

# Potential of N-Heterocyclic Carbene Derivatives from $\text{Au}_{13}(\text{dppe})_5\text{Cl}_2$ Gold Superatoms. Evaluation of Electronic, Optical and Chiroptical Properties from Relativistic DFT

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Table S1. HOMO-LUMO gap calculated at both GGA-PBE and hybrid-PBE0 level (frozen electron TZ2P quality basis sets). Values in eV. Page 2.

Table S2. Structural parameters obtained for  $[\text{Au}_{13}\text{Cl}_2(\text{L})_5]^{3+}$  involving different ligands (L) along the 1-7 series at the  $T_1$  excited state. Page 2.

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Figure S2. Far infrared region for optical absorption spectrum. Note, only clusters 5 and 6 shows peaks within this region. For numbering see full text. Page 4.

Figure S3. Far infrared region for circular dichroism spectrum. Note, only clusters 5 and 6 shows peaks within this region. For numbering see full text. Page 4.

Figure S4. Structural rearrangement in 7, from  $\sim D_{5h}/\sim D_{5d}$   $\text{Au}_{13}\text{Cl}_2$  core transformation at the excited state. Page 5.

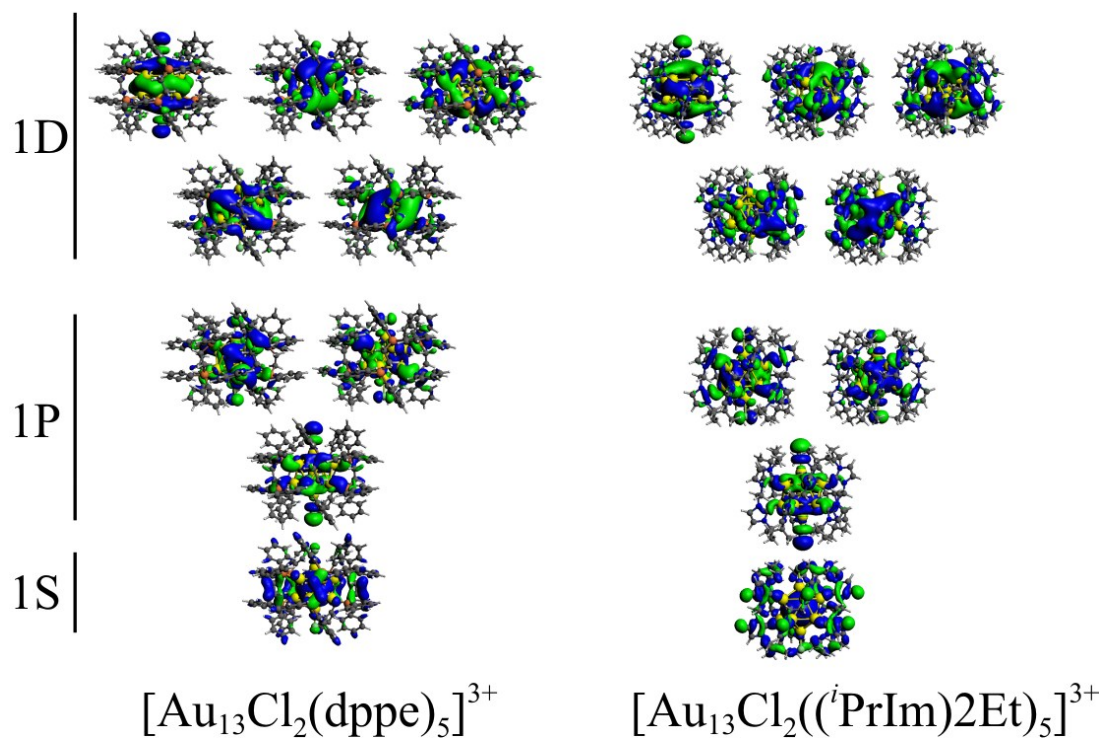
Table S3. Coordinates in Angstrom for optimized structures in multiple Xmol format. Page 6.

**Table S1. HOMO-LUMO gap calculated at both GGA-PBE and hybrid-PBE0 level (frozen electron TZ2P quality basis sets). Values in eV.**

	<b>GGA PBE</b>	<b>hybrid PBE0</b>
<b>1</b>	1.875	3.235
<b>2</b>	1.901	3.494
<b>3</b>	1.908	3.392
<b>4</b>	1.731	3.383
<b>5</b>	1.757	3.114
<b>6</b>	0.380	2.462
<b>7</b>	1.541	3.023

**Table S2. Structural parameters obtained for  $[\text{Au}_{13}\text{Cl}_2(\text{L})_5]^{3+}$  involving different ligands (L) along the 1-7 series at the  $T_1$  excited state.**

	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>	<b>7</b>
Au-Au	2.697	2.711	2.752	2.675	2.623	2.728	2.758
Au-Au(L)	2.718	2.682	2.790	2.666	2.700	2.740	2.775
Au- Au(Cl)	2.592	2.855	2.561	2.721	2.648	2.666	2.672
Au(Cl)- Au(Cl)	5.184	5.711	5.123	5.443	5.295	5.343	5.342
Au-L	2.292	1.945	2.044	1.972	1.957	1.919	1.959
Au-Cl	2.261	2.302	2.271	2.273	2.238	2.169	2.248



**Figure S1.** Comparison of isosurfaces related to superatomic shells.

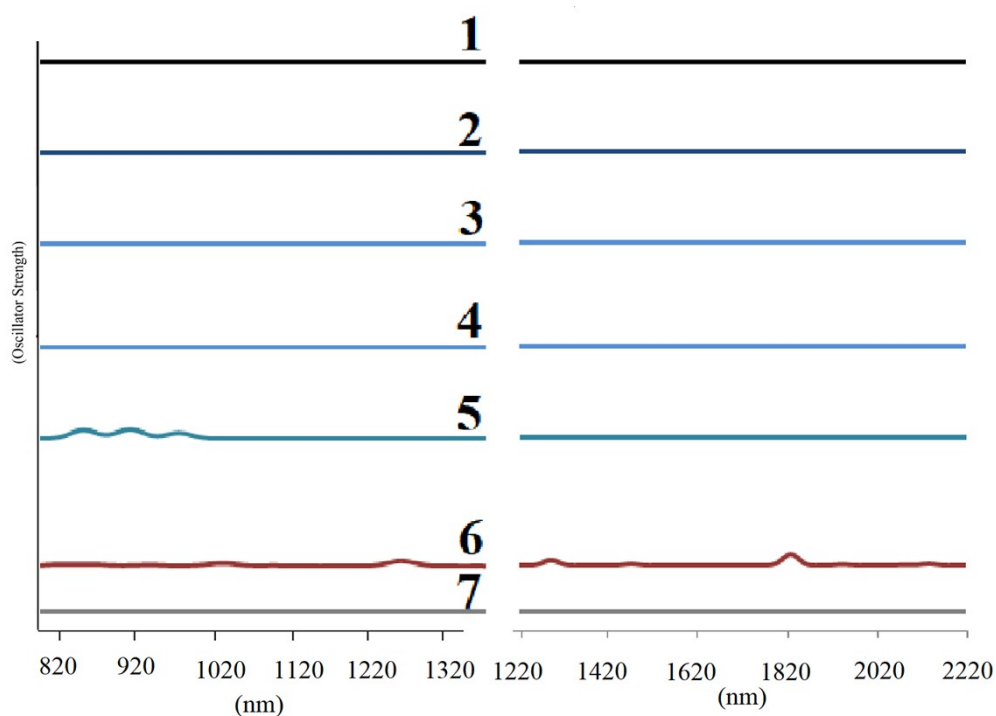


Figure S2. Far infrared region for optical absorption spectrum. Note, only clusters 5 and 6 shows peaks within this region. For numbering see full text.

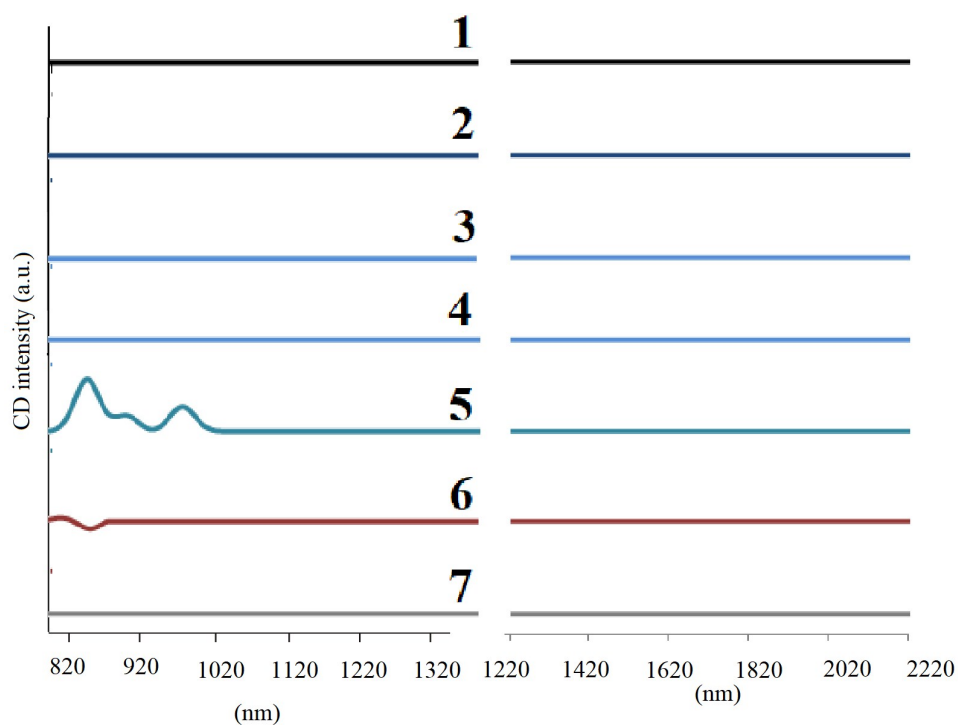


Figure S3. Far infrared region for circular dichroism spectrum. Note, only clusters 5 and 6 shows peaks within this region. For numbering see full text. Values between  $\pm 500 \times 10^{-40} \text{esu}^2 \text{cm}^2$ .

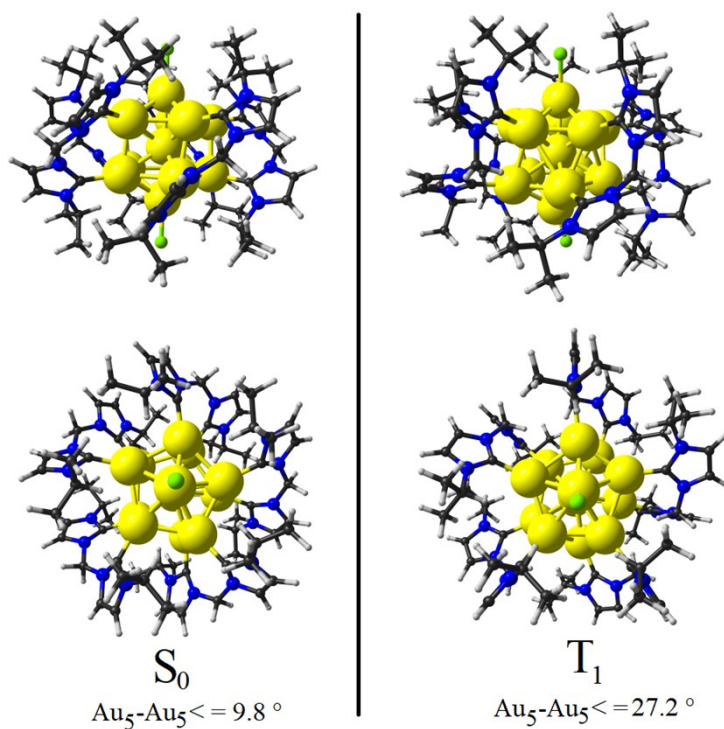


Figure S4. Structural rearrangement in **7**, from  $\sim D_{5h}/\sim D_{5d}$   $Au_{13}Cl_2$  core transformation at the excited state, denoting the twist of each  $Au_5$  rings of  $9.8^\circ$  to  $27.2^\circ$  from ground state ( $S_0$ ) to the first excited triplet-state ( $T_1$ ).

Table S3. Coordinates in Angstrom for optimized structures in multiple Xmol format.

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1 dppe S0 Ground State

Au	0.0000	0.0000	-2.5480
Au	-1.3845	1.9244	1.1549
Au	1.4024	1.9114	1.1549
Au	-0.0111	2.3707	-1.1549
Au	-0.0111	-2.3707	1.1549
Au	0.0000	0.0000	0.0000
Au	-1.3845	-1.9244	-1.1549
Au	2.2512	0.7431	-1.1549
Au	2.2512	-0.7431	1.1549
Au	-2.2581	0.7220	-1.1549
Au	-2.2581	-0.7220	1.1549
Au	1.4024	-1.9114	-1.1549
Au	0.0000	0.0000	2.5480
P	-1.9552	-3.9264	-1.8186
P	3.1301	3.0729	1.8186
P	-0.7261	4.3258	-1.8186
P	3.1301	-3.0729	-1.8186
P	3.8897	-2.0273	1.8186
P	-0.7261	-4.3258	1.8186
Cl	0.0000	0.0000	-4.7488
Cl	0.0000	0.0000	4.7488
P	-4.3384	0.6462	-1.8186
P	-4.3384	-0.6462	1.8186
P	3.8897	2.0273	-1.8186
P	-1.9552	3.9264	1.8186
C	3.0796	4.7853	1.9045
C	-3.5995	4.4076	1.9045
C	-4.7444	3.2099	-2.2453
C	-6.6012	2.0166	-1.6407
C	-4.7444	-3.2099	2.2453
C	-1.6415	-3.0201	3.9059
C	-6.7660	-4.2536	2.0545
C	-2.3929	-5.1746	3.6925
C	-3.3796	0.6279	3.9059
C	-6.7660	4.2536	-2.0545
C	-1.6415	3.0201	-3.9059
C	4.1552	5.5116	1.6407
C	-6.6012	-2.0166	1.6407
C	5.5027	1.4501	-1.9045
C	1.9516	5.3855	2.2453
C	-5.3042	2.0613	-1.9045
C	-5.4763	-4.3009	2.3186
C	5.7250	-0.1919	2.2453
C	-1.9037	-4.8331	0.6504
C	-0.4472	3.4082	3.9059
C	-3.9578	5.6550	1.6407
C	4.9775	-2.7798	-3.6925
C	2.9736	7.4182	2.0545
C	-2.3929	5.1746	-3.6925
C	-5.7348	1.4695	4.7390
C	4.0083	-3.3040	0.6504
C	-5.3042	-2.0613	1.9045
C	-4.4776	0.2663	3.2638
C	4.1009	6.8233	1.7180
C	1.9025	6.6984	2.3186
C	-5.6608	0.6768	3.6925
C	-1.1304	-4.3408	-3.2638
C	3.4659	2.8474	-3.2638
C	-0.4472	-3.4082	-3.9059
C	3.7790	2.4164	3.2638
C	-1.9037	4.8331	-0.6504
C	-5.4763	4.3009	-2.3186
C	-1.3007	5.0290	0.6504

C	4.0083	3.3040	-0.6504
C	5.7250	0.1919	-2.2453
C	-5.1848	-0.3170	-0.6504
C	3.7790	-2.4164	-3.2638
C	3.1032	1.4785	3.9059
C	-1.3007	-5.0290	-0.6504
C	-0.3745	5.9082	4.7390
C	-3.1697	-5.0000	4.7390
C	-1.6370	-4.1762	3.2638
C	5.5027	-1.4501	1.9045
C	-1.1304	4.3408	3.2638
C	-7.3283	-3.1098	1.7180
C	0.2801	3.7276	4.9545
C	-3.4586	1.4183	4.9545
C	-3.1697	5.0000	-4.7390
C	4.1819	-3.8748	3.6925
C	3.1032	-1.4785	-3.9059
C	-5.1848	0.3170	0.6504
C	4.3809	2.7911	0.6504
C	3.4659	-2.8474	3.2638
C	4.9775	2.7798	3.6925
C	4.1819	3.8748	-3.6925
C	1.5866	-5.5041	2.2453
C	-1.6370	4.1762	-3.2638
C	5.5033	-2.1819	-4.7390
C	6.9584	0.2606	2.3186
C	-4.5189	3.5203	2.2453
C	5.5033	2.1819	4.7390
C	4.8347	-1.2310	-5.3645
C	-4.6349	1.8459	5.3645
C	4.8347	1.2310	5.3645
C	-3.1878	-3.8377	5.3645
C	6.9584	-0.2606	-2.3186
C	-3.1878	3.8377	-5.3645
C	1.9546	-7.7493	2.0545
C	7.7566	-1.7916	1.7180
C	3.7757	-4.5597	4.7390
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C	3.7757	4.5597	-4.7390
C	7.9740	0.5357	-2.0545
C	1.9644	3.1804	-4.9545
C	7.9740	-0.5357	2.0545
C	0.3213	-5.6815	1.9045
C	6.5258	-2.2486	1.6407
C	7.7566	1.7916	-1.7180
C	4.1009	-6.8233	-1.7180
C	-4.4776	-0.2663	-3.2638
C	-6.1362	-5.1204	-2.0545
C	-3.3796	-0.6279	-3.9059
C	-5.7348	-1.4695	-4.7390
C	-3.9578	-5.6550	-1.6407
C	1.9025	-6.6984	-2.3186
C	-5.2221	-6.0087	-1.7180
C	-4.5189	-3.5203	-2.2453
C	1.9516	-5.3855	-2.2453
C	3.0796	-4.7853	-1.9045
C	2.9736	-7.4182	-2.0545
C	4.1552	-5.5116	-1.6407
C	-3.4586	-1.4183	-4.9545
C	-5.6608	-0.6768	-3.6925
C	0.6930	-7.9306	1.7180
C	-3.5995	-4.4076	-1.9045
C	-5.7826	-3.8792	-2.3186
C	6.5258	2.2486	-1.6407
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C	3.6317	0.8855	4.9545

C	-4.6349	-1.8459	-5.3645
C	1.5866	5.5041	-2.2453
C	0.6930	7.9306	-1.7180
C	-0.1220	6.9013	-1.6407
C	-0.1220	-6.9013	1.6407
C	2.3651	-2.4944	3.9059
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C	4.3809	-2.7911	-0.6504
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C	2.3981	-6.5373	2.3186
C	-5.7826	3.8792	2.3186
C	-6.1362	5.1204	2.0545
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H	-0.4802	2.4167	3.5796
H	-1.6704	6.3252	3.2125
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H	1.0134	7.1612	2.5975
H	2.9343	8.4553	2.1174
H	4.9503	7.3883	1.5177
H	5.0517	5.0569	1.3704
H	2.5960	8.5652	-2.1174
H	3.3894	6.3892	-2.5975
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H	-1.1145	7.0604	-1.3704
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H	6.3705	3.2417	-1.3704
H	8.5565	2.4249	-1.5177
H	8.9482	0.1779	-2.1174
H	7.1239	-1.2491	-2.5975
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H	5.0693	-4.1353	3.2125
H	-1.0320	-2.2374	3.5796
H	-2.4146	-1.9353	5.4491
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H	-6.6618	1.7948	5.0785



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H	1.9357	-4.5454	2.4689
H	5.0517	-5.0569	-1.3704
H	4.9503	-7.3883	-1.5177
H	2.9343	-8.4553	-2.1174
H	1.0134	-7.1612	-2.5975
H	1.1057	-4.8151	-2.4689
H	-0.4802	-2.4167	-3.5796
H	0.8159	-2.9850	-5.4491
H	0.9016	-5.2353	-6.1892
H	-0.3516	-6.8904	-5.0785
H	-1.6704	-6.3252	-3.2125
H	2.1500	-1.2035	-3.5796
H	3.0910	-0.1465	-5.4491
H	5.2577	-0.7603	-6.1892
H	6.4445	-2.4636	-5.0785
H	5.4994	-3.5433	-3.2125
H	5.0693	4.1353	-3.2125
H	1.8090	1.6729	-3.5796
H	1.0945	2.8944	-5.4491
H	2.3478	4.7654	-6.1892
H	4.3345	5.3677	-5.0785
H	3.0735	-3.7888	0.6404
H	4.6871	-4.0225	1.0010
H	4.5531	-1.7523	-0.6404
H	5.2740	-3.2147	-1.0010
H	-1.4276	-6.0092	-1.0010
H	-2.6536	-4.0939	0.6404
H	-6.1563	-0.4992	-1.0010
H	-4.7135	1.2586	0.6404
H	-2.6536	4.0939	-0.6404
H	-1.4276	6.0092	1.0010
H	3.0735	3.7888	-0.6404
H	4.5531	1.7523	0.6404

H	4.6871	4.0225	-1.0010
H	5.2740	3.2147	1.0010
H	-0.2595	-4.8718	-0.6404
H	-2.3772	-5.7007	1.0010
H	-4.7135	-1.2586	-0.6404
H	-6.1563	0.4992	1.0010
H	-2.3772	5.7007	-1.0010
H	-0.2595	4.8718	0.6404

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2 NHC S0 Ground State

Au	-1.4874	1.9095	1.2098
Au	0.0810	2.4191	-1.2098
N	0.4211	4.6971	-3.0759
N	-0.4276	5.2818	-1.2989
C	0.0558	4.2463	-1.9202
C	0.1554	5.9836	-3.1821
H	0.3745	6.5339	-4.0223
C	-0.3802	6.3533	-2.0654
H	-0.7069	7.2775	-1.7544
C	1.0628	3.9241	-4.0695
H	1.1879	2.9928	-3.6180
C	0.2181	3.7722	-5.2364
H	0.6902	3.1500	-5.9260
H	0.0323	4.6881	-5.6997
H	-0.6867	3.3261	-4.9808
C	2.3583	4.4958	-4.3888
H	2.9546	4.5877	-3.5399
H	2.2636	5.4351	-4.8311
H	2.8499	3.8813	-5.0706
C	-0.9338	5.2371	-0.0084
N	-2.7586	4.5244	1.2989
N	-3.1016	3.5525	3.0759
C	-2.5411	3.4025	1.9202
C	-3.4268	5.3634	2.0654
H	-3.7057	6.3031	1.7544
C	-3.6428	4.7495	3.1821
H	-4.1435	5.0659	4.0223
C	-2.3228	4.7858	0.0084
C	-3.1664	2.5500	4.0695
H	-2.7201	1.7230	3.6180
C	-2.3937	2.9236	5.2364
H	-2.7817	3.7738	5.6997
H	-1.3995	3.0945	4.9808
H	-2.4099	2.1427	5.9260
C	-4.5505	2.2510	4.3888
H	-4.5870	1.4649	5.0706
H	-5.0869	1.9749	3.5399
H	-5.0260	3.0666	4.8311
H	-0.8410	6.1844	0.4136
H	-0.3559	4.5632	0.5368
H	-2.9548	5.4976	-0.4136
H	-2.3942	3.9009	-0.5368
Au	2.3257	-0.6705	1.2098
Au	1.3564	-2.0046	-1.2098
N	2.4202	-4.0476	-3.0759
N	3.4505	-4.0217	-1.2989
C	2.4508	-3.4682	-1.9202
C	3.3914	-4.9322	-3.1821
H	3.5376	-5.5062	-4.0223
C	4.0420	-4.9165	-2.0654
H	4.8495	-5.4721	-1.7544
C	1.4467	-3.7994	-4.0695
H	0.7981	-3.1194	-3.6180
C	2.0408	-3.1800	-5.2364
H	1.2931	-2.9541	-5.9260
H	2.7295	-3.8117	-5.6997
H	2.5106	-2.2872	-4.9808
C	0.7347	-5.0233	-4.3888

H	0.3063	-5.4482	-3.5399
H	1.3634	-5.7276	-4.8311
H	-0.0242	-4.8152	-5.0706
C	3.8338	-3.6880	-0.0084
N	4.8911	-2.0389	1.2989
N	4.5973	-1.0510	3.0759
C	4.0558	-1.2591	1.9202
C	5.9249	-2.3248	2.0654
H	6.7029	-2.9212	1.7544
C	5.7388	-1.7013	3.1821
H	6.3299	-1.6629	4.0223
C	4.6922	-2.5065	0.0084
C	4.0605	-0.2018	4.0695
H	3.2134	0.2049	3.6180
C	3.6550	-0.9583	5.2364
H	4.4687	-1.4180	5.6997
H	2.9511	-1.6810	4.9808
H	3.2091	-0.3170	5.9260
C	5.0045	0.8536	4.3888
H	4.5720	1.5110	5.0706
H	5.2762	1.3923	3.5399
H	5.8686	0.4733	4.8311
H	4.3155	-4.5090	0.4136
H	2.9701	-3.4825	0.5368
H	5.6219	-2.7109	-0.4136
H	4.2298	-1.7486	-0.5368
Au	1.3564	2.0046	1.2098
Au	2.3257	0.6705	-1.2098
N	4.5973	1.0510	-3.0759
N	4.8911	2.0389	-1.2989
C	4.0558	1.2591	-1.9202
C	5.7388	1.7013	-3.1821
H	6.3299	1.6629	-4.0223
C	5.9249	2.3248	-2.0654
H	6.7029	2.9212	-1.7544
C	4.0605	0.2018	-4.0695
H	3.2134	-0.2049	-3.6180
C	3.6550	0.9583	-5.2364
H	3.2091	0.3170	-5.9260
H	4.4687	1.4180	-5.6997
H	2.9511	1.6810	-4.9808
C	5.0045	-0.8536	-4.3888
H	5.2762	-1.3923	-3.5399
H	5.8686	-0.4733	-4.8311
H	4.5720	-1.5110	-5.0706
C	4.6922	2.5065	-0.0084
N	3.4505	4.0217	1.2989
N	2.4202	4.0476	3.0759
C	2.4508	3.4682	1.9202
C	4.0420	4.9165	2.0654
H	4.8495	5.4721	1.7544
C	3.3914	4.9322	3.1821
H	3.5376	5.5062	4.0223
C	3.8338	3.6880	0.0084
C	1.4467	3.7994	4.0695
H	0.7981	3.1194	3.6180
C	2.0408	3.1800	5.2364
H	2.7295	3.8117	5.6997
H	2.5106	2.2872	4.9808
H	1.2931	2.9541	5.9260
C	0.7347	5.0233	4.3888
H	-0.0242	4.8152	5.0706
H	0.3063	5.4482	3.5399
H	1.3634	5.7276	4.8311
H	5.6219	2.7109	0.4136
H	4.2298	1.7486	0.5368
H	4.3155	4.5090	-0.4136
H	2.9701	3.4825	-0.5368

Au	0.0810	-2.4191	1.2098
Au	-1.4874	-1.9095	-1.2098
N	-3.1016	-3.5525	-3.0759
N	-2.7586	-4.5244	-1.2989
C	-2.5411	-3.4025	-1.9202
C	-3.6428	-4.7495	-3.1821
H	-4.1435	-5.0659	-4.0223
C	-3.4268	-5.3634	-2.0654
H	-3.7057	-6.3031	-1.7544
C	-3.1664	-2.5500	-4.0695
H	-2.7201	-1.7230	-3.6180
C	-2.3937	-2.9236	-5.2364
H	-2.4099	-2.1427	-5.9260
H	-2.7817	-3.7738	-5.6997
H	-1.3995	-3.0945	-4.9808
C	-4.5505	-2.2510	-4.3888
H	-5.0869	-1.9749	-3.5399
H	-5.0260	-3.0666	-4.8311
H	-4.5870	-1.4649	-5.0706
C	-2.3228	-4.7858	-0.0084
N	-0.4276	-5.2818	1.2989
N	0.4211	-4.6971	3.0759
C	0.0558	-4.2463	1.9202
C	-0.3802	-6.3533	2.0654
H	-0.7069	-7.2775	1.7544
C	0.1554	-5.9836	3.1821
H	0.3745	-6.5339	4.0223
C	-0.9338	-5.2371	0.0084
C	1.0628	-3.9241	4.0695
H	1.1879	-2.9928	3.6180
C	0.2181	-3.7722	5.2364
H	0.0323	-4.6881	5.6997
H	-0.6867	-3.3261	4.9808
H	0.6902	-3.1500	5.9260
C	2.3583	-4.4958	4.3888
H	2.8499	-3.8813	5.0706
H	2.9546	-4.5877	3.5399
H	2.2636	-5.4351	4.8311
H	-2.9548	-5.4976	0.4136
H	-2.3942	-3.9009	0.5368
H	-0.8410	-6.1844	-0.4136
H	-0.3559	-4.5632	-0.5368
Au	0.0000	0.0000	-2.6495
Au	-2.2756	-0.8245	1.2098
Au	-2.2756	0.8245	-1.2098
Au	0.0000	0.0000	0.0000
Au	0.0000	0.0000	2.6495
Cl	0.0000	0.0000	-4.8989
Cl	0.0000	0.0000	4.8989
N	-4.3371	1.8520	-3.0759
N	-5.1554	1.2254	-1.2989
C	-4.0213	1.3653	-1.9202
C	-5.6428	1.9968	-3.1821
H	-6.0984	2.3753	-4.0223
C	-6.1599	1.6017	-2.0654
H	-7.1398	1.5765	-1.7544
C	-3.4036	2.2234	-4.0695
H	-2.4792	2.0546	-3.6180
C	-3.5202	1.3731	-5.2364
H	-2.7825	1.6298	-5.9260
H	-4.4487	1.4794	-5.6997
H	-3.3755	0.3747	-4.9808
C	-3.5470	3.6321	-4.3888
H	-3.4501	4.2277	-3.5399
H	-4.4696	3.8324	-4.8311
H	-2.8107	3.9098	-5.0706
C	-5.2693	0.7302	-0.0084
N	-5.1554	-1.2254	1.2989

N	-4.3371	-1.8520	3.0759
C	-4.0213	-1.3653	1.9202
C	-6.1599	-1.6017	2.0654
H	-7.1398	-1.5765	1.7544
C	-5.6428	-1.9968	3.1821
H	-6.0984	-2.3753	4.0223
C	-5.2693	-0.7302	0.0084
C	-3.4036	-2.2234	4.0695
H	-2.4792	-2.0546	3.6180
C	-3.5202	-1.3731	5.2364
H	-4.4487	-1.4794	5.6997
H	-3.3755	-0.3747	4.9808
H	-2.7825	-1.6298	5.9260
C	-3.5470	-3.6321	4.3888
H	-2.8107	-3.9098	5.0706
H	-3.4501	-4.2277	3.5399
H	-4.4696	-3.8324	4.8311
H	-6.1416	1.1113	0.4136
H	-4.4498	1.0716	0.5368
H	-6.1416	-1.1113	-0.4136
H	-4.4498	-1.0716	-0.5368

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3 NHC-iPr S0 Ground State

Au	2.30394	0.91143	1.24165
Au	2.30394	-0.91143	-1.24165
N	4.13516	-2.282945	-3.079425
N	5.143395	-1.372845	-1.218565
C	4.11274	-1.631055	-1.960895
C	2.87641	-2.47741	-3.74262
H	2.185	-1.932015	-3.18003
C	2.85019	-1.94655	-5.095515
H	1.867605	-1.97714	-5.44692
H	3.4466	-2.484725	-5.76555
H	3.139465	-0.946105	-5.12183
C	2.47912	-3.87334	-3.705285
H	2.536975	-4.25011	-2.734765
H	3.050165	-4.47811	-4.338745
H	1.48846	-3.951145	-4.01356
C	4.95691	-0.73416	0.025175
N	5.143395	1.372845	1.218565
N	4.13516	2.282945	3.079425
C	4.11274	1.631055	1.960895
C	4.95691	0.73416	-0.025175
C	2.87641	2.47741	3.74262
C	2.85019	1.94655	5.095515
H	3.4466	2.484725	5.76555
H	3.139465	0.946105	5.12183
H	1.867605	1.97714	5.44692
C	2.47912	3.87334	3.705285
H	1.48846	3.951145	4.01356
H	2.536975	4.25011	2.734765
H	3.050165	4.47811	4.338745
H	5.722705	-1.059155	0.650085
H	4.056025	-1.06362	0.43852
H	5.722705	1.059155	-0.650085
H	4.056025	1.06362	-0.43852
H	2.185	1.932015	3.18003
C	5.14938	3.003045	3.828975
H	4.578715	3.39017	4.60636
C	5.672355	4.2047	3.18155
C	6.12674	2.17873	4.53815
H	5.64509	1.41037	5.053525
H	6.874485	1.751515	3.953045
H	6.601075	2.783595	5.246945
H	6.367375	4.044435	2.422405
H	6.146405	4.785435	3.911245
H	4.889365	4.76805	2.784165
C	5.14938	-3.003045	-3.828975

H	4.578715	-3.39017	-4.60636
C	5.672355	-4.2047	-3.18155
C	6.12674	-2.17873	-4.53815
H	5.64509	-1.41037	-5.053525
H	6.874485	-1.751515	-3.953045
H	6.601075	-2.783595	-5.246945
H	6.367375	-4.044435	-2.422405
H	6.146405	-4.785435	-3.911245
H	4.889365	-4.76805	-2.784165
C	6.4923	1.734985	1.48618
H	6.44746	2.30565	2.339565
C	7.072655	2.584095	0.453055
C	7.34502	0.596315	1.79398
H	6.92949	0.002185	2.54429
H	7.532455	0.00057	0.9595
H	8.271745	0.942875	2.13256
H	7.332765	2.06112	-0.4123
H	7.9534	3.011975	0.817665
H	6.423045	3.35597	0.18734
C	6.4923	-1.734985	-1.48618
H	6.44746	-2.30565	-2.339565
C	7.072655	-2.584095	-0.453055
C	7.34502	-0.596315	-1.79398
H	6.92949	-0.002185	-2.54429
H	7.532455	-0.00057	-0.9595
H	8.271745	-0.942875	-2.13256
H	7.332765	-2.06112	0.4123
H	7.9534	-3.011975	-0.817665
H	6.423045	-3.35597	-0.18734
Au	1.578805	-1.909595	1.24165
Au	-0.15485	-2.47285	-1.24165
N	-0.89338	-4.63828	-3.079425
N	0.283765	-5.315915	-1.218565
C	-0.280345	-4.41541	-1.960895
C	-1.467275	-3.50113	-3.74262
H	-1.16223	-2.675105	-3.18003
C	-0.97052	-3.312175	-5.095515
H	-1.303305	-2.38716	-5.44692
H	-1.29808	-4.045765	-5.76555
H	0.070395	-3.278165	-5.12183
C	-2.91764	-3.55471	-3.705285
H	-3.25812	-3.72609	-2.734765
H	-3.316355	-4.28469	-4.338745
H	-3.297735	-2.636535	-4.01356
C	0.83353	-4.94114	0.025175
N	2.89503	-4.467375	1.218565
N	3.44907	-3.22734	3.079425
C	2.822165	-3.407365	1.960895
C	2.23003	-4.48742	-0.025175
C	3.24501	-1.970015	3.74262
C	2.73201	-2.10919	5.095515
H	3.428265	-2.51009	5.76555
H	1.869885	-2.69344	5.12183
H	2.45746	-1.165175	5.44692
C	4.449895	-1.1609	3.705285
H	4.217715	-0.194655	4.01356
H	4.826095	-1.099435	2.734765
H	5.20144	-1.517055	4.338745
H	0.761045	-5.76992	0.650085
H	0.24187	-4.186175	0.43852
H	2.77571	-5.11537	-0.650085
H	2.26499	-3.52887	-0.43852
H	2.512655	-1.48105	3.18003
C	4.447235	-3.969385	3.828975
H	4.639135	-3.30695	4.60636
C	5.751775	-4.09545	3.18155
C	3.9653	-5.153655	4.53815
H	3.08579	-4.93297	5.053525

H	3.79012	-5.99678	3.953045
H	4.687205	-5.41785	5.246945
H	5.81419	-4.80586	2.422405
H	6.4505	-4.36677	3.911245
H	6.04561	-3.176705	2.784165
C	-1.26483	-5.825305	-3.828975
H	-1.80937	-5.402175	-4.60636
C	-2.24599	-6.69408	-3.18155
C	-0.17879	-6.500185	-4.53815
H	0.403085	-5.804595	-5.053525
H	0.458565	-7.079305	-3.953045
H	-0.607525	-7.138205	-5.246945
H	-1.87891	-7.3055	-2.422405
H	-2.65183	-7.32431	-3.911245
H	-3.023755	-6.12351	-2.784165
C	3.65636	-5.63844	1.48618
H	4.185225	-5.419465	2.339565
C	4.64322	-5.927905	0.453055
C	2.83689	-6.801335	1.79398
H	2.14339	-6.589675	2.54429
H	2.32826	-7.163665	0.9595
H	3.45287	-7.575585	2.13256
H	4.22617	-6.336975	-0.4123
H	5.32228	-6.63347	0.817665
H	5.17655	-5.071575	0.18734
C	0.356155	-6.710705	-1.48618
H	-0.20045	-6.84437	-2.339565
C	-0.27208	-7.525045	-0.453055
C	1.70259	-7.16984	-1.79398
H	2.13921	-6.591005	-2.54429
H	2.32712	-7.164045	-0.9595
H	1.659365	-8.158315	-2.13256
H	0.30571	-7.610735	0.4123
H	-0.40679	-8.4949	-0.817665
H	-1.20688	-7.14571	-0.18734
Au	-1.328195	-2.091615	1.24165
Au	-2.3997	-0.616835	-1.24165
N	-4.6873	-0.583585	-3.079425
N	-4.968025	-1.91254	-1.218565
C	-4.285925	-1.09782	-1.960895
C	-3.783185	0.313595	-3.74262
H	-2.90339	0.27873	-3.18003
C	-3.45002	-0.10051	-5.095515
H	-2.673015	0.50179	-5.44692
H	-4.248875	-0.015675	-5.76555
H	-3.095955	-1.079865	-5.12183
C	-4.282315	1.67637	-3.705285
H	-4.550595	1.947215	-2.734765
H	-5.09979	1.83008	-4.338745
H	-3.52659	2.32161	-4.01356
C	-4.441725	-2.319615	0.025175
N	-3.354165	-4.13383	1.218565
N	-2.00355	-4.277565	3.079425
C	-2.36854	-3.73692	1.960895
C	-3.57865	-3.507495	-0.025175
C	-0.870865	-3.69493	3.74262
C	-1.16166	-3.250045	5.095515
H	-1.32791	-4.036075	5.76555
H	-1.98379	-2.610695	5.12183
H	-0.348745	-2.69724	5.44692
C	0.271035	-4.59078	3.705285
H	1.118245	-4.071415	4.01356
H	0.44574	-4.929645	2.734765
H	0.16454	-5.415665	4.338745
H	-5.25236	-2.50686	0.650085
H	-3.90659	-1.52361	0.43852
H	-4.007195	-4.220565	-0.650085
H	-2.6562	-3.244535	-0.43852

H	-0.63213	-2.84734	3.18003
C	-2.40084	-5.45623	3.828975
H	-1.71152	-5.434	4.60636
C	-2.117645	-6.735785	3.18155
C	-3.676025	-5.363795	4.53815
H	-3.737965	-4.45911	5.053525
H	-4.53207	-5.45775	3.953045
H	-3.70424	-6.131965	5.246945
H	-2.774	-7.014705	2.422405
H	-2.15973	-7.484195	3.911245
H	-1.153015	-6.73132	2.784165
C	-5.93104	-0.597265	-3.828975
H	-5.696865	0.051395	-4.60636
C	-7.060495	0.067545	-3.18155
C	-6.237225	-1.83863	-4.53815
H	-5.396	-2.17702	-5.053525
H	-6.5911	-2.62371	-3.953045
H	-6.976515	-1.628015	-5.246945
H	-7.52856	-0.470535	-2.422405
H	-7.785345	0.25878	-3.911245
H	-6.758205	0.983535	-2.784165
C	-4.23263	-5.219775	1.48618
H	-3.860895	-5.655065	2.339565
C	-4.20299	-6.24777	0.453055
C	-5.591795	-4.79978	1.79398
H	-5.60481	-4.074835	2.54429
H	-6.093585	-4.42795	0.9595
H	-6.13776	-5.624855	2.13256
H	-4.720835	-5.97759	-0.4123
H	-4.66412	-7.111605	0.817665
H	-3.22373	-6.4904	0.18734
C	-6.27228	-2.41243	-1.48618
H	-6.57134	-1.924415	-2.339565
C	-7.240805	-2.066535	-0.453055
C	-6.2928	-3.834865	-1.79398
H	-5.607375	-4.07132	-2.54429
H	-6.09425	-4.427	-0.9595
H	-7.24622	-4.09925	-2.13256
H	-7.14381	-2.642615	0.4123
H	-8.204865	-2.2382	-0.817665
H	-7.168985	-1.060295	-0.18734
Au	-2.3997	0.616835	1.24165
Au	-1.328195	2.091615	-1.24165
N	-2.00355	4.277565	-3.079425
N	-3.354165	4.13383	-1.218565
C	-2.36854	3.73692	-1.960895
C	-0.870865	3.69493	-3.74262
H	-0.63213	2.84734	-3.18003
C	-1.16166	3.250045	-5.095515
H	-0.348745	2.69724	-5.44692
H	-1.32791	4.036075	-5.76555
H	-1.98379	2.610695	-5.12183
C	0.271035	4.59078	-3.705285
H	0.44574	4.929645	-2.734765
H	0.16454	5.415665	-4.338745
H	1.118245	4.071415	-4.01356
C	-3.57865	3.507495	0.025175
N	-4.968025	1.91254	1.218565
N	-4.6873	0.583585	3.079425
C	-4.285925	1.09782	1.960895
C	-4.441725	2.319615	-0.025175
C	-3.783185	-0.313595	3.74262
C	-3.45002	0.10051	5.095515
H	-4.248875	0.015675	5.76555
H	-3.095955	1.079865	5.12183
H	-2.673015	-0.50179	5.44692
C	-4.282315	-1.67637	3.705285
H	-3.52659	-2.32161	4.01356



H	-4.550595	-1.947215	2.734765
H	-5.09979	-1.83008	4.338745
H	-4.007195	4.220565	0.650085
H	-2.6562	3.244535	0.43852
H	-5.25236	2.50686	-0.650085
H	-3.90659	1.52361	-0.43852
H	-2.90339	-0.27873	3.18003
C	-5.93104	0.597265	3.828975
H	-5.696865	-0.051395	4.60636
C	-7.060495	-0.067545	3.18155
C	-6.237225	1.83863	4.53815
H	-5.396	2.17702	5.053525
H	-6.5911	2.62371	3.953045
H	-6.976515	1.628015	5.246945
H	-7.52856	0.470535	2.422405
H	-7.785345	-0.25878	3.911245
H	-6.758205	-0.983535	2.784165
C	-2.40084	5.45623	-3.828975
H	-1.71152	5.434	-4.60636
C	-2.117645	6.735785	-3.18155
C	-3.676025	5.363795	-4.53815
H	-3.737965	4.45911	-5.053525
H	-4.53207	5.45775	-3.953045
H	-3.70424	6.131965	-5.246945
H	-2.774	7.014705	-2.422405
H	-2.15973	7.484195	-3.911245
H	-1.153015	6.73132	-2.784165
C	-6.27228	2.41243	1.48618
H	-6.57134	1.924415	2.339565
C	-7.240805	2.066535	0.453055
C	-6.2928	3.834865	1.79398
H	-5.607375	4.07132	2.54429
H	-6.09425	4.427	0.9595
H	-7.24622	4.09925	2.13256
H	-7.14381	2.642615	-0.4123
H	-8.204865	2.2382	0.817665
H	-7.168985	1.060295	0.18734
C	-4.23263	5.219775	-1.48618
H	-3.860895	5.655065	-2.339565
C	-4.20299	6.24777	-0.453055
C	-5.591795	4.79978	-1.79398
H	-5.60481	4.074835	-2.54429
H	-6.093585	4.42795	-0.9595
H	-6.13776	5.624855	-2.13256
H	-4.720835	5.97759	0.4123
H	-4.66412	7.111605	-0.817665
H	-3.22373	6.4904	-0.18734
Au	-0.15485	2.47285	1.24165
Au	1.578805	1.909595	-1.24165
N	3.44907	3.22734	-3.079425
N	2.89503	4.467375	-1.218565
C	2.822165	3.407365	-1.960895
C	3.24501	1.970015	-3.74262
H	2.512655	1.48105	-3.18003
C	2.73201	2.10919	-5.095515
H	2.45746	1.165175	-5.44692
H	3.428265	2.51009	-5.76555
H	1.869885	2.69344	-5.12183
C	4.449895	1.1609	-3.705285
H	4.826095	1.099435	-2.734765
H	5.20144	1.517055	-4.338745
H	4.217715	0.194655	-4.01356
C	2.23003	4.48742	0.025175
N	0.283765	5.315915	1.218565
N	-0.89338	4.63828	3.079425
C	-0.280345	4.41541	1.960895
C	0.83353	4.94114	-0.025175
C	-1.467275	3.50113	3.74262

C	-0.97052	3.312175	5.095515
H	-1.29808	4.045765	5.76555
H	0.070395	3.278165	5.12183
H	-1.303305	2.38716	5.44692
C	-2.91764	3.55471	3.705285
H	-3.297735	2.636535	4.01356
H	-3.25812	3.72609	2.734765
H	-3.316355	4.28469	4.338745
H	2.77571	5.11537	0.650085
H	2.26499	3.52887	0.43852
H	0.761045	5.76992	-0.650085
H	0.24187	4.186175	-0.43852
Au	0	0	-2.597395
Au	0	0	0
Au	0	0	2.597395
Cl	0	0	-4.864
Cl	0	0	4.864
H	-1.16223	2.675105	3.18003
C	-1.26483	5.825305	3.828975
H	-1.80937	5.402175	4.60636
C	-2.24599	6.69408	3.18155
C	-0.17879	6.500185	4.53815
H	0.403085	5.804595	5.053525
H	0.458565	7.079305	3.953045
H	-0.607525	7.138205	5.246945
H	-1.87891	7.3055	2.422405
H	-2.65183	7.32431	3.911245
H	-3.023755	6.12351	2.784165
C	4.447235	3.969385	-3.828975
H	4.639135	3.30695	-4.60636
C	5.751775	4.09545	-3.18155
C	3.9653	5.153655	-4.53815
H	3.08579	4.93297	-5.053525
H	3.79012	5.99678	-3.953045
H	4.687205	5.41785	-5.246945
H	5.81419	4.80586	-2.422405
H	6.4505	4.36677	-3.911245
H	6.04561	3.176705	-2.784165
C	0.356155	6.710705	1.48618
H	-0.20045	6.84437	2.339565
C	-0.27208	7.525045	0.453055
C	1.70259	7.16984	1.79398
H	2.13921	6.591005	2.54429
H	2.32712	7.164045	0.9595
H	1.659365	8.158315	2.13256
H	0.30571	7.610735	-0.4123
H	-0.40679	8.4949	0.817665
H	-1.20688	7.14571	0.18734
C	3.65636	5.63844	-1.48618
H	4.185225	5.419465	-2.339565
C	4.64322	5.927905	-0.453055
C	2.83689	6.801335	-1.79398
H	2.14339	6.589675	-2.54429
H	2.32826	7.163665	-0.9595
H	3.45287	7.575585	-2.13256
H	4.22617	6.336975	0.4123
H	5.32228	6.63347	-0.817665
H	5.17655	5.071575	-0.18734

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4 Benzo S0 Ground State

Au	2.2794	0.8265	1.2211
Au	2.2794	-0.8265	-1.2211
N	4.3061	-1.8214	-3.1290
N	5.1570	-1.1766	-1.3454
C	4.0241	-1.3589	-1.9554
C	5.6265	-1.9144	-3.2856
C	6.1704	-1.4947	-2.1400
C	3.3203	-2.2463	-4.0474

H	2.4252	-2.0381	-3.5535
C	3.3506	-1.4716	-5.2732
H	2.5614	-1.7718	-5.8842
H	4.2378	-1.6006	-5.8029
H	3.2167	-0.4597	-5.0729
C	3.4160	-3.6786	-4.2701
H	3.3693	-4.2022	-3.3706
H	4.2990	-3.9416	-4.7550
H	2.6232	-3.9893	-4.8698
C	5.2650	-0.7290	-0.0399
N	5.1570	1.1766	1.3454
N	4.3061	1.8214	3.1290
C	4.0241	1.3589	1.9554
C	6.1704	1.4947	2.1400
C	5.6265	1.9144	3.2856
C	5.2650	0.7290	0.0399
C	3.3203	2.2463	4.0474
H	2.4252	2.0381	3.5535
C	3.3506	1.4716	5.2732
H	4.2378	1.6006	5.8029
H	3.2167	0.4597	5.0729
H	2.5614	1.7718	5.8842
C	3.4160	3.6786	4.2701
H	2.6232	3.9893	4.8698
H	3.3693	4.2022	3.3706
H	4.2990	3.9416	4.7550
H	6.1281	-1.1340	0.3778
H	4.4419	-1.0909	0.4853
H	6.1281	1.1340	-0.3778
H	4.4419	1.0909	-0.4853
C	6.3967	-2.3114	-4.2933
C	7.4847	-1.4549	-1.9605
C	7.7061	-2.2695	-4.1149
C	8.2433	-1.8494	-2.9685
C	7.4847	1.4549	1.9605
C	6.3967	2.3114	4.2933
C	7.7061	2.2695	4.1149
C	8.2433	1.8494	2.9685
H	6.0030	-2.6386	-5.1895
H	8.3274	-2.5699	-4.8839
H	9.2718	-1.8297	-2.8674
H	7.9057	-1.1319	-1.0724
H	7.9057	1.1319	1.0724
H	9.2718	1.8297	2.8674
H	8.3274	2.5699	4.8839
H	6.0030	2.6386	5.1895
Au	-0.0817	2.4233	1.2211
Au	1.4905	1.9124	-1.2211
N	3.0630	3.5325	-3.1290
N	2.7126	4.5410	-1.3454
C	2.5359	3.4073	-1.9554
C	3.5594	4.7595	-3.2856
C	3.3283	5.4065	-2.1400
C	3.1623	2.4636	-4.0474
H	2.6878	1.6767	-3.5535
C	2.4350	2.7318	-5.2732
H	2.4766	1.8885	-5.8842
H	2.8318	3.5358	-5.8029
H	1.4313	2.9173	-5.0729
C	4.5541	2.1121	-4.2701
H	5.0378	1.9058	-3.3706
H	5.0771	2.8706	-4.7550
H	4.6047	1.2621	-4.8698
C	2.3203	4.7820	-0.0399
N	0.4746	5.2681	1.3454
N	-0.4017	4.6581	3.1290
C	-0.0488	4.2471	1.9554
C	0.4853	6.3303	2.1400

C	-0.0821	5.9426	3.2856
C	0.9337	5.2326	0.0399
C	-1.1103	3.8519	4.0474
H	-1.1890	2.9363	3.5535
C	-0.3642	3.6414	5.2732
H	-0.2126	4.5249	5.8029
H	0.5568	3.2014	5.0729
H	-0.8935	2.9836	5.8842
C	-2.4429	4.3856	4.2701
H	-2.9835	3.7276	4.8698
H	-2.9555	4.5030	3.3706
H	-2.4201	5.3067	4.7550
H	2.9722	5.4777	0.3778
H	2.4102	3.8874	0.4853
H	0.8152	6.1785	-0.3778
H	0.3351	4.5616	-0.4853
C	4.1750	5.3694	-4.2933
C	3.6966	6.6687	-1.9605
C	4.5397	6.6277	-4.1149
C	4.3062	7.2685	-2.9685
C	0.9292	7.5679	1.9605
C	-0.2215	6.7979	4.2933
C	0.2230	8.0303	4.1149
C	0.7885	8.4114	2.9685
H	4.3645	4.8937	-5.1895
H	5.0174	7.1257	-4.8839
H	4.6053	8.2526	-2.8674
H	3.5196	7.1690	-1.0724
H	1.3665	7.8686	1.0724
H	1.1250	9.3834	2.8674
H	0.1291	8.7140	4.8839
H	-0.6545	6.5245	5.1895
Au	-2.3299	0.6711	1.2211
Au	-1.3582	2.0085	-1.2211
N	-2.4131	4.0046	-3.1290
N	-3.4805	3.9831	-1.3454
C	-2.4569	3.4647	-1.9554
C	-3.4267	4.8559	-3.2856
C	-4.1134	4.8362	-2.1400
C	-1.3658	3.7688	-4.0474
H	-0.7640	3.0744	-3.5535
C	-1.8457	3.1601	-5.2732
H	-1.0308	2.9389	-5.8842
H	-2.4877	3.7858	-5.8029
H	-2.3322	2.2627	-5.0729
C	-0.6014	4.9839	-4.2701
H	-0.2558	5.3801	-3.3706
H	-1.1613	5.7157	-4.7550
H	0.2227	4.7694	-4.8698
C	-3.8310	3.6845	-0.0399
N	-4.8636	2.0793	1.3454
N	-4.5543	1.0574	3.1290
C	-4.0543	1.2660	1.9554
C	-5.8706	2.4177	2.1400
C	-5.6771	1.7584	3.2856
C	-4.6880	2.5050	0.0399
C	-4.0064	0.1343	4.0474
H	-3.1600	-0.2234	3.5535
C	-3.5757	0.7788	5.2732
H	-4.3692	1.1961	5.8029
H	-2.8726	1.5189	5.0729
H	-3.1136	0.0722	5.8842
C	-4.9258	-0.9681	4.2701
H	-4.4672	-1.6856	4.8698
H	-5.1958	-1.4193	3.3706
H	-5.7948	-0.6619	4.7550
H	-4.2912	4.5194	0.3778
H	-2.9523	3.4934	0.4853

H	-5.6243	2.6845	-0.3778
H	-4.2348	1.7283	-0.4853
C	-3.8165	5.6298	-4.2933
C	-5.2000	5.5764	-1.9605
C	-4.9005	6.3656	-4.1149
C	-5.5820	6.3414	-2.9685
C	-6.9104	3.2223	1.9605
C	-6.5336	1.8900	4.2933
C	-7.5684	2.6935	4.1149
C	-7.7560	3.3492	2.9685
H	-3.3055	5.6631	-5.1895
H	-5.2264	6.9739	-4.8839
H	-6.4255	6.9301	-2.8674
H	-5.7305	5.5626	-1.0724
H	-7.0612	3.7311	1.0724
H	-8.5765	3.9696	2.8674
H	-8.2475	2.8156	4.8839
H	-6.4075	1.3937	5.1895
Au	-1.3582	-2.0085	1.2211
Au	-2.3299	-0.6711	-1.2211
N	-4.5543	-1.0574	-3.1290
N	-4.8636	-2.0793	-1.3454
C	-4.0543	-1.2660	-1.9554
C	-5.6771	-1.7584	-3.2856
C	-5.8706	-2.4177	-2.1400
C	-4.0064	-0.1343	-4.0474
H	-3.1600	0.2234	-3.5535
C	-3.5757	-0.7788	-5.2732
H	-3.1136	-0.0722	-5.8842
H	-4.3692	-1.1961	-5.8029
H	-2.8726	-1.5189	-5.0729
C	-4.9258	0.9681	-4.2701
H	-5.1958	1.4193	-3.3706
H	-5.7948	0.6619	-4.7550
H	-4.4672	1.6856	-4.8698
C	-4.6880	-2.5050	-0.0399
N	-3.4805	-3.9831	1.3454
N	-2.4131	-4.0046	3.1290
C	-2.4569	-3.4647	1.9554
C	-4.1134	-4.8362	2.1400
C	-3.4267	-4.8559	3.2856
C	-3.8310	-3.6845	0.0399
C	-1.3658	-3.7688	4.0474
H	-0.7640	-3.0744	3.5535
C	-1.8457	-3.1601	5.2732
H	-2.4877	-3.7858	5.8029
H	-2.3322	-2.2627	5.0729
H	-1.0308	-2.9389	5.8842
C	-0.6014	-4.9839	4.2701
H	0.2227	-4.7694	4.8698
H	-0.2558	-5.3801	3.3706
H	-1.1613	-5.7157	4.7550
H	-5.6243	-2.6845	0.3778
H	-4.2348	-1.7283	0.4853
H	-4.2912	-4.5194	-0.3778
H	-2.9523	-3.4934	-0.4853
C	-6.5336	-1.8900	-4.2933
C	-6.9104	-3.2223	-1.9605
C	-7.5684	-2.6935	-4.1149
C	-7.7560	-3.3492	-2.9685
C	-5.2000	-5.5764	1.9605
C	-3.8165	-5.6298	4.2933
C	-4.9005	-6.3656	4.1149
C	-5.5820	-6.3414	2.9685
H	-6.4075	-1.3937	-5.1895
H	-8.2475	-2.8156	-4.8839
H	-8.5765	-3.9696	-2.8674
H	-7.0612	-3.7311	-1.0724

H	-5.7305	-5.5626	1.0724
H	-6.4255	-6.9301	2.8674
H	-5.2264	-6.9739	4.8839
H	-3.3055	-5.6631	5.1895
Au	1.4905	-1.9124	1.2211
Au	-0.0817	-2.4233	-1.2211
N	-0.4017	-4.6581	-3.1290
N	0.4746	-5.2681	-1.3454
C	-0.0488	-4.2471	-1.9554
C	-0.0821	-5.9426	-3.2856
C	0.4853	-6.3303	-2.1400
C	-1.1103	-3.8519	-4.0474
H	-1.1890	-2.9363	-3.5535
C	-0.3642	-3.6414	-5.2732
H	-0.8935	-2.9836	-5.8842
H	-0.2126	-4.5249	-5.8029
H	0.5568	-3.2014	-5.0729
C	-2.4429	-4.3856	-4.2701
H	-2.9555	-4.5030	-3.3706
H	-2.4201	-5.3067	-4.7550
H	-2.9835	-3.7276	-4.8698
C	0.9337	-5.2326	-0.0399
N	2.7126	-4.5410	1.3454
N	3.0630	-3.5325	3.1290
C	2.5359	-3.4073	1.9554
C	3.3283	-5.4065	2.1400
C	3.5594	-4.7595	3.2856
C	2.3203	-4.7820	0.0399
C	3.1623	-2.4636	4.0474
H	2.6878	-1.6767	3.5535
C	2.4350	-2.7318	5.2732
H	2.8318	-3.5358	5.8029
H	1.4313	-2.9173	5.0729
H	2.4766	-1.8885	5.8842
C	4.5541	-2.1121	4.2701
H	4.6047	-1.2621	4.8698
H	5.0378	-1.9058	3.3706
H	5.0771	-2.8706	4.7550
H	0.8152	-6.1785	0.3778
H	0.3351	-4.5616	0.4853
H	2.9722	-5.4777	-0.3778
H	2.4102	-3.8874	-0.4853
Au	0.0000	0.0000	-2.6491
Au	0.0000	0.0000	0.0000
Au	0.0000	0.0000	2.6491
Cl	0.0000	0.0000	-4.8955
Cl	0.0000	0.0000	4.8955
C	-0.2215	-6.7979	-4.2933
C	0.9292	-7.5679	-1.9605
C	0.2230	-8.0303	-4.1149
C	0.7885	-8.4114	-2.9685
C	3.6966	-6.6687	1.9605
C	4.1750	-5.3694	4.2933
C	4.5397	-6.6277	4.1149
C	4.3062	-7.2685	2.9685
H	-0.6545	-6.5245	-5.1895
H	0.1291	-8.7140	-4.8839
H	1.1250	-9.3834	-2.8674
H	1.3665	-7.8686	-1.0724
H	3.5196	-7.1690	1.0724
H	4.6053	-8.2526	2.8674
H	5.0174	-7.1257	4.8839
H	4.3645	-4.8937	5.1895
255			
5 BenzoN S0 Ground State			
Au	2.2776	0.8139	1.2215
Au	2.2776	-0.8139	-1.2215
N	4.2717	-1.7775	-3.1604

N	5.1548	-1.1396	-1.3707
C	4.0114	-1.3273	-1.9723
C	5.5845	-1.8541	-3.3281
C	6.1446	-1.4405	-2.1893
C	3.2914	-2.2096	-4.0873
H	2.3906	-2.0003	-3.6048
C	3.3571	-1.4500	-5.3188
H	2.5915	-1.7665	-5.9503
H	4.2676	-1.5933	-5.8022
H	3.2086	-0.4359	-5.1399
C	3.4212	-3.6398	-4.2994
H	3.3636	-4.1629	-3.4001
H	4.3253	-3.8677	-4.7627
H	2.6513	-3.9671	-4.9199
C	5.3026	-0.7270	-0.0544
N	5.1548	1.1396	1.3707
N	4.2717	1.7775	3.1604
C	4.0114	1.3273	1.9723
C	6.1446	1.4405	2.1893
C	5.5845	1.8541	3.3281
C	5.3026	0.7270	0.0544
C	3.2914	2.2096	4.0873
H	2.3906	2.0003	3.6048
C	3.3571	1.4500	5.3188
H	4.2676	1.5933	5.8022
H	3.2086	0.4359	5.1399
H	2.5915	1.7665	5.9503
C	3.4212	3.6398	4.2994
H	2.6513	3.9671	4.9199
H	3.3636	4.1629	3.4001
H	4.3253	3.8677	4.7627
H	6.1961	-1.1239	0.3016
H	4.5031	-1.1162	0.4863
H	6.1961	1.1239	-0.3016
H	4.5031	1.1162	-0.4863
N	6.2520	-2.2267	-4.3311
N	7.3827	-1.3683	-1.9878
C	7.5146	-2.1574	-4.1433
C	8.0679	-1.7387	-3.0017
N	7.3827	1.3683	1.9878
N	6.2520	2.2267	4.3311
C	7.5146	2.1574	4.1433
C	8.0679	1.7387	3.0017
H	8.1170	-2.4464	-4.9339
H	9.0979	-1.7080	-2.9054
H	9.0979	1.7080	2.9054
H	8.1170	2.4464	4.9339
Au	-0.0702	2.4177	1.2215
Au	1.4778	1.9147	-1.2215
N	3.0106	3.5133	-3.1604
N	2.6767	4.5503	-1.3707
C	2.5020	3.4049	-1.9723
C	3.4891	4.7382	-3.3281
C	3.2688	5.3988	-2.1893
C	3.1186	2.4475	-4.0873
H	2.6411	1.6555	-3.6048
C	2.4164	2.7447	-5.3188
H	2.4808	1.9188	-5.9503
H	2.8341	3.5663	-5.8022
H	1.4060	2.9169	-5.1399
C	4.5189	2.1290	-4.2994
H	4.9986	1.9125	-3.4001
H	5.0151	2.9183	-4.7627
H	4.5922	1.2956	-4.9199
C	2.3301	4.8184	-0.0544
N	0.5091	5.2546	1.3707
N	-0.3705	4.6119	3.1604
C	-0.0228	4.2252	1.9723

C	0.5289	6.2890	2.1893
C	-0.0377	5.8841	3.3281
C	0.9472	5.2678	0.0544
C	-1.0844	3.8131	4.0873
H	-1.1637	2.8917	3.6048
C	-0.3416	3.6409	5.3188
H	-0.1967	4.5511	5.8022
H	0.5770	3.1863	5.1399
H	-0.8792	3.0106	5.9503
C	-2.4045	4.3786	4.2994
H	-2.9536	3.7474	4.9199
H	-2.9197	4.4854	3.4001
H	-2.3418	5.3087	4.7627
H	2.9837	5.5455	0.3016
H	2.4530	3.9378	0.4863
H	0.8458	6.2402	-0.3016
H	0.3300	4.6275	-0.4863
N	4.0498	5.2579	-4.3311
N	3.5827	6.5985	-1.9878
C	4.3739	6.4801	-4.1433
C	4.1468	7.1356	-3.0017
N	0.9800	7.4442	1.9878
N	-0.1858	6.6340	4.3311
C	0.2704	7.8135	4.1433
C	0.8395	8.2103	3.0017
H	4.8350	6.9637	-4.9339
H	4.4358	8.1248	-2.9054
H	1.1870	9.1804	2.9054
H	0.1815	8.4757	4.9339
Au	-2.3210	0.6804	1.2215
Au	-1.3643	1.9972	-1.2215
N	-2.4110	3.9489	-3.1604
N	-3.5005	3.9518	-1.3707
C	-2.4651	3.4317	-1.9723
C	-3.4281	4.7825	-3.3281
C	-4.1244	4.7771	-2.1893
C	-1.3640	3.7223	-4.0873
H	-0.7583	3.0234	-3.6048
C	-1.8637	3.1463	-5.3188
H	-1.0582	2.9524	-5.9503
H	-2.5160	3.7974	-5.8022
H	-2.3397	2.2386	-5.1399
C	-0.6284	4.9556	-4.2994
H	-0.2743	5.3450	-3.4001
H	-1.2258	5.6714	-4.7627
H	0.1869	4.7678	-4.9199
C	-3.8626	3.7050	-0.0544
N	-4.8402	2.1080	1.3707
N	-4.5006	1.0727	3.1604
C	-4.0255	1.2840	1.9723
C	-5.8178	2.4463	2.1893
C	-5.6078	1.7825	3.3281
C	-4.7172	2.5286	0.0544
C	-3.9616	0.1470	4.0873
H	-3.1097	-0.2132	3.6048
C	-3.5683	0.8002	5.3188
H	-4.3891	1.2193	5.8022
H	-2.8520	1.5334	5.1399
H	-3.1349	0.0941	5.9503
C	-4.9072	-0.9338	4.2994
H	-4.4767	-1.6511	4.9199
H	-5.1681	-1.3908	3.4001
H	-5.7726	-0.5868	4.7627
H	-4.3521	4.5513	0.3016
H	-2.9870	3.5498	0.4863
H	-5.6734	2.7327	-0.3016
H	-4.2991	1.7439	-0.4863
N	-3.7491	5.4763	-4.3311



N	-5.1685	5.4464	-1.9878
C	-4.8114	6.1623	-4.1433
C	-5.5051	6.1488	-3.0017
N	-6.7770	3.2325	1.9878
N	-6.3668	1.8733	4.3311
C	-7.3475	2.6717	4.1433
C	-7.5490	3.3355	3.0017
H	-5.1288	6.7503	-4.9339
H	-6.3564	6.7294	-2.9054
H	-8.3643	3.9658	2.9054
H	-8.0048	2.7918	4.9339
Au	-1.3643	-1.9972	1.2215
Au	-2.3210	-0.6804	-1.2215
N	-4.5006	-1.0727	-3.1604
N	-4.8402	-2.1080	-1.3707
C	-4.0255	-1.2840	-1.9723
C	-5.6078	-1.7825	-3.3281
C	-5.8178	-2.4463	-2.1893
C	-3.9616	-0.1470	-4.0873
H	-3.1097	0.2132	-3.6048
C	-3.5683	-0.8002	-5.3188
H	-3.1349	-0.0941	-5.9503
H	-4.3891	-1.2193	-5.8022
H	-2.8520	-1.5334	-5.1399
C	-4.9072	0.9338	-4.2994
H	-5.1681	1.3908	-3.4001
H	-5.7726	0.5868	-4.7627
H	-4.4767	1.6511	-4.9199
C	-4.7172	-2.5286	-0.0544
N	-3.5005	-3.9518	1.3707
N	-2.4110	-3.9489	3.1604
C	-2.4651	-3.4317	1.9723
C	-4.1244	-4.7771	2.1893
C	-3.4281	-4.7825	3.3281
C	-3.8626	-3.7050	0.0544
C	-1.3640	-3.7223	4.0873
H	-0.7583	-3.0234	3.6048
C	-1.8637	-3.1463	5.3188
H	-2.5160	-3.7974	5.8022
H	-2.3397	-2.2386	5.1399
H	-1.0582	-2.9524	5.9503
C	-0.6284	-4.9556	4.2994
H	0.1869	-4.7678	4.9199
H	-0.2743	-5.3450	3.4001
H	-1.2258	-5.6714	4.7627
H	-5.6734	-2.7327	0.3016
H	-4.2991	-1.7439	0.4863
H	-4.3521	-4.5513	-0.3016
H	-2.9870	-3.5498	-0.4863
N	-6.3668	-1.8733	-4.3311
N	-6.7770	-3.2325	-1.9878
C	-7.3475	-2.6717	-4.1433
C	-7.5490	-3.3355	-3.0017
N	-5.1685	-5.4464	1.9878
N	-3.7491	-5.4763	4.3311
C	-4.8114	-6.1623	4.1433
C	-5.5051	-6.1488	3.0017
H	-8.0048	-2.7918	-4.9339
H	-8.3643	-3.9658	-2.9054
H	-6.3564	-6.7294	2.9054
H	-5.1288	-6.7503	4.9339
Au	1.4778	-1.9147	1.2215
Au	-0.0702	-2.4177	-1.2215
N	-0.3705	-4.6119	-3.1604
N	0.5091	-5.2546	-1.3707
C	-0.0228	-4.2252	-1.9723
C	-0.0377	-5.8841	-3.3281
C	0.5289	-6.2890	-2.1893

C	-1.0844	-3.8131	-4.0873
H	-1.1637	-2.8917	-3.6048
C	-0.3416	-3.6409	-5.3188
H	-0.8792	-3.0106	-5.9503
H	-0.1967	-4.5511	-5.8022
H	0.5770	-3.1863	-5.1399
C	-2.4045	-4.3786	-4.2994
H	-2.9197	-4.4854	-3.4001
H	-2.3418	-5.3087	-4.7627
H	-2.9536	-3.7474	-4.9199
C	0.9472	-5.2678	-0.0544
N	2.6767	-4.5503	1.3707
N	3.0106	-3.5133	3.1604
C	2.5020	-3.4049	1.9723
C	3.2688	-5.3988	2.1893
C	3.4891	-4.7382	3.3281
C	2.3301	-4.8184	0.0544
C	3.1186	-2.4475	4.0873
H	2.6411	-1.6555	3.6048
C	2.4164	-2.7447	5.3188
H	2.8341	-3.5663	5.8022
H	1.4060	-2.9169	5.1399
H	2.4808	-1.9188	5.9503
C	4.5189	-2.1290	4.2994
H	4.5922	-1.2956	4.9199
H	4.9986	-1.9125	3.4001
H	5.0151	-2.9183	4.7627
H	0.8458	-6.2402	0.3016
H	0.3300	-4.6275	0.4863
H	2.9837	-5.5455	-0.3016
H	2.4530	-3.9378	-0.4863
Au	0.0000	0.0000	-2.6502
Au	0.0000	0.0000	0.0000
Au	0.0000	0.0000	2.6502
Cl	0.0000	0.0000	-4.8868
Cl	0.0000	0.0000	4.8868
N	-0.1858	-6.6340	-4.3311
N	0.9800	-7.4442	-1.9878
C	0.2704	-7.8135	-4.1433
C	0.8395	-8.2103	-3.0017
N	3.5827	-6.5985	1.9878
N	4.0498	-5.2579	4.3311
C	4.3739	-6.4801	4.1433
C	4.1468	-7.1356	3.0017
H	0.1815	-8.4757	-4.9339
H	1.1870	-9.1804	-2.9054
H	4.4358	-8.1248	2.9054
H	4.8350	-6.9637	4.9339

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6 NHC-O S0 Ground State

Au	-1.485325	1.898575	1.227115
Au	0.093195	2.41224	-1.228825
N	0.50521	4.619945	-3.10156
N	-0.415435	5.24077	-1.298745
C	0.085405	4.2256	-1.94712
C	0.268185	5.943675	-3.284245
O	0.51433	6.581315	-4.19976
C	-0.37297	6.369845	-2.033665
O	-0.751355	7.404015	-1.726435
C	1.190825	3.805985	-4.046335
H	1.225785	2.870615	-3.579125
C	0.4408	3.69132	-5.282285
H	0.95418	3.052825	-5.928475
H	0.335825	4.6151	-5.75472
H	-0.499035	3.27237	-5.113945
C	2.5384	4.31224	-4.24593
H	3.058145	4.38634	-3.34248
H	2.5308	5.24894	-4.703925

H	3.05748	3.65997	-4.87331
C	-0.907725	5.212555	-0.00057
N	-2.716335	4.494545	1.337505
N	-3.11524	3.419715	3.11714
C	-2.536595	3.36547	1.965835
C	-3.4219	5.370255	2.080595
O	-3.72039	6.434445	1.78923
C	-3.704335	4.626025	3.314645
O	-4.290295	4.978475	4.22997
C	-2.30128	4.7766	0.04237
C	-3.197225	2.34555	4.046145
H	-2.67767	1.57282	3.569245
C	-2.523865	2.67577	5.28713
H	-2.97749	3.48346	5.76593
H	-1.51525	2.882965	5.12392
H	-2.57127	1.851645	5.925055
C	-4.5866	1.96517	4.237475
H	-4.62726	1.12328	4.851935
H	-5.04925	1.73489	3.32975
H	-5.12943	2.72213	4.70592
H	-0.81453	6.179655	0.379335
H	-0.313025	4.558575	0.55309
H	-2.930655	5.525105	-0.320625
H	-2.41984	3.91096	-0.52763
Au	2.32237	-0.65531	1.2274
Au	1.34235	-2.00127	-1.22683
N	2.29406	-4.032275	-3.102415
N	3.414395	-3.992185	-1.30682
C	2.410815	-3.46351	-1.95073
C	3.261635	-4.965555	-3.288995
O	3.43178	-5.626945	-4.2047
C	4.036835	-4.934015	-2.042405
O	4.94931	-5.551705	-1.737645
C	1.25457	-3.779575	-4.040825
H	0.67678	-3.04589	-3.569625
C	1.785335	-3.24425	-5.279625
H	0.99123	-3.041235	-5.925625
H	2.420125	-3.92445	-5.750065
H	2.289405	-2.3465	-5.11575
C	0.46474	-4.9837	-4.23548
H	0.096615	-5.35135	-3.32918
H	1.020585	-5.73439	-4.69832
H	-0.344565	-4.764155	-4.8564
C	3.805415	-3.675455	-0.013015
N	4.84842	-2.024925	1.31176
N	4.54575	-0.942115	3.10517
C	4.04016	-1.22683	1.95339
C	5.934555	-2.33016	2.047915
O	6.800575	-3.012165	1.744295
C	5.72907	-1.579375	3.292795
O	6.4106	-1.53748	4.2085
C	4.66545	-2.49527	0.018525
C	3.98924	-0.029545	4.044435
H	3.113055	0.296495	3.57504
C	3.6442	-0.698915	5.283805
H	4.488085	-1.088035	5.757095
H	2.94956	-1.458915	5.11974
H	3.201215	-0.007315	5.92724
C	4.89592	1.08965	4.237665
H	4.442105	1.79246	4.860675
H	5.131235	1.553725	3.331745
H	5.781795	0.7885	4.697845
H	4.310625	-4.50737	0.362615
H	2.944145	-3.50341	0.549955
H	5.611555	-2.721465	-0.35834
H	4.237095	-1.728525	-0.54416
Au	1.34919	2.0026	1.228445
Au	2.318285	0.665855	-1.230725

N	4.51155	0.969095	-3.141365
N	4.825335	2.063115	-1.35603
C	4.01964	1.25077	-1.982745
C	5.68765	1.613955	-3.345045
O	6.360535	1.57035	-4.267115
C	5.900735	2.37329	-2.106435
O	6.765425	3.06242	-1.815925
C	3.953235	0.04465	-4.06847
H	3.07895	-0.27721	-3.592235
C	3.602495	0.698725	-5.314775
H	3.156755	-0.00152	-5.946905
H	4.444195	1.081955	-5.796995
H	2.907665	1.460245	-5.15755
C	4.86077	-1.076065	-4.252295
H	5.0996	-1.530165	-3.342005
H	5.74465	-0.779095	-4.71922
H	4.40534	-1.786475	-4.8659
C	4.66792	2.514935	-0.052345
N	3.42969	3.982495	1.320785
N	2.31819	4.008145	3.12284
C	2.42459	3.45382	1.96327
C	4.05859	4.914445	2.0634
O	4.97135	5.532705	1.7613
C	3.28928	4.936295	3.313885
O	3.46522	5.58847	4.235195
C	3.80247	3.68961	0.01539
C	1.284875	3.747275	4.065905
H	0.704995	3.016155	3.5929
C	1.824	3.203115	5.297105
H	2.457175	3.882365	5.771725
H	2.33187	2.309545	5.1224
H	1.033695	2.98908	5.94358
C	0.49533	4.94912	4.27557
H	-0.30913	4.7234	4.900005
H	0.119985	5.323895	3.37554
H	1.053455	5.696865	4.74088
H	5.62077	2.741035	0.30704
H	4.25657	1.737645	0.508345
H	4.29685	4.530265	-0.354445
H	2.932935	3.52279	-0.5358
Au	0.085595	-2.404735	1.229775
Au	-1.48485	-1.89525	-1.22968
N	-3.094435	-3.42969	-3.127685
N	-2.71681	-4.48932	-1.33418
C	-2.5346	-3.36376	-1.96764
C	-3.66529	-4.643885	-3.328705
O	-4.228355	-5.010015	-4.25296
C	-3.398435	-5.37719	-2.08468
O	-3.69018	-6.4429	-1.792365
C	-3.174615	-2.359515	-4.06182
H	-2.66399	-1.58194	-3.583305
C	-2.48919	-2.68964	-5.296345
H	-2.5365	-1.867795	-5.93712
H	-2.934265	-3.501415	-5.776095
H	-1.48067	-2.89028	-5.12411
C	-4.56494	-1.98854	-4.26645
H	-5.03728	-1.757595	-3.363665
H	-5.09884	-2.750915	-4.73632
H	-4.605695	-1.149405	-4.884805
C	-2.330635	-4.755035	-0.02698
N	-0.474905	-5.22044	1.355555
N	0.46569	-4.582705	3.141935
C	0.053295	-4.204035	1.97999
C	-0.45239	-6.334885	2.1128
O	-0.85082	-7.36782	1.827325
C	0.20197	-5.89684	3.351885
O	0.439565	-6.52023	4.27918
C	-0.946105	-5.212935	0.04921

C	1.173535	-3.766655	4.068375
H	1.221985	-2.83936	3.58682
C	0.43567	-3.62007	5.308125
H	0.318535	-4.534635	5.794905
H	-0.49742	-3.18649	5.141115
H	0.965105	-2.98053	5.93997
C	2.51275	-4.295235	4.26512
H	3.049595	-3.64363	4.877775
H	3.023565	-4.393655	3.359295
H	2.49109	-5.224145	4.738125
H	-2.978535	-5.48682	0.33763
H	-2.44568	-3.877425	0.524685
H	-0.863075	-6.189535	-0.308465
H	-0.331645	-4.5809	-0.50844
Au	0.00266	0.002565	-2.654585
Au	-2.26062	-0.828115	1.229585
Au	-2.26081	0.82878	-1.228635
Au	0.003135	0.002945	-0.000285
Au	0.00399	0.00437	2.654015
Cl	0.01045	0.006365	-4.87122
Cl	0.00988	0.008835	4.870745
N	-4.218095	1.880715	-3.129965
N	-5.111	1.17686	-1.34406
C	-3.98297	1.361635	-1.97296
C	-5.54952	2.04497	-3.3326
O	-6.07107	2.47228	-4.254955
C	-6.165785	1.55268	-2.09399
O	-7.270255	1.49397	-1.805
C	-3.225155	2.302895	-4.057545
H	-2.327405	2.05865	-3.57922
C	-3.319205	1.56028	-5.299385
H	-2.551225	1.869125	-5.93427
H	-4.227785	1.732895	-5.781035
H	-3.1939	0.53827	-5.136745
C	-3.31151	3.74091	-4.248495
H	-3.24178	4.253435	-3.341055
H	-4.20318	4.011375	-4.71637
H	-2.528045	4.05061	-4.86343
C	-5.24666	0.708415	-0.043795
N	-5.10739	-1.21771	1.31366
N	-4.223985	-1.90608	3.1103
C	-3.9843	-1.38244	1.95586
C	-6.16436	-1.61006	2.052
O	-7.26598	-1.56997	1.74971
C	-5.555125	-2.091425	3.29821
O	-6.08076	-2.52681	4.214485
C	-5.236305	-0.75107	0.01216
C	-3.234275	-2.308595	4.050325
H	-2.33548	-2.05675	3.577985
C	-3.348465	-1.55743	5.28542
H	-4.260655	-1.734225	5.75871
H	-3.23095	-0.535515	5.11575
H	-2.584855	-1.854115	5.931515
C	-3.302865	-3.746135	4.252675
H	-2.519115	-4.04035	4.87521
H	-3.220785	-4.26512	3.349605
H	-4.19387	-4.02458	4.71694
H	-6.14992	1.082145	0.320435
H	-4.45588	1.09117	0.518415
H	-6.12997	-1.13829	-0.36138
H	-4.433745	-1.12176	-0.541405

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7 NHC-Me S0 Ground State

Au	2.0591	1.2407	-1.3139
Au	1.8163	1.5749	1.3139
N	2.4368	4.1342	2.4261
N	3.6733	3.8552	0.8005
C	2.8533	3.2177	1.6039

C	2.9851	5.3004	2.1682
H	2.7917	6.1492	2.7141
C	3.7545	5.1348	1.1511
H	4.3668	5.8042	0.6678
C	1.5464	3.8966	3.5036
H	0.9738	3.0833	3.1898
C	2.2836	3.5315	4.6959
H	1.6160	3.2780	5.4551
H	2.8770	4.3198	5.0321
H	2.8889	2.7063	4.5140
C	0.6806	5.0360	3.7201
H	0.1525	5.2836	2.8583
H	1.2036	5.8717	4.0573
H	-0.0041	4.7964	4.4659
C	4.7482	3.4497	0.0000
N	4.8016	2.3022	-0.8005
N	4.6848	1.0400	-2.4261
C	3.9418	1.7193	-1.6039
C	6.0436	1.9840	-1.1511
H	6.8695	2.3594	-0.6678
C	5.9634	1.2011	-2.1682
H	6.7109	0.7548	-2.7141
C	4.1838	0.2666	-3.5036
H	3.2333	-0.0267	-3.1898
C	4.0644	1.0805	-4.6959
H	4.9975	1.4013	-5.0321
H	3.4666	1.9111	-4.5140
H	3.6168	0.5239	-5.4551
C	4.9998	-0.9089	-3.7201
H	4.5604	-1.4861	-4.4659
H	5.0721	-1.4877	-2.8583
H	5.9561	-0.6698	-4.0573
H	5.5719	3.3539	0.6308
H	4.9115	4.2628	-0.6308
Au	-2.3951	0.2065	-1.3139
Au	-2.3951	-0.2065	1.3139
N	-4.4014	-1.9124	2.4261
N	-5.2377	-0.9598	0.8005
C	-4.1997	-0.9260	1.6039
C	-5.5305	-2.5336	2.1682
H	-5.8729	-3.3339	2.7141
C	-6.0556	-1.9473	1.1511
H	-6.9444	-2.1290	0.6678
C	-3.5415	-2.2435	3.5036
H	-2.6002	-1.9221	3.1898
C	-3.9233	-1.5148	4.6959
H	-3.2341	-1.7021	5.4551
H	-4.8667	-1.8038	5.0321
H	-3.9278	-0.4914	4.5140
C	-3.5106	-3.6741	3.7201
H	-3.2290	-4.1849	2.8583
H	-4.4249	-4.0428	4.0573
H	-2.8159	-3.8827	4.4659
C	-5.8691	0.0000	0.0000
N	-5.2377	0.9598	-0.8005
N	-4.4014	1.9124	-2.4261
C	-4.1997	0.9260	-1.6039
C	-6.0556	1.9473	-1.1511
H	-6.9444	2.1290	-0.6678
C	-5.5305	2.5336	-2.1682
H	-5.8729	3.3339	-2.7141
C	-3.5415	2.2435	-3.5036
H	-2.6002	1.9221	-3.1898
C	-3.9233	1.5148	-4.6959
H	-4.8667	1.8038	-5.0321
H	-3.9278	0.4914	-4.5140
H	-3.2341	1.7021	-5.4551
C	-3.5106	3.6741	-3.7201

H	-2.8159	3.8827	-4.4659
H	-3.2290	4.1849	-2.8583
H	-4.4249	4.0428	-4.0573
H	-6.4791	0.5617	0.6308
H	-6.4791	-0.5617	-0.6308
Au	-0.5437	2.3418	-1.3139
Au	-0.9366	2.2141	1.3139
N	-3.1789	3.5950	2.4261
N	-2.5314	4.6848	0.8005
C	-2.1784	3.7079	1.6039
C	-4.1185	4.4769	2.1682
H	-4.9856	4.5553	2.7141
C	-3.7232	5.1575	1.1511
H	-4.1708	5.9466	0.6678
C	-3.2281	2.6748	3.5036
H	-2.6315	1.8789	3.1898
C	-2.6530	3.2632	4.6959
H	-2.6182	2.5498	5.4551
H	-3.2194	4.0710	5.0321
H	-1.6811	3.5837	4.5140
C	-4.5791	2.2035	3.7201
H	-4.9779	1.7777	2.8583
H	-5.2124	2.9591	4.0573
H	-4.5629	1.4782	4.4659
C	-1.8136	5.5818	0.0000
N	-0.7058	5.2780	-0.8005
N	0.4587	4.7769	-2.4261
C	-0.4171	4.2802	-1.6039
C	-0.0193	6.3609	-1.1511
H	-0.1211	7.2625	-0.6678
C	0.7005	6.0427	-2.1682
H	1.3559	6.6157	-2.7141
C	1.0393	4.0614	-3.5036
H	1.0246	3.0668	-3.1898
C	0.2283	4.1994	-4.6959
H	0.2117	5.1859	-5.0321
H	-0.7464	3.8874	-4.5140
H	0.6194	3.6017	-5.4551
C	2.4094	4.4742	-3.7201
H	2.8225	3.8779	-4.4659
H	2.9822	4.3642	-2.8583
H	2.4776	5.4577	-4.0573
H	-1.4679	6.3356	0.6308
H	-2.5364	5.9884	-0.6308
Au	-0.9366	-2.2141	-1.3139
Au	-0.5437	-2.3418	1.3139
N	0.4587	-4.7769	2.4261
N	-0.7058	-5.2780	0.8005
C	-0.4171	-4.2802	1.6039
C	0.7005	-6.0427	2.1682
H	1.3559	-6.6157	2.7141
C	-0.0193	-6.3609	1.1511
H	-0.1211	-7.2625	0.6678
C	1.0393	-4.0614	3.5036
H	1.0246	-3.0668	3.1898
C	0.2283	-4.1994	4.6959
H	0.6194	-3.6017	5.4551
H	0.2117	-5.1859	5.0321
H	-0.7464	-3.8874	4.5140
C	2.4094	-4.4742	3.7201
H	2.9822	-4.3642	2.8583
H	2.4776	-5.4577	4.0573
H	2.8225	-3.8779	4.4659
C	-1.8136	-5.5818	0.0000
N	-2.5314	-4.6848	-0.8005
N	-3.1789	-3.5950	-2.4261
C	-2.1784	-3.7079	-1.6039
C	-3.7232	-5.1575	-1.1511

H	-4.1708	-5.9466	-0.6678
C	-4.1185	-4.4769	-2.1682
H	-4.9856	-4.5553	-2.7141
C	-3.2281	-2.6748	-3.5036
H	-2.6315	-1.8789	-3.1898
C	-2.6530	-3.2632	-4.6959
H	-3.2194	-4.0710	-5.0321
H	-1.6811	-3.5837	-4.5140
H	-2.6182	-2.5498	-5.4551
C	-4.5791	-2.2035	-3.7201
H	-4.5629	-1.4782	-4.4659
H	-4.9779	-1.7777	-2.8583
H	-5.2124	-2.9591	-4.0573
H	-2.5364	-5.9884	0.6308
H	-1.4679	-6.3356	-0.6308
Au	0.0000	0.0000	2.6754
Au	1.8163	-1.5749	-1.3139
Au	2.0591	-1.2407	1.3139
Au	0.0000	0.0000	0.0000
Au	0.0000	0.0000	-2.6754
Cl	0.0000	0.0000	4.9216
Cl	0.0000	0.0000	-4.9216
N	4.6848	-1.0400	2.4261
N	4.8016	-2.3022	0.8005
C	3.9418	-1.7193	1.6039
C	5.9634	-1.2011	2.1682
H	6.7109	-0.7548	2.7141
C	6.0436	-1.9840	1.1511
H	6.8695	-2.3594	0.6678
C	4.1838	-0.2666	3.5036
H	3.2333	0.0267	3.1898
C	4.0644	-1.0805	4.6959
H	3.6168	-0.5239	5.4551
H	4.9975	-1.4013	5.0321
H	3.4666	-1.9111	4.5140
C	4.9998	0.9089	3.7201
H	5.0721	1.4877	2.8583
H	5.9561	0.6698	4.0573
H	4.5604	1.4861	4.4659
C	4.7482	-3.4497	0.0000
N	3.6733	-3.8552	-0.8005
N	2.4368	-4.1342	-2.4261
C	2.8533	-3.2177	-1.6039
C	3.7545	-5.1348	-1.1511
H	4.3668	-5.8042	-0.6678
C	2.9851	-5.3004	-2.1682
H	2.7917	-6.1492	-2.7141
C	1.5464	-3.8966	-3.5036
H	0.9738	-3.0833	-3.1898
C	2.2836	-3.5315	-4.6959
H	2.8770	-4.3198	-5.0321
H	2.8889	-2.7063	-4.5140
H	1.6160	-3.2780	-5.4551
C	0.6806	-5.0360	-3.7201
H	-0.0041	-4.7964	-4.4659
H	0.1525	-5.2836	-2.8583
H	1.2036	-5.8717	-4.0573
H	4.9115	-4.2628	0.6308
H	5.5719	-3.3539	-0.6308

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1 dppe T1 Excited State

Au	0.0098	0.0139	-2.5918
Au	-1.4468	2.0132	1.2132
Au	1.4607	1.9903	1.1789
Au	0.0044	2.4886	-1.2196
Au	-0.0119	-2.4505	1.2204
Au	0.0044	0.0196	0.0001
Au	-1.4197	-1.9710	-1.1775



Au	2.3225	0.7938	-1.1883
Au	2.3261	-0.7538	1.1798
Au	-2.3329	0.7570	-1.1813
Au	-2.3265	-0.7163	1.1887
Au	1.4712	-1.9651	-1.2140
Au	0.0026	0.0165	2.5921
P	-2.0120	-4.0491	-1.8675
P	3.2167	3.2588	1.8524
P	-0.8058	4.5401	-1.8595
P	3.2284	-3.3030	-1.8250
P	4.0173	-2.0969	1.8782
P	-0.6673	-4.5618	1.8358
Cl	0.0022	0.0208	-4.8528
Cl	0.0066	0.0130	4.8534
P	-4.5029	0.7552	-1.8541
P	-4.4953	-0.7061	1.8585
P	4.0572	2.0939	-1.8605
P	-2.0178	4.1407	1.8471
C	3.1334	4.9929	1.9168
C	-3.7015	4.5388	1.9876
C	-4.9231	3.2937	-2.4914
C	-6.7234	2.2398	-1.4976
C	-4.8546	-3.2505	2.4981
C	-1.5095	-3.4135	4.1022
C	-6.8254	-4.4174	2.2662
C	-2.1518	-5.6048	3.7932
C	-3.7018	0.4103	4.1516
C	-6.9146	4.4137	-2.2146
C	-1.6336	3.3766	-4.1197
C	4.1537	5.7582	1.5300
C	-6.6918	-2.2427	1.5296
C	5.6659	1.4418	-1.9561
C	2.0550	5.5647	2.4482
C	-5.4544	2.2077	-1.9209
C	-5.5571	-4.3626	2.6647
C	5.8019	-0.2573	2.5517
C	-1.8843	-5.0221	0.6480
C	-0.6539	3.7156	4.1055
C	-4.1781	5.7299	1.6130
C	5.0316	-3.3044	-3.7928
C	3.0225	7.6371	2.1970
C	-2.2773	5.5719	-3.8323
C	-6.1703	0.8686	5.0226
C	4.1350	-3.4090	0.7078
C	-5.4184	-2.1794	1.9330
C	-4.7441	0.0843	3.3879
C	4.0965	7.0746	1.6698
C	2.0034	6.8818	2.5850
C	-5.9830	0.3081	3.8354
C	-1.3173	-4.5110	-3.3928
C	3.7807	2.9025	-3.3743
C	-0.6748	-3.6158	-4.1414
C	3.8688	2.7533	3.3852
C	-1.9877	5.0753	-0.6723
C	-5.6529	4.3893	-2.6361
C	-1.3952	5.2728	0.6543
C	4.1766	3.3929	-0.6724
C	5.8330	0.2392	-2.5129
C	-5.3321	-0.2654	-0.6759
C	3.8893	-2.7771	-3.3471
C	3.2170	1.8636	4.1321
C	-1.3339	-5.1808	-0.6999
C	-0.9402	6.2039	4.9719
C	-2.7806	-5.5762	4.9544
C	-1.5211	-4.5162	3.3518
C	5.6264	-1.4529	1.9836
C	-1.2935	4.6119	3.3532
C	-7.3893	-3.3585	1.6956

C	-0.1579	4.0655	5.2822
C	-3.8953	0.9659	5.3425
C	-2.8776	5.5461	-5.0132
C	4.5958	-3.8086	3.8364
C	3.2340	-1.8959	-4.1013
C	-5.3443	0.2954	0.6791
C	4.4934	2.9246	0.6805
C	3.7276	-2.8946	3.3957
C	5.0001	3.2960	3.8435
C	4.6330	3.8344	-3.8011
C	1.5801	-5.7886	2.5143
C	-1.6571	4.4814	-3.3740
C	5.5153	-2.9392	-4.9711
C	7.0257	0.2181	2.7350
C	-4.5213	3.6548	2.5665
C	5.4788	2.9325	5.0236
C	4.8596	-2.0579	-5.7174
C	-5.1275	1.1950	5.7779
C	4.8294	2.0378	5.7575
C	-2.7715	-4.4727	5.6922
C	7.0537	-0.2503	-2.6802
C	-2.8518	4.4411	-5.7515
C	1.9873	-8.0398	2.2810
C	7.9131	-1.6791	1.7852
C	4.4009	-4.3969	5.0044
C	2.4901	-3.1568	5.3168
C	-2.2312	3.3589	-5.3051
C	3.3496	-4.0706	5.7452
C	4.4372	4.4217	-4.9706
C	8.1139	0.4513	-2.2934
C	2.5612	3.1419	-5.3160
C	8.0824	-0.4919	2.3545
C	0.3902	-5.9368	1.9340
C	6.6920	-2.1591	1.5988
C	7.9534	1.6456	-1.7348
C	4.1361	-7.1170	-1.7151
C	-4.7377	-0.0439	-3.3829
C	-6.2465	-5.1328	-2.2916
C	-3.6892	-0.3813	-4.1320
C	-6.1503	-0.8507	-5.0179
C	-4.1331	-5.6753	-1.5833
C	2.0446	-6.9183	-2.6534
C	-5.4048	-6.0027	-1.7507
C	-4.5438	-3.6005	-2.5016
C	2.0876	-5.6052	-2.4780
C	3.1612	-5.0370	-1.9196
C	3.0681	-7.6758	-2.2765
C	4.1834	-5.8047	-1.5329
C	-3.8722	-0.9579	-5.3136
C	-5.9733	-0.2731	-3.8380
C	0.8072	-8.1931	1.7020
C	-3.6924	-4.4729	-1.9585
C	-5.8149	-3.9335	-2.6658
C	6.7356	2.1412	-1.5672
C	3.7201	-1.5373	-5.2827
C	3.6999	1.5039	5.3124
C	-5.1013	-1.1910	-5.7568
C	1.4926	5.6464	-2.5600
C	0.8064	8.1137	-1.8555
C	-0.0331	7.1098	-1.6413
C	0.0123	-7.1476	1.5252
C	2.6786	-2.5657	4.1468
C	0.3026	5.8683	-1.9981
C	4.4877	-2.9632	-0.6418
C	-5.4518	6.0330	1.8226
C	2.3711	-6.8380	2.6854
C	-5.7940	3.9641	2.7730
C	-6.2610	5.1514	2.4048

C	-7.4485	3.3390	-1.6451
C	-2.1350	-3.3936	5.2682
C	2.7489	2.5545	-4.1428
C	-0.3021	5.3067	5.7163
C	-0.1796	-3.9673	-5.3198
C	-0.3274	-5.2096	-5.7556
C	2.3280	6.6550	-2.7703
C	3.4030	4.0752	-5.7286
C	-1.4738	-5.7580	-3.8418
C	1.9861	7.8877	-2.4223
C	-0.9716	-6.1049	-5.0151
C	-1.4400	5.8602	3.7966
H	-1.0617	7.1702	5.3158
H	0.0749	5.5773	6.6408
H	0.3315	3.3606	5.8604
H	-0.5559	2.7395	3.7803
H	-1.9674	6.5583	3.2422
H	1.2628	4.9802	2.7703
H	1.1662	7.3154	3.0024
H	2.9836	8.6639	2.3080
H	4.8945	7.6604	1.3713
H	5.0039	5.3396	1.1234
H	2.6352	8.6756	-2.5943
H	3.2438	6.4719	-3.2143
H	0.5353	9.0750	-1.5869
H	-0.9511	7.3100	-1.2080
H	1.7612	4.6883	-2.8474
H	7.1513	1.1419	3.1847
H	9.0377	-0.1240	2.5050
H	5.4986	4.0188	3.2954
H	6.3532	3.3586	5.3768
H	2.3251	1.4559	3.7980
H	3.1837	0.8135	5.8828
H	5.2020	1.7642	6.6823
H	8.7343	-2.2360	1.4910
H	6.5830	-3.0902	1.1604
H	4.9835	0.2951	2.8671
H	6.6337	3.0777	-1.1382
H	8.7786	2.1954	-1.4352
H	9.0662	0.0716	-2.4295
H	7.1743	-1.1792	-3.1207
H	5.0098	-0.3074	-2.8283
H	2.0129	-1.8400	3.8260
H	1.6733	-2.8922	5.8931
H	3.2074	-4.5251	6.6629
H	5.0791	-5.1004	5.3445
H	5.4384	-4.0445	3.2842
H	-1.0027	-2.5718	3.7818
H	-2.1155	-2.5333	5.8434
H	-3.2567	-4.4575	6.6026
H	-3.2687	-6.4211	5.2902
H	-2.1368	-6.4824	3.2433
H	-2.7377	0.2210	3.8235
H	-3.0787	1.2103	5.9286
H	-5.2790	1.6198	6.7117
H	-7.1323	1.0362	5.3680
H	-6.8044	0.0212	3.2739
H	-4.1608	2.7316	2.8708
H	-3.5631	6.4347	1.1673
H	-5.8119	6.9616	1.5384
H	-7.2530	5.3950	2.5740
H	-6.4181	3.2755	3.2303
H	-7.1615	1.4117	-1.0589
H	-8.4344	3.3546	-1.3194
H	-7.4853	5.2675	-2.3333
H	-5.2339	5.2226	-3.0871
H	-3.9434	3.2769	-2.8386
H	-1.1353	2.5333	-3.7848

H	-2.2709	6.4505	-3.2841
H	-2.2002	2.4978	-5.8793
H	-3.3111	4.4281	-6.6793
H	-3.3536	6.3935	-5.3651
H	-2.7270	-0.1842	-3.8006
H	-3.0499	-1.2139	-5.8862
H	-5.2456	-1.6309	-6.6839
H	-7.1095	-1.0224	-5.3692
H	-6.7992	0.0196	-3.2866
H	-4.2102	-2.6683	-2.8121
H	-3.4921	-6.3707	-1.1675
H	-5.7372	-6.9405	-1.4638
H	-7.2372	-5.3951	-2.4260
H	-6.4655	-3.2543	-3.0935
H	-8.3784	-3.3978	1.3865
H	-7.1543	-1.4256	1.0927
H	-5.1141	-5.1837	3.1149
H	-7.3750	-5.2830	2.4045
H	-3.8701	-3.2092	2.8241
H	-0.9075	-7.2916	1.0822
H	0.5003	-9.1305	1.3974
H	2.6029	-8.8588	2.4230
H	3.2878	-6.7159	3.1437
H	1.8804	-4.8564	2.8482
H	5.0290	-5.3900	-1.1031
H	4.9383	-7.7040	-1.4271
H	3.0389	-8.6999	-2.4243
H	1.2117	-7.3487	-3.0950
H	1.2933	-5.0184	-2.7926
H	-0.5674	-2.6397	-3.8114
H	0.3137	-3.2630	-5.8955
H	0.0520	-5.4810	-6.6777
H	-1.0978	-7.0713	-5.3604
H	-2.0076	-6.4543	-3.2913
H	2.3364	-1.4966	-3.7726
H	3.1991	-0.8567	-5.8630
H	5.2356	-1.7848	-6.6438
H	6.3987	-3.3543	-5.3145
H	5.5326	-4.0195	-3.2356
H	5.4626	4.0866	-3.2356
H	2.0958	1.8169	-3.8320
H	1.7582	2.8615	-5.9054
H	3.2590	4.5301	-6.6466
H	5.1000	5.1429	-5.2984
H	3.2055	-3.8854	0.7368
H	4.8174	-4.1094	1.0691
H	4.6393	-1.9308	-0.6921
H	5.3802	-3.3937	-0.9644
H	-1.4782	-6.1489	-1.0591
H	-2.6096	-4.2715	0.6937
H	-6.2988	-0.4485	-1.0211
H	-4.8743	1.2271	0.7255
H	-2.7373	4.3484	-0.6686
H	-1.5505	6.2441	0.9991
H	3.2577	3.8869	-0.7157
H	4.6388	1.8909	0.7186
H	4.8819	4.0834	-1.0075
H	5.3816	3.3436	1.0302
H	-0.3016	-5.0238	-0.7288
H	-2.3603	-5.8915	0.9710
H	-4.8416	-1.1869	-0.7178
H	-6.3187	0.4541	1.0154
H	-2.4445	5.9459	-1.0180
H	-0.3595	5.1402	0.6502

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2 NHC T1 Excited State

Au	-1.4597	1.8749	1.2489
Au	0.0769	2.3744	-1.2454

N	0.4709	4.6824	-3.0667
N	-0.3897	5.2388	-1.2849
C	0.1040	4.2148	-1.9191
C	0.1948	5.9684	-3.1586
H	0.4110	6.5307	-3.9905
C	-0.3487	6.3189	-2.0391
H	-0.6855	7.2366	-1.7195
C	1.1050	3.9222	-4.0755
H	1.2553	2.9929	-3.6264
C	0.2354	3.7563	-5.2224
H	0.7003	3.1432	-5.9262
H	0.0212	4.6697	-5.6786
H	-0.6540	3.2913	-4.9468
C	2.3822	4.5165	-4.4243
H	2.9914	4.6328	-3.5865
H	2.2615	5.4475	-4.8789
H	2.8754	3.9040	-5.1077
C	-0.8968	5.1804	0.0057
N	-2.7356	4.4828	1.3124
N	-3.1242	3.5154	3.0854
C	-2.5416	3.3587	1.9412
C	-3.4107	5.3273	2.0658
H	-3.6712	6.2705	1.7507
C	-3.6556	4.7171	3.1793
H	-4.1688	5.0409	4.0096
C	-2.2887	4.7364	0.0232
C	-3.2075	2.5183	4.0830
H	-2.7518	1.6899	3.6433
C	-2.4549	2.8955	5.2624
H	-2.8599	3.7384	5.7238
H	-1.4600	3.0805	5.0213
H	-2.4699	2.1118	5.9475
C	-4.5982	2.2215	4.3777
H	-4.6498	1.4389	5.0628
H	-5.1183	1.9418	3.5201
H	-5.0813	3.0405	4.8056
H	-0.7947	6.1216	0.4391
H	-0.3195	4.4980	0.5407
H	-2.9172	5.4466	-0.4057
H	-2.3639	3.8487	-0.5169
Au	2.2577	-0.6635	1.3004
Au	1.3045	-1.9950	-1.2515
N	2.4193	-4.0012	-3.1301
N	3.4664	-3.9362	-1.3612
C	2.4470	-3.4129	-1.9780
C	3.4051	-4.8681	-3.2351
H	3.5552	-5.4487	-4.0700
C	4.0672	-4.8268	-2.1254
H	4.8902	-5.3616	-1.8193
C	1.4368	-3.7764	-4.1206
H	0.7856	-3.0957	-3.6727
C	2.0153	-3.1652	-5.2996
H	1.2598	-2.9590	-5.9865
H	2.7095	-3.7941	-5.7592
H	2.4726	-2.2608	-5.0621
C	0.7352	-5.0119	-4.4192
H	0.3228	-5.4335	-3.5600
H	1.3674	-5.7134	-4.8637
H	-0.0350	-4.8199	-5.0933
C	3.8424	-3.5977	-0.0691
N	4.8677	-1.9357	1.2560
N	4.6057	-0.9913	3.0635
C	4.0351	-1.1871	1.9204
C	5.9295	-2.2149	1.9862
H	6.7088	-2.7921	1.6416
C	5.7656	-1.6173	3.1209
H	6.3793	-1.5845	3.9445
C	4.6490	-2.3806	-0.0401

C	4.0794	-0.1801	4.0950
H	3.2300	0.2479	3.6670
C	3.6793	-0.9812	5.2348
H	4.4950	-1.4625	5.6726
H	2.9706	-1.6888	4.9547
H	3.2373	-0.3674	5.9529
C	5.0334	0.8568	4.4464
H	4.6077	1.4936	5.1519
H	5.3063	1.4224	3.6155
H	5.8963	0.4560	4.8728
H	4.3579	-4.4031	0.3424
H	2.9719	-3.4362	0.4810
H	5.5744	-2.5289	-0.4928
H	4.1406	-1.6277	-0.5503
Au	1.2454	1.9878	1.3362
Au	2.2538	0.5806	-1.3702
N	4.5592	1.0277	-3.1144
N	4.8074	1.9896	-1.3124
C	3.9925	1.2163	-1.9671
C	5.6995	1.6860	-3.1838
H	6.3071	1.6656	-4.0121
C	5.8562	2.2925	-2.0529
H	6.6209	2.8912	-1.7168
C	4.0490	0.1910	-4.1338
H	3.1944	-0.2280	-3.7065
C	3.6605	0.9636	-5.2955
H	3.2312	0.3299	-6.0033
H	4.4799	1.4358	-5.7360
H	2.9454	1.6769	-5.0433
C	5.0060	-0.8537	-4.4505
H	5.2747	-1.3938	-3.6014
H	5.8706	-0.4634	-4.8844
H	4.5855	-1.5124	-5.1391
C	4.5915	2.4198	-0.0120
N	3.4023	3.9439	1.3319
N	2.4140	3.9907	3.1361
C	2.4177	3.4018	1.9851
C	4.0126	4.8449	2.0763
H	4.8145	5.3940	1.7411
C	3.3872	4.8760	3.2068
H	3.5525	5.4601	4.0358
C	3.7433	3.6064	0.0311
C	1.4648	3.7506	4.1563
H	0.8124	3.0570	3.7310
C	2.0906	3.1524	5.3179
H	2.7921	3.7925	5.7509
H	2.5517	2.2540	5.0657
H	1.3611	2.9380	6.0304
C	0.7486	4.9723	4.4730
H	-0.0022	4.7643	5.1637
H	0.3089	5.3880	3.6245
H	1.3768	5.6848	4.9048
H	5.5167	2.6012	0.4293
H	4.1183	1.6474	0.5030
H	4.2148	4.4251	-0.4058
H	2.8605	3.4098	-0.4866
Au	0.1419	-2.3754	1.2595
Au	-1.4252	-1.8432	-1.3215
N	-3.1347	-3.4891	-3.0646
N	-2.7762	-4.4130	-1.2640
C	-2.5523	-3.3145	-1.9234
C	-3.6906	-4.6817	-3.1278
H	-4.2050	-5.0186	-3.9525
C	-3.4652	-5.2649	-1.9966
H	-3.7488	-6.1922	-1.6564
C	-3.1939	-2.5196	-4.0927
H	-2.7884	-1.6654	-3.6529
C	-2.3679	-2.9063	-5.2184

H	-2.3888	-2.1525	-5.9382
H	-2.7084	-3.7886	-5.6594
H	-1.3768	-3.0260	-4.9249
C	-4.5742	-2.2760	-4.4693
H	-5.1538	-2.0075	-3.6462
H	-5.0043	-3.1126	-4.9200
H	-4.6121	-1.5015	-5.1640
C	-2.3375	-4.6434	0.0315
N	-0.4767	-5.2174	1.3527
N	0.3840	-4.6614	3.1345
C	0.0268	-4.1957	1.9819
C	-0.4467	-6.2948	2.1111
H	-0.7911	-7.2104	1.7947
C	0.0971	-5.9430	3.2295
H	0.3064	-6.5037	4.0651
C	-0.9721	-5.1583	0.0588
C	1.0235	-3.9066	4.1427
H	1.1490	-2.9663	3.7089
C	0.1756	-3.7762	5.3112
H	-0.0112	-4.7010	5.7577
H	-0.7288	-3.3244	5.0622
H	0.6462	-3.1649	6.0113
C	2.3180	-4.4879	4.4534
H	2.8080	-3.8875	5.1490
H	2.9171	-4.5641	3.6038
H	2.2196	-5.4369	4.8768
H	-2.9991	-5.3060	0.4870
H	-2.3656	-3.7349	0.5406
H	-0.9190	-6.1122	-0.3545
H	-0.3580	-4.5170	-0.4875
Au	0.0039	0.0013	-2.8531
Au	-2.1571	-0.8346	1.3727
Au	-2.1767	0.8839	-1.3101
Au	0.0071	0.0012	0.0018
Au	0.0097	-0.0024	2.8578
Cl	-0.0449	0.0103	-5.1550
Cl	0.0514	0.0033	5.1598
N	-4.2955	1.7925	-3.1454
N	-5.0723	1.1800	-1.3440
C	-3.9531	1.3229	-1.9909
C	-5.6029	1.9285	-3.2237
H	-6.0790	2.2943	-4.0595
C	-6.0945	1.5396	-2.0943
H	-7.0680	1.5069	-1.7642
C	-3.3901	2.1612	-4.1656
H	-2.4527	1.9729	-3.7485
C	-3.5593	1.3258	-5.3376
H	-2.8426	1.5821	-6.0495
H	-4.5034	1.4473	-5.7663
H	-3.4149	0.3226	-5.0991
C	-3.5276	3.5771	-4.4613
H	-3.3917	4.1594	-3.6078
H	-4.4646	3.7950	-4.8662
H	-2.8129	3.8540	-5.1662
C	-5.1549	0.7102	-0.0428
N	-5.0419	-1.2231	1.2987
N	-4.2850	-1.8520	3.1068
C	-3.9321	-1.3657	1.9614
C	-6.0718	-1.6002	2.0311
H	-7.0402	-1.5720	1.6872
C	-5.5943	-1.9976	3.1648
H	-6.0791	-2.3763	3.9888
C	-5.1147	-0.7469	-0.0009
C	-3.3865	-2.2265	4.1328
H	-2.4464	-2.0901	3.7018
C	-3.5100	-1.3479	5.2791
H	-4.4591	-1.4076	5.7094
H	-3.3123	-0.3620	5.0113

H	-2.8087	-1.6215	6.0004
C	-3.5755	-3.6242	4.4757
H	-2.8531	-3.9123	5.1677
H	-3.4901	-4.2378	3.6378
H	-4.5063	-3.7902	4.9161
H	-6.0307	1.0777	0.3829
H	-4.3383	1.0873	0.4839
H	-5.9564	-1.1602	-0.4538
H	-4.2647	-1.0756	-0.5060

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3	NHC-iPr	T1	Excited	State
Au	2.3380	1.0570	1.3453	
Au	2.2762	-0.9507	-1.2779	
N	4.1433	-2.3430	-3.0062	
N	5.1399	-1.3690	-1.1676	
C	4.1158	-1.6648	-1.9025	
C	2.8873	-2.5663	-3.6698	
H	2.1746	-2.0812	-3.0806	
C	2.8316	-1.9659	-4.9902	
H	1.8545	-2.0332	-5.3529	
H	3.4624	-2.4306	-5.6818	
H	3.0631	-0.9511	-4.9544	
C	2.5381	-3.9752	-3.6968	
H	2.6658	-4.4083	-2.7569	
H	3.0807	-4.5258	-4.4006	
H	1.5294	-4.0611	-3.9463	
C	4.9451	-0.7053	0.0637	
N	5.2462	1.4067	1.2354	
N	4.2893	2.3798	3.0984	
C	4.2439	1.7221	1.9870	
C	5.0018	0.7641	0.0015	
C	3.0357	2.6203	3.7580	
C	2.9759	2.0486	5.0921	
H	3.6248	2.5049	5.7709	
H	3.1731	1.0248	5.0764	
H	2.0073	2.1559	5.4599	
C	2.6893	4.0330	3.7485	
H	1.6830	4.1320	3.9926	
H	2.8211	4.4403	2.7977	
H	3.2340	4.5983	4.4384	
H	5.6785	-1.0508	0.7166	
H	4.0190	-0.9949	0.4511	
H	5.7589	1.0548	-0.6495	
H	4.1007	1.1247	-0.3832	
H	2.3228	2.1221	3.1765	
C	5.3322	3.0599	3.8510	
H	4.7740	3.4756	4.6237	
C	5.9128	4.2292	3.1966	
C	6.2673	2.1918	4.5591	
H	5.7502	1.4526	5.0828	
H	6.9842	1.7254	3.9692	
H	6.7779	2.7714	5.2584	
H	6.6071	4.0287	2.4454	
H	6.4038	4.7947	3.9253	
H	5.1615	4.8237	2.7873	
C	5.1725	-3.0370	-3.7673	
H	4.6032	-3.4304	-4.5416	
C	5.7238	-4.2312	-3.1269	
C	6.1265	-2.1921	-4.4766	
H	5.6223	-1.4463	-5.0041	
H	6.8567	-1.7360	-3.8920	
H	6.6225	-2.7932	-5.1739	
H	6.4169	-4.0587	-2.3691	
H	6.2090	-4.7984	-3.8582	
H	4.9558	-4.8138	-2.7310	
C	6.6111	1.7265	1.4825	
H	6.5922	2.2940	2.3399	
C	7.1997	2.5641	0.4436	



C	7.4347	0.5619	1.7772
H	7.0143	-0.0213	2.5348
H	7.5900	-0.0394	0.9397
H	8.3763	0.8800	2.1006
H	7.4307	2.0399	-0.4281
H	8.0965	2.9652	0.7953
H	6.5687	3.3564	0.1944
C	6.4855	-1.7517	-1.4261
H	6.4341	-2.3238	-2.2771
C	7.0438	-2.6107	-0.3894
C	7.3639	-0.6339	-1.7364
H	6.9616	-0.0264	-2.4825
H	7.5719	-0.0443	-0.9044
H	8.2780	-1.0064	-2.0809
H	7.2982	-2.0950	0.4809
H	7.9233	-3.0490	-0.7460
H	6.3819	-3.3768	-0.1377
Au	1.5685	-1.8874	1.2495
Au	-0.1998	-2.4530	-1.2379
N	-0.9601	-4.6265	-3.0427
N	0.2381	-5.3000	-1.1929
C	-0.3342	-4.3976	-1.9316
C	-1.5410	-3.4938	-3.7063
H	-1.2788	-2.6664	-3.1206
C	-0.9944	-3.2804	-5.0352
H	-1.3658	-2.3808	-5.4104
H	-1.2434	-4.0376	-5.7127
H	0.0453	-3.1812	-5.0073
C	-2.9968	-3.5725	-3.7209
H	-3.3672	-3.8101	-2.7767
H	-3.3688	-4.2623	-4.4159
H	-3.3798	-2.6382	-3.9755
C	0.8076	-4.9209	0.0404
N	2.8871	-4.4308	1.1973
N	3.4860	-3.1697	3.0312
C	2.8398	-3.3566	1.9239
C	2.2027	-4.4643	-0.0353
C	3.3199	-1.8985	3.6811
C	2.7234	-2.0183	4.9985
H	3.3422	-2.5028	5.6890
H	1.8078	-2.5170	4.9560
H	2.5190	-1.0624	5.3661
C	4.5664	-1.1501	3.7158
H	4.3524	-0.1606	3.9557
H	5.0295	-1.1517	2.7821
H	5.2427	-1.5043	4.4293
H	0.7484	-5.7465	0.6708
H	0.2223	-4.1648	0.4605
H	2.7380	-5.0968	-0.6644
H	2.2275	-3.5097	-0.4575
H	2.6522	-1.3657	3.0794
C	4.4478	-3.9403	3.8066
H	4.6464	-3.2766	4.5803
C	5.7602	-4.1116	3.1824
C	3.9168	-5.0993	4.5175
H	3.0529	-4.8352	5.0397
H	3.6971	-5.9335	3.9346
H	4.6342	-5.3947	5.2212
H	5.8120	-4.8233	2.4248
H	6.4375	-4.4048	3.9232
H	6.0919	-3.2033	2.7907
C	-1.3187	-5.8174	-3.7993
H	-1.8707	-5.3970	-4.5728
C	-2.2923	-6.6981	-3.1531
C	-0.2252	-6.4748	-4.5145
H	0.3254	-5.7719	-5.0551
H	0.4421	-7.0195	-3.9301
H	-0.6489	-7.1408	-5.2029

H	-1.9219	-7.2978	-2.3881
H	-2.6845	-7.3376	-3.8816
H	-3.0820	-6.1362	-2.7639
C	3.6493	-5.6002	1.4704
H	4.1715	-5.3806	2.3271
C	4.6445	-5.8846	0.4437
C	2.8357	-6.7694	1.7707
H	2.1308	-6.5662	2.5123
H	2.3398	-7.1370	0.9313
H	3.4561	-7.5365	2.1165
H	4.2332	-6.2850	-0.4278
H	5.3196	-6.5938	0.8094
H	5.1825	-5.0273	0.1912
C	0.3021	-6.6954	-1.4589
H	-0.2523	-6.8261	-2.3147
C	-0.3361	-7.5055	-0.4270
C	1.6465	-7.1685	-1.7615
H	2.0954	-6.5959	-2.5102
H	2.2680	-7.1704	-0.9239
H	1.5929	-8.1558	-2.1004
H	0.2356	-7.5908	0.4439
H	-0.4712	-8.4753	-0.7914
H	-1.2736	-7.1227	-0.1691
Au	-1.3063	-2.0951	1.2420
Au	-2.4824	-0.5842	-1.3434
N	-4.8717	-0.5403	-3.0627
N	-5.0911	-1.9014	-1.2095
C	-4.4573	-1.0541	-1.9516
C	-4.0017	0.4114	-3.6986
H	-3.1623	0.4697	-3.0771
C	-3.5440	-0.0305	-5.0035
H	-2.8423	0.6522	-5.3671
H	-4.3126	-0.1022	-5.7099
H	-3.0542	-0.9494	-4.9419
C	-4.5943	1.7382	-3.7485
H	-4.9967	2.0017	-2.8235
H	-5.3358	1.8347	-4.4777
H	-3.8466	2.4260	-3.9736
C	-4.5255	-2.2858	0.0258
N	-3.3906	-4.1020	1.1897
N	-1.9997	-4.2920	3.0205
C	-2.3823	-3.7298	1.9157
C	-3.6364	-3.4561	-0.0409
C	-0.8535	-3.7272	3.6777
C	-1.1588	-3.2145	5.0020
H	-1.4096	-3.9636	5.6912
H	-1.9355	-2.5159	4.9664
H	-0.3207	-2.7084	5.3692
C	0.2661	-4.6559	3.7013
H	1.1325	-4.1268	3.9442
H	0.4143	-5.0832	2.7612
H	0.1590	-5.4197	4.4107
H	-5.3133	-2.4825	0.6768
H	-3.9940	-1.4738	0.4113
H	-4.0499	-4.1641	-0.6811
H	-2.7208	-3.1627	-0.4491
H	-0.5708	-2.9123	3.0865
C	-2.4121	-5.4622	3.7828
H	-1.7151	-5.4457	4.5530
C	-2.1504	-6.7479	3.1366
C	-3.6782	-5.3500	4.5040
H	-3.7085	-4.4576	5.0439
H	-4.5409	-5.4024	3.9246
H	-3.7206	-6.1363	5.1934
H	-2.8126	-7.0142	2.3779
H	-2.2031	-7.4970	3.8677
H	-1.1843	-6.7594	2.7374
C	-6.0905	-0.6363	-3.8525

H	-5.8682	0.0153	-4.6315
C	-7.2753	-0.0328	-3.2444
C	-6.3015	-1.9044	-4.5430
H	-5.4297	-2.1952	-5.0370
H	-6.6134	-2.6993	-3.9473
H	-7.0411	-1.7546	-5.2680
H	-7.7247	-0.5867	-2.4860
H	-7.9922	0.1002	-3.9921
H	-7.0428	0.9060	-2.8574
C	-4.2513	-5.2024	1.4550
H	-3.8688	-5.6352	2.3049
C	-4.2053	-6.2274	0.4182
C	-5.6179	-4.8109	1.7699
H	-5.6456	-4.0885	2.5226
H	-6.1314	-4.4476	0.9389
H	-6.1435	-5.6486	2.1084
H	-4.7175	-5.9613	-0.4511
H	-4.6594	-7.0961	0.7781
H	-3.2213	-6.4605	0.1610
C	-6.3845	-2.4366	-1.4671
H	-6.6910	-1.9675	-2.3293
C	-7.3584	-2.0912	-0.4391
C	-6.3774	-3.8636	-1.7540
H	-5.6801	-4.1009	-2.4935
H	-6.1782	-4.4402	-0.9090
H	-7.3224	-4.1480	-2.0990
H	-7.2414	-2.6419	0.4407
H	-8.3192	-2.2971	-0.7957
H	-7.3135	-1.0757	-0.2015
Au	-2.4089	0.6127	1.2645
Au	-1.2875	2.1483	-1.2573
N	-2.0025	4.2791	-3.0835
N	-3.3660	4.1184	-1.2306
C	-2.3714	3.7283	-1.9683
C	-0.8723	3.6998	-3.7498
H	-0.6089	2.8669	-3.1757
C	-1.1920	3.2179	-5.0813
H	-0.3681	2.6969	-5.4588
H	-1.4257	3.9833	-5.7561
H	-1.9836	2.5386	-5.0518
C	0.2653	4.6073	-3.7460
H	0.4164	5.0052	-2.7944
H	0.1711	5.3916	-4.4309
H	1.1223	4.0747	-4.0004
C	-3.5993	3.4783	0.0021
N	-4.9942	1.8676	1.1606
N	-4.7309	0.5116	3.0081
C	-4.3254	1.0357	1.8941
C	-4.4584	2.2890	-0.0734
C	-3.8463	-0.4189	3.6536
C	-3.4079	0.0391	4.9614
H	-4.1784	0.0733	5.6682
H	-2.9627	0.9815	4.9043
H	-2.6754	-0.6108	5.3224
C	-4.4190	-1.7543	3.7051
H	-3.6646	-2.4320	3.9437
H	-4.8039	-2.0316	2.7753
H	-5.1671	-1.8578	4.4299
H	-4.0352	4.1802	0.6340
H	-2.6790	3.2128	0.4209
H	-5.2624	2.4843	-0.7041
H	-3.9183	1.4983	-0.4909
H	-3.0016	-0.4660	3.0388
C	-5.9549	0.5755	3.7913
H	-5.7190	-0.0716	4.5696
C	-7.1196	-0.0632	3.1804
C	-6.2039	1.8319	4.4922
H	-5.3436	2.1389	4.9967

H	-6.5312	2.6249	3.9035
H	-6.9439	1.6547	5.2092
H	-7.5835	0.4744	2.4178
H	-7.8365	-0.2156	3.9287
H	-6.8558	-0.9973	2.7971
C	-2.4024	5.4613	-3.8297
H	-1.7090	5.4444	-4.6035
C	-2.1254	6.7407	-3.1768
C	-3.6728	5.3662	-4.5441
H	-3.7117	4.4778	-5.0898
H	-4.5325	5.4208	-3.9590
H	-3.7157	6.1570	-5.2273
H	-2.7793	7.0129	-2.4129
H	-2.1754	7.4910	-3.9039
H	-1.1582	6.7430	-2.7864
C	-6.2948	2.3717	1.4374
H	-6.5856	1.8888	2.2964
C	-7.2706	2.0175	0.4139
C	-6.3158	3.7964	1.7386
H	-5.6127	4.0431	2.4693
H	-6.1442	4.3860	0.8963
H	-7.2619	4.0546	2.1008
H	-7.1754	2.5837	-0.4592
H	-8.2326	2.1956	0.7838
H	-7.2022	1.0063	0.1619
C	-4.2270	5.2192	-1.4892
H	-3.8565	5.6483	-2.3457
C	-4.1675	6.2446	-0.4539
C	-5.5975	4.8282	-1.7852
H	-5.6349	4.1153	-2.5463
H	-6.0954	4.4517	-0.9508
H	-6.1318	5.6684	-2.1032
H	-4.6771	5.9797	0.4181
H	-4.6195	7.1163	-0.8100
H	-3.1802	6.4709	-0.2026
Au	-0.1549	2.4971	1.2257
Au	1.5911	1.9200	-1.2331
N	3.5217	3.1766	-3.0235
N	2.9497	4.4511	-1.1889
C	2.8911	3.3728	-1.9070
C	3.3468	1.8990	-3.6531
H	2.6773	1.3805	-3.0394
C	2.7393	1.9998	-4.9687
H	2.5216	1.0417	-5.3173
H	3.3556	2.4624	-5.6750
H	1.8297	2.5093	-4.9296
C	4.5893	1.1433	-3.6802
H	5.0529	1.1583	-2.7465
H	5.2678	1.4823	-4.4025
H	4.3719	0.1491	-3.9040
C	2.2751	4.4985	0.0477
N	0.3158	5.3284	1.2085
N	-0.8788	4.6449	3.0574
C	-0.2620	4.4217	1.9379
C	0.8805	4.9562	-0.0265
C	-1.4567	3.5080	3.7116
C	-0.9204	3.2926	5.0424
H	-1.1894	4.0400	5.7231
H	0.1210	3.2116	5.0221
H	-1.2785	2.3839	5.4080
C	-2.9114	3.5777	3.7044
H	-3.2967	2.6424	3.9535
H	-3.2637	3.8166	2.7537
H	-3.2978	4.2671	4.3918
H	2.8149	5.1374	0.6662
H	2.3010	3.5482	0.4799
H	0.8204	5.7836	-0.6547
H	0.2938	4.2013	-0.4492

Au	-0.0168	0.0174	-2.5638
Au	-0.0057	0.0236	-0.0024
Au	0.0029	0.0344	2.5587
Cl	-0.0627	-0.0075	-4.8342
Cl	0.0732	0.0494	4.8286
H	-1.1780	2.6838	3.1300
C	-1.2396	5.8302	3.8170
H	-1.7966	5.4061	4.5844
C	-2.2087	6.7191	3.1723
C	-0.1501	6.4819	4.5405
H	0.3929	5.7744	5.0824
H	0.5243	7.0248	3.9621
H	-0.5757	7.1496	5.2266
H	-1.8314	7.3312	2.4191
H	-2.6101	7.3489	3.9049
H	-2.9935	6.1612	2.7691
C	4.4791	3.9337	-3.8144
H	4.6693	3.2612	-4.5831
C	5.7968	4.1062	-3.2031
C	3.9451	5.0869	-4.5321
H	3.0803	4.8180	-5.0501
H	3.7250	5.9222	-3.9526
H	4.6572	5.3809	-5.2385
H	5.8596	4.8275	-2.4560
H	6.4684	4.3839	-3.9541
H	6.1267	3.2029	-2.8008
C	0.3837	6.7202	1.4858
H	-0.1642	6.8448	2.3457
C	-0.2605	7.5371	0.4640
C	1.7291	7.1910	1.7835
H	2.1822	6.6111	2.5233
H	2.3455	7.2006	0.9427
H	1.6769	8.1754	2.1317
H	0.3073	7.6272	-0.4087
H	-0.3951	8.5054	0.8352
H	-1.1986	7.1545	0.2099
C	3.7124	5.6151	-1.4785
H	4.2187	5.3899	-2.3438
C	4.7244	5.8967	-0.4667
C	2.8978	6.7864	-1.7713
H	2.1776	6.5797	-2.4982
H	2.4200	7.1630	-0.9247
H	3.5139	7.5484	-2.1354
H	4.3281	6.3036	0.4092
H	5.3987	6.5994	-0.8446
H	5.2594	5.0355	-0.2177

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Au	2.2103	1.0916	1.1952
Au	2.4222	-0.5598	-1.2375
N	4.4325	-0.8353	-3.4060
N	5.2485	-0.0392	-1.6702
C	4.1573	-0.5268	-2.1803
C	5.6958	-0.5222	-3.6925
C	6.2148	-0.0034	-2.5765
C	3.5108	-1.4501	-4.2798
H	2.6458	-1.5392	-3.7040
C	3.2054	-0.6034	-5.4175
H	2.4348	-1.0395	-5.9662
H	4.0250	-0.4719	-6.0464
H	2.8658	0.3282	-5.1000
C	3.9731	-2.7754	-4.6528
H	4.0857	-3.3831	-3.8143
H	4.8839	-2.7457	-5.1562
H	3.2783	-3.2158	-5.2908
C	5.3476	0.4371	-0.3773
N	4.8424	2.2836	0.9973
N	4.0789	2.6442	2.8966

C	3.8016	2.1052	1.7553
C	5.7970	2.9227	1.6594
C	5.3077	3.1607	2.8785
C	4.9358	1.8351	-0.3063
C	3.1725	2.6890	3.9778
H	2.3364	2.1739	3.6283
C	3.6863	1.9772	5.1316
H	4.4677	2.4820	5.5986
H	4.0208	1.0307	4.8582
H	2.9133	1.8582	5.8202
C	2.7946	4.0576	4.2781
H	2.1042	4.0568	5.0575
H	2.3545	4.5183	3.4541
H	3.6083	4.6321	4.5801
H	6.3248	0.3070	-0.0451
H	4.7146	-0.1349	0.2202
H	5.5982	2.4516	-0.8198
H	3.9952	1.9277	-0.7442
C	6.4332	-0.6225	-4.7952
C	7.4658	0.4331	-2.5178
C	7.6795	-0.1826	-4.7379
C	8.1903	0.3345	-3.6198
C	7.0143	3.3070	1.3012
C	6.0387	3.8032	3.7851
C	7.2518	4.1883	3.4281
C	7.7341	3.9460	2.2067
H	6.0614	-1.0228	-5.6710
H	8.2739	-0.2446	-5.5814
H	9.1709	0.6603	-3.6138
H	7.8665	0.8273	-1.6498
H	7.3903	3.1200	0.3567
H	8.6880	4.2638	1.9668
H	7.8434	4.6865	4.1140
H	5.6883	3.9977	4.7359
Au	-0.4799	2.3263	1.3030
Au	1.3595	2.0488	-1.6652
N	2.8445	4.0958	-3.1028
N	2.3787	4.7725	-1.1944
C	2.3058	3.7428	-1.9794
C	3.2457	5.3661	-3.0463
C	2.9415	5.7990	-1.8203
C	3.0272	3.2053	-4.1829
H	2.6237	2.3121	-3.8226
C	2.2656	3.6112	-5.3491
H	2.3661	2.8860	-6.0912
H	2.5957	4.5172	-5.7428
H	1.2544	3.6987	-5.1174
C	4.4368	3.0040	-4.4633
H	4.9508	2.6941	-3.6117
H	4.8933	3.8668	-4.8256
H	4.5389	2.2636	-5.1890
C	1.9107	4.7932	0.1060
N	0.0258	5.1790	1.4563
N	-0.8608	4.5391	3.2241
C	-0.4722	4.1410	2.0569
C	-0.0126	6.2406	2.2499
C	-0.5980	5.8375	3.3808
C	0.5049	5.1721	0.1596
C	-1.5625	3.7112	4.1295
H	-1.4865	2.7643	3.6992
C	-0.9333	3.6616	5.4342
H	-0.9890	4.5684	5.9411
H	0.0601	3.3674	5.3572
H	-1.4203	2.9440	6.0109
C	-2.9590	4.1065	4.1849
H	-3.4817	3.4516	4.8040
H	-3.3946	4.0807	3.2393
H	-3.0725	5.0668	4.5716

H	2.4995	5.4510	0.6583
H	2.0233	3.8369	0.5039
H	0.3546	6.1171	-0.2507
H	-0.0547	4.4828	-0.3850
C	3.8345	6.1755	-3.9212
C	3.2127	7.0352	-1.4235
C	4.1006	7.4107	-3.5269
C	3.7983	7.8347	-2.2975
C	0.4043	7.4889	2.0774
C	-0.8057	6.6966	4.3749
C	-0.3885	7.9393	4.2055
C	0.2100	8.3307	3.0783
H	4.0762	5.8701	-4.8765
H	4.5552	8.0625	-4.1872
H	4.0272	8.8060	-2.0260
H	2.9837	7.3643	-0.4707
H	0.8563	7.7995	1.2008
H	0.5219	9.3120	2.9856
H	-0.5321	8.6254	4.9653
H	-1.2743	6.4201	5.2525
Au	-2.2784	0.2533	1.2021
Au	-1.4690	1.7818	-1.2457
N	-2.8861	3.4463	-3.2464
N	-3.9555	3.2628	-1.4736
C	-2.8180	2.9841	-2.0402
C	-4.0794	3.9981	-3.4666
C	-4.7659	3.8728	-2.3274
C	-1.7932	3.4323	-4.1397
H	-1.0416	2.9597	-3.5914
C	-2.0661	2.6307	-5.3175
H	-1.2184	2.6173	-5.9244
H	-2.8552	3.0097	-5.8812
H	-2.2722	1.6447	-5.0561
C	-1.3727	4.7892	-4.4435
H	-1.1523	5.3159	-3.5727
H	-2.0981	5.3187	-4.9697
H	-0.5162	4.7633	-5.0347
C	-4.2593	2.9546	-0.1587
N	-5.0017	1.2464	1.2834
N	-4.5446	0.3635	3.1085
C	-4.0899	0.5683	1.9149
C	-6.0274	1.5057	2.0821
C	-5.7382	0.9374	3.2563
C	-4.8922	1.6441	-0.0385
C	-3.8738	-0.4323	4.0620
H	-3.0156	-0.7420	3.5555
C	-3.4627	0.3410	5.2184
H	-4.2738	0.7219	5.7493
H	-2.8403	1.1253	4.9349
H	-2.9162	-0.2708	5.8614
C	-4.6691	-1.5996	4.4009
H	-4.1249	-2.2136	5.0417
H	-4.9116	-2.1496	3.5502
H	-5.5533	-1.3470	4.8883
H	-4.8643	3.7086	0.2277
H	-3.3637	2.9411	0.3717
H	-5.8414	1.6350	-0.4663
H	-4.2998	0.9415	-0.5278
C	-4.6334	4.5776	-4.5277
C	-6.0120	4.3094	-2.2050
C	-5.8780	5.0114	-4.4071
C	-6.5583	4.8805	-3.2649
C	-7.1548	2.1746	1.8844
C	-6.5845	1.0303	4.2782
C	-7.7065	1.7021	4.0819
C	-7.9897	2.2649	2.9054
H	-4.1268	4.6892	-5.4202
H	-6.3341	5.4638	-5.2180

H	-7.5285	5.2333	-3.2094
H	-6.5409	4.2138	-1.3215
H	-7.3789	2.6106	0.9744
H	-8.8784	2.7797	2.7904
H	-8.3822	1.7894	4.8593
H	-6.3856	0.6033	5.1970
Au	-0.9076	-2.2489	1.6482
Au	-2.1317	-0.9106	-1.3372
N	-4.2764	-1.7597	-3.1833
N	-4.3645	-2.7487	-1.3567
C	-3.7035	-1.8567	-2.0286
C	-5.3073	-2.6025	-3.2590
C	-5.3542	-3.2446	-2.0875
C	-3.9058	-0.8059	-4.1582
H	-3.0408	-0.3776	-3.7639
C	-3.5616	-1.4232	-5.4234
H	-3.1970	-0.6876	-6.0639
H	-4.3782	-1.8753	-5.8841
H	-2.8045	-2.1239	-5.2988
C	-4.9363	0.2100	-4.2811
H	-5.1223	0.6692	-3.3645
H	-5.8315	-0.1865	-4.6362
H	-4.6239	0.9401	-4.9549
C	-4.0624	-3.1284	-0.0609
N	-2.7217	-4.5352	1.2607
N	-1.8237	-4.5794	3.1350
C	-1.8483	-3.9378	2.0100
C	-3.2783	-5.5511	1.9106
C	-2.7002	-5.5828	3.1153
C	-3.0255	-4.1525	-0.0326
C	-0.9168	-4.2760	4.1745
H	-0.3789	-3.4684	3.7896
C	-1.5996	-3.8375	5.3772
H	-2.1925	-4.5868	5.7917
H	-2.1985	-3.0087	5.1821
H	-0.8908	-3.5614	6.0904
C	-0.0035	-5.3795	4.4096
H	0.7231	-5.0834	5.0949
H	0.4776	-5.6655	3.5313
H	-0.4876	-6.2126	4.8028
H	-4.9355	-3.4651	0.3941
H	-3.7261	-2.2863	0.4523
H	-3.3174	-4.9973	-0.5658
H	-2.1585	-3.7718	-0.4668
C	-6.2011	-2.8667	-4.2076
C	-6.2696	-4.1678	-1.8271
C	-7.1124	-3.7895	-3.9492
C	-7.1471	-4.4317	-2.7797
C	-4.2018	-6.4330	1.5524
C	-3.0457	-6.5079	4.0062
C	-3.9693	-7.3843	3.6506
C	-4.5371	-7.3519	2.4425
H	-6.1973	-2.3791	-5.1169
H	-7.8161	-4.0154	-4.6720
H	-7.8759	-5.1454	-2.6150
H	-6.3055	-4.6623	-0.9196
H	-4.6403	-6.4154	0.6169
H	-5.2523	-8.0576	2.1988
H	-4.2567	-8.1114	4.3257
H	-2.6203	-6.5519	4.9461
Au	1.8225	-1.6774	1.2339
Au	0.3456	-2.4216	-1.2030
N	0.0886	-4.8752	-2.8568
N	0.7993	-5.2719	-0.9456
C	0.3769	-4.3212	-1.7249
C	0.3409	-6.1831	-2.8115
C	0.8019	-6.4333	-1.5845
C	-0.4354	-4.1697	-3.9601



H	-0.4841	-3.1821	-3.6311
C	0.4652	-4.2186	-5.0952
H	0.1434	-3.5271	-5.8051
H	0.4960	-5.1581	-5.5423
H	1.4306	-3.9578	-4.8072
C	-1.7737	-4.6319	-4.2769
H	-2.4200	-4.4992	-3.4712
H	-1.7876	-5.6364	-4.5468
H	-2.1408	-4.0860	-5.0835
C	1.2388	-5.0775	0.3490
N	3.0023	-4.2967	1.6737
N	3.2343	-3.1604	3.3959
C	2.7946	-3.1171	2.1792
C	3.5488	-5.1044	2.5708
C	3.7065	-4.3752	3.6786
C	2.6353	-4.6566	0.3919
C	3.2186	-2.0554	4.2721
H	2.7914	-1.2936	3.7020
C	2.3585	-2.2949	5.4160
H	2.7285	-3.0408	6.0421
H	1.3991	-2.5551	5.1053
H	2.2730	-1.4148	5.9663
C	4.5738	-1.6787	4.6358
H	4.5440	-0.8648	5.2836
H	5.1283	-1.4138	3.7950
H	5.0765	-2.4470	5.1264
H	1.0921	-5.9587	0.8826
H	0.6510	-4.3324	0.7790
H	3.2733	-5.4069	0.0580
H	2.7562	-3.8218	-0.2195
Au	0.1196	0.0228	-2.7332
Au	0.0809	-0.0134	-0.0110
Au	0.0693	-0.0722	2.7089
Cl	-0.3052	-0.7284	-4.8384
Cl	0.3827	0.6231	4.8498
C	0.2201	-7.1664	-3.7001
C	1.1577	-7.6519	-1.1986
C	0.5739	-8.3813	-3.3164
C	1.0356	-8.6235	-2.0857
C	3.9116	-6.3792	2.5096
C	4.2419	-4.9146	4.7702
C	4.6038	-6.1857	4.7098
C	4.4436	-6.9081	3.5995
H	-0.1295	-7.0027	-4.6568
H	0.4923	-9.1647	-3.9863
H	1.3040	-9.5872	-1.8238
H	1.5146	-7.8414	-0.2474
H	3.7926	-6.9409	1.6492
H	4.7420	-7.8975	3.5905
H	5.0219	-6.6292	5.5452
H	4.3755	-4.3774	5.6411
255			
5 BenzoN T1 Excited State			
Au	2.3025	0.7476	1.2724
Au	2.2554	-0.8594	-1.1504
N	4.2260	-1.8291	-3.1170
N	5.1314	-0.9643	-1.4383
C	3.9822	-1.3006	-1.9584
C	5.5308	-1.8189	-3.3441
C	6.1047	-1.2607	-2.2773
C	3.2400	-2.3698	-3.9746
H	2.3456	-2.1643	-3.4774
C	3.2399	-1.6926	-5.2557
H	2.4658	-2.0724	-5.8400
H	4.1373	-1.8426	-5.7602
H	3.0689	-0.6726	-5.1403
C	3.4241	-3.8049	-4.0895
H	3.4104	-4.2640	-3.1548

H	4.3257	-4.0294	-4.5587
H	2.6540	-4.2063	-4.6641
C	5.3124	-0.4511	-0.1625
N	5.0929	1.4600	1.1747
N	4.3052	2.0014	3.0402
C	3.9857	1.5559	1.8637
C	6.1156	1.8269	1.9199
C	5.6155	2.1754	3.1087
C	5.1855	1.0029	-0.1311
C	3.3729	2.3292	4.0531
H	2.4529	2.0868	3.6264
C	3.5779	1.5149	5.2342
H	4.5041	1.7057	5.6673
H	3.5036	0.5030	5.0029
H	2.8346	1.7343	5.9309
C	3.4346	3.7527	4.3320
H	2.7035	4.0022	5.0307
H	3.2713	4.3135	3.4683
H	4.3598	4.0120	4.7306
H	6.2568	-0.7417	0.1629
H	4.5826	-0.8737	0.4484
H	6.0131	1.4583	-0.5678
H	4.3185	1.2927	-0.6297
N	6.1815	-2.2334	-4.3408
N	7.3417	-1.0752	-2.1485
C	7.4418	-2.0522	-4.2255
C	8.0100	-1.4848	-3.1579
N	7.3364	1.8707	1.6184
N	6.3261	2.5914	4.0630
C	7.5713	2.6392	3.7728
C	8.0650	2.2889	2.5828
H	8.0305	-2.3698	-5.0144
H	9.0373	-1.3593	-3.1208
H	9.0823	2.3482	2.4054
H	8.2080	2.9708	4.5174
Au	-0.2537	2.3903	1.3582
Au	1.5192	1.8269	-1.2848
N	2.9169	3.5032	-3.2098
N	2.6085	4.5204	-1.4012
C	2.4543	3.3759	-2.0053
C	3.3489	4.7438	-3.3840
C	3.1468	5.3903	-2.2346
C	3.0191	2.4440	-4.1479
H	2.5606	1.6436	-3.6603
C	2.2872	2.7400	-5.3626
H	2.3589	1.9224	-6.0037
H	2.6784	3.5750	-5.8453
H	1.2765	2.8876	-5.1638
C	4.4166	2.1377	-4.3932
H	4.9231	1.9330	-3.5061
H	4.8930	2.9266	-4.8778
H	4.4783	1.2987	-5.0079
C	2.2988	4.7691	-0.0718
N	0.5327	5.1946	1.4193
N	-0.2879	4.5939	3.2548
C	-0.0187	4.1966	2.0502
C	0.6407	6.2270	2.2354
C	0.1111	5.8484	3.4019
C	0.9093	5.1804	0.0848
C	-0.9956	3.8229	4.2130
H	-1.1135	2.9002	3.7407
C	-0.2241	3.6397	5.4254
H	-0.0333	4.5495	5.8936
H	0.6714	3.1480	5.2292
H	-0.7689	3.0395	6.0799
C	-2.2972	4.4163	4.4580
H	-2.8413	3.7951	5.0941
H	-2.8349	4.5305	3.5726

H	-2.2050	5.3457	4.9183
H	2.9435	5.5116	0.2664
H	2.4667	3.8900	0.4588
H	0.7606	6.1363	-0.2972
H	0.2863	4.5059	-0.4049
N	3.8618	5.2842	-4.4003
N	3.4332	6.5979	-2.0371
C	4.1563	6.5135	-4.2175
C	3.9465	7.1570	-3.0648
N	1.1387	7.3592	2.0131
N	0.0465	6.6025	4.4093
C	0.5487	7.7589	4.1991
C	1.0841	8.1291	3.0319
H	4.5793	7.0139	-5.0185
H	4.2045	8.1542	-2.9748
H	1.4790	9.0796	2.9212
H	0.5276	8.4253	4.9918
Au	-2.3775	0.6292	1.1471
Au	-1.4457	1.9524	-1.2408
N	-2.2596	4.1855	-2.9888
N	-3.2574	4.1969	-1.1452
C	-2.3044	3.6105	-1.8238
C	-3.1902	5.1239	-3.0603
C	-3.8276	5.1268	-1.8862
C	-1.3130	3.8845	-3.9948
H	-0.7268	3.1360	-3.5647
C	-1.9660	3.3560	-5.1759
H	-1.2403	3.0829	-5.8719
H	-2.5915	4.0672	-5.6092
H	-2.5165	2.5033	-4.9440
C	-0.5012	5.0551	-4.2738
H	-0.0405	5.4107	-3.4093
H	-1.0785	5.8186	-4.6831
H	0.2389	4.8061	-4.9619
C	-3.6378	3.8711	0.1465
N	-4.7708	2.2465	1.4235
N	-4.5306	1.0431	3.1240
C	-4.0239	1.3182	1.9597
C	-5.7386	2.5761	2.2555
C	-5.5911	1.8061	3.3383
C	-4.6037	2.7762	0.1534
C	-4.0395	0.0455	3.9984
H	-3.2289	-0.3560	3.4778
C	-3.5647	0.6327	5.2371
H	-4.3444	1.0791	5.7636
H	-2.8169	1.3342	5.0532
H	-3.1490	-0.1146	5.8328
C	-5.0515	-0.9757	4.2031
H	-4.6619	-1.7319	4.8050
H	-5.3521	-1.3981	3.2983
H	-5.8874	-0.5824	4.6834
H	-4.0467	4.7252	0.5786
H	-2.7824	3.5866	0.6674
H	-5.5353	3.1064	-0.1727
H	-4.2629	2.0092	-0.4635
N	-3.4783	5.9071	-4.0077
N	-4.7781	5.8968	-1.5924
C	-4.4464	6.6962	-3.7246
C	-5.0799	6.6927	-2.5502
N	-6.6472	3.4326	2.1066
N	-6.3609	1.8587	4.3372
C	-7.2927	2.7253	4.1999
C	-7.4341	3.4920	3.1146
H	-4.7342	7.3626	-4.4645
H	-5.8560	7.3544	-2.3804
H	-8.2101	4.1751	3.0597
H	-7.9591	2.8166	4.9869
Au	-1.3177	-1.9999	1.2659

Au	-2.4411	-0.5311	-1.3289
N	-4.4196	-1.2778	-3.3602
N	-4.7489	-2.3033	-1.5603
C	-3.9529	-1.4596	-2.1610
C	-5.5031	-2.0185	-3.5306
C	-5.7067	-2.6777	-2.3866
C	-3.8941	-0.3535	-4.2962
H	-3.0417	0.0194	-3.8238
C	-3.5042	-1.0116	-5.5275
H	-3.0759	-0.3062	-6.1628
H	-4.3256	-1.4368	-6.0064
H	-2.7849	-1.7426	-5.3477
C	-4.8486	0.7206	-4.5106
H	-5.0847	1.2009	-3.6158
H	-5.7256	0.3615	-4.9442
H	-4.4344	1.4217	-5.1602
C	-4.6255	-2.7123	-0.2422
N	-3.3524	-4.0745	1.2037
N	-2.3737	-4.0626	3.0573
C	-2.3897	-3.5148	1.8816
C	-3.9700	-4.9606	1.9611
C	-3.3452	-4.9580	3.1405
C	-3.6693	-3.8051	-0.1198
C	-1.4068	-3.7991	4.0588
H	-0.7863	-3.0858	3.6170
C	-2.0213	-3.2306	5.2401
H	-2.6831	-3.9023	5.6820
H	-2.5219	-2.3475	5.0102
H	-1.2762	-2.9980	5.9298
C	-0.6538	-5.0075	4.3423
H	0.1054	-4.7874	5.0203
H	-0.2191	-5.3954	3.4784
H	-1.2632	-5.7361	4.7679
H	-5.5680	-3.0078	0.0836
H	-4.2993	-1.8959	0.3155
H	-4.0610	-4.6773	-0.5292
H	-2.7860	-3.5513	-0.6078
N	-6.2452	-2.1416	-4.5436
N	-6.6428	-3.4936	-2.1895
C	-7.2028	-2.9706	-4.3596
C	-7.3977	-3.6300	-3.2144
N	-4.9519	-5.6923	1.6759
N	-3.6808	-5.7005	4.1043
C	-4.6791	-6.4486	3.8320
C	-5.3013	-6.4454	2.6480
H	-7.8465	-3.1184	-5.1574
H	-8.1906	-4.2875	-3.1232
H	-6.1057	-7.0732	2.4851
H	-5.0040	-7.0825	4.5836
Au	1.5814	-1.8359	1.3198
Au	-0.1935	-2.3812	-1.3343
N	-0.4739	-4.6959	-3.1013
N	0.3199	-5.2429	-1.2397
C	-0.1667	-4.2466	-1.9241
C	-0.1518	-5.9788	-3.1801
C	0.3578	-6.3238	-1.9960
C	-1.1277	-3.9407	-4.1072
H	-1.2586	-3.0055	-3.6628
C	-0.2903	-3.7977	-5.2803
H	-0.7802	-3.1945	-5.9746
H	-0.0991	-4.7209	-5.7227
H	0.6080	-3.3303	-5.0412
C	-2.4185	-4.5335	-4.4063
H	-3.0012	-4.6285	-3.5476
H	-2.3062	-5.4725	-4.8418
H	-2.9276	-3.9241	-5.0811
C	0.7133	-5.1889	0.0891
N	2.4697	-4.6057	1.5315

N	2.8217	-3.5805	3.3256
C	2.3329	-3.4542	2.1297
C	3.0225	-5.4744	2.3566
C	3.2536	-4.8213	3.4981
C	2.1277	-4.8618	0.2138
C	2.9628	-2.5182	4.2524
H	2.4996	-1.7133	3.7771
C	2.2656	-2.8007	5.4908
H	2.6672	-3.6331	5.9699
H	1.2493	-2.9474	5.3215
H	2.3563	-1.9770	6.1212
C	4.3730	-2.2315	4.4474
H	4.4720	-1.4170	5.0878
H	4.8400	-1.9985	3.5459
H	4.8624	-3.0415	4.8818
H	0.5118	-6.1170	0.5162
H	0.1400	-4.4539	0.5543
H	2.7192	-5.6523	-0.1152
H	2.3396	-4.0063	-0.3417
Au	0.0254	-0.0096	-2.6442
Au	-0.0125	-0.0027	0.0027
Au	-0.0626	0.0262	2.6500
Cl	-0.1123	0.0436	-4.8767
Cl	0.1081	0.0035	4.8817
N	-0.2665	-6.7832	-4.1442
N	0.7796	-7.4733	-1.7082
C	0.1597	-7.9558	-3.8689
C	0.6721	-8.2939	-2.6818
N	3.2956	-6.6851	2.1595
N	3.7828	-5.3597	4.5084
C	4.0640	-6.5942	4.3254
C	3.8267	-7.2419	3.1822
H	0.0947	-8.6629	-4.6230
H	1.0042	-9.2596	-2.5186
H	4.0756	-8.2423	3.0921
H	4.4983	-7.0939	5.1210

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6 NHC-O T1 Excited State

Au	-1.4838	1.9511	1.1992
Au	0.1183	2.4129	-1.2204
N	0.4950	4.6628	-3.1060
N	-0.4312	5.2853	-1.3149
C	0.0623	4.2500	-1.9425
C	0.2484	5.9654	-3.2763
O	0.5125	6.5089	-4.1938
C	-0.3764	6.3793	-2.0663
O	-0.7588	7.3495	-1.7111
C	1.1988	3.8274	-4.0211
H	1.2327	2.8681	-3.5653
C	0.4555	3.7081	-5.2757
H	0.9746	3.0544	-5.9233
H	0.3544	4.6153	-5.7404
H	-0.4900	3.2813	-5.1141
C	2.5483	4.3275	-4.2277
H	3.0483	4.3956	-3.3316
H	2.5378	5.2404	-4.6734
H	3.0731	3.6612	-4.8503
C	-0.9307	5.2450	-0.0106
N	-2.7317	4.4707	1.3172
N	-3.0903	3.3965	3.0824
C	-2.5135	3.3806	1.9456
C	-3.4300	5.3765	2.0244
O	-3.7625	6.4447	1.7417
C	-3.7138	4.6272	3.3224
O	-4.3019	4.9861	4.2495
C	-2.3266	4.7823	0.0144
C	-3.1934	2.3653	4.0286
H	-2.6654	1.5919	3.5771

C	-2.5442	2.6913	5.2888
H	-3.0326	3.4961	5.7598
H	-1.5413	2.9299	5.1467
H	-2.5973	1.8668	5.9254
C	-4.5762	1.9471	4.1926
H	-4.6247	1.1211	4.8299
H	-5.0201	1.7169	3.2793
H	-5.1405	2.7252	4.6430
H	-0.8544	6.1874	0.3523
H	-0.3388	4.5910	0.5537
H	-2.9551	5.5152	-0.3374
H	-2.4287	3.9199	-0.5483
Au	2.3285	-0.6489	1.2075
Au	1.3827	-2.0078	-1.2128
N	2.3086	-4.0030	-3.1087
N	3.4430	-3.9793	-1.3193
C	2.4270	-3.4432	-1.9419
C	3.2823	-4.9294	-3.3107
O	3.4510	-5.5977	-4.2706
C	4.0721	-4.9220	-2.0575
O	4.9864	-5.5585	-1.7439
C	1.2683	-3.7586	-4.0485
H	0.7025	-3.0162	-3.5799
C	1.7900	-3.2471	-5.2980
H	0.9891	-3.0331	-5.9315
H	2.3999	-3.9433	-5.7784
H	2.3176	-2.3567	-5.1522
C	0.4615	-4.9543	-4.2180
H	0.0926	-5.3059	-3.3108
H	1.0081	-5.7254	-4.6741
H	-0.3390	-4.7414	-4.8475
C	3.8348	-3.6871	-0.0202
N	4.8413	-2.0227	1.2993
N	4.5122	-0.9526	3.1039
C	4.0238	-1.2605	1.9560
C	5.9535	-2.3754	2.0359
O	6.8183	-3.0528	1.7551
C	5.6880	-1.5929	3.3342
O	6.3705	-1.5916	4.2747
C	4.6967	-2.5035	0.0159
C	3.9663	-0.0678	4.0433
H	3.1014	0.2770	3.5652
C	3.5990	-0.7530	5.2734
H	4.4348	-1.1468	5.7486
H	2.9136	-1.5070	5.0837
H	3.1523	-0.0694	5.9148
C	4.8783	1.0462	4.2677
H	4.4249	1.7448	4.8946
H	5.1294	1.5211	3.3684
H	5.7608	0.7287	4.7320
H	4.3461	-4.5138	0.3364
H	2.9916	-3.5214	0.5354
H	5.6565	-2.7212	-0.3536
H	4.2741	-1.7300	-0.5491
Au	1.3472	1.9923	1.1977
Au	2.2690	0.6154	-1.1993
N	4.5044	0.9819	-3.0934
N	4.8079	2.0322	-1.3447
C	4.0379	1.2422	-1.9456
C	5.7030	1.6381	-3.3399
O	6.3456	1.6065	-4.2764
C	5.9119	2.3817	-2.1069
O	6.7602	3.0677	-1.8317
C	3.9725	0.0619	-4.0530
H	3.1027	-0.2831	-3.5703
C	3.6069	0.7047	-5.2961
H	3.1590	0.0020	-5.9317
H	4.4408	1.0993	-5.7847

H	2.9053	1.4649	-5.1321
C	4.8898	-1.0505	-4.2561
H	5.1440	-1.5191	-3.3477
H	5.7752	-0.7389	-4.7285
H	4.4420	-1.7692	-4.8806
C	4.6902	2.5287	-0.0862
N	3.4334	3.9858	1.3009
N	2.3255	4.0144	3.1076
C	2.4276	3.4448	1.9418
C	4.0773	4.9328	2.0423
O	4.9828	5.5469	1.7475
C	3.2970	4.9505	3.3073
O	3.4699	5.5985	4.2394
C	3.8186	3.6854	0.0148
C	1.2929	3.7593	4.0487
H	0.7181	3.0229	3.5791
C	1.8329	3.2310	5.2884
H	2.4562	3.9237	5.7578
H	2.3552	2.3451	5.1215
H	1.0418	3.0136	5.9315
C	0.5026	4.9628	4.2434
H	-0.3021	4.7424	4.8763
H	0.1233	5.3196	3.3391
H	1.0629	5.7178	4.6949
H	5.6311	2.7515	0.3094
H	4.2833	1.7707	0.4962
H	4.3105	4.5358	-0.3567
H	2.9743	3.5302	-0.5440
Au	0.0319	-2.4027	1.2073
Au	-1.4484	-1.9279	-1.2007
N	-3.0929	-3.4133	-3.1267
N	-2.7219	-4.4887	-1.3112
C	-2.5011	-3.3840	-1.9401
C	-3.6786	-4.6550	-3.3193
O	-4.2347	-5.0333	-4.2552
C	-3.4184	-5.3851	-2.0538
O	-3.7323	-6.4628	-1.7505
C	-3.1746	-2.3835	-4.0470
H	-2.6591	-1.6013	-3.5829
C	-2.4959	-2.7187	-5.2931
H	-2.5409	-1.8921	-5.9336
H	-2.9581	-3.5264	-5.7690
H	-1.4905	-2.9339	-5.1251
C	-4.5570	-1.9990	-4.2548
H	-5.0326	-1.7625	-3.3513
H	-5.1057	-2.7673	-4.7199
H	-4.6012	-1.1578	-4.8815
C	-2.3241	-4.7636	-0.0048
N	-0.4555	-5.2339	1.3533
N	0.4626	-4.5984	3.1122
C	0.0506	-4.2342	1.9549
C	-0.4790	-6.3304	2.1318
O	-0.9076	-7.3315	1.8648
C	0.1577	-5.8808	3.3509
O	0.3443	-6.4726	4.2986
C	-0.9396	-5.2348	0.0496
C	1.1869	-3.7698	4.0343
H	1.2902	-2.8743	3.5382
C	0.4171	-3.5621	5.2598
H	0.2525	-4.4433	5.7536
H	-0.4749	-3.1024	5.0493
H	0.9567	-2.9373	5.8807
C	2.5013	-4.3620	4.2890
H	3.0467	-3.7161	4.8899
H	3.0156	-4.5062	3.4076
H	2.4197	-5.2573	4.7812
H	-2.9772	-5.4889	0.3516
H	-2.4353	-3.9074	0.5258

H	-0.8744	-6.2009	-0.3008
H	-0.3449	-4.6228	-0.5146
Au	0.0395	0.0205	-2.6791
Au	-2.2720	-0.8430	1.2205
Au	-2.2758	0.8256	-1.1714
Au	-0.0081	0.0260	-0.0132
Au	0.0782	0.0029	2.6633
Cl	0.0023	0.0061	-4.8476
Cl	0.0116	0.0125	4.8431
N	-4.2168	1.8758	-3.0880
N	-5.0962	1.1741	-1.3213
C	-4.0041	1.3735	-1.9665
C	-5.5584	2.0460	-3.3463
O	-6.0726	2.4407	-4.2508
C	-6.1998	1.5355	-2.0723
O	-7.2940	1.4596	-1.7888
C	-3.2466	2.3096	-4.0347
H	-2.3476	2.0939	-3.5426
C	-3.3172	1.5675	-5.2751
H	-2.5428	1.8852	-5.9002
H	-4.2256	1.7286	-5.7595
H	-3.1869	0.5464	-5.1045
C	-3.3498	3.7564	-4.2293
H	-3.2881	4.2766	-3.3356
H	-4.2426	4.0093	-4.7058
H	-2.5731	4.0699	-4.8478
C	-5.2428	0.7288	-0.0588
N	-5.1011	-1.1976	1.3274
N	-4.1782	-1.8921	3.0894
C	-3.9613	-1.3924	1.9663
C	-6.2007	-1.6249	2.0887
O	-7.2580	-1.5496	1.7741
C	-5.5020	-2.0888	3.3372
O	-6.0587	-2.5235	4.2745
C	-5.2409	-0.7615	0.0801
C	-3.1989	-2.3123	4.0308
H	-2.3292	-2.0647	3.5608
C	-3.3021	-1.5578	5.2766
H	-4.2092	-1.7376	5.7662
H	-3.1924	-0.5400	5.1063
H	-2.5353	-1.8561	5.9057
C	-3.2746	-3.7560	4.2407
H	-2.4928	-4.0442	4.8436
H	-3.2149	-4.2713	3.3498
H	-4.1604	-4.0238	4.7281
H	-6.1391	1.0984	0.3150
H	-4.4907	1.0772	0.5577
H	-6.1245	-1.1174	-0.3352
H	-4.4808	-1.1081	-0.5415

200

7 NHC-Me T1 Excited State

Au	2.2783	0.8245	-1.0989
Au	1.7876	1.6617	1.5971
N	2.8115	4.4183	1.9692
N	4.1862	3.2498	0.9987
C	2.9881	3.2221	1.5163
C	3.8677	5.1763	1.7441
H	3.9259	6.1583	2.0412
C	4.7345	4.4432	1.1336
H	5.6801	4.6692	0.8008
C	1.6720	4.8374	2.6815
H	1.0332	4.0139	2.6315
C	2.0222	5.1012	4.0632
H	1.1697	5.3692	4.5984
H	2.6995	5.8896	4.1412
H	2.4388	4.2587	4.5122
C	1.0473	5.9732	2.0267
H	0.8056	5.7539	1.0377



H	1.6638	6.8130	2.0414
H	0.1714	6.2239	2.5299
C	4.8211	2.1455	0.4546
N	4.8923	2.1486	-0.9242
N	4.4403	1.7976	-2.8913
C	3.9859	1.6190	-1.6977
C	5.8944	2.6349	-1.6313
H	6.7193	3.0798	-1.2055
C	5.6074	2.4106	-2.8690
H	6.1383	2.6300	-3.7205
C	3.8298	1.2879	-4.0591
H	2.8625	1.0310	-3.7647
C	3.7601	2.2978	-5.0953
H	4.7002	2.5414	-5.4743
H	3.3041	3.1670	-4.7480
H	3.1881	1.9284	-5.8824
C	4.5213	0.0904	-4.4930
H	3.9982	-0.3324	-5.2876
H	4.5686	-0.6063	-3.7199
H	5.4906	0.3010	-4.8148
H	4.2773	1.3080	0.7486
H	5.7908	2.1012	0.8298
Au	-2.3128	0.4117	-1.4987
Au	-2.3243	-0.6317	1.1045
N	-4.9333	-1.7058	2.0468
N	-5.1840	0.0455	1.0158
C	-4.2689	-0.7719	1.4588
C	-6.2309	-1.4841	1.9815
H	-6.9283	-2.1094	2.4025
C	-6.3921	-0.3795	1.3345
H	-7.2519	0.1286	1.0883
C	-4.3383	-2.7683	2.7586
H	-3.3223	-2.6696	2.5425
C	-4.5475	-2.5848	4.1851
H	-4.0825	-3.3543	4.7089
H	-5.5614	-2.6068	4.4265
H	-4.1406	-1.6830	4.5086
C	-4.8189	-4.0455	2.2686
H	-4.6586	-4.1474	1.2433
H	-5.8357	-4.1771	2.4615
H	-4.3123	-4.8151	2.7544
C	-4.9041	1.2588	0.4129
N	-5.0755	1.2915	-0.9592
N	-4.6744	1.2877	-2.9734
C	-4.1143	1.1022	-1.8242
C	-6.2051	1.5962	-1.5728
H	-7.0809	1.7976	-1.0725
C	-5.9483	1.5935	-2.8367
H	-6.5659	1.7856	-3.6357
C	-3.9814	1.2271	-4.2041
H	-3.0751	0.7732	-3.9543
C	-4.6912	0.3959	-5.1549
H	-5.5864	0.8310	-5.4662
H	-4.8987	-0.5428	-4.7563
H	-4.0984	0.2655	-6.0004
C	-3.7227	2.5635	-4.7024
H	-3.1599	2.5014	-5.5759
H	-3.1839	3.1223	-4.0078
H	-4.6080	3.0660	-4.9279
H	-3.9053	1.4740	0.6197
H	-5.5236	1.9827	0.8324
Au	-0.0794	2.2855	-1.2225
Au	-1.1505	1.8699	1.4001
N	-2.3255	3.9506	3.0929
N	-2.5089	4.4309	1.1026
C	-2.0471	3.5173	1.9106
C	-2.9498	5.1105	3.0324
H	-3.2614	5.6209	3.8690

C	-3.0677	5.4153	1.7830
H	-3.5025	6.2338	1.3345
C	-2.1130	3.1931	4.2730
H	-1.3538	2.5251	4.0162
C	-1.6736	4.0339	5.3639
H	-1.4006	3.4262	6.1623
H	-2.4288	4.6673	5.7035
H	-0.8473	4.6082	5.0993
C	-3.3082	2.4345	4.5932
H	-3.5772	1.8203	3.7968
H	-4.1057	3.0632	4.8314
H	-3.1128	1.8224	5.4121
C	-2.5081	4.3055	-0.2761
N	-1.4276	4.8788	-0.9224
N	0.2732	5.0890	-2.0473
C	-0.4446	4.1992	-1.4483
C	-1.3130	6.1638	-1.1990
H	-1.9941	6.8685	-0.8897
C	-0.2427	6.2928	-1.9050
H	0.1784	7.1346	-2.3196
C	1.4207	4.8077	-2.8187
H	1.5284	3.7729	-2.7290
C	1.1799	5.1560	-4.2058
H	1.0247	6.1805	-4.3243
H	0.3525	4.6480	-4.5814
H	2.0078	4.9004	-4.7822
C	2.5848	5.4668	-2.2543
H	3.4324	5.1989	-2.7979
H	2.7310	5.1888	-1.2613
H	2.5003	6.5048	-2.3013
H	-3.3795	4.7426	-0.6409
H	-2.4875	3.2909	-0.5036
Au	-1.3623	-2.0791	-1.2879
Au	-0.2622	-2.4012	1.2985
N	-0.3402	-4.8320	2.9637
N	-0.3609	-5.2863	0.9594
C	-0.3013	-4.2865	1.7956
C	-0.4096	-6.1450	2.8674
H	-0.4466	-6.7618	3.6878
C	-0.4254	-6.4347	1.6095
H	-0.4730	-7.3464	1.1351
C	-0.2391	-4.1053	4.1759
H	-0.5305	-3.1348	3.9250
C	-1.1449	-4.6352	5.1746
H	-1.1799	-3.9734	5.9760
H	-0.8292	-5.5575	5.5451
H	-2.1100	-4.7406	4.7998
C	1.1406	-4.0761	4.6288
H	1.7559	-3.6455	3.9077
H	1.4888	-5.0331	4.8527
H	1.2018	-3.4971	5.4915
C	-0.3140	-5.1471	-0.4184
N	-1.5454	-5.0380	-1.0379
N	-3.1330	-4.2698	-2.0833
C	-2.0348	-3.9201	-1.5010
C	-2.3296	-6.0572	-1.3388
H	-2.1180	-7.0273	-1.0739
C	-3.3266	-5.5708	-1.9964
H	-4.1419	-6.0452	-2.4073
C	-3.9788	-3.3813	-2.7808
H	-3.5571	-2.4449	-2.5897
C	-3.9244	-3.6525	-4.2042
H	-4.2778	-4.6073	-4.4278
H	-2.9530	-3.5631	-4.5658
H	-4.5253	-2.9710	-4.7116
C	-5.3267	-3.4228	-2.2400
H	-5.9104	-2.7046	-2.7198
H	-5.3329	-3.2192	-1.2177

H	-5.7812	-4.3470	-2.3997
H	0.1781	-5.9776	-0.8085
H	0.2133	-4.2757	-0.6355
Au	0.1463	-0.0592	2.7852
Au	1.6483	-1.8603	-1.1029
Au	2.3194	-0.9855	1.5541
Au	0.0742	-0.0708	0.0631
Au	0.0533	-0.1238	-2.6051
Cl	-0.8224	-0.4567	4.7886
Cl	0.6951	-0.2014	-4.7788
N	4.8976	-1.8661	2.6060
N	4.1342	-3.3272	1.3845
C	3.8822	-2.1367	1.8558
C	5.7628	-2.8598	2.6107
H	6.6333	-2.8390	3.1557
C	5.2850	-3.7814	1.8452
H	5.6602	-4.7056	1.6012
C	5.0031	-0.7093	3.4109
H	4.2243	-0.1026	3.0693
C	4.7608	-1.0421	4.8013
H	4.7586	-0.1719	5.3718
H	5.5028	-1.6689	5.1803
H	3.8365	-1.5060	4.9170
C	6.2769	-0.0487	3.1987
H	6.4424	0.1474	2.1886
H	7.0761	-0.6149	3.5544
H	6.2850	0.8533	3.7212
C	3.2311	-4.0826	0.6574
N	3.4353	-4.1201	-0.7107
N	3.1636	-3.7906	-2.7210
C	2.7890	-3.3700	-1.5610
C	4.1979	-4.9925	-1.3435
H	4.7902	-5.6780	-0.8579
C	4.0234	-4.7822	-2.6058
H	4.4391	-5.2553	-3.4170
C	2.6128	-3.3228	-3.9405
H	2.3309	-2.3380	-3.7438
C	3.5986	-3.3432	-5.0012
H	3.8477	-4.3142	-5.2904
H	4.4683	-2.8387	-4.7328
H	3.1941	-2.8698	-5.8357
C	1.4248	-4.0882	-4.2721
H	0.9837	-3.6775	-5.1218
H	0.7292	-4.0445	-3.4975
H	1.6598	-5.0855	-4.4708
H	2.2886	-3.6782	0.8275
H	3.2734	-5.0593	1.0153