.5067660	-5.2703617	-0.1676942
				H	-0.8369154	-4.5323681	1.4031294
				H	0.8161803	-4.6685538	0.8363690
				Ir	-0.1192425	-0.1609977	-0.1602344
				C	1.1795532	0.9312922	1.1944077
				H	1.7707764	0.2512336	1.7996388
				C	-0.1655968	1.1067007	1.6003137
				H	-0.4868163	0.5697143	2.4870003
				C	2.0223318	2.0265319	0.5689629

H	2.8786692	1.5693383	0.0674663	C	-1.4490249	-1.5161864	-1.9796732
H	1.4717558	2.5593026	-0.2112293	H	-1.8826867	-3.5138553	-1.4975789
C	-0.9889708	2.3496914	1.3056882	C	-1.3310800	-2.6476642	-1.1640085
H	-0.9910355	2.5760922	0.2306470	C	-0.6289238	-2.8144627	0.0353859
H	-2.0283188	2.1125527	1.5473498	N	-0.8343684	-0.3557438	-1.7530701
C	2.5105925	3.0272200	1.6541940	N	0.1259097	-1.8751437	0.6043710
H	3.5987393	3.1291721	1.6023638	C	-2.3462127	-1.6629791	-3.1949407
H	2.3033455	2.5897474	2.6346113	H	-2.7298486	-2.6791006	-3.2635086
C	-0.5850327	3.6514360	2.0530329	H	-1.8092152	-1.4324497	-4.1167270
H	-1.5031705	4.2214049	2.2230379	H	-3.1947724	-0.9775506	-3.1477259
C	1.9029631	4.4400586	1.5954757	C	-0.7621924	-4.1718875	0.7009715
H	2.4343281	5.0263824	0.8371147	H	-1.3675358	-4.8376142	0.0887564
H	-0.1972600	3.4049360	3.0467567	H	-1.2301470	-4.0880659	1.6838458
H	2.1144458	4.9332702	2.5508745	H	0.2129051	-4.6364182	0.8579147
C	0.3985964	4.5674077	1.2925280	Ir	0.5134873	0.0682011	-0.1648704
H	0.2303654	4.4309289	0.2191827	H	-0.3920184	0.9109412	0.7426772
H	0.1289651	5.6098722	1.4903467	C	2.2292399	1.3152581	-0.0580036
C	0.4368022	-2.1858841	1.8732822	C	2.0897540	0.7593665	1.2537622
C	1.3099104	-2.4714556	4.4981276	C	1.2601608	2.0749136	-0.7884141
C	-0.5021200	-2.1549926	2.9188937	H	1.5148714	2.0868767	-1.8467466
C	1.8087064	-2.3564622	2.1285994	H	3.0215960	0.8743200	-0.6639887
C	2.2245335	-2.4988874	3.4528554	H	2.8392307	-0.0138545	1.4139736
C	-0.0417634	-2.3000932	4.2283905	C	1.8210464	1.4195276	2.5991406
H	3.2803737	-2.6298659	3.6625135	H	1.7871332	0.6025607	3.3260371
H	-0.7565036	-2.2777744	5.0436675	H	2.7256713	1.9913806	2.8555080
H	1.6504019	-2.5810280	5.5211360	C	0.5745836	3.3964509	-0.4696462
C	-1.0046422	0.2884549	-2.8463038	H	1.3477396	4.1767870	-0.5364901
C	-1.3888250	2.5426564	-4.4391477	H	-0.0965383	3.5900652	-1.3117516
C	0.0612218	0.7759739	-3.6307701	C	-0.2336052	3.6472073	0.8044433
C	-2.2607854	0.9298406	-2.8531862	H	-0.6956277	4.6312744	0.6693885
C	-2.4302382	2.0555738	-3.6592675	C	0.6099264	2.3101970	2.8805867
C	-0.1548073	1.9051007	-4.4211154	H	0.6403635	2.5145835	3.9563921
H	-3.3919118	2.5565345	-3.6694536	H	-0.3126973	1.7434316	2.7183155
H	0.6595745	2.2886408	-5.0256862	H	-1.0675110	2.9398249	0.8598888
H	-1.5376555	3.4205873	-5.0569723	C	0.5087319	3.6578095	2.1495530
C	-3.3999385	0.4172825	-2.0105207	H	-0.0297186	4.3442516	2.8104632
H	-4.2562562	1.0900246	-2.0723732	H	1.5079680	4.0928118	2.0236473
H	-3.1005729	0.3204556	-0.9643924	C	0.7246276	-2.1830038	1.8726455
H	-3.7284424	-0.5745782	-2.3330512	C	1.9069000	-2.7600312	4.3324463
C	1.4067094	0.0979306	-3.6215949	C	2.0237441	-2.7202282	1.9107428
H	2.1277064	0.6672649	-4.2093272	C	0.0140768	-1.9336398	3.0598072
H	1.3547255	-0.9110140	-4.0400394	C	0.6244768	-2.2297604	4.2799893
H	1.7843748	-0.0068769	-2.6019186	C	2.5971688	-3.0017791	3.1512216
C	2.8116320	-2.3888422	1.0052078	H	0.0815308	-2.0392913	5.1995196
H	2.6961405	-1.5217673	0.3516297	H	3.5988723	-3.4162693	3.1867726
H	2.6838247	-3.2725706	0.3735352	H	2.3663321	-2.9838656	5.2880965
H	3.8287618	-2.4045836	1.3985332	C	-1.1168086	0.7304291	-2.6488826
C	-1.9727571	-1.9839803	2.6414509	C	-1.6427262	2.8520048	-4.3822686
H	-2.5250572	-1.8403517	3.5710074	C	-2.2086796	1.5792132	-2.3959755
H	-2.3918667	-2.8592452	2.1362254	C	-0.2871056	0.9384043	-3.7652889
H	-2.1517613	-1.1310224	1.9838502	C	-0.5672805	2.0051533	-4.6200413
=====				C	-2.4538874	2.6348974	-3.2761223
71	XyNacnacIr_24.xyz			H	0.0690650	2.1703112	-5.4827628
				H	-3.2945786	3.2934539	-3.0860961

H	-1.8468916	3.6763630	-5.0554862	C	0.5889111	4.4491038	2.4046280
C	0.8836529	0.0309794	-4.0447945	H	0.3480832	4.6801499	1.3620187
H	1.5781871	0.0049952	-3.2009222	H	0.3888865	5.3752969	2.9530573
H	1.4304871	0.3693976	-4.9259205	H	0.4378098	1.3115278	-1.1706227
H	0.5707263	-1.0020203	-4.2202394	H	-1.0509786	1.3533648	-0.6530814
C	-3.1067609	1.3592588	-1.2065666	C	0.4384257	-2.1062141	1.8158510
H	-3.8484550	2.1555681	-1.1320872	C	1.2868587	-2.4298883	4.4547776
H	-2.5331708	1.3298679	-0.2784291	C	-0.5090838	-2.1102808	2.8569240
H	-3.6426707	0.4079204	-1.2687295	C	1.8091262	-2.2656512	2.0920555
C	2.7906611	-2.9930961	0.6421023	C	2.2119933	-2.4248963	3.4193304
H	2.2891437	-3.7299663	0.0086603	C	-0.0633889	-2.2739993	4.1694153
H	2.8980056	-2.0879787	0.0383573	H	3.2671911	-2.5478673	3.6381741
H	3.7883430	-3.3709844	0.8697236	H	-0.7892194	-2.2788061	4.9753982
C	-1.3806168	-1.3647401	3.0275371	H	1.6164885	-2.5539430	5.4795854
H	-1.4126087	-0.4285725	2.4670173	C	-1.0971003	0.2485552	-3.2150353
H	-1.7428582	-1.1767141	4.0390288	C	-1.6507811	2.1270071	-5.1948974
H	-2.0874962	-2.0413406	2.5390670	C	-0.0752390	0.6506984	-4.0912279
=====				C	-2.3923508	0.7827369	-3.3178403
73				C	-2.6484782	1.7219181	-4.3181144
XyNacnacIr_26.xyz				C	-0.3746253	1.5923515	-5.0769207
C	-0.9705546	-1.9928751	-2.4533409	H	-3.6451037	2.1408617	-4.4035968
H	-0.9243499	-4.0280719	-1.9542257	H	0.4086254	1.9097867	-5.7565248
C	-0.7338817	-3.0427794	-1.5565053	H	-1.8661900	2.8581414	-5.9652870
C	-0.2936215	-3.0184494	-0.2299117	C	-3.4864304	0.3703850	-2.3673782
N	-0.8034943	-0.7042054	-2.1731512	H	-4.4121312	0.9002501	-2.5956376
N	0.0038514	-1.9150907	0.4627988	H	-3.2089674	0.5851984	-1.3326147
C	-1.4524812	-2.3971039	-3.8340846	H	-3.6919936	-0.7023023	-2.4165069
H	-1.5358659	-3.4795126	-3.9061834	C	1.3206285	0.0961903	-3.9714531
H	-0.7679848	-2.0499293	-4.6098989	H	1.3459312	-0.9884714	-4.1068281
H	-2.4268449	-1.9591211	-4.0576060	H	1.7372009	0.2948317	-2.9811885
C	-0.1612081	-4.3776276	0.4347756	H	1.9760013	0.5427903	-4.7202354
H	-0.4365628	-5.1709563	-0.2568615	C	2.8299449	-2.2978338	0.9822651
H	-0.8008952	-4.4507593	1.3158634	H	2.6847595	-1.4799748	0.2741956
H	0.8600578	-4.5558351	0.7751560	H	2.7645753	-3.2228437	0.4013542
Ir	-0.1540988	0.1099474	-0.3592230	H	3.8405477	-2.2347055	1.3877921
C	1.1842222	1.0302618	1.1509431	C	-1.9819607	-1.9659936	2.5684617
H	1.7712939	0.2015308	1.5328735	H	-2.3841457	-2.8518691	2.0679343
C	-0.1258003	1.1203186	1.6370435	H	-2.1816239	-1.1218307	1.9056831
H	-0.4203671	0.3559382	2.3472875	H	-2.5427763	-1.8261331	3.4935003
C	2.0390143	2.2227648	0.7868884	=====			
H	2.8304014	1.9023914	0.1053144	73			
H	1.4589053	2.9742282	0.2495544	XyNacnacIr_27.xyz			
C	-0.9105260	2.4081916	1.7829348	C	-0.4102060	-1.4104907	-2.5539487
H	-0.9315346	2.9608254	0.8422361	H	0.1137438	-3.4415497	-2.7228742
H	-1.9491250	2.1400808	1.9947501	C	0.2229718	-2.5760307	-2.0862270
C	2.6588983	2.8268131	2.0778179	C	1.0715150	-2.7588145	-0.9938865
H	3.7402050	2.9351865	1.9529768	N	-0.4454815	-0.2762688	-1.8702045
H	2.5317674	2.1029532	2.8879514	N	1.3880199	-1.8239307	-0.0816929
C	-0.3984534	3.3656236	2.8942978	C	-1.0338156	-1.4918962	-3.9344710
H	-1.2712635	3.8763239	3.3108710	H	-0.9344871	-2.4955257	-4.3437234
C	2.1020135	4.1902169	2.5322274	H	-0.5470462	-0.7935288	-4.6196064
H	2.6074652	4.9838439	1.9705812	H	-2.0921412	-1.2287841	-3.9164063
H	0.0326949	2.7920126	3.7215123	C	1.7278007	-4.1227792	-0.8861931
H	2.3987024	4.3352227	3.5769264	H	1.3419004	-4.7860449	-1.6574664

H	1.5502124	-4.5820157	0.0868938	H	1.4515514	0.6572337	-3.8584187
H	2.8108070	-4.0505706	-1.0060131	H	1.7491369	1.4875374	-2.3452120
Ir	0.5977296	0.0214971	0.0386686	H	1.7024666	2.4059175	-3.8599321
H	1.6929334	0.3245819	1.1446133	C	-3.3458402	0.0835271	-1.7054929
C	-0.5575401	0.6818510	1.6362847	H	-3.7931225	-0.5761671	-2.4568323
H	0.0152769	0.7744916	2.5532707	H	-4.1693518	0.5756648	-1.1846289
C	-0.5311551	1.9394395	0.8203556	H	-2.8122117	-0.5500417	-1.0001367
H	0.2137867	1.8260293	-0.0938647	=====			
H	-1.4765785	2.1256310	0.3142447	75			
C	-1.9087109	0.0390167	1.9066116	XyNacnacIr_29.xyz			
H	-1.7896530	-0.6922072	2.7119657	C	-0.3544174	-1.8944124	-2.6041918
H	-2.2452704	-0.5247043	1.0335229	H	-0.2468628	-3.9081866	-2.0315653
C	0.0038822	3.1955002	1.5260384	C	-0.0347080	-2.9065915	-1.6889590
H	-0.2011859	4.0650113	0.8931416	C	0.5952872	-2.8399949	-0.4389166
H	1.0908639	3.1218478	1.6125697	N	-0.1827702	-0.5960238	-2.3730071
C	-3.0340910	1.0253379	2.2936146	N	0.9361509	-1.7188006	0.2024661
H	-3.9016325	0.4170729	2.5694504	C	-0.9001844	-2.3534155	-3.9428930
H	-3.3462378	1.5907841	1.4091955	H	-1.0370163	-3.4328737	-3.9540201
C	-0.5766016	3.4315176	2.9315624	H	-0.2192385	-2.0842268	-4.7533035
H	-0.2298421	4.4193009	3.2508358	H	-1.8562148	-1.8781610	-4.1672803
H	-0.1268485	2.7242964	3.6353212	C	0.9362702	-4.1795952	0.1885689
C	-2.7573625	2.0177943	3.4403781	H	0.6487915	-4.9936235	-0.4732851
H	-2.1678491	1.5286588	4.2249735	H	0.4288219	-4.3185500	1.1434903
H	-3.7235939	2.2461970	3.9011218	H	2.0070464	-4.2563209	0.3865987
C	-2.1097551	3.3786336	3.0917967	Ir	0.6362935	0.2202929	-0.5320610
H	-2.5970361	3.7944381	2.2016389	H	1.8289184	0.6673926	0.3805243
H	-2.3676900	4.0599416	3.9083450	C	-0.1325161	1.1235365	1.2924479
C	2.3945440	-2.1561764	0.8992741	H	0.2333648	0.4824007	2.0959554
C	4.3442375	-2.7776369	2.7864774	C	0.3805458	2.5497664	1.5338016
C	2.0156374	-2.7539885	2.1115177	H	1.4435806	2.5651205	1.2928301
C	3.7399382	-1.8600192	0.6256300	H	-0.0934155	3.2376069	0.8219179
C	4.7014472	-2.1812539	1.5841357	H	1.0500215	1.6307274	-1.2701646
C	3.0088317	-3.0580374	3.0436267	H	0.1060015	1.7035288	-1.0508282
H	5.7424482	-1.9540742	1.3822943	C	-1.6541201	0.9826944	1.1762455
H	2.7248640	-3.5188805	3.9833685	H	-1.8632637	0.0316852	0.6773890
H	5.1032557	-3.0203297	3.5210157	H	-2.0415072	1.7572361	0.5048150
C	-1.0490033	0.8759028	-2.4728952	C	0.2445228	3.1301432	2.9617167
C	-2.1829996	3.2067493	-3.5214240	H	1.0976165	3.8012542	3.1013018
C	-2.4330343	1.0971893	-2.3494515	H	0.3826660	2.3308002	3.6989442
C	-0.2334181	1.8137058	-3.1405049	C	-2.4943704	0.9874729	2.4804061
C	-0.8199176	2.9693400	-3.6547386	H	-1.9220974	0.5297913	3.2939891
C	-2.9777010	2.2718866	-2.8753202	H	-3.3420666	0.3174463	2.3060997
H	-0.1949685	3.6923212	-4.1674361	C	-1.0204283	3.9401958	3.3023937
H	-4.0437783	2.4466269	-2.7745743	H	-0.7327632	4.6984777	4.0386132
H	-2.6208910	4.1131623	-3.9227596	H	-1.3433401	4.5009737	2.4163473
C	4.1432519	-1.1782328	-0.6551072	C	-3.0741111	2.3327115	2.9525356
H	3.6907230	-0.1848115	-0.7194854	H	-4.0071065	2.1159474	3.4838856
H	3.8159401	-1.7304898	-1.5395033	H	-3.3659798	2.9304902	2.0802411
H	5.2270813	-1.0676865	-0.7065776	C	-2.2179220	3.1871370	3.8946625
C	0.5714859	-3.0464794	2.4199899	H	-1.8708072	2.5621974	4.7274817
H	0.4737435	-3.5003872	3.4068107	H	-2.8809451	3.9351549	4.3439872
H	0.1217713	-3.7254822	1.6911327	C	1.6567119	-1.8547668	1.4463478
H	-0.0219231	-2.1313477	2.3965831	C	3.0829900	-2.0338456	3.8392351
C	1.2461733	1.5810293	-3.3112619	C	3.0641282	-1.7793693	1.4275318

C	0.9663401	-2.0468343	2.6540757	H	1.1178733	0.1360366	-2.4362149
C	1.7004063	-2.1249824	3.8417734	C	0.4465177	1.7774033	-1.2661955
C	3.7557686	-1.8700903	2.6338871	H	-0.3564460	1.9298455	-1.9712594
H	1.1694735	-2.2622352	4.7778273	C	-1.2705805	0.7805982	2.6616502
H	4.8385534	-1.8113353	2.6246942	H	-1.0799251	-0.2088257	3.0588591
H	3.6366496	-2.0949411	4.7688676	H	-2.2857668	0.7657723	2.2535905
C	-0.4557928	0.3280743	-3.4385029	C	1.9180719	0.0965226	2.6594803
C	-0.9429060	2.1999100	-5.4492448	H	2.8235578	0.7145601	2.7248058
C	0.5826368	0.6938767	-4.3151622	H	2.2762619	-0.8807775	2.3413008
C	-1.7358883	0.8964495	-3.5634359	C	2.8182717	0.7024432	-1.2421749
C	-1.9582263	1.8299620	-4.5772866	H	3.1465500	-0.3395996	-1.1814645
C	0.3172172	1.6322404	-5.3135911	H	3.0490094	1.1478540	-0.2749241
H	-2.9435026	2.2720678	-4.6778888	C	0.9112342	3.0971401	-0.6911726
H	1.1144084	1.9201528	-5.9902271	H	1.7679985	2.9824793	-0.0271123
H	-1.1318764	2.9284773	-6.2289519	H	0.1242667	3.5706790	-0.0966600
C	-2.8545750	0.5136430	-2.6295483	C	3.6690739	1.4101354	-2.3190945
H	-3.7481894	1.1026257	-2.8399069	H	4.7129833	1.1278208	-2.1438518
H	-2.5737967	0.6714922	-1.5871341	H	3.4126812	1.0117301	-3.3081889
H	-3.1221850	-0.5426319	-2.7224531	C	1.2955120	4.0828889	-1.8168409
C	1.9606152	0.0972336	-4.1842175	H	1.7235224	4.9770626	-1.3483692
H	2.6414397	0.5421001	-4.9110000	H	0.3841998	4.4121129	-2.3273245
H	1.9564120	-0.9841355	-4.3474328	C	3.5952162	2.9470680	-2.3662830
H	2.3694222	0.2569260	-3.1833624	H	4.4060068	3.2823371	-3.0206205
C	-0.5317549	-2.2184337	2.7103444	H	3.8342760	3.3518646	-1.3755590
H	-0.8032449	-3.2784362	2.7578443	C	2.2713488	3.5556419	-2.8816381
H	-1.0271597	-1.7937730	1.8406804	H	2.5026835	4.3950001	-3.5449400
H	-0.9411206	-1.7475269	3.6053780	H	1.7599253	2.8197839	-3.5090461
C	3.8253075	-1.6161402	0.1374336	C	-1.2272164	1.8344653	3.7993650
H	3.5827898	-2.4036492	-0.5808544	H	-1.7761192	1.4374015	4.6611739
H	3.5812850	-0.6678930	-0.3469127	H	-1.7808920	2.7211147	3.4708072
H	4.8999368	-1.6456174	0.3220123	C	1.3711794	-0.0532400	4.0890566
=====							
93							
XyNacnacIr_COE_2.xyz							
C	-2.0324029	-1.7983486	-2.0929431	H	2.1274624	-0.6081674	4.6545393
H	-2.3935989	-3.8093388	-1.6509493	H	0.4948381	-0.6963292	4.0953312
C	-1.8838694	-2.9286436	-1.2909630	C	0.1706308	2.2942854	4.2372822
C	-1.2001537	-3.0982376	-0.0870315	H	0.6800669	2.7453816	3.3813156
N	-1.3825739	-0.6492243	-1.9141972	H	0.0439985	3.1051545	4.9633769
N	-0.5899380	-2.1344268	0.6163963	C	1.0874226	1.2392009	4.8747287
C	-3.0092682	-1.9560894	-3.2472500	H	2.0431827	1.7290604	5.0989512
H	-3.5231259	-2.9125377	-3.1742161	H	0.6684363	0.9493798	5.8463782
H	-2.5073294	-1.9108806	-4.2148415	C	-0.0998097	-2.6039193	1.8874983
H	-3.7571514	-1.1615166	-3.2433530	C	0.8091440	-3.7213696	4.2844175
C	-1.2022982	-4.5362535	0.4191459	C	1.2303507	-3.0550371	1.9907656
H	-1.6222651	-5.1947771	-0.3382723	C	-0.9833654	-2.7424442	2.9753346
H	-1.7878578	-4.6526497	1.3313780	C	-0.5044680	-3.2919983	4.1675640
H	-0.1930190	-4.8788067	0.6493617	C	1.6654224	-3.6047574	3.1964892
Ir	-0.1327361	-0.1476598	-0.1879702	H	-1.1827745	-3.3936804	5.0084497
C	1.0708893	0.7408848	1.5589612	H	2.6895343	-3.9531824	3.2765125
H	1.6865155	1.4377710	1.0196533	H	1.1633704	-4.1506468	5.2144778
C	-0.2888332	1.1229197	1.5721571	C	-1.6672420	0.3564900	-2.9061106
H	-0.5159812	2.0891878	1.1350417	C	-2.2371838	2.3520164	-4.7799044
C	1.3353326	0.7170361	-1.5461739	C	-2.6434489	1.3349692	-2.6176815
				C	-1.0048620	0.3589144	-4.1455641
				C	-1.2975469	1.3744196	-5.0630609
				C	-2.9116966	2.3210842	-3.5632786

H	-0.7802385	1.3839839	-6.0170247	H	3.2343027	0.2647550	-0.5646189
H	-3.6589758	3.0751658	-3.3412083	C	-1.8530725	0.9524537	-1.6813243
H	-2.4523660	3.1300209	-5.5033327	C	-2.7405575	2.9307958	-3.4344050
C	2.1563273	-3.0110049	0.8029551	C	-2.8255590	1.8735311	-1.2530945
H	3.1799437	-3.2406103	1.1031187	C	-1.3167435	1.0226563	-2.9780403
H	2.1344999	-2.0325961	0.3204766	C	-1.7759983	2.0188419	-3.8413068
H	1.8604479	-3.7394309	0.0413666	C	-3.2554803	2.8563478	-2.1457782
C	-2.4515281	-2.4014922	2.8694163	H	-1.3645765	2.0791129	-4.8431672
H	-2.6564054	-1.7135937	2.0530027	H	-4.0059582	3.5696585	-1.8226436
H	-2.8144535	-1.9580834	3.7989365	H	-3.0863865	3.6992485	-4.1158449
H	-3.0463410	-3.3040908	2.6931813	C	0.4886224	-1.8454910	2.6648790
C	-0.0245138	-0.7171412	-4.5543470	C	1.9689293	-2.2964617	4.9841458
H	0.2089703	-1.3979118	-3.7382858	C	-0.0488904	-1.4815315	3.9125145
H	0.9088702	-0.2786600	-4.9155544	C	1.7623471	-2.4336308	2.5718526
H	-0.4316798	-1.3141021	-5.3767977	C	2.4866730	-2.6511895	3.7453071
C	-3.3844135	1.3215145	-1.3072207	C	0.7094194	-1.7156265	5.0607540
H	-2.6878660	1.3800686	-0.4677143	H	3.4711481	-3.1019397	3.6805634
H	-3.9520306	0.3965313	-1.1740675	H	0.3018035	-1.4368480	6.0263967
H	-4.0813201	2.1588803	-1.2498022	H	2.5447473	-2.4701685	5.8856788
=====							
67							
XyNacnacIr_TS_1_2.xyz							
C	-2.1003512	-1.2512546	-0.8966782	C	-0.2731409	0.0394289	-3.4444002
H	-2.5111842	-3.2320059	-0.3385216	H	0.4898166	-0.1240209	-2.6817868
C	-1.8967023	-2.3772524	-0.0993412	H	0.2088669	0.3934947	-4.3570312
C	-1.0672578	-2.5288993	1.0182465	H	-0.7059955	-0.9420177	-3.6615772
N	-1.4274832	-0.0955334	-0.7935728	C	-3.4111549	1.7942738	0.1326381
N	-0.2551897	-1.5803035	1.4634616	H	-2.6237400	1.7649434	0.8886255
C	-3.2116220	-1.3796813	-1.9247281	H	-4.0056671	0.8858287	0.2685618
H	-3.6421677	-2.3781993	-1.8890630	H	-4.0595715	2.6498424	0.3267524
H	-2.8569413	-1.1929029	-2.9385786	C	2.3411966	-2.8287795	1.2375748
H	-4.0074516	-0.6566003	-1.7341152	H	1.8416602	-3.7099963	0.8237410
C	-1.1585552	-3.8528917	1.7523621	H	3.4018544	-3.0658855	1.3322970
H	-1.8328785	-4.5295682	1.2309406	H	2.2177573	-2.0316493	0.5017524
H	-1.5305104	-3.7150804	2.7700138	C	-1.4147321	-0.8532270	4.0191995
H	-0.1830752	-4.3339546	1.8371720	H	-1.6324363	-0.5808415	5.0526917
Ir	0.0729755	0.3199096	0.6096558	H	-2.2019103	-1.5313880	3.6780501
H	0.5102000	0.7520654	2.1027508	H	-1.4893168	0.0420805	3.3977815
C	1.7621605	1.5837430	0.2864500	=====			
C	1.9121335	1.0267556	1.6269963	67			
C	0.6794919	2.4970870	0.1003664	XyNacnacIr_TS_2_3.xyz			
H	2.6369960	0.2305341	1.7524246	C	-2.4103602	-0.7622178	-1.3324627
C	0.2094631	3.4347256	1.2032551	H	-3.0435371	-2.6889267	-0.7880949
H	0.7531937	4.3883563	1.1426508	C	-2.3650157	-1.8946259	-0.5152916
H	-0.8502093	3.6665716	1.0761791	C	-1.6163012	-2.1188922	0.6447914
H	1.9264223	1.7121456	2.4728555	N	-1.6610716	0.3296552	-1.1630768
H	0.3352548	3.0451780	2.2111385	N	-0.7219041	-1.2643552	1.1354041
C	0.5201537	3.1597169	-1.2518598	C	-3.4290738	-0.8026816	-2.4575529
H	0.7518208	2.5091607	-2.0900096	H	-3.9332934	-1.7667796	-2.4759263
H	1.1847966	4.0322988	-1.3144196	H	-2.9653729	-0.6372506	-3.4305990
H	-0.4974814	3.5234400	-1.3927668	H	-4.1835881	-0.0228787	-2.3331430
C	2.7863874	1.2395661	-0.7632840	C	-1.9014199	-3.4153886	1.3803743
H	3.5918805	1.9841998	-0.7541802	H	-2.6521061	-3.9960097	0.8477471
H	2.3681152	1.2228787	-1.7681016	H	-2.2710359	-3.2196763	2.3893788
				H	-1.0051343	-4.0273025	1.4876614
				Ir	-0.2317553	0.6378924	0.3555975
				H	0.3240401	0.9456259	1.8328604

C	1.3328409	2.0184062	-0.0753721	C	-2.6223924	-0.7898148	-0.7637785
C	1.7146804	1.4427949	1.2256458	H	-3.1935429	-2.7647467	-0.3388281
C	0.1271847	2.7653186	-0.0719421	C	-2.4929214	-1.9904421	-0.0641251
H	-0.2147085	3.1671353	-1.0167517	C	-1.6217052	-2.3147874	0.9841847
C	1.7973496	2.3834615	2.4337456	N	-1.8327484	0.2800560	-0.6045432
H	1.8188733	1.8192195	3.3685431	N	-0.7270882	-1.4737888	1.4871024
H	2.7284590	2.9570633	2.3689711	C	-3.7826420	-0.7197356	-1.7404699
H	-0.1851748	3.3397507	0.7912489	H	-4.3397956	-1.6542713	-1.7318144
H	0.9713142	3.0900860	2.4805261	H	-3.4518288	-0.5264153	-2.7609798
C	2.2042090	1.9092153	-1.2977562	H	-4.4652620	0.0899816	-1.4737402
H	1.6351021	2.1550392	-2.1938354	C	-1.7622930	-3.7051186	1.5728132
H	2.6383787	0.9177206	-1.4245392	H	-2.5042844	-4.2782297	1.0201161
H	3.0311811	2.6261559	-1.2254237	H	-2.0697815	-3.6642338	2.6198783
C	2.8554858	0.4449684	1.2577065	H	-0.8155904	-4.2473677	1.5445493
H	3.8129001	0.9807424	1.2460178	Ir	-0.3276273	0.4860612	0.8321336
H	2.8381179	-0.2429655	0.4166748	H	0.0736708	0.8028727	2.3575059
H	2.8225456	-0.1427136	2.1755691	C	1.3685573	1.7733916	0.6080066
C	-1.8874608	1.4164429	-2.0769779	C	1.4967936	1.1315987	1.9148863
C	-2.2842243	3.5483978	-3.8300773	C	0.2256619	2.6093412	0.4909544
C	-2.8011051	2.4310300	-1.7403703	H	0.0075676	3.0680805	-0.4640952
C	-1.1743160	1.4613421	-3.2873496	H	2.2366796	0.3451001	2.0222670
C	-1.3850068	2.5400988	-4.1495950	H	-0.1177042	3.1786481	1.3491233
C	-2.9862809	3.4876071	-2.6322209	H	1.4644268	1.7783569	2.7924927
H	-0.8338523	2.5838895	-5.0829647	C	2.4664930	1.5911735	-0.4261905
H	-3.6872595	4.2751061	-2.3774514	H	2.6765672	0.5173375	-0.4920618
H	-2.4361956	4.3791524	-4.5093439	C	3.7495847	2.2850797	0.0767398
C	-0.0519580	-1.6381176	2.3520600	H	4.0779841	1.8855930	1.0380877
C	1.2905029	-2.3170650	4.7021227	H	3.5856820	3.3596516	0.1954856
C	1.1088214	-2.4292955	2.2864115	H	4.5616878	2.1462580	-0.6412742
C	-0.5522624	-1.1955651	3.5914379	C	2.1098386	2.1048687	-1.8212494
C	0.1368615	-1.5437278	4.7536603	H	2.9027893	1.8489799	-2.5281025
C	1.7660950	-2.7566360	3.4744999	H	2.0025005	3.1924030	-1.8242198
H	-0.2422659	-1.2042926	5.7114816	H	1.1803924	1.6759383	-2.1881543
H	2.6656068	-3.3612958	3.4287053	C	-2.1015387	1.4170749	-1.4441533
H	1.8139629	-2.5765808	5.6149332	C	-2.5786513	3.6370583	-3.0642543
C	-3.5532798	2.3929350	-0.4363447	C	-2.8840646	2.4788856	-0.9550103
H	-2.8619114	2.3351847	0.4078417	C	-1.5708980	1.4545428	-2.7457459
H	-4.2024593	1.5158150	-0.3651296	C	-1.8167586	2.5784675	-3.5380873
H	-4.1751900	3.2821196	-0.3242175	C	-3.1098348	3.5795828	-1.7813297
C	-0.2164941	0.3621826	-3.6731892	H	-1.4031709	2.6168115	-4.5401867
H	-0.7472520	-0.5193394	-4.0473667	H	-3.7098423	4.4027019	-1.4089163
H	0.3770867	0.0304022	-2.8211466	H	-2.7596326	4.5025015	-3.6909140
H	0.4558621	0.6967925	-4.4647652	C	0.0490108	-1.9096191	2.6158990
C	-1.8142455	-0.3763637	3.6758364	C	1.5999742	-2.6884899	4.7979632
H	-2.0171972	-0.0884594	4.7082883	C	-0.4215520	-1.6745684	3.9202483
H	-2.6808869	-0.9308681	3.3048717	C	1.2915027	-2.5306509	2.3981064
H	-1.7429119	0.5267226	3.0654477	C	2.0516864	-2.9143241	3.5042477
C	1.6378419	-2.9387256	0.9692840	C	0.3716532	-2.0716685	4.9980590
H	2.6959558	-3.1925177	1.0510463	H	3.0115032	-3.3930395	3.3430995
H	1.1113442	-3.8433057	0.6477397	H	0.0162147	-1.8925405	6.0069580
H	1.5090920	-2.2017410	0.1766088	H	2.2031321	-2.9897103	5.6464312
=====				C	-0.7780704	0.3009655	-3.3100680
67	XyNacnacIr_TS_3_4.xyz			H	-0.1457452	-0.1654129	-2.5546008
				H	-0.1510779	0.6331980	-4.1387774

H	-1.4347384	-0.4848593	-3.6974487	C	1.3951715	-2.9634327	2.4182354
C	-3.4718510	2.4366026	0.4305506	C	2.2370771	-3.1182013	3.5201848
H	-2.6886617	2.3096183	1.1814838	C	4.1724749	-2.9352958	2.1128697
H	-4.1580035	1.5940154	0.5536298	H	1.7990562	-3.2508833	4.5036093
H	-4.0226521	3.3538969	0.6432308	H	5.2505984	-2.9229723	1.9945591
C	1.7990431	-2.7829337	1.0018994	H	4.2593048	-3.2239230	4.2409077
H	1.2119992	-3.5503576	0.4886183	C	-1.1233406	-0.1395998	-2.8028553
H	2.8365796	-3.1191402	1.0236776	C	-2.3656197	1.9165793	-4.2216665
H	1.7299388	-1.8815263	0.3893668	C	-0.4322822	0.4994289	-3.8472808
C	-1.7526666	-1.0101664	4.1628838	C	-2.4300206	0.2515922	-2.4610395
H	-1.9044524	-0.8330673	5.2284528	C	-3.0343415	1.2811735	-3.1835167
H	-2.5847164	-1.6229541	3.8042588	C	-1.0730402	1.5247642	-4.5445978
H	-1.8236703	-0.0560970	3.6359151	H	-4.0425888	1.5855497	-2.9245075
=====				H	-0.5460167	2.0195511	-5.3532058
69				H	-2.8485638	2.7135433	-4.7748623
XyNacnacIr_TS_6_7.xyz				C	-3.1704375	-0.4132848	-1.3290017
C	-0.6150821	-2.4399579	-2.4819426	H	-3.2795178	-1.4899361	-1.4809268
C	-0.0468507	-3.5583597	-1.8620458	H	-4.1676865	0.0146680	-1.2187479
C	0.7509022	-3.6335201	-0.7097199	H	-2.6408862	-0.2867696	-0.3803726
N	-0.4839620	-1.1845471	-2.0529914	C	0.9767385	0.1067158	-4.2064932
N	1.1189167	-2.5810940	0.0096783	H	1.3154963	0.6534734	-5.0874776
C	-1.4396732	-2.7131845	-3.7261773	H	1.0676435	-0.9620560	-4.4128990
H	-1.4629888	-3.7799049	-3.9396416	H	1.6624322	0.3194320	-3.3825971
H	-1.0292907	-2.1955369	-4.5953479	C	-0.1008213	-2.9688950	2.6019022
H	-2.4665322	-2.3616874	-3.6090115	H	-0.3586232	-3.1246880	3.6503484
C	1.1923941	-5.0228010	-0.2882853	H	-0.5858756	-3.7524527	2.0145846
H	0.7898287	-5.7743314	-0.9647948	H	-0.5433857	-2.0218935	2.2811280
H	0.8566550	-5.2543161	0.7245134	C	3.9908837	-2.5912808	-0.3737433
H	2.2806034	-5.1097219	-0.2844349	H	3.6360690	-1.6733174	-0.8464975
C	0.7890312	1.3361967	0.9385623	H	3.7385028	-3.4063567	-1.0574656
C	0.1451342	1.5494576	-0.3505913	H	5.0778289	-2.5462027	-0.2942742
H	-0.9237831	1.7478437	-0.3313426	=====			
Ir	0.6145836	-0.5297434	-0.3810910	69			
H	1.8915064	-0.1189659	-1.1301109	XyNacnacIr_TS_7_8.xyz			
H	1.4204338	-0.0030275	0.9818086	C	-0.0489572	-1.5237373	-2.7296708
H	-0.2604405	-4.5046317	-2.3362402	C	0.4569579	-2.7236140	-2.2205336
C	2.1016835	2.0864950	1.2766423	C	0.9960751	-2.9733667	-0.9526718
H	2.4847205	1.6490446	2.2062258	N	-0.1361939	-0.4056861	-2.0144524
C	1.7989634	3.5720207	1.5482395	N	1.1311737	-2.0587428	0.0056121
H	2.7178112	4.0934086	1.8258982	C	-0.4918802	-1.5247136	-4.1785457
H	1.0857768	3.7120480	2.3615648	H	-0.3495971	-2.5094809	-4.6197481
H	0.6609371	2.1649447	-1.0812232	H	0.0811603	-0.8006538	-4.7625011
H	1.3947921	4.0565153	0.6560799	H	-1.5430288	-1.2503950	-4.2809403
C	-0.1472490	1.2199065	2.1383191	C	1.4660002	-4.3899061	-0.6836809
H	0.3507676	0.7692608	2.9994209	H	1.2678721	-5.0204613	-1.5481799
H	-1.0238702	0.6178444	1.8945959	H	0.9590173	-4.8226855	0.1806982
H	-0.5065480	2.2097658	2.4297446	H	2.5365360	-4.4243251	-0.4718090
C	3.2077863	1.9679533	0.2255558	Ir	0.5460585	-0.1284065	-0.0729961
H	4.0890496	2.5241172	0.5543506	H	1.6227486	0.2048578	1.0986290
H	2.8981138	2.3813722	-0.7370740	C	0.5727638	0.8469421	1.8790355
H	3.5041799	0.9305466	0.0709883	H	1.3865635	1.0883189	2.5683546
C	1.9690838	-2.7921958	1.1457487	C	0.1114424	2.0649147	1.0844433
C	3.6184496	-3.1039498	3.3752531	H	-0.1120648	1.7396799	-0.0011083
C	3.3663102	-2.7790276	0.9843061	H	0.4464083	-3.5649065	-2.8974182

C	-1.2383039	2.6842621	1.5471609	C	0.9487952	-2.5985927	-1.7906778
H	-1.4296962	3.5249151	0.8697159	N	-0.1417931	-0.1336823	-3.2481426
C	-1.1494843	3.2465859	2.9740164	N	1.1491014	-1.5790609	-0.9512272
H	-0.9466174	2.4542988	3.6995836	C	-0.7883781	-1.6449302	-5.0770513
H	-2.0982614	3.7116426	3.2519587	H	-0.7512098	-2.7066341	-5.3119558
H	-0.1989558	0.3301403	2.4453683	H	-0.2654746	-1.0975177	-5.8632387
H	-0.3722267	4.0052973	3.0760485	H	-1.8294231	-1.3189074	-5.1085309
C	1.2160074	3.1197363	0.9374064	C	1.4101302	-3.9892527	-1.3956024
H	2.1229684	2.6714797	0.5314563	H	1.1945647	-4.7045859	-2.1865020
H	1.4620982	3.5609604	1.9054037	H	0.9213335	-4.3275186	-0.4807115
H	0.9050323	3.9234539	0.2658383	H	2.4838466	-4.0031482	-1.1991908
C	-2.4227214	1.7227578	1.4255764	Ir	0.6627919	0.4783406	-1.3995370
H	-2.5121869	1.3255225	0.4148286	H	1.8178002	1.0016239	-0.4564215
H	-3.3532014	2.2425041	1.6679082	C	0.7482799	1.1292780	0.7513742
H	-2.3314318	0.8766441	2.1108936	H	1.4183921	0.5011987	1.3328226
C	1.7579551	-2.4413713	1.2432175	H	0.2473834	-3.4287538	-3.5830186
C	2.9606154	-3.1267145	3.6587580	C	0.9297214	2.6115812	1.1281901
C	0.9609865	-2.8991476	2.3067209	H	1.7673244	3.0188634	0.5502511
C	3.1525868	-2.3216540	1.3793187	H	-0.2865947	1.7296489	-1.4212316
C	3.7343062	-2.6701279	2.5990736	H	1.1034351	1.8385724	-2.0459134
C	1.5843993	-3.2381906	3.5087499	C	1.3326763	2.7877876	2.6248122
H	4.8088073	-2.5793417	2.7151052	H	1.3087517	3.8690133	2.8088704
H	0.9777869	-3.5909524	4.3357104	C	0.3550780	2.1356091	3.6125373
H	3.4287911	-3.3918696	4.5995918	H	0.6325153	2.3807539	4.6412455
C	-0.6967710	0.7698971	-2.6163624	H	-0.6711454	2.4769345	3.4602232
C	-1.7831020	3.1089313	-3.6790339	H	-0.2692519	0.8026574	0.9749032
C	0.1547862	1.7351200	-3.1882373	H	0.3638780	1.0463780	3.5235344
C	-2.0904756	0.9670428	-2.5851260	C	-0.3023478	3.4601953	0.7897583
C	-2.6128772	2.1462760	-3.1194992	H	-0.1553529	4.4989070	1.0979290
C	-0.4101906	2.8980482	-3.7131157	H	-1.1973110	3.0851678	1.2937927
H	-3.6851401	2.3077349	-3.0918319	H	-0.5063050	3.4580331	-0.2814552
H	0.2397354	3.6467112	-4.1529283	C	2.7691647	2.3226434	2.8987374
H	-2.2041173	4.0204795	-4.0870816	H	3.4778768	2.8079358	2.2222358
C	4.0066846	-1.8247858	0.2421749	H	2.8803280	1.2419154	2.7803441
H	3.6279889	-0.8772328	-0.1472746	H	3.0655593	2.5681934	3.9222772
H	4.0115677	-2.5255218	-0.5976707	C	1.7697430	-1.8779499	0.3086456
H	5.0387050	-1.6878355	0.5679745	C	2.9632241	-2.3954397	2.7753797
C	-0.5329417	-3.0262086	2.1608437	C	0.9690735	-2.2471523	1.4042265
H	-0.9977645	-3.2367512	3.1251161	C	3.1643247	-1.7568574	0.4436138
H	-0.8054731	-3.8350976	1.4764002	C	3.7411097	-2.0220023	1.6868928
H	-0.9640169	-2.1123866	1.7461322	C	1.5866733	-2.5049968	2.6293460
C	1.6448904	1.5205151	-3.2450315	H	4.8160993	-1.9317005	1.7980958
H	1.9063515	0.6981938	-3.9176530	H	0.9747307	-2.7892078	3.4785009
H	2.0395902	1.2533521	-2.2617746	H	3.4274364	-2.5958986	3.7337590
H	2.1502654	2.4186585	-3.6030540	C	-0.6836203	0.9121629	-4.0785087
C	-3.0140484	-0.0718169	-2.0008638	C	-1.7161327	2.9765967	-5.6362133
H	-3.9909971	0.3614182	-1.7805448	C	0.1548029	1.5753759	-4.9902719
H	-2.6031001	-0.5037108	-1.0874671	C	-2.0320184	1.2789099	-3.9342478
H	-3.1747058	-0.9027752	-2.6953334	C	-2.5298855	2.3145733	-4.7263651
=====				C	-0.3837570	2.6061465	-5.7619685
71				H	-3.5695274	2.6047391	-4.6211364
XyNacnacIr_TS_9_10.xyz				H	0.2563670	3.1248452	-6.4671147
C	-0.1714455	-1.3779094	-3.7173244	H	-2.1177907	3.7800469	-6.2424986
C	0.3385040	-2.4971552	-3.0450640	C	-2.9288392	0.5858623	-2.9410848

H	-3.0113522	-0.4863072	-3.1384529	C	2.6080971	-2.9760278	3.1575920
H	-3.9329829	1.0106962	-2.9700129	C	0.5492699	-2.8093377	1.8867123
H	-2.5409547	0.6856474	-1.9242907	C	2.6583942	-2.0143084	0.9320085
C	1.6074467	1.2010391	-5.1328511	C	3.3084617	-2.4001764	2.1044139
H	1.7352724	0.1673451	-5.4659598	C	1.2394406	-3.1790807	3.0432778
H	2.1315257	1.2857911	-4.1781126	H	4.3785076	-2.2445454	2.1891027
H	2.1003840	1.8493408	-5.8583398	H	0.6903175	-3.6311916	3.8623451
C	4.0301991	-1.3563602	-0.7231901	H	3.1283333	-3.2665392	4.0629710
H	5.0723143	-1.2670757	-0.4142212	C	-1.2386826	1.1638487	-2.8705329
H	3.7108537	-0.4021305	-1.1484340	C	-2.1998588	3.5628624	-3.9174761
H	3.9820269	-2.0866625	-1.5357332	C	-2.6008793	1.4875242	-2.7292997
C	-0.5277220	-2.3675736	1.2711986	C	-0.3543502	2.0372747	-3.5308821
H	-0.9897109	-2.5095295	2.2488605	C	-0.8567021	3.2325866	-4.0474687
H	-0.8156603	-3.2150349	0.6421353	C	-3.0613625	2.6934227	-3.2609932
H	-0.9612638	-1.4792946	0.8081487	H	-0.1808449	3.9115564	-4.5559894
=====				H	-4.1096392	2.9505068	-3.1538795
69	XyNacnacIr_TS_13_8a.xyz			H	-2.5728222	4.4962584	-4.3227642
C	-0.7311533	-1.1580148	-3.0135982	C	1.1061715	1.6975093	-3.6757019
C	-0.2231201	-2.3780987	-2.5550855	H	1.2576275	0.8274996	-4.3210419
C	0.4006979	-2.6603141	-1.3345521	H	1.6554019	2.5346288	-4.1087501
N	-0.7378101	-0.0473465	-2.2846795	H	1.5452264	1.4456050	-2.7074195
N	0.5713430	-1.7821918	-0.3466423	C	-3.5505577	0.5568495	-2.0193508
C	-1.2739932	-1.1310918	-4.4284675	H	-3.1414156	0.2320285	-1.0601560
H	-1.2282248	-2.1238986	-4.8720835	H	-3.7354627	-0.3525392	-2.5987154
H	-0.7008979	-0.4471277	-5.0587011	H	-4.5124555	1.0430041	-1.8501238
H	-2.3101250	-0.7888530	-4.4539828	C	-0.9317729	-3.0679881	1.7754381
C	0.9354012	-4.0702281	-1.1661987	H	-1.3807222	-3.1732298	2.7645453
H	0.7099705	-4.6650425	-2.0491253	H	-1.1345601	-3.9936930	1.2267361
H	0.5020911	-4.5676990	-0.2974365	H	-1.4356120	-2.2642344	1.2393837
H	2.0178868	-4.0679053	-1.0217446	C	3.4338212	-1.3987866	-0.2028724
Ir	-0.0312115	0.1689463	-0.3281543	H	3.4447620	-2.0485350	-1.0828891
H	0.8913858	0.3414636	0.9909642	H	4.4684249	-1.2167033	0.0910767
C	-0.1859429	1.2131195	1.6255724	H	2.9801322	-0.4571604	-0.5199485
C	-0.7446986	2.1883395	0.6087343	=====			
H	-0.3085127	3.1880993	0.6648168	71	XyNacnacIr_TS_14_10.xyz		
H	-0.4149401	1.9604264	-0.4980710	C	0.1709470	-1.4740025	-3.7663324
H	-0.2854489	-3.2030369	-3.2489873	C	0.8501743	-2.5799456	-3.2502487
C	-1.2398278	0.5160927	2.4782334	C	1.6030100	-2.7291431	-2.0726903
H	-0.7920396	-0.3030245	3.0434617	N	0.1206545	-0.2684075	-3.1962553
H	-1.6895232	1.2090222	3.1972125	N	1.7697795	-1.7906643	-1.1472208
C	0.9600024	1.7966467	2.5160485	C	-0.5435891	-1.6947575	-5.0870119
H	1.3451794	0.9516126	3.0982947	H	-0.4508810	-2.7322327	-5.4013765
H	-1.8290877	2.2597955	0.6131326	H	-0.1326468	-1.0576328	-5.8723607
H	-2.0384692	0.1079451	1.8615181	H	-1.6039985	-1.4493654	-5.0092263
C	0.4365835	2.8456368	3.5139108	C	2.2768001	-4.0822714	-1.9076962
H	1.2674553	3.2462332	4.0991331	H	2.0679887	-4.7212095	-2.7631525
H	-0.2876836	2.4343192	4.2171000	H	1.9446656	-4.5966909	-1.0055077
H	-0.0334910	3.6885249	2.9985192	H	3.3590545	-3.9662621	-1.8204672
C	2.1373434	2.3854285	1.7287922	Ir	1.0487402	0.3155011	-1.3886706
H	2.9431344	2.6586450	2.4142715	H	2.1013848	0.7244821	-0.2696739
H	1.8524804	3.2919906	1.1869949	C	0.8756296	1.2358842	0.7454502
H	2.5346172	1.6764062	1.0016207	H	0.8006344	-3.4645471	-3.8670046
C	1.2692115	-2.2159290	0.8351224	C	1.0306099	2.7829106	0.6911633

H	0.3762211	3.1266457	-0.1124347	71			
H	0.3864073	1.7249519	-1.6439531		XyNacnacIr_TS_23_24.xyz		
H	2.1048868	1.1838871	-2.0987106	C	-2.0338039	-1.6501649	-1.9009300
C	-0.5933136	0.8305281	0.9147318	H	-2.5064144	-3.6238234	-1.3590428
H	-0.7530982	-0.2344396	0.7231218	C	-1.9047004	-2.7721604	-1.0787165
H	-1.2533654	1.4043342	0.2651641	C	-1.1622365	-2.9228575	0.0982930
C	0.5494636	3.4697460	1.9870561	N	-1.3671186	-0.5035855	-1.7370936
H	0.5549913	4.5528955	1.8440856	N	-0.3552554	-1.9891855	0.5919744
H	1.2034365	3.2517207	2.8343612	C	-3.0344996	-1.7742666	-3.0353206
H	-0.9107191	0.9940589	1.9527467	H	-3.4539053	-2.7779666	-3.0615376
H	-0.4676552	3.1836700	2.2596082	H	-2.5755598	-1.5654396	-4.0026089
C	1.6913334	0.6191164	1.8883211	H	-3.8546905	-1.0629719	-2.9176445
H	2.7535823	0.8577621	1.8279448	C	-1.3380494	-4.2334640	0.8411243
H	1.6021036	-0.4638023	1.9017531	H	-1.9891627	-4.9023997	0.2817090
H	1.3180295	0.9889067	2.8481238	H	-1.7794140	-4.0712536	1.8269571
C	2.4483967	3.2678414	0.3666322	H	-0.3831266	-4.7352684	1.0034828
H	3.1634883	2.9798433	1.1417638	Ir	0.0841944	-0.1261274	-0.2706318
H	2.4637330	4.3586699	0.3033392	H	0.7026257	0.2723931	1.1703954
H	2.8017348	2.8748827	-0.5864093	C	1.6637466	1.1942384	-0.7712871
C	2.5522099	-2.1505316	-0.0010785	C	2.0789444	0.5486932	0.4716388
C	4.0596380	-2.8111314	2.2565807	C	0.5029551	1.9965267	-0.8905698
C	3.9213819	-1.8268298	0.0425338	H	0.2672677	2.1698611	-1.9371453
C	1.9401538	-2.8132862	1.0796464	H	2.1920257	0.9112426	-1.6760486
C	2.7110073	-3.1338975	2.1985226	H	2.7277850	-0.2962546	0.2514249
C	4.6544865	-2.1637151	1.1810596	C	-0.0468278	3.1618369	-0.0833454
H	2.2397693	-3.6376494	3.0355902	H	0.5548075	4.0464913	-0.3428049
H	5.7098428	-1.9162979	1.2182953	H	-1.0341242	3.3626425	-0.5099722
H	4.6445192	-3.0634614	3.1332320	C	2.6342496	1.2368439	1.7331251
C	-0.5588243	0.7815652	-3.9116787	H	3.1603850	0.4574305	2.2911887
C	-1.8736391	2.8457585	-5.2492744	H	3.4087871	1.9338313	1.3885483
C	0.1470840	1.5676586	-4.8392318	C	-0.2166283	3.1270881	1.4373851
C	-1.9200380	1.0201755	-3.6552424	H	-0.7674205	2.2262957	1.7227286
C	-2.5598217	2.0569493	-4.3353902	H	-0.8694329	3.9713106	1.6828760
C	-0.5302352	2.5970340	-5.4951881	C	1.7246212	1.9521587	2.7334415
H	-3.6100828	2.2450627	-4.1411321	H	2.3500688	2.1709586	3.6055532
H	0.0091736	3.2086478	-6.2101649	H	0.9608859	1.2514573	3.0900140
H	-2.3837624	3.6485700	-5.7685717	C	1.0491282	3.2578032	2.3011048
C	-2.6858526	0.1851262	-2.6617465	H	0.7700926	3.7868448	3.2179191
H	-3.7291036	0.5009918	-2.6193779	H	1.7786041	3.9047398	1.7978347
H	-2.2618570	0.2762192	-1.6591091	C	0.2969405	-2.2591941	1.8449051
H	-2.6657076	-0.8781369	-2.9136879	C	1.6033318	-2.7100697	4.2658551
C	1.6074763	1.3310009	-5.1230327	C	1.5600947	-2.8762655	1.8467063
H	1.9469519	1.9704018	-5.9388870	C	-0.3174476	-1.8680978	3.0478471
H	1.8146321	0.2936584	-5.3953955	C	0.3533653	-2.1039388	4.2486992
H	2.2192713	1.5465601	-4.2432389	C	2.1977421	-3.0910736	3.0699428
C	0.4787293	-3.1859062	1.0482380	H	-0.1136592	-1.8036225	5.1803784
H	0.2978608	-4.0752862	0.4365901	H	3.1745060	-3.5627780	3.0788804
H	-0.1326395	-2.3903243	0.6216339	H	2.1122327	-2.8830446	5.2069330
H	0.1153609	-3.4025061	2.0538414	C	-1.6921234	0.5703605	-2.6353997
C	4.6025226	-1.1530086	-1.1205449	C	-2.2945638	2.6736288	-4.3630550
H	4.1361379	-0.1948592	-1.3554343	C	-2.7072986	1.4800818	-2.2926900
H	4.5397990	-1.7564261	-2.0302762	C	-0.9737381	0.7093505	-3.8358746
H	5.6574688	-0.9836194	-0.9012262	C	-1.2910155	1.7696497	-4.6867724
=====				C	-2.9947289	2.5249036	-3.1724448

H	-0.7386275	1.8851298	-5.6129865	C	-0.4088228	3.0857697	2.7891755
H	-3.7763724	3.2311946	-2.9143466	H	-0.9217105	3.6383899	3.5822282
H	-2.5275547	3.4922863	-5.0338052	H	2.3382152	2.4580646	2.9661244
C	0.1166671	-0.2628091	-4.2080607	H	-0.0885568	2.1453235	3.2495185
H	0.8178684	-0.4083554	-3.3838002	C	0.8381199	3.8829763	2.3493300
H	0.6664838	0.0916723	-5.0809371	H	0.6017341	4.4894690	1.4673881
H	-0.2848866	-1.2520598	-4.4473782	H	1.0859717	4.5990718	3.1387458
C	2.2165948	-3.3125626	0.5618764	C	0.9479227	-2.3758666	1.5079558
H	3.2725399	-3.5340641	0.7237664	C	1.6998576	-2.3657393	4.1986525
H	1.7499657	-4.2162142	0.1574685	C	-0.0391405	-2.2947308	2.5076726
H	2.1262697	-2.5470830	-0.2105903	C	2.3117525	-2.4682840	1.8535277
C	-1.6704026	-1.2051443	3.0484354	C	2.6645946	-2.4631767	3.2025119
H	-1.9512098	-0.9036632	4.0585134	C	0.3606151	-2.2846306	3.8467949
H	-2.4505029	-1.8707563	2.6679227	H	3.7125599	-2.5357333	3.4720536
H	-1.6756277	-0.3231936	2.4036752	H	-0.3970192	-2.2145137	4.6199932
C	-3.4714923	1.3358418	-1.0023902	H	1.9921691	-2.3559826	5.2420924
H	-4.0760810	0.4242916	-0.9866607	C	-0.2739535	-0.2518185	-3.6909025
H	-4.1420619	2.1834538	-0.8544929	C	-0.7045487	1.5018946	-5.8123216
H	-2.7908763	1.2710756	-0.1508660	C	0.7844310	0.0505602	-4.5636039
=====							
73							
XyNacnacIr_TS_26_27.xyz							
C	-0.3067827	-2.4618348	-2.7878083	C	-1.5431015	0.3233785	-3.8672818
C	-0.1717217	-3.4691873	-1.8431271	C	-1.7387175	1.1984915	-4.9366440
C	0.2375328	-3.4143658	-0.4901211	C	0.5466391	0.9303125	-5.6202883
N	-0.0528312	-1.1493410	-2.5819405	H	-2.7154375	1.6486995	-5.0772366
N	0.5774494	-2.3027114	0.1284517	H	1.3592189	1.1712125	-6.2969959
C	-0.7651140	-2.9007465	-4.1653906	H	-0.8713185	2.1839578	-6.6378573
H	-0.9227398	-3.9770465	-4.1878171	C	-2.6725847	0.0202299	-2.9178948
H	-0.0282748	-2.6421783	-4.9280977	H	-2.9572838	-1.0356852	-2.9385443
H	-1.6956414	-2.4079782	-4.4522304	H	-3.5554240	0.6094142	-3.1696237
C	0.2764132	-4.7432290	0.2432056	H	-2.3867397	0.2441595	-1.8875732
H	0.0809197	-5.5676898	-0.4399358	C	2.1576191	-0.5308822	-4.3550863
H	-0.4706296	-4.7762319	1.0388678	H	2.1512549	-1.6239680	-4.3685630
H	1.2470185	-4.9055883	0.7150107	H	2.5582239	-0.2325362	-3.3822638
C	1.3106835	0.8851905	0.9621409	H	2.8419057	-0.1880971	-5.1324117
H	1.6602903	0.2429099	1.7669817	C	3.3759365	-2.5938704	0.7933684
C	-0.1188467	0.8536362	0.7438688	H	3.2810174	-3.5310172	0.2369665
H	-0.6557809	0.1733493	1.3999464	H	4.3697241	-2.5719268	1.2425717
Ir	0.6565512	-0.3081329	-0.8618768	H	3.3065343	-1.7921187	0.0557203
H	0.7553851	1.0645287	-1.6565997	C	-1.5107588	-2.2633430	2.1716553
H	2.0164836	0.1645001	-0.1230371	H	-1.9247880	-3.2758761	2.1190835
H	-0.4117064	-4.4595708	-2.2007365	H	-1.7002714	-1.7928224	1.2078519
C	-0.9168614	2.0950379	0.4268938	H	-2.0720072	-1.7292109	2.9404510
H	-0.3212625	2.7861645	-0.1698140	=====			
H	-1.7723260	1.8242794	-0.1982144	73			
C	2.1343590	2.1636064	0.8316069	XyNacnacIr_TS_27_8a.xyz			
H	3.1753166	1.8824371	0.6423940	C	0.5728457	-1.1809834	-2.9799410
H	1.8150262	2.7280569	-0.0458598	C	1.2072566	-2.3404985	-2.5231625
C	-1.4463702	2.7960575	1.6937668	C	1.7574932	-2.5988196	-1.2624025
H	-2.2445057	2.1860871	2.1318242	N	0.3523515	-0.1193931	-2.2120424
H	-1.9179394	3.7368715	1.3883744	N	1.7582502	-1.7454114	-0.2381225
C	2.1122477	3.0637950	2.0802199	C	0.1591421	-1.1559092	-4.4375629
H	2.9452563	3.7677856	1.9811426	H	0.4215054	-2.0936700	-4.9237317
				H	0.6555354	-0.3417578	-4.9708498
				H	-0.9144980	-0.9983971	-4.5513244
				C	2.4206244	-3.9528449	-1.0888529

H	2.3815547	-4.5102180	-2.0226100	H	2.3522114	1.7301991	-2.3257989
H	1.9288966	-4.5468574	-0.3168849	C	4.5440331	-1.0457645	0.1227714
H	3.4663155	-3.8507525	-0.7924013	H	4.6564458	-1.6471163	-0.7839805
Ir	0.9906535	0.1356305	-0.2357975	H	5.5420670	-0.7955035	0.4852733
H	2.0123801	0.4021832	0.9782653	H	4.0327456	-0.1286798	-0.1784007
C	0.9391929	1.1967142	1.6950399	C	0.3045101	-3.3557800	1.7232075
H	1.8360459	1.5237292	2.2339114	H	0.2956398	-4.3795172	1.3333816
C	0.5552943	2.3406678	0.7548424	H	-0.2206444	-2.7291995	1.0048955
H	1.4689946	2.8652499	0.4784798	H	-0.2568257	-3.3662198	2.6592557
H	0.1359774	1.9440311	-0.2337769	=====			
H	1.3113869	-3.1345903	-3.2472811	73			
C	-0.0032155	0.7061467	2.7957368	XyNacnacIr_TS_27_8b.xyz			
H	0.5849026	0.0372285	3.4316286	C	0.1488420	-1.2219466	-3.5377208
H	-0.2205582	1.5766993	3.4315709	C	0.7849378	-2.4083983	-3.1597786
C	-0.4572481	3.4130152	1.2325518	C	1.3496028	-2.7378400	-1.9215635
H	-0.2490756	3.6150303	2.2891929	N	-0.0603552	-0.2053076	-2.7057278
H	-0.1994334	4.3317545	0.6982204	N	1.3658951	-1.9328050	-0.8614233
C	-1.3115624	-0.0173513	2.4655178	C	-0.2967349	-1.1128441	-4.9818711
H	-1.0716056	-0.9843287	2.0229015	H	-0.0700104	-2.0309064	-5.5208038
H	-1.8024362	-0.2289825	3.4238762	H	0.2074019	-0.2853802	-5.4868212
C	-1.9630780	3.1976885	1.0347807	H	-1.3685100	-0.9225562	-5.0599949
H	-2.1539506	2.9775943	-0.0218345	C	1.9954520	-4.1057549	-1.8139523
H	-2.4403644	4.1651489	1.2270967	H	1.8796210	-4.6498733	-2.7492793
C	-2.3179642	0.6835730	1.5463934	H	1.5488827	-4.6987504	-1.0136749
H	-1.9470099	0.6424304	0.5202372	H	3.0618065	-4.0281750	-1.5918745
H	-3.2320800	0.0817143	1.5528289	Ir	0.5441535	-0.0873774	-0.7180611
C	-2.6685067	2.1420528	1.8956266	H	1.4798254	0.1858248	0.5737103
H	-2.4764983	2.3392764	2.9569231	C	0.3035734	0.6340740	1.3354405
H	-3.7444906	2.2885888	1.7611741	H	-0.3966913	-0.0844875	1.7512567
C	2.4182427	-2.1444796	0.9790001	C	-0.3852830	1.7468462	0.5655204
C	3.6870684	-2.8363848	3.3641300	H	0.1282886	2.6954981	0.7393462
C	1.7167579	-2.8787335	1.9501251	H	-0.2010924	1.6642561	-0.5816387
C	3.7654515	-1.7826919	1.1812829	H	0.8717122	-3.1621290	-3.9282922
C	4.3782704	-2.1346156	2.3832009	C	1.2621356	1.1088276	2.4438913
C	2.3694569	-3.2074242	3.1412242	H	2.1613756	1.5492787	2.0008275
H	5.4132423	-1.8554905	2.5479326	H	1.5951085	0.2303933	3.0053019
H	1.8294842	-3.7648890	3.8992199	C	-1.9080268	1.8969430	0.7528831
H	4.1774885	-3.0972244	4.2948056	H	-2.1843569	2.9228912	0.4900899
C	-0.3129228	1.0212189	-2.7750572	H	-2.4141668	1.2549015	0.0300618
C	-1.6067326	3.2888058	-3.7605964	C	0.6694564	2.1465505	3.4145699
C	0.4488988	2.0978736	-3.2706128	H	1.4128702	2.2934724	4.2040122
C	-1.7200625	1.0708163	-2.7864058	H	0.5899166	3.1161595	2.9105973
C	-2.3467776	2.2160848	-3.2819021	C	-2.4805550	1.5628291	2.1405493
C	-0.2188879	3.2230881	-3.7554602	H	-3.5583340	1.7424589	2.0691717
H	-3.4305063	2.2627455	-3.2873266	C	-0.6868775	1.8199493	4.0682818
H	0.3619736	4.0567899	-4.1348394	H	-0.6837417	2.2653755	5.0677117
H	-2.1087333	4.1722334	-4.1379264	H	-0.7782429	0.7393033	4.2296013
C	-2.5499370	-0.0885254	-2.2960517	H	-2.3809657	0.4900550	2.3340808
H	-2.6431222	-0.8652201	-3.0620243	C	-1.9545047	2.3416675	3.3599980
H	-3.5592411	0.2390196	-2.0422969	H	-1.8081743	3.3955967	3.0928595
H	-2.1016657	-0.5605097	-1.4223110	H	-2.7545773	2.3380706	4.1068819
C	1.9543317	2.0395251	-3.2952509	C	2.0236330	-2.3818610	0.3367992
H	2.3730570	3.0109704	-3.5622833	C	3.2741355	-3.1859368	2.6907078
H	2.3140052	1.3085904	-4.0259119	C	3.3881475	-2.0998504	0.5254811

C	1.2798381	-3.0606628	1.3174428	H	1.5807530	2.6832127	0.5645630
C	1.9262673	-3.4548605	2.4902080	H	-0.2416290	1.5909665	-1.3342530
C	3.9950276	-2.5125814	1.7123439	H	1.3750602	1.5488366	-1.7720016
H	1.3602659	-3.9773304	3.2538511	C	-0.9658813	0.4054746	1.2061567
H	5.0467216	-2.2983328	1.8683369	H	-1.1213156	-0.5236724	0.6518642
H	3.7608376	-3.4974580	3.6076503	H	-1.6689801	1.1257485	0.7791299
C	-0.7313543	0.9660962	-3.1915593	C	1.0105566	2.8727176	2.6086203
C	-2.0392906	3.2786501	-4.0378310	H	1.6294020	3.7708294	2.5145964
C	0.0222153	2.0546901	-3.6699389	H	1.6427649	2.1372272	3.1206988
C	-2.1364118	1.0300673	-3.1365829	C	-1.3612010	0.0981563	2.6699771
C	-2.7711244	2.1975434	-3.5641754	H	-0.5245154	-0.3892097	3.1830838
C	-0.6529074	3.2020285	-4.0886176	H	-2.1539005	-0.6551741	2.6191586
H	-3.8534222	2.2555244	-3.5209572	C	-0.1767808	3.2473585	3.5104701
H	-0.0792198	4.0454966	-4.4570865	H	0.2006463	3.9556060	4.2557082
H	-2.5469856	4.1789690	-4.3639798	H	-0.9160921	3.8060791	2.9231659
C	-2.9491292	-0.1354894	-2.6325174	C	-1.8973925	1.2498527	3.5362975
H	-2.9760551	-0.9537240	-3.3585666	H	-2.5454735	0.7988394	4.2952576
H	-3.9796769	0.1672266	-2.4407105	H	-2.5545860	1.8864359	2.9314052
H	-2.5230670	-0.5497950	-1.7167411	C	-0.8837903	2.1267029	4.2855335
C	1.5260450	1.9893625	-3.7297253	H	-0.1315424	1.4846629	4.7607057
H	1.8694588	1.2370325	-4.4455009	H	-1.4249540	2.6035239	5.1098547
H	1.9420159	1.7059884	-2.7595757	C	-0.6367974	0.8439816	-3.9349541
H	1.9421725	2.9521272	-4.0298853	C	-1.7554021	2.9528906	-5.3718991
C	-0.1834425	-3.3579331	1.1164939	C	0.1810477	1.6210018	-4.7732705
H	-0.3400336	-4.1214788	0.3484701	C	-2.0089478	1.1175037	-3.8083918
H	-0.7206440	-2.4679402	0.7813899	C	-2.5498895	2.1763074	-4.5388209
H	-0.6333569	-3.7215191	2.0415100	C	-0.3999938	2.6730166	-5.4832050
C	4.1794198	-1.3572254	-0.5190993	H	-3.6083942	2.3932580	-4.4459702
H	4.2476431	-1.9199697	-1.4541538	H	0.2248768	3.2793138	-6.1298123
H	5.1942600	-1.1647192	-0.1683863	H	-2.1902423	3.7736271	-5.9303180
H	3.7017363	-0.4057770	-0.7649675	C	2.0759670	-2.0765208	0.2248104
=====				C	3.4447920	-2.5459702	2.6162954
75							
XyNacnacIr_TS_29_10.xyz				C	1.4139708	-2.7000490	1.2971121
C	0.0375013	-1.4262126	-3.7372916	C	3.4334959	-1.7098986	0.3393752
C	0.6402065	-2.5514510	-3.1580792	C	4.0960048	-1.9507210	1.5417594
C	1.2748223	-2.7111238	-1.9185223	C	2.1162913	-2.9193339	2.4862099
N	-0.0542073	-0.2263957	-3.1670932	H	5.1390545	-1.6680959	1.6331647
N	1.3711542	-1.7643786	-0.9871138	H	1.6049362	-3.3930278	3.3177534
C	-0.5392313	-1.6285238	-5.1260723	H	3.9735332	-2.7207015	3.5459837
H	-0.4282703	-2.6647997	-5.4383557	C	1.6567504	1.3455593	-4.9048397
H	-0.0416043	-0.9914619	-5.8594998	H	2.1208256	2.0634861	-5.5820984
H	-1.5987424	-1.3686174	-5.1541993	H	1.8561127	0.3425091	-5.2915132
C	1.8916037	-4.0746379	-1.6657119	H	2.1586756	1.4081486	-3.9367742
H	1.7995805	-4.7079760	-2.5455618	C	-2.8857421	0.3028531	-2.8932522
H	1.4096219	-4.5801320	-0.8274112	H	-3.9212419	0.6404111	-2.9537177
H	2.9493769	-3.9833742	-1.4120471	H	-2.5547931	0.3911660	-1.8554396
Ir	0.6455702	0.2828648	-1.2483521	H	-2.8627626	-0.7617936	-3.1393362
H	1.6354259	0.6304532	-0.0571676	C	-0.0141753	-3.1787333	1.1943048
C	0.4712785	0.8945748	0.9589515	H	-0.5542502	-2.9941578	2.1246396
H	1.1298796	0.3254472	1.6221482	H	-0.0518718	-4.2582470	1.0132262
H	0.6317554	-3.4351272	-3.7784863	H	-0.5509929	-2.6962078	0.3800257
C	0.7191200	2.3968059	1.1697574	C	4.1734992	-1.0895645	-0.8178617
H	-0.1220879	2.9620661	0.7557436	H	5.1956341	-0.8409587	-0.5295651
				H	3.6777102	-0.1833490	-1.1710926

H	4.2219179	-1.7680735	-1.6744307
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XyNacnacRh_1.xyz

C	-0.6352735	-1.4643094	-2.2769210
H	-0.7813893	-3.5113722	-1.8039428
C	-0.5780742	-2.5372736	-1.3848785
C	-0.3110673	-2.5087900	-0.0111405
N	-0.3866957	-0.2136007	-1.9155350
N	-0.0518450	-1.4154301	0.7094628
C	-1.0121459	-1.7775959	-3.7111765
H	-1.1575249	-2.8484117	-3.8424255
H	-0.2411465	-1.4453337	-4.4089682
H	-1.9354843	-1.2682568	-3.9965925
C	-0.3418231	-3.8625082	0.6808718
H	-0.5503821	-4.6484208	-0.0422744
H	-1.1084306	-3.8990622	1.4569130
H	0.6084540	-4.0877051	1.1675806
Rh	0.1030904	0.4823705	-0.0323758
C	1.2186647	1.9599882	1.0290626
C	0.0579726	1.8766657	1.8182655
C	1.1148065	2.7048882	-0.2795351
H	2.0429177	2.6856101	-0.8459299
H	0.3155487	2.2740288	-0.9473581
C	-1.1545967	2.7641107	1.5887582
H	-1.2785755	3.1030247	0.5624620
H	-2.0714673	2.2433014	1.8736882
H	0.7775209	3.7403345	-0.1652914
H	-1.0876921	3.6569053	2.2286674
C	2.6131919	1.7268695	1.5516268
H	3.0242053	2.6579804	1.9644570
H	3.2821160	1.4014604	0.7523514
H	2.6427030	0.9804597	2.3419521
C	0.1523921	1.4627621	3.2692109
H	0.8949435	0.6954629	3.4664941
H	-0.8063109	1.0965344	3.6359969
H	0.4091896	2.3414206	3.8767679
C	0.1817105	-1.6166445	2.1075087
C	0.6210068	-2.0868457	4.8205975
C	1.4879751	-1.8668223	2.5659086
C	-0.9044315	-1.6004315	3.0008020
C	-0.6647729	-1.8453425	4.3528861
C	1.6869148	-2.0922962	3.9294801
H	-1.4983632	-1.8361724	5.0469036
H	2.6917737	-2.2826918	4.2911949
H	0.7918816	-2.2694490	5.8751715
C	-0.4930607	0.8276338	-2.8916236
C	-0.6681094	2.9198957	-4.7283863
C	-1.7123720	1.5138819	-3.0507933
C	0.6402326	1.1896694	-3.6453498
C	0.5309340	2.2386920	-4.5587798
C	-1.7781686	2.5567114	-3.9764122
H	1.4003713	2.5238747	-5.1411929
H	-2.7139628	3.0899791	-4.1040215

H	-0.7357408	3.7336369	-5.4409935
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XyNacnacRh_2.xyz

C	-1.8021356	-0.9176352	-1.7945257
H	-2.4115615	-2.8642858	-1.2961881
C	-1.7679684	-2.0567030	-0.9807901
C	-1.0476642	-2.2963227	0.1976007
N	-1.0822029	0.1799060	-1.5853708
N	-0.1860097	-1.4466617	0.7512743
C	-2.7441452	-0.9786292	-2.9843018
H	-3.2154314	-1.9575138	-3.0486234
H	-2.2174678	-0.7849072	-3.9202741
H	-3.5286188	-0.2230629	-2.9047948
C	-1.3077854	-3.6391724	0.8605014
H	-2.0114304	-4.2252398	0.2725817
H	-1.7206868	-3.5097764	1.8630362
H	-0.3881240	-4.2155571	0.9741232
Rh	0.2535384	0.4994792	0.0146288
H	-0.7360248	1.2292213	0.8790882
C	1.9294447	1.8546680	0.1877981
C	1.7549530	1.3997581	1.5255523
C	0.8700913	2.5360619	-0.4650633
H	0.9948206	2.7902026	-1.5104241
C	1.0221968	2.2454950	2.5539871
H	0.5096403	1.6170858	3.2848117
H	1.7505105	2.8496043	3.1121012
H	0.2199756	3.2115648	0.0743118
H	0.2925898	2.9279498	2.1231666
C	2.8437357	0.5784512	2.1822430
H	3.6470747	1.2361022	2.5423351
H	3.2954557	-0.1614101	1.5250432
H	2.4529766	0.0482329	3.0505333
C	3.1457749	1.4680479	-0.6266258
H	3.9985098	2.0821613	-0.3165556
H	2.9788488	1.6477866	-1.6888807
H	3.4424727	0.4266437	-0.4946575
C	0.4283378	-1.8465292	1.9803095

C	1.6343784	-2.6421868	4.3707910	H	0.3052642	2.1678210	-0.4754474
C	1.6394967	-2.5615092	1.9476001	C	2.4652111	1.1693527	2.0162375
C	-0.1810879	-1.5272809	3.2086535	H	2.9623819	2.0266723	2.4881025
C	0.4411720	-1.9306173	4.3912674	H	3.1547695	0.7598556	1.2774797
C	2.2237847	-2.9536748	3.1526380	H	2.3042431	0.4202356	2.7910461
H	-0.0253430	-1.6882524	5.3401258	H	-0.0640062	0.8568837	3.0223718
H	3.1562561	-3.5073826	3.1308122	H	-0.8741963	2.1390912	2.0093288
H	2.1013751	-2.9513409	5.2984975	C	2.4182389	2.5773867	-0.5951186
C	-1.2717162	1.2890654	-2.4717518	H	3.2162226	3.0634086	-0.0271558
C	-1.5888824	3.4777661	-4.1768677	H	2.2693455	3.1471734	-1.5139029
C	-2.2514398	2.2577957	-2.1869676	H	2.7544884	1.5787087	-0.8702319
C	-0.4503843	1.4141745	-3.6072709	C	0.6743992	3.9749285	0.5702804
C	-0.6255751	2.5143683	-4.4475787	H	1.4134782	4.4441524	1.2255303
C	-2.3922216	3.3439474	-3.0520915	H	-0.2866754	3.9912798	1.0825424
H	0.0047653	2.6132902	-5.3247718	H	0.5900841	4.5803590	-0.3350101
H	-3.1462832	4.0931188	-2.8361354	C	-0.1846733	-1.7428264	2.3357028
H	-1.7130170	4.3269878	-4.8385532	C	0.3443904	-2.1402318	5.0440607
C	0.6070283	0.3860512	-3.9177940	C	1.0918256	-2.1752806	2.7373725
H	1.3200989	0.2865284	-3.0950732	C	-1.1999280	-1.5139101	3.2823853
H	1.1600269	0.6626846	-4.8165014	C	-0.9145220	-1.7192548	4.6326013
H	0.1812375	-0.6080339	-4.0772468	C	1.3366364	-2.3656621	4.0989269
C	-3.1291780	2.1457308	-0.9682707	H	-1.6912659	-1.5416136	5.3684785
H	-2.5354424	2.1893842	-0.0515197	H	2.3198503	-2.6959586	4.4166123
H	-3.6723068	1.1982103	-0.9355129	H	0.5505398	-2.2919778	6.0972270
H	-3.8592024	2.9558271	-0.9449002	C	-0.5566600	0.7594615	-2.6633243
C	2.3001740	-2.9114665	0.6387673	C	-0.3519024	2.8436542	-4.5079122
H	2.4650815	-2.0236339	0.0233229	C	-1.6200428	1.6732292	-2.8034198
H	1.6895153	-3.5908726	0.0378240	C	0.6082711	0.8872564	-3.4447918
H	3.2638746	-3.3928262	0.8114506	C	0.6896749	1.9363471	-4.3617677
C	-1.4928182	-0.7877667	3.2585413	C	-1.4963840	2.7079574	-3.7315433
H	-1.7904550	-0.6015700	4.2913925	H	1.5852713	2.0410622	-4.9648014
H	-2.2956543	-1.3499871	2.7736876	H	-2.3112082	3.4150025	-3.8440524
H	-1.4309482	0.1684547	2.7354845	H	-0.2719926	3.6543516	-5.2228456
=====							
67							
XyNacnacRh_3.xyz							
C	-1.0898043	-1.4735787	-2.0305277	C	-2.8725082	1.5387143	-1.9760338
H	-1.5629988	-3.4687509	-1.5465396	H	-2.6387632	1.4795509	-0.9101705
C	-1.1912445	-2.5423573	-1.1346869	H	-3.4224809	0.6258208	-2.2215874
C	-0.8883544	-2.5648244	0.2323403	H	-3.5382586	2.3863991	-2.1448233
N	-0.6362405	-0.2772633	-1.6817544	C	1.7466822	-0.0910582	-3.3070274
N	-0.4490340	-1.5265113	0.9437095	H	2.6489926	0.2975618	-3.7816335
C	-1.5445320	-1.7235727	-3.4547243	H	1.5135341	-1.0504860	-3.7791539
H	-1.8841826	-2.7508929	-3.5738866	H	1.9603857	-0.3061396	-2.2588991
H	-0.7404537	-1.5407959	-4.1700112	C	2.1722079	-2.4525936	1.7240628
H	-2.3655164	-1.0559146	-3.7264954	H	2.2233204	-1.6613637	0.9746457
C	-1.1083326	-3.8957930	0.9319091	H	3.1440471	-2.5457177	2.2113601
H	-1.4691868	-4.6383727	0.2230094	H	1.9840050	-3.3846117	1.1817826
H	-1.8385384	-3.8070998	1.7384608	C	-2.5662019	-1.0491000	2.8528048
H	-0.1870738	-4.2698948	1.3815706	H	-2.4979006	-0.1404602	2.2502180
Rh	-0.0809652	0.3365405	0.2159942	H	-3.1968040	-0.8512804	3.7207202
C	1.1504064	1.5951303	1.4189887	H	-3.0719783	-1.7934484	2.2316346
C	-0.0592378	1.4306779	2.1054085	=====			
C	1.1258808	2.5425705	0.2243732	67			
				XyNacnacRh_4.xyz			
				C	-2.1704327	-0.8511259	-1.4043161
				H	-2.8907042	-2.7549493	-0.8785297

C	-2.1729040	-1.9985461	-0.5980069	H	1.3611665	-3.5105900	0.0722596
C	-1.3828985	-2.3119855	0.5164151	H	2.9883877	-3.4361401	0.7562701
N	-1.3521885	0.1836058	-1.2418331	H	2.2126330	-1.9819666	0.1170948
N	-0.4588616	-1.5091782	1.0351604	C	-1.5596655	-0.9302773	3.6607004
C	-3.1908044	-0.8272894	-2.5287074	H	-1.5069538	0.0681168	3.2193651
H	-3.7687359	-1.7491672	-2.5412255	H	-1.8007632	-0.8280297	4.7195108
H	-2.7127153	-0.7056940	-3.5016947	H	-2.3941066	-1.4382547	3.1710988
H	-3.8810648	0.0108407	-2.4119758	C	0.1561815	0.0524550	-3.7107797
C	-1.6273371	-3.6717695	1.1461539	H	0.9032211	0.3183620	-4.4602254
H	-2.3894613	-4.2182060	0.5940325	H	-0.4556525	-0.7527295	-4.1311350
H	-1.9535845	-3.5758933	2.1835499	H	0.6650014	-0.3686692	-2.8435751
H	-0.7143416	-4.2702875	1.1597155				
Rh	0.0116458	0.4180483	0.3484364	69			
H	-0.9569422	1.1583067	1.2290619		XyNacnacRh_5.xyz		
C	1.7500474	1.6898768	0.6799801	C	-0.9409401	-1.6445813	-2.1614404
C	1.3947177	1.0974075	1.9170771	H	-1.2984157	-3.6314526	-1.5876869
C	0.7686341	2.4693893	0.0204114	C	-1.0224828	-2.6608274	-1.2044148
H	0.9474189	2.8130926	-0.9900915	C	-0.8140706	-2.6030898	0.1772759
H	2.0775256	0.3846943	2.3659196	N	-0.6548426	-0.3818679	-1.8796435
H	0.7837875	1.6416786	2.6273549	N	-0.4409602	-1.5237520	0.8716888
H	0.1158580	3.1098831	0.6012794	C	-1.2186723	-2.0518732	-3.5971253
C	3.0906925	1.3241933	0.0523263	H	-1.4326429	-3.1172207	-3.6557649
H	3.3229529	0.2997123	0.3637433	H	-0.3654745	-1.8355829	-4.2427950
C	4.1698767	2.2411096	0.6639016	H	-2.0696502	-1.5055757	-4.0081903
H	5.1576122	1.9712355	0.2820632	C	-1.0632517	-3.9153514	0.9070999
H	4.1905673	2.1612479	1.7519711	H	-1.3921490	-4.6802869	0.2070802
H	3.9805744	3.2861089	0.4045109	H	-1.8305639	-3.8002541	1.6745396
C	3.1457631	1.3839740	-1.4760696	H	-0.1671954	-4.2769626	1.4123190
H	4.1216813	1.0392727	-1.8259776	Rh	-0.2443426	0.4193032	0.0051235
H	3.0070442	2.4029980	-1.8439898	C	1.0124200	1.7220386	1.4943773
H	2.3849442	0.7554580	-1.9397991	C	-0.2779303	1.4822895	1.9505620
C	-1.4448552	1.2782521	-2.1619175	H	-0.4488646	0.7475907	2.7227367
C	-1.5328502	3.4473963	-3.9203823	C	1.3512615	3.1157084	0.9418935
C	-0.6826922	1.2509019	-3.3446967	H	0.4473845	3.5112834	0.4720795
C	-2.2673581	2.3822921	-1.8675643	C	1.6856296	4.0729269	2.1058648
C	-2.2951622	3.4549646	-2.7592494	H	2.6086244	3.7869743	2.6152310
C	-0.7359890	2.3475187	-4.2067722	H	0.8826070	4.0944383	2.8451015
H	-2.9270967	4.3076426	-2.5355390	H	0.1136271	1.7832534	-0.8455175
H	-0.1439693	2.3317630	-5.1156182	H	-0.7445426	1.8694566	-0.5807622
H	-1.5629294	4.2917847	-4.5988972	H	1.8235913	5.0883038	1.7255705
C	0.2501341	-1.9464191	2.2002553	H	-1.0245145	2.2667705	1.8819655
C	1.6845514	-2.7429715	4.4590669	C	2.1918316	0.9378140	2.0123179
C	1.4772251	-2.6170942	2.0470153	H	2		

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C	-0.9409401	-1.6445813	-2.1614404
H	-1.2984157	-3.6314526	-1.5876869
C	-1.0224828	-2.6608274	-1.2044148
C	-0.8140706	-2.6030898	0.1772759
N	-0.6548426	-0.3818679	-1.8796435
N	-0.4409602	-1.5237520	0.8716888
C	-1.2186723	-2.0518732	-3.5971253
H	-1.4326429	-3.1172207	-3.6557649
H	-0.3654745	-1.8355829	-4.2427950
H	-2.0696502	-1.5055757	-4.0081903
C	-1.0632517	-3.9153514	0.9070999
H	-1.3921490	-4.6802869	0.2070802
H	-1.8305639	-3.8002541	1.6745396
H	-0.1671954	-4.2769626	1.4123190
Rh	-0.2443426	0.4193032	0.0051235
C	1.0124200	1.7220386	1.4943773
C	-0.2779303	1.4822895	1.9505620
H	-0.4488646	0.7475907	2.7227367
C	1.3512615	3.1157084	0.9418935
H	0.4473845	3.5112834	0.4720795
C	1.6856296	4.0729269	2.1058648
H	2.6086244	3.7869743	2.6152310
H	0.8826070	4.0944383	2.8451015
H	0.1136271	1.7832534	-0.8455175
H	-0.7445426	1.8694566	-0.5807622
H	1.8235913	5.0883038	1.7255705
H	-1.0245145	2.2667705	1.8819655
C	2.1918316	0.9378140	2.0123179
H	2.7778000	1.5554685	2.7021269
H	2.8649019	0.6325840	1.2090225
H	1.8736215	0.0548959	2.5569274
C	2.4790175	3.1367960	-0.0970977
H	2.6176797	4.1490694	-0.4844397
H	2.2649731	2.4803540	-0.9423102
H	3.4296222	2.8205571	0.3390724
C	-0.2673791	-1.7342117	2.2804588
C	0.0681894	-2.1309885	5.0254538
C	0.9627713	-2.2083601	2.7721869
C	-1.3392047	-1.4825007	3.1596952
C	-1.1490338	-1.6826041	4.5273593

C	1.1111445	-2.3946621	4.1486259	H	3.2068668	3.8714659	1.6516589
H	-1.9702522	-1.4849722	5.2077102	H	0.4218087	1.5677374	-0.8527397
H	2.0606976	-2.7528630	4.5318471	H	-1.1773966	1.1548360	0.0491243
H	0.2004616	-2.2781531	6.0909040	H	-0.3479018	1.6459586	2.4144904
C	-0.6265704	0.5576804	-2.9667809	H	1.8828036	3.9739449	2.8197215
C	-0.5455188	2.4459318	-5.0161766	C	-0.1890387	3.8648353	0.9249875
C	0.5835961	0.7985086	-3.6413087	H	-0.1912712	4.9166749	0.6300165
C	-1.7961229	1.2591537	-3.3103359	H	-0.5807160	3.8141925	1.9442132
C	-1.7335807	2.1996629	-4.3397090	H	-0.8715126	3.3283860	0.2673483
C	0.6023338	1.7471862	-4.6650740	C	2.7833542	1.2722042	0.9394681
H	-2.6310349	2.7457268	-4.6095407	H	3.4653930	1.6482720	1.7089733
H	1.5326797	1.9395517	-5.1884301	H	3.1826581	1.5739081	-0.0307563
H	-0.5139538	3.1811165	-5.8116910	H	2.8070038	0.1835528	1.0021791
C	1.8401728	0.0552850	-3.2679773	C	-0.3966718	-1.7761547	2.3554666
H	2.0372729	0.1287668	-2.1958100	C	-0.3130486	-1.9593784	5.1433390
H	2.6984452	0.4519184	-3.8121968	C	0.7581365	-2.2712965	2.9902495
H	1.7647479	-1.0122609	-3.4941631	C	-1.5098712	-1.3717221	3.1162305
C	-3.0923744	1.0142356	-2.5815520	C	-1.4480123	-1.4733271	4.5064093
H	-3.8704441	1.6874236	-2.9441828	C	0.7801726	-2.3540429	4.3840022
H	-2.9764321	1.1614279	-1.5048061	H	-2.3049661	-1.1640366	5.0950514
H	-3.4471191	-0.0115918	-2.7129793	H	1.6698454	-2.7332000	4.8751794
C	2.1002425	-2.5551377	1.8432145	H	-0.2808691	-2.0288714	6.2242237
H	2.1426362	-1.8831142	0.9872104	C	-0.2907967	0.4167439	-2.9826588
H	1.9918516	-3.5691714	1.4447017	C	-0.1174049	2.2119768	-5.1114943
H	3.0547705	-2.5159788	2.3707892	C	-1.4327200	1.1338874	-3.3814397
C	-2.6784204	-1.0292030	2.6388917	C	0.9374005	0.5972078	-3.6431030
H	-2.5797062	-0.1595078	1.9864092	C	1.0029215	1.4975059	-4.7066262
H	-3.3475876	-0.7793402	3.4634864	C	-1.3230870	2.0278314	-4.4481123
H	-3.1603653	-1.8081529	2.0409824	H	1.9475122	1.6378781	-5.2209534
=====				H	-2.2003458	2.5843254	-4.7598895
69				H	-0.0510091	2.9075302	-5.9398647
XyNacnacRh_6.xyz				C	2.1710414	-0.1488233	-3.2059777
C	-0.7483854	-1.7462082	-2.1248643	H	2.0247028	-1.2315411	-3.2137885
H	-1.2740192	-3.6912700	-1.5569575	H	2.4479548	0.1200483	-2.1827956
C	-0.9532965	-2.7390883	-1.1619643	H	3.0133892	0.0840775	-3.8587780
C	-0.8405652	-2.6890253	0.2371503	C	-2.7490614	0.9688518	-2.6684368
N	-0.3678808	-0.4955195	-1.8737438	H	-2.6761193	1.3016376	-1.6294828
N	-0.4213917	-1.6385654	0.9320579	H	-3.0740395	-0.0733464	-2.6330555
C	-0.9958009	-2.1651318	-3.5643242	H	-3.5285174	1.5511981	-3.1614031
H	-1.2450132	-3.2231216	-3.6143499	C	1.9552345	-2.7189562	2.1902629
H	-0.1171596	-1.9862133	-4.1865429	H	2.2625655	-1.9631239	1.4648646
H	-1.8147422	-1.5967034	-4.0089361	H	1.7465457	-3.6254717	1.6146630
C	-1.2557986	-3.9600714	0.9621081	H	2.8002495	-2.9306746	2.8470327
H	-1.5382323	-4.7341367	0.2514335	C	-2.7498824	-0.8365577	2.4488022
H	-2.1069392	-3.7714222	1.6199231	H	-2.5194679	0.0281668	1.8228115
H	-0.4539732	-4.3456726	1.5930960	H	-3.4912899	-0.5426716	3.1931020
Rh	0.0764940	0.3184596	-0.0114730	H	-3.2102027	-1.5774221	1.7894555
C	1.3861083	1.8178123	1.1584374	=====			
C	0.5229712	1.1487061	2.0098127	69			
H	0.8751217	0.3011244	2.5789563	XyNacnacRh_7.xyz			
C	1.2343648	3.3100577	0.8385439	C	-0.2687469	-1.1162289	-2.6094041
H	1.5923295	3.4592342	-0.1850418	H	0.4957268	-3.0483974	-2.9641189
C	2.1541377	4.1288801	1.7718956	C	0.3626932	-2.3033252	-2.1936864
H	2.0493306	5.1936578	1.5528119	C	0.8238840	-2.6736579	-0.9260449

N	-0.5097852	-0.0990712	-1.8013416	H	4.5926296	-1.5665377	1.2003639
N	0.7590558	-1.9206571	0.1747090	H	3.2895698	-0.4500226	0.7626014
C	-0.6921568	-1.0469802	-4.0647629	H	3.5494849	-1.8924597	-0.1903308
H	-0.4191852	-1.9591484	-4.5922534	C	1.1202686	2.0114514	-2.9270678
H	-0.2250865	-0.2006065	-4.5722232	H	1.5560119	2.9512090	-3.2691043
H	-1.7719495	-0.9075991	-4.1522386	H	1.4269804	1.2274710	-3.6251961
C	1.4267970	-4.0630113	-0.8167527	H	1.5587204	1.7518813	-1.9611849
H	1.3952387	-4.5672183	-1.7804653	C	-3.3874134	0.0766222	-1.6314121
H	0.8870941	-4.6728486	-0.0896686	H	-3.2676758	-0.8577024	-2.1852316
H	2.4648987	-4.0213984	-0.4817714	H	-3.1059236	-0.1397412	-0.5971267
Rh	0.0343996	-0.0316409	0.2701028	H	-4.4451093	0.3430766	-1.6437571
H	1.4171538	0.5753272	0.2202168	=====			
C	0.1232172	0.4549132	2.2832180	49			
H	1.1039802	0.6269920	2.7170741	XyNacnacRh_8.xyz			
C	-0.6280416	1.6682908	1.8158859	C	-0.9826970	-1.0193344	-1.4346363
H	-0.6368990	1.6585328	0.6243048	H	-0.9803776	-3.0179066	-0.7525183
C	0.0270258	3.0518850	2.0973381	C	-0.6554919	-2.0182001	-0.5031088
H	0.0016039	3.1559638	3.1897716	C	0.0389651	-1.8863437	0.7104700
C	1.4899924	3.1430772	1.6511976	N	-0.6577989	0.2577531	-1.2787922
H	1.9101965	4.1073654	1.9477125	N	0.5048915	-0.7287959	1.1617640
H	1.5714928	3.0674220	0.5634519	C	-1.7444119	-1.4277222	-2.6776090
H	-0.4564592	-0.2199114	2.9128159	H	-1.9404379	-2.4984222	-2.6709109
H	2.1126000	2.3634632	2.0896445	H	-1.1833136	-1.1872236	-3.5836805
C	-2.1153859	1.6267828	2.1957767	H	-2.7007856	-0.9041274	-2.7472050
H	-2.5127985	0.6172725	2.0758977	C	0.2630893	-3.1320436	1.5411950
H	-2.7256255	2.3002490	1.5936476	H	-0.1687750	-4.0018603	1.0494431
H	-2.2335906	1.9043772	3.2472552	H	-0.1911466	-3.0363846	2.5302649
C	-0.7674932	4.2160410	1.4878348	H	1.3281224	-3.3193539	1.6969229
H	-0.8610674	4.1012134	0.4030693	Rh	0.3188222	0.9808996	0.2450131
H	-0.2548311	5.1624783	1.6746738	C	1.2127344	-0.5694608	2.3866599
H	-1.7717150	4.3021982	1.9045044	C	2.6074870	-0.1290405	4.7571401
C	1.2775371	-2.4401147	1.4071676	C	2.6216937	-0.6541608	2.3910245
C	2.2481913	-3.4329118	3.8268846	C	0.5014185	-0.2527672	3.5639749
C	0.4078705	-3.1170234	2.2817133	C	1.2212383	-0.0391030	4.7393343
C	2.6300673	-2.2505679	1.7425830	C	3.2980459	-0.4322569	3.5903949
C	3.0939885	-2.7559445	2.9585214	H	0.6845986	0.2045687	5.6494249
C	0.9132622	-3.6086000	3.4852978	H	4.3804084	-0.4949902	3.6048190
H	4.1368453	-2.6160099	3.2216817	H	3.1502468	0.0437308	5.6791617
H	0.2478094	-4.1348326	4.1610461	C	-0.9793526	1.2876239	-2.2076088
H	2.6268920	-3.8214715	4.7649893	C	-1.5493947	3.3879170	-3.9461200
C	-1.1527188	1.0719582	-2.3060046	C	-0.0575150	1.6196231	-3.2236420
C	-2.4078528	3.4099241	-3.1756892	C	-2.1802480	2.0129072	-2.0524641
C	-0.3791167	2.1246495	-2.8313777	C	-2.4452701	3.0585440	-2.9365905
C	-2.5522931	1.1910750	-2.2090998	C	-0.3659072	2.6733401	-4.0838017
C	-3.1603370	2.3662143	-2.6520730	H	-3.3651125	3.6218692	-2.8264064
C	-1.0270724	3.2837833	-3.2606005	H	0.3352151	2.9364907	-4.8678907
H	-4.2387106	2.4605314	-2.5825647	H	-1.7706164	4.2058866	-4.6217990
H	-0.4356771	4.0974207	-3.6667022	C	-3.1607510	1.6679637	-0.9621469
H	-2.8946270	4.3170428	-3.5141294	H	-3.9608199	2.4080324	-0.9165484
C	-1.0478764	-3.3039955	1.9398725	H	-2.6642735	1.6197842	0.0100211
H	-1.5535616	-3.8814630	2.7149332	H	-3.6185567	0.6884054	-1.1267581
H	-1.5580444	-2.3409443	1.8478353	C	1.2301118	0.8544916	-3.3844794
H	-1.1864500	-3.8206757	0.9872013	H	1.0492237	-0.1780806	-3.6960007
C	3.5680976	-1.5054367	0.8305896	H	1.7754572	0.8025340	-2.4390662

H	1.8652709	1.3249360	-4.1360543	C	1.4624426	-1.6322257	4.1834299
C	-1.0015796	-0.1513919	3.5601936	H	4.6540758	-1.2113100	3.1485032
H	-1.3473267	0.5129461	2.7645284	H	0.8758782	-1.7144067	5.0923298
H	-1.3637419	0.2229379	4.5186102	H	3.3224901	-1.3830720	5.2267111
H	-1.4705736	-1.1230149	3.3803427	C	-0.8625260	-0.0274818	-3.1729973
C	3.3842494	-0.9813597	1.1338494	C	-1.8050972	1.6752057	-5.1735228
H	3.0822292	-0.3283350	0.3114677	C	0.0038111	0.3829803	-4.2036957
H	3.1952264	-2.0066575	0.8029853	C	-2.1961877	0.4196229	-3.1358169
H	4.4575299	-0.8748473	1.2968326	C	-2.6480092	1.2686373	-4.1471777
=====							
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XyNacnacRh_9.xyz							
C	-0.4383048	-2.1676859	-2.2331503	C	-0.4885267	1.2330658	-5.1949971
H	-0.0767585	-4.1109930	-1.5237984	H	-3.6750578	1.6164379	-4.1228286
C	0.0436806	-3.0679793	-1.2717637	H	0.1747037	1.5528668	-5.9913481
C	0.6798495	-2.8308770	-0.0459990	H	-2.1708476	2.3367983	-5.9498036
N	-0.3622970	-0.8488224	-2.1128424	C	-3.1250912	-0.0038716	-2.0268579
N	0.9336319	-1.6333613	0.4872588	H	-3.3199918	-1.0798800	-2.0450621
C	-1.0603588	-2.7791528	-3.4747115	H	-4.0834823	0.5099632	-2.1107879
H	-1.0619168	-3.8656719	-3.4129780	H	-2.6989575	0.2173414	-1.0461143
H	-0.5137969	-2.4843895	-4.3729022	C	1.4411074	-0.0702615	-4.2379718
H	-2.0886334	-2.4377290	-3.6084434	H	1.5280105	-1.1570015	-4.3185825
C	1.1267762	-4.0748419	0.7034156	H	1.9714023	0.2123445	-3.3244394
H	0.9434190	-4.9645975	0.1049258	H	1.9627323	0.3720264	-5.0875893
H	0.5972026	-4.1850263	1.6504945	C	3.8057612	-1.3080676	0.5913065
H	2.1909790	-4.0290385	0.9406064	H	4.8664432	-1.2616664	0.8420727
Rh	0.5366095	0.1704032	-0.4301453	H	3.5445476	-0.4122671	0.0223188
H	1.6379923	0.8241493	0.4351269	H	3.6512806	-2.1575735	-0.0786208
C	-0.3629614	1.0845010	1.2435836	C	-0.6756200	-1.9724834	2.9188177
H	0.1261813	0.6689965	2.1209645	H	-0.8930390	-3.0442780	2.9800573
C	-0.4257193	2.6159233	1.3482966	H	-1.1369471	-1.6004499	2.0066502
H	0.5272627	3.0221041	0.9936054	H	-1.1635844	-1.4998281	3.7730373
H	0.8406115	1.6093761	-1.2662203	=====			
H	-0.0042353	1.6047215	-1.1731607	51			
C	-0.5202630	3.0537674	2.8433980	XyNacnacRh_10.xyz			
H	0.3069460	2.5431516	3.3501706	C	-1.0717926	-0.9307100	-1.5542128
C	-1.8179572	2.6181771	3.5369748	C	-0.6746610	-1.9768919	-0.7134403
H	-1.7787061	2.8556130	4.6033597	C	0.0695320	-1.9018626	0.4753623
H	-2.6888044	3.1326406	3.1221916	N	-0.7663018	0.3308562	-1.2992843
H	-1.3664644	0.6541660	1.1635588	N	0.5383800	-0.7818527	1.0220385
H	-1.9880056	1.5434908	3.4446045	C	-1.8755236	-1.2679994	-2.7900698
C	-1.5419895	3.2180866	0.4834882	H	-2.0417226	-2.3412415	-2.8630720
H	-1.4167324	2.9646447	-0.5715049	H	-1.3620851	-0.9354007	-3.6951584
H	-1.5632673	4.3076955	0.5473542	H	-2.8468509	-0.7682380	-2.7749476
H	-2.5238625	2.8450152	0.7857802	C	0.3497308	-3.2189431	1.1758805
C	-0.2910567	4.5601653	3.0233188	H	-0.0912227	-4.0439171	0.6199365
H	0.6318697	4.8839895	2.5344736	H	-0.0604095	-3.2266750	2.1875274
H	-0.2113213	4.8128190	4.0840633	H	1.4223159	-3.3998583	1.2684487
H	-1.1138150	5.1501113	2.6112129	Rh	0.2757967	1.0384599	0.2538011
C	1.5754747	-1.5963736	1.7748680	H	1.4744219	1.7614063	1.2143568
C	2.8339984	-1.4468632	4.2614795	H	0.7280217	1.8489311	1.6752970
C	0.8119708	-1.7169925	2.9489116	H	-0.9776255	-2.9685464	-1.0152954
C	2.9714091	-1.4172663	1.8405170	C	1.2862638	-0.8440147	2.2424039
C	3.5796417	-1.3472131	3.0925964	C	2.7462982	-0.8979323	4.6114647
				C	0.6129771	-0.7303817	3.4723116
				C	2.6861915	-0.9716288	2.1891607
				C	3.3979760	-0.9992964	3.3888654

C	1.3642255	-0.7626341	4.6476037	H	-2.0041335	2.8964040	1.3190651
H	4.4775648	-1.0968461	3.3590698	H	0.1536380	1.8947159	-1.1172761
H	0.8551515	-0.6753399	5.6010718	H	-0.6922131	1.8674238	-0.8385130
H	3.3147615	-0.9189957	5.5339041	H	-0.8798549	4.0781174	1.9769342
C	-1.1460238	1.4259891	-2.1248949	H	2.3809904	3.8944724	0.7369788
C	-1.8256425	3.6545412	-3.6551188	C	-0.2833664	1.6783236	3.0315749
C	-2.3520721	2.1113541	-1.8616929	H	0.3486670	0.8701154	3.3771191
C	-0.2723366	1.8656453	-3.1432488	H	-1.3226221	1.3670000	3.1422879
C	-0.6353294	2.9807657	-3.8981729	H	-0.1352011	2.5272728	3.7133045
C	-2.6726995	3.2214558	-2.6428218	C	2.4358921	1.4303075	1.8198072
H	0.0286730	3.3248267	-4.6832315	H	2.9276818	2.1815082	2.4528692
H	-3.5975533	3.7531867	-2.4490331	H	3.1895491	1.0603943	1.1218424
H	-2.0895584	4.5213318	-4.2495936	H	2.1297343	0.6123564	2.4596982
C	1.0226429	1.1464906	-3.4199070	C	0.2262124	-1.4885248	2.2585197
H	0.8502775	0.1353525	-3.7995772	C	0.2751334	-1.7851570	5.0374123
H	1.6104034	1.6870807	-4.1629018	C	1.4491592	-1.7194538	2.9141150
H	1.6172246	1.0402199	-2.5096863	C	-0.9779141	-1.4458804	2.9910181
C	-3.2822506	1.6553068	-0.7672895	C	-0.9329370	-1.5982227	4.3751293
H	-2.7538919	1.5557914	0.1837535	C	1.4525518	-1.8472430	4.3065572
H	-3.7156101	0.6754745	-0.9873525	H	-1.8577558	-1.5617307	4.9406124
H	-4.1024507	2.3632660	-0.6416108	H	2.3960288	-2.0114391	4.8167001
C	3.4093989	-1.0620529	0.8712267	H	0.2958350	-1.8907108	6.1158429
H	3.1341501	-1.9624769	0.3149825	C	-0.6617472	0.4744146	-3.0564795
H	4.4890732	-1.0797672	1.0257822	C	-1.2575461	2.2232508	-5.1453020
H	3.1583289	-0.2133956	0.2297704	C	0.3800045	0.9922389	-3.8468034
C	-0.8826907	-0.5630062	3.5277120	C	-1.9991607	0.8328138	-3.3022256
H	-1.2152289	-0.4166974	4.5562055	C	-2.2761536	1.7082522	-4.3535117
H	-1.4064872	-1.4345834	3.1253897	C	0.0596310	1.8651723	-4.8880618
H	-1.2017604	0.2934542	2.9282872	H	-3.3055707	1.9892128	-4.5482720
=====				H	0.8581543	2.2693375	-5.5008903
69	XyNacnacRh_11.xyz			H	-1.4888972	2.9031086	-5.9569992
C	-0.3144318	-1.6965645	-2.1932106	C	-3.1151601	0.2963730	-2.4434241
H	-0.1082783	-3.6850414	-1.5606311	H	-4.0739051	0.7162105	-2.7510431
C	-0.0932397	-2.6640154	-1.2109719	H	-2.9510210	0.5350048	-1.3893114
C	0.0646153	-2.5085943	0.1703456	H	-3.1891036	-0.7927578	-2.5028689
N	-0.3555268	-0.3945089	-1.9522896	C	1.8164929	0.6250835	-3.5781648
N	0.1703661	-1.3507118	0.8311083	H	2.0092485	-0.4350527	-3.7656266
C	-0.5508531	-2.2126218	-3.6010972	H	2.0797114	0.8040523	-2.5328603
H	-0.4425264	-3.2951381	-3.6313856	H	2.4872510	1.2039362	-4.2147395
H	0.1511675	-1.7744418	-4.3122753	C	-2.2984683	-1.2554934	2.2917411
H	-1.5532241	-1.9573240	-3.9516850	H	-2.2770204	-0.3828945	1.6349460
C	0.0810747	-3.8225738	0.9411171	H	-3.1048112	-1.1347812	3.0168148
H	-0.0340202	-4.6614840	0.2582018	H	-2.5442653	-2.1108623	1.6555604
H	-0.7307999	-3.8611930	1.6695922	C	2.7421102	-1.9036677	2.1557000
H	1.0080275	-3.9601319	1.4974950	H	2.7020642	-1.4513214	1.1672636
Rh	0.0352933	0.5739286	-0.1378920	H	2.9631736	-2.9676789	2.0202612
C	1.2923014	2.0815508	1.0758246	H	3.5814260	-1.4728534	2.7051307
C	0.0040371	2.1509262	1.6236968	=====			
C	1.8374970	3.1502766	0.1392436	69	XyNacnacRh_12.xyz		
H	2.5540147	2.7253538	-0.5667956	C	-0.3912119	-1.5546068	-2.2569483
H	1.0806415	3.6850468	-0.4290562	H	-0.3181189	-3.5845839	-1.7694972
C	-0.9747365	3.2562408	1.2545631	C	-0.2452426	-2.5960831	-1.3419132
H	-0.8329114	3.6798732	0.2636691	C	-0.0463783	-2.5689215	0.0497194

N	-0.3527708	-0.2559883	-1.9578278	H	2.0636601	-0.2967831	-3.4654289
N	0.1181185	-1.4741138	0.7827037	H	2.1757737	1.0768915	-2.3834317
C	-0.6121492	-1.9707379	-3.7012945	H	2.6307151	1.2585162	-4.0842125
H	-0.5742856	-3.0542996	-3.7928465	C	-2.2648875	-1.4977828	2.3938646
H	0.1452358	-1.5408899	-4.3589889	H	-2.2896093	-0.6222144	1.7428960
H	-1.5795028	-1.6264586	-4.0715936	H	-3.0198367	-1.3827126	3.1728833
C	-0.0376562	-3.9413046	0.7098589	H	-2.5555431	-2.3493878	1.7717064
H	-0.1894005	-4.7243564	-0.0301150	C	2.7627002	-2.0413346	1.9088841
H	-0.8261812	-4.0215033	1.4602905	H	2.6921994	-1.4517830	0.9969274
H	0.9042337	-4.1341922	1.2247483	H	2.9281052	-3.0799909	1.6041810
Rh	-0.0225758	0.6207423	-0.1219006	H	3.6478426	-1.7256103	2.4639943
C	1.2124924	2.1319346	1.1745365	=====			
C	-0.0561250	2.1581117	1.7426873	69			
C	1.7242328	3.2454708	0.2786148	XyNacnacRh_13.xyz			
H	2.4278997	2.8628598	-0.4629555	C	-0.8751857	-1.1175450	-2.1448274
H	0.9439527	3.7855702	-0.2479088	H	-0.6335183	-3.2048165	-2.1087866
C	-1.0440132	3.2673440	1.4253010	C	-0.3855160	-2.3048149	-1.5660630
H	-0.9853455	3.6304363	0.4038406	C	0.4858210	-2.5028201	-0.4882245
H	-2.0675409	2.9300355	1.5999704	N	-0.7008726	0.0815363	-1.6174073
H	-0.0606423	1.9259973	-0.9275512	N	0.9348610	-1.5646481	0.3545969
H	-1.4401916	1.1357837	-0.0417639	C	-1.5981192	-1.2717093	-3.4709442
H	2.2750116	3.9648858	0.8998055	H	-1.5881829	-2.3083193	-3.8018906
H	-0.8659667	4.1136351	2.1015533	H	-1.1292387	-0.6565482	-4.2420401
C	-0.3504487	1.5459925	3.0913987	H	-2.6371310	-0.9452498	-3.3958077
H	0.3027301	0.7277479	3.3692331	C	0.9985854	-3.9249154	-0.3244634
H	-1.3801677	1.1927248	3.1493562	H	0.5984408	-4.5619132	-1.1101167
H	-0.2436683	2.3304152	3.8526727	H	0.7170146	-4.3504908	0.6392739
C	2.3659230	1.3955522	1.8204139	H	2.0886420	-3.9550708	-0.3771042
H	2.9050006	2.0857134	2.4825322	Rh	0.4393092	0.3874544	0.2440495
H	3.0846711	1.0629140	1.0678321	H	1.5378780	0.6467018	1.3078483
H	2.0651046	0.5380253	2.4110304	C	-0.7949869	0.8851590	1.8690759
C	0.2548376	-1.6926896	2.1893073	C	-1.2310258	2.2481154	1.2919800
C	0.4887571	-2.0795889	4.9496751	H	-1.9791457	2.0415491	0.5238661
C	1.5216247	-1.9197361	2.7595101	C	-1.9605059	-0.0905621	1.9449514
C	-0.8991393	-1.6922535	2.9997751	H	-1.6646562	-1.0375736	2.3903819
C	-0.7615007	-1.8891681	4.3724438	H	-2.3919449	-0.2946195	0.9656196
C	1.6174489	-2.0963072	4.1426956	C	-1.8755405	3.2122232	2.3013328
H	-1.6482877	-1.8855000	4.9970063	H	-2.7331002	2.7543920	2.7995523
H	2.5944562	-2.2598132	4.5852697	H	-2.2313666	4.1102666	1.7884321
H	0.5803661	-2.2205942	6.0201780	H	-2.7575788	0.3258919	2.5775300
C	-0.5856228	0.6794802	-3.0266299	H	-1.1668190	3.5257405	3.0705625
C	-1.0182350	2.5153175	-5.0820720	C	-0.0903759	0.9831481	3.2184578
C	0.5099046	1.1930804	-3.7432716	H	0.6757705	1.7588600	3.2334850
C	-1.8972871	1.0816466	-3.3337065	H	0.3955525	0.0416115	3.4731102
C	-2.0906002	2.0029178	-4.3647294	H	-0.8138285	1.2070337	4.0148215
C	0.2724198	2.1082738	-4.7686042	C	-0.0406117	2.9268639	0.5883483
H	-3.1001344	2.3178831	-4.6056245	H	0.7057136	3.2816000	1.2983426
H	1.1139843	2.5063406	-5.3250214	H	-0.3795493	3.7642628	-0.0265651
H	-1.1867740	3.2271855	-5.8815759	H	0.5184146	2.2981814	-0.1540738
C	-3.0792289	0.5581933	-2.5614867	C	1.9476277	-1.9298710	1.3141941
H	-4.0127617	0.9048902	-3.0064532	C	3.9626863	-2.5660833	3.1462498
H	-3.0481310	0.8970797	-1.5219625	C	1.6156375	-2.5547794	2.5273597
H	-3.1023151	-0.5330620	-2.5263414	C	3.2962156	-1.6516940	1.0029193
C	1.9200759	0.7847634	-3.4056403	C	4.2837414	-1.9747173	1.9293895

C	2.6392809	-2.8559589	3.4318886	C	-0.9202058	2.9472264	1.1435633
H	5.3194228	-1.7590984	1.6911639	H	-1.3865262	2.9034129	0.1535032
H	2.3820377	-3.3352541	4.3707408	C	-1.8140802	0.6290819	1.6842536
H	4.7427009	-2.8086172	3.8585289	H	-1.5767954	-0.4304616	1.7528053
C	-1.1177961	1.2395233	-2.3445600	H	-2.4970847	0.7652164	0.8465748
C	-1.8251993	3.6126836	-3.6550536	H	-2.3560177	0.8921528	2.6020574
C	-0.1518502	1.9513138	-3.0919195	H	-0.3306830	1.8270152	3.6702387
C	-2.4428209	1.7095498	-2.2797613	C	-1.9841144	3.5700489	2.0773892
C	-2.7710645	2.8998802	-2.9359107	H	-1.6330634	3.6218873	3.1106751
C	-0.5239259	3.1292439	-3.7355479	H	-2.9234609	3.0170752	2.0645632
H	-3.7920485	3.2632647	-2.8798789	H	-2.1990055	4.5919169	1.7546850
H	0.2184214	3.6729915	-4.3095251	C	0.2734161	3.9111242	1.0678846
H	-2.0981879	4.5332400	-4.1574092	H	1.1110407	3.5019328	0.5033517
C	-3.5365179	0.9581605	-1.5584985	H	0.6424877	4.1609134	2.0651498
H	-4.2798794	0.5829268	-2.2690112	H	-0.0298145	4.8476095	0.5928339
H	-4.0678603	1.6097786	-0.8600859	C	-1.1183305	0.3858392	-2.8325293
H	-3.1497289	0.1082780	-1.0021310	C	-1.6777976	2.1116442	-4.9629447
C	1.2634737	1.4455297	-3.2136411	C	-0.1597328	0.5848460	-3.8490200
H	1.8472996	2.0966686	-3.8655525	C	-2.3594083	1.0442917	-2.8918357
H	1.2993532	0.4334544	-3.6240545	C	-2.6181335	1.8998998	-3.9662322
H	1.7639015	1.4019146	-2.2420860	C	-0.4564442	1.4517730	-4.8995086
C	3.6802254	-1.0032649	-0.3004337	H	-3.5786308	2.4021539	-4.0162871
H	4.7645159	-0.9955798	-0.4197899	H	0.2813820	1.6064334	-5.6792691
H	3.3233322	0.0302575	-0.3361484	H	-1.8957671	2.7799266	-5.7875873
H	3.2445646	-1.5181930	-1.1594476	C	1.8157460	-1.5950730	1.7055872
C	0.2049034	-2.9475345	2.8938497	C	3.8038158	-1.7614135	3.6699174
H	-0.1482743	-2.3811443	3.7597039	C	1.4632490	-1.8788141	3.0374866
H	0.1626469	-4.0052940	3.1682910	C	3.1734847	-1.4352615	1.3513311
H	-0.4940372	-2.7805505	2.0788635	C	4.1459081	-1.5170785	2.3447818
=====				C	2.4732902	-1.9487464	4.0028223
71	XyNacnacRh_14.xyz			H	5.1880538	-1.3937010	2.0714416
C	-1.0631384	-1.7481023	-1.7975901	H	2.1987559	-2.1609740	5.0309105
H	-0.9282847	-3.7179178	-1.0935288	H	4.5727719	-1.8192319	4.4313182
C	-0.6081635	-2.7089538	-0.8803948	C	-3.4179204	0.8649797	-1.8315400
C	0.3144502	-2.6052583	0.1714908	H	-4.4149965	0.9107010	-2.2747174
N	-0.7751593	-0.4567738	-1.7239799	H	-3.3620609	1.6613444	-1.0832664
N	0.8159493	-1.4731428	0.6747206	H	-3.3182125	-0.0805967	-1.3017766
C	-1.8879348	-2.2756332	-2.9581265	C	1.1707507	-0.1229128	-3.8107522
H	-2.0671118	-3.3437349	-2.8524474	H	1.0559827	-1.2098194	-3.8201325
H	-1.3768256	-2.1041571	-3.9081177	H	1.7290624	0.1195253	-2.9026517
H	-2.8508257	-1.7663996	-3.0246201	H	1.7790303	0.1588464	-4.6710588
C	0.7957802	-3.9389943	0.7237091	C	3.5897338	-1.1982076	-0.0767385
H	0.3927733	-4.7593385	0.1342327	H	3.1612790	-1.9413731	-0.7531701
H	0.4954222	-4.0849558	1.7613533	H	4.6759506	-1.2382201	-0.1692778
H	1.8852739	-3.9983487	0.6987675	H	3.2487983	-0.2206415	-0.4273746
Rh	0.4000502	0.4290452	-0.1043925	C	0.0429392	-2.1401436	3.4850018
H	1.5815663	0.9688063	0.7354474	H	-0.0283016	-3.1160411	3.9731967
C	-0.5562218	1.4845907	1.5435713	H	-0.6645823	-2.1249957	2.6608705
C	0.2665348	1.4518729	2.8279282	H	-0.2825372	-1.3954187	4.2154934
H	0.5810749	0.4441737	3.0795127	=====			
H	1.1656105	2.0619376	2.7583935	71	XyNacnacRh_23.xyz		
H	0.8366408	1.8275557	-0.9268275	C	-0.9917397	-2.0584181	-2.3491017
H	-0.0106821	1.8740359	-0.9011190	H	-0.9944508	-4.1229333	-1.9125509

C	-0.7833072	-3.1483091	-1.4980068	H	-4.2296484	1.1188146	-2.0104254
C	-0.3347541	-3.1335870	-0.1682541	H	-3.0867309	0.3022793	-0.9254304
N	-0.7741006	-0.8141709	-1.9571183	H	-3.7157604	-0.5406778	-2.3252594
N	-0.0124186	-2.0451223	0.5319916	C	1.4336743	0.1379839	-3.5632248
C	-1.4804582	-2.3295533	-3.7545774	H	2.1622078	0.7226066	-4.1263477
H	-1.6120654	-3.3974486	-3.9199686	H	1.3788233	-0.8559142	-4.0159244
H	-0.7734119	-1.9496105	-4.4957192	H	1.8062939	-0.0043232	-2.5463274
H	-2.4339758	-1.8305420	-3.9421849	C	2.8082285	-2.4160034	1.0286892
C	-0.2186915	-4.4904224	0.5047762	H	2.6888941	-1.5566052	0.3653248
H	-0.5175607	-5.2785583	-0.1832997	H	2.6890252	-3.3063470	0.4046145
H	-0.8512725	-4.5507371	1.3922145	H	3.8246792	-2.4203553	1.4245613
H	0.8033426	-4.6893948	0.8320963	C	-1.9786782	-1.9959698	2.6466181
Rh	-0.1115413	-0.1591038	-0.1579659	H	-2.5359563	-1.8576478	3.5740951
C	1.1901571	0.9208048	1.2052386	H	-2.3988663	-2.8641723	2.1306560
H	1.7907515	0.2224566	1.7785225	H	-2.1524995	-1.1368493	1.9951144
C	-0.1365811	1.0831449	1.6214472				
H	-0.4567065	0.5131094	2.4866673	71			
C	2.0089396	1.9956803	0.5215911	XyNacnacRh_24.xyz			
H	2.8650933	1.5292665	0.0289343	C	-1.4700342	-1.4869863	-1.9555759
H	1.4401125	2.4890155	-0.2717417	H	-1.9406178	-3.4702446	-1.4461798
C	-0.9995866	2.2899729	1.3061095	C	-1.3667561	-2.6126845	-1.1274269
H	-1.0396923	2.4715444	0.2228975	C	-0.6493836	-2.7866804	0.0637892
H	-2.0242782	2.0402754	1.5919994	N	-0.8316190	-0.3376501	-1.7538312
C	2.5005919	3.0508647	1.5540627	N	0.1330709	-1.8648239	0.6179839
H	3.5841859	3.1745680	1.4681921	C	-2.3762572	-1.6364375	-3.1655437
H	2.3289983	2.6493450	2.5562419	H	-2.7848375	-2.6439050	-3.2151232
C	-0.6064270	3.6322988	1.9857563	H	-1.8348304	-1.4362404	-4.0920959
H	-1.5324078	4.1924979	2.1452885	H	-3.2072603	-0.9293757	-3.1301971
C	1.8580877	4.4461246	1.4513291	C	-0.7936817	-4.1437762	0.7308937
H	2.3643253	5.0142981	0.6627072	H	-1.4280615	-4.7972653	0.1351188
H	-0.1978015	3.4383874	2.9826433	H	-1.2315957	-4.0533468	1.7267463
H	2.0724247	4.9804433	2.3835508	H	0.1770382	-4.6265993	0.8592649
C	0.3472790	4.5287903	1.1666902	Rh	0.5142062	0.0590751	-0.1717237
H	0.1653159	4.3392445	0.1037396	H	-0.4063406	0.8505831	0.7145141
H	0.0597799	5.5738494	1.3199659	C	2.2046937	1.3292643	-0.0438100
C	0.4301659	-2.2078453	1.8835329	C	2.0847493	0.7700542	1.2553048
C	1.2946106	-2.4964026	4.5166531	C	1.2521980	2.0828568	-0.7781807
C	-0.5099604	-2.1737999	2.9297377	H	1.5014626	2.0913420	-1.8372445
C	1.8013073	-2.3802977	2.1485040	H	2.9741715	0.8628199	-0.6603183
C	2.2124188	-2.5242900	3.4741822	H	2.8310539	-0.0063675	1.4106936
C	-0.0554521	-2.3210773	4.2410652	C	1.7720898	1.3939435	2.6049092
H	3.2674231	-2.6574345	3.6873622	H	1.7340845	0.5623427	3.3142290
H	-0.7734549	-2.2968381	5.0535815	H			

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C	-1.4700342	-1.4869863	-1.9555759
H	-1.9406178	-3.4702446	-1.4461798
C	-1.3667561	-2.6126845	-1.1274269
C	-0.6493836	-2.7866804	0.0637892
N	-0.8316190	-0.3376501	-1.7538312
N	0.1330709	-1.8648239	0.6179839
C	-2.3762572	-1.6364375	-3.165543
H	-2.7848375	-2.6439050	-3.2151232
H	-1.8348304	-1.4362404	-4.0920959
H	-3.2072603	-0.9293757	-3.1301971
C	-0.7936817	-4.1437762	0.7308937
H	-1.4280615	-4.7972653	0.1351188
H	-1.2315957	-4.0533468	1.7267463
H	0.1770382	-4.6265993	0.8592649
Rh	0.5142062	0.0590751	-0.1717237
H	-0.4063406	0.8505831	0.7145141
C	2.2046937	1.3292643	-0.0438100
C	2.0847493	0.7700542	1.2553048
C	1.2521980	2.0828568	-0.7781807
H	1.5014626	2.0913420	-1.8372445
H	2.9741715	0.8628199	-0.6603183
H	2.8310539	-0.0063675	1.4106936
C	1.7720898	1.3939435	2.6049092
H	1.7340845	0.5623427	3.3142290
H	2.6659416	1.9694415	2.8908778
C	0.5141736	3.3726619	-0.4618711
H	1.2614448	4.1781191	-0.5306484
H	-0.1607403	3.5424533	-1.3055985
C	-0.3014543	3.6011881	0.8111264
H	-0.7827770	4.5761794	0.6782028
C	0.5478208	2.2675738	2.8805169
H	0.5653349	2.4625112	3.9583003
H	-0.3656882	1.6911928	2.7031490
H	-1.1201647	2.8762928	0.8615781
C	0.4362709	3.6186794	2.1582948
H	-0.1136924	4.2950730	2.8199734

H	1.4304698	4.0669852	2.0391782	H	1.7957884	0.1124989	1.5186081
C	0.7519524	-2.1771826	1.8707748	C	-0.0618731	1.1004716	1.6308351
C	1.9839645	-2.7586186	4.3081285	H	-0.3831296	0.3547637	2.3466647
C	2.0515524	-2.7172559	1.8843867	C	2.1245983	2.1029225	0.7131878
C	0.0679231	-1.9261857	3.0741241	H	2.8990781	1.7259568	0.0411495
C	0.7027236	-2.2237377	4.2816455	H	1.5712261	2.8568721	0.1498330
C	2.6490578	-3.0018136	3.1125417	C	-0.8242650	2.4053104	1.7415663
H	0.1796299	-2.0308318	5.2122383	H	-0.8708414	2.9277804	0.7835570
H	3.6496424	-3.4204700	3.1273137	H	-1.8593670	2.1625653	1.9959208
H	2.4619406	-2.9848020	5.2541113	C	2.7791500	2.7454272	1.9691121
C	-1.0907590	0.7397869	-2.6605663	H	3.8592767	2.8310613	1.8190683
C	-1.5650008	2.8575132	-4.4175269	H	2.6554511	2.0540454	2.8072167
C	-2.1685465	1.6124364	-2.4244537	C	-0.2687529	3.4031741	2.7957195
C	-0.2488913	0.9253013	-3.7731807	H	-1.1209088	3.9622370	3.1930310
C	-0.5035952	1.9886386	-4.6396845	C	2.2524619	4.1353903	2.3792946
C	-2.3872636	2.6652368	-3.3151302	H	2.7760921	4.8983892	1.7923867
H	0.1412036	2.1336215	-5.4998741	H	0.1531980	2.8580246	3.6462411
H	-3.2164663	3.3414975	-3.1364550	H	2.5517638	4.3081798	3.4188715
H	-1.7494289	3.6791442	-5.0997523	C	0.7468387	4.4273329	2.2413581
C	0.9089250	-0.0038911	-4.0343202	H	0.5077087	4.6073999	1.1880514
H	1.6193306	-0.0001373	-3.2028712	H	0.5755815	5.3881860	2.7371931
H	1.4432905	0.2921706	-4.9381344	H	0.2040079	1.4497359	-1.1445492
H	0.5849939	-1.0405524	-4.1580886	H	-0.6242638	1.5393956	-0.8669071
C	-3.0813014	1.4183303	-1.2418928	C	0.3569891	-2.0904983	1.8382567
H	-3.7712350	2.2579833	-1.1461352	C	1.2103609	-2.4382525	4.4729139
H	-2.5138344	1.3244145	-0.3145373	C	-0.5820605	-2.0506211	2.8864682
H	-3.6782251	0.5058306	-1.3318664	C	1.7208731	-2.3108932	2.1054784
C	2.7925452	-2.9895230	0.6003381	C	2.1268965	-2.4799756	3.4307246
H	2.2575331	-3.6936525	-0.0421984	C	-0.1343505	-2.2266561	4.1966576
H	2.9243257	-2.0760356	0.0136474	H	3.1772609	-2.6486086	3.6424635
H	3.7798176	-3.4053320	0.8067342	H	-0.8536942	-2.1968846	5.0079089
C	-1.3265722	-1.3561152	3.0713682	H	1.5421717	-2.5706604	5.4960071
H	-1.3849157	-0.4541770	2.4597466	C	-1.0882223	0.2492154	-3.1691824
H	-1.6445067	-1.1113209	4.0857124	C	-1.5353895	2.2000771	-5.1095252
H	-2.0542922	-2.0585201	2.6545805	C	-2.3499199	0.8640302	-3.2570229
=====							
73							
XyNacnacRh_25.xyz							
C	-1.0755421	-1.9967075	-2.4150802	H	0.5073116	1.8765075	-5.6815999
H	-1.1160032	-4.0280579	-1.8808599	H	-3.5237939	2.3156151	-4.3110989
C	-0.8810543	-3.0432095	-1.5062049	H	-1.7093312	2.9582250	-5.8640817
C	-0.4289526	-3.0009051	-0.1830587	C	1.3152919	-0.0236835	-3.9301088
N	-0.8432511	-0.7208734	-2.1391793	H	1.7210655	0.0875426	-2.9212765
N	-0.0805957	-1.8996677	0.4858402	H	2.0102665	0.4289755	-4.6387259
C	-1.5853467	-2.3880565	-3.7898716	H	1.2822924	-1.0979022	-4.1310749
H	-1.7234348	-3.4655557	-3.8538561	C	-3.4603740	0.4958605	-2.3072101
H	-0.8886444	-2.0816387	-4.5724271	H	-3.1445146	0.6141515	-1.2674184
H	-2.5383149	-1.9037517	-4.0114637	H	-3.7652031	-0.5483461	-2.4187891
C	-0.3454227	-4.3509975	0.5111280	H	-4.3373203	1.1213884	-2.4798362
H	-0.6644054	-5.1436052	-0.1622018	C	2.7292801	-2.4010501	0.9877584
H	-0.9759416	-4.3818865	1.4011498	H	2.6379932	-3.3451352	0.4416944
H	0.6717764	-4.5689751	0.8403108	H	3.7455411	-2.3455048	1.3808697
Rh	-0.1408559	0.0378405	-0.3237985	H	2.5902697	-1.6063468	0.2530152
C	1.2338594	0.9571034	1.1386056	C	-2.0495627	-1.8478323	2.6068205

H	-2.5983442	-1.6799460	3.5346317
H	-2.4897006	-2.7198470	2.1140381
H	-2.2176239	-1.0010312	1.9386748

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XyNacnacRh_27.xyz

C	-0.4105865	-1.3943134	-2.6193313
H	0.1462063	-3.4163072	-2.7742744
C	0.2378864	-2.5460626	-2.1415623
C	1.0644957	-2.7197148	-1.0247117
N	-0.4502302	-0.2480237	-1.9574940
N	1.3529428	-1.7895601	-0.1092893
C	-1.0513998	-1.5046668	-3.9906773
H	-0.9657461	-2.5179551	-4.3787032
H	-0.5673171	-0.8253527	-4.6967834
H	-2.1069245	-1.2308143	-3.9644224
C	1.7201502	-4.0847379	-0.9016510
H	1.3979551	-4.7335149	-1.7133960
H	1.4728832	-4.5672510	0.0444312
H	2.8082431	-4.0011468	-0.9379262
Rh	0.6021448	0.0850931	-0.0793515
H	1.7493553	0.4391153	0.9055249
C	-0.4015941	0.6937019	1.6088228
H	0.2395967	0.7998599	2.4773494
C	-0.5055945	1.9543560	0.8027060
H	0.1461866	1.8833800	-0.1593821
H	-1.5039181	2.0956542	0.3905318
C	-1.6923830	-0.0254670	1.9632986
H	-1.4806774	-0.7484725	2.7553298
H	-2.0562951	-0.6060756	1.1104621
C	0.0078271	3.2335275	1.4850143
H	-0.2804489	4.0942613	0.8729990
H	1.1005013	3.2175189	1.5043998
C	-2.8485399	0.8931693	2.4239452
H	-3.6587647	0.2328712	2.7496598
H	-3.2490702	1.4394192	1.5635695
C	-0.4971146	3.4324281	2.9247663
H	-0.1866193	4.4365757	3.2297759
H	0.0324629	2.7481021	3.5948112
C	-2.5597241	1.8978084	3.5567033
H	-1.8967870	1.4414189	4.3014170
H	-3.5076950	2.0697960	4.0759471
C	-2.0124790	3.2937713	3.1766370
H	-2.5751392	3.6827757	2.3194245
H	-2.2586158	3.9582467	4.0104025
C	2.2935652	-2.1206482	0.9300590
C	4.1312608	-2.6992189	2.9481731
C	1.8559756	-2.7462683	2.1088469
C	3.6503563	-1.7890195	0.7532410
C	4.5524115	-2.0895013	1.7723267
C	2.7918215	-3.0211900	3.1089298
H	5.5984907	-1.8350406	1.6413218
H	2.4569749	-3.4964206	4.0249733
H	4.8443515	-2.9201111	3.7338579

C	-1.0680696	0.8915494	-2.5593319
C	-2.2267405	3.2092637	-3.6139036
C	-2.4476157	1.1218461	-2.3967963
C	-0.2692908	1.8214473	-3.2576524
C	-0.8675325	2.9690293	-3.7768204
C	-3.0046254	2.2877128	-2.9279822
H	-0.2549039	3.6840854	-4.3151020
H	-4.0666126	2.4680910	-2.7983687
H	-2.6746557	4.1087508	-4.0196132
C	4.1258215	-1.0980312	-0.4969157
H	3.6836736	-0.1008494	-0.5771984
H	3.8402195	-1.6397222	-1.4016273
H	5.2116852	-0.9946109	-0.4895104
C	0.4173221	-3.1494895	2.3087095
H	0.1540863	-3.1242317	3.3679464
H	0.2378739	-4.1720175	1.9584044
H	-0.2622550	-2.4983824	1.7636133
C	1.2080202	1.5887031	-3.4469640
H	1.4090584	0.6579459	-3.9839296
H	1.7259895	1.5091525	-2.4870042
H	1.6558786	2.4075614	-4.0118206
C	-3.3363612	0.1252698	-1.6961656
H	-3.7016339	-0.6394873	-2.3893463
H	-4.2126742	0.6179237	-1.2718478
H	-2.8070393	-0.3975061	-0.9014753

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XyNacnacRh_29.xyz

C	-0.3943643	-1.8891670	-2.5754325
H	-0.2958818	-3.9009645	-1.9870052
C	-0.0758821	-2.8978995	-1.6538471
C	0.5693251	-2.8243800	-0.4109523
N	-0.2129668	-0.5942615	-2.3517613
N	0.9222263	-1.7054575	0.2243264
C	-0.9397935	-2.3564934	-3.9127270
H	-1.0976566	-3.4332257	-3.9120734
H	-0.2450307	-2.1120102	-4.7195481
H	-1.8835834	-1.8656489	-4.1537450
C	0.9147104	-4.1647407	0.2166198
H	0.6177067	-4.9794667	-0.4399758
H	0.4177374	-4.3006615	1.1774096
H	1.9875264	-4.2439562	0.4020678
Rh	0.6233180	0.2058060	-0.5135508
H	1.8260515	0.6410887	0.3357020
C	-0.1141994	1.1086769	1.2840350
H	0.2398612	0.4538313	2.0799893
C	0.4099789	2.5277283	1.5304303
H	1.4765049	2.5345529	1.3050698
H	-0.0482092	3.2234465	0.8162352
H	1.0126027	1.6838085	-1.2403112
H	0.1787661	1.7527001	-1.0908032
C	-1.6268594	0.9703349	1.1147064
H	-1.8205886	0.0234386	0.6007292
H	-1.9940882	1.7528336	0.4413457

C	0.2601744	3.1043130	2.9586822	C	-1.7671997	-2.9886362	-1.3626824
H	1.1035758	3.7867136	3.1017884	C	-1.1065656	-3.1429045	-0.1411678
H	0.4063556	2.3054205	3.6944008	N	-1.3869556	-0.6703206	-1.9234586
C	-2.5120507	0.9604478	2.3894028	N	-0.5536814	-2.1661896	0.5831563
H	-1.9805349	0.4639640	3.2070014	C	-2.9593300	-2.0122571	-3.2815113
H	-3.3698254	0.3192045	2.1648930	H	-3.4276975	-2.9933405	-3.2347035
C	-1.0157550	3.8964951	3.2961160	H	-2.4727844	-1.9117601	-4.2527079
H	-0.7427130	4.6409154	4.0514048	H	-3.7428981	-1.2535039	-3.2413012
H	-1.3295554	4.4735123	2.4175321	C	-1.0752374	-4.5827018	0.3619006
C	-3.0724857	2.3059560	2.8812430	H	-1.4636875	-5.2530221	-0.4019920
H	-4.0175267	2.0935698	3.3924134	H	-1.6717079	-4.7150899	1.2652176
H	-3.3400167	2.9277877	2.0181199	H	-0.0601513	-4.8960867	0.6083428
C	-2.2176057	3.1251132	3.8559753	Rh	-0.1207432	-0.1810375	-0.2163534
H	-1.8771950	2.4725385	4.6698739	C	1.0731507	0.7905067	1.6080204
H	-2.8812126	3.8595894	4.3257402	H	1.6980887	1.4053641	0.9861345
C	1.6590197	-1.8363574	1.4552273	C	-0.2718889	1.1334464	1.5752906
C	3.1218000	-2.0012783	3.8303517	H	-0.5300962	2.0237585	1.0133395
C	3.0668032	-1.7589315	1.4179837	C	1.3574302	0.6863376	-1.6150252
C	0.9884574	-2.0261789	2.6753221	H	1.0823831	0.0560975	-2.4515705
C	1.7397489	-2.0967324	3.8526105	C	0.5272360	1.7663799	-1.3342326
C	3.7762307	-1.8422381	2.6142963	H	-0.3377846	1.9088614	-1.9628643
H	1.2229292	-2.2328995	4.7967178	C	-1.2804310	0.8193075	2.6461943
H	4.8586331	-1.7823437	2.5886711	H	-1.1057676	-0.1638821	3.0670076
H	3.6889531	-2.0569576	4.7520522	H	-2.2827815	0.7984067	2.2093766
C	-0.4710405	0.3315486	-3.4138446	C	1.9047653	0.1672587	2.7226368
C	-0.9206785	2.2250697	-5.4172896	H	2.7891958	0.8128223	2.8138025
C	0.5806129	0.7019049	-4.2741893	H	2.3013701	-0.7958962	2.4020297
C	-1.7463619	0.9094519	-3.5536792	C	2.8364642	0.6177038	-1.3098819
C	-1.9496149	1.8527174	-4.5625779	H	3.1298110	-0.4341841	-1.2489605
C	0.3344142	1.6492633	-5.2686147	H	3.0800534	1.0563141	-0.3417361
H	-2.9314047	2.3000653	-4.6740949	C	1.0360099	3.0652476	-0.7583417
H	1.1421438	1.9377756	-5.9324527	H	1.9019604	2.9185990	-0.1128485
H	-1.0951926	2.9605969	-6.1936285	H	0.2739750	3.5551198	-0.1450217
C	-2.8830694	0.5227328	-2.6429415	C	3.7127808	1.2965893	-2.3868000
H	-3.7627541	1.1345847	-2.8467241	H	4.7459349	0.9777271	-2.2111460
H	-2.6136853	0.6450834	-1.5931424	H	3.4416733	0.9056887	-3.3745265
H	-3.1703367	-0.5248377	-2.7693737	C	1.4341526	4.0459917	-1.8841696
C	1.9538731	0.0978801	-4.1278622	H	1.8848283	4.9277956	-1.4141237
H	2.6417552	0.5277129	-4.8569743	H	0.5285999	4.3971215	-2.3897741
H	1.9425786	-0.9854815	-4.2735653	C	3.6945787	2.8356053	-2.4364594
H	2.3602954	0.2683303	-3.1274778	H	4.5159642	3.1378015	-3.0935223
C	-0.5076725	-2.2059990	2.7554838	H	3.9522348	3.2339580	-1.4478497
H	-0.7710555	-3.2666602	2.8245891	C	2.3950965	3.4954960	-2.9510404
H	-1.0177471	-1.7999224	1.8854859	H	2.6591684	4.3329997	-3.6041744
H	-0.9077615	-1.7232154	3.6483969	H	1.8614764	2.7842854	-3.5880567
C	3.8091469	-1.6002453	0.1168468	C	-1.2690930	1.8913168	3.7677135
H	3.5365727	-2.3742402	-0.6045742	H	-1.8619437	1.5139457	4.6087767
H	3.5776496	-0.6421077	-0.3549129	H	-1.7935186	2.7813912	3.4029718
H	4.8859168	-1.6535445	0.2823643	C	1.3208056	-0.0122196	4.1328930
=====				H	2.0679390	-0.5648238	4.7118948
93				H	0.4549576	-0.6680522	4.1026876
XyNacnacRh_COE_2.xyz				C	0.1149152	2.3343782	4.2611291
C	-1.9762648	-1.8430267	-2.1323120	H	0.6609377	2.7853375	3.4278759
H	-2.2293057	-3.8853663	-1.7468615	H	-0.0317300	3.1421755	4.9866412

C	0.9979763	1.2673402	4.9258030	Rh	0.0327303	0.3249347	0.6483102
H	1.9420487	1.7528250	5.2021589	H	0.2975832	0.7865761	2.1096428
H	0.5340715	0.9624851	5.8718393	C	1.7187812	1.6296390	0.3388412
C	-0.1032394	-2.6014058	1.8741228	C	1.8204156	1.0217469	1.6540674
C	0.7326925	-3.6439686	4.3316194	C	0.6853992	2.5634813	0.1282883
C	1.2324676	-3.0145665	2.0434141	H	2.5397371	0.2195997	1.7742769
C	-1.0248188	-2.7288638	2.9326182	C	0.1254559	3.4427782	1.2319500
C	-0.5837237	-3.2421652	4.1544186	H	0.6073806	4.4297158	1.1903776
C	1.6300320	-3.5304636	3.2771558	H	-0.9438692	3.6113601	1.0872994
H	-1.2919536	-3.3380957	4.9709166	H	1.8026340	1.6683384	2.5284320
H	2.6573514	-3.8541608	3.4061669	H	0.2633478	3.0505126	2.2365736
H	1.0577307	-4.0459636	5.2841984	C	0.5300740	3.2240808	-1.2217673
C	-1.7350813	0.3675876	-2.8525541	H	0.7801641	2.5797932	-2.0594858
C	-2.3984660	2.4662750	-4.5822770	H	1.1811717	4.1073074	-1.2747916
C	-2.7211449	1.3076367	-2.4784122	H	-0.4920218	3.5721231	-1.3710496
C	-1.1153539	0.4592440	-4.1123018	C	2.7223818	1.2368480	-0.7174043
C	-1.4545075	1.5233886	-4.9548436	H	3.5476055	1.9591851	-0.7276202
C	-3.0346971	2.3465022	-3.3507646	H	2.2984705	1.2148551	-1.7199059
H	-0.9686981	1.6006983	-5.9221192	H	3.1478684	0.2552516	-0.5052003
H	-3.7888308	3.0697472	-3.0601787	C	-1.8389707	0.9370887	-1.7071418
H	-2.6473044	3.2842413	-5.2482751	C	-2.6338056	2.9224794	-3.5016967
C	2.2047263	-2.9652161	0.8932389	C	-2.8031867	1.8846618	-1.3158349
H	3.2210331	-3.1653461	1.2366450	C	-1.2642941	0.9882928	-2.9896591
H	2.1791859	-1.9945456	0.3951470	C	-1.6768703	1.9871562	-3.8730261
H	1.9574417	-3.7097995	0.1302248	C	-3.1870817	2.8686120	-2.2280021
C	-2.4896861	-2.4101434	2.7527451	H	-1.2372550	2.0295398	-4.8638777
H	-2.6525649	-1.6570265	1.9853692	H	-3.9320657	3.5996176	-1.9323973
H	-2.9275843	-2.0601237	3.6894894	H	-2.9439523	3.6919430	-4.1988916
H	-3.0488494	-3.3021908	2.4508074	C	0.5131542	-1.8485957	2.6611455
C	-0.1264452	-0.5660313	-4.6197716	C	2.0741149	-2.3338811	4.9233623
H	0.1197683	-1.3135998	-3.8686288	C	0.0214996	-1.5019644	3.9331194
H	0.8004109	-0.0883545	-4.9469848	C	1.7829327	-2.4367947	2.5182562
H	-0.5336255	-1.0919630	-5.4890443	C	2.5476256	-2.6716461	3.6622577
C	-3.4324178	1.1903864	-1.1565052	C	0.8185008	-1.7534119	5.0509923
H	-2.7210440	1.1931041	-0.3276658	H	3.5281392	-3.1234572	3.5568315
H	-3.9894485	0.2521836	-1.0826137	H	0.4442361	-1.4892188	6.0341711
H	-4.1361437	2.0135140	-1.0230143	H	2.6801571	-2.5213974	5.8019812
=====				C	-0.2324366	-0.0237800	-3.4186082
67	XyNacnacRh_TS_1_2.xyz			H	0.5349237	-0.1612386	-2.6546371
C	-2.1384359	-1.2413713	-0.8737921	H	0.2476411	0.2851469	-4.3485886
H	-2.5737662	-3.2045163	-0.2662462	H	-0.6745717	-1.0103624	-3.5874531
C	-1.9471736	-2.3528242	-0.0480218	C	-3.4298270	1.8284448	0.0532755
C	-1.0984504	-2.5025631	1.0565445	H	-2.6673164	1.7761125	0.8332084
N	-1.4532022	-0.0979060	-0.7961096	H	-4.0562551	0.9397883	0.1753461
N	-0.2675329	-1.5662662	1.4917617	H	-4.0561927	2.7046452	0.2273909
C	-3.2428320	-1.3857615	-1.9082647	C	2.3140503	-2.8153711	1.1596302
H	-3.6877773	-2.3772157	-1.8534422	H	1.7786709	-3.6711254	0.7378206
H	-2.8724838	-1.2286561	-2.9220240	H	3.3699008	-3.0831893	1.2189229
H	-4.0302315	-0.6466975	-1.7459455	H	2.1945987	-1.9979728	0.4455992
C	-1.1830858	-3.8305141	1.7880247	C	-1.3373869	-0.8716150	4.0975699
H	-1.8858265	-4.4953326	1.2895379	H	-1.5376080	-0.6587811	5.1484625
H	-1.5126378	-3.6929729	2.8200310	H	-2.1356131	-1.5198294	3.7268298
H	-0.2115109	-4.3252548	1.8324880	H	-1.4151780	0.0606347	3.5327034
				=====			

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XyNacnacRh_TS_2_3.xyz

C	-2.4381658	-0.7305249	-1.2937824
H	-3.1131361	-2.6287083	-0.6991473
C	-2.4160594	-1.8437837	-0.4461508
C	-1.6479105	-2.0760718	0.7017709
N	-1.6756866	0.3518414	-1.1496615
N	-0.7322877	-1.2407932	1.1817598
C	-3.4419243	-0.7947582	-2.4328991
H	-3.9767699	-1.7424006	-2.4176362
H	-2.9547343	-0.6895693	-3.4034724
H	-4.1720278	0.0140678	-2.3602342
C	-1.9332976	-3.3768482	1.4331512
H	-2.7134682	-3.9382537	0.9226792
H	-2.2607306	-3.1861599	2.4574632
H	-1.0447129	-4.0059928	1.5003229
Rh	-0.2818392	0.6757759	0.4256091
H	0.1293454	0.9926757	1.8892911
C	1.2214345	2.1216603	0.0036645
C	1.6441232	1.4585106	1.2400633
C	0.0125847	2.8323397	0.0761814
H	-0.3856137	3.2684127	-0.8301654
C	1.7609065	2.3032038	2.5128161
H	1.7773745	1.6718480	3.4034311
H	2.7066488	2.8569547	2.4822756
H	-0.3277927	3.2943001	0.9934047
H	0.9551756	3.0272893	2.6212083
C	2.0297103	2.0699713	-1.2659708
H	1.4196176	2.3545587	-2.1228163
H	2.4640074	1.0892879	-1.4575319
H	2.8580027	2.7858076	-1.1978913
C	2.7833436	0.4622939	1.1687255
H	3.7420896	0.9975321	1.1649351
H	2.7445147	-0.1697440	0.2849352
H	2.7772382	-0.1845300	2.0463231
C	-1.8457565	1.4015272	-2.1091871
C	-2.1262432	3.4747578	-3.9589011
C	-2.7485148	2.4497618	-1.8499992
C	-1.0874374	1.3861321	-3.2942050
C	-1.2400387	2.4342884	-4.2045917
C	-2.8744617	3.4752770	-2.7877288
H	-0.6549914	2.4280500	-5.1183225
H	-3.5675524	4.2863530	-2.5913610
H	-2.2334303	4.2810848	-4.6751468
C	-0.0202469	-1.6439423	2.3597404
C	1.4132109	-2.3859674	4.6395603
C	1.1337892	-2.4386621	2.2310843
C	-0.4666395	-1.2299849	3.6299665
C	0.2661700	-1.6097098	4.7550889
C	1.8369160	-2.7970998	3.3832481
H	-0.0742505	-1.2944027	5.7355967
H	2.7300998	-3.4053622	3.2867763
H	1.9704061	-2.6710843	5.5243956
C	-3.5594144	2.4742510	-0.5810321

H	-2.9126783	2.4293448	0.2985615
H	-4.2331728	1.6158326	-0.5112154
H	-4.1634764	3.3811364	-0.5271684
C	-0.1445002	0.2498508	-3.6002732
H	-0.6858679	-0.6481677	-3.9142240
H	0.4408566	-0.0325424	-2.7247196
H	0.5368604	0.5201126	-4.4085435
C	-1.7193966	-0.4071566	3.7863438
H	-1.9128471	-0.1987474	4.8396828
H	-2.5941463	-0.9185411	3.3760044
H	-1.6432499	0.5424057	3.2506006
C	1.6031257	-2.9223750	0.8821175
H	2.6547214	-3.2115626	0.9200320
H	1.0363760	-3.7981895	0.5495063
H	1.4726479	-2.1579503	0.1161240

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XyNacnacRh_TS_3_4.xyz

C	-2.6727118	-0.7733579	-0.7433028
H	-3.2707071	-2.7274417	-0.2528027
C	-2.5563165	-1.9561353	-0.0062137
C	-1.6620688	-2.2764243	1.0254058
N	-1.8724341	0.2865519	-0.6166691
N	-0.7445899	-1.4471349	1.5033200
C	-3.8260589	-0.7250664	-1.7307873
H	-4.3890564	-1.6559747	-1.7058224
H	-3.4815359	-0.5577937	-2.7518251
H	-4.5062929	0.0954391	-1.4918172
C	-1.7953305	-3.6674020	1.6185393
H	-2.5721203	-4.2293089	1.1034981
H	-2.0467601	-3.6248296	2.6802083
H	-0.8584656	-4.2221806	1.5402318
Rh	-0.3809783	0.5072469	0.8530150
H	-0.1895287	0.8750856	2.3487061
C	1.3172438	1.8150347	0.6896552
C	1.3643555	1.1467448	1.9791162
C	0.2016710	2.6450184	0.4971927
H	0.0197479	3.0950977	-0.4686950
H	2.0912838	0.3526879	2.1156499
H	-0.2498909	3.1585310	1.3382289
H	1.2716285	1.7679374	2.8694108
C	2.4335198	1.5831226	-0.3162160
H	2.6086944	0.5022462	-0.3661174
C	3.7269648	2.2338027	0.2178776
H	4.0102171	1.8344784	1.1933747
H	3.6009206	3.3152542	0.3189335
H	4.5534835	2.0541156	-0.4740011
C	2.1351098	2.0942165	-1.7262982
H	2.9421763	1.8085287	-2.4051088
H	2.0609099	3.1844714	-1.7423101
H	1.2050710	1.6898326	-2.1206791
C	-2.1106784	1.4030546	-1.4825936
C	-2.5131594	3.6069682	-3.1491102
C	-2.8901016	2.4849588	-1.0317392

C	-1.5437022	1.4164219	-2.7702963	C	0.9723513	4.0034101	2.1194515
C	-1.7530383	2.5307094	-3.5859175	H	1.8932906	3.7119178	2.6302368
C	-3.0786397	3.5760979	-1.8798751	H	0.1637321	4.0041118	2.8528022
H	-1.3121394	2.5483383	-4.5769958	H	-0.3846960	1.5508268	-0.8519232
H	-3.6765952	4.4131659	-1.5358321	H	-1.5492185	1.7096378	-0.4930795
H	-2.6658556	4.4647807	-3.7936141	H	1.1070068	5.0274905	1.7623130
C	0.0833196	-1.8954086	2.5839929	H	-1.6819840	2.1653887	1.9136276
C	1.7484887	-2.6978194	4.6750454	C	1.5431216	0.8537621	1.9000984
C	-0.3176252	-1.6780394	3.9149644	H	2.1595537	1.4467871	2.5852258
C	1.3156128	-2.5103965	2.2967580	H	2.1815598	0.5764835	1.0590416
C	2.1330928	-2.9056957	3.3566975	H	1.2430941	-0.0478375	2.4260761
C	0.5304873	-2.0873528	4.9452885	C	1.7806385	3.1368070	-0.1056108
H	3.0838977	-3.3806418	3.1399979	H	1.8944415	4.1603956	-0.4705139
H	0.2261030	-1.9237710	5.9734239	H	1.5783220	2.4958705	-0.9654346
H	2.3945666	-3.0092495	5.4874448	H	2.7397915	2.8342398	0.3220508
C	-0.7472646	0.2446346	-3.2890333	C	-1.3559742	0.4856841	-2.9913409
H	-0.1014505	-0.1796009	-2.5194413	C	-1.2129918	2.3242309	-5.0818519
H	-0.1325738	0.5422796	-4.1399591	C	-2.4936574	1.2383589	-3.3312244
H	-1.3997260	-0.5668227	-3.6275918	C	-0.1466733	0.6502313	-3.6892302
C	-3.5143191	2.4703157	0.3386290	C	-0.0964826	1.5751817	-4.7332184
H	-2.7576699	2.3237279	1.1129244	C	-2.4001718	2.1529962	-4.3815595
H	-4.2304000	1.6512034	0.4491999	H	0.8335812	1.7078821	-5.2753988
H	-4.0410041	3.4059578	0.5321691	H	-3.2734104	2.7381225	-4.6491242
C	1.7513103	-2.7430557	0.8731713	H	-1.1577604	3.0393873	-5.8942921
H	1.1074595	-3.4642005	0.3621328	C	-1.0133495	-1.8363200	2.2695225
H	2.7722118	-3.1257139	0.8397982	C	-0.5884793	-2.2302702	5.0036182
H	1.7013760	-1.8211658	0.2894821	C	0.2234870	-2.3351904	2.7200825
C	-1.6319393	-1.0143910	4.2360394	C	-2.0453178	-1.5534984	3.1862979
H	-1.7655294	-0.9299598	5.3154501	C	-1.8113612	-1.7541995	4.5472904
H	-2.4817026	-1.5716603	3.8333417	C	0.4164878	-2.5203822	4.0909542
H	-1.6913056	-0.0134462	3.8005375	H	-2.6024445	-1.5333758	5.2557733
=====				H	1.3704218	-2.8997046	4.4418064
69	XyNacnacRh_TS_5_6.xyz			H	-0.4217359	-2.3773495	6.0642348
C	-1.7807966	-1.6868790	-2.1568535	C	1.3182665	-2.7073720	1.7508402
H	-2.2370055	-3.6523172	-1.5840716	H	1.3890883	-1.9975117	0.9271210
C	-1.9028895	-2.7006906	-1.1992505	H	1.1368344	-3.6894540	1.3024824
C	-1.6604712	-2.6705900	0.1779445	H	2.2830030	-2.7554262	2.2585651
N	-1.4162481	-0.4399328	-1.8916979	C	-3.3883364	-1.0615809	2.7118796
N	-1.2252314	-1.6144899	0.8698908	H	-3.2881044	-0.1956455	2.0544861
C	-2.1057484	-2.0827688	-3.5865928	H	-4.0199196	-0.7897440	3.5588835
H	-2.3778130	-3.1351358	-3.6371845	H	-3.9154910	-1.8261068	2.1337638
H	-1.2535637	-1.9143191	-4.2475657	C	1.0773608	-0.1466557	-3.3189709
H	-2.9328692	-1.4925021	-3.9851696	H	1.3259744	-0.0170099	-2.2628450
C	-1.9419979	-3.9797571	0.9004566	H	1.9336774	0.1611093	-3.9207333
H	-2.3179480	-4.7261184	0.2039103	H	0.9288556	-1.2194118	-3.4705374
H	-2.6827817	-3.8425371	1.6901515	C	-3.7887853	1.0778390	-2.5779035
H	-1.0461280	-4.3780384	1.3785622	H	-3.6536067	1.2801206	-1.5123504
Rh	-0.9454454	0.3591156	-0.0250758	H	-4.1812048	0.0599970	-2.6489236
C	0.3472205	1.6595452	1.4585992	H	-4.5467198	1.7586505	-2.9678205
C	-0.9227219	1.3917037	1.9441618	=====			
H	-1.0643193	0.6261473	2.6922030	69	XyNacnacRh_TS_6_7.xyz		
C	0.6546108	3.0687575	0.9325961	C	-0.6104803	-2.4150033	-2.4658802
H	-0.2589265	3.4486301	0.4690988	C	-0.0390483	-3.5352626	-1.8456498

C	3.1262846	-2.2821626	1.4352340	H	0.0852975	1.9491640	-1.5964140
C	3.6627221	-2.6212838	2.6780577	H	0.8778106	1.9866756	-1.9364242
C	1.4773899	-3.1483446	3.5239225	C	1.3465903	2.8702112	2.4553404
H	4.7340891	-2.5438433	2.8277830	H	1.1454276	3.9372930	2.6143258
H	0.8390333	-3.4817441	4.3349309	C	0.6663303	2.1023252	3.5970201
H	3.2827907	-3.3111678	4.6772340	H	1.0485813	2.4412269	4.5637027
C	-0.7236453	0.7507093	-2.6760587	H	-0.4157111	2.2498862	3.6041358
C	-1.8567180	3.0685193	-3.7418707	H	-0.1053384	0.5466669	0.9819182
C	0.1055145	1.7236498	-3.2685943	H	0.8580246	1.0286507	3.5273773
C	-2.1192725	0.9358040	-2.6186192	C	-0.6423747	3.1133060	0.8841283
C	-2.6648173	2.1021420	-3.1567138	H	-0.6610014	4.1859661	1.0955608
C	-0.4821150	2.8744258	-3.7954905	H	-1.3461733	2.6256180	1.5637636
H	-3.7382709	2.2514649	-3.1120397	H	-1.0268236	2.9708279	-0.1281974
H	0.1511503	3.6269461	-4.2528136	C	2.8691610	2.6909602	2.5155456
H	-2.2960413	3.9697493	-4.1533582	H	3.3674698	3.2650119	1.7294330
C	4.0250720	-1.8075171	0.3236445	H	3.1611334	1.6436421	2.4018923
H	3.7269049	-0.8163909	-0.0273974	H	3.2614273	3.0337052	3.4769907
H	3.9811310	-2.4666407	-0.5473874	C	1.7024463	-1.8944822	0.3396738
H	5.0617993	-1.7630876	0.6600210	C	2.7802685	-2.4437666	2.8522341
C	-0.5903599	-2.9311245	2.1028968	C	0.8497242	-2.2564775	1.3977272
H	-1.0874156	-3.1453276	3.0500161	C	3.0929542	-1.8062321	0.5325908
H	-0.8502039	-3.7295018	1.4016800	C	3.6113319	-2.0861827	1.7980738
H	-1.0039119	-2.0101793	1.6862911	C	1.4096753	-2.5281564	2.6473662
C	1.5977314	1.5276506	-3.3459515	H	4.6827907	-2.0224863	1.9538589
H	1.8607070	0.6964783	-4.0066824	H	0.7572318	-2.8052442	3.4683130
H	2.0166888	1.2861021	-2.3661398	H	3.1996240	-2.6559033	3.8287576
H	2.0848552	2.4257306	-3.7282317	C	-0.6278145	0.9262145	-4.0358613
C	-3.0175079	-0.1047173	-1.9991489	C	-1.6347021	3.0731105	-5.5030289
H	-4.0157236	0.3008996	-1.8278847	C	0.2140889	1.6114429	-4.9307819
H	-2.6174302	-0.4662284	-1.0505596	C	-1.9676653	1.3175674	-3.8638581
H	-3.1254702	-0.9819655	-2.6443445	C	-2.4526999	2.3927680	-4.6102093
=====				C	-0.3108354	2.6816649	-5.6568051
71	XyNacnacRh_TS_9_10.xyz			H	-3.4851523	2.6998786	-4.4827386
C	-0.1386649	-1.3762463	-3.7274098	H	0.3323359	3.2151422	-6.3484109
C	0.3614928	-2.4997361	-3.0569871	H	-2.0258982	3.9074500	-6.0733669
C	0.9448139	-2.5959865	-1.7878731	C	-2.8670072	0.6023180	-2.8882371
N	-0.0952293	-0.1426159	-3.2412398	H	-3.0012952	-0.4507116	-3.1501921
N	1.1383846	-1.5824653	-0.9427117	H	-3.8524339	1.0693796	-2.8602127
C	-0.7575552	-1.6264657	-5.0897150	H	-2.4485836	0.6174737	-1.8783840
H	-0.7129516	-2.6836402	-5.3442773	C	1.6574768	1.2122405	-5.1008366
H	-0.2434082	-1.0603209	-5.8686787	H	1.7573197	0.2094471	-5.5258172
H	-1.8023263	-1.3097046	-5.1103258	H	2.1794056	1.1917511	-4.1409252
C	1.3824467	-3.9918038	-1.3771023	H	2.1731192	1.9084961	-5.7636598
H	1.1891754	-4.7019226	-2.1784547	C	4.0166379	-1.4256756	-0.5953829
H	0.8570721	-4.3310529	-0.4829665	H	5.0540210	-1.4261102	-0.2582926
H	2.4481842	-4.0168805	-1.1425098	H	3.7791891	-0.4339827	-0.9883881
Rh	0.7364019	0.4056016	-1.3775813	H	3.9345378	-2.1155217	-1.4392911
H	1.9562672	0.8950122	-0.5699792	C	-0.6404889	-2.3690538	1.1983626
C	0.8321803	1.0393367	0.7140527	H	-1.1493052	-2.4727336	2.1576893
H	1.6164194	0.5492207	1.2852311	H	-0.9037597	-3.2391069	0.5891128
H	0.2764571	-3.4323962	-3.5942814	H	-1.0456442	-1.4978779	0.6812653
C	0.7739002	2.5426700	1.0423332	=====			
H	1.4198043	3.0831466	0.3408695	69	XyNacnacRh_TS_11_12.xyz		

C	-0.9879260	-1.7867220	-2.3007854	H	-4.7936679	0.5416694	-2.7022327
H	-0.7683524	-3.7891685	-1.7269336	H	-3.6266558	0.4076086	-1.3736175
C	-0.7525523	-2.7794196	-1.3456744	H	-3.8538013	-0.9363371	-2.4711600
C	-0.5984707	-2.6719124	0.0418976	C	1.0649812	0.6063244	-3.7375660
N	-1.0248731	-0.4866054	-2.0422372	H	1.3781460	0.8367108	-2.7162933
N	-0.4860485	-1.5357540	0.7345546	H	1.6922129	1.1682606	-4.4311162
C	-1.2516498	-2.2765330	-3.7141113	H	1.2667488	-0.4576764	-3.8885544
H	-1.1161435	-3.3547939	-3.7725826	C	-2.9755470	-1.4185224	2.1512077
H	-0.5837805	-1.8028605	-4.4349222	H	-2.9316198	-0.5360546	1.5086454
H	-2.2707369	-2.0409253	-4.0284895	H	-3.2217509	-2.2602865	1.4972985
C	-0.5964280	-4.0085639	0.7716394	H	-3.7935713	-1.2969465	2.8630141
H	-0.7138303	-4.8279881	0.0656966	C	2.0568487	-2.1590090	2.1043803
H	-1.4125521	-4.0601083	1.4948912	H	2.0371335	-1.7253022	1.1068552
H	0.3265943	-4.1668477	1.3293858	H	2.2765138	-3.2261809	1.9934710
Rh	-0.5814298	0.4660519	-0.2393745	H	2.8885029	-1.7210328	2.6600913
C	0.7157681	1.9378327	1.0169650	=====			
C	-0.5699540	2.0368799	1.5530969	69			
C	1.3019021	3.0114786	0.1139278	XyNacnacRh_TS_12_13.xyz			
H	2.0332107	2.5859397	-0.5758188	C	-0.6103658	-2.4596336	-2.4955864
H	0.5665409	3.5578517	-0.4703130	C	-0.3884233	-3.5193518	-1.6134685
C	-1.5003476	3.1855419	1.1967527	C	0.3405074	-3.5741610	-0.4102855
H	-1.3517487	3.5929270	0.2005783	N	-0.2405600	-1.1931857	-2.2812946
H	-2.5439168	2.8744799	1.2783008	N	0.8280833	-2.5217419	0.2345274
H	-0.2825792	1.6701908	-1.1629779	C	-1.2746809	-2.8299435	-3.8109413
H	-1.4652968	1.6151375	-0.7562739	H	-1.5341214	-3.8865864	-3.8253544
H	-1.3537886	4.0025909	1.9158746	H	-0.6096571	-2.6265168	-4.6530614
H	1.8361982	3.7395711	0.7393040	H	-2.1815226	-2.2489358	-3.9806637
C	-0.9074865	1.5106887	2.9294015	C	0.5905771	-4.9769053	0.1228171
H	-0.3028761	0.6742093	3.2569024	H	0.1464364	-5.7235470	-0.5323177
H	-1.9560174	1.2186160	2.9963721	H	0.1776566	-5.1078861	1.1236290
H	-0.7620562	2.3267537	3.6504743	H	1.6614709	-5.1775036	0.1970537
C	1.8244026	1.2006354	1.7329346	C	1.0317480	0.9898155	1.1473853
H	2.3646807	1.9056545	2.3791023	C	-0.2109210	1.2210126	0.4688398
H	2.5503266	0.8062768	1.0189155	Rh	0.7320058	-0.4244016	-0.5507882
H	1.4754947	0.3853670	2.3545389	H	1.0787777	0.7755128	-1.4422425
C	-0.4553259	-1.7013247	2.1583340	H	2.1542527	-0.1848265	-0.0474809
C	-0.4604902	-2.0029501	4.9397354	H	-0.7490298	-4.4756957	-1.9620395
C	0.7511803	-1.9558335	2.8363522	C	-0.4592113	2.4947043	-0.3187815
C	-1.6708378	-1.6376188	2.8720770	H	0.4395523	2.9146023	-0.7606185
C	-1.6530267	-1.7924175	4.2563622	H	-1.1757286	2.3224090	-1.1228563
C	0.7274036	-2.0862769	4.2286060	C	2.1666334	1.9947357	0.9874791
H	-2.5869531	-1.7392723	4.8054924	H	3.1089106	1.5629196	1.3304004
H	1.6588623	-2.2687723	4.7545897	H	2.3091759	2.3264885	-0.0377738
H	-0.4604439	-2.1101822	6.0182139	H	-0.8943985	3.2502134	0.3500333
C	-1.3877553	0.3939275	-3.1217198	H	1.9675223	2.8767981	1.6089258
C	-2.1015194	2.1481928	-5.1689108	C	1.0531697	0.3859536	2.5357783
C	-0.3889556	0.9414752	-3.9460416	H	2.0060215	-0.1016372	2.7414387
C	-2.7410600	0.7232240	-3.3141508	H	0.2651785	-0.3378480	2.7116535
C	-3.0772926	1.6024249	-4.3448085	H	0.9342132	1.1928739	3.2716365
C	-0.7681686	1.8166510	-4.9654030	C	-1.5040348	0.6940542	1.0655875
H	-4.1195852	1.8612693	-4.4974056	H	-1.4259977	-0.3204644	1.4498545
H	-0.0025384	2.2433099	-5.6044242	H	-2.3056263	0.7168424	0.3268997
H	-2.3785789	2.8301055	-5.9644900	H	-1.8151958	1.3393030	1.8983045
C	-3.8131752	0.1550150	-2.4205997	C	1.6201238	-2.7857506	1.4005508

C	3.1896006	-3.2057122	3.6804422	H	-0.3614358	2.0368816	-0.5396291
C	1.0054793	-2.9643061	2.6534196	H	-0.2622994	-3.1946586	-3.2240909
C	3.0252853	-2.8494198	1.2853995	C	-1.2322502	0.5033609	2.3006289
C	3.7877236	-3.0542959	2.4347396	H	-0.8236188	-0.3318938	2.8708918
C	1.8072951	-3.1667140	3.7792029	H	-1.7245838	1.1792823	3.0093542
H	4.8677706	-3.1028187	2.3468401	C	0.9929116	1.7085759	2.5013452
H	1.3315122	-3.2930338	4.7462525	H	1.3446361	0.8131106	3.0259722
H	3.7981858	-3.3614489	4.5635474	H	-1.7096052	2.4013043	0.5730935
C	-0.4133632	-0.2603720	-3.3629078	H	-1.9996126	0.1172885	1.6306511
C	-0.6800349	1.6130953	-5.4214296	C	0.4508371	2.6839797	3.5641259
C	0.6629787	-0.0272192	-4.2432842	H	1.2646847	3.0200200	4.2106727
C	-1.6251667	0.4335284	-3.5231503	H	-0.3060101	2.2301110	4.2039056
C	-1.7346141	1.3705595	-4.5545376	H	0.0132318	3.5740525	3.1017633
C	0.5087433	0.9095828	-5.2632855	C	2.2092194	2.3423418	1.8138853
H	-2.6668663	1.9131531	-4.6734288	H	2.9809238	2.5654371	2.5542502
H	1.3365879	1.0908048	-5.9404269	H	1.9550194	3.2839259	1.3188132
H	-0.7813232	2.3427389	-6.2163647	H	2.6463213	1.6815269	1.0639134
C	-2.8194360	0.1711026	-2.6389050	C	1.2643143	-2.1778644	0.8613527
H	-3.5054995	-0.5466563	-3.1013287	C	2.5443479	-2.9259338	3.2257406
H	-3.3871086	1.0886209	-2.4703068	C	0.5209061	-2.7728204	1.8968126
H	-2.5259723	-0.2421940	-1.6759501	C	2.6513986	-1.9745993	0.9972614
C	1.9684324	-0.7620127	-4.0851305	C	3.2704656	-2.3527985	2.1885043
H	1.8342590	-1.8465412	-4.0989082	C	1.1807107	-3.1353740	3.0733405
H	2.4383600	-0.5191115	-3.1284276	H	4.3376309	-2.1945832	2.3003614
H	2.6586514	-0.4953651	-4.8867955	H	0.6109745	-3.5880018	3.8780545
C	3.7090390	-2.7337411	-0.0530498	H	3.0406079	-3.2105206	4.1462612
H	4.7865130	-2.8638181	0.0561603	C	-1.2705509	1.1640438	-2.8890634
H	3.5253699	-1.7625703	-0.5179427	C	-2.2809937	3.5501582	-3.9266202
H	3.3470686	-3.4853493	-0.7591875	C	-2.6299338	1.4832814	-2.7078064
C	-0.4956692	-2.9708908	2.8155798	C	-0.4134927	2.0411867	-3.5816649
H	-0.7887658	-2.4775445	3.7448002	C	-0.9398746	3.2281770	-4.0933391
H	-0.8840621	-3.9937320	2.8645122	C	-3.1155255	2.6804277	-3.2362385
H	-0.9972689	-2.4784366	1.9844541	H	-0.2848974	3.9074035	-4.6283941
=====				H	-4.1620753	2.9308266	-3.0999146
69				H	-2.6730753	4.4766437	-4.3295286
XyNacnacRh_TS_13_8a.xyz				C	1.0455864	1.7127266	-3.7662291
C	-0.7370357	-1.1541242	-3.0103403	H	1.1868122	0.8314279	-4.3982477
C	-0.2042157	-2.3608172	-2.5404460	H	1.5717951	2.5466764	-4.2328690
C	0.4265954	-2.6274347	-1.3172871	H	1.5222255	1.4853327	-2.8095578
N	-0.7427265	-0.0306509	-2.3057824	C	-3.5498397	0.5546267	-1.9572891
N	0.5983688	-1.7472759	-0.3347056	H	-3.1332161	0.2842727	-0.9843888
C	-1.3129256	-1.1643669	-4.4132523	H	-3.7070251	-0.3847801	-2.4944622
H	-1.2595896	-2.1627657	-4.8432191	H	-4.5255172	1.0181989	-1.8051854
H	-0.7690559	-0.4786324	-5.0669152	C	-0.9537523	-3.0507857	1.7470579
H	-2.3556017	-0.8410278	-4.4168824	H	-1.4339419	-3.1268569	2.7242607
C	0.9625523	-4.0379482	-1.1433605	H	-1.1291859	-3.9981349	1.2263460
H	0.7679490	-4.6294257	-2.0357386	H	-1.4510924	-2.2739396	1.1679745
H	0.5045128	-4.5421921	-0.2912607	C	3.4598699	-1.3707327	-0.1207084
H	2.0395030	-4.0300335	-0.9635925	H	3.4649314	-2.0122331	-1.0065867
Rh	0.0372817	0.2180541	-0.3770136	H	4.4945772	-1.2192688	0.1900816
H	1.0925289	0.4340077	0.7506201	H	3.0402256	-0.4135342	-0.4386173
C	-0.1272343	1.2205244	1.5334966	=====			
C	-0.6298461	2.2675678	0.5564782	69			
H	-0.1395485	3.2370260	0.6582481	XyNacnacRh_TS_13_8b.xyz			

C	0.1119507	-0.7067212	-3.2337503	H	-3.6399476	1.4059361	-1.7449522
C	0.6897628	-1.9063901	-2.8055537	H	-2.2519921	0.4640716	-1.1730625
C	1.3534858	-2.1616823	-1.5965451	H	-2.9599735	0.1178170	-2.7378552
N	0.1068036	0.3798459	-2.4797595	C	1.8773577	2.2421601	-3.8065984
N	1.5254563	-1.2874291	-0.6057989	H	2.3789830	1.8914585	-2.9021380
C	-0.4996189	-0.6669063	-4.6169997	H	2.4031056	3.1203843	-4.1829037
H	-0.4150548	-1.6357487	-5.1060172	H	1.9807207	1.4461205	-4.5494313
H	-0.0032150	0.0801535	-5.2408874	C	4.3856619	-0.8246458	-0.4391819
H	-1.5554615	-0.3918422	-4.5738686	H	4.3065384	-1.3930585	-1.3696671
C	1.9395643	-3.5547004	-1.4453080	H	5.4420926	-0.7453399	-0.1793934
H	1.7272800	-4.1500962	-2.3309259	H	4.0006411	0.1745765	-0.6580783
H	1.5342143	-4.0744279	-0.5764115	C	0.0474056	-2.6336753	1.4835855
H	3.0222789	-3.5116169	-1.3108701	H	-0.1330496	-3.4933589	0.8306514
Rh	0.9232965	0.6330349	-0.6179981	H	-0.4951510	-1.7927461	1.0517906
H	2.1240359	1.0278767	0.2944939	H	-0.3827088	-2.8698734	2.4576504
C	0.9750283	1.6359593	1.2773454	=====			
H	1.8846963	2.0103070	1.7526811	71			
H	0.6413840	-2.7323988	-3.4992423	XyNacnacRh_TS_14_10.xyz			
C	0.0582224	1.1063604	2.3962036	C	0.1063025	-1.4878092	-3.7536026
H	0.3799706	0.0823479	2.6111849	C	0.7221364	-2.6061084	-3.1827596
C	-1.4374575	1.0244498	1.9885751	C	1.4804049	-2.7138466	-2.0098080
H	-1.4501753	0.4966847	1.0282817	N	0.1356801	-0.2737853	-3.2214990
C	-2.1022698	2.3911720	1.7723067	N	1.6949899	-1.7437648	-1.1174355
H	-1.5684169	3.0065589	1.0455092	C	-0.6046351	-1.7151877	-5.0750413
H	-3.1219750	2.2621832	1.4002042	H	-0.5698953	-2.7668585	-5.3526442
H	0.5378639	2.5188954	0.7690803	H	-0.1449039	-1.1319308	-5.8755561
H	-2.1672502	2.9570306	2.7052563	H	-1.6495792	-1.4048822	-5.0215334
C	0.2886739	1.9247604	3.6814154	C	2.1054881	-4.0833057	-1.7883236
H	1.3268794	1.8322111	4.0086432	H	1.9389620	-4.7188606	-2.6553164
H	-0.3440696	1.5817852	4.5032249	H	1.6836150	-4.5821284	-0.9147471
H	0.0876019	2.9876542	3.5243038	H	3.1802236	-4.0042101	-1.6178929
C	-2.2639667	0.1935281	2.9802564	Rh	1.0513357	0.2573726	-1.3824690
H	-1.8152332	-0.7870207	3.1543386	H	2.1783686	0.7781230	-0.4489849
H	-3.2768579	0.0335222	2.6008436	C	0.9346272	1.1046293	0.7624038
H	-2.3574284	0.6938049	3.9478804	H	0.6332727	-3.5180239	-3.7535775
C	-0.4251089	1.6236101	-2.9256092	C	0.8660493	2.6641365	0.7074118
C	-1.4283179	4.1163358	-3.6756712	H	0.1136989	2.9240779	-0.0429102
C	-1.7810633	1.9313893	-2.6869262	H	0.3376652	1.7512613	-1.6370944
C	0.4300606	2.5653863	-3.5380270	H	1.1531317	1.8080480	-1.9555030
C	-0.0941252	3.8046093	-3.9051844	C	-0.4425646	0.5093429	1.0658639
C	-2.2611592	3.1836134	-3.0712047	H	-0.4574019	-0.5706320	0.9303204
H	0.5567399	4.5335126	-4.3752598	H	-1.2276394	0.9435113	0.4444008
H	-3.3017673	3.4279346	-2.8885276	C	0.3676535	3.	

H	2.5720655	2.9804681	-0.6371240	C	1.5886330	1.2431871	-0.7363632
C	2.5237892	-2.0950989	0.0018469	C	1.9966691	0.5524331	0.4755425
C	4.1629854	-2.7539071	2.1687491	C	0.4619816	2.0661464	-0.8593289
C	3.8951024	-1.7665277	-0.0306352	H	0.2125624	2.2389062	-1.9023469
C	1.9812612	-2.7728933	1.1084394	H	2.0659409	0.9247872	-1.6580961
C	2.8188750	-3.0913081	2.1813636	H	2.6323452	-0.2944166	0.2236236
C	4.6927167	-2.0980906	1.0630772	C	-0.1327910	3.1853613	-0.0282573
H	2.4001826	-3.6088784	3.0382563	H	0.4211987	4.0978349	-0.2994021
H	5.7470324	-1.8447388	1.0413071	H	-1.1374234	3.3448191	-0.4313534
H	4.7978228	-3.0042470	3.0105804	C	2.5527674	1.1702298	1.7667532
C	-0.4687024	0.8013146	-3.9563309	H	3.0116501	0.3464741	2.3203866
C	-1.6109936	2.9566103	-5.3105706	H	3.3827724	1.8214526	1.4611139
C	0.3064826	1.5379656	-4.8710777	C	-0.2578634	3.1419689	1.4952592
C	-1.8123172	1.1406298	-3.7162425	H	-0.8125445	2.2477676	1.7934015
C	-2.3651757	2.2214033	-4.4053903	H	-0.8943196	3.9921515	1.7617915
C	-0.2845262	2.6125363	-5.5373862	C	1.6703896	1.9248251	2.7616193
H	-3.4006512	2.4881582	-4.2236019	H	2.3042522	2.1271719	3.6317498
H	0.3085253	3.1861585	-6.2414203	H	0.8835611	1.2529326	3.1234597
H	-2.0539147	3.7951721	-5.8349210	C	1.0359870	3.2487154	2.3208003
C	-2.6478653	0.3583509	-2.7358768	H	0.8013801	3.8071835	3.2323598
H	-3.6247346	0.8253791	-2.6043399	H	1.7740272	3.8575608	1.7840156
H	-2.1590447	0.2915785	-1.7617154	C	0.3299309	-2.2482577	1.8428815
H	-2.8117053	-0.6702862	-3.0690367	C	1.7288384	-2.7307377	4.2084974
C	1.7492779	1.1862149	-5.1292314	C	1.5921205	-2.8668542	1.7907921
H	2.2102442	1.9191211	-5.7927556	C	-0.2365163	-1.8732807	3.0749148
H	1.8519264	0.2019484	-5.5950184	C	0.4795128	-2.1240430	4.2461718
H	2.3225165	1.1465771	-4.1998205	C	2.2758369	-3.0980484	2.9858716
C	0.5289655	-3.1825578	1.1799679	H	0.0481490	-1.8364062	5.1989828
H	0.4300344	-4.2723062	1.1545630	H	3.2510952	-3.5720629	2.9517035
H	-0.0529862	-2.7776350	0.3551552	H	2.2728735	-2.9162948	5.1273072
H	0.0777988	-2.8459549	2.1166681	C	-1.6751920	0.5598376	-2.6691791
C	4.5094486	-1.1016997	-1.2347152	C	-2.1843065	2.6556514	-4.4408374
H	4.0263199	-0.1471728	-1.4540985	C	-2.6806972	1.4968547	-2.3688178
H	4.3956488	-1.7157186	-2.1324089	C	-0.9220808	0.6699522	-3.8525864
H	5.5748601	-0.9292013	-1.0755632	C	-1.1924721	1.7256616	-4.7250633
=====				C	-2.9207813	2.5361090	-3.2687741
71	XyNacnacRh_TS_23_24.xyz			H	-0.6128860	1.8169857	-5.6374447
C	-2.0622032	-1.6346796	-1.8815173	H	-3.6942350	3.2619424	-3.0415548
H	-2.5563914	-3.5905794	-1.2937374	H	-2.3807800	3.4704181	-5.1278252
C	-1.9447173	-2.7399768	-1.0321793	C	0.1560042	-0.3307601	-4.1822664
C	-1.1844986	-2.8870006	0.1363871	H	0.8486963	-0.4601039	-3.3477942
N	-1.3883737	-0.4932736	-1.7428849	H	0.7201721	-0.0140471	-5.0606644
N	-0.3661697	-1.9616215	0.6219917	H	-0.2580071	-1.3215773	-4.3913904
C	-3.0534069	-1.7826808	-3.0227444	C	2.1975498	-3.2912735	0.4770572
H	-3.4893004	-2.7797829	-3.0241956	H	3.2533808	-3.5374556	0.6001729
H	-2.5771246	-1.6110890	-3.9893330	H	1.6986518	-4.1760386	0.0694616
H	-3.8623769	-1.0539547	-2.9389291	H	2.1009573	-2.5098661	-0.2786543
C	-1.3517891	-4.2018112	0.8776845	C	-1.5890726	-1.2122295	3.1365558
H	-2.0285533	-4.8611041	0.3375297	H	-1.8404826	-0.9436875	4.1636217
H	-1.7565660	-4.0401280	1.8790684	H	-2.3797939	-1.8652983	2.7570905
H	-0.3970952	-4.7146509	1.0045083	H	-1.6154648	-0.3093173	2.5217502
Rh	0.0310652	-0.0933902	-0.2286934	C	-3.4844850	1.3850142	-1.0993483
H	0.4849133	0.3390879	1.1999993	H	-4.1158431	0.4917928	-1.0940272
				H	-4.1340506	2.2527966	-0.9761062

H	-2.8320754	1.3061965	-0.2269085
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XyNacnacRh_TS_26_27.xyz

C	-0.2648123	-2.4733962	-2.8107084
C	-0.0950961	-3.4807510	-1.8644934
C	0.2790033	-3.4091927	-0.5047328
N	-0.0640278	-1.1615238	-2.5967950
N	0.5581555	-2.2875199	0.1311035
C	-0.7055991	-2.9298345	-4.1899949
H	-0.8248285	-4.0112054	-4.2153374
H	0.0215620	-2.6424682	-4.9518036
H	-1.6532869	-2.4695708	-4.4755561
C	0.3510071	-4.7389468	0.2273358
H	0.1677016	-5.5673150	-0.4543165
H	-0.3864576	-4.7881109	1.0308018
H	1.3296112	-4.8808649	0.6897342
C	1.3451449	0.8862890	0.9034892
H	1.7681370	0.2085661	1.6405558
C	-0.0783632	0.8563456	0.8030545
H	-0.5709494	0.1374483	1.4511518
Rh	0.6004509	-0.3024404	-0.8472123
H	0.6438800	1.0466527	-1.6290622
H	1.9882176	0.1977094	-0.3341480
H	-0.2900077	-4.4795539	-2.2263245
C	-0.9122774	2.0776552	0.5180738
H	-0.3618386	2.7748387	-0.1138595
H	-1.7998171	1.7906427	-0.0528883
C	2.1604479	2.1640817	0.7304427
H	3.1893548	1.8855390	0.4822365
H	1.7920825	2.7357065	-0.1229298
C	-1.3740308	2.7804948	1.8121278
H	-2.1400579	2.1666991	2.2989492
H	-1.8692245	3.7159539	1.5290169
C	2.2040289	3.0559208	1.9852814
H	3.0307997	3.7606347	1.8468176
C	-0.2741089	3.0810816	2.8419130
H	-0.7410422	3.6412489	3.6577147
H	2.4756285	2.4448936	2.8544874
H	0.0724310	2.1450002	3.2918816
C	0.9456797	3.8744708	2.3248826
H	0.6584556	4.4785522	1.4564237
H	1.2393127	4.5931615	3.0959613
C	0.8826931	-2.3569878	1.5190850
C	1.5367343	-2.3528520	4.2377549
C	-0.1406684	-2.3008037	2.4849555
C	2.2348634	-2.4201212	1.9152523
C	2.5385887	-2.4203694	3.2766160
C	0.2094125	-2.2943951	3.8375848
H	3.5774940	-2.4740609	3.5839661
H	-0.5769741	-2.2462670	4.5834350
H	1.7905459	-2.3482375	5.2912752
C	-0.2989195	-0.2647449	-3.6965435
C	-0.7511744	1.5026675	-5.8059828

C	0.7581650	0.0693685	-4.5607790
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C	-1.5772112	0.2913445	-3.8751192
C	-1.7835467	1.1719368	-4.9377898
C	0.5098143	0.9534806	-5.6112371
H	-2.7679710	1.6050337	-5.0795845
H	1.3215633	1.2157104	-6.2813386
H	-0.9269936	2.1878862	-6.6270527
C	-2.7034873	-0.0336930	-2.9290390
H	-2.9439441	-1.1003073	-2.9210504
H	-3.6070952	0.5120895	-3.2044601
H	-2.4390566	0.2320764	-1.9021255
C	2.1415050	-0.4836011	-4.3436475
H	2.1584492	-1.5764826	-4.3551281
H	2.5293232	-0.1774658	-3.3677322
H	2.8243417	-0.1267620	-5.1160678
C	3.3393595	-2.5063630	0.8931208
H	3.2697039	-3.4214643	0.2983090
H	4.3154098	-2.4971801	1.3803055
H	3.2961797	-1.6783605	0.1821718
C	-1.5980940	-2.2931953	2.0917193
H	-1.9713346	-3.3103069	1.9327878
H	-1.7692003	-1.7497519	1.1628477
H	-2.2083106	-1.8467074	2.8786473

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XyNacnacRh_TS_27_8a.xyz

C	0.5772487	-1.3375604	-3.0237497
C	1.2312132	-2.4602291	-2.5018207
C	1.8006703	-2.6312239	-1.2320597
N	0.3620929	-0.2404993	-2.3148819
N	1.7900702	-1.7337633	-0.2469139
C	0.1381032	-1.3995978	-4.4719073
H	0.3873594	-2.3641064	-4.9106145
H	0.6254030	-0.6171804	-5.0586407
H	-0.9376153	-1.2432784	-4.5695654
C	2.5085867	-3.9555556	-1.0015008
H	2.4449106	-4.5761173	-1.8929044
H	2.0722719	-4.5070166	-0.1678301
H	3.5629666	-3.8029083	-0.7627819
Rh	0.9893930	0.1155440	-0.3702062
H	2.0493252	0.5605229	0.6772063
C	0.7879978	1.0452309	1.5746384
H	1.6290501	1.2385928	2.2489469
C	0.4240003	2.3884056	0.9226321
H	1.3567991	2.8494509	0.5923957
H	-0.1777146	2.2427947	0.0048778
H	1.3410046	-3.2959609	-3.1767495
C	-0.2503969	0.3446841	2.4558443
H	0.2274531	-0.5509199	2.8609348
H	-0.4168605	0.9885895	3.3317071
C	-0.3119488	3.4179200	1.8261404
H	-0.0189934	3.2415009	2.8666462
H	0.0793009	4.4076425	1.5725898
C	-1.6143605	-0.0658972	1.8879421

H	-1.4675604	-0.8145245	1.1053731	H	-0.0710320	-2.0789800	-5.5038027
H	-2.1500399	-0.5746549	2.6987572	H	0.1646414	-0.3259643	-5.5054898
C	-1.8405319	3.5066888	1.7235801	H	-1.3910460	-0.9922429	-5.0507424
H	-2.1075760	3.7254763	0.6824529	C	2.0056194	-4.0679970	-1.7642489
H	-2.1515646	4.3846502	2.3010040	H	1.9076440	-4.6183884	-2.6978380
C	-2.5320783	1.0363675	1.3325630	H	1.5441016	-4.6552849	-0.9682882
H	-2.2061573	1.3253229	0.3307879	H	3.0669702	-3.9876460	-1.5210937
H	-3.5199992	0.5868694	1.1930892	Rh	0.5913671	-0.0200733	-0.7578027
C	-2.6746278	2.3070648	2.1946503	H	1.6366853	0.3283568	0.3442480
H	-2.4473278	2.0835102	3.2430167	C	0.3408532	0.6499590	1.2492348
H	-3.7220424	2.6233850	2.1837975	H	-0.3678950	-0.0927461	1.6093565
C	2.4705672	-2.0498446	0.9777973	C	-0.3373283	1.8100978	0.5463706
C	3.7868093	-2.6092851	3.3741822	H	0.1891101	2.7410659	0.7705255
C	1.7964957	-2.7481729	1.9954358	H	-0.1710867	1.7555688	-0.5881250
C	3.8120814	-1.6511367	1.1463233	H	0.8917407	-3.1599663	-3.8889108
C	4.4488816	-1.9381166	2.3530614	C	1.2975800	1.0330018	2.3863039
C	2.4727787	-3.0130714	3.1888202	H	2.2038667	1.4978391	1.9841253
H	5.4802471	-1.6318358	2.4893511	H	1.6216673	0.1145649	2.8846469
H	1.9546931	-3.5453187	3.9794736	C	-1.8596089	1.9708363	0.7486140
H	4.2960574	-2.8202483	4.3072574	H	-2.1214023	3.0163771	0.5567850
C	-0.2826389	0.8954790	-2.8898971	H	-2.3794432	1.3901444	-0.0164004
C	-1.5324339	3.1819306	-3.8914681	C	0.7152774	2.0066449	3.4300901
C	0.4983302	1.9422140	-3.4226690	H	1.4575607	2.0859293	4.2305745
C	-1.6888020	0.9924607	-2.8613404	H	0.6512788	3.0112932	2.9967347
C	-2.2924792	2.1446520	-3.3666031	C	-2.4385265	1.5519112	2.1104332
C	-0.1475924	3.0751293	-3.9181761	H	-3.5142376	1.7479159	2.0503543
H	-3.3737726	2.2261487	-3.3433880	C	-0.6482367	1.6559744	4.0552770
H	0.4475880	3.8832040	-4.3292759	H	-0.6435104	2.0334515	5.0824260
H	-2.0172687	4.0713737	-4.2766178	H	-0.7557787	0.5684756	4.1433944
C	-2.5372732	-0.1276608	-2.3156638	H	-2.3508046	0.4677066	2.2336639
H	-2.6111761	-0.9581255	-3.0246681	C	-1.9049579	2.2424971	3.3789672
H	-3.5507654	0.2204661	-2.1128012	H	-1.7406194	3.3088895	3.1799595
H	-2.1170308	-0.5371469	-1.3968139	H	-2.7079354	2.2043337	4.1219799
C	2.0012505	1.8410903	-3.4744005	C	2.0047391	-2.3287061	0.3738747
H	2.4381916	2.7807055	-3.8152738	C	3.1970163	-3.1356521	2.7605525
H	2.3271786	1.0518183	-4.1579889	C	3.3673161	-2.0573494	0.5947262
H	2.4164922	1.5925317	-2.4948243	C	1.2353337	-2.9977289	1.3423490
C	4.5604584	-0.9410906	0.0491765	C	1.8516619	-3.3933485	2.5306472
H	4.6062837	-1.5412048	-0.8634652	C	3.9444098	-2.4716530	1.7957979
H	5.5822532	-0.7217735	0.3616949	H	1.2642656	-3.9087599	3.2829026
H	4.0665538	-0.0057301	-0.2255263	H	4.9945192	-2.2667382	1.9737111
C	0.3873747	-3.2509291	1.8115716	H	3.6610661	-3.4495789	3.6883110
H	0.3787800	-4.2438959	1.3494673	C	-0.7540405	0.9653742	-3.2237344
H	-0.1933597	-2.5937421	1.1677825	C	-2.0917054	3.2628478	-4.0732066
H	-0.1202313	-3.3407205	2.7735060	C	-0.0164756	2.0578929	-3.7203501
=====							
73							
XyNacnacRh_TS_27_8b.xyz							
C	0.1455922	-1.2207962	-3.5374182	C	-2.1593156	1.0229313	-3.1479333
C	0.7984427	-2.3922150	-3.1352578	C	-2.8085058	2.1809183	-3.5787350
C	1.3618944	-2.6985821	-1.8884469	C	-0.7054999	3.1958693	-4.1412010
N	-0.0675513	-0.1878761	-2.7321265	H	-3.8905302	2.2314948	-3.5208254
N	1.3784124	-1.8845886	-0.8376105	H	-0.1433046	4.0400981	-4.5255487
C	-0.3141629	-1.1560104	-4.9807187	H	-2.6106042	4.1556893	-4.4020299
				C	-2.9566103	-0.1420911	-2.6184836
				H	-2.9727495	-0.9774036	-3.3250969
				H	-3.9908088	0.1512953	-2.4324067

H	-2.5280592	-0.5314631	-1.6928592	C	-0.9149365	2.1250951	4.2575690
C	1.4874260	2.0049059	-3.7971915	H	-0.2336403	1.4574487	4.8000792
H	1.8308754	1.2293076	-4.4872745	H	-1.4823821	2.6564495	5.0297934
H	1.9228911	1.7647485	-2.8238394	C	-0.6436722	0.8085545	-3.9346862
H	1.8895769	2.9600294	-4.1380185	C	-1.7583832	2.9535939	-5.3260157
C	-0.2245653	-3.2885774	1.1089767	C	0.1774718	1.6131126	-4.7458873
H	-0.3696952	-4.0372812	0.3247024	C	-2.0181377	1.0787911	-3.8102275
H	-0.7579813	-2.3938071	0.7816877	C	-2.5566413	2.1549173	-4.5174575
H	-0.6922872	-3.6672801	2.0188290	C	-0.4008363	2.6806098	-5.4342833
C	4.1897620	-1.3262370	-0.4335993	H	-3.6162802	2.3678148	-4.4267805
H	4.2309973	-1.8664793	-1.3829723	H	0.2267434	3.3057223	-6.0602259
H	5.2121821	-1.1859674	-0.0801434	H	-2.1915036	3.7869808	-5.8665913
H	3.7569349	-0.3477289	-0.6570683	C	2.0512031	-2.0170950	0.2356792
=====							
75							
XyNacnacRh_TS_29_10.xyz							
C	0.0270351	-1.4606467	-3.7432229	C	3.4318343	-2.4937970	2.6179919
C	0.6324177	-2.5717934	-3.1420751	C	1.3954494	-2.6471088	1.3077872
C	1.2639031	-2.6844900	-1.8963353	C	3.4074940	-1.6464327	0.3453816
N	-0.0594823	-0.2623816	-3.1799801	C	4.0763178	-1.8907009	1.5439070
N	1.3410513	-1.7221461	-0.9782671	C	2.1036170	-2.8705814	2.4924581
C	-0.5369612	-1.6767446	-5.1353696	H	5.1193491	-1.6067263	1.6317308
H	-0.4201392	-2.7149220	-5.4401592	H	1.5975978	-3.3498735	3.3239900
H	-0.0325262	-1.0430932	-5.8678282	H	3.9657519	-2.6726860	3.5439592
H	-1.5971572	-1.4201103	-5.1766123	C	1.6550343	1.3419541	-4.8668600
C	1.9127062	-4.0295552	-1.6162351	H	2.1402793	2.1165756	-5.4620452
H	1.8237365	-4.6826355	-2.4818750	H	1.8559298	0.3784313	-5.3435507
H	1.4517328	-4.5282324	-0.7625045	H	2.1324405	1.3042730	-3.8847931
H	2.9717651	-3.9123883	-1.3789419	C	-2.8993137	0.2339632	-2.9263138
Rh	0.6405914	0.2257580	-1.2556520	H	-3.9226664	0.6120459	-2.9303136
H	1.6841423	0.6848825	-0.2095689	H	-2.5366298	0.2278552	-1.8954199
C	0.5200015	0.8178685	0.9131876	H	-2.9252426	-0.8097835	-3.2506586
H	1.1462153	0.1724999	1.5312100	C	-0.0316702	-3.1283288	1.2063548
H	0.6405127	-3.4697058	-3.7415474	H	-0.5603700	-2.9759522	2.1487867
C	0.8709891	2.2906717	1.1991793	H	-0.0674398	-4.2016837	0.9909747
H	0.1004526	2.9397397	0.7667269	H	-0.5783867	-2.6213198	0.4142675
H	1.7882251	2.5347451	0.6584656	C	4.1409910	-1.0174908	-0.8108655
H	-0.1458522	1.7149694	-1.4001172	H	5.1771145	-0.8101370	-0.5398970
H	0.6675617	1.8432281	-1.6866953	H	3.6663246	-0.0851878	-1.1255945
C	-0.9524205	0.4382316	1.1480751	H	4.1447610	-1.6696632	-1.6884594
H	-1.1794343	-0.4544948	0.5626495	=====			
H	-1.5998778	1.2250291	0.7473303				
C	1.1104448	2.6972180	2.6704140				
H	1.8263384	3.5248480	2.6451094				
H	1.6244452	1.8858435	3.1985915				
C	-1.3784073	0.1254059	2.6060788				
H	-0.5564229	-0.3711647	3.1336022				
H	-2.1766333	-0.6205968	2.5384105				
C	-0.0922687	3.1769504	3.5019185				
H	0.2953164	3.8716986	4.2545502				
H	-0.7582169	3.7747594	2.8673474				
C	-1.9209289	1.2810947	3.4642919				
H	-2.6086497	0.8424193	4.1952348				
H	-2.5382772	1.9394037	2.8405555				

Cartesian coordinates for benzene/H₂
reactivity.

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13CHD.xyz

C	0.5769451	-1.2222396	0.5040652
H	0.9551740	-2.0766578	1.0547644
C	0.1916762	-1.3465516	-0.7718267
H	0.2363625	-2.3077320	-1.2719312
C	-0.2717024	-0.1825462	-1.5292393
H	-0.3712114	-0.2690017	-2.6056289
C	-0.5907732	0.9568865	-0.9034331
H	-0.9691872	1.8076847	-1.4595827
C	-0.5138875	1.0485830	0.6003758
H	-1.4926691	0.7633727	1.0146925
H	-0.3401759	2.0795615	0.9177980
C	0.5755735	0.1298967	1.1730281
H	1.5635313	0.5908286	1.0232580
H	0.4503441	0.0279154	2.2536600

14

14CHD.xyz

C	0.1817621	0.0052544	-1.4847743
C	-0.1818470	-0.0052545	1.4847603
C	0.0836086	-1.2506065	-0.6640090
C	0.0780634	1.2552752	-0.6558255
C	-0.0835461	1.2506033	0.6640244
C	-0.0779942	-1.2552718	0.6558418
H	0.1509845	-2.1927780	-1.1997700
H	0.1412738	2.2012146	-1.1854141
H	-0.1508057	2.1927722	1.1997918
H	-0.1410846	-2.2012081	1.1854375
H	-0.5988827	0.0060538	-2.2586439
H	1.1259515	0.0091818	-2.0476382
H	-1.1261335	-0.0091860	2.0474484
H	0.5986498	-0.0060504	2.2587709

12

Bz.xyz

H	-0.0000038	-0.0000002	-2.4761105
C	-0.0000015	0.0000001	-1.3924248
C	-0.0000019	-0.0000000	1.3924248
C	0.0000027	-1.2058847	-0.6962199
C	-0.0000011	1.2058848	-0.6962199
C	0.0000008	1.2058847	0.6962199
C	0.0000016	-1.2058848	0.6962199
H	0.0000026	-2.1443929	-1.2380592
H	0.0000011	2.1443930	-1.2380592
H	0.0000036	2.1443929	1.2380593
H	-0.0000004	-2.1443930	1.2380592
H	-0.0000036	0.0000000	2.4761105

2

H2.xyz

H	0.0000000	0.0000000	-0.3721230
H	0.0000000	0.0000000	0.3721230

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XyNacnacIr_1.xyz

C	-0.9747368	-0.9889756	-1.4322201
H	-0.9661028	-2.9781297	-0.7429947
C	-0.6412594	-1.9782790	-0.4935754
C	0.0518924	-1.8595270	0.7214662
N	-0.6542734	0.2965926	-1.2868429
N	0.5248081	-0.7027914	1.1848887
C	-1.7361275	-1.4028760	-2.6717052
H	-1.9270045	-2.4743497	-2.6568559
H	-1.1783277	-1.1677456	-3.5812244
H	-2.6958630	-0.8857753	-2.7435895
C	0.2729042	-3.1073258	1.5471481
H	-0.1625608	-3.9714895	1.0487725
H	-0.1820410	-3.0183932	2.5365155
H	1.3367595	-3.3021638	1.7017426
Ir	0.3205461	0.9814278	0.2442042
C	1.2342135	-0.5667310	2.4211141
C	2.6202869	-0.2014374	4.8027375
C	2.6402563	-0.6738025	2.4257648
C	0.5177691	-0.2721796	3.5994030
C	1.2353616	-0.0945078	4.7822854
C	3.3132782	-0.4877261	3.6332633
H	0.6979880	0.1346626	5.6955461
H	4.3945148	-0.5648427	3.6514748
H	3.1609397	-0.0558146	5.7306851
C	-0.9903176	1.3158266	-2.2345130
C	-1.5976081	3.3628856	-4.0141942
C	-2.2019063	2.0222063	-2.0878256
C	-0.0778308	1.6312902	-3.2622493
C	-0.4054358	2.6615591	-4.1436889
C	-2.4850821	3.0440877	-2.9940126
H	0.2875793	2.9166343	-4.9374159
H	-3.4119665	3.5970894	-2.8922061
H	-1.8330030	4.1630295	-4.7062591
C	3.4040248	-0.9855796	1.1656388
H	3.1093244	-0.3145221	0.3554928
H	3.2063796	-2.0037135	0.8175614
H	4.4775218	-0.8923812	1.3348953
C	-0.9839231	-0.1557041	3.5919995
H	-1.3179981	0.5240169	2.8047225
H	-1.3451908	0.2071117	4.5550816
H	-1.4605684	-1.1207554	3.3966720
C	-3.1736101	1.6859812	-0.9872145
H	-2.6698621	1.6580106	-0.0182795
H	-3.6233604	0.6999812	-1.1356999
H	-3.9800629	2.4194513	-0.9500845
C	1.2170978	0.8774121	-3.4158016
H	1.0446959	-0.1591952	-3.7194229
H	1.7608765	0.8401987	-2.4691168

H	1.8470044	1.3472593	-4.1720837
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XyNacnacIr_3.xyz

C	-1.0201267	-0.8504110	-1.5790943
H	-0.8999745	-2.8926848	-1.0833743
C	-0.6175921	-1.9041590	-0.7533486
C	0.1053026	-1.8614625	0.4490766
N	-0.7407507	0.4162746	-1.2928475
N	0.5610153	-0.7602216	1.0533276
C	-1.7964884	-1.1858806	-2.8319114
H	-1.9423841	-2.2605374	-2.9242800
H	-1.2742236	-0.8286105	-3.7222074
H	-2.7755523	-0.7017410	-2.8258994
C	0.3863109	-3.1985898	1.1085086
H	-0.0400496	-4.0044434	0.5148853
H	-0.0397370	-3.2459707	2.1120308
H	1.4583331	-3.3750594	1.2110707
Ir	0.3179062	1.0885256	0.3842862
H	1.6789576	1.6346680	0.9826420
H	0.2752973	1.7549194	1.8206324
C	1.2913015	-0.8831122	2.2884676
C	2.7014876	-1.1048234	4.6701113
C	2.6886932	-1.0220104	2.2477069
C	0.5916355	-0.8429786	3.5060178
C	1.3204822	-0.9588605	4.6898633
C	3.3759994	-1.1345257	3.4564506
H	0.7940656	-0.9289507	5.6371928
H	4.4547560	-1.2418520	3.4406236
H	3.2518314	-1.1914633	5.5996163
C	-1.1482161	1.4952641	-2.1350132
C	-1.8890131	3.6795841	-3.6993858
C	-2.3804691	2.1374685	-1.8946766
C	-0.2786658	1.9541700	-3.1459832
C	-0.6721776	3.0467438	-3.9187733
C	-2.7318112	3.2263851	-2.6926442
H	-0.0098802	3.4062700	-4.6983652
H	-3.6775725	3.7261480	-2.5151517
H	-2.1766462	4.5294295	-4.3070747
C	-0.9024552	-0.6602970	3.5478264
H	-1.2600735	-0.6658621	4.5780918
H	-1.4289722	-1.4483693	3.0030343
H	-1.1892986	0.2859054	3.0830787
C	3.4398373	-1.0301263	0.9426527
H	3.1042272	-1.8314374	0.2792368
H	3.2862782	-0.0928533	0.4027799
H	4.5083117	-1.1616597	1.1169047
C	-3.3041966	1.6651652	-0.8015620
H	-2.7892887	1.6260477	0.1614594
H	-3.6815919	0.6568677	-0.9943567
H	-4.1627039	2.3316298	-0.7111238
C	1.0491277	1.2855552	-3.3930688
H	0.9282492	0.2550130	-3.7387665
H	1.6444306	1.2391664	-2.4779718

H	1.6160739	1.8277522	-4.1506950
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XyNacnacIr_11.xyz

C	1.4791302	-3.9549151	0.9297392
H	0.3249957	-5.5657382	1.6353921
C	0.2607032	-4.5598346	1.2492877
C	-1.0315192	-4.0480980	1.1058538
N	1.6034361	-2.7104415	0.4717293
N	-1.3101358	-2.8199419	0.6717267
C	2.7173491	-4.8085436	1.1327014
H	2.4432232	-5.7711856	1.5598199
H	3.4338327	-4.3242772	1.7981558
H	3.2369502	-4.9853495	0.1889589
C	-2.1628844	-4.9878648	1.4797486
H	-1.7615648	-5.9251674	1.8601696
H	-2.7973698	-5.2083122	0.6191278
H	-2.8104675	-4.5520869	2.2422574
Ir	0.0662356	-1.3283092	0.1905297
H	-0.0273239	-1.4478992	-1.3415859
C	-1.4742137	3.9584145	-0.9244907
H	-0.3166438	5.5764375	-1.6070781
C	-0.2537926	4.5693063	-1.2239513
C	1.0383759	4.0618697	-1.0647611
N	-1.6001996	2.7126679	-0.4699531
N	1.3155503	2.8323775	-0.6338764
C	-2.7129817	4.8065967	-1.1463113
H	-2.4363122	5.7718321	-1.5658876
H	-3.2499815	4.9779248	-0.2113673
H	-3.4151918	4.3206778	-1.8256788
C	2.1711077	5.0082844	-1.4171008
H	1.7714377	5.9456572	-1.7991004
H	2.8321810	4.5790740	-2.1716776
H	2.7913599	5.2274948	-0.5458357
Ir	-0.0620115	1.3352872	-0.1722488
H	1.1928199	0.0506592	-0.0651686
H	0.0227686	1.4524382	1.3605882
H	-1.1882015	-0.0438102	0.0814589
C	-2.9289465	2.2857035	-0.1261844
C	2.7044015	2.5190085	-0.4358697
C	-2.7004208	-2.5018278	0.4932070
C	2.9277622	-2.2911203	0.1022617
C	-5.4396858	-2.0961745	0.2248882
C	-3.3309131	-2.8248347	-0.7210093
C	-3.4225702	-1.9363026	1.5577601
C	-4.7958445	-1.7505600	1.4053722
C	-4.7056974	-2.6136300	-0.8336579
C	-2.5573100	-3.4092451	-1.8743401
C	-2.7405783	-1.5472988	2.8439818
H	-5.3637466	-1.3267257	2.2255716
H	-5.2037579	-2.8724102	-1.7619113
H	-6.5092038	-1.9512579	0.1259554
C	5.5644406	-1.6828708	-0.5449840
C	3.4030961	-2.5683221	-1.1914282

C	3.7491985	-1.6726270	1.0599653	XyNacnacIr_13.xyz		
C	5.0696521	-1.3849002	0.7175569	C	-0.8199798	-0.3046095 -1.3217419
C	4.7289602	-2.2554010	-1.4943122	H	-0.7886037	-2.3464173 -0.8436493
C	2.5210511	-3.2109365	-2.2302582	C	-0.4624411	-1.3778513 -0.4956138
C	3.2290564	-1.3354334	2.4333254	C	0.2502051	-1.3949708 0.7101593
H	5.7145680	-0.9190656	1.4537465	N	-0.5190716	0.9716867 -1.0797995
H	5.1093282	-2.4784858	-2.4854391	N	0.7427527	-0.3136004 1.3152059
H	6.5957249	-1.4590207	-0.7920817	C	-1.6041477	-0.6579233 -2.5702372
C	5.4409242	2.1219334	-0.1275940	H	-1.7696152	-1.7316190 -2.6291077
C	3.3149238	2.8373050	0.7898192	H	-1.0762339	-0.3377527 -3.4702783
C	3.4452199	1.9629478	-1.4925323	H	-2.5731223	-0.1557153 -2.5816190
C	4.8166563	1.7812349	-1.3199899	C	0.4567382	-2.7572117 1.3425477
C	4.6886740	2.6304616	0.9224788	H	-0.0000200	-3.5360610 0.7355424
C	2.5222228	3.4126459	1.9347253	H	0.0223420	-2.7966410 2.3430418
C	2.7849803	1.5796834	-2.7917109	H	1.5188922	-2.9819127 1.4546856
H	5.3986349	1.3645045	-2.1339194	Ir	0.5662692	1.6777032 0.6019443
H	5.1714542	2.8862319	1.8596094	H	1.8935278	2.1018561 1.3501482
H	6.5093688	1.9805338	-0.0129359	H	-0.1448286	3.0873876 0.5145807
C	-5.5746928	1.6643603	0.4688416	H	0.6772427	2.2521767 2.0711370
C	-3.4305276	2.5589660	1.1583005	H	1.0740500	2.9373761 -0.2082678
C	-3.7283470	1.6635074	-1.1000917	C	-0.9592280	1.9632819 -2.0271690
C	-5.0538780	1.3692864	-0.7838421	C	1.4540390	-0.4948656 2.5544372
C	-4.7605963	2.2398005	1.4348339	C	2.8401093	-0.7716614 4.9530741
C	-2.5709196	3.2034637	2.2145937	C	0.7520873	-0.4268122 3.7695722
C	-3.1794375	1.3292650	-2.4629948	C	2.8457119	-0.6860947 2.5298517
H	-5.6821128	0.9007426	-1.5327014	C	3.5203603	-0.8257196 3.7436674
H	-5.1611730	2.4595519	2.4187264	C	1.4660203	-0.5711453 4.9601435
H	-6.6094895	1.4352929	0.6955530	C	-0.7352204	-0.1858778 3.8006807
H	-2.7891812	2.2101964	-2.9791020	C	3.6068165	-0.7231073 1.2296806
H	-2.3548087	0.6156014	-2.3856990	H	4.5946465	-0.9734003 3.7347881
H	-3.9538759	0.8844890	-3.0891302	H	0.9329395	-0.5195411 5.9030808
H	-2.1855566	4.1753034	1.8951435	H	3.3794418	-0.8802034 5.8866619
H	-1.6986294	2.5868084	2.4428630	C	-1.7791150	3.9323804 -3.8165874
H	-3.1395106	3.3512489	3.1338457	C	-0.1132430	2.3282219 -3.0878862
H	-2.0625449	-4.3461780	-1.6052950	C	-2.2058346	2.5853996 -1.8459895
H	-1.7691135	-2.7291613	-2.2049871	C	-2.5986072	3.5676530 -2.7564776
H	-3.2192024	-3.6073514	-2.7185781	C	-0.5451954	3.3153438 -3.9750247
H	-3.4662609	-1.1605013	3.5604963	C	1.2399490	1.6887060 -3.2640553
H	-1.9917544	-0.7703864	2.6672825	C	-3.1000051	2.2222594 -0.6884650
H	-2.2204436	-2.3893706	3.3076471	H	-3.5590543	4.0536318 -2.6247218
H	4.0191216	-0.8987813	3.0455544	H	0.1011850	3.6040115 -4.7965011
H	2.8403941	-2.2136420	2.9552212	H	-2.0986548	4.6981544 -4.5135332
H	2.4098014	-0.6140133	2.3724899	H	-3.3840403	1.1666249 -0.7010452
H	1.6484800	-2.5899833	-2.4454241	H	-4.0146848	2.8158382 -0.7102587
H	2.1357289	-4.1795242	-1.9009659	H	-2.5982164	2.3968780 0.2665974
H	3.0725557	-3.3648184	-3.1588708	H	1.1702399	0.6068463 -3.4058821
H	3.1709790	3.6081343	2.7896870	H	1.8675903	1.8461377 -2.3832382
H	1.7315461	2.7282352	2.2501655	H	1.7518532	2.1081425 -4.1309732
H	2.0283370	4.3494789	1.6636636	H	-1.0964205	-0.1523517 4.8292246
H	3.5234116	1.2011198	-3.4995398	H	-1.2911689	-0.9665982 3.2746145
H	2.2681794	2.4226331	-3.2574737	H	-0.9915177	0.7586459 3.3141073
H	2.0372286	0.7981028	-2.6319430	H	3.4761351	0.2067321 0.6703559
=====				H	3.2664824	-1.5295069 0.5745523
53				H	4.6721305	-0.8674998 1.4135172

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XyNacnacRh_1.xyz
C   -0.9823278   -1.0195958   -1.4348179
H   -0.9788546   -3.0183290   -0.7531540
C   -0.6544323   -2.0185106   -0.5035762
C    0.0401407   -1.8865661    0.7099314
N   -0.6580835    0.2576209   -1.2787072
N    0.5056344   -0.7288972    1.1613730
C   -1.7440220   -1.4280821   -2.6777715
H   -1.9394606   -2.4988959   -2.6713177
H   -1.1831739   -1.1870537   -3.5838618
H   -2.7006974   -0.9049948   -2.7471062
C    0.2648406   -3.1322977    1.5404583
H   -0.1663575   -4.0022865    1.0484205
H   -0.1897554   -3.0371073    2.5294209
H    1.3299416   -3.3189823    1.6964729
Rh   0.3185508    0.9809041    0.2450210
C    1.2138568   -0.5695106    2.3860441
C    2.6094104   -0.1289175    4.7560320
C    2.6228394   -0.6540359    2.3899089
C    0.5029229   -0.2529357    3.5636174
C    1.2231500   -0.0391386    4.7387170
C    3.2995924   -0.4320899    3.5890395
H    0.6868019    0.2044760    5.6489988
H    4.3819686   -0.4947325    3.6030882
H    3.1524832    0.0439209    5.6778615
C   -0.9807369    1.2876929   -2.2069121
C   -1.5530488    3.3885242   -3.9440557
C   -2.1822649    2.0118085   -2.0510863
C   -0.0594002    1.6211569   -3.2229234
C   -0.3689105    2.6751560   -4.0823594
C   -2.4484423    3.0576988   -2.9345570
H    0.3318569    2.9394739   -4.8663776
H   -3.3687806    3.6201134   -2.8238499
H   -1.7751494    4.2067152   -4.6191852
C    3.3849737   -0.9809410    1.1324014
H    3.0842692   -0.3262076    0.3108430
H    3.1940654   -2.0054106    0.8000173
H    4.4584423   -0.8765944    1.2956800
C   -1.0001060   -0.1519350    3.5604513
H   -1.3464149    0.5116818    2.7644336
H   -1.3619270    0.2230389    4.5187518
H   -1.4688949   -1.1238508    3.3816089
C   -3.1621306    1.6654112   -0.9606593
H   -2.6652242    1.6170585    0.0113139
H   -3.6192280    0.6855506   -1.1256880
H   -3.9627980    2.4048335   -0.9143462
C    1.2287519    0.8570994   -3.3847098
H    1.0485892   -0.1742933   -3.7008122
H    1.7725836    0.8015276   -2.4386155
H    1.8649562    1.3307291   -4.1334566
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XyNacnacRh_2.xyz
C   -1.0777741   -0.9051424   -1.5652846
C   -0.6880931   -1.9638162   -0.7367462
C    0.0561643   -1.9077834    0.4530745
N   -0.7639060    0.3512474   -1.2953687
N    0.5323020   -0.7974406    1.0130191
C   -1.8832262   -1.2223608   -2.8053422
H   -2.0564937   -2.2935486   -2.8912213
H   -1.3672530   -0.8823723   -3.7062458
H   -2.8512382   -0.7163866   -2.7845378
C    0.3273428   -3.2348812    1.1380531
H   -0.1191309   -4.0502572    0.5724180
H   -0.0829114   -3.2517620    2.1495505
H    1.3986772   -3.4241283    1.2284852
Rh   0.2820458    1.0335316    0.2663524
H    1.4849159    1.7372412    1.2359149
H    0.7388562    1.8242177    1.6975348
H   -0.9976592   -2.9497915   -1.0503090
C    1.2794432   -0.8790253    2.2326902
C    2.7384095   -0.9709517    4.6012316
C    0.6065724   -0.7756810    3.4637484
C    2.6785219   -1.0151766    2.1781918
C    3.3897590   -1.0618973    3.3776332
C    1.3572516   -0.8269845    4.6387185
H    4.4686983   -1.1661652    3.3468899
H    0.8485028   -0.7477686    5.5930801
H    3.3064593   -1.0068388    5.5234726
C   -1.1354325    1.4585903   -2.1083096
C   -1.7983568    3.7096489   -3.6126854
C   -2.3367809    2.1493318   -1.8377566
C   -0.2580208    1.9039832   -3.1209619
C   -0.6126709    3.0303843   -3.8629708
C   -2.6490752    3.2707451   -2.6059838
H    0.0542532    3.3789112   -4.6435777
H   -3.5702654    3.8067142   -2.4064534
H   -2.0557729    4.5851873   -4.1971067
C   -0.8879752   -0.5990853    3.5208275
H   -1.2197173   -0.4620746    4.5507771
H   -1.4174253   -1.4625917    3.1088214
H   -1.2013100    0.2660201    2.9309950
C    3.4015523   -1.0945896    0.8594427
H    3.1212405   -1.9867818    0.2928567
H    4.4809649   -1.1204248    1.0139333
H    3.1557612   -0.2372183    0.2277834
C   -3.2708281    1.6870686   -0.7492650
H   -2.7437579    1.5718956    0.2005686
H   -3.7115481    0.7134851   -0.9813406
H   -4.0855478    2.3995737   -0.6151590
C    1.0320927    1.1790982   -3.4052287
H    1.6251191    1.0577154   -2.4960196
H    0.8529919    0.1740095   -3.7971124
H    1.6242727    1.7243256   -4.1410779
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XyNacnacRh_4.xyz				C	1.7114912	0.6868700	-3.3459983
C	-0.8449331	-1.1450593	-1.9642488	H	2.0608249	0.4870022	-2.3313155
H	-1.0885753	-3.2111139	-1.6269730	H	2.4962893	1.2041994	-3.9000298
C	-0.7530477	-2.2931158	-1.1681006	H	1.5620178	-0.2889054	-3.8184353
C	-0.3127995	-2.4000360	0.1565967	C	-2.9510418	1.5679519	-1.5597354
N	-0.4785947	0.0691768	-1.5722948	H	-2.6253493	1.5943836	-0.5167458
N	0.1364766	-1.3821747	0.8806894	H	-3.3341237	0.5598357	-1.7369571
C	-1.4159707	-1.3365700	-3.3570528	H	-3.7772564	2.2691774	-1.6856228
H	-1.6345849	-2.3872446	-3.5377768	=====			
H	-0.7209158	-0.9909653	-4.1243178	63			
H	-2.3379741	-0.7662779	-3.4880837	XyNacnacRh_5.xyz			
C	-0.3784832	-3.7830457	0.7778385	C	-0.8658863	-1.4390018	-1.9923294
H	-0.7318362	-4.5111384	0.0501825	H	-0.9886637	-3.4713950	-1.4654861
H	-1.0540722	-3.7991883	1.6356984	C	-0.7218489	-2.4964732	-1.0861126
H	0.5991776	-4.1041035	1.1416351	C	-0.2801071	-2.4674388	0.2401582
Rh	0.3035080	0.5735171	0.2632874	N	-0.5891359	-0.1725606	-1.7145417
C	-0.4479210	3.2480899	1.2308028	N	0.0953694	-1.3721498	0.9001905
C	-0.1581476	2.5713924	2.3729688	C	-1.3746061	-1.8052932	-3.3745137
C	0.3322419	2.9611315	0.0535217	H	-1.5557221	-2.8762466	-3.4410190
C	0.9118854	1.6066080	2.3392456	H	-0.6565812	-1.5278049	-4.1485246
H	-1.2609392	3.9612442	1.1750870	H	-2.3044512	-1.2827696	-3.6068918
H	-0.7257337	2.7115346	3.2845165	C	-0.2413425	-3.8136295	0.9438602
H	0.0484617	3.4179175	-0.8848596	H	-0.5770940	-4.6022206	0.2737358
H	1.0871951	0.9907622	3.2108261	H	-0.8799989	-3.8202300	1.8288098
C	1.6025957	2.3619336	0.1485742	H	0.7668965	-4.0576055	1.2829893
H	2.3109785	2.4201292	-0.6661214	C	1.5257910	1.5315345	1.7150712
C	1.9053479	1.6537159	1.3427350	H	2.0586246	0.6322473	1.9808581
H	2.8534164	1.1508967	1.4737874	C	0.1966923	1.7220278	2.1471805
C	-0.6259741	1.1606944	-2.4844852	H	-0.2919875	0.9691798	2.7453112
C	-0.8708130	3.3444497	-4.2016789	Rh	0.1044237	0.5569808	0.0787967
C	-1.8158342	1.9118604	-2.4882094	H	-0.3092230	2.0927928	-0.4509700
C	0.4416021	1.4981057	-3.3366820	H	0.5117084	1.9739543	-0.7193109
C	0.2995430	2.5965935	-4.1864527	C	-0.3682594	3.0253700	2.0975924
C	-1.9190543	2.9984810	-3.3573625	H	-1.3758630	3.1774865	2.4663170
H	1.1197816	2.8646731	-4.8436507	C	2.2670204	2.6474884	1.2402766
H	-2.8331557	3.5822452	-3.3658103	H	3.3002607	2.5069353	0.9452202
H	-0.9657085	4.1941322	-4.8676505	C	0.3625091	4.0860381	1.6204775
C	0.5552156	-1.6263438	2.2262860	H	-0.0718131	5.0784594	1.5937660
C	1.4006448	-2.0124727	4.8557812	C	1.6947467	3.8950086	1.1869821
C	1.9012481	-1.9447058	2.4841404	H	2.2688564	4.7428297	0.8322243
C	-0.3697038	-1.5005573	3.2793108	C	-0.7839611	0.8065953	-2.7476217
C	0.0730976	-1.7011951	4.5872053	C	-1.1355721	2.7637832	-4.6987639
C	2.3043980	-2.1309964	3.8076981	C	0.2812977	1.1265675	-3.6075021
H	-0.6342138	-1.6061510	5.4039377	C	-2.0208136	1.4668431	-2.8512906
H	3.3414275	-2.3727961	4.0141687	C	-2.1766187	2.4422768	-3.8372144
H	1.7292394	-2.1608026	5.8777770	C	0.0831350	2.1080497	-4.5797615
C	2.8912108	-2.0949226	1.3579767	H	-3.1272250	2.9572671	-3.9236940
H	2.8043442	-1.2751050	0.6425162	H	0.8997638	2.3615510	-5.2469926
H	3.9117184	-2.1284284	1.7426392	H	-1.2723745	3.5250816	-5.4578421
H	2.7208346	-3.0166932	0.7932646	C	0.5192143	-1.5489618	2.2569201
C	-1.8057935	-1.1353591	3.0085749	C	1.3535094	-1.8515245	4.9039394
H	-2.3018652	-1.8700875	2.3695732	C	-0.4230826	-1.4643794	3.2996636
H	-1.8741994	-0.1775237	2.4866380	C	1.8773849	-1.7928745	2.5371213
H	-2.3675982	-1.0656253	3.9411706	C	2.2737240	-1.9394784	3.8674817

C	0.0153903	-1.6168547	4.6161723	C	-2.0572891	1.9767644	-2.2970594
H	3.3191688	-2.1252892	4.0888374	C	-0.0684942	1.3309151	-3.5640800
H	-0.7061510	-1.5502570	5.4232831	C	-0.2820209	2.4171673	-4.4135704
H	1.6780236	-1.9647065	5.9316097	C	-2.2334164	3.0519775	-3.1689182
C	-3.1545154	1.1430990	-1.9133788	H	0.4071548	2.5887182	-5.2333332
H	-3.4971045	0.1109315	-2.0268790	H	-3.0723492	3.7218041	-3.0144109
H	-4.0050985	1.8010640	-2.0965679	H	-1.5098070	4.1152882	-4.8910894
H	-2.8440079	1.2512099	-0.8710053	C	0.7805342	-1.7784164	2.0527478
C	1.6155388	0.4385905	-3.4796878	C	1.9761003	-2.2802065	4.5249016
H	2.0108638	0.5355586	-2.4653438	C	0.0562513	-1.5441376	3.2363106
H	2.3361786	0.8638858	-4.1795526	C	2.1029057	-2.2577446	2.1039902
H	1.5436839	-0.6337304	-3.6808304	C	2.6810350	-2.5052106	3.3488828
C	2.8886979	-1.9240158	1.4260397	C	0.6742341	-1.8020069	4.4615573
H	2.7643584	-1.1444414	0.6721460	H	3.6983846	-2.8784771	3.3927027
H	2.7840991	-2.8782014	0.9004015	H	0.1200761	-1.6252861	5.3769653
H	3.9043730	-1.8764304	1.8218038	H	2.4392149	-2.4766680	5.4845664
C	-1.8864447	-1.2433816	3.0093136	C	-1.3567299	-1.0229929	3.1976713
H	-2.3567895	-2.1486266	2.6131820	H	-2.0232428	-1.6797085	2.6335316
H	-2.4221735	-0.9660721	3.9184176	H	-1.4060327	-0.0464895	2.7096678
H	-2.0367877	-0.4666439	2.2574776	H	-1.7569549	-0.9240273	4.2073372
=====				C	2.8916322	-2.4950533	0.8416789
63	XyNacnacRh_7.xyz			H	3.0109469	-1.5715163	0.2682739
C	-1.3274441	-1.1446792	-1.8518717	H	2.4007878	-3.2097456	0.1766705
H	-1.7457225	-3.1502498	-1.3772931	H	3.8851987	-2.8791373	1.0757760
C	-1.2157130	-2.2761008	-1.0292780	C	1.1150390	0.4224994	-3.7789465
C	-0.5376317	-2.4373047	0.1865317	H	1.7793375	0.4230800	-2.9099778
N	-0.7399579	0.0206061	-1.6063327	H	1.6929364	0.7429702	-4.6466357
N	0.1886808	-1.4945124	0.7814327	H	0.8153729	-0.6163966	-3.9371228
C	-2.1800443	-1.3048186	-3.0977091	C	-3.0083439	1.7685302	-1.1476378
H	-2.5482748	-2.3253092	-3.1826435	H	-2.4849450	1.8339127	-0.1908726
H	-1.6125478	-1.0641585	-3.9985790	H	-3.4810541	0.7837297	-1.1756206
H	-3.0376221	-0.6290549	-3.0784467	H	-3.7973241	2.5215792	-1.1611756
C	-0.6548770	-3.8031095	0.8396147	=====			
H	-1.2332739	-4.4786948	0.2126370	63	XyNacnacRh_8.xyz		
H	-1.1418200	-3.7357534	1.8144738	C	-1.2737746	-1.1241525	-1.8104706
H	0.3283845	-4.2450638	1.0109861	C	-1.1524512	-2.2676781	-1.0129595
Rh	0.4844209	0.4404441	0.0574959	C	-0.5497530	-2.4090424	0.2422244
H	-0.5583591	1.0424754	0.9550555	N	-0.8510105	0.0878345	-1.4598129
C	2.0961926	1.8067279	0.2493867	N	-0.0063728	-1.4110225	0.9343451
C	1.9064915	1.3076508	1.5594399	C	-1.9282831	-1.3258465	-3.1655148
C	1.0668303	2.6220971	-0.2727266	H	-2.2467503	-2.3595426	-3.2851519
H	1.1146870	2.9463693	-1.3040660	H	-1.2401693	-1.0822428	-3.9775465
H	2.9087147	1.4586550	-0.3821259	H	-2.7987808	-0.6792905	-3.2882082
H	2.6383619	0.6093065	1.9493590	C	-0.5258988	-3.8159462	0.8127640
C	1.2373057	2.1908674	2.6007730	H	-1.0377705	-4.5068575	0.1457191
H	2.0094252	2.6351607	3.2498684	H	-1.0084024	-3.8580614	1.7906864
H	0.6264262	1.5814548	3.2767681	H	0.4977997	-4.1689412	0.9529886
C	0.3058905	3.4553187	0.6712050	Rh	0.0341471	0.5982371	0.3624108
H	-0.3242841	4.2361483	0.2597787	C	-0.3220529	2.6430388	0.8862367
C	0.4055066	3.2905998	1.9972069	C	0.0960683	1.9084383	2.0536361
H	-0.1237968	3.9525267	2.6741841	C	0.6033182	2.7051227	-0.1642579
C	-0.9680182	1.1108829	-2.5046963	C	1.3776930	1.3443125	1.9970174
C	-1.3570692	3.2758033	-4.2232096	H	-1.3360214	3.0093390	0.7921294

H	-0.5943076	1.7068047	2.8621761	H	-1.7535950	-2.7308955	-3.2566306
H	0.2488767	3.0900610	-1.1122530	H	-0.6616358	-1.5440515	-3.9805458
H	1.6425638	0.6416957	2.7771276	H	-2.2797947	-1.0631025	-3.5144881
C	2.0924134	2.8242576	0.0726665	C	-0.7384155	-3.6481563	1.2087083
H	2.6242742	2.4729856	-0.8144482	H	-1.1575110	-4.4140113	0.5590895
H	2.3489648	3.8869743	0.1717277	H	-1.3994420	-3.5267940	2.0688403
C	2.5400069	2.0368730	1.3208853	H	0.2160661	-4.0096342	1.5957507
H	3.0231836	2.7032873	2.0472102	Rh	0.2403070	0.5996591	0.2269661
H	3.2938136	1.2921552	1.0555100	C	1.6702075	1.4661124	1.6849129
H	-1.5532864	-3.1750675	-1.4395582	H	2.2145622	0.7410263	2.2743523
C	-1.0208058	1.1495397	-2.4062782	C	0.3888032	1.8473483	2.0556136
C	-1.3136349	3.2730410	-4.1924970	H	-0.0726312	1.4218368	2.9363271
C	-2.1870735	1.9343492	-2.3679154	C	1.3339151	2.4082161	-0.4477752
C	-0.0002650	1.4237353	-3.3350493	H	1.6207053	2.4038723	-1.4905031
C	-0.1669804	2.4885272	-4.2209104	C	0.0524304	2.7893824	-0.0771778
C	-2.3126036	2.9934971	-3.2692545	H	-0.6667009	3.0847543	-0.8289475
H	0.6176597	2.7059493	-4.9375230	C	2.3904685	2.2835339	0.6314650
H	-3.2082450	3.6048132	-3.2421314	H	3.2662436	1.7510452	0.2580778
H	-1.4262156	4.0993721	-4.8844382	C	-0.2246837	3.0615619	1.3877268
C	0.5993054	-1.7291025	2.1929801	H	-1.2977649	3.1089411	1.5778678
C	1.7997776	-2.2634847	4.6547247	H	0.2120423	4.0107109	1.7381085
C	1.9638235	-2.0682876	2.2432106	H	2.7367945	3.2595566	1.0080555
C	-0.1664127	-1.6561724	3.3703682	C	0.2831105	-1.4293079	2.4586581
C	0.4543022	-1.9252958	4.5919533	C	0.9908606	-1.6664124	5.1483105
C	2.5445721	-2.3339499	3.4836553	C	-0.6689342	-1.1508881	3.4569831
H	-0.1302351	-1.8670562	5.5038028	C	1.5893615	-1.8234822	2.8033629
H	3.5967387	-2.5934911	3.5283496	C	1.9225356	-1.9367339	4.1542637
H	2.2665617	-2.4684126	5.6109610	C	-0.2947817	-1.2762417	4.7960011
C	1.2573626	0.5947145	-3.3673203	H	2.9278964	-2.2404754	4.4254802
H	1.9733687	1.0073917	-4.0793987	H	-1.0247427	-1.0629469	5.5694388
H	1.0569885	-0.4410510	-3.6554113	H	1.2658555	-1.7577859	6.1924814
H	1.7258618	0.5537827	-2.3813137	C	-0.5219934	0.8389584	-2.6816078
C	-3.2907792	1.6384588	-1.3850218	C	-0.5572782	2.7036391	-4.7584127
H	-2.8979868	1.4893339	-0.3777429	C	0.5995050	0.9674350	-3.5220816
H	-3.8268468	0.7203683	-1.6440444	C	-1.6601170	1.6434115	-2.8765454
H	-4.0185622	2.4509265	-1.3663461	C	-1.6575816	2.5690998	-3.9214728
C	2.7906726	-2.1314361	0.9852959	C	0.5612150	1.9055552	-4.5551253
H	3.8409476	-2.3065108	1.2224577	H	-2.5323892	3.1913726	-4.0764069
H	2.4596823	-2.9323610	0.3184080	H	1.4230213	2.0087202	-5.2056488
H	2.7089050	-1.2035220	0.4148206	H	-0.5707548	3.4281071	-5.5641453
C	-1.6322282	-1.3080599	3.3238737	C	-2.0718654	-0.7368897	3.0944809
H	-2.0136285	-1.1101914	4.3267621	H	-2.6281039	-0.4386062	3.9843955
H	-2.2272052	-2.1222487	2.8986885	H	-2.0703121	0.0920579	2.3834362
H	-1.8148593	-0.4348923	2.6950049	H	-2.6230579	-1.5504014	2.6141186
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63							
XyNacnacRh_9.xyz							
C	-0.9291049	-1.3310593	-1.8385993	C	-1.7535950	-2.7308955	-3.2566306
H	-1.3474203	-3.3048618	-1.2473280	H	-0.6616358	-1.5440515	-3.9805458
C	-0.9631545	-2.3609349	-0.8910173	H	-2.2797947	-1.0631025	-3.5144881
C	-0.5692041	-2.3422788	0.4521876	C	-0.7384155	-3.6481563	1.2087083
N	-0.4928828	-0.0979508	-1.5998792	H	-1.1575110	-4.4140113	0.5590895
N	-0.0719627	-1.2808779	1.0800054	H	-1.3994420	-3.5267940	2.0688403
C	-1.4351583	-1.6908204	-3.2245019	H	0.2160661	-4.0096342	1.5957507
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63							
XyNacnacRh_9.xyz							
C	-0.9291049	-1.3310593	-1.8385993	C	-1.7535950	-2.7308955	-3.2566306
H	-1.3474203	-3.3048618	-1.2473280	H	-0.6616358	-1.5440515	-3.9805458
C	-0.9631545	-2.3609349	-0.8910173	H	-2.2797947	-1.0631025	-3.5144881
C	-0.5692041	-2.3422788	0.4521876	C	-0.7384155	-3.6481563	1.2087083
N	-0.4928828	-0.0979508	-1.5998792	H	-1.1575110	-4.4140113	0.5590895
N	-0.0719627	-1.2808779	1.0800054	H	-1.3994420	-3.5267940	2.0688403
C	-1.4351583	-1.6908204	-3.2245019	H	0.2160661	-4.0096342	1.5957507
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63							
XyNacnacRh_9.xyz							
C	-0.9291049	-1.3310593	-1.8385993	C	-1.7535950	-2.7308955	-3.2566306
H	-1.3474203	-3.3048618	-1.2473280	H	-0.6616358	-1.5440515	-3.9805458
C	-0.9631545	-2.3609349	-0.8910173	H	-2.2797947	-1.0631025	-3.5144881
C	-0.5692041	-2.3422788	0.4521876	C	-0.7384155	-3.6481563	1.2087083
N	-0.4928828	-0.0979508	-1.5998792	H	-1.1575110	-4.4140113	0.5590895
N	-0.0719627	-1.2808779	1.0800054	H	-1.3994420	-3.5267940	2.0688403
C	-1.4351583	-1.6908204	-3.2245019	H	0.2160661	-4.0096342	1.5957507
=====							
63							
XyNacnacRh_9.xyz							
C	-0.9291049	-1.3310593	-1.8385993	C	-1.7535950	-2.7308955	-3.2566306
H	-1.3474203	-3.3048618	-1.2473280	H	-0.6616358	-1.5440515	-3.9805458
C	-0.9631545	-2.3609349	-0.8910173	H	-2.2797947	-1.0631025	-3.5144881
C	-0.5692041	-2.3422788	0.4521876	C	-0.7384155	-3.6481563	1.2087083
N	-0.4928828	-0.0979508	-1.5998792	H	-1.1575110	-4.4140113	0.5590895
N	-0.0719627	-1.2808779	1.0800054	H	-1.3994420	-3.5267940	2.0688403
C	-1.4351583	-1.6908204	-3.2245019	H	0.2160661	-4.0096342	1.5957507
=====							
63							
XyNacnacRh_9.xyz							
C	-0.9291049	-1.3310593	-1.8385993	C	-1.7535950	-2.7308955	-3.2566306
H	-1.3474203	-3.3048618	-1.2473280	H	-0.6616358	-1.5440515	-3.9805458
C	-0.9631545	-2.3609349	-0.8910173	H	-2.2797947	-1.0631025	-3.5144881
C	-0.5692041	-2.3422788	0.4521876	C	-0.7384155	-3.6481563	1.2087083
N	-0.4928828	-0.0979508	-1.5998792	H	-1.1575110	-4.4140113	0.5590895
N	-0.0719627	-1.2808779	1.0800054	H	-1.3994420	-3.5267940	2.0688403
C	-1.4351583	-1.6908204	-3.2245019	H	0.2160661	-4.0096342	1.5957507
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63							
XyNacnacRh_9.xyz							
C	-0.9291049	-1.3310593	-1.8385993	C	-1.7535950	-2.7308955	-3.2566306
H	-1.3474203	-3.3048618	-1.2473280	H	-0.6616358	-1.5440515	-3.9805458
C	-0.9631545	-2.3609349	-0.8910173	H	-2.2797947	-1.0631025	-3.5144881
C	-0.5692041	-2.3422788	0.4521876	C	-0.7384155	-3.6481563	1.2087083
N	-0.4928828	-0.0979508	-1.5998792	H	-1.1575110	-4.4140113	0.5590895
N	-0.0719627	-1.2808779	1.0800054	H	-1.3994420	-3.5267940	2.0688403
C	-1.4351583	-1.6908204	-3.2245019	H	0.2160661	-4.0096342	1.5957507
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63							
XyNacnacRh_9.xyz							
C	-0.9291049	-1.3310593	-1.8385993	C	-1.7535950	-2.7308955	-3.2566306
H	-1.3474203	-3.3048618	-1.2473280	H	-0.6616358	-1.5440515	-3.9805458
C	-0.9631545	-2.3609349	-0.8910173	H	-2.2797947	-1.0631025	-3.5144881
C	-0.5692041	-2.3422788	0.4521876	C	-0.7384155	-3.6481563	1.2087083
N	-0.4928828	-0.0979508	-1.5998792	H	-1.1575110	-4.4140113	0.5590895
N	-0.0719627	-1.2808779	1.0800054	H	-1.3994420	-3.5267940	2.0688403
C	-1.4351583	-1.6908204	-3.2245019	H	0.2160661	-4.0096342	1.5957507
=====							
63							
XyNacnacRh_9.xyz							
C	-0.9291049	-1.3310593	-1.8385993	C	-1.7535950	-2.7308955	-3.2566306
H	-1.3474203	-3.3048618	-1.2473280	H	-0.6616358	-1.5440515	-3.9805458
C	-0.9631545	-2.3609349	-0.8910173	H	-2.2797947	-1.0631025	-3.5144881
C	-0.5692041	-2.3422788	0.4521876	C	-0.7384155	-3.6481563	1.2087083
N	-0.4928828	-0.0979508	-1.5998792	H	-1.1575110	-4.4140113	0.5590895
N	-0.0719627	-1.2808779	1.0800054	H	-1.3994420	-3.5267940	2.0688403
C	-1.4351583	-1.6908204	-3.2245019	H	0.2160661	-4.0096342	1.5957507
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63							
XyNacnacRh_9.xyz							
C	-0.9291049	-1.3310593	-1.8385993	C	-1.7535950	-2.7308955	-3.2566306
H	-1.3474203	-3.3048618	-1.2473280	H	-0.6616358	-1.5440515	-3.9805458
C	-0.9631545	-2.3609349	-0.8910173	H	-2.2797947	-1.0631025	-3.5144881
C	-0.5692041	-2.3422788	0.4521876	C	-0.7384155	-3.6481563	1.2087083
N	-0.4928828	-0.0979508	-1.5998792	H	-1.1575110	-4.4140113	0.5590895
N	-0.0719627	-1.2808779	1.0800054	H	-1.3994420	-3.5267940	2.0688403
C	-1.4351583	-1.6908204	-3.2245019	H	0.2160661	-4.0096342	1.5957507
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63							
XyNacnacRh_9.xyz							
C	-0.9291049	-1.3310593	-1.8385993	C	-1.7535950	-2.7308955	-3.2566306
H	-1.3474203	-3.3048618	-1.2473280	H	-0.6616358	-1.5440515	-3.9805458
C	-0.9631545	-2.3609349	-0.8910173	H	-2.2797947	-1.0631025	-3.5144881
C	-0.5692041	-2.3422788	0.4521876	C	-0.7384155	-3.6481563	1.2087083
N	-0.4928828	-0.0979508	-1.5998792	H	-1.1575110	-4.4140113	0.5590895
N	-0.0719627	-1.2808779	1.0800054	H	-1.3994420	-3.5267940	2.0688403
C	-1.4351583	-1.6908204	-3.2245019	H	0.2160661	-4.0096342	1.5957507
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63							
XyNacnacRh_9.xyz							
C	-0.9291049	-1.3310593	-1.8385993	C	-1.7535950	-2.7308955	-3.2566306
H	-1.3474203	-3.3048618	-1.2473280	H	-0.6616358	-1.5440515	-3.9805458
C	-0.9631545	-2.3609349	-0.8910173	H	-2.2797947	-1.0631025	-3.5144881
C	-0.5692041	-2.3422788	0.4521876	C	-0.7384155	-3.6481563	1.2087083
N	-0.4928828	-0.0979508	-1.5998792	H	-1.1575110	-4.4140113	0.5590895
N							

H	2.6782673	-1.3240412	1.0071626
H	2.3519313	-3.0332368	1.1773272

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XyNacnacRh_10_x.xyz

Rh	1.5678753	-0.5461024	-1.3252293
Rh	-1.5701211	0.5607214	1.2995514
C	0.5343342	-0.3317146	0.9929271
H	1.0254405	-0.7983947	1.8344177
C	-0.2023012	-1.1437137	0.0898686
H	-0.3389083	-2.1890028	0.3256011
C	-0.5340025	-0.6525151	-1.2300194
H	-1.0420800	-1.2845208	-1.9441117
C	-0.3012610	0.7223878	-1.4173735
H	-0.5523966	1.1820663	-2.3627207
C	-0.2347156	1.5864987	-0.2240644
H	-0.3522393	2.6521537	-0.3615717
C	0.4340134	1.1073953	0.9162375
N	2.1664137	-0.4027994	-3.2700768
N	3.4065452	-1.3378546	-0.7952302
C	3.6080895	-0.6547925	-5.2439454
H	2.8552216	-1.1606550	-5.8508687
H	4.5844252	-1.0650765	-5.4944119
H	3.5925120	0.3974530	-5.5359907
C	3.3310164	-0.8180109	-3.7601319
C	4.3600288	-1.3926389	-3.0021079
H	5.2442142	-1.6752448	-3.5537903
C	4.4085774	-1.6140253	-1.6216353
C	5.6988404	-2.1876757	-1.0690763
H	6.1687882	-1.4943234	-0.3677618
H	6.4033530	-2.3915265	-1.8733185
H	5.5201420	-3.1148112	-0.5215332
C	1.2235336	0.1893490	-4.1712934
C	0.2720893	-0.6215295	-4.8157529
C	-0.6595472	-0.0161306	-5.6622108
H	-1.3986664	-0.6344717	-6.1601702
C	-0.6508194	1.3561864	-5.8748440
H	-1.3798189	1.8099325	-6.5360760
C	0.2953085	2.1455449	-5.2314452
H	0.3013875	3.2184299	-5.3904217
C	1.2387921	1.5822884	-4.3720176
C	0.2599454	-2.1154942	-4.6168171
H	-0.6666209	-2.5477813	-4.9973809
H	0.3705457	-2.3772458	-3.5631463
H	1.0892962	-2.5982207	-5.1428877
C	2.2336868	2.4547624	-3.6530421
H	2.1171897	2.3644099	-2.5696048
H	2.1021034	3.5010967	-3.9322871
H	3.2652225	2.1705699	-3.8751359
C	3.5702866	-1.5767923	0.6043859
C	4.0393441	-0.5424844	1.4362753
C	4.1397067	-0.7789025	2.8078612
H	4.4996562	0.0137272	3.4548162
C	3.7825646	-2.0064017	3.3525640

H	3.8643206	-2.1730121	4.4202895
C	3.3173296	-3.0177342	2.5213679
H	3.0327927	-3.9752336	2.9437254
C	3.2035294	-2.8240045	1.1437711
C	4.4086972	0.8019130	0.8653526
H	5.2112103	0.7270771	0.1274851
H	4.7377983	1.4786341	1.6551580
H	3.5585146	1.2555260	0.3490469
C	2.6958119	-3.9321507	0.2580468
H	1.9304685	-3.5685028	-0.4301144
H	2.2767260	-4.7424651	0.8557630
H	3.4937781	-4.3534527	-0.3609372
N	-2.9292125	-0.7093664	2.2138532
N	-2.6049060	2.1874832	1.9809496
C	-4.8825180	-1.4014413	3.5404682
H	-5.3488524	-2.0030034	2.7570308
H	-5.6699550	-0.9420261	4.1350085
H	-4.3262624	-2.0922570	4.1768443
C	-3.9734632	-0.3418059	2.9481254
C	-4.3102753	0.9900075	3.2121318
H	-5.1818020	1.1389421	3.8319115
C	-3.6847362	2.1579392	2.7565101
C	-4.3215590	3.4668161	3.1883035
H	-3.6158771	4.0924963	3.7377077
H	-5.1821795	3.2772409	3.8267400
H	-4.6538428	4.0497825	2.3269611
C	-2.6908483	-2.1024837	1.9982724
C	-3.2349887	-2.7354934	0.8649490
C	-2.9468204	-4.0836131	0.6473114
H	-3.3615188	-4.5774688	-0.2247695
C	-2.1383037	-4.7955944	1.5250390
H	-1.9234323	-5.8418013	1.3409341
C	-1.6056429	-4.1584861	2.6390768
H	-0.9717925	-4.7102786	3.3246602
C	-1.8691452	-2.8117453	2.8943851
C	-4.0978469	-1.9736273	-0.1073580
H	-4.9964484	-1.5736471	0.3690940
H	-4.4105579	-2.6172985	-0.9308244
H	-3.5613989	-1.1149494	-0.5192932
C	-1.2795910	-2.1353954	4.1051795
H	-0.5765308	-2.7973877	4.6125068
H	-2.0504120	-1.8487823	4.8264461
H	-0.7603297	-1.2147820	3.8295495
C	-2.0860068	3.4641928	1.5905213
C	-1.1117005	4.0905444	2.3883133
C	-0.5929130	5.3180719	1.9708331
H	0.1609098	5.8058181	2.5793914
C	-1.0275110	5.9188900	0.7966616
H	-0.6155346	6.8723438	0.4873753
C	-1.9906113	5.2885169	0.0177350
H	-2.3278692	5.7517597	-0.9031204
C	-2.5303728	4.0585546	0.3949100
C	-0.6415557	3.4644514	3.6760142
H	-1.4091732	3.5182227	4.4541590

H	0.2457868	3.9760611	4.0520474	C	-2.8076709	-0.3281235	-3.6834645
H	-0.4136756	2.4050267	3.5429363	C	-0.9676286	-1.8630025	-4.1880437
C	-3.5483040	3.3719172	-0.4770306	C	-0.6624388	-1.0920784	-5.3103711
H	-3.7581616	3.9672114	-1.3666458	C	-2.4649243	0.4167203	-4.8135411
H	-4.4917274	3.2030413	0.0481465	H	0.1694245	-1.3860716	-5.9412385
H	-3.1913140	2.3875438	-0.7907228	H	-3.0429227	1.3018980	-5.0559993
H	0.9328152	1.7391440	1.6368130	H	-1.1490678	0.6311751	-6.4983821
=====							
110							
XyNacnacRh_10.xyz							
C	-3.2393494	-3.2399704	-2.3210621	C	-0.8590676	-3.9041390	2.3087048
H	-4.3687280	-4.8423476	-1.5434429	C	-0.4554353	-3.8383556	3.6425607
C	-3.6539574	-4.0784695	-1.2752844	C	-2.2628588	-2.3398723	4.1578679
C	-3.2570296	-4.0554937	0.0660004	H	0.4161279	-4.4014818	3.9584495
N	-2.3673883	-2.2391641	-2.2095551	H	-2.8021456	-1.7308929	4.8754413
N	-2.3880601	-3.1740151	0.5383327	H	-0.8201342	-3.0223122	5.5965395
C	-3.8495501	-3.5258618	-3.6823308	C	-0.1875171	3.7926844	1.6803759
H	-4.5417263	-4.3628836	-3.6168715	C	-2.8057217	4.3610044	2.4603734
H	-3.0825965	-3.7713237	-4.4194117	C	-0.5753301	3.5880000	3.0173006
H	-4.3918303	-2.6607244	-4.0680372	C	-1.1062142	4.2778748	0.7313254
C	-3.8556690	-5.0904325	0.9943716	C	-2.4098984	4.5586174	1.1427755
H	-4.5515872	-5.7339938	0.4590000	C	-1.8906786	3.8764171	3.3862413
H	-4.3888197	-4.6155650	1.8209768	H	-3.1231693	4.9316519	0.4156607
H	-3.0780218	-5.7158111	1.4387562	H	-2.1963075	3.7177937	4.4149697
Rh	-1.4473282	-1.6880743	-0.5044957	H	-3.8230634	4.5805614	2.7627008
C	-0.8113512	0.8370716	0.5644722	C	4.2013653	0.7800162	-0.1640194
C	-0.0461956	0.1688320	1.5432087	C	5.6470065	-1.4200809	-1.0881469
C	-0.8838696	0.3546091	-0.8156854	C	4.2994052	0.5440823	-1.5477782
C	1.0807582	-0.5980119	1.0874790	C	4.8196181	-0.0836670	0.7587534
H	-1.5725198	1.5269270	0.9029226	C	5.5368645	-1.1797924	0.2754332
H	-0.2675165	0.2648127	2.5965883	C	5.0300120	-0.5600507	-1.9889767
H	-1.5048347	0.8945796	-1.5167660	H	6.0143527	-1.8503744	0.9819397
H	1.7418291	-1.0880862	1.7879868	H	5.1097508	-0.7474945	-3.0543994
C	0.1920358	-0.4513434	-1.2482557	H	6.2082743	-2.2747309	-1.4475124
H	0.4057939	-0.5680007	-2.3009996	C	-3.9061164	-1.5775189	2.4089300
C	1.2938293	-0.6419385	-0.3002905	H	-4.7340623	-2.2214958	2.0995809
H	2.2024850	-1.1038527	-0.6630263	H	-3.6726095	-0.9399295	1.5532370
C	2.0803363	4.3970908	1.3445888	H	-4.2585907	-0.9488735	3.2276598
H	4.0600813	5.0690696	1.0975436	C	-0.0866996	-4.7371661	1.3187690
C	3.4219025	4.2042388	0.9929248	H	0.7906472	-5.1807643	1.7914672
C	4.0457043	3.0472624	0.5106423	H	0.2407832	-4.1347316	0.4679482
N	1.1437895	3.4568195	1.2760485	H	-0.6935819	-5.5482710	0.9074969
N	3.4294069	1.8854648	0.3168201	C	-3.9788169	0.0815634	-2.8283095
C	1.7070179	5.7871486	1.8264050	H	-4.3239523	1.0800940	-3.1006805
H	2.5817943	6.4345608	1.8395476	H	-3.7202718	0.0714236	-1.7677684
H	1.2840675	5.7577663	2.8323938	H	-4.8231859	-0.6043310	-2.9467583
H	0.9519780	6.2417394	1.1817520	C	-0.1518929	-3.0852868	-3.8568581
C	5.5250817	3.1670608	0.1932563	H	0.2283550	-3.0384395	-2.8335971
H	5.8811320	4.1730959	0.4070240	H	0.6905418	-3.1835634	-4.5429242
H	5.7239691	2.9470660	-0.8575801	H	-0.7464710	-4.0006621	-3.9218722
H	6.1158725	2.4600729	0.7788543	C	-0.7020391	4.4718310	-0.7068682
Rh	1.4290548	1.4967883	0.6704400	H	0.0958074	5.2116199	-0.8120700
C	-2.0494066	-1.4727962	-3.3761503	H	-1.5516647	4.8065497	-1.3039148
C	-1.4019583	0.0415153	-5.6249382	H	-0.3181708	3.5424494	-1.1352477

C	0.4067594	3.0749890	4.0388652	C	-3.3184461	-2.7878921	-0.7184826
H	1.1562590	3.8307154	4.2937318	C	-3.4337512	-1.9138299	1.5646135
H	0.9579501	2.2124390	3.6591345	C	-4.8075441	-1.7407695	1.4041852
H	-0.1057753	2.7937248	4.9601639	C	-4.6940531	-2.5881200	-0.8395494
C	4.7202434	0.1671024	2.2414513	C	-2.5310255	-3.3541354	-1.8710396
H	5.0939248	-0.6901665	2.8036094	C	-2.7646657	-1.5272725	2.8581750
H	3.6895424	0.3681581	2.5405653	H	-5.3849604	-1.3268505	2.2228843
H	5.3039640	1.0419994	2.5441836	H	-5.1831768	-2.8441825	-1.7733136
C	3.6140033	1.4496978	-2.5374313	H	-6.5110644	-1.9521046	0.1129600
H	3.7676359	1.0926465	-3.5568266	C	5.5622533	-1.6670989	-0.5510133
H	3.9859195	2.4759835	-2.4797252	C	3.3878577	-2.5280580	-1.1865091
H	2.5395418	1.5000630	-2.3437698	C	3.7584892	-1.6479983	1.0670481
=====							
102							
XyNacnacRh_11.xyz							
C	1.4793144	-3.9202962	0.9463431	C	3.2520124	-1.3139260	2.4462661
H	0.3259427	-5.5324950	1.6525698	H	5.7336520	-0.9153114	1.4504831
C	0.2613523	-4.5250106	1.2706197	H	5.0842679	-2.4436597	-2.4936826
C	-1.0314912	-4.0144207	1.1224135	H	6.5941068	-1.4524157	-0.8039809
N	1.6062189	-2.6759842	0.4939579	C	5.4418868	2.1017760	-0.1326216
N	-1.3128953	-2.7867924	0.6943968	C	3.3068356	2.7889489	0.7851895
C	2.7160117	-4.7802432	1.1370304	C	3.4524361	1.9433726	-1.5069058
H	2.4441572	-5.7415538	1.5686058	C	4.8243832	1.7704812	-1.3312770
H	3.4421489	-4.2965768	1.7923245	C	4.6811741	2.5895865	0.9211764
H	3.2229121	-4.9592518	0.1866993	C	2.5050893	3.3416637	1.9343920
C	-2.1618609	-4.9614352	1.4837107	C	2.8007094	1.5721691	-2.8137945
H	-1.7615757	-5.8959505	1.8719434	H	5.4127765	1.3678634	-2.1477693
H	-2.7822135	-5.1864033	0.6138735	H	5.1581612	2.8355631	1.8639162
H	-2.8228243	-4.5263934	2.2349572	H	6.5111684	1.9682124	-0.0159906
Rh	0.0675232	-1.3126939	0.2301404	C	-5.5755173	1.6508708	0.4667118
H	-0.0267517	-1.4191870	-1.2728166	C	-3.4191980	2.5185146	1.1524705
C	-1.4733113	3.9281172	-0.9335172	C	-3.7361467	1.6420822	-1.1105397
H	-0.3145105	5.5499338	-1.6079590	C	-5.0628636	1.3588793	-0.7901672
C	-0.2525378	4.5395308	-1.2333641	C	-4.7505492	2.2094740	1.4334147
C	1.0396765	4.0313009	-1.0716931	C	-2.5471087	3.1425390	2.2102729
N	-1.6029357	2.6810598	-0.4891045	C	-3.1973965	1.3128490	-2.4785683
N	1.3185810	2.8001792	-0.6524794	H	-5.6990451	0.9011442	-1.5390809
C	-2.7101516	4.7835496	-1.1427291	H	-5.1438608	2.4242574	2.4213408
H	-2.4349016	5.7476360	-1.5658257	H	-6.6118796	1.4317055	0.6961418
H	-3.2348922	4.9567121	-0.2010727	H	-2.8156693	2.1964751	-2.9965214
H	-3.4221436	4.2991720	-1.8128478	H	-2.3687404	0.6030588	-2.4102432
C	2.1720786	4.9850797	-1.4078957	H	-3.9748979	0.8657096	-3.0992157
H	1.7742997	5.9235838	-1.7890708	H	-2.1573389	4.1160902	1.9018072
H	2.8426922	4.5609039	-2.1568114	H	-1.6772233	2.5164129	2.4222097
H	2.7817401	5.2003067	-0.5281031	H	-3.1067480	3.2808567	3.1362835
Rh	-0.0641517	1.3213462	-0.2097582	H	-2.0355448	-4.2929337	-1.6099626
H	1.1512143	0.0496770	-0.0624856	H	-1.7416581	-2.6665998	-2.1835814
H	0.0183441	1.4244652	1.2941409	H	-3.1828972	-3.5427169	-2.7250460
H	-1.1478289	-0.0415272	0.0796327	H	-3.4958163	-1.1325391	3.5647537
C	-2.9261811	2.2544630	-0.1381736	H	-2.0067122	-0.7576017	2.6897616
C	2.7026018	2.4852316	-0.4482271	H	-2.2579320	-2.3726450	3.3307233
C	-2.6984251	-2.4707525	0.5036356	H	4.0466856	-0.8740632	3.0501499
C	2.9241672	-2.2578421	0.1138122	H	2.8732164	-2.1939433	2.9724726
C	-5.4406252	-2.0861171	0.2177096	H	2.4287642	-0.5964450	2.3954424

H	1.6184672	-2.5278149	-2.4185407	H	-3.9708173	2.8321441	-0.6418044
H	2.1071424	-4.1260844	-1.9018137	H	-2.5693790	2.2758136	0.2926304
H	3.0310800	-3.2975738	-3.1600573	H	1.1550845	0.5888820	-3.4567080
H	3.1465893	3.5214614	2.7981161	H	1.8558573	1.7299845	-2.3296024
H	1.7126915	2.6501740	2.2300232	H	1.7958098	2.1204590	-4.0589574
H	2.0118680	4.2828944	1.6776460	H	-1.1091805	-0.0832487	4.7914726
H	3.5426704	1.1937021	-3.5180465	H	-1.2973218	-1.0154098	3.3033174
H	2.2930566	2.4210709	-3.2789822	H	-1.0334937	0.7122675	3.2077277
H	2.0466381	0.7944904	-2.6658344	H	3.3895501	0.1669974	0.5839780
=====				H	3.2863772	-1.5803198	0.5872428
53	XyNacnacRh_12.xyz			H	4.6570628	-0.7911815	1.3729775
C	-0.8296100	-0.3418933	-1.3282524	=====			
H	-0.8047050	-2.3924633	-0.8593531	63	XyNacnacRh_TS_6_7.xyz		
C	-0.4786419	-1.4237567	-0.5115304	C	-0.7409670	-1.5000195	-1.9668228
C	0.2354092	-1.4261579	0.6929428	C	-0.5538628	-2.5386512	-1.0580457
N	-0.5213267	0.9255933	-1.0720279	C	-0.0925472	-2.5197766	0.2768521
N	0.7196661	-0.3377863	1.2829793	N	-0.4876430	-0.2002613	-1.7344602
C	-1.6147803	-0.6750462	-2.5826425	N	0.2590145	-1.4249391	0.9211676
H	-1.7865083	-1.7472953	-2.6517467	C	-1.2680164	-1.9046993	-3.3320674
H	-1.0836197	-0.3513478	-3.4797050	H	-1.4224277	-2.9808165	-3.3784180
H	-2.5817896	-0.1686579	-2.5904002	H	-0.5733788	-1.6190511	-4.1240923
C	0.4532374	-2.7799713	1.3413958	H	-2.2143856	-1.4084388	-3.5544438
H	0.0002932	-3.5673555	0.7423442	C	-0.0136938	-3.8711273	0.9669380
H	0.0191819	-2.8139391	2.3424151	H	-0.2437182	-4.6759808	0.2714005
H	1.5168596	-2.9987307	1.4529564	H	-0.7170397	-3.9292602	1.8002757
Rh	0.5308435	1.5775690	0.5666810	H	0.9810740	-4.0447224	1.3815103
H	1.7343690	2.1097150	1.6214364	C	1.1556707	1.7285835	1.7785629
H	0.0391916	3.1638030	0.2733820	H	1.6004580	1.0435576	2.4966612
H	0.9840976	2.2019613	2.0662151	C	-0.3060979	1.7255639	1.7110149
H	0.7894900	3.0715844	-0.1715995	H	-0.8387663	0.9917180	2.3011697
C	-0.9460743	1.9372552	-1.9994392	Rh	0.2870021	0.5824401	-0.0125080
C	1.4345922	-0.4871567	2.5201240	H	0.3640207	1.9381346	-0.7771971
C	2.8331171	-0.6882869	4.9207454	H	1.6551880	1.1478101	0.6663296
C	0.7363685	-0.4016796	3.7373444	H	-0.8020571	-3.5197385	-1.4351892
C	2.8296538	-0.6594133	2.4962900	C	1.8255265	3.0354116	1.6688840
C	3.5106456	-0.7609613	3.7104334	H	2.9004873	3.0705197	1.8018622
C	1.4559307	-0.5078875	4.9286232	C	-0.9889747	2.9614536	1.4466938
C	-0.7547425	-0.1858015	3.7649500	H	-2.0725838	2.9526581	1.4168257
C	3.5835488	-0.7197257	1.1929084	C	-0.3078434	4.1276225	1.2871414
H	4.5869324	-0.8938279	3.7016101	H	-0.8411858	5.0503157	1.0939168
H	0.9256039	-0.4427935	5.8723578	C	1.1192328	4.1598623	1.4163912
H	3.3770876	-0.7670030	5.8546622	H	1.6310844	5.1122816	1.3397001
C	-1.7308678	3.9610903	-3.7452115	C	0.6784823	-1.5317289	2.2795977
C	-0.0915286	2.3155850	-3.0497651	C	1.5299153	-1.5804379	4.9431344
C	-2.1849747	2.5738980	-1.8090927	C	-0.2697739	-1.4719907	3.3191314
C	-2.5602733	3.5833329	-2.6970559	C	2.0550701	-1.6252047	2.5751579
C	-0.5053149	3.3298211	-3.9147970	C	2.4575678	-1.6510333	3.9102123
C	1.2503346	1.6557360	-3.2365607	C	0.1784788	-1.4926295	4.6423096
C	-3.0885689	2.1910723	-0.6654369	H	3.5148812	-1.7271917	4.1398111
H	-3.5142435	4.0800244	-2.5578408	H	-0.5500436	-1.4405759	5.4443535
H	0.1477088	3.6283921	-4.7275193	H	1.8601197	-1.5950858	5.9750294
H	-2.0363991	4.7480807	-4.4245961	C	-0.7566602	0.7325873	-2.7957010
H	-3.4282562	1.1544401	-0.7410210	C	-1.2775210	2.5634294	-4.8326906

C	0.2596697	1.0614514	-3.7090008	H	1.7665383	1.8428869	3.2719417
C	-2.0269363	1.3264515	-2.8871113	C	-0.9979894	1.0753876	-2.4951250
C	-2.2680911	2.2385424	-3.9150306	C	-1.4179701	3.2287439	-4.2200976
C	-0.0228327	1.9776967	-4.7223731	C	-2.1110465	1.9144824	-2.3027883
H	-3.2464398	2.7009886	-3.9902686	C	-0.0905700	1.3154659	-3.5428651
H	0.7573797	2.2364933	-5.4300163	C	-0.3186704	2.3986363	-4.3942944
H	-1.4802920	3.2732558	-5.6261227	C	-2.3048755	2.9828296	-3.1787040
C	3.0790532	-1.7183052	1.4726634	H	0.3791684	2.5899810	-5.2024067
H	4.0895702	-1.6825367	1.8819342	H	-3.1613150	3.6326747	-3.0353541
H	2.9657217	-0.9104479	0.7466292	H	-1.5811055	4.0653335	-4.8892026
H	2.9799134	-2.6501874	0.9084803	C	0.6413659	-1.7713084	2.1279835
C	-1.7520715	-1.4317010	3.0355312	C	1.7621926	-2.2473159	4.6378868
H	-2.1650962	-2.4421515	2.9488390	C	1.9689155	-2.2266567	2.2218976
H	-1.9764567	-0.9214826	2.0993029	C	-0.1254737	-1.5450583	3.2856472
H	-2.2887027	-0.9358589	3.8463551	C	0.4538478	-1.7924784	4.5310262
C	-3.1045997	1.0084988	-1.8841232	C	2.5107504	-2.4588082	3.4872585
H	-3.3803865	-0.0495820	-1.8933008	H	-0.1330381	-1.6233136	5.4273707
H	-4.0039666	1.5913749	-2.0879797	H	3.5342815	-2.8092907	3.5658401
H	-2.7669180	1.2324401	-0.8689221	H	2.1965377	-2.4338933	5.6131144
C	1.6382203	0.4708747	-3.5799305	C	1.1038184	0.4209829	-3.7577242
H	1.6283203	-0.6212453	-3.6236143	H	1.6367812	0.2338907	-2.8236601
H	2.0815568	0.7394979	-2.6165694	H	1.7945182	0.8663246	-4.4751800
H	2.2892987	0.8353442	-4.3757710	H	0.8114363	-0.5599766	-4.1449259
=====				C	-3.0655999	1.6814531	-1.1609218
63	XyNacnacRh_TS_7_8.xyz			H	-3.5425453	0.6996725	-1.2185022
C	-1.2705458	-1.1941435	-1.8732751	H	-3.8515512	2.4379974	-1.1554658
H	-1.6114614	-3.2256390	-1.4522999	H	-2.5421604	1.7144177	-0.2018385
C	-1.1434949	-2.3318955	-1.0671546	C	-1.5396427	-1.0338643	3.1926052
C	-0.5374481	-2.4685881	0.1893735	H	-2.1797720	-1.7012530	2.6102003
N	-0.7552317	-0.0016359	-1.5843571	H	-1.5739365	-0.0618600	2.6933114
N	0.0845584	-1.4901087	0.8368502	H	-1.9767453	-0.9287478	4.1865236
C	-2.0779767	-1.3699471	-3.1468321	C	2.7965560	-2.4666971	0.9851110
H	-2.4028688	-2.4027412	-3.2555956	H	3.8414362	-2.6384473	1.2481364
H	-1.4983029	-1.0938585	-4.0291013	H	2.4482987	-3.3402594	0.4254736
H	-2.9627538	-0.7295951	-3.1405397	H	2.7382452	-1.6198876	0.2979607
C	-0.6393025	-3.8400023	0.8329712	=====			
H	-1.1446816	-4.5376954	0.1680657	63	XyNacnacRh_TS_7_9.xyz		
H	-1.1970021	-3.7933307	1.7707974	C	-1.2848469	-1.1847992	-1.8328995
H	0.3457348	-4.2428759	1.0737821	H	-1.6332078	-3.2204960	-1.4441394
Rh	0.3535590	0.4587125	0.1503971	C	-1.1481309	-2.3383778	-1.0533932
H	0.5302926	0.8009014	1.6555328	C	-0.5131178	-2.5039072	0.1861139
C	1.8412138	1.9000720	-0.1596946	N	-0.7503456	-0.0004820	-1.5375098
C	2.0717641	1.3903910	1.1735590	N	0.1334929	-1.5424739	0.8322999
C	0.6894825	2.7021062	-0.2628538	C	-2.1267994	-1.3298541	-3.0882139
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H	2.4722847	1.6544396	-1.0036584	H	-1.5683642	-1.0412384	-3.9801379
H	2.8779931	0.6765946	1.3050104	H	-3.0065718	-0.6840126	-3.0470269
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C	0.2255898	3.4670062	0.8979842	H	-1.1447169	-4.5655800	0.1453466
H	0.4985298	3.9881696	2.9277737	H	-1.1338932	-3.8528712	1.7634657
C	0.8154665	3.3676318	2.0973027	H	0.3789994	-4.3040017	1.0048235
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C	1.9295819	1.8352600	-0.0956632
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C	0.3059668	3.5629610	0.8240937
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C	1.8512481	2.3657581	2.3398563
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C	-1.5025296	3.2890282	-4.0736182
C	-2.1291922	1.9295847	-2.1653703
C	-0.1530366	1.3607303	-3.4882569
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H	0.7332314	-0.5121596	-4.1233727
C	-1.4383632	-1.1288932	3.2326730
H	-2.0979284	-1.7994676	2.6757562
H	-1.4869202	-0.1602849	2.7283586
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C	2.8457807	-2.5234322	0.9026577
H	2.7909909	-1.6530487	0.2447954
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H	3.8918868	-2.7221730	1.1403477

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