Electronic Supplementary Information

Oxidatively Induced Reactivity in Rh(III)-Catalyzed 7-Azaindole Synthesis: Insights into the Role of the Silver Additive

Ho Ryu,[a,b] Bimal Pudasaini,[b] Dasol Cho,[a,b] Sungwoo Hong,[b,a,*] and Mu-Hyun Baik[b,a,*]

[a]Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea

[b]Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science (IBS), Daejeon 34141, Republic of Korea

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Computational Results

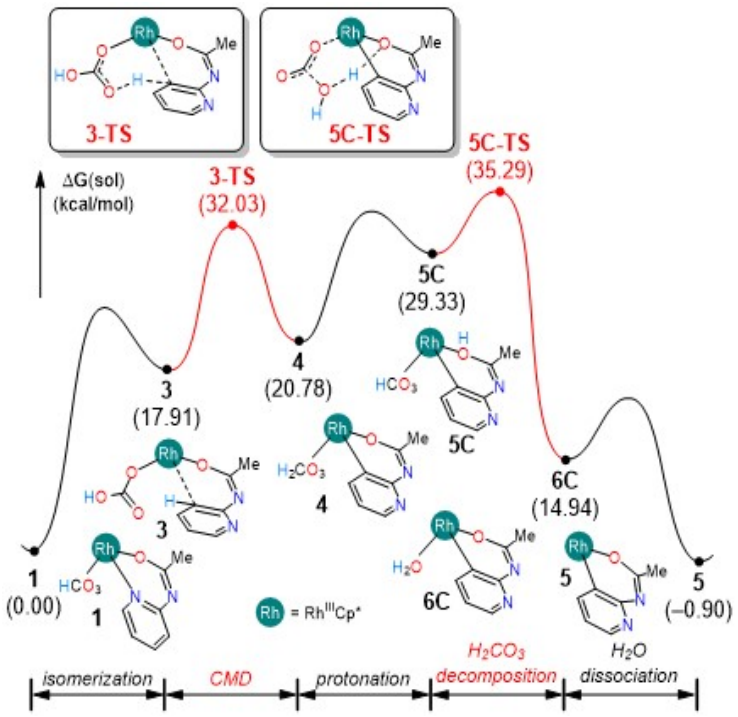


Figure S1. Energy profile of carbonic acid decomposition pathway.

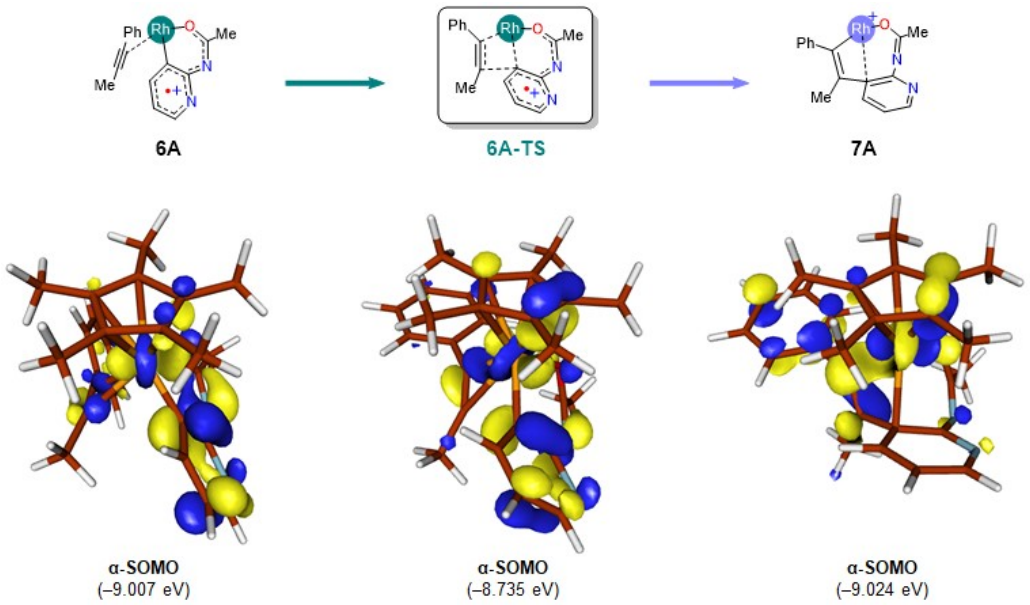


Figure S2. The frontier orbitals of **6A**, **6A-TS**, and **7A**. The SOMO orbital of **7A** does not feature over the pyridyl ligand.

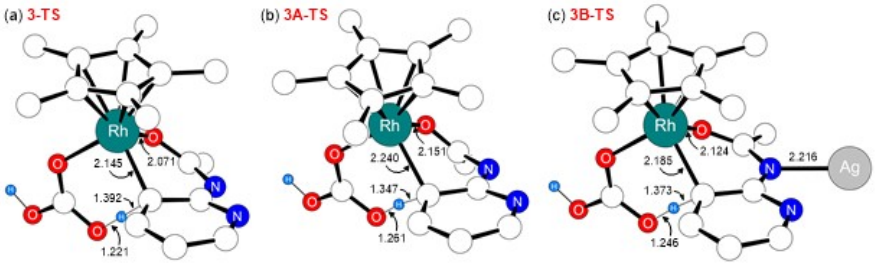


Figure S3. Comparison of DFT-optimized geometries of the transition states, **3-TS**, **3A-TS**, and **3B-TS** for C–H activation. Nonessential hydrogen atoms are omitted for clarity.

Table S1. Overall barriers of neutral, oxidized, and Ag(pyridine)-coordinated Rh complexes relative to each starting complex.

	3-TS	**3A-TS**	**3B-TS**
$\Delta G^{\ddagger}$ from starting complex	32.03	28.10	28.80

In the **3B-TS**, coordinating Ag^{+} to the amide attenuates a donating ability of the O-donor of the amide to the Rh(III) center. As the Rh(III) becomes more electrophilic, the step barrier for CMD is to be lower than the **3-TS** that is in the case without the Lewis acid.

We found that intermediate **6** is oxidized by an external oxidant, Ag^{+} at –0.68 V of an oxidation potential. Intermediate **6** has the lowest oxidation potential among Rh(III) intermediates. We found that the energy trend of HOMO for intermediates is correlated by the oxidation potential.

Additionally, we found that coordinating the $Ag(pyridine)^{+}$ to the nitrogen of the amide of the 2-amidopyridine is an exergonic process with 2.7 kcal/mol downhill (Figure S4).

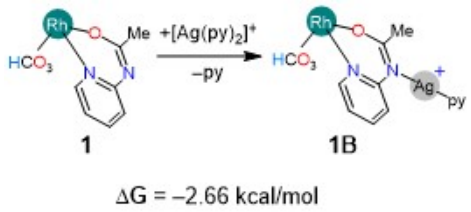


Figure S4. Thermodynamic change with coordination of $Ag(pyridine)_2$ to complex **1**.

As the Lewis acid coordinates the pyridine, the meta-C–H proton becomes acidic. The barrier for CMD of **3B-TS** is now only 28.8 kcal/mol uphill relative to the starting complex **1B**, which is around 3.2 kcal/mol lower in energy than the case without Lewis acid coordination, **3-TS**.

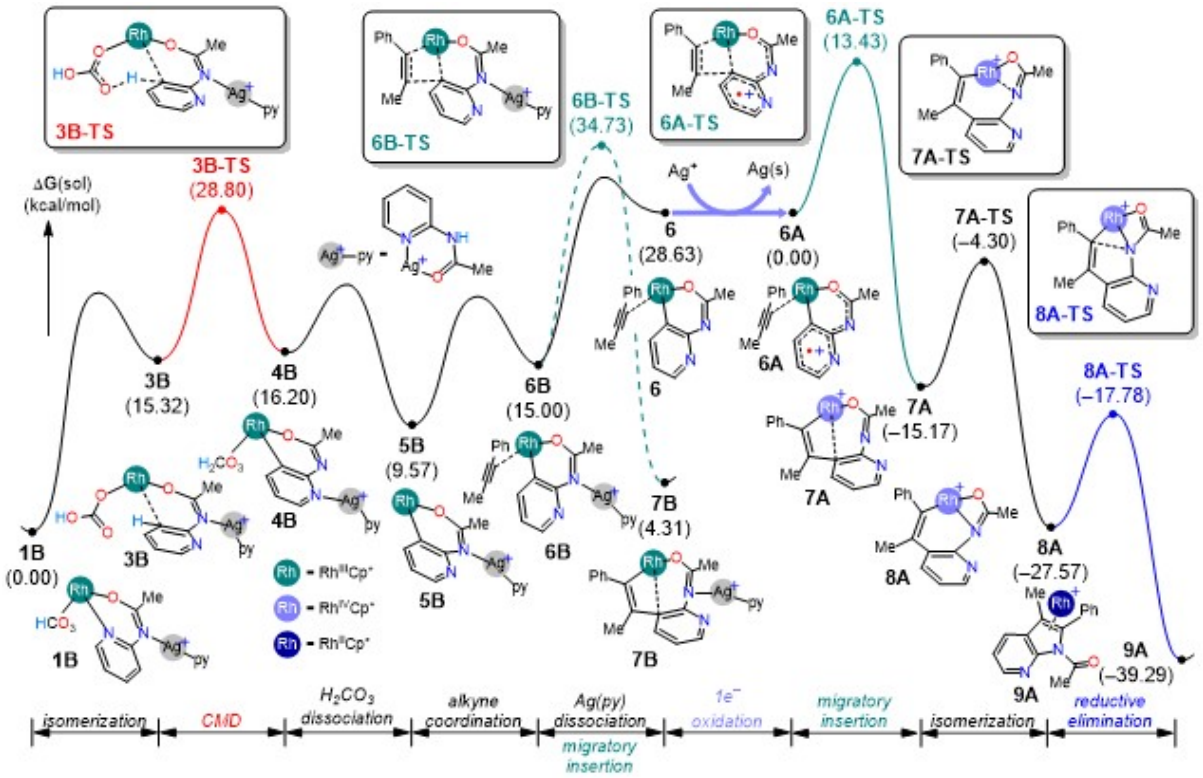


Figure S5. Reaction profile(s) illustrating the role of the [Ag(pyridine)]$^+$ is acted as a Lewis acid in the catalysis to form the 7-azaindole. Energies are in kcal/mol. (This profile will compare the oxidation path from complex 7 in scheme 2, with the path in Figure 1.)

As the [Ag(pyridine)]$^+$ coordinates to the N of amide, the O of carbonyl relatively weakly coordinates to the Rh center, as we found in the transition state structure analysis shown in Figure S3. The distance between the Rh center and O of amide is slightly elongated at the **3B-TS** compared to that of **3-TS**. This structural difference originates from increasing the electrophilicity of the Rh center. The meta-C of 2-amidopyridine more strongly interacts with the Rh center at the transition state **3B-TS**, lowering the activation barrier. The same result is observed at **3A-TS**. As the pyridyl ligand oxidizes, the O of carbonyl of amide is weakly donating so that the Rh center becomes more electrophilic. This strengthens the interaction between the Rh and the meta-C of 2-amidopyridine resulting in lowering the free energy of **3A-TS**.

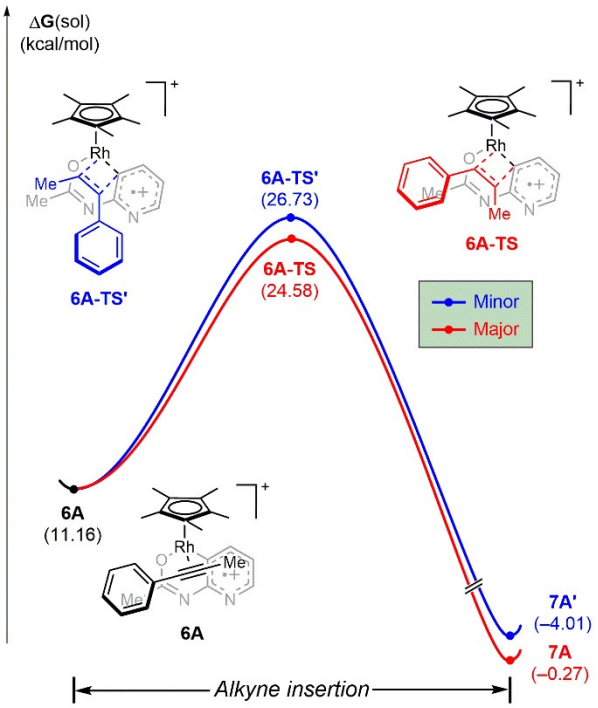
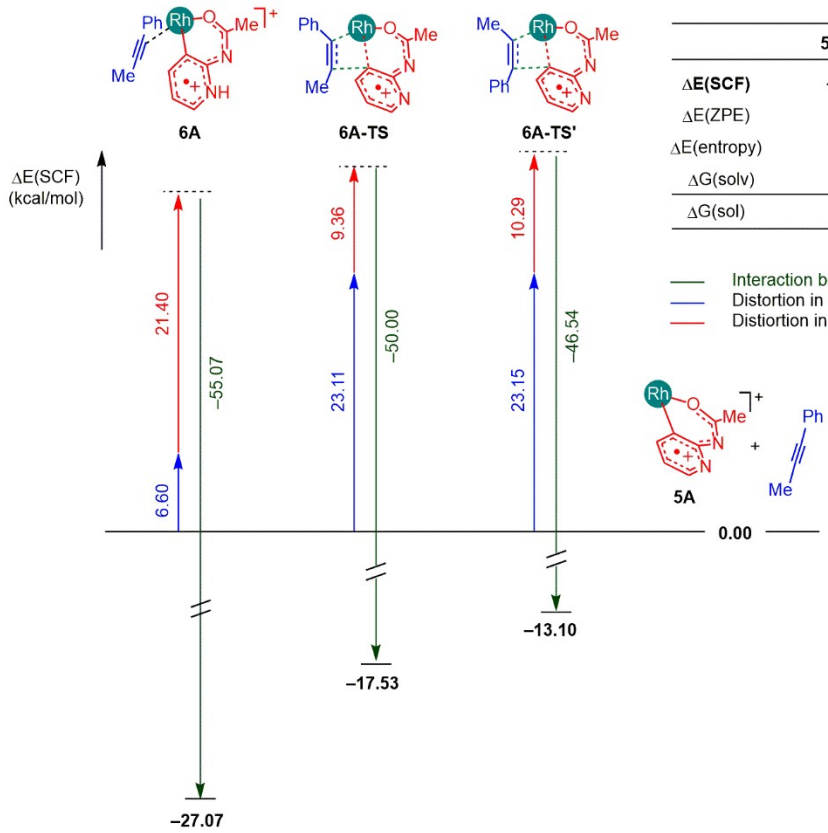


Figure S6. Energy profile for explaining the regioselectivity.

Figure S6 illustrates the free energy profile of the regio-determining step. In this alkyne insertion step, the orientation of the alkyne determines the regioselectivity, as the major product is formed as the reaction proceeds via **6A-TS** (highlighted in red color). We anticipate the formation of the minor product could occur via a somewhat more sterically congested transition state, **6A-TS'** (highlighted in blue). Quantitative inspection of the two transition states suggests that the difference in the transition state energies arises from the interaction between the Rh center and the C_{alkyne} due to the substitution effect of a phenyl group versus a methyl group, resulting in the difference of 2.2 kcal/mol. As shown in Figure S7 below, the decomposition of energy into fragment interactions and distortion components reveals that the energy difference largely originates from the interaction between the metal fragment and substrate in the transition states. In **6A-TS**, the interaction energy between the metal fragment and substrate is 50.0 kcal/mol, whereas the interaction energy is 46.5 kcal/mol in **6A-TS'.** Consistent with the experimental observations, the reaction path involving **6A-TS** will eventually lead to the formation of 2-aryl-7-azaindole.



	5A → 6A	5A → 6A-TS	5A → 6A-TS'
ΔE(SCF)	**−27.07**	**−17.53**	**−13.10**
ΔE(ZPE)	1.79	1.68	1.20
ΔE(entropy)	16.89	20.76	19.96
ΔG(solv)	8.63	8.51	7.51
ΔG(sol)	0.24	13.42	15.57

Figure S7. Distortion-interaction analysis to reveal the origins of the regioselectivity.

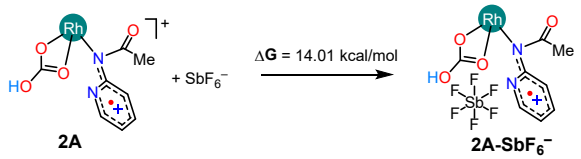


Figure S8. Thermodynamic change with coordination of SbF_6^- to complex **2A-SbF_6^-**.

In the experimental conditions, counter ion SbF_6^- is not expected to bind to Ag^+, nor to cationic Rh complexes. Although the weak coordinating property of the counterion is not expected to alter the course of the reaction pathway, we evaluated the binding energy of the **2A** and SbF_6^- in 1,2-DCE solutions to support our argument. As expected, the non-coordinating SbF_6^- shows the association energy of +14.01 kcal/mol. As Ag^+ is expected to reduce and precipitate out of organic solution (1,2-DCE), only the cationic form, **2A**, is plausible.

Table S2. NPA charge analysis of **2** and **2A**. Values are the summation of charges of each fragment.

	2	**2A**	Difference
pyridyl ligand	–0.612	0.174	0.785
RhCp*HCO_3	0.612	0.826	0.215

Table S3. NPA charge analysis of **6** and **6A**. Values are the summation of charges of each fragment.

	6	**6A**	Difference
pyridyl ligand	–0.836	–0.169	0.667
RhCp*HCO_3	0.836	1.169	0.333

Natural Population Analysis of 2, 2A, 6, and 6A

2

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population Core	Valence	Rydberg	Total
O	1	-0.64792	2.00000	6.62688	0.02103	8.64792
N	2	-0.64625	2.00000	5.61233	0.03393	7.64625
N	3	-0.50340	2.00000	5.47130	0.03210	7.50340
C	4	0.66885	2.00000	3.29497	0.03619	5.33115
C	5	-0.15838	2.00000	4.14389	0.01450	6.15838
C	6	-0.28035	2.00000	4.26526	0.01509	6.28035
C	7	-0.24964	2.00000	4.23462	0.01502	6.24964
C	8	0.04579	2.00000	3.93296	0.02126	5.95421
C	9	0.38332	2.00000	3.58983	0.02685	5.61668
H	10	0.20403	0.00000	0.79403	0.00193	0.79597
H	11	0.17277	0.00000	0.82499	0.00223	0.82723
H	12	0.20129	0.00000	0.79678	0.00193	0.79871
C	13	-0.02918	2.00000	4.00474	0.02445	6.02918
C	14	0.04499	2.00000	3.93064	0.02437	5.95501
C	15	0.04720	2.00000	3.92791	0.02489	5.95280
C	16	-0.01602	2.00000	3.99134	0.02468	6.01602
C	17	0.03899	2.00000	3.93615	0.02486	5.96101
C	18	-0.61320	2.00000	4.60058	0.01261	6.61320
C	19	-0.61608	2.00000	4.60309	0.01299	6.61608
C	20	-0.61955	2.00000	4.60584	0.01372	6.61955
C	21	-0.62327	2.00000	4.61001	0.01327	6.62327
C	22	-0.63229	2.00000	4.61868	0.01361	6.63229
H	23	0.21588	0.00000	0.78220	0.00192	0.78412
H	24	0.21558	0.00000	0.78279	0.00164	0.78442
H	25	0.23313	0.00000	0.76507	0.00180	0.76687
H	26	0.22968	0.00000	0.76864	0.00168	0.77032
H	27	0.22189	0.00000	0.77638	0.00173	0.77811
H	28	0.21993	0.00000	0.77831	0.00176	0.78007
H	29	0.21428	0.00000	0.78385	0.00187	0.78572
H	30	0.23824	0.00000	0.76006	0.00171	0.76176
H	31	0.22874	0.00000	0.76941	0.00185	0.77126
H	32	0.23940	0.00000	0.75841	0.00220	0.76060
H	33	0.21725	0.00000	0.78063	0.00212	0.78275
H	34	0.21957	0.00000	0.77871	0.00172	0.78043
H	35	0.25509	0.00000	0.74251	0.00240	0.74491
H	36	0.22869	0.00000	0.76958	0.00174	0.77131
H	37	0.21716	0.00000	0.78104	0.00180	0.78284
Rh	38	0.79170	35.99975	8.17556	0.03300	44.20830
H	39	0.22315	0.00000	0.77462	0.00223	0.77685
C	40	0.96256	2.00000	2.99031	0.04713	5.03744
O	41	-0.70416	2.00000	6.68145	0.02271	8.70416
O	42	-0.64040	2.00000	6.61405	0.02635	8.64040
O	43	-0.66118	2.00000	6.64017	0.02102	8.66118
H	44	0.48699	0.00000	0.50944	0.00357	0.51301

C 45	-0.68393	2.00000	4.67183	0.01211	6.68393
H 46	0.20759	0.00000	0.79044	0.00196	0.79241
H 47	0.22486	0.00000	0.77372	0.00143	0.77514
H 48	0.22660	0.00000	0.77142	0.00198	0.77340
* Total *	0.00000	83.99967	137.38738	0.61295	222.00000

2A

Summary of Natural Population Analysis:

	Natural	Natural Population				Natural Spin
Atom No	Charge	Core	Valence	Rydberg	Total	Density
O 1	-0.52594	2.00000	6.50314	0.02280	8.52594	0.03647
N 2	-0.41855	2.00000	5.38318	0.03537	7.41855	0.53385
N 3	-0.41745	2.00000	5.38720	0.03025	7.41745	0.13960
C 4	0.70189	2.00000	3.26364	0.03448	5.29811	-0.02092
C 5	-0.16068	2.00000	4.14590	0.01478	6.16068	-0.10863
C 6	-0.16208	2.00000	4.14812	0.01396	6.16208	0.27420
C 7	-0.18503	2.00000	4.17131	0.01372	6.18503	0.25563
C 8	0.07731	2.00000	3.90203	0.02066	5.92269	-0.05688
C 9	0.33389	2.00000	3.64124	0.02487	5.66611	-0.09922
H 10	0.22885	0.00000	0.76965	0.00150	0.77115	-0.00824
H 11	0.20161	0.00000	0.79653	0.00186	0.79839	0.00159
H 12	0.23188	0.00000	0.76644	0.00167	0.76812	0.00308
C 13	0.01939	2.00000	3.95561	0.02500	5.98061	-0.00343
C 14	0.06321	2.00000	3.91192	0.02488	5.93679	-0.00291
C 15	0.04403	2.00000	3.93094	0.02503	5.95597	-0.00291
C 16	0.00449	2.00000	3.97082	0.02469	5.99551	-0.00209
C 17	0.05962	2.00000	3.91555	0.02484	5.94038	-0.00176
C 18	-0.62371	2.00000	4.61053	0.01319	6.62371	0.00051
C 19	-0.62315	2.00000	4.60977	0.01338	6.62315	0.00027
C 20	-0.62151	2.00000	4.60814	0.01338	6.62151	0.00016
C 21	-0.62777	2.00000	4.61443	0.01334	6.62777	0.00019
C 22	-0.63360	2.00000	4.62027	0.01333	6.63360	0.00042
H 23	0.23635	0.00000	0.76203	0.00161	0.76365	-0.00006
H 24	0.22646	0.00000	0.77200	0.00154	0.77354	-0.00003
H 25	0.24082	0.00000	0.75753	0.00165	0.75918	-0.00011
H 26	0.23251	0.00000	0.76591	0.00158	0.76749	-0.00005
H 27	0.24174	0.00000	0.75673	0.00152	0.75826	-0.00016
H 28	0.23042	0.00000	0.76790	0.00167	0.76958	-0.00006
H 29	0.23508	0.00000	0.76321	0.00172	0.76492	-0.00026
H 30	0.23835	0.00000	0.76008	0.00157	0.76165	-0.00011
H 31	0.22684	0.00000	0.77152	0.00163	0.77316	-0.00001
H 32	0.24522	0.00000	0.75318	0.00160	0.75478	-0.00010
H 33	0.23516	0.00000	0.76302	0.00182	0.76484	-0.00023
H 34	0.22507	0.00000	0.77341	0.00152	0.77493	0.00000
H 35	0.24545	0.00000	0.75271	0.00184	0.75455	-0.00009
H 36	0.22486	0.00000	0.77345	0.00170	0.77514	-0.00012
H 37	0.24019	0.00000	0.75819	0.00162	0.75981	-0.00049

Rh 38	0.76638	35.99977	8.20144	0.03241	44.23362	0.05919
H 39	0.22750	0.00000	0.77059	0.00191	0.77250	-0.00756
C 40	0.96229	2.00000	2.99161	0.04610	5.03771	0.00039
O 41	-0.70684	2.00000	6.68350	0.02334	8.70684	0.00067
O 42	-0.64036	2.00000	6.61380	0.02656	8.64036	0.00250
O 43	-0.63882	2.00000	6.61701	0.02181	8.63882	0.00046
H 44	0.49806	0.00000	0.49867	0.00327	0.50194	0.00000
C 45	-0.70408	2.00000	4.69248	0.01160	6.70408	0.00376
H 46	0.24306	0.00000	0.75538	0.00156	0.75694	0.00348
H 47	0.23605	0.00000	0.76269	0.00126	0.76395	0.00002
H 48	0.26554	0.00000	0.73286	0.00160	0.73446	-0.00004
* Total *	1.00000	83.99970	136.39729	0.60301	221.00000	1.00000

6

Summary of Natural Population Analysis:

	Natural	Natural Population			
Atom No	Charge	Core	Valence	Rydberg	Total
O 1	-0.69746	2.00000	6.67464	0.02282	8.69746
N 2	-0.56755	2.00000	5.53972	0.02783	7.56755
N 3	-0.41814	2.00000	5.39019	0.02796	7.41814
C 4	0.61337	2.00000	3.35439	0.03224	5.38663
C 5	-0.24928	2.00000	4.23056	0.01872	6.24928
C 6	-0.27690	2.00000	4.26085	0.01605	6.27690
C 7	-0.13182	2.00000	4.10157	0.03026	6.13182
C 8	0.02987	2.00000	3.94805	0.02209	5.97013
C 9	0.30239	2.00000	3.67368	0.02394	5.69761
H 10	0.19906	0.00000	0.79864	0.00230	0.80094
H 11	0.17491	0.00000	0.82291	0.00218	0.82509
H 12	0.18945	0.00000	0.80762	0.00293	0.81055
C 13	-0.04675	2.00000	4.02233	0.02442	6.04675
C 14	-0.02219	2.00000	3.99810	0.02410	6.02219
C 15	-0.00389	2.00000	3.97829	0.02561	6.00389
C 16	-0.02289	2.00000	3.99860	0.02429	6.02289
C 17	-0.00077	2.00000	3.97452	0.02625	6.00077
C 18	-0.61376	2.00000	4.60073	0.01303	6.61376
C 19	-0.61820	2.00000	4.60598	0.01222	6.61820
C 20	-0.61639	2.00000	4.60348	0.01291	6.61639
C 21	-0.62314	2.00000	4.61069	0.01245	6.62314
C 22	-0.61787	2.00000	4.60473	0.01314	6.61787
H 23	0.21471	0.00000	0.78290	0.00239	0.78529
H 24	0.21327	0.00000	0.78502	0.00171	0.78673
H 25	0.21310	0.00000	0.78513	0.00178	0.78690
H 26	0.21607	0.00000	0.78217	0.00176	0.78393
H 27	0.21541	0.00000	0.78260	0.00198	0.78459
H 28	0.21932	0.00000	0.77873	0.00195	0.78068
H 29	0.21702	0.00000	0.78100	0.00197	0.78298
H 30	0.21387	0.00000	0.78440	0.00172	0.78613

H 31	0.23468	0.00000	0.76357	0.00174	0.76532
H 32	0.24776	0.00000	0.74987	0.00237	0.75224
H 33	0.21109	0.00000	0.78703	0.00188	0.78891
H 34	0.20999	0.00000	0.78830	0.00171	0.79001
H 35	0.22903	0.00000	0.76884	0.00213	0.77097
H 36	0.22331	0.00000	0.77509	0.00160	0.77669
H 37	0.21219	0.00000	0.78581	0.00200	0.78781
Rh 38	0.64901	35.99965	8.31865	0.03270	44.35099
C 39	-0.11850	1.99999	4.09756	0.02095	6.11850
C 40	-0.16918	2.00000	4.15501	0.01418	6.16918
C 41	-0.13812	2.00000	4.12261	0.01551	6.13812
H 42	0.20491	0.00000	0.79294	0.00215	0.79509
H 43	0.22416	0.00000	0.77366	0.00218	0.77584
C 44	-0.20553	2.00000	4.19079	0.01474	6.20553
C 45	-0.20263	2.00000	4.18779	0.01484	6.20263
H 46	0.20445	0.00000	0.79358	0.00197	0.79555
H 47	0.20890	0.00000	0.78909	0.00200	0.79110
C 48	-0.18748	2.00000	4.17261	0.01488	6.18748
H 49	0.20456	0.00000	0.79359	0.00185	0.79544
C 50	0.00008	1.99999	3.97855	0.02138	5.99992
C 51	0.00610	1.99999	3.97066	0.02325	5.99390
C 52	-0.64263	2.00000	4.62846	0.01418	6.64263
H 53	0.22592	0.00000	0.77171	0.00237	0.77408
H 54	0.24859	0.00000	0.74957	0.00184	0.75141
H 55	0.21877	0.00000	0.77940	0.00182	0.78123
C 56	-0.63451	2.00000	4.62362	0.01089	6.63451
H 57	0.20428	0.00000	0.79384	0.00187	0.79572
H 58	0.22004	0.00000	0.77811	0.00185	0.77996
H 59	0.20593	0.00000	0.79231	0.00176	0.79407
* Total *	0.00000	93.99954	157.33484	0.66562	252.00000

6A

Summary of Natural Population Analysis:

	Natural	Natural Population				Natural Spin
Atom No	Charge	Core	Valence	Rydberg	Total	Density
O 1	-0.59927	2.00000	6.57472	0.02454	8.59927	0.12512
N 2	-0.45096	2.00000	5.42357	0.02739	7.45096	0.27006
N 3	-0.37964	2.00000	5.35099	0.02866	7.37964	0.05802
C 4	0.67568	2.00000	3.29254	0.03178	5.32432	0.00064
C 5	-0.25667	2.00000	4.23810	0.01858	6.25667	-0.07878
C 6	-0.17000	2.00000	4.15508	0.01492	6.17000	0.21179
C 7	-0.06504	2.00000	4.03501	0.03004	6.06504	0.23263
C 8	0.07506	2.00000	3.90380	0.02114	5.92494	0.01683
C 9	0.32135	2.00000	3.65520	0.02345	5.67865	0.01977
H 10	0.22053	0.00000	0.77765	0.00182	0.77947	-0.00634
H 11	0.20043	0.00000	0.79765	0.00192	0.79957	-0.00076
H 12	0.20945	0.00000	0.78785	0.00270	0.79055	0.00205

C 13	0.00155	2.00000	3.97380	0.02466	5.99845	-0.00512
C 14	-0.00732	2.00000	3.98290	0.02442	6.00732	-0.00178
C 15	-0.00462	2.00000	3.97776	0.02686	6.00462	0.00303
C 16	0.00113	2.00000	3.97384	0.02503	5.99887	-0.00306
C 17	0.02793	2.00000	3.94562	0.02645	5.97207	0.01166
C 18	-0.62679	2.00000	4.61295	0.01385	6.62679	0.00023
C 19	-0.62628	2.00000	4.61357	0.01271	6.62628	0.00014
C 20	-0.62269	2.00000	4.60949	0.01320	6.62269	-0.00008
C 21	-0.62812	2.00000	4.61543	0.01269	6.62812	0.00016
C 22	-0.62410	2.00000	4.61061	0.01349	6.62410	0.00015
H 23	0.23766	0.00000	0.76027	0.00208	0.76234	-0.00046
H 24	0.22363	0.00000	0.77480	0.00158	0.77637	-0.00004
H 25	0.21938	0.00000	0.77894	0.00168	0.78062	-0.00009
H 26	0.22204	0.00000	0.77640	0.00156	0.77796	0.00000
H 27	0.23217	0.00000	0.76611	0.00172	0.76783	-0.00022
H 28	0.23090	0.00000	0.76735	0.00175	0.76910	-0.00008
H 29	0.23876	0.00000	0.75942	0.00182	0.76124	-0.00006
H 30	0.21771	0.00000	0.78072	0.00158	0.78229	0.00012
H 31	0.23132	0.00000	0.76706	0.00162	0.76868	-0.00006
H 32	0.24577	0.00000	0.75231	0.00192	0.75423	-0.00018
H 33	0.23031	0.00000	0.76803	0.00166	0.76969	-0.00017
H 34	0.21896	0.00000	0.77946	0.00158	0.78104	-0.00001
H 35	0.23179	0.00000	0.76650	0.00171	0.76821	0.00046
H 36	0.22579	0.00000	0.77269	0.00152	0.77421	0.00004
H 37	0.23383	0.00000	0.76437	0.00180	0.76617	0.00043
Rh 38	0.63794	35.99967	8.33111	0.03128	44.36206	0.09847
C 39	-0.14261	1.99999	4.12143	0.02119	6.14261	0.00129
C 40	-0.15370	2.00000	4.13951	0.01419	6.15370	0.00021
C 41	-0.15398	2.00000	4.13926	0.01473	6.15398	0.00457
H 42	0.20689	0.00000	0.79086	0.00226	0.79311	-0.00001
H 43	0.22384	0.00000	0.77409	0.00207	0.77616	-0.00015
C 44	-0.19106	2.00000	4.17640	0.01467	6.19106	0.00325
C 45	-0.19078	2.00000	4.17588	0.01491	6.19078	-0.00104
H 46	0.21771	0.00000	0.78048	0.00181	0.78229	-0.00010
H 47	0.22217	0.00000	0.77605	0.00178	0.77783	0.00003
C 48	-0.16669	2.00000	4.15194	0.01475	6.16669	0.00393
H 49	0.21936	0.00000	0.77896	0.00168	0.78064	-0.00013
C 50	0.00923	1.99999	3.96920	0.02158	5.99077	0.01305
C 51	0.02803	1.99999	3.94813	0.02385	5.97197	0.01729
C 52	-0.64570	2.00000	4.63093	0.01478	6.64570	-0.00063
H 53	0.24609	0.00000	0.75177	0.00214	0.75391	0.00006
H 54	0.24303	0.00000	0.75522	0.00175	0.75697	0.00007
H 55	0.22847	0.00000	0.76990	0.00163	0.77153	0.00077
C 56	-0.65563	2.00000	4.64412	0.01152	6.65563	0.00017
H 57	0.23856	0.00000	0.76010	0.00134	0.76144	0.00166
H 58	0.23911	0.00000	0.75952	0.00137	0.76089	-0.00022
H 59	0.22812	0.00000	0.77034	0.00153	0.77188	0.00143
* Total *	1.00000	93.99956	156.33777	0.66267	251.00000	1.00000

Table S4. Mulliken spin densities of 6A and 7A.

Atomic Spin Densities of **6A**

Atom	O1	N2	N3	C4	C5
Spin	0.12421	0.2748	0.05735	0.00289	-0.11614
Atom	C6	C7	C8	C9	H10
Spin	0.24636	0.27024	0.00493	-0.00067	-0.01502
Atom	H11	H12	C13	C14	C15
Spin	-0.00241	0.00465	-0.0065	-0.0015	0.00158
Atom	C16	C17	C18	C19	C20
Spin	-0.00371	0.01554	0.00033	0.00023	0.00011
Atom	C21	C22	H23	H24	H25
Spin	0.0003	-0.00069	-0.00043	-0.00003	-0.00012
Atom	H26	H27	H28	H29	H30
Spin	0.00001	-0.00021	0.00003	-0.00009	0.00015
Atom	H31	H32	H33	H34	H35
Spin	-0.00019	-0.00054	-0.00011	-0.00002	0.00089
Atom	H36	H37	Rh38	C39	C40
Spin	0.00001	0.00044	0.09881	0.00113	-0.00055
Atom	C41	H42	H43	C44	C45
Spin	0.00424	-0.00005	-0.0001	0.00358	-0.00133
Atom	H46	H47	C48	H49	C50
Spin	-0.00028	0.00005	0.00463	-0.00032	0.0118
Atom	C51	C52	H53	H54	H55
Spin	0.02041	-0.00062	-0.00009	-0.00077	0.00122
Atom	C56	H57	H58	H59	
Spin	-0.00174	0.00203	-0.00058	0.00184	

Atomic Spin Densities of **7A**

Atom	O1	N2	N3	C4	C5
Spin	0.07547	0.02592	0.00699	-0.01373	0.00379
Atom	C6	C7	C8	C9	H10
Spin	0.00199	-0.00765	-0.00225	0.00004	-0.00005
Atom	H11	H12	C13	C14	C15
Spin	0.00013	0.00018	-0.00376	-0.00138	-0.01276
Atom	C16	C17	C18	C19	C20
Spin	0.08121	0.04576	0.00009	0.00017	0.00033
Atom	C21	C22	H23	H24	H25
Spin	-0.00688	-0.00462	-0.00099	-0.00035	0.00048

Atom	H26	H27	H28	H29	H30
Spin	0.00017	0.00004	0	-0.00085	-0.00012
Atom	H31	H32	H33	H34	H35
Spin	-0.00009	-0.00002	0.00471	0.0044	-0.00009
Atom	H36	H37	Rh38	C39	C40
Spin	0.00291	0.00306	0.3311	-0.00783	0.05773
Atom	C41	H42	H43	C44	C45
Spin	0.06399	-0.00339	-0.00484	-0.03066	-0.03765
Atom	H46	H47	C48	H49	C50
Spin	0.00133	0.00184	0.08746	-0.0056	0.13239
Atom	C51	C52	H53	H54	H55
Spin	0.18309	0.01097	0.00244	0.0122	-0.0011
Atom	C56	H57	H58	H59	
Spin	0.00459	0.00116	-0.00081	-0.00068	

Computed Energy Components for DFT-Optimized Structures

	E(SCF)/(eV)	**ZPE/(kcal/mol)**	**S(gas)/(cal/mol·K)**	**G(solv)/(kcal/mol)**
	cc-pVTZ(-f)/LACV3P	6-31G**/LACVP	6-31G**/LACVP	6-31G**/LACVP
1	-33204.090	242.45	178.66	-18.55
2	-33203.492	241.86	180.54	-18.87
3	-33203.059	241.57	181.45	-22.52
3-TS	-33202.461	238.31	176.92	-20.57
4	-33203.113	241.24	177.26	-19.59
5	-25988.158	215.47	160.17	-16.76
6	-35453.961	303.77	200.46	-17.61
6-TS	-35453.484	303.32	196.03	-15.16
7	-35455.074	304.97	192.99	-12.67
7-TS	-35454.430	304.53	190.92	-11.01
8	-35455.570	305.45	195.89	-10.29
9	-35454.813	305.09	196.03	-10.60
9-TS	-35454.488	304.32	193.35	-8.92
10	-35455.195	305.63	199.21	-8.77
2A	-33197.066	241.06	185.73	-45.76
2A'	-33197.137	241.15	185.55	-45.55
3A-TS	-33195.750	237.81	179.87	-48.15
4A	-33196.461	241.32	182.94	-47.34
5A	-25981.365	214.86	162.54	-46.26
6A	-35447.742	303.25	207.26	-42.04
6A-TS	-35447.328	303.14	196.61	-41.92
6A-TS′	-35447.136	302.66	198.83	-42.92
7A	-35448.633	304.79	195.91	-42.32
7A′	-35448.462	304.70	195.58	-42.56
7A-TS	-35448.336	304.53	194.17	-38.67
8A	-35449.305	305.49	199.86	-38.49
8A-TS	-35448.902	304.19	196.87	-37.78
9A	-35449.918	305.78	197.38	-37.27
1B	-49588.652	334.08	252.52	-52.63
3B	-49588.012	333.44	253.26	-51.16
3B-TS	-49587.672	330.79	238.83	-48.10
4B	-49588.348	334.02	245.58	-45.90

5B	-42373.445	307.42	233.25	-41.19
6B	-51839.488	395.79	275.31	-40.43
6B-TS	-51838.734	395.17	270.36	-39.27
7B	-51840.102	396.81	269.19	-40.21
5C	-33202.660	241.21	178.30	-21.09
5C-TS	-33202.352	238.96	177.74	-20.18
6C	-28069.318	231.85	165.51	-17.99

XYZ Coordinates

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  O  -0.601265788  -2.228587151  -0.291156709
  N   1.079713821  -2.121599197  -1.947880864
  N   1.952474236  -0.870195329  -0.053437024
  C  -0.063079081  -2.515488863  -1.423392296
  C   4.315976143  -0.532304347  -1.469083428
  C   4.211231709  -0.062918350  -0.149614409
  C   3.247068882  -1.193845034  -2.034913540
  C   3.016938210  -0.255194187   0.517257512
  C   2.041135788  -1.393546939  -1.310505390
  H   5.036217213   0.431477726   0.351164579
  H   2.878393888   0.040762160   1.550664902
  H   5.233301163  -0.391809285  -2.034410000
  C  -0.963488102   0.499136001   2.464065552
  C  -1.876148939   0.097267739   1.436928868
  C   0.067792311   1.315700769   1.869573236
  C  -1.426393390   0.697134078   0.188840479
  C  -0.239981428   1.447197676   0.459315866
  C  -1.016147971   0.112823315   3.908446550
  C  -3.073105812  -0.794438004   1.557983041
  C   1.160321712   2.021631479   2.612011433
  C  -2.115655661   0.513903499  -1.127138138
  C   0.566596568   2.232513666  -0.529969513
  H  -1.524950504   0.893964052   4.486798286
  H  -1.557245851  -0.825019360   4.048284054
  H  -0.005533883  -0.014683301   4.300400257
  H  -3.025089025  -1.588877916   0.806010902
  H  -4.001513481  -0.231054410   1.404885650
  H  -3.118873119  -1.267477155   2.540546894
  H   0.763376832   2.898930550   3.138175249
  H   1.619473100   1.346121430   3.335715532
  H   1.939649105   2.369612932   1.929363132
  H  -1.479588270   0.815692365  -1.961315036
  H  -3.036749840   1.107695103  -1.164853096
  H  -2.381591558  -0.537214398  -1.268041134
  H   0.363224357   1.913968921  -1.554373622
  H   1.637712955   2.108695745  -0.349882632
  H   0.331983685   3.300745249  -0.451462388
 Rh   0.111160554  -0.694111109   0.920464098
  H   3.284122944  -1.599584579  -3.038992643
  C   1.574664354  -1.997277617   3.111911297
  O   2.090733051  -0.914624393   3.435225725
  O   0.716370523  -2.240832567   2.189697266
  O   1.912081480  -3.131089449   3.798665285
  H   2.556505442  -2.835418940   4.458113670
  C  -0.897990406  -3.454567194  -2.271286726
  H  -0.385701329  -3.697185516  -3.202082872
  H  -1.097874403  -4.368672371  -1.703180790
  H  -1.867691755  -2.992774248  -2.489425421

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2
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  O  -0.578474700  -2.639305115  -2.245607853
  N   0.025329642  -2.165440798  -0.059646193
  N   2.285194159  -1.842477679   0.394623548
  C  -0.884532392  -2.391189098  -1.074165463
  C   3.011331081  -4.201938152  -0.884828210
  C   3.984574318  -3.426229477  -0.241320327
  C   1.687719941  -3.795594454  -0.873627782
  C   3.557380199  -2.259341240   0.378315091
  C   1.347106695  -2.594512939  -0.207300603
  H   5.030041218  -3.716704130  -0.225995928
  H   4.269448280  -1.610770226   0.889049530
  H   3.288458109  -5.123307705  -1.390769958
  C   0.201982737   1.805995464   1.435361385
  C  -1.034907460   1.687827110   0.737672925
  C   1.252513051   1.293859005   0.562338054
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  C   0.654954314   0.879616380  -0.672470152
  C   0.438378572   2.350040913   2.810831070
  C  -2.394486427   2.052939177   1.243607402
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  C  -1.778424978   0.846923411  -1.641820669
  C   1.344611287   0.319639236  -1.877312064
  H   0.930125952   3.329083681   2.762501955
  H  -0.496611029   2.467787266   3.362292528
  H   1.082125068   1.676005840   3.383056641
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  H  -2.724508286   2.997546196   0.794530749
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H	-1.465977430	0.035386551	-2.302379131
H	-1.896101594	1.755036831	-2.246419430
H	-2.755931616	0.588309705	-1.228962541
H	0.816072166	-0.555626988	-2.267195702
H	2.361749887	0.009681865	-1.639931679
H	1.380556226	1.080487609	-2.666900635
Rh	-0.166876271	-0.320043296	0.975105047
H	0.921771348	-4.369601250	-1.377703786
C	-0.756288767	-1.648776889	3.044619322
O	-1.682701468	-1.233183622	2.265949249
O	0.447879285	-1.335573554	2.861451149
O	-1.075721383	-2.435416222	4.085253716
H	-2.030754566	-2.592083693	4.035280704
C	-2.353351116	-2.381398439	-0.674962223
H	-2.953181982	-1.983672500	-1.496462584
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3

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O	-0.295968175	-2.040455103	-0.200084001
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C	0.392830133	-2.881947994	-0.895231009
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C	4.478835583	-0.971077383	1.241676688
C	2.345946550	-2.086946726	1.050915003
C	4.531448841	-1.005992889	-0.172467530
C	2.524172783	-2.113207817	-0.382788807
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C	-0.685132980	1.162730694	1.484763265
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C	-1.866665602	1.067882299	2.396133661
C	2.952138186	1.851949453	0.748897195
C	-1.791860819	0.625972331	-0.836302280
C	1.206832528	0.998349726	-1.788298965
H	0.812305868	2.731678724	3.633500576
H	0.527326167	1.026383162	4.033206940
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H	-2.786181927	0.860381305	1.846274257
H	-1.997808337	2.001348019	2.954581499
H	-1.705167532	0.253754228	3.110520601
H	3.004695892	2.942756414	0.641162872
H	3.478797913	1.574437737	1.662976265
H	3.479322195	1.405759692	-0.095033973
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H	-1.852365017	1.334725380	-1.668963194
H	-2.743198156	0.634268105	-0.302332193
H	0.539548516	0.364934951	-2.376448631
H	2.203413963	0.553405464	-1.839486837
H	1.240064025	1.990068913	-2.256628990
Rh	0.570186257	-0.588822663	1.033347964
H	1.668425441	-2.820055723	1.491039395
C	-0.359993815	-2.859224081	2.860729456
O	-0.156012416	-1.572915792	2.762967587
O	0.083319239	-3.764112473	2.166656256
O	-1.167198062	-3.178738594	3.921872377
H	-1.414113164	-2.340329885	4.336861134
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H	0.196879789	-4.592720032	-2.189905882
H	-0.665839791	-4.677590370	-0.623053312
H	-1.321117401	-3.671479225	-1.919729233

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3-TS

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O	-0.317289859	-2.059553623	-0.163241521
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C	3.125203848	-1.403822899	2.239525318
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C	2.111691236	-1.842599750	1.358262658
C	4.748482227	-2.068086863	0.630481005
C	2.535055876	-2.487736940	0.142942190
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H	5.783699989	-2.101222992	0.286602080
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C	0.670672297	1.604756117	1.587780237
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C	1.118625164	0.862641335	-0.564611733
C	0.805148125	2.093595266	2.997328281
C	-1.938175678	1.689193726	1.516383290
C	3.189460516	1.504052401	0.887173116
C	-1.302838922	0.682788372	-1.518098950
C	1.842749834	0.465233445	-1.815166831
H	0.689328730	3.183569670	3.047604084
H	0.038881470	1.644867182	3.635355234
H	1.781590462	1.838884830	3.415474892
H	-2.754766464	1.443368793	0.834986687
H	-2.054286957	2.732867718	1.831372619
H	-2.038820505	1.054299712	2.402751446
H	3.491998672	2.481774807	0.490862250
H	3.449213028	1.472907186	1.946517229
H	3.774616957	0.735100746	0.380195409
H	-1.281099200	-0.401198894	-1.682633758
H	-1.044804096	1.178195596	-2.459948778
H	-2.322628021	0.965228498	-1.249393344
H	1.237404823	-0.225181833	-2.406877518
H	2.782033920	-0.042246297	-1.583672047
H	2.066140652	1.343367577	-2.434480906
Rh	0.473300993	-0.514631271	0.966584086
H	1.173239827	-2.612761974	2.038597584

C	-0.585620761	-2.489540577	2.977810621
O	-0.716790617	-1.283533812	2.627577305
O	0.360589921	-3.275578022	2.663445473
O	-1.523887634	-3.021629572	3.782347679
H	-2.190339804	-2.331378698	3.918413877
C	-0.439255953	-4.100232124	-1.332143545
H	0.196294084	-4.770066261	-1.911403775
H	-0.961007953	-4.674896240	-0.558521271
H	-1.200882196	-3.644620895	-1.972273827

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4

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O	-0.184227273	-2.467598915	0.353821784
N	1.936300397	-3.281015635	-0.290078938
N	3.764369249	-3.319420576	1.103846550
C	0.664984941	-3.160881519	-0.429676175
C	2.991844893	-1.037358165	2.502950191
C	4.169502735	-1.707105875	2.845313787
C	2.199399233	-1.514212489	1.459324121
C	4.503814697	-2.841044664	2.105814695
C	2.616970301	-2.686160326	0.782733023
H	4.805461407	-1.361088395	3.655502558
H	5.415373325	-3.394785881	2.329806566
H	2.688465357	-0.150900170	3.056099653
C	0.692247808	1.635627151	1.009809732
C	-0.698261917	1.428234220	0.565583169
C	1.564099312	1.122429252	-0.000279241
C	-0.671555161	0.707099617	-0.631154954
C	0.737820923	0.420562267	-0.951438606
C	1.081813216	2.434634686	2.217001200
C	-1.890162468	1.861956358	1.363737702
C	3.054234028	1.257506132	-0.061050646
C	-1.824281096	0.156027943	-1.413927197
C	1.216079950	-0.266055882	-2.196123600
H	0.994031549	3.511350155	2.023124218
H	0.435961813	2.194951534	3.066621304
H	2.114027977	2.230167627	2.510534763
H	-2.823201895	1.512018681	0.917857051
H	-1.935298920	2.955069304	1.439275980
H	-1.834333658	1.462189794	2.382092953
H	3.326097250	2.176456451	-0.594937027
H	3.494557858	1.297153234	0.937283635
H	3.504646063	0.410789400	-0.582715809
H	-1.793961525	-0.939879894	-1.404749155
H	-1.782992840	0.484969646	-2.458329678
H	-2.783732176	0.468901932	-0.996638834
H	0.455193043	-0.949334621	-2.579032898
H	2.115007877	-0.855656147	-2.001490355
H	1.440763593	0.464736581	-2.983203411
Rh	0.499887913	-0.552135527	0.947725713
H	-0.444751114	-2.970108986	1.689617395
C	-0.512903571	-2.122536421	3.405979872
O	-0.221530616	-0.977714717	3.003739119
O	-0.632011235	-3.192100286	2.694686890
O	-0.751781523	-2.335609198	4.704127789
H	-0.611486793	-1.489655256	5.154902458
C	-0.028004700	-3.858808041	-1.573436499
H	0.696852386	-4.369647026	-2.207847834
H	-0.749693215	-4.582930565	-1.179208398
H	-0.597946107	-3.134243727	-2.166501045

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O	3.748417616	2.393520594	-0.290382624
N	5.611860752	0.981935740	-0.036467351
N	7.607882023	1.291931033	0.995621443
C	4.424908638	1.292222381	-0.474989235
C	6.869937897	3.692355633	2.206628561
C	8.130220413	3.165609837	2.420448780
C	5.943943501	3.046889305	1.356401920
C	8.441262245	1.953427076	1.776470542
C	6.359542370	1.804220319	0.769834638
H	9.424431801	1.501371861	1.917075992
H	8.859054565	3.659715176	3.056802034
H	6.597414494	4.628122330	2.683937311
C	4.084307194	6.038424492	1.580400705
C	3.674828768	5.193408012	2.645318985
C	3.123419046	5.873783588	0.481145680
C	2.514192343	4.445034504	2.174603939
C	2.133714914	4.946521759	0.874441564
C	5.191054344	7.048162937	1.583243728
C	4.231490612	5.118360519	4.034545422
C	3.217017889	6.607356548	-0.820505321
C	1.742867708	3.439193010	2.969874144
C	1.017102599	4.386703491	0.042041250
H	5.736923695	7.038331985	0.635998487
H	4.790318966	8.059679031	1.727284551
H	5.910400867	6.856894493	2.382056952
H	4.372479439	4.082111359	4.352067471
H	3.545905590	5.599938869	4.742722034
H	5.195626736	5.624319077	4.112843990
H	4.242070675	6.594213009	-1.202503085
H	2.569844961	6.165595531	-1.580458045
H	2.927657604	7.658296108	-0.690929592
H	1.292324543	2.688174009	2.316517115
H	2.383829832	2.926367521	3.690277815
H	0.934551299	3.933133841	3.526167870
H	1.275916338	3.381566286	-0.313506871
H	0.818529427	5.011107922	-0.831989348
H	0.090795398	4.317129612	0.621498883
Rh	4.203639984	3.909309149	0.927374899
C	3.694091320	0.278270900	-1.326508999
H	4.319140911	-0.597787738	-1.497520328
H	2.764073372	-0.020448379	-0.829325318
H	3.414263248	0.730200350	-2.284399986

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O	-0.119900540	-1.845253706	-0.315487593
N	1.918141484	-2.902191877	-0.885526657
N	4.092808723	-2.348413467	-0.488845468
C	0.629855871	-2.773025751	-0.857640564
C	3.516207933	0.085836001	0.692320108

C	4.846318245	-0.311625808	0.535026550
C	2.467901468	-0.730573356	0.266778916
C	5.068336487	-1.551406622	-0.060587011
C	2.796925068	-1.969681382	-0.347293794
H	5.670867920	0.314781994	0.863336980
H	6.083200932	-1.923200488	-0.204354838
H	3.299955606	1.042420745	1.159868836
C	0.379716337	2.208183050	0.552886605
C	-1.001930475	1.723095179	0.610524416
C	0.926155925	1.841000795	-0.714755774
C	-1.258790731	0.987757087	-0.556947291
C	-0.033182319	0.989965260	-1.359121323
C	0.991970718	3.143909931	1.552084088
C	-1.926825047	1.980768681	1.758404493
C	2.233789921	2.272458076	-1.305031538
C	-2.479213953	0.200772747	-0.920898974
C	0.094145693	0.348605186	-2.706564426
H	0.722794890	4.185508251	1.331741929
H	0.642446935	2.923847198	2.564343214
H	2.082967997	3.078000546	1.547687054
H	-2.869462967	1.443134189	1.641827345
H	-2.153670549	3.050124168	1.845469594
H	-1.468814135	1.661241651	2.700691462
H	2.060950994	3.043737650	-2.065681696
H	2.903831482	2.688673496	-0.551011264
H	2.750135183	1.434320092	-1.777177215
H	-2.207778215	-0.856297433	-1.024682999
H	-2.899040461	0.542175829	-1.874220729
H	-3.255393028	0.277760267	-0.156703576
H	-0.394482374	-0.628322840	-2.703406811
H	1.141503096	0.199865133	-2.976249695
H	-0.377845407	0.967304647	-3.480206966
Rh	0.548163116	-0.069603965	0.476420015
C	-1.251272917	-1.962113142	2.419909000
C	-2.528375864	-1.488355637	2.769027472
C	-1.102498174	-3.294738770	1.992675066
H	-2.640962362	-0.465255290	3.109175444
H	-0.117936075	-3.655004740	1.719576836
C	-3.635131598	-2.328761578	2.681528330
C	-2.213900089	-4.128344059	1.913092971
H	-4.618309498	-1.954900146	2.953219414
H	-2.090887308	-5.155007839	1.580951929
C	-3.482145548	-3.648039818	2.249182463
H	-4.347848415	-4.300374031	2.178864479
C	0.900289178	-0.422675759	2.719959259
C	-0.109477647	-1.100108266	2.481716871
C	2.003456116	0.109120078	3.534590244
H	1.822360635	-0.109966286	4.592412949
H	2.947067976	-0.353800505	3.234205961
H	2.110197067	1.190763116	3.413297892
C	-0.203606725	-3.836049557	-1.547880054
H	-0.707887352	-3.396186352	-2.417040825
H	0.426891178	-4.663800716	-1.872200131
H	-0.987510026	-4.193233490	-0.872247040

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O	-0.141006842	-1.556524754	-1.128042579
N	1.930088162	-2.677805901	-1.220389724
N	4.007361889	-1.702476740	-1.223269820
C	0.637880504	-2.583430052	-1.339128017
C	3.339665413	0.158791319	0.738710105
C	4.646527290	0.089693978	0.261400968
C	2.353619337	-0.675579250	0.203487858
C	4.909082890	-0.849152029	-0.739785850
C	2.736639023	-1.661654830	-0.753883898
H	5.430979729	0.732590377	0.649750113
H	5.910243034	-0.929740489	-1.164161801
H	3.076810122	0.859974861	1.526575804
C	0.236316085	2.143812895	0.870686829
C	-1.114027619	1.622307301	0.832639277
C	0.742910087	2.181687355	-0.488013327
C	-1.383671165	1.220784307	-0.502458572
C	-0.222121879	1.574206114	-1.323279142
C	0.882137835	2.774899721	2.067944765
C	-2.044085503	1.524711728	2.004035711
C	2.061465025	2.743509293	-0.923136115
C	-2.623631239	0.582124412	-1.048476696
C	-0.134863287	1.302789092	-2.793286324
H	0.539405525	3.809838533	2.196729660
H	0.637945771	2.229063749	2.983063698
H	1.970109463	2.801521301	1.970805168
H	-2.781307936	0.731408775	1.865151048
H	-2.581457138	2.470705032	2.147181273
H	-1.501872778	1.305778027	2.927607775
H	1.954107881	3.794377327	-1.219482183
H	2.803468943	2.695479631	-0.124215968
H	2.468018532	2.189964771	-1.772339702
H	-2.354202271	-0.284480482	-1.661000371
H	-3.184272528	1.284638762	-1.677855134
H	-3.282284021	0.236491859	-0.249074832
H	-0.327948183	0.241723865	-2.984828711
H	0.852637827	1.545143366	-3.191571712
H	-0.879812896	1.889870644	-3.344359875
Rh	0.350222051	-0.008308955	0.198408023
C	-1.351432323	-1.804900289	2.133922100
C	-1.683750510	-1.756774664	3.498140335
C	-2.328855515	-2.191764116	1.198482990
H	-0.931578755	-1.447925568	4.218320370
H	-2.057042360	-2.207583189	0.148087263
C	-2.971371651	-2.089508057	3.917859316
C	-3.609645605	-2.528220415	1.627549648
H	-3.221624851	-2.043375969	4.974203587
H	-4.358129501	-2.828075647	0.899078012
C	-3.937227726	-2.475212097	2.986088991
H	-4.940360546	-2.730664730	3.315603733
C	1.228341579	-1.540309906	1.783924222
C	-0.032237563	-1.422525406	1.677425146
C	2.342734098	-2.172154427	2.527425289
H	1.912387133	-2.784309626	3.329197168
H	2.943831682	-2.807530642	1.870695353
H	3.007126093	-1.424460292	2.970211029
C	-0.110563904	-3.806286812	-1.827598333
H	0.582466185	-4.600820065	-2.105594158
H	-0.781257331	-4.162050724	-1.036459208

H	-0.736084521	-3.537613392	-2.685750961

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6A-TS'

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O	-0.756451218	-2.385089860	0.366871603
N	0.990388657	-3.298284837	-0.898044873
N	2.464278669	-2.352015844	-2.357116341
C	-0.008270367	-3.356269078	-0.030278891
C	2.356044563	0.161492335	-1.110668281
C	3.226876775	-0.061533207	-2.159690906
C	1.472023459	-0.863440227	-0.714368262
C	3.214910227	-1.345276441	-2.760061660
C	1.608407834	-2.174945081	-1.305055157
H	3.903866554	0.708503876	-2.515301181
H	3.882648253	-1.555271760	-3.594902686
H	2.319991610	1.120561192	-0.603603109
C	-2.089649692	1.206441890	0.300815442
C	-2.633130115	0.044536095	-0.294565090
C	-1.024580462	1.700032848	-0.571264599
C	-1.951179770	-0.174861827	-1.568311561
C	-1.018388789	0.891289999	-1.764376667
C	-2.580681050	1.875099868	1.546924960
C	-3.692712706	-0.861171422	0.245190682
C	-0.276316811	2.985068642	-0.386306815
C	-2.266576487	-1.280871774	-2.525975889
C	-0.208444737	1.125577491	-2.999658898
H	-3.429925365	2.524637716	1.302873865
H	-2.922970883	1.151127191	2.290120749
H	-1.815421096	2.503581548	2.003788619
H	-3.299092667	-1.879800417	0.340338406
H	-4.550859322	-0.896772999	-0.435312422
H	-4.046094280	-0.536664389	1.225260249
H	-0.864164363	3.824905311	-0.776052412
H	-0.073420757	3.189227519	0.667246593
H	0.677098299	2.974716580	-0.918866255
H	-1.420022501	-1.502812175	-3.179288756
H	-3.118152370	-1.003162682	-3.160091742
H	-2.532914524	-2.195670214	-1.991442226
H	0.102597786	0.186067166	-3.462179483
H	0.688335131	1.710747058	-2.793629609
H	-0.809775845	1.677511294	-3.732129228
Rh	-0.384447220	-0.375418214	0.021914976
C	1.596437980	-0.809570534	1.426385272
C	0.722948015	0.047598844	1.789010758
C	-0.355399604	-4.722404580	0.504410902
H	-0.471540723	-5.424756943	-0.325088133
H	0.476257825	-5.081590719	1.119562894
H	-1.265697511	-4.686787165	1.104153212
C	0.417918630	0.965463329	2.912283241
H	-0.598248729	0.806547573	3.280392174
H	1.124929830	0.798013783	3.731816084
H	0.502988280	2.011329000	2.599647366
C	2.426896103	-1.941996927	1.739099801
C	1.931559474	-2.892157860	2.654596855
C	3.711212575	-2.102024975	1.185710087
C	2.720774411	-3.979593263	3.017722556
C	4.491132681	-3.189334487	1.557408909
C	3.996884577	-4.129636459	2.468658420
H	0.931947655	-2.768315972	3.058545964
H	4.078944538	-1.378259718	0.466224249
H	2.340093601	-4.712167398	3.722704272
H	5.482046406	-3.313482627	1.132483061
H	4.607323642	-4.983627602	2.746364951

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O	-1.010213852	-2.467218399	-0.204885960
N	1.051443338	-3.318187952	-0.875898421
N	1.881546378	-1.996734619	-2.600168228
C	-0.120870724	-3.414292097	-0.324399769
C	2.566235304	0.065442309	-0.829704762
C	2.879452229	0.168629721	-2.173961401
C	1.901561379	-1.079889178	-0.336082995
C	2.507842779	-0.901703477	-3.008149385
C	1.577750683	-2.121274471	-1.279727221
H	3.401342869	1.030902624	-2.576495647
H	2.741886854	-0.860431433	-4.072471142
H	2.829118967	0.851643384	-0.126661360
C	-1.548784494	1.425716758	0.242446482
C	-2.457073689	0.377347857	-0.159275636
C	-0.707710803	1.697090507	-0.880047500
C	-2.277807951	0.141664669	-1.598955035
C	-1.213451743	0.939835668	-2.035130739
C	-1.519549131	2.101177216	1.578374863
C	-3.559018135	-0.222396746	0.657157540
C	0.360155851	2.744532347	-0.970824718
C	-3.049555063	-0.889177024	-2.362921715
C	-0.611302555	1.008844614	-3.403498650
H	-2.233353376	2.934594393	1.597636938
H	-1.781047702	1.409174442	2.381510973
H	-0.527570903	2.501035213	1.801181912
H	-3.676575661	-1.282140613	0.415005952
H	-4.511440277	0.282945514	0.449021250
H	-3.352705956	-0.143620074	1.726272225
H	-0.051335581	3.683144331	-1.364792347
H	0.800200939	2.954200983	0.007085164
H	1.160550475	2.424036980	-1.641858101
H	-2.730627060	-0.943228066	-3.405845165
H	-4.123944759	-0.671754599	-2.342598438
H	-2.893087387	-1.874806166	-1.909537911
H	-1.060792923	0.278248996	-4.078922272
H	0.465134263	0.809911668	-3.367732286
H	-0.746141315	2.006953001	-3.838873148
Rh	-0.469404876	-0.437480301	-0.276483566
C	-0.203296989	-0.846210957	2.794645548
C	0.275204182	-0.059991699	3.857166767
C	-1.377085805	-1.600135684	2.988585472
H	1.173417330	0.533382952	3.709821224
H	-1.743589044	-2.198738337	2.159775257
C	-0.398903221	-0.028885841	5.078904629
C	-2.043624163	-1.570224762	4.211079121
H	-0.018456275	0.587998867	5.888874531
H	-2.944894552	-2.162734747	4.347229004
C	-1.560686231	-0.781464756	5.260526180

H	-2.086802244	-0.753731608	6.210779190
C	1.688624144	-1.255840659	1.145956516
C	0.461691439	-0.859989047	1.494135976
C	2.766453028	-1.872124195	1.997218966
H	3.021831512	-2.869398832	1.617386103
H	3.686804056	-1.273689389	1.980126262
H	2.434800386	-1.967235804	3.035063028
C	-0.557093203	-4.754016876	0.221126884
H	0.128500238	-5.545516968	-0.084178776
H	-0.583056092	-4.696825981	1.315474749
H	-1.571394444	-4.983187199	-0.119324945

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O	-0.726712215	-2.497831029	-0.177906822
N	1.339322108	-3.096911272	-1.051837124
N	2.339930524	-1.617405113	-2.507793065
C	0.223407483	-3.354723341	-0.426425984
C	2.433285101	0.420504056	-0.566555533
C	2.925643558	0.640971534	-1.831822760
C	1.855182510	-0.840944742	-0.236370084
C	2.864726504	-0.431062607	-2.756429402
C	1.824210733	-1.862950614	-1.273789271
H	3.390648460	1.580758558	-2.108925671
H	3.287301898	-0.301759384	-3.752596047
H	2.498339306	1.178391100	0.208716430
C	-1.771150457	1.353077800	0.172335037
C	-2.552283795	0.193345136	-0.172111348
C	-0.890758252	1.620136361	-0.928340521
C	-2.239149480	-0.167557523	-1.555203944
C	-1.218921415	0.692333437	-2.014046863
C	-1.936638560	2.198069978	1.396136577
C	-3.638352713	-0.435455611	0.640703889
C	0.022577390	2.797401165	-1.063516310
C	-2.855764823	-1.327676620	-2.267663260
C	-0.560873515	0.702592467	-3.356603557
H	-2.664027707	2.993747428	1.193696217
H	-2.314073366	1.619229430	2.241458213
H	-1.000235901	2.677520317	1.690656773
H	-3.690325242	-1.509906389	0.449606919
H	-4.610306539	0.002099533	0.379076546
H	-3.480133459	-0.284604236	1.710903988
H	-0.519242894	3.631072518	-1.527725597
H	0.392472737	3.138501757	-0.094049415
H	0.880170644	2.565450844	-1.698001241
H	-2.499698466	-1.409303363	-3.295621377
H	-3.946558550	-1.228764032	-2.286318300
H	-2.610311270	-2.258032388	-1.742822679
H	-0.764544446	-0.211358868	-3.916420006
H	0.524210948	0.803643567	-3.262000297
H	-0.917205531	1.555105767	-3.947670308
Rh	-0.428770935	-0.420486780	-0.120068867
C	1.622241330	-1.169632618	1.215047199
C	0.479321890	-0.529043655	1.651440529
C	-0.060115641	-4.770169027	0.000704739
H	0.696827735	-5.449139016	-0.391897401
H	-0.062394505	-4.816285933	1.095177916
H	-1.053354468	-5.072183802	-0.343183268
C	0.030626388	-0.194725522	3.023978028
H	-0.851732433	-0.789404947	3.294878521
H	0.819264162	-0.368000393	3.763565574
H	-0.273764304	0.854755171	3.085720968
C	2.437928541	-2.160554907	1.892743154
C	1.977626276	-2.843476154	3.042105404
C	3.719588273	-2.471654442	1.382268230
C	2.785356093	-3.781313478	3.671059699
C	4.525894785	-3.401268354	2.023376847
C	4.061211956	-4.059403532	3.167831351
H	0.977084099	-2.660432129	3.415682200
H	4.080353015	-1.966539475	0.492462630
H	2.422042893	-4.304864922	4.549745164
H	5.514781553	-3.619827932	1.632819809
H	4.690919207	-4.792026836	3.663422948

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O	-1.161285281	-2.986656666	0.086140499
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N	1.822986603	-2.713329077	-3.044315100
C	-0.220408991	-3.773559809	-0.338751704
C	3.610866547	-1.208989739	-1.520502687
C	3.841259718	-1.401488423	-2.888012171
C	2.491461992	-1.753369212	-0.900074065
C	2.888231277	-2.120584965	-3.599755049
C	1.648994684	-2.599971771	-1.708548188
H	4.705143452	-0.971817672	-3.384328604
H	2.980026960	-2.241369486	-4.678934574
H	4.290111065	-0.591158450	-0.938578784
C	-2.047876358	0.311732620	-0.609001100
C	-2.436410427	-0.449072361	-1.808892727
C	-0.814382195	1.013965368	-0.902933598
C	-1.394917369	-0.340946615	-2.735416412
C	-0.349302590	0.520974994	-2.153944492
C	-2.914541483	0.513692379	0.594350100
C	-3.674371481	-1.287266850	-1.895309687
C	-0.169328436	2.060799360	-0.051616412
C	-1.242112279	-1.035518289	-4.052917480
C	0.907754123	0.914900899	-2.864032269
H	-3.590308189	1.366256833	0.444020361
H	-3.525763273	-0.372407407	0.783250928
H	-2.314861536	0.699835777	1.487876058
H	-3.731529474	-1.821345329	-2.845969200
H	-4.573322296	-0.668096542	-1.796189427
H	-3.687478065	-2.031633854	-1.091577530
H	-0.537328005	3.054164648	-0.337703407
H	-0.389340043	1.906904578	1.005978584
H	0.916661918	2.053027153	-0.169971719
H	-0.346092612	-1.668594122	-4.049209595
H	-1.132289171	-0.303995907	-4.862294197
H	-2.103165627	-1.668019772	-4.278885841
H	1.311712503	0.077196665	-3.435944796
H	1.678388357	1.232823849	-2.159364700
H	0.714617074	1.741619945	-3.560351133
Rh	-0.510713637	-1.158518791	-0.730014563

C	0.357787013	-0.671777487	2.124205828
C	0.915316284	0.435698420	2.791790962
C	-0.727492511	-1.333214879	2.733592987
H	1.745038629	0.962586403	2.329464436
H	-1.173844457	-2.177209139	2.218176603
C	0.410816699	0.866876900	4.019611359
C	-1.222143650	-0.906830788	3.963797331
H	0.854755998	1.728652000	4.511629581
H	-2.055935860	-1.436271191	4.418368816
C	-0.660676956	0.197507367	4.612209797
H	-1.056025743	0.532646716	5.567263603
C	2.130914927	-1.421590209	0.503421307
C	0.854364276	-1.091894388	0.803585649
C	3.258974075	-1.457984924	1.518441081
H	2.883722305	-1.381886840	2.540375471
H	3.827076435	-2.390541792	1.421317697
H	3.971446991	-0.635884702	1.367268920
C	-0.296645522	-5.207441807	0.136129826
H	-1.288916588	-5.614818573	-0.081995785
H	0.469437093	-5.820914268	-0.339650333
H	-0.164474934	-5.228217602	1.223147392

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O	-0.886975706	-3.253811359	-1.008996129
N	0.780735672	-2.219003201	-1.991114736
N	2.713162899	-2.024779320	-3.299052954
C	0.253841579	-3.364380360	-1.564263344
C	4.163525581	-1.147166491	-1.077066183
C	4.769895077	-1.243599176	-2.330316782
C	2.812091112	-1.478823185	-0.920717478
C	4.008173466	-1.689667463	-3.405896902
C	2.146528482	-1.927618384	-2.096106291
H	5.812663555	-0.973321319	-2.467730045
H	4.445073605	-1.781873822	-4.398787022
H	4.741747856	-0.801817060	-0.225726306
C	-2.335951328	0.368351281	-0.710505962
C	-2.424544811	-0.101341143	-2.098188162
C	-1.155340075	1.145636201	-0.583296597
C	-1.276910543	0.329293460	-2.786227226
C	-0.421835452	1.026797533	-1.825953126
C	-3.396780968	0.165938303	0.330083668
C	-3.553842306	-0.934183359	-2.625717640
C	-0.751376271	1.975343347	0.593451738
C	-0.885393858	0.061036047	-4.208234787
C	0.867676258	1.709869146	-2.171008587
H	-4.178320885	0.933420360	0.252373934
H	-3.877201557	-0.809307039	0.211116433
H	-2.976711512	0.202785417	1.337810040
H	-3.358756781	-1.278791308	-3.643446445
H	-4.490880966	-0.363431543	-2.632892370
H	-3.709147215	-1.818857312	-1.999593019
H	-1.090042114	3.009999037	0.452579379
H	-1.183141351	1.597965598	1.521409750
H	0.334301770	1.991284490	0.715614438
H	0.093777359	-0.427385956	-4.255783558
H	-0.825478435	0.995827854	-4.779173851
H	-1.605367064	-0.592406154	-4.704426765
H	1.439665675	1.116558671	-2.889743090
H	1.490635514	1.847862124	-1.284233928
H	0.683643997	2.696266413	-2.617101669
Rh	-0.540197194	-0.976865113	-1.035120845
C	0.079840019	-1.163688421	1.816954970
C	0.394033790	-0.200757980	2.792832613
C	-0.981276035	-2.052954674	2.082480907
H	1.205002666	0.495696574	2.602676630
H	-1.233018041	-2.799009562	1.334453940
C	-0.331587046	-0.116347954	3.982125998
C	-1.695722222	-1.975471139	3.275253296
H	-0.076394208	0.645078182	4.715099812
H	-2.506470919	-2.675751448	3.460446835
C	-1.381294847	-1.001981854	4.228950024
H	-1.948235750	-0.936375737	5.153708458
C	2.122041225	-1.415081501	0.390365005
C	0.780343831	-1.221122026	0.517433226
C	3.038068771	-1.581369638	1.596690774
H	2.473975420	-1.816896319	2.499570370
H	3.763911724	-2.384988308	1.425715923
H	3.615059137	-0.669481397	1.801874757
C	0.960976660	-4.686280727	-1.691212773
H	1.837337971	-4.689913273	-1.032660842
H	0.288300574	-5.494589329	-1.402912736
H	1.317167759	-4.831396580	-2.714955807

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O	-0.851005793	-2.964907169	-2.393712759
N	1.275315046	-2.263259172	-2.028071642
N	3.330939054	-3.382366419	-2.443903685
C	0.358849555	-3.223742008	-2.388406754
C	4.576178074	-1.728410363	-0.574146748
C	5.326061726	-2.643962622	-1.321717143
C	3.196656942	-1.646742225	-0.753148913
C	4.650981903	-3.458919764	-2.219460726
C	2.617979765	-2.484836102	-1.757116199
H	6.401618481	-2.720399380	-1.198846340
H	5.189133644	-4.198309898	-2.811070204
H	5.076581478	-1.098750591	0.154042020
C	-1.585214019	0.268800288	-1.916405797
C	-0.728488147	0.210934624	-3.083675623
C	-1.015724778	1.210353017	-1.010823846
C	0.328989267	1.151582599	-2.930502653
C	0.191165239	1.729010105	-1.619711995
C	-2.840861320	-0.527079880	-1.743565321
C	-0.979426503	-0.609444201	-4.312479019
C	-1.590878963	1.675936341	0.295502514
C	1.385711193	1.472790360	-3.946052074
C	1.061985373	2.804802656	-1.041516662
H	-3.600857019	-0.226932973	-2.476314306
H	-2.620842934	-1.587193012	-1.891978741
H	-3.270121098	-0.388985217	-0.747418284
H	-0.041517839	-1.000797629	-4.716631889
H	-1.447088480	0.008840175	-5.090301991
H	-1.620876670	-1.461144805	-4.093384743

H	-2.132836819	2.622119188	0.169809103
H	-2.286939383	0.946259439	0.713353634
H	-0.808993518	1.839717388	1.042491794
H	2.293502331	1.856545806	-3.472128630
H	1.037957549	2.233503819	-4.658462524
H	1.664020419	0.585319936	-4.521348476
H	2.101311684	2.690785646	-1.361157179
H	1.044364929	2.790918827	0.051373579
H	0.719897151	3.796187639	-1.366584420
Rh	0.571855903	-0.443404198	-1.270730138
C	0.340802372	-1.203465581	1.721525431
C	1.029254556	-1.230464220	2.955537796
C	-1.059255362	-1.395967484	1.724998116
H	2.108006239	-1.121966124	2.965799809
H	-1.571656823	-1.430825114	0.769305170
C	0.334127992	-1.395680547	4.147981167
C	-1.748223543	-1.566968918	2.919233561
H	0.872798800	-1.406260371	5.091366768
H	-2.823783398	-1.718150496	2.907679558
C	-1.055027008	-1.558947206	4.134087086
H	-1.593532443	-1.695394874	5.067820549
C	2.346949100	-0.753474474	0.082782261
C	1.024058819	-1.063300729	0.464849502
C	3.069002390	0.346400231	0.850203335
H	3.753154039	-0.058671594	1.606783748
H	3.664906502	0.956107140	0.163127035
H	2.355586052	0.998763680	1.358589530
C	0.808588684	-4.623910427	-2.782287359
H	1.442792177	-5.077793598	-2.016283512
H	-0.092290081	-5.220847130	-2.933236837
H	1.408041120	-4.598253727	-3.694841146

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O	-0.931216359	-2.920465708	-2.041735649
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C	0.266266704	-3.207529783	-2.076451778
C	4.647362232	-1.373619080	-1.075324416
C	5.313996792	-2.199860573	-1.995781541
C	3.264164448	-1.466290474	-0.987806737
C	4.572829247	-3.081073523	-2.771329641
C	2.606122017	-2.371631384	-1.867461085
H	6.394397259	-2.161532640	-2.094902754
H	5.063249111	-3.740660906	-3.484057665
H	5.201073647	-0.688628912	-0.439909995
C	-1.453331470	0.596303642	-2.033182144
C	-0.534306943	0.601844847	-3.165383339
C	-0.924984992	1.472278237	-1.057867169
C	0.490602285	1.566267252	-2.939368010
C	0.317983180	2.024653673	-1.586479783
C	-2.728375196	-0.188533172	-1.972887039
C	-0.736983418	-0.229897231	-4.397503376
C	-1.532257080	1.798177958	0.274865955
C	1.560804367	1.994004011	-3.900922298
C	1.167583466	3.055535078	-0.902338564
H	-3.472615957	0.213300228	-2.673378706
H	-2.546367884	-1.235410929	-2.227625132
H	-3.168112755	-0.153525978	-0.971870661
H	0.180819288	-0.306662560	-4.985555172
H	-1.513400078	0.207761630	-5.038601875
H	-1.053337812	-1.240013957	-4.123552799
H	-2.271715641	2.604706764	0.187727332
H	-2.035945177	0.928042352	0.705472350
H	-0.772173762	2.124488354	0.989504039
H	2.487146854	2.255780697	-3.381114721
H	1.251712680	2.872627497	-4.484015942
H	1.800221443	1.197243690	-4.610528946
H	2.200405598	3.013625622	-1.258492708
H	1.182345986	2.907675028	0.180945784
H	0.788500726	4.067815304	-1.095336795
Rh	0.658206642	-0.150106683	-1.388048410
C	0.317031920	-1.987772822	1.116735578
C	0.994152367	-2.524181604	2.231604338
C	-1.078173757	-2.159579754	1.004350066
H	2.071914196	-2.411903858	2.300389290
H	-1.573874474	-1.778393388	0.119673230
C	0.285236299	-3.184921026	3.228660822
C	-1.776628137	-2.842027426	1.994430423
H	0.807440758	-3.586820841	4.092226982
H	-2.849459648	-2.982974529	1.900412798
C	-1.099632978	-3.345681667	3.109507084
H	-1.650353312	-3.871535063	3.884803295
C	2.366585732	-0.779711843	-0.056355134
C	1.039760232	-1.294813991	0.082843848
C	2.963832617	0.058771312	1.055015326
H	3.702593803	-0.509344757	1.637557268
H	3.478154659	0.932527065	0.638577104
H	2.190926552	0.420956582	1.737770557
C	0.714862883	-4.619937420	-2.405238628
H	1.443950057	-4.984353065	-1.675726771
H	-0.169931889	-5.258056641	-2.414610147
H	1.215445876	-4.643425465	-3.375608921

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O	-1.003939271	-3.184041023	-1.539068937
N	1.228377104	-2.764410973	-1.348743200
N	3.052519798	-3.613644123	-2.724562168
C	0.140656441	-3.536498785	-1.783317566
C	4.536706924	-1.415842414	-1.723267436
C	5.105214119	-2.336808920	-2.620182753
C	3.212759495	-1.605984211	-1.352663398
C	4.336256504	-3.393885851	-3.094126940
C	2.547805786	-2.741099834	-1.874814391
H	6.136504650	-2.231309652	-2.942551851
H	4.753829956	-4.116755962	-3.790613890
H	5.111147881	-0.579834402	-1.334541321
C	-1.371394873	0.753070474	-2.504169226
C	-0.209850669	1.203855395	-3.287099123
C	-1.201077223	1.198787451	-1.188241243
C	0.626766622	2.001006603	-2.477214813
C	0.106290266	1.870703578	-1.126662850
C	-2.493317366	-0.069485828	-3.063735962

C	-0.041570056	0.921377301	-4.750504494
C	-2.147462845	1.092253923	-0.031790927
C	1.835871935	2.790922880	-2.880966663
C	0.604465485	2.616903305	0.073414154
H	-3.021716118	0.466322064	-3.862515450
H	-2.123016357	-1.011483312	-3.481911182
H	-3.220255852	-0.329270959	-2.291091442
H	0.994108260	1.060945511	-5.070136547
H	-0.673414469	1.585974455	-5.354312420
H	-0.333435178	-0.106590152	-4.987885475
H	-2.573607445	2.075333834	0.209361851
H	-2.975473881	0.413030833	-0.248443604
H	-1.646242619	0.719247699	0.865781188
H	2.606961250	2.761496544	-2.105195045
H	1.586690187	3.846548557	-3.057500124
H	2.280261993	2.398947239	-3.799670935
H	1.691215754	2.728280783	0.056250010
H	0.329824209	2.105132580	0.999436855
H	0.164194718	3.622651577	0.104961433
Rh	0.642413914	-0.140248448	-1.656028867
C	0.391572744	-1.981459975	0.929988146
C	1.171716452	-2.348443985	2.037222385
C	-0.998711228	-1.908503056	1.085763931
H	2.249219656	-2.427119732	1.925630093
H	-1.599939227	-1.659173608	0.222398102
C	0.583094001	-2.613622665	3.273806334
C	-1.589441657	-2.174639225	2.320022583
H	1.205714941	-2.893715620	4.119530201
H	-2.669687033	-2.112813473	2.422740936
C	-0.801723063	-2.522532940	3.419714212
H	-1.264619350	-2.727665663	4.381317139
C	2.299974203	-0.878672898	-0.472151995
C	1.073794127	-1.665007949	-0.361400962
C	2.853637695	0.020906178	0.604257703
H	3.589400291	-0.504638195	1.228607178
H	3.360297203	0.885856092	0.161457360
H	2.060994864	0.390312016	1.257094026
C	0.442431629	-4.815813541	-2.531429768
H	-0.492962599	-5.369678974	-2.617959976
H	0.851447523	-4.596492290	-3.521074057
H	1.204440355	-5.407791615	-2.019457817

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O	-0.941248477	-2.133062840	-2.115454197
N	0.164456576	-2.074794769	-0.121905558
N	2.376166582	-2.020877600	0.493741482
C	-0.915613413	-2.523089170	-0.967375696
C	2.890272856	-4.396357059	-0.936978698
C	3.890838385	-3.768906832	-0.192233130
C	1.620846152	-3.837353468	-0.957191586
C	3.574002266	-2.574150324	0.494472414
C	1.384817600	-2.648569345	-0.202726394
H	4.895867825	-4.174000740	-0.142279163
H	4.343835831	-2.053431273	1.060442328
H	3.098268270	-5.304162025	-1.493966341
C	0.236615464	1.812227964	1.495146513
C	-0.993210018	1.783447385	0.762436926
C	1.297367573	1.339884996	0.611407578
C	-0.720642686	1.255985975	-0.563085496
C	0.705603838	1.019331336	-0.655229509
C	0.447661519	2.250915766	2.909499884
C	-2.341484547	2.165105581	1.280167818
C	2.739726305	1.258137345	0.989865422
C	-1.700363874	1.115240932	-1.684773922
C	1.414470911	0.504495502	-1.866554260
H	0.947981954	3.226064444	2.928970575
H	-0.495722473	2.343251467	3.449357271
H	1.077766180	1.536220551	3.445538044
H	-3.125762463	1.548004389	0.837386191
H	-2.550530434	3.211629391	1.027637601
H	-2.398575068	2.058832407	2.364623308
H	3.173890829	2.265294313	1.004666448
H	2.852890730	0.824836731	1.986459374
H	3.305042267	0.645890176	0.288140476
H	-1.483694553	0.234406918	-2.292734146
H	-1.650193810	1.997743964	-2.334449530
H	-2.723855257	1.030663371	-1.314452291
H	0.794974685	-0.217419714	-2.402724743
H	2.354856491	0.020701442	-1.597908854
H	1.639635444	1.338582873	-2.541391611
Rh	-0.165332615	-0.254351884	0.909093142
H	0.823026419	-4.289134502	-1.536328554
C	-0.881323278	-1.599510908	2.930584669
O	-1.753242373	-1.242229462	2.059127569
O	0.331735283	-1.271844983	2.795485735
O	-1.240131140	-2.330733061	3.981782436
H	-2.198587894	-2.476527214	3.942963123
C	-1.937739372	-3.389466286	-0.298384547
H	-2.730865717	-3.635451794	-1.005332112
H	-1.460853577	-4.306033611	0.068329953
H	-2.337979794	-2.861756086	0.573386908

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O	0.455900759	-2.036888838	-1.848177314
N	1.256615520	-1.965065956	0.304309130
N	3.074305058	-3.300863743	-0.190172359
C	0.588506937	-2.634383202	-0.806556225
C	4.442020416	-2.312029362	2.070383549
C	5.041121483	-3.228477001	1.201808929
C	3.153308868	-1.875692606	1.799754620
C	4.302077770	-3.697175503	0.090776980
C	2.497459888	-2.381992817	0.638363481
H	6.046767712	-3.596356153	1.375115395
H	4.740745544	-4.425373554	-0.588105023
H	4.969151497	-1.955439568	2.949503183
C	0.171389535	1.834306240	1.653616071
C	-0.912634909	1.568415761	0.763273418
C	1.414221287	1.550212145	0.945091486
C	-0.356886566	1.126173019	-0.512481987
C	1.075171590	1.165264726	-0.403245360
C	0.075661995	2.291193008	3.073236227
C	-2.372827053	1.696165919	1.053433418

C	2.793186665	1.757748961	1.487868190
C	-1.143770576	0.803888857	-1.740057826
C	2.039072275	0.843885601	-1.499068975
H	0.209860101	3.378191710	3.121583700
H	-0.893786788	2.048169136	3.510232210
H	0.846306980	1.826367378	3.691613436
H	-2.921413898	0.824877918	0.686506331
H	-2.773434639	2.582871437	0.548589110
H	-2.566809893	1.796530724	2.121994495
H	3.132309914	2.778094769	1.270873427
H	2.818674803	1.623167992	2.571720123
H	3.508392096	1.065002322	1.040568709
H	-0.629428744	0.065763026	-2.356191874
H	-1.288000584	1.715193868	-2.333465815
H	-2.130304337	0.411309808	-1.485092402
H	1.689804673	-0.005561636	-2.086820602
H	3.031198502	0.613089502	-1.107074857
H	2.133361816	1.714071393	-2.159636736
Rh	0.245629385	-0.279003382	1.054139137
H	2.624671936	-1.202034712	2.462214708
C	-0.805743515	-1.849844813	2.733639717
O	-1.358663797	-1.705839753	1.591380954
O	0.246889606	-1.200649261	3.029180765
O	-1.305858374	-2.685861111	3.636230230
H	-2.111999989	-3.085955381	3.272761822
C	-0.010290878	-3.967466593	-0.469589233
H	-0.391684085	-4.430396557	-1.380334735
H	0.724090993	-4.616877079	0.011351568
H	-0.832758725	-3.789009094	0.232294574

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O	0.132006213	-2.150609732	-0.532799363
N	2.269291639	-3.005424738	-0.370823801
N	4.175493717	-2.306785107	0.667258918
C	0.943559885	-3.112353086	-0.619350195
C	2.678942442	-1.369238019	2.881234884
C	4.068160057	-1.377694726	2.901884794
C	1.985552073	-1.839150786	1.751769304
C	4.762688160	-1.824809551	1.741259694
C	2.802751064	-2.380141258	0.678485632
H	4.628467560	-1.042800426	3.769508362
H	5.850765228	-1.784763217	1.718182325
H	2.119835377	-1.004348278	3.738594532
C	1.084621429	1.486088514	1.509766102
C	-0.315445691	1.535837054	1.190169930
C	1.805633783	1.129270196	0.295544565
C	-0.478483945	1.185135365	-0.201308131
C	0.840550244	0.955248415	-0.752795756
C	1.696978331	1.879113674	2.817188501
C	-1.439929128	1.837972760	2.127617836
C	3.291677713	1.072435141	0.138745070
C	-1.771859527	1.123425364	-0.948701978
C	1.129248142	0.579706430	-2.169445276
H	1.787548661	2.970663309	2.867074728
H	1.082326412	1.556421399	3.660240889
H	2.694094896	1.454893112	2.938422918
H	-2.136650324	0.995112300	2.165215254
H	-1.989592671	2.718629599	1.778366685
H	-1.084247470	2.033622742	3.139801025
H	3.665367603	2.050590277	-0.186730638
H	3.782181025	0.821693182	1.079607010
H	3.593467951	0.332754523	-0.605468750
H	-1.754689217	0.334702790	-1.704443932
H	-1.961275578	2.075254679	-1.459944606
H	-2.607361078	0.929895282	-0.273095280
H	0.353476197	-0.078122176	-2.566187143
H	2.091139078	0.073150977	-2.264102936
H	1.156972647	1.483237147	-2.790569305
Rh	0.429718733	-0.515110016	0.832053959
H	0.859093487	-2.534865379	2.000790596
C	-1.145846844	-2.598983526	2.254760027
O	-1.208899021	-1.381965280	1.883146405
O	-0.097462684	-3.313879967	2.260458708
O	-2.256037712	-3.190035582	2.686549902
H	-2.985949755	-2.554353237	2.622355461
C	0.445018113	-4.446461678	-1.087815166
H	1.245003819	-5.040525436	-1.529891253
H	0.061365131	-4.969450474	-0.202385396
H	-0.382470429	-4.312869072	-1.787819624

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O	-0.267630994	-2.492261887	0.337787539
N	1.800100207	-3.451508760	-0.059276547
N	3.662152052	-3.544146299	1.246992588
C	0.559763372	-3.157573462	-0.406000823
C	3.141063452	-1.008270502	2.357468605
C	4.232512474	-1.759273052	2.765693426
C	2.267626762	-1.506908655	1.378970861
C	4.450034142	-3.029129028	2.161800861
C	2.569608450	-2.825783491	0.845987022
H	4.922586918	-1.391401649	3.519040346
H	5.320724487	-3.620236158	2.440367222
H	2.948763132	-0.041185152	2.812844515
C	0.685815334	1.606894135	1.003385067
C	-0.702887356	1.351004124	0.573334873
C	1.567315221	1.156399608	-0.033388987
C	-0.657559156	0.657193899	-0.640640259
C	0.758976698	0.443797052	-0.990334034
C	1.048445702	2.392883778	2.223160982
C	-1.901488543	1.732999086	1.383587003
C	3.042443037	1.385316849	-0.119670287
C	-1.798376322	0.111593142	-1.439229131
C	1.243028641	-0.153261140	-2.275798798
H	0.851781368	3.459168911	2.056992054
H	0.451687217	2.074354172	3.081858873
H	2.104840994	2.285237551	2.477510691
H	-2.824341774	1.338965774	0.954992235
H	-1.990880847	2.823562622	1.445736289
H	-1.811320186	1.349903226	2.405261040
H	3.232417822	2.321268797	-0.658371031
H	3.499647617	1.471823096	0.867727399
H	3.544623613	0.578759074	-0.657159805

H	-1.739706874	-0.980547547	-1.494181395
H	-1.770972610	0.501443326	-2.462415695
H	-2.762471914	0.371995360	-1.000384331
H	0.544365764	-0.901415765	-2.654915810
H	2.220726013	-0.625882030	-2.156804323
H	1.338191748	0.627881408	-3.040245056
Rh	0.562200546	-0.572463214	0.918996811
H	-0.607007504	-2.937018633	1.889270186
C	-0.577127159	-1.942365766	3.495118141
O	-0.142160818	-0.881786644	3.002589226
O	-0.789771557	-3.058419228	2.860768557
O	-0.878077209	-2.039236784	4.778517246
H	-0.682469606	-1.190869689	5.205681324
C	0.038592510	-3.732408047	-1.689160585
H	0.853562474	-4.073928833	-2.327951670
H	-0.601945221	-4.590624809	-1.452048182
H	-0.583837450	-2.998404980	-2.206216812

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O	3.931851625	2.534219980	-0.572903574
N	5.428389549	0.955360055	0.230643213
N	7.425673962	1.071027875	1.293866634
C	4.272275448	1.328995943	-0.331267864
C	6.930415630	3.691988230	2.192872763
C	8.129747391	3.049610376	2.473355532
C	5.931853771	3.045754910	1.446758270
C	8.319581032	1.723422647	1.997810245
C	6.237937450	1.695328712	0.998089254
H	9.241647720	1.191435814	2.225122929
H	8.910010338	3.537123203	3.049958229
H	6.781054974	4.710041523	2.537074327
C	3.986822605	6.069252014	1.633402228
C	3.689077854	5.073099613	2.599877834
C	3.006820679	5.957501888	0.527622998
C	2.633643389	4.241132736	2.028983116
C	2.167016268	4.868909836	0.787855923
C	4.989151001	7.172706127	1.747966051
C	4.258074760	4.917074203	3.974996090
C	2.997038841	6.861282825	-0.662523150
C	1.973500371	3.082856655	2.699536085
C	1.065925956	4.315599918	-0.060281329
H	5.488544464	7.359661102	0.793628991
H	4.486241817	8.102100372	2.042677402
H	5.752202511	6.955320835	2.497483969
H	4.459411621	3.870099306	4.212295055
H	3.538282394	5.296818256	4.709689140
H	5.184237957	5.479957581	4.101076126
H	4.005940437	6.993715286	-1.065696597
H	2.360359907	6.477588654	-1.460687518
H	2.629730463	7.854924679	-0.377832532
H	1.556337833	2.387446642	1.967901230
H	2.668588877	2.542573690	3.345447779
H	1.146743178	3.446317196	3.324017763
H	1.321701765	3.308491230	-0.407269418
H	0.880840003	4.935996056	-0.938006043
H	0.135753095	4.249330997	0.513561606
Rh	4.336575031	4.051974297	0.764440238
C	3.370352745	0.224750489	-0.799851775
H	3.817334652	-0.257712990	-1.675916553
H	3.285765171	-0.543520629	-0.024749495
H	2.388039112	0.618336856	-1.061487794

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6A

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O	-0.265330344	-1.645060778	-0.500262380
N	1.558652639	-3.103912830	-0.345539302
N	3.762512207	-2.793383360	-0.008480417
C	0.278130740	-2.786572933	-0.606260419
C	3.520722628	-0.035666782	0.431442380
C	4.765050411	-0.644281507	0.407455266
C	2.352710009	-0.784672141	0.209714040
C	4.821363926	-2.048046589	0.194987774
C	2.517394304	-2.203670979	-0.041430186
H	5.676256657	-0.077690013	0.575014293
H	5.781612873	-2.562050343	0.212832361
H	3.449220419	1.025156260	0.644878209
C	0.424392521	2.317361116	0.626461029
C	-0.973639727	1.859791160	0.664288402
C	0.950066686	2.043640852	-0.674315631
C	-1.261959910	1.238710880	-0.557912529
C	-0.039391998	1.272219539	-1.374668002
C	1.041414022	3.198767662	1.666959882
C	-1.874260068	2.048135757	1.844211578
C	2.243702173	2.529729366	-1.249819517
C	-2.520268917	0.556515813	-0.991557598
C	0.047393896	0.772436321	-2.782703400
H	0.794005096	4.247601032	1.458259821
H	0.658093393	2.968366861	2.663599968
H	2.130995750	3.116870403	1.682658315
H	-2.876754522	1.661661625	1.652579784
H	-1.966803551	3.111164331	2.091804266
H	-1.473182559	1.536534905	2.725394726
H	2.046996593	3.366542339	-1.930345058
H	2.926177740	2.891576290	-0.478277564
H	2.753025293	1.749094725	-1.819772243
H	-2.335842133	-0.514796019	-1.131133914
H	-2.867690802	0.963668227	-1.947073936
H	-3.321196079	0.674141943	-0.259589732
H	-0.490222573	-0.172410607	-2.890846014
H	1.083642364	0.615841329	-3.089940310
H	-0.404305577	1.498350501	-3.470277309
Rh	0.539279461	0.061495643	0.365510255
C	-1.043534875	-2.089592934	2.322925568
C	-2.389708757	-1.766950250	2.076720476
C	-0.659711421	-3.439364910	2.449740648
H	-2.676162004	-0.727683604	1.966965318
H	0.382266372	-3.685612679	2.623007774
C	-3.336086035	-2.779155970	1.962303281
C	-1.617034435	-4.445028305	2.341303110
H	-4.374900818	-2.528993607	1.769652843
H	-1.319019198	-5.483984947	2.441157579
C	-2.952522039	-4.118539810	2.095017910
H	-3.695548534	-4.905383110	2.005587578

C	0.940288603	-0.346229583	2.628109217
C	-0.034584008	-1.079848289	2.409827232
C	2.030153036	0.247070566	3.417042494
H	1.872539878	0.021999316	4.476314545
H	2.990054369	-0.177191436	3.109533310
H	2.086440325	1.330050588	3.295828104
C	-0.599042654	-3.896888733	-1.120494246
H	-0.650443435	-3.830204248	-2.214253664
H	-0.176220804	-4.865631580	-0.855438352
H	-1.610868454	-3.791073799	-0.723333359

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6A-TS

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O	-0.130141005	-1.583125710	-1.137863398
N	1.918484807	-2.665590525	-1.216261029
N	3.996030569	-1.728464842	-1.252047777
C	0.596704781	-2.639011621	-1.248419642
C	3.356886387	0.140315160	0.744798362
C	4.628416061	0.088386424	0.212978452
C	2.341938496	-0.689323664	0.219451457
C	4.885232449	-0.868293703	-0.805787861
C	2.722407103	-1.696326137	-0.752606690
H	5.422129631	0.737760186	0.568526566
H	5.883619785	-0.944864154	-1.234219074
H	3.118246078	0.832469225	1.546361566
C	0.218975112	2.109863520	0.919315934
C	-1.134529233	1.574225426	0.849148095
C	0.739199102	2.195886374	-0.422796428
C	-1.399167061	1.229923487	-0.500382245
C	-0.223949239	1.592154145	-1.293984532
C	0.845141828	2.684114456	2.152760267
C	-2.071889400	1.452523232	2.007807970
C	2.035270691	2.816953897	-0.840735734
C	-2.640362501	0.619839191	-1.072141290
C	-0.126833007	1.423120737	-2.776560783
H	0.438549250	3.683630705	2.351271391
H	0.640997946	2.065456390	3.030301332
H	1.927169919	2.787982225	2.048036575
H	-2.826629877	0.682791352	1.840634108
H	-2.586119652	2.408627748	2.164098978
H	-1.542190194	1.204783320	2.930219173
H	1.875286818	3.868442059	-1.108117223
H	2.777497530	2.788753986	-0.041007109
H	2.461577892	2.312134504	-1.710455060
H	-2.383836031	-0.217183650	-1.728630781
H	-3.191108704	1.358266711	-1.666538715
H	-3.302413464	0.246026695	-0.289786249
H	-0.501379550	0.441427916	-3.077418327
H	0.901128709	1.520474553	-3.129800081
H	-0.734267235	2.183633804	-3.282401085
Rh	0.393651575	0.007337285	0.133894041
C	-1.363409400	-1.789131522	2.095373392
C	-1.669210911	-1.746393681	3.467759609
C	-2.355696440	-2.160026550	1.169170976
H	-0.904865623	-1.448985577	4.179363728
H	-2.111078501	-2.170611858	0.112921715
C	-2.949404001	-2.080702305	3.903985739
C	-3.630378246	-2.494201899	1.617186785
H	-3.181887388	-2.046971560	4.963945389
H	-4.392959595	-2.785376787	0.900996447
C	-3.931068182	-2.453065872	2.982418299
H	-4.928506374	-2.708699703	3.326555252
C	1.224400520	-1.537963152	1.756836414
C	-0.038075019	-1.431420684	1.649380326
C	2.322253466	-2.146958828	2.553716660
H	1.860677123	-2.750463247	3.342476606
H	2.959208965	-2.787935734	1.938293099
H	2.952570915	-1.383534551	3.018543005
C	-0.129541665	-3.926889181	-1.525769114
H	0.567851245	-4.725060463	-1.778044105
H	-0.705258429	-4.206286907	-0.635734022
H	-0.843162537	-3.778600216	-2.341909170

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7A

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O	-0.968454480	-2.536342382	-0.407260954
N	1.154749155	-3.312249660	-0.934606493
N	2.015661716	-1.966263413	-2.621370316
C	-0.040959802	-3.473664045	-0.470929325
C	2.500874996	0.141290426	-0.822324157
C	2.879474163	0.249798596	-2.144782066
C	1.855792046	-1.038995862	-0.371446133
C	2.607110739	-0.842070818	-2.999080420
C	1.650325179	-2.098990679	-1.324851751
H	3.396145344	1.126441002	-2.520686626
H	2.899210691	-0.791643977	-4.047143936
H	2.701603174	0.933156371	-0.106580295
C	-1.625046849	1.339288831	0.309310913
C	-2.536388397	0.311494410	-0.146241829
C	-0.743746519	1.642933965	-0.771353066
C	-2.286249638	0.080069773	-1.561237812
C	-1.175855637	0.877384126	-1.943109274
C	-1.667013645	2.015675306	1.641553044
C	-3.680536032	-0.276949227	0.613248467
C	0.296915680	2.717982769	-0.797607422
C	-3.044313908	-0.908944309	-2.386936188
C	-0.550712407	0.980797052	-3.294760466
H	-2.353176832	2.869904280	1.589166641
H	-2.021775723	1.346815705	2.426919937
H	-0.685344100	2.390747786	1.936609507
H	-3.815985203	-1.330113411	0.353771210
H	-4.607372761	0.252074540	0.357424617
H	-3.531963110	-0.200452611	1.690826416
H	-0.156454250	3.662546396	-1.122870326
H	0.734958649	2.881306410	0.189595550
H	1.098815799	2.477289677	-1.497843981
H	-2.678565979	-0.948024392	-3.413915873
H	-4.108668804	-0.649933994	-2.408447742
H	-2.948105335	-1.910259128	-1.952784061
H	-0.922996640	0.213501498	-3.975023031
H	0.537338197	0.880562723	-3.233344078
H	-0.762791812	1.963471770	-3.733389378
Rh	-0.504576862	-0.554996252	-0.270280123
C	-0.165458560	-0.658634245	2.821031570

C	0.399540454	0.133196816	3.842647791
C	-1.382412910	-1.334463358	3.064162970
H	1.333077788	0.655540347	3.655389309
H	-1.801638246	-1.953371644	2.276580572
C	-0.239295110	0.245231628	5.073902130
C	-2.009466887	-1.223866940	4.299808025
H	0.200103581	0.855047941	5.857336521
H	-2.935740232	-1.758873343	4.487172127
C	-1.444339156	-0.428102583	5.304041862
H	-1.939739585	-0.338108510	6.266070366
C	1.639832854	-1.268495917	1.100555420
C	0.467578977	-0.773861945	1.532692432
C	2.600409269	-2.122777462	1.881122112
H	2.691558361	-3.105990410	1.407058716
H	3.596914768	-1.663922548	1.878680348
H	2.266815662	-2.249351025	2.913347960
C	-0.486289382	-4.823417187	0.023388909
H	0.286714643	-5.573172092	-0.146008760
H	-0.712594509	-4.760182858	1.093336105
H	-1.407415628	-5.116750717	-0.488784105

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7A-TS

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O	-1.079582095	-3.020431995	-0.069440059
N	0.855914772	-3.681480169	-1.065399051
N	1.690662861	-2.806299448	-3.008948565
C	-0.174422666	-3.904177904	-0.300757617
C	3.634189367	-1.391987324	-1.537608981
C	3.776328802	-1.590581656	-2.894316435
C	2.473300934	-1.847176194	-0.871875465
C	2.725764513	-2.245393753	-3.594611645
C	1.597928643	-2.740354300	-1.639961123
H	4.633658409	-1.205034852	-3.435569525
H	2.755181074	-2.303308725	-4.681669235
H	4.373836517	-0.821202397	-0.984914362
C	-2.091369867	0.277122676	-0.616245568
C	-2.409531116	-0.458910882	-1.849327803
C	-0.878159761	1.051267624	-0.844748437
C	-1.352564335	-0.262897313	-2.742127657
C	-0.360921770	0.628813028	-2.098685503
C	-3.005860329	0.394857645	0.557035685
C	-3.610296011	-1.337537289	-2.005659103
C	-0.330640554	2.107317448	0.060420774
C	-1.160334110	-0.860244036	-4.099164486
C	0.881865263	1.113050461	-2.774079800
H	-3.737143040	1.193002224	0.372490138
H	-3.558143139	-0.533930123	0.717608452
H	-2.460258722	0.633050740	1.471240759
H	-3.619908571	-1.838873148	-2.974574804
H	-4.529913902	-0.749730408	-1.914024115
H	-3.625288963	-2.108161211	-1.227650046
H	-0.802593946	3.069201708	-0.173499838
H	-0.528312504	1.880049825	1.109199166
H	0.748314261	2.223797560	-0.062454537
H	-0.267691880	-1.494668603	-4.120721340
H	-1.027124882	-0.067967959	-4.844898701
H	-2.013847589	-1.470724702	-4.397303581
H	1.355088234	0.310883045	-3.345993042
H	1.607172370	1.496334553	-2.053991556
H	0.637906194	1.921115279	-3.474968433
Rh	-0.474692583	-1.115379333	-0.753845930
C	0.401268631	-0.634151936	2.086182594
C	1.043167353	0.407188773	2.790078640
C	-0.756898880	-1.215827346	2.648734808
H	1.919021845	0.883950353	2.362358809
H	-1.252971292	-2.016492128	2.109264135
C	0.537640393	0.853651524	4.008825779
C	-1.235115767	-0.788391292	3.883259058
H	1.030509830	1.668496370	4.530681133
H	-2.112251043	-1.262268662	4.314226627
C	-0.596334636	0.252891421	4.563281059
H	-0.979705215	0.594587445	5.519979954
C	2.175403357	-1.445530772	0.488456219
C	0.866401374	-1.104985714	0.782557547
C	3.326162100	-1.349277735	1.470840812
H	2.971460819	-1.451189637	2.497971296
H	4.067424297	-2.129660845	1.278194070
H	3.840297461	-0.382082701	1.402775764
C	-0.356159270	-5.269758701	0.302837729
H	-1.343369246	-5.652968407	0.029620359
H	0.416540235	-5.961896420	-0.032336663
H	-0.326531440	-5.179694653	1.393261552

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8A

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O	-0.985500395	-3.235409260	-1.135435700
N	0.804678977	-2.205016136	-1.793789029
N	2.625337124	-2.106225491	-3.257696867
C	0.157485008	-3.356043577	-1.708177209
C	4.187480927	-0.911140740	-1.266833425
C	4.707087517	-1.134437561	-2.541028023
C	2.866170168	-1.273991227	-0.979252040
C	3.894991636	-1.744239688	-3.496093988
C	2.139138460	-1.875339746	-2.038396358
H	5.723374844	-0.847018838	-2.788699627
H	4.268280983	-1.947106719	-4.496901989
H	4.806841373	-0.456883341	-0.500163674
C	-2.325446844	0.465288997	-0.728331923
C	-2.375116348	-0.133636102	-2.046838522
C	-1.086640239	1.176997662	-0.599530518
C	-1.137686253	0.129856944	-2.700121880
C	-0.307358772	0.909684956	-1.779367328
C	-3.429143429	0.437741548	0.283521056
C	-3.524606943	-0.924552083	-2.584260225
C	-0.711103082	2.109384775	0.503444850
C	-0.723709583	-0.278812557	-4.077870369
C	1.023378372	1.504842401	-2.118403912
H	-4.085333347	1.308588862	0.156647339
H	-4.045154095	-0.457693785	0.175676301
H	-3.035431862	0.459673703	1.302610636
H	-3.247566938	-1.486923099	-3.476704597
H	-4.352870941	-0.255087972	-2.847140551
H	-3.898283958	-1.634389639	-1.840872169
H	-1.047685146	3.122164488	0.248960510

H	-1.175552249	1.828753114	1.449501753
H	0.370836943	2.146755934	0.645998597
H	0.293927401	-0.680465817	-4.083112717
H	-0.747402608	0.589265168	-4.747899055
H	-1.386227489	-1.041566849	-4.489657879
H	1.576498032	0.870528102	-2.813562632
H	1.636260152	1.644793034	-1.226082087
H	0.882980943	2.483281851	-2.594677925
Rh	-0.565444708	-1.042326570	-0.837081552
C	0.136784852	-1.129402995	1.786452413
C	0.191443041	-0.092487782	2.747982502
C	-0.777589202	-2.196883440	1.990031838
H	0.902361214	0.714932978	2.610394239
H	-0.805751920	-3.014621973	1.276062250
C	-0.636094689	-0.121648885	3.861996651
C	-1.619155169	-2.204048395	3.101132393
H	-0.572438002	0.668554306	4.604369640
H	-2.313035011	-3.026703358	3.244086742
C	-1.554640889	-1.169272304	4.035076141
H	-2.204270601	-1.178654194	4.905107498
C	2.272365093	-1.167620420	0.371580124
C	0.943665445	-1.108542800	0.576526582
C	3.232438326	-1.208348274	1.547470093
H	2.703033447	-1.318997383	2.494063854
H	3.939768076	-2.037225485	1.440620184
H	3.822345018	-0.284699827	1.600208879
C	0.686315715	-4.672146797	-2.181935787
H	1.156874776	-5.193740368	-1.340480804
H	-0.143319488	-5.286164284	-2.538888216
H	1.425590873	-4.530854225	-2.971980333

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8A-TS

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O	-1.324314713	-2.828423262	-1.035261393
N	0.694903433	-2.051668882	-1.301190853
N	2.554723740	-2.371243477	-2.743426323
C	-0.140092075	-3.119483471	-1.342540622
C	3.911651373	-0.400738180	-1.219799638
C	4.503977776	-0.987483025	-2.331714392
C	2.617162943	-0.813768625	-0.854293108
C	3.800096273	-1.968188405	-3.047152042
C	1.996988654	-1.801755786	-1.679767847
H	5.501041412	-0.701277316	-2.648670435
H	4.254932404	-2.447647333	-3.910371065
H	4.437968254	0.351974815	-0.640712559
C	-2.555700541	0.801865816	-1.204250574
C	-2.374291420	0.277332246	-2.560889006
C	-1.400787234	1.571591973	-0.855022848
C	-1.087785244	0.652734220	-3.003964424
C	-0.438838184	1.394615889	-1.918908238
C	-3.812091827	0.655906558	-0.402696252
C	-3.396356106	-0.532624483	-3.295124292
C	-1.208655477	2.386034966	0.386803687
C	-0.430920780	0.331639051	-4.309454918
C	0.905465364	2.044253826	-2.025197744
H	-4.567500114	1.373744965	-0.745628655
H	-4.236606598	-0.345749050	-0.511887372
H	-3.636186838	0.839322388	0.659509957
H	-2.969787598	-1.024019718	-4.171332836
H	-4.220702171	0.107293367	-3.632300854
H	-3.821034908	-1.306958795	-2.649865627
H	-1.554115534	3.413876772	0.221075833
H	-1.773147106	1.975906014	1.227195501
H	-0.156679466	2.430745125	0.677791774
H	0.590991676	-0.029587768	-4.158167362
H	-0.373433053	1.229800105	-4.936348915
H	-0.979543269	-0.431957752	-4.863243580
H	1.629142165	1.384207487	-2.510240555
H	1.299479961	2.313224077	-1.043220878
H	0.835324109	2.961370707	-2.622709274
Rh	-0.830488920	-0.558943272	-1.082059860
C	0.079028487	-1.646161318	1.621981740
C	-1.294196010	-1.710924864	1.946604729
C	1.002022743	-2.321535826	2.456747293
H	-2.011210918	-1.209296346	1.305365205
H	2.057397366	-2.306578159	2.202572584
C	-1.723914742	-2.400912762	3.074020863
C	0.568869531	-3.013496637	3.579103470
H	-2.781201601	-2.438059330	3.316701174
H	1.286681294	-3.529241562	4.209413052
C	-0.795234859	-3.052733183	3.890423059
H	-1.133407474	-3.597322464	4.766983509
C	1.869208694	-0.445544302	0.309388667
C	0.548321784	-0.950486481	0.434385210
C	2.469596863	0.421859294	1.384016395
H	1.810549259	0.509318590	2.248926401
H	3.435194016	0.024500631	1.719419837
H	2.659768105	1.430936933	0.995204628
C	0.328344554	-4.502104282	-1.666583061
H	0.936471105	-4.877412319	-0.835058331
H	-0.532016158	-5.156119347	-1.808959126
H	0.962216616	-4.483664989	-2.556646585

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9A

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O	-1.055129766	-3.271238327	-1.453534245
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N	2.724516153	-3.283358812	-3.042357445
C	0.092854626	-3.636354208	-1.534804463
C	4.383859158	-1.228082299	-1.961748719
C	4.780229092	-1.993519425	-3.057378292
C	3.135166168	-1.515776992	-1.398823023
C	3.931911469	-2.992308855	-3.559852600
C	2.385937452	-2.566578388	-1.987050056
H	5.742030621	-1.826200724	-3.529937267
H	4.234630108	-3.587602615	-4.416518688
H	5.016454220	-0.444893956	-1.556034446
C	-1.399081826	0.565726876	-2.089355469
C	-0.656363368	0.551990449	-3.335289001
C	-0.662707448	1.351457953	-1.161260724
C	0.454970479	1.455981374	-3.232304335
C	0.517319679	1.876613975	-1.862080693
C	-2.688828230	-0.158888295	-1.860242724
C	-1.097372174	-0.182680890	-4.563044071

C	-1.051853418	1.687241793	0.244162887
C	1.394729614	1.842561722	-4.331470966
C	1.492622733	2.848687172	-1.275123596
H	-3.447638273	0.175874382	-2.576841593
H	-2.562895298	-1.238096356	-1.989728928
H	-3.076112509	0.026532762	-0.856854200
H	-0.266597688	-0.365310252	-5.247923851
H	-1.852406740	0.403794855	-5.102114201
H	-1.550496459	-1.143319130	-4.303537846
H	-1.679955721	2.587063074	0.252799571
H	-1.610583425	0.877643585	0.716092885
H	-0.175993010	1.894044638	0.863913715
H	2.388539076	2.084785938	-3.946883678
H	1.019896984	2.727847338	-4.860967159
H	1.503427267	1.042427540	-5.067852497
H	2.450761318	2.823909521	-1.799369454
H	1.674575090	2.643735647	-0.217725500
H	1.097625017	3.869746685	-1.348022223
Rh	0.716856718	-0.300856739	-1.778403401
C	0.362679720	-1.910864830	1.038157225
C	1.068911791	-2.182880402	2.221817255
C	-1.035774827	-1.817057252	1.085207343
H	2.150602341	-2.272555351	2.194312572
H	-1.585554004	-1.623208523	0.176084086
C	0.391272008	-2.349676371	3.427943230
C	-1.710244775	-1.985921621	2.292414665
H	0.949835718	-2.561333418	4.334634781
H	-2.793437719	-1.913055062	2.316102266
C	-1.000221491	-2.248150349	3.466271162
H	-1.529197216	-2.375929832	4.405914783
C	2.357990503	-0.959969461	-0.309096694
C	1.156706214	-1.720041752	-0.199035421
C	2.884195805	0.022066880	0.695335746
H	3.641916752	-0.440872580	1.338076234
H	3.355222225	0.870170772	0.189889714
H	2.082446814	0.396042645	1.334842443
C	0.545661330	-5.035808086	-1.821699142
H	-0.333887041	-5.669050217	-1.933482170
H	1.160861135	-5.054093361	-2.725255251
H	1.171728253	-5.395993233	-0.997463644

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1B

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C	4.579995632	-1.734937310	-1.160545111
C	4.448979855	-0.960997462	-0.004175353
C	3.445044279	-2.275935173	-1.740450501
C	3.181060791	-0.776948869	0.519063950
C	2.167741060	-2.036337137	-1.187083125
H	5.307257652	-0.529198587	0.497773945
H	3.013619184	-0.248456284	1.451560855
H	5.557590008	-1.932953358	-1.590423942
C	-0.774786234	0.771046221	2.055721998
C	-1.734778762	0.151711851	1.190202713
C	0.267833769	1.346044540	1.241508722
C	-1.323653936	0.411638021	-0.184941903
C	-0.100819990	1.144963861	-0.153266132
C	-0.810970128	0.789102316	3.549459219
C	-2.979993343	-0.576965034	1.589148164
C	1.428253293	2.146034718	1.745221853
C	-2.078244925	-0.043483101	-1.394679904
C	0.686617374	1.628447175	-1.331871390
H	-1.308319807	1.705699205	3.889949799
H	-1.364508748	-0.064588733	3.944887877
H	0.199028224	0.762295127	3.959227562
H	-3.119436741	-1.471921206	0.976613939
H	-3.860090971	0.064887635	1.461363912
H	-2.937950850	-0.892404318	2.632920980
H	1.108489156	3.167098045	1.986568451
H	1.845545650	1.682066917	2.639970779
H	2.219283819	2.214809179	0.994360745
H	-1.441360235	-0.065872125	-2.281932354
H	-2.917137861	0.633249700	-1.595428824
H	-2.486637831	-1.045147896	-1.240041256
H	0.457195789	1.050473690	-2.229859829
H	1.760509133	1.550806642	-1.144466758
H	0.457212031	2.680361271	-1.535883307
Rh	0.207483053	-0.801847339	0.827507257
H	3.521377325	-2.926292181	-2.605838537
C	1.545507073	-1.623634577	3.312917948
O	2.121510983	-0.525112987	3.380821466
O	0.744462371	-2.050131321	2.398128271
O	1.729397774	-2.551650047	4.287313461
H	2.344177246	-2.148297310	4.918169498
C	-1.060557246	-3.756985903	-2.046545029
H	-0.563751757	-4.598381042	-2.537814140
H	-1.845274925	-4.129582405	-1.387398362
H	-1.522881746	-3.135365486	-2.823484659
Ag	1.262497663	-2.744548798	-4.035061836
O	0.265123129	-3.580514193	-5.986076832
N	1.774080515	-3.053067446	-7.655537128
N	2.722887516	-1.942245364	-5.759633064
C	0.644653022	-3.662475586	-7.152289391
C	4.645750523	-0.786961615	-7.434304714
C	4.651703835	-0.518372715	-6.061888695
C	3.675462484	-1.630127788	-7.949505329
C	3.678176880	-1.113666773	-5.277276039
C	2.725597858	-2.193774223	-7.077580929
H	5.393122196	0.133542970	-5.613956928
H	3.652593374	-0.941882253	-4.205458164
H	5.385769844	-0.342692614	-8.092424393
H	3.641876698	-1.853693604	-9.011632919
H	1.931709409	-3.217543125	-8.640346527
C	-0.147512913	-4.442887783	-8.180780411
H	-0.788405180	-3.754824877	-8.744023323
H	0.494128734	-4.972822189	-8.891345024
H	-0.783313513	-5.158917904	-7.660652161

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3B

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O	0.857206643	-0.132901117	-0.829178751

N	1.772552133	-2.077911615	-1.707817912
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C	1.056212187	-0.954231024	-1.784992933
C	1.393134236	-3.525101662	1.683486700
C	2.648035765	-4.112166882	1.795862317
C	1.073189974	-2.787793159	0.529890478
C	3.533886433	-3.959190130	0.720211864
C	2.055618525	-2.677040577	-0.495780915
H	2.928672314	-4.709622860	2.656541824
H	4.512972355	-4.435849190	0.752710879
H	0.639590919	-3.651502848	2.455336094
C	1.223578572	0.634632289	3.140156507
C	1.407812357	1.508157492	1.995221615
C	2.273709059	-0.331432819	3.127756596
C	2.637647629	1.115845680	1.330657244
C	3.157565832	-0.034266844	2.000835896
C	0.071597181	0.721359551	4.087469578
C	0.527310371	2.660111666	1.632684946
C	2.508148909	-1.394135714	4.154597282
C	3.193829060	1.781344295	0.112823680
C	4.440946102	-0.739148855	1.693039298
H	0.009257256	1.726662874	4.516629219
H	-0.860149622	0.517995000	3.547934532
H	0.163396746	0.002894914	4.903014183
H	0.609673083	2.898666382	0.570301712
H	0.805478692	3.552066326	2.207589865
H	-0.517017901	2.423727274	1.849282622
H	3.147258759	-0.999846160	4.953586578
H	1.571934700	-1.730158687	4.604938030
H	3.008445740	-2.262318611	3.723525524
H	4.028418541	1.217619300	-0.307095736
H	3.547795773	2.787671089	0.362948030
H	2.420475245	1.869560480	-0.655677974
H	4.647209644	-0.747980416	0.620760858
H	4.413853645	-1.775624275	2.032788038
H	5.274789333	-0.239724189	2.201440334
Rh	1.123742700	-0.470427006	1.221390605
H	0.038408708	-2.554295063	0.268800825
C	-1.778795958	-0.984946012	0.489253759
O	-0.962718129	-0.565685868	1.426951528
O	-1.516149044	-1.689383507	-0.478384644
O	-3.059602022	-0.577681601	0.682607591
H	-3.075912952	-0.037028212	1.485213280
C	0.438965291	-0.570759833	-3.100550413
H	0.588001192	0.494158447	-3.293405771
H	0.817103922	-1.165155292	-3.933550835
H	-0.637068987	-0.747207046	-2.990140676
Ag	2.937183142	-3.077886820	-3.309020281
O	2.888377428	-3.693462849	-5.594515800
N	4.764915943	-5.027409554	-5.835119247
N	5.034512520	-4.205006123	-3.608990908
C	3.572901487	-4.473886013	-6.251993656
C	7.584557056	-5.338693619	-3.513373137
C	7.076895714	-4.651849747	-2.407696009
C	6.806202888	-5.452199936	-4.654622078
C	5.804363728	-4.107853413	-2.503317595
C	5.527136803	-4.867300034	-4.664707661
H	7.653760910	-4.541704178	-1.496318460
H	5.345409393	-3.579549551	-1.672627211
H	8.575348854	-5.782131195	-3.487632990
H	7.175814152	-5.980939865	-5.528007507
H	5.207966805	-5.621422291	-6.522670269
C	3.162696838	-4.884585381	-7.652570724
H	3.341610432	-5.947407246	-7.844019890
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H	3.732274771	-4.303342342	-8.386743546

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3B-TS

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C	0.833602250	-0.040643457	-1.980943441
C	0.812059283	-3.506414175	0.673948467
C	1.307194352	-4.670895576	0.096521623
C	0.778128088	-2.293100357	-0.044363834
C	1.792113185	-4.580165386	-1.212480545
C	1.256571531	-2.336235523	-1.384959579
H	1.315590143	-5.619214535	0.623673797
H	2.206715345	-5.456901550	-1.707768917
H	0.423152864	-3.522441626	1.689771891
C	2.892563820	-1.037558913	2.491576910
C	2.597398520	0.373176724	2.659047365
C	3.545796156	-1.198349118	1.209317327
C	2.987482071	1.061521411	1.467808127
C	3.562890291	0.078374296	0.558813632
C	2.709013462	-2.094086647	3.538508177
C	1.911165595	0.948752284	3.857600927
C	4.144333839	-2.456158876	0.665924430
C	2.818181515	2.511382580	1.136625290
C	4.124910831	0.389525175	-0.794139624
H	3.571979284	-2.122997046	4.215362549
H	1.818830848	-1.895552516	4.141618729
H	2.601023674	-3.083930254	3.089099646
H	1.725879312	2.017753839	3.743119001
H	2.523469687	0.796905398	4.753201962
H	0.947489262	0.454316556	4.015130997
H	5.177160263	-2.550024509	1.025960684
H	3.590785503	-3.338706017	0.992666125
H	4.164951324	-2.444546700	-0.426199615
H	2.305269718	2.619721174	0.174948722
H	3.791601658	3.009431601	1.059331536
H	2.226111650	3.031944990	1.891603231
H	3.491883278	1.113554955	-1.314552903
H	4.218585014	-0.501878500	-1.417684555
H	5.120999813	0.836604893	-0.689564586
Rh	1.476554990	-0.466325581	0.930593669
H	-0.431688547	-1.666851163	0.124417946
C	-1.482467532	-0.422510505	1.292761207
O	-0.403637171	-0.064809069	1.863948226
O	-1.577997327	-1.216208816	0.310738087
O	-2.635673523	0.055470645	1.768804312
H	-2.424718142	0.661445975	2.495577574
C	0.579934299	0.895507395	-3.140908957
H	1.529653430	1.346464992	-3.453813553

H	0.156487271	0.358725786	-3.992374420
H	-0.091785938	1.696052670	-2.827679873
Ag	2.338947296	-2.030164480	-4.041557789
O	4.790680408	-2.408331156	-3.047438860
N	4.797074318	-4.298919678	-4.362482548
N	3.540429831	-2.822010279	-5.760960102
C	5.000647068	-3.607148886	-3.177610159
C	4.663388252	-4.015517712	-8.024419785
C	3.749138594	-2.968928099	-8.159925461
C	5.022439003	-4.434740543	-6.751685619
C	3.220470905	-2.407384396	-7.007546425
C	4.444350719	-3.811621189	-5.635783195
H	3.445370436	-2.601412296	-9.133475304
H	2.498468876	-1.600183845	-7.065551758
H	5.099086761	-4.490935326	-8.897744179
H	5.750847816	-5.227142334	-6.610581875
H	5.136883736	-5.250472546	-4.370292187
C	5.471579552	-4.475328445	-2.026442289
H	5.942237854	-5.412716866	-2.337357283
H	6.176731586	-3.898744583	-1.424781799
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4B

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C	1.340373993	-3.942344666	0.697273314
C	3.320778370	-0.185811594	1.585057378
C	4.704463482	-0.329598218	1.734073639
C	2.539191961	-1.251221418	1.135524988
C	5.280725479	-1.542965770	1.377449870
C	3.192541599	-2.476597071	0.900871217
H	5.325511456	0.488896012	2.083077431
H	6.354731560	-1.696970463	1.407165289
H	2.851967573	0.770062864	1.806500196
C	0.170277670	0.842901826	-0.403152287
C	-1.128478885	0.145520389	-0.391011834
C	1.079237700	0.079071246	-1.202952743
C	-0.977321923	-1.067020893	-1.073235273
C	0.426275939	-1.168751717	-1.508240581
C	0.398889631	2.211767912	0.159277692
C	-2.340696096	0.670335889	0.314564109
C	2.456610441	0.475737572	-1.633928418
C	-1.978069186	-2.166443110	-1.248999953
C	0.982878864	-2.281900406	-2.344661713
H	0.000464775	2.979621410	-0.515419602
H	-0.101249024	2.325488091	1.124847412
H	1.463245273	2.412149191	0.302187145
H	-3.158259630	-0.052925117	0.311454117
H	-2.697383165	1.590617537	-0.162421331
H	-2.105619907	0.909223735	1.357007861
H	2.406384468	1.002170324	-2.594589233
H	2.931242943	1.139728308	-0.908876240
H	3.100333214	-0.397960812	-1.758129358
H	-1.631453753	-3.077148676	-0.746934652
H	-2.120285988	-2.398530722	-2.310262918
H	-2.948391199	-1.900034666	-0.827190816
H	0.436256737	-3.209165335	-2.158064365
H	2.038104773	-2.471448183	-2.133326769
H	0.884992301	-2.044373512	-3.411625385
Rh	0.594986677	-1.049901247	0.629853725
H	0.221029282	-2.875002623	2.663206577
C	0.058758233	-1.278939605	3.680581570
O	0.146277070	-0.485469580	2.723858833
O	0.108783327	-2.575613976	3.622323751
O	-0.109507240	-0.841167152	4.923139572
H	-0.126062870	0.127707392	4.895143032
C	0.833691716	-5.324421883	0.368671566
H	1.639231443	-5.963729382	0.004364096
H	0.387513906	-5.775096893	1.261556983
H	0.036055479	-5.254114151	-0.379748553
Ag	4.941895008	-4.564872742	-0.055022817
O	4.035437584	-4.571817398	-2.498714209
N	3.822726965	-6.854760647	-2.293313265
N	5.769373417	-6.467189789	-0.971391261
C	3.391658545	-5.592442989	-2.687319517
C	6.860342026	-8.882528305	-1.859317899
C	7.569882870	-8.072483063	-0.970068216
C	5.617881775	-8.459344864	-2.308493376
C	6.989515305	-6.880787849	-0.562594831
C	5.100475788	-7.240862846	-1.845031261
H	8.548915863	-8.355110168	-0.600428045
H	7.504111290	-6.221906662	0.128453687
H	7.275263786	-9.822887421	-2.208355904
H	5.052826405	-9.049383163	-3.023308754
H	3.253727913	-7.624070168	-2.620048046
C	2.026797056	-5.595928192	-3.350137472
H	1.942773700	-6.373035431	-4.116825581
H	1.251326799	-5.774721146	-2.597225189
H	1.861327767	-4.620727539	-3.805175066

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5B

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O	0.649319470	-0.490451187	-1.390759945
N	2.744399071	-1.506615281	-1.470389366
N	4.248507500	-2.022285461	0.140923306
C	1.622535348	-1.069463611	-2.005525112
C	2.787332058	-0.933514953	2.221678972
C	3.996517897	-1.565583944	2.479072809
C	2.264305115	-0.836055219	0.915401518
C	4.701180935	-2.085488558	1.388157964
C	3.047634602	-1.429795265	-0.112795651
H	4.391390324	-1.653731108	3.486142397
H	5.664803028	-2.574261427	1.521715403
H	2.226984262	-0.519664466	3.052825689
C	-0.738591671	0.487945944	2.336900711
C	-1.647889733	0.556471586	1.175034404
C	0.240423039	1.504292607	2.190712690
C	-1.208263993	1.582795858	0.321153671
C	0.022110008	2.115133047	0.886543453
C	-0.952657700	-0.403790861	3.519273996
C	-2.823073864	-0.349327862	0.986170948
C	1.252525210	1.966763258	3.192890167

C	-1.762740016	1.976366282	-1.014923573
C	0.812155426	3.245386124	0.312101007
H	-1.735333920	0.010173554	4.167372227
H	-1.272570372	-1.402255535	3.210874557
H	-0.044325534	-0.510357261	4.115464211
H	-3.206389904	-0.309056729	-0.034584954
H	-3.633851290	-0.066795476	1.669319153
H	-2.557627439	-1.387442708	1.207407713
H	0.958557427	2.946273804	3.588295937
H	1.325085282	1.282170773	4.039501667
H	2.245730400	2.067835331	2.748386383
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H	-1.903029323	3.060455084	-1.073763132
H	-2.727091789	1.501691222	-1.203704238
H	0.785561323	3.229218960	-0.779899120
H	1.853923440	3.209783792	0.637356281
H	0.385955125	4.201509476	0.644665301
Rh	0.497856677	0.047206718	0.548226178
C	1.403303862	-1.250330210	-3.487917185
H	2.271677732	-1.689265609	-3.980228901
H	0.533175707	-1.895758748	-3.646353722
H	1.175656676	-0.281640619	-3.942881823
Ag	4.485869884	-2.702180862	-2.356071472
O	5.006811619	-4.284310818	-4.066752434
N	7.039455891	-5.158841610	-3.392832994
N	6.854980469	-3.222377300	-2.018981457
C	5.853319168	-5.173676491	-4.095146656
C	9.529398918	-3.500586033	-1.266882777
C	8.754226685	-2.460664272	-0.744243681
C	8.952129364	-4.389232635	-2.161655188
C	7.429831505	-2.366433859	-1.149018884
C	7.602383137	-4.215018749	-2.513536930
H	9.165131569	-1.744811654	-0.041166484
H	6.774353981	-1.593361259	-0.759440660
H	10.570527077	-3.615338802	-0.981503785
H	9.529193878	-5.205726147	-2.585518122
H	7.638532162	-5.954006195	-3.568762779
C	5.670975685	-6.410089970	-4.956364632
H	6.414133072	-6.429528236	-5.761342049
H	5.785007477	-7.325748920	-4.365880489
H	4.673836708	-6.385132313	-5.393896580

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6B

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N	3.793459892	-2.647547722	-1.128346324
C	0.271258563	-2.487068176	-1.081436157
C	3.814595938	-0.412815481	0.478601038
C	5.020288944	-0.998492479	0.087049514
C	2.580435038	-0.930887222	0.072304547
C	4.952386856	-2.122667074	-0.727989137
C	2.622571230	-2.085783243	-0.742288768
H	5.976803780	-0.596221805	0.405484855
H	5.852699280	-2.626428366	-1.072892427
H	3.840616465	0.460942298	1.122587919
C	1.065332174	2.184487581	1.142077923
C	-0.382597059	1.947020531	1.111467123
C	1.566147804	2.033295155	-0.190434799
C	-0.728250623	1.535490751	-0.188189417
C	0.496185124	1.508520126	-0.992270112
C	1.810014606	2.727744579	2.323862314
C	-1.299738169	2.155085087	2.274600744
C	2.924469471	2.400979996	-0.701490581
C	-2.067843914	1.113388300	-0.703256130
C	0.548641205	1.179883718	-2.452477932
H	1.640948653	3.806852579	2.427174568
H	1.477614999	2.250277281	3.249490738
H	2.886759996	2.567508698	2.228638649
H	-2.246209383	1.628142118	2.145313978
H	-1.513345599	3.223987341	2.396705866
H	-0.848685741	1.798263311	3.203403473
H	2.853200436	3.339109182	-1.265244603
H	3.641958714	2.556238890	0.105931483
H	3.326904058	1.636619091	-1.369627833
H	-1.998246551	0.109587602	-1.135629773
H	-2.413783789	1.796804070	-1.487245560
H	-2.817673683	1.087768197	0.088806093
H	-0.105221048	0.333813161	-2.678654909
H	1.562018871	0.917032957	-2.763834476
H	0.216217667	2.033210516	-3.056164265
Rh	0.837625325	0.019663999	0.578499079
C	-1.387945175	-1.122969508	2.761653900
C	-1.838442922	-0.831752241	4.064285278
C	-2.320211887	-1.488055348	1.775142312
H	-1.117993116	-0.546706319	4.824915886
H	-1.965617895	-1.703548074	0.775653601
C	-3.195161343	-0.902171135	4.368873119
C	-3.675482988	-1.549811840	2.090057135
H	-3.532582998	-0.673648775	5.375414848
H	-4.390634537	-1.828539968	1.321139097
C	-4.118521690	-1.256921291	3.382299423
H	-5.177108765	-1.304936051	3.619991541
C	1.251023293	-0.988823175	2.670408487
C	0.024585046	-1.021294594	2.501476288
C	2.566620350	-1.213848233	3.279822826
H	2.429852724	-1.609603405	4.291608810
H	3.154735565	-1.927411199	2.697607994
H	3.141778708	-0.285143584	3.345461607
C	-0.795055509	-3.362323523	-1.703998327
H	-1.553318143	-2.727347136	-2.170746326
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H	-1.292720914	-3.928837061	-0.907931924
Ag	2.453839540	-4.498725891	-2.411494970
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N	1.706646204	-7.763562679	-3.452021599
N	3.528527260	-6.229672432	-3.472616434
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H	5.798480988	-8.944555283	-5.060482979
H	3.406739473	-9.422728539	-4.560891151
H	1.521559238	-8.752709389	-3.359213829
C	-0.720928192	-7.644610882	-3.221497774
H	-0.734434545	-8.698950768	-3.513249874
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6B-TS

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O	-0.273803353	-1.028334856	-1.188053131
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C	0.264388651	-2.001660347	-1.814434171
C	3.655699492	-0.226435885	0.408741146
C	4.869988441	-0.409188092	-0.247962698
C	2.469402075	-0.789463401	-0.089075513
C	4.865310192	-1.203110695	-1.393694282
C	2.572149038	-1.587888122	-1.260676146
H	5.790778637	0.026738176	0.125953287
H	5.781723976	-1.401322246	-1.946461558
H	3.618384600	0.339015186	1.335434079
C	0.943826556	2.120886087	1.380048633
C	-0.466642976	1.795553327	1.464503765
C	1.263913155	2.411053896	-0.009261081
C	-0.965742946	1.729292274	0.135955155
C	0.117870994	2.122017860	-0.778912425
C	1.837650180	2.388779402	2.553816795
C	-1.238124132	1.559508562	2.726405144
C	2.583558798	2.916380405	-0.504283726
C	-2.352725029	1.387282491	-0.311891794
C	-0.042637445	2.189782381	-2.265713453
H	1.653721094	3.394378662	2.952840567
H	1.660902739	1.674755335	3.362174034
H	2.893102169	2.338272333	2.276101351
H	-2.078192472	0.882075369	2.561679602
H	-1.632589459	2.507446289	3.111514330
H	-0.608274281	1.118824482	3.502635241
H	2.685140133	3.987426758	-0.291834712
H	3.419882774	2.403512716	-0.022493180
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H	-2.315491676	0.683175862	-1.148802757
H	-2.887687445	2.284831762	-0.645033777
H	-2.926604271	0.923437059	0.492009312
H	-0.482016653	1.259202838	-2.638964891
H	0.913127303	2.342302561	-2.771052599
H	-0.711764634	3.011725187	-2.546547651
Rh	0.630668044	0.194207236	0.304699719
C	-0.984246492	-1.802820563	2.142638445
C	-1.051369786	-2.063477039	3.521288633
C	-2.156098366	-1.868224263	1.367024779
H	-0.148689345	-2.001625299	4.122117996
H	-2.089639187	-1.653156400	0.305653632
C	-2.272066355	-2.387857676	4.111491203
C	-3.368993521	-2.202608347	1.963300943
H	-2.318386316	-2.583497524	5.178725243
H	-4.268936634	-2.260476828	1.357508540
C	-3.431415796	-2.459151030	3.336228132
H	-4.380136013	-2.712728739	3.799744368
C	1.510459065	-1.750271082	1.392602205
C	0.273144037	-1.448620439	1.514517665
C	2.579775095	-2.636667967	1.918023229
H	2.119383335	-3.337962627	2.623200417
H	3.068855047	-3.199084759	1.117077351
H	3.350423336	-2.067893028	2.447679758
C	-0.704317212	-2.860996723	-2.596310616
H	-0.221588224	-3.734715700	-3.036621094
H	-1.508823276	-3.187206030	-1.930650592
H	-1.160108685	-2.259981632	-3.390316963
Ag	2.670158863	-3.605998993	-3.382407904
N	4.717419624	-3.263586760	-4.806235790
O	3.048652172	-5.643108368	-4.468032837
N	5.202991009	-5.538772583	-5.308874607
C	4.051569939	-6.187330246	-4.929854870
C	7.180743217	-2.502977848	-5.888467789
C	6.309832573	-1.540966868	-5.368903637
C	6.802977562	-3.836994648	-5.863217831
C	5.100792885	-1.971920848	-4.839674950
C	5.552874565	-4.174403191	-5.314327240
H	6.563151360	-0.486552358	-5.371140480
H	4.401419163	-1.271532893	-4.395342350
H	8.140813828	-2.216936111	-6.307022572
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C	4.088439941	-7.692804337	-5.100977421
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7B

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C	3.202876329	-0.172836348	0.911422610
C	4.145703793	0.562670171	0.207017004
C	2.268991947	-0.982713342	0.231563911
C	4.140426159	0.453138024	-1.187988520
C	2.325603962	-0.978541851	-1.195603013
H	4.881713867	1.179315686	0.712125242
H	4.884421825	0.981778085	-1.781670332
H	3.174188614	-0.157050207	1.997082472
C	0.565138459	2.332682133	1.341950178
C	-0.726403534	1.815398812	1.671200871
C	0.552477837	2.764526844	-0.068454914
C	-1.469544888	1.743651867	0.433598459
C	-0.683313549	2.412345886	-0.618400693
C	1.675054908	2.639789343	2.300127506
C	-1.234965801	1.430947185	3.024952412
C	1.715666771	3.412708998	-0.752739131
C	-2.886187077	1.295067430	0.267654151
C	-1.157569408	2.555188179	-2.031491756
H	1.584085941	3.670010090	2.667079926

H	1.654860020	1.972534776	3.164613008
H	2.650191307	2.545853376	1.816279888
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H	-1.790673494	2.267906189	3.465471506
H	-0.417621464	1.174142599	3.702237129
H	1.914688468	4.402347565	-0.324075222
H	2.625529289	2.815148830	-0.631541431
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H	-3.566254377	2.153614283	0.338952154
H	-3.165354729	0.570216894	1.033572316
H	-1.424499631	1.574214697	-2.439292669
H	-0.392274112	2.992725372	-2.675557375
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C	-0.991266608	-1.833310246	1.964018106
C	-0.936021984	-2.161449432	3.329280615
C	-2.208617687	-1.997548819	1.275674462
H	-0.001538089	-2.029705048	3.867659330
H	-2.246701241	-1.738212705	0.221724540
C	-2.067426205	-2.644268990	3.987930059
C	-3.334157705	-2.484601736	1.935837150
H	-2.011119127	-2.892677307	5.044016361
H	-4.265472889	-2.614778996	1.391146779
C	-3.268605471	-2.806526661	3.295212030
H	-4.148365498	-3.181505203	3.809912443
C	1.352378130	-1.895657539	1.003395200
C	0.177695468	-1.312326670	1.258882284
C	1.817143202	-3.287427425	1.344043016
H	1.030755997	-3.836605072	1.867288470
H	2.079077244	-3.836336374	0.430234313
H	2.711243629	-3.270973921	1.980126739
C	-0.662654638	-2.663371801	-2.738278389
H	-0.064798482	-3.439155817	-3.220551968
H	-1.373268127	-3.133629560	-2.051302910
H	-1.244885445	-2.127314329	-3.493924856
Ag	2.547547579	-2.656156063	-3.697752476
N	4.338361263	-2.411286354	-5.188570976
O	2.261810541	-4.533508301	-5.171664238
N	4.124825001	-4.379638195	-6.534179211
C	2.971590996	-4.978538513	-6.068788052
C	6.628639698	-1.704307675	-6.620778561
C	6.159852028	-0.882552743	-5.592147827
C	5.940859795	-2.868463755	-6.922149181
C	5.019485950	-1.275480151	-4.910149574
C	4.789221287	-3.191924810	-6.181878567
H	6.666621208	0.038024981	-5.326072693
H	4.610819817	-0.680263340	-4.097879410
H	7.519886971	-1.440922618	-7.181858540
H	6.281591415	-3.524367332	-7.717879772
H	4.582989216	-4.883466721	-7.280421734
C	2.637016773	-6.296824932	-6.738308430
H	3.062307835	-6.403319836	-7.739941597
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H	1.551267385	-6.388276577	-6.793260574

Frequencies

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9-TS

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1194.74 1217.26 1218.19 1249.42 1297.28 1330.35
1332.49 1342.72 1363.06 1375.99 1381.72 1398.63
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3A-TS

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5A

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6A-TS

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7A
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7A'
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7A-TS
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8A
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3213.86 3218.86 3222.74

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8A-TS

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218.21 222.39 246.89 264.81 275.37 290.11
302.30 306.61 313.68 314.82 334.85 381.74
396.17 412.06 417.26 422.32 429.64 444.81
491.11 521.14 525.71 534.31 560.86 565.28
568.21 582.97 587.66 587.96 603.10 614.21
615.82 628.72 659.27 691.12 698.43 756.50
781.77 805.75 808.68 811.16 820.49 832.35
844.58 856.73 958.12 961.62 965.38 967.68
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1100.90 1119.99 1128.61 1159.38 1171.97 1175.17
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1437.14 1439.51 1447.88 1458.21 1461.09 1471.33
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9A

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173.49 175.61 182.79 192.87 201.15 219.73
227.87 240.11 251.05 264.92 280.59 288.82
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488.50 496.34 535.12 545.57 559.70 563.17
572.30 578.25 587.40 596.69 607.81 611.95
627.44 651.10 673.88 701.49 719.49 764.90
772.87 806.88 811.32 812.24 813.16 840.09
870.18 951.27 955.53 955.92 963.74 976.87
990.72 993.88 995.55 1016.27 1020.47 1034.27
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1062.94 1067.11 1071.58 1096.42 1100.03 1103.61
1114.78 1130.11 1132.94 1152.06 1162.07 1175.54
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3215.74 3225.61 3276.56

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1B

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613.26 625.57 634.00 645.70 660.68 697.53
703.65 710.17 752.40 757.89 794.58 796.51
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3B

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3227.16 3622.46 3808.56

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3B-TS

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4B

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5B

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407.68 418.79 422.16 440.84 464.14 478.59
526.37 526.95 537.84 546.08 564.71 566.35

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640.61 644.41 668.79 696.77 721.17 751.61
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6B

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5.43 9.62 15.91 21.24 23.99 27.53
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150.31 152.38 156.58 158.32 163.97 166.24
168.72 175.92 179.02 180.64 187.33 192.72
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472.83 511.33 526.92 533.36 538.09 557.62
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757.11 782.54 794.22 798.36 809.08 812.60
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1014.50 1014.91 1036.38 1036.82 1045.86 1047.10
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7B

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