

SUPPORTING INFORMATION

To Bend or Not to Bend! The Dilemma of Allenes

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Contents

Table S1. NBO Analysis for $R_2C=C=CR_2$ ($R = H, NH_2$)

Table S2. Absolute Energies of **1 – 8** (a.u, ZPE corrected values, which have been scaled by a factor of 0.9153, 0.9806, and 0.9661 for HF, B3LYP, and MP2(full) levels respectively).

Table S3. Absolute Energies for rotational transition states of **1 – 8** (a.u, ZPE corrected values, which have been scaled by a factor of 0.9806, and 0.9661 for B3LYP and MP2(full) levels respectively).

Figure S1. 3-D structural geometries of diprotonated species of **1 – 8** optimized at MP2(full)/6-31+G* level of theory. All distances are in angstrom ($\text{\AA}$) units and angles are in degrees. $i = 0$ represents the minimum.

Figure S2. 3-D structural geometries of two units of BH_3 complexes of **3 – 8** optimized at MP2(full)/6-31+G* level of theory. All distances are in angstrom ($\text{\AA}$) units and angles are in degrees. $i = 0$ represents the minimum.

Figure S3. 3-D structural geometries of two units of $AuCl$ complexes of **3 – 8** optimized at MP2(full)/6-31+G* level of theory. All distances are in angstrom ($\text{\AA}$) units and angles are in degrees. $i = 0$ represents the minimum.

Table S1: NBO Analysis for R₂C=C=CR₂ (R = H, NH₂)

Structure	interaction	second-order interaction			occupancy	
		E ⁽²⁾ ^a	E _i - E _j ^b	F _{ij} ^b	ρ _{n(N)}	ρ _{π*}
2	n _{N4} — π* _{C2-C1}	27.80	0.73	0.128	1.92 _(N4)	
3	n _{N4} — π* _{C2-C1}	25.27	0.74	0.124	1.92 _(N4)	0.162
	n _{N5} — π* _{C2-C1}	25.27	0.74	0.124	1.92 _(N5)	
4	n _{N4} — π* _{C2-C1}	30.96	0.73	0.134	1.91 _(N4)	0.102
	n _{N5} — π* _{C3-C1}	30.96	0.73	0.134	1.91 _(N5)	
4a	n _{N4} — π* _{C2-C1}	67.24	0.61	0.184	1.76 _(N4)	0.178
	n _{N5} — LP* _{C3}	129.91	0.35	0.219	1.76 _(N5)	
	n _{C1} — σ* _{C2-H6}	19.76	0.99	0.128	1.86 _(C1)	
	n _{C1} — σ* _{C3-H7}	19.76	0.99	0.128		
	LP* _{C3} — π* _{C2-C1}	34.14	0.26	0.124	0.75 _(C3)	0.178
	π _{C2-C1} — LP* _{C3}	233.23	0.21	0.214	1.53 _(C2-C1)	
5	n _{N4} — π* _{C2-C1}	27.64	0.74	0.130	1.92 _(N4)	0.165
	n _{N5} — π* _{C2-C1}	28.97	0.73	0.133	1.92 _(N5)	
	n _{N6} — π* _{C3-C1}	33.57	0.72	0.139	1.91 _(N6)	0.103
5a	n _{N4} — π* _{C2-C1}	34.30	0.71	0.143	1.89 _(N4)	0.204
	n _{N5} — π* _{C2-C1}	33.07	0.71	0.140	1.89 _(N5)	
	n _{N6} — π* _{C3-C1}	34.32	0.71	0.140	1.90 _(N6)	0.103
6	n _{N4} — π* _{C2-C1}	29.31	0.74	0.134	1.92 _(N4)	0.165
	n _{N5} — π* _{C2-C1}	29.31	0.74	0.134	1.92 _(N5)	
	n _{N6} — π* _{C3-C1}	29.31	0.74	0.134	1.92 _(N6)	
	n _{N7} — π* _{C3-C1}	29.31	0.74	0.134	1.92 _(N7)	
6b	n _{N4} — π* _{C2-C1}	34.22	0.70	0.142	1.89 _(N4)	0.211
	n _{N5} — π* _{C2-C1}	36.65	0.70	0.147	1.89 _(N5)	
	n _{N7} — π* _{C3-C1}	31.20	0.72	0.136	1.90 _(N6)	0.177
	n _{N6} — π* _{C3-C1}	31.47	0.72	0.138	1.91 _(N7)	
6c	n _{N4} — π* _{C2-C1}	36.27	0.70	0.146	1.89 _(N4)	0.223
	n _{N5} — π* _{C2-C1}	35.92	0.69	0.145	1.89 _(N5)	
	n _{N7} — π* _{C3-C1}	36.27	0.70	0.146	1.89 _(N6)	
	n _{N6} — π* _{C3-C1}	35.92	0.69	0.145	1.89 _(N7)	
6d	n _{N4} — π* _{C2-C1}	38.02	0.70	0.150	1.89 _(N4)	0.216
	n _{N5} — π* _{C2-C1}	32.45	0.70	0.138	1.89 _(N5)	
	n _{N7} — π* _{C3-C1}	43.24	0.67	0.156	1.89 _(N6)	0.215
	n _{N6} — π* _{C3-C1}	33.91	0.69	0.141	1.89 _(N7)	

Table S2: Absolute Energies of **1 – 8** (a.u, ZPE corrected values, which have been scaled by a factor of 0.9153, 0.9806, and 0.9661 for HF, B3LYP, and MP2(full) levels respectively)

	B3LYP/6-31+G*	MP2(full)/6-31+G*	G2MP2
1	-116.610853180	-116.203136620	-116.439757000
2	-171.945009657	-171.382134021	-171.708602000
3	-227.286393517	-226.570586850	-226.985555000
4	-227.284383437	-226.566643654	-226.981629000
4a	-227.263177110	-226.544936006	-226.955708000
5	-282.627777934	-281.757698680	-282.260759000
5a	-282.624043922	-281.753669696	-282.258857000
6	-337.972090250	-336.949996568	-337.541047000
6a	-337.971876095	-336.949572051	-337.540862000
6b	-337.968312597	-336.945852145	-337.538890000
6c	-337.964978051	-336.943354774	-337.536945000
6d	-337.963470451	-336.941014588	-
6e	-	-336.935261326	-337.530336000
7	-416.531410029	-415.226779469	-415.978911000
7a	-416.524345604	-415.219001663	-415.973219000
8	-652.206457718	-650.060667471	-
8a	-652.201876803	-650.047481540	-

Table S3: Absolute Energies for rotational transition states of **1 – 8** (a.u, ZPE corrected values, which have been scaled by a factor of 0.9806, and 0.9661 for B3LYP and MP2(full) levels respectively)

	B3LYP/6-31+G*	MP2(full)/6-31+G*	G2MP2
1-RT	-116.496348323	-116.088019095	-116.325305000
2-RT	-171.892448177	-171.328664292	-171.651353000
3-RT	-227.248639137	-226.531160899	-226.945419000
4-RT	-227.245815587	-226.525977747	-226.939679000
5-RT	-282.607475914	-281.735474402	-282.235745000
6-RT	-337.949430440	-336.926647096	-337.514977000
7-RT	-416.506294222	-415.199494408	-415.948960000
8-RT	-652.159243595	-650.009498831	

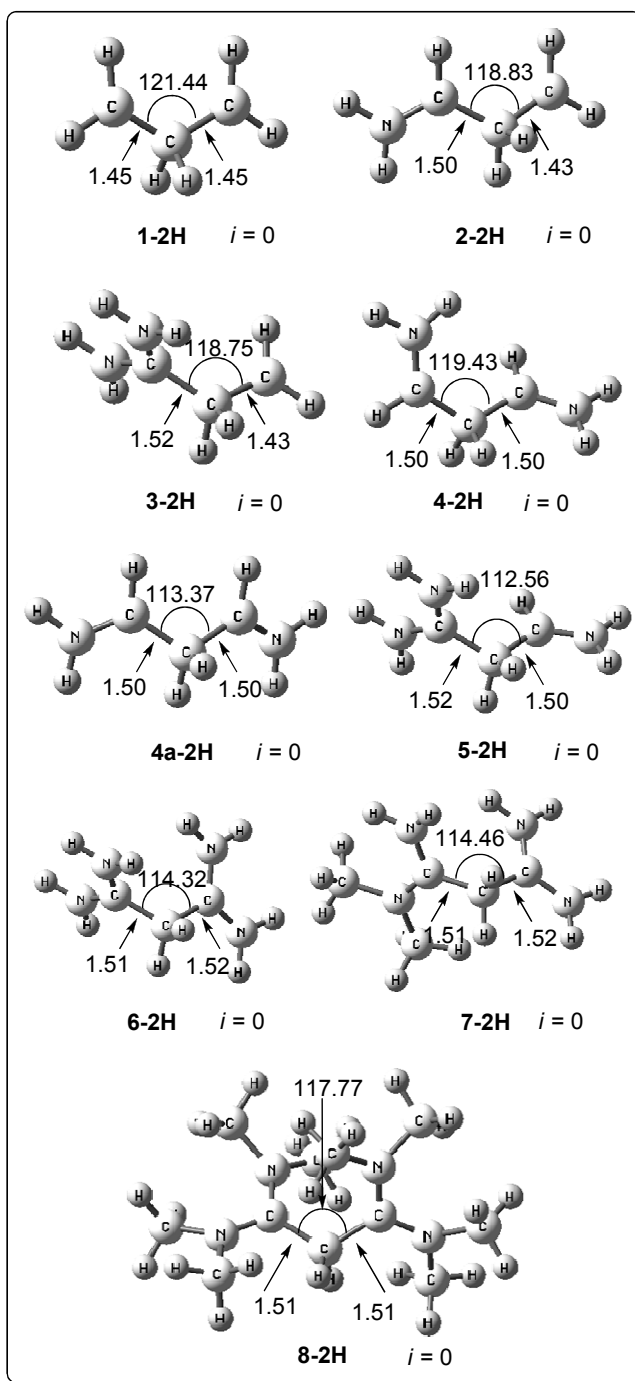


Figure S1: 3-D structural geometries of diprotonated species of **1** – **8** optimized at MP2(full)/6-31+G* level of theory. All distances are in angstrom (Å) units and angles are in degrees. $i = 0$ represents the minimum.

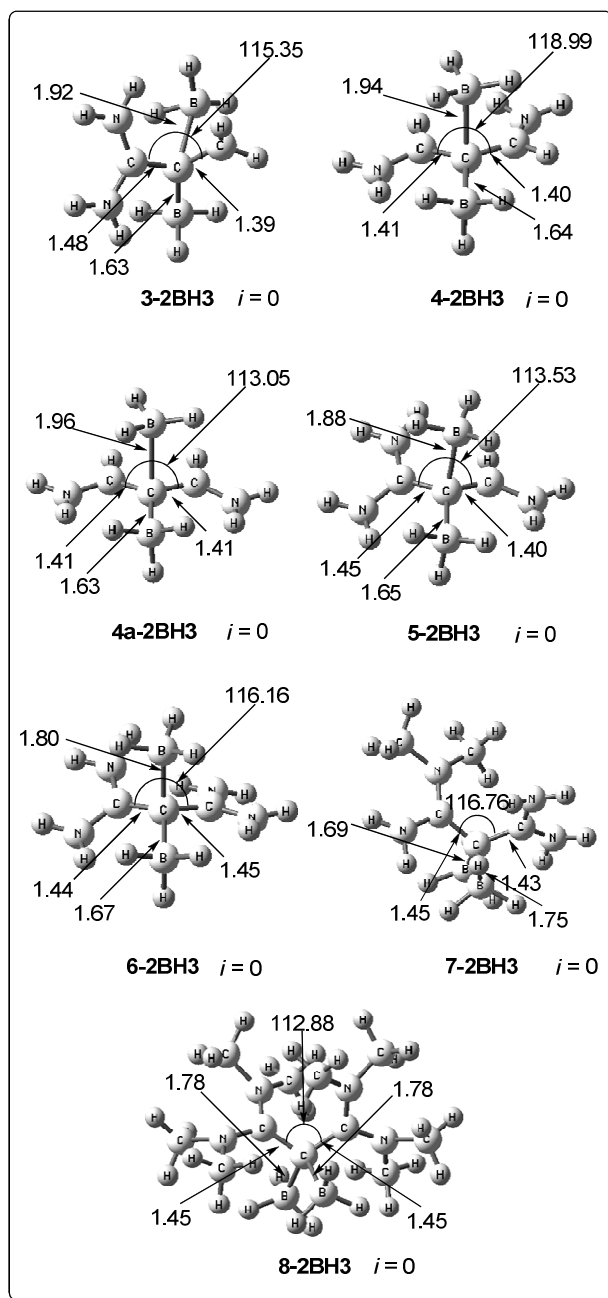


Figure S2: 3-D structural geometries of two units of BH_3 complexes of **3** – **8** optimized at MP2(full)/6-31+G* level of theory. All distances are in angstrom ($\text{\AA}$) units and angles are in degrees. $i = 0$ represents the minimum.

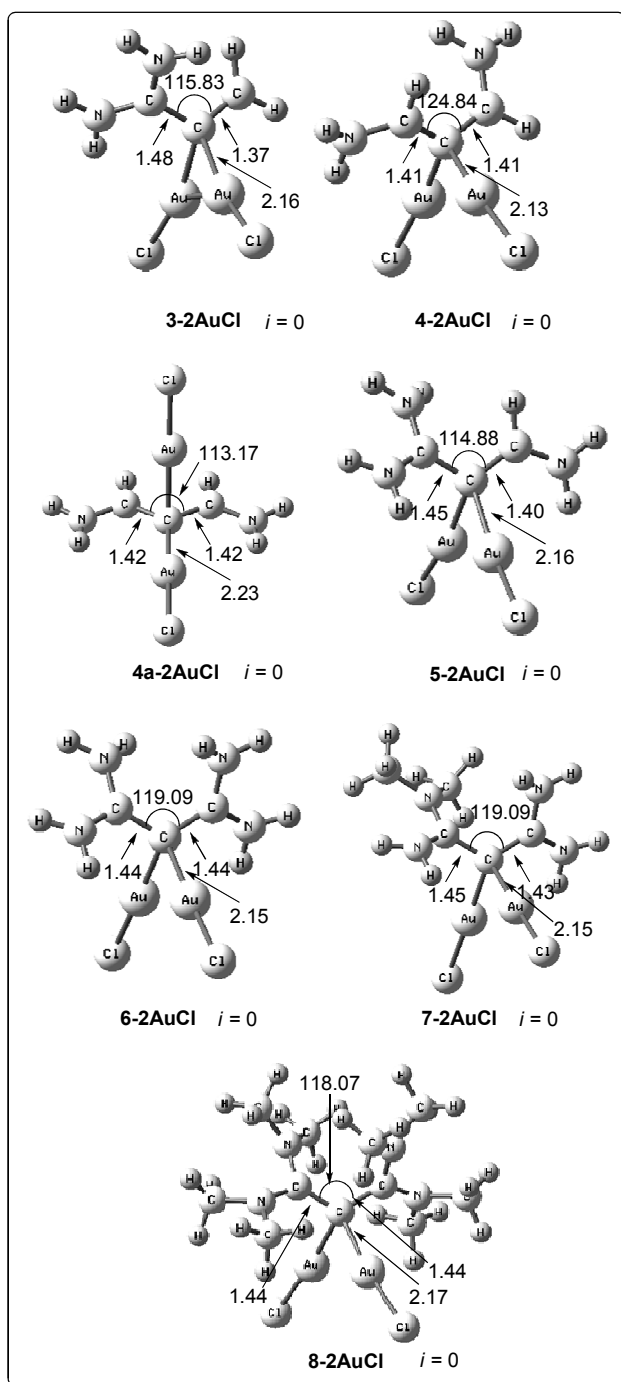


Figure S3: 3-D structural geometries of two units of AuCl complexes of **3** – **8** optimized at MP2(full)/6-31+G* level of theory. All distances are in angstrom (Å) units and angles are in degrees. $i = 0$ represents the minimum.

Cartesian coordinates of the optimized minima, rotational transition states, protonated species, dicoordinated BH3 and AuCl species of 1 – 8.

1-mp2

C	-1.314084	-0.000001	0.000000
C	0.000000	0.000003	0.000000
C	1.314084	-0.000001	0.000000
H	1.877131	0.903606	0.214491
H	1.877123	-0.903612	-0.214492
H	-1.877126	-0.214493	0.903610
H	-1.877128	0.214491	-0.903609

1-RT-mp2

C	-1.013727	0.200096	0.023798
C	-0.002804	-0.758088	-0.163128
C	1.011855	0.173275	0.028355
H	1.072919	1.164886	-0.441102
H	1.819104	-0.045931	0.730440
H	-0.931457	1.283124	-0.157855
H	-1.932504	-0.093780	0.534363

1-RT-mp2 (open shell)

C	0.000000	-1.272933	-0.092985
C	0.000000	0.000000	0.386588
C	0.000000	1.272933	-0.092985
H	0.000000	-1.466188	-1.166196
H	0.000000	-2.134208	0.564340
H	0.000000	1.466188	-1.166196
H	0.000000	2.134208	0.564340

2-mp2

H	-2.495759	-0.065683	0.481738
H	-0.876859	1.575468	-0.053656
C	0.659227	0.165524	0.019717
N	-1.712132	-0.361552	-0.094312
C	-0.610347	0.521321	-0.008276
H	2.460606	-0.367239	-0.925538
C	1.927933	-0.184590	0.006090
H	-1.463608	-1.322178	0.127979
H	2.499666	-0.303036	0.924479

2-RT-mp2

N	-1.700690	-0.075382	0.000004
H	1.872848	1.192919	0.000159
H	-2.486561	0.564756	0.000108
H	-0.319186	1.421909	0.000206
C	-0.439575	0.323232	0.000049
C	1.805067	0.089782	-0.000001
H	2.772697	-0.412091	-0.000080
H	-1.868818	-1.079670	-0.000138
C	0.623483	-0.606373	-0.000095

2-RT-mp2 (open shell)

H	-2.376244	0.968299	0.003872
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H	0.555778	1.503304	-0.020865
C	0.544807	0.413871	0.007858
C	-1.972935	-0.044934	0.004761
H	-2.688101	-0.859139	0.006018
C	-0.639907	-0.267441	0.005133
N	1.792921	-0.195029	-0.085928
H	2.558197	0.320286	0.334555
H	1.808125	-1.176527	0.171409

3-mp2

H	-1.883557	-1.189738	0.695291
C	0.913571	-0.000005	-0.000029
N	-1.211270	-1.163026	-0.070982
C	-0.408587	-0.000001	0.000000
H	2.808680	-0.096389	-0.919121
C	2.230772	-0.000003	0.000010
H	-0.653531	-2.013184	-0.079827
H	2.808624	0.096390	0.919175
N	-1.211261	1.163031	0.070989
H	-0.653505	2.013178	0.079844
H	-1.883531	1.189764	-0.695298

3-RT-mp2

C	-1.965546	-0.095214	0.001896
C	-0.822604	-0.828979	-0.000182
H	-2.938415	-0.584996	0.005208
C	0.399341	-0.042447	0.001058
N	0.521225	1.301495	-0.032989
N	1.533925	-0.750958	0.013000
H	1.397679	1.784184	0.125044
H	-0.320705	1.854812	0.061755
H	2.465889	-0.359052	-0.053776
H	1.398471	-1.757117	-0.011022
H	-2.056108	1.008257	-0.003918

3-RT-mp2 (open shell)

C	-0.415058	-0.055860	-0.013410
C	0.857261	-0.545240	-0.026085
C	2.147685	-0.125001	0.013530
H	2.408728	0.931508	0.086110
N	-1.558544	-0.854816	0.089232
H	-2.268650	-0.613160	-0.600801
H	-1.350984	-1.848679	0.069657
H	2.973418	-0.825820	-0.020076
N	-0.731777	1.311553	-0.079367
H	-1.354672	1.602590	0.673867
H	0.085081	1.913015	-0.122023

4-mp2

H	-1.635123	-1.047535	1.143595
H	3.176229	0.075809	0.207462
H	-3.176236	0.075792	-0.207432
H	1.992127	0.961527	0.990520
H	-1.992152	0.961465	-0.990569
C	1.270787	-0.385574	-0.356951
N	-2.257027	0.500641	-0.124027
N	2.257022	0.500653	0.124010

C	-1.270780	-0.385552	0.356968
H	1.635148	-1.047602	-1.143531
C	0.000000	-0.393626	-0.000005

4a-mp2

H	1.110567	1.431440	-0.000015
H	-3.201369	0.414880	-0.000123
H	3.201369	0.414881	0.000177
H	-2.490528	-1.180108	-0.000004
H	2.490528	-1.180108	0.000163
C	-1.126551	0.326037	-0.000049
N	2.378689	-0.172031	0.000030
N	-2.378689	-0.172031	-0.000040
C	1.126551	0.326037	0.000022
H	-1.110567	1.431440	-0.000116
C	0.000000	-0.472740	0.000025

4-RT-mp2

H	0.621010	-1.332675	-0.009216
H	-2.980656	-0.572354	0.102266
H	2.884391	-0.929005	-0.001333
H	-1.522505	-1.476045	0.061208
H	2.629314	0.806378	0.004857
C	-1.273038	0.595776	0.003292
N	2.253963	-0.137988	0.003155
N	-1.977417	-0.576820	-0.027992
C	0.913843	-0.264895	-0.001505
H	-1.962479	1.445086	0.004634
C	0.091712	0.846165	0.000120

5-mp2

C	-1.610178	0.042228	0.502677
C	-0.329930	-0.027395	0.185633
N	-2.685889	0.054414	-0.405203
H	-1.931974	0.169045	1.539442
C	0.984209	-0.007387	0.027410
H	-3.529531	-0.388669	-0.053527
H	-2.442121	-0.293976	-1.328077
N	1.792821	-1.155088	-0.145102
N	1.774455	1.162822	-0.030749
H	2.610100	-1.124902	0.463692
H	1.268944	-2.012984	0.006151
H	2.383136	1.166152	-0.848558
H	1.207137	2.005623	-0.006068

5a-mp2

C	0.998283	-0.012045	-0.020273
N	1.832838	-1.136793	0.061994
N	1.701590	1.201103	0.056233
C	-1.545857	-0.012563	0.437659
H	2.713638	-1.059287	-0.441280
H	1.348438	-1.992591	-0.188101
H	2.559656	1.236020	-0.490332
H	1.109292	1.997103	-0.158141
N	-2.753622	0.080098	-0.273097
H	-3.541637	-0.374518	0.177999
H	-2.670695	-0.196440	-1.247393
H	-1.686947	0.036706	1.521845

C	-0.335324	-0.085034	-0.099137
5-RT			
C	-0.946359	-0.074082	-0.001049
N	-2.023993	-0.913790	0.063070
N	-1.326696	1.260092	-0.069656
C	1.378906	0.244893	-0.007904
H	-2.908980	-0.623368	-0.339803
H	-1.771748	-1.889175	-0.059428
H	-2.176528	1.513796	0.425596
H	-0.585707	1.935022	0.074846
N	2.674625	-0.172989	-0.035295
H	3.434252	0.462165	0.171738
H	2.829313	-1.165525	0.111796
H	1.327998	1.349474	-0.050402
C	0.331427	-0.636741	0.002090
6-mp2			
C	-1.322380	-0.000003	0.000034
N	-2.134149	0.942011	0.675210
C	1.322379	-0.000004	-0.000037
H	-2.866472	0.486053	1.218484
H	-1.583350	1.559452	1.265336
H	-1.583474	-1.559452	-1.265252
N	2.134208	-0.942030	0.675055
H	2.866550	-0.486070	1.218301
H	1.583453	-1.559492	1.265200
H	2.866486	0.486089	-1.218454
C	0.000000	-0.000019	-0.000010
N	-2.134217	-0.941998	-0.675087
N	2.134160	0.942031	-0.675171
H	-2.866571	-0.486025	-1.218306
H	1.583369	1.559495	-1.265281
6a-mp2			
C	1.322451	-0.000335	-0.000599
N	2.137790	-0.956647	-0.650619
C	-1.322417	-0.000973	-0.000761
H	1.591127	-1.582505	-1.235603
H	2.876516	-0.512632	-1.195209
H	2.867613	0.519225	1.202483
N	-2.133885	-0.652276	0.958179
H	-2.872298	-1.199011	0.516205
H	-1.584106	-1.235878	1.582585
H	-2.870809	1.200122	-0.514495
C	0.000014	-0.003707	-0.003165
N	2.130294	0.960067	0.653343
N	-2.134365	0.652104	-0.958138
H	1.577461	1.583318	1.235368
H	-1.584635	1.234721	-1.583541
6b-mp2			
C	1.273682	-0.047532	-0.122482
N	2.213363	-1.003627	0.284873
C	-1.270868	-0.078435	-0.036130
N	-2.373195	-0.081594	-0.911399
N	-1.701489	0.145877	1.293274
N	1.801761	1.252481	-0.163521

H	3.141999	-0.907063	-0.120073
H	1.863414	-1.949032	0.168100
H	-3.153218	-0.631984	-0.555360
H	-2.110080	-0.390822	-1.842462
H	-2.363764	0.918538	1.350633
H	-0.917429	0.296055	1.923240
H	1.220941	1.888429	-0.699591
H	2.778776	1.324925	-0.437384
C	-0.010102	-0.330868	-0.393003

6c-mp2

C	0.000000	0.649773	0.000000
C	1.241786	0.129596	-0.056353
C	-1.241786	0.129596	0.056353
N	-1.573484	-1.045142	0.752437
N	1.573484	-1.045142	-0.752436
N	2.329026	0.676525	0.632837
N	-2.329026	0.676524	-0.632837
H	-0.836580	-1.334704	1.388334
H	-2.477805	-1.040016	1.219416
H	0.836581	-1.334703	-1.388336
H	2.477807	-1.040017	-1.219414
H	3.233141	0.602597	0.173385
H	2.142641	1.625550	0.939301
H	-2.142642	1.625550	-0.939301
H	-3.233141	0.602596	-0.173385

6d-mp2

C	-0.011294	-0.594463	0.111224
C	1.248445	-0.127954	0.079423
C	-1.253160	-0.103702	-0.031322
N	-1.583203	0.916079	-0.933564
N	1.659040	1.038411	0.754013
N	2.280680	-0.705488	-0.669421
N	-2.390688	-0.733575	0.508195
H	-0.847235	1.600223	-1.072096
H	-2.506412	1.326720	-0.842876
H	1.091915	1.238064	1.570739
H	2.651985	1.102793	0.964394
H	3.170568	-0.808333	-0.185794
H	1.990126	-1.584490	-1.085768
H	-2.130056	-1.434187	1.196406
H	-3.085636	-0.092071	0.884492

6e-mp2

C	-0.000012	-0.773881	0.000054
C	-1.207602	-0.154706	-0.072991
C	1.207588	-0.154742	0.073009
N	1.454417	1.008784	0.789830
N	-1.454374	1.008792	-0.789840
N	-2.347586	-0.695377	0.483248
N	2.347554	-0.695414	-0.483281
H	0.692657	1.434254	1.296440
H	2.359781	1.454798	0.831964
H	-0.692429	1.434560	-1.295922
H	-2.359856	1.454515	-0.832509
H	-3.274799	-0.327520	0.330951
H	-2.238199	-1.505282	1.075152
H	2.238115	-1.505065	-1.075520

H	3.274811	-0.327783	-0.330700
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6-RT

H	2.348143	1.590515	-0.069389
H	-2.232081	1.402259	0.772925
H	0.646159	1.772462	0.086793
H	-1.370135	1.785599	-0.593660
C	1.219902	-0.137840	-0.061782
N	-1.362991	1.233279	0.264815
N	1.424403	1.209246	-0.253136
C	-1.172834	-0.169611	-0.019653
C	0.012099	-0.819830	-0.184248
N	-2.375236	-0.878040	0.020592
N	2.358935	-0.872735	0.133520
H	2.180324	-1.855295	0.313017
H	-2.236583	-1.857769	-0.216774
H	-3.164831	-0.455003	-0.462220
H	3.158221	-0.461323	0.602865

7-mp2

N	1.671554	-0.410533	-0.262852
C	0.700473	0.615811	-0.223784
C	-1.862344	0.066031	0.078332
N	-2.574484	-0.545364	-0.981580
H	-3.476153	-0.094565	-1.135566
H	-2.035164	-0.557989	-1.842872
N	-2.716929	0.263483	1.188718
H	-3.232724	-0.585328	1.419881
N	1.278407	1.896302	-0.412112
C	2.767756	-0.242748	0.696964
H	2.425273	-0.434965	1.728099
H	3.562818	-0.952116	0.451690
H	3.159681	0.771415	0.643657
C	1.115614	-1.753758	-0.200109
H	0.646584	-1.964934	0.775334
H	0.360507	-1.877843	-0.978238
H	1.924248	-2.470030	-0.368088
H	1.893905	1.908822	-1.225300
H	0.560927	2.612174	-0.497120
H	-2.202968	0.597283	1.999753
C	-0.587628	0.418141	0.032523

7a-mp2

C	0.612638	-0.333164	-0.283465
C	1.917678	-0.145341	-0.025669
C	-0.535064	0.357078	-0.087209
N	-0.612697	1.762749	-0.238728
N	2.408521	0.505564	1.124374
N	2.939218	-0.503499	-0.918604
N	-1.728626	-0.246973	0.295601
H	0.285770	2.122245	-0.553232
H	-1.342367	2.086019	-0.870473
H	1.706608	0.567884	1.855900
H	3.281459	0.133808	1.493915
H	3.783513	-0.875202	-0.488606
H	2.595446	-1.128886	-1.640663
C	-2.980632	0.353420	-0.142705
H	-3.805788	-0.193511	0.317840
H	-3.042923	1.389391	0.194734

H	-3.109757	0.311239	-1.238376
C	-1.721434	-1.700878	0.259048
H	-1.660189	-2.085078	-0.772121
H	-0.858938	-2.073988	0.810498
H	-2.636863	-2.065503	0.732090

7-RT

H	3.339495	-1.271111	0.023245
H	-1.016315	-1.986561	-1.043777
H	1.691570	-1.755470	-0.200630
H	-0.299199	-2.221277	0.433230
C	1.897050	0.204625	0.100417
N	-0.284797	-1.652848	-0.415007
N	2.354844	-1.082906	0.189159
C	-0.445871	-0.241030	-0.118947
C	0.562245	0.637480	0.159212
N	-1.775163	0.184615	-0.265451
N	2.862800	1.166194	0.069938
H	2.506182	2.109560	-0.033925
H	3.800578	0.972005	-0.261739
C	-1.999131	1.623690	-0.192720
H	-1.274280	2.129810	-0.827955
H	-3.018031	1.824010	-0.539842
H	-1.877441	2.010440	0.829504
C	-2.801161	-0.545746	0.478552
H	-3.786043	-0.269919	0.092157
H	-2.683641	-1.623675	0.367215
H	-2.765458	-0.297320	1.552956

8-mp2

C	-1.328515	-0.002084	-0.001176
N	-2.122220	-0.778159	0.885039
C	1.328483	-0.002660	0.001583
N	2.120275	-0.779533	-0.885735
C	-0.000012	-0.007669	0.001541
N	-2.112056	0.780568	-0.891233
N	2.114052	0.779096	0.890633
C	-1.339900	1.501590	-1.890848
H	-0.670981	2.256006	-1.441389
H	-0.731868	0.802135	-2.465416
H	-2.037191	2.003754	-2.567559
C	-3.031752	1.684718	-0.193136
H	-3.712521	2.127394	-0.926263
H	-3.608895	1.132686	0.548222
H	-2.485445	2.496177	0.319250
C	-3.047674	-1.673820	0.183776
H	-3.735391	-2.109802	0.914425
H	-3.616751	-1.116658	-0.559963
H	-2.507017	-2.490546	-0.326230
C	-1.360125	-1.505872	1.887486
H	-0.696139	-2.265948	1.440238
H	-0.748113	-0.811763	2.464337
H	-2.064180	-2.002069	2.561588
C	1.344080	1.499280	1.892526
H	0.674285	2.254203	1.445232
H	0.737226	0.799233	2.467662
H	2.042851	2.000754	2.568232
C	3.032446	1.683615	0.191350
H	3.715499	2.124867	0.923221
H	3.607183	1.132134	-0.552299

H	2.485306	2.496134	-0.318463
C	3.046902	-1.674965	-0.185586
H	3.732531	-2.112222	-0.917429
H	3.618152	-1.117285	0.556081
H	2.506921	-2.490709	0.326667
C	1.356027	-1.508025	-1.886021
H	0.693132	-2.267837	-1.436710
H	0.742635	-0.814474	-2.462011
H	2.058658	-2.004608	-2.561316

8a-mp2

C	-0.038230	-0.052825	-0.258337
C	1.268960	0.062969	-0.000476
C	-1.338744	-0.143327	0.046123
N	-1.953523	0.692517	1.042345
N	1.928497	-0.707734	0.976554
N	2.109501	0.972989	-0.710601
N	-2.201226	-1.071415	-0.543028
C	-2.370280	1.982591	0.484255
H	-2.983463	1.829137	-0.406077
H	-2.965423	2.519126	1.230982
H	-1.503036	2.603370	0.205133
C	-1.084306	0.906315	2.196916
H	-0.800062	-0.057329	2.624624
H	-0.166651	1.462429	1.943438
H	-1.645349	1.471814	2.947845
C	1.330351	-1.992918	1.296244
H	0.254814	-1.890558	1.442047
H	1.504197	-2.731681	0.493980
H	1.775883	-2.370257	2.221492
C	3.380348	-0.717282	1.061260
H	3.841228	-1.473906	0.402975
H	3.766175	0.268252	0.804504
H	3.663543	-0.954595	2.091967
C	2.733083	0.323098	-1.867761
H	3.224390	-0.602887	-1.563798
H	1.981615	0.081639	-2.638961
H	3.485601	0.992508	-2.297594
C	1.415563	2.185375	-1.128655
H	0.604474	1.980697	-1.846973
H	0.992389	2.680335	-0.252300
H	2.145621	2.854705	-1.595116
C	-1.655201	-1.776596	-1.688625
H	-2.356508	-2.562293	-1.982777
H	-1.484919	-1.100577	-2.544247
H	-0.699805	-2.230932	-1.421125
C	-3.617717	-0.759331	-0.664344
H	-3.965505	-0.298250	0.259481
H	-3.829536	-0.090232	-1.516350
H	-4.165380	-1.693413	-0.819652

8-RT

H	1.254989	0.243546	0.011550
N	-1.611028	-1.125123	0.043145
N	1.611023	-1.125128	-0.043064
C	-1.254991	0.243545	-0.011550
C	0.000000	0.827177	-0.000016
N	-2.371175	1.069890	-0.151434
N	2.371176	1.069899	0.151383
C	-2.217325	2.449491	-0.588116

H	-1.382118	2.519129	-1.283775
H	-3.151775	2.768408	-1.070930
H	-2.007489	3.124210	0.255354
C	-3.597705	0.836234	0.601994
H	-4.481302	0.820330	-0.051985
H	-3.544381	-0.107952	1.143992
H	-3.738862	1.640668	1.340591
C	-2.693452	-1.701775	-0.737268
H	-2.357867	-2.649754	-1.184330
H	-3.595306	-1.923150	-0.140391
H	-2.973443	-1.017622	-1.541187
C	-1.137181	-1.952022	1.136743
H	-1.931743	-2.104025	1.889824
H	-0.830504	-2.944161	0.778553
H	-0.285438	-1.473880	1.619050
C	1.137203	-1.952074	-1.136637
H	0.830582	-2.944220	-0.778417
H	0.285426	-1.473988	-1.618941
H	1.931758	-2.104057	-1.889729
C	2.693459	-1.701728	0.737372
H	3.595322	-1.923104	0.140507
H	2.973432	-1.017540	1.541268
H	2.357892	-2.649699	1.184466
C	2.217321	2.449528	0.587973
H	2.007450	3.124186	-0.255536
H	1.382135	2.519205	1.283654
H	3.151781	2.768490	1.070737
C	3.597685	0.836212	-0.602070
H	4.481304	0.820395	0.051880
H	3.544371	-0.108024	-1.143980
H	3.738792	1.640583	-1.340747

1-H-mp2

C	1.183779	-0.213430	0.000050
C	0.000000	0.502009	-0.000101
C	-1.183778	-0.213429	0.000019
H	-2.151364	0.282602	0.000166
H	-1.181732	-1.301706	-0.000033
H	2.151362	0.282605	0.000115
H	1.181728	-1.301707	-0.000127
H	0.000001	1.587302	0.000067

2-H-mp2

H	2.548438	-0.542982	0.000052
H	0.418068	-1.464447	-0.000326
C	-0.639108	0.448654	-0.000118
N	1.741862	0.080124	0.000095
C	0.525237	-0.380771	-0.000121
H	-1.976039	-1.216506	0.001190
C	-1.857856	-0.135834	-0.000191
H	1.939057	1.081509	0.000282
H	-2.765238	0.459030	0.000526
H	-0.526958	1.530239	0.000186

3-H-mp2

H	-1.530382	1.748030	-0.122365
C	0.868693	-0.574131	0.285624
N	-0.642559	1.302771	0.093612

C	-0.467350	-0.009710	0.063788
H	2.945121	-0.450169	-0.065863
C	1.970357	-0.003172	-0.227124
H	0.107826	1.904849	0.415231
H	1.936343	0.893416	-0.839975
N	-1.479979	-0.834624	-0.155175
H	-1.309585	-1.827826	-0.276252
H	-2.440529	-0.519963	-0.260933
H	0.918768	-1.503287	0.847370

4-H-mp2

H	2.101328	1.087811	0.365165
H	-2.488106	-1.131608	0.039312
H	2.488108	-1.131608	-0.039380
H	-0.881587	-1.445514	0.559318
H	0.881544	-1.445545	-0.559230
C	-1.242489	0.471517	-0.108688
N	1.524991	-0.813446	-0.092431
N	-1.524994	-0.813439	0.092429
C	1.242495	0.471513	0.108674
H	-2.101307	1.087810	-0.365245
C	0.000000	1.089295	0.000029
H	0.000009	2.172899	-0.000019

4a-H-mp2

H	1.170688	-1.457846	0.000000
H	-3.233929	-0.412090	0.000000
H	3.233929	-0.412090	0.000000
H	-2.543972	1.172789	0.000000
H	2.543972	1.172789	0.000000
C	-1.191741	-0.369212	0.000000
N	2.400988	0.166791	0.000000
N	-2.400988	0.166791	0.000000
C	1.191741	-0.369212	0.000000
H	-1.170688	-1.457846	0.000000
C	0.000000	0.343189	0.000000
H	0.000000	1.430634	0.000000

5-H-mp2

C	-1.015495	-0.039501	0.049916
N	-2.021976	-0.897906	-0.140458
N	-1.294529	1.273647	0.079757
C	1.395207	0.238562	-0.151534
H	-2.995483	-0.624460	-0.062778
H	-1.831723	-1.869471	-0.355528
H	-2.202514	1.633685	-0.193951
H	-0.674821	1.916535	0.555831
N	2.673941	-0.121170	-0.018007
H	3.421969	0.460294	-0.374480
H	2.941009	-1.008412	0.394812
H	1.248258	1.214220	-0.611153
C	0.311965	-0.525589	0.208161
H	0.441189	-1.545230	0.558943

6-H-mp2

C	-1.245155	-0.114750	0.048186
N	-1.386983	1.211219	0.312029
C	1.245249	-0.114516	-0.047937

H	-2.317868	1.612012	0.356684
H	-0.695945	1.658465	0.905374
H	-2.308796	-1.759488	-0.560106
N	2.366037	-0.806652	0.221640
H	3.285175	-0.468528	-0.037343
H	2.309238	-1.759309	0.559629
H	2.317585	1.612167	-0.358505
C	0.000043	-0.755578	0.000626
N	-2.365851	-0.806742	-0.222384
N	1.386861	1.211228	-0.312173
H	-3.284936	-0.469294	0.037703
H	0.694115	1.659075	-0.903051
H	0.000169	-1.839411	0.000586

7-H-mp2

N	-1.737750	0.243377	0.041205
C	-0.518964	-0.283279	-0.136054
C	1.937066	0.150950	-0.016098
N	2.295248	-1.056222	0.497424
H	3.222739	-1.153748	0.897034
H	1.573073	-1.597974	0.961445
N	2.943874	1.018157	-0.264915
H	3.911295	0.721331	-0.221325
N	-0.391828	-1.650923	-0.144298
C	-2.966401	-0.521910	-0.191142
H	-3.296166	-1.039464	0.716072
H	-3.747102	0.174928	-0.497754
H	-2.821648	-1.237871	-1.002380
C	-1.906169	1.644445	0.434367
H	-1.056184	1.960761	1.038866
H	-2.002329	2.293698	-0.442429
H	-2.813416	1.722992	1.035316
H	-1.214285	-2.221400	0.015393
H	0.263782	-2.048281	-0.811275
H	2.763685	1.843951	-0.821933
C	0.618179	0.534350	-0.283495
H	0.467485	1.553024	-0.618412

8-H-mp2

C	-1.251329	-0.270177	-0.103379
N	-2.368306	-0.888252	0.366152
C	1.251127	-0.270415	0.103731
N	2.367760	-0.888798	-0.366177
C	-0.000185	-0.908174	0.000488
N	-1.420153	0.948246	-0.683117
N	1.420562	0.948102	0.683115
C	-0.505392	1.469769	-1.689791
H	0.177285	2.214597	-1.264702
H	0.073186	0.653683	-2.124508
H	-1.092491	1.949604	-2.479546
C	-2.487488	1.864505	-0.281543
H	-3.283938	1.921821	-1.031085
H	-2.908100	1.542700	0.671914
H	-2.060069	2.865113	-0.161838
C	-3.630025	-0.858532	-0.379170
H	-4.420611	-0.352169	0.183505
H	-3.483898	-0.358404	-1.336469
H	-3.943052	-1.889771	-0.572048
C	-2.266953	-1.962186	1.350075
H	-2.130448	-2.940802	0.871842

H	-1.432827	-1.769373	2.025591
H	-3.194673	-1.985705	1.927617
C	0.506677	1.470067	1.690358
H	-0.176099	2.215010	1.265644
H	-0.071802	0.654235	2.125679
H	1.094499	1.949890	2.479583
C	2.487933	1.863955	0.280719
H	3.284860	1.921158	1.029764
H	2.907862	1.541836	-0.672934
H	2.060749	2.864672	0.161084
C	3.629834	-0.859073	0.378543
H	4.420238	-0.353012	-0.184659
H	3.484243	-0.358622	1.335757
H	3.942780	-1.890306	0.571590
C	2.265755	-1.962955	-1.349784
H	2.129304	-2.941431	-0.871245
H	1.431351	-1.770158	-2.024960
H	3.193199	-1.986780	-1.927758
H	-0.000323	-1.993581	0.000876

1-2H-mp2

C	0.000000	1.268798	-0.259593
C	0.000000	0.000000	0.451859
C	0.000000	-1.268798	-0.259593
H	0.000000	-2.204165	0.311871
H	0.000000	-1.347253	-1.352686
H	0.000000	2.204165	0.311871
H	0.000000	1.347253	-1.352686
H	0.809789	0.000000	1.242797
H	-0.809789	0.000000	1.242797

2-2H-mp2

H	-2.615489	0.491950	-0.135806
H	-0.582092	1.478110	0.365784
C	0.627054	-0.423692	0.166522
N	-1.768293	-0.095233	-0.136430
C	-0.621023	0.411669	0.136308
H	2.016082	1.261853	-0.269776
C	1.869513	0.179380	-0.203426
H	-1.919161	-1.088276	-0.361909
H	2.751441	-0.453981	-0.338870
H	0.950734	-0.558048	1.260381
H	0.523274	-1.469123	-0.161220

3-2H-mp2

H	2.106276	-1.218723	-0.384036
C	-0.925377	-0.009780	0.540619
N	1.126298	-1.155376	-0.096803
C	0.523723	-0.000251	0.098221
H	-2.999853	-0.009505	-0.145200
C	-1.952239	0.001463	-0.460453
H	0.673764	-2.049726	0.085940
H	-1.754732	0.023556	-1.536435
N	1.114688	1.162287	-0.088937
H	0.655042	2.050752	0.104314
H	2.093424	1.237244	-0.377585
H	-1.171541	0.822071	1.247828
H	-1.165921	-0.852633	1.235030

4-2H-mp2

H	-2.119514	1.302085	-0.012043
H	2.903960	-0.954292	0.041381
H	-2.945556	-0.822323	-0.191140
H	2.467235	0.398548	-0.962458
H	-1.389945	-1.579055	-0.162380
C	1.044555	-0.230310	0.357299
N	-1.925959	-0.707183	-0.123466
N	2.190081	-0.264357	-0.227284
C	-1.415645	0.469024	-0.015039
H	0.877539	-0.969958	1.142400
C	0.033132	0.835639	0.077854
H	0.111749	1.564684	0.906231
H	0.273421	1.414977	-0.827423

4a-2H-mp2

H	-0.644097	1.367459	1.308858
H	-0.591715	0.031661	-3.185254
H	-0.591715	0.031661	3.185254
H	0.300239	-1.234192	-2.392526
H	0.300239	-1.234192	2.392526
C	-0.146255	0.398503	-1.253126
N	-0.146255	-0.311767	2.324623
N	-0.146255	-0.311767	-2.324623
C	-0.146255	0.398503	1.253126
H	-0.644097	1.367459	-1.308858
C	0.558867	-0.026887	0.000000
H	0.791796	-1.097804	0.000000
H	1.528767	0.511961	0.000000

5-2H-mp2

C	-1.062885	0.035801	0.110902
N	-1.740480	-1.072417	-0.118318
N	-1.532012	1.229059	-0.195998
C	1.388712	-0.271380	-0.330707
H	-2.677993	-1.068546	-0.524326
H	-1.406977	-1.982152	0.193007
H	-2.466758	1.369075	-0.583990
H	-1.015245	2.080620	0.011249
N	2.606373	0.106488	-0.158847
H	3.325014	-0.084403	-0.867994
H	2.931107	0.592697	0.685541
H	1.163937	-0.786950	-1.265310
C	0.326520	-0.069894	0.710234
H	0.536598	0.808025	1.332733
H	0.359078	-0.937441	1.388651

6-2H-mp2

C	-1.262237	-0.196000	0.125586
N	-1.988501	0.841980	0.506731
C	1.266480	0.092824	0.035663
H	-2.915049	1.033235	0.120332
H	-1.746950	1.379057	1.337466
H	-1.081443	-1.803820	-1.124328
N	2.403426	-0.561038	0.156150
H	3.276630	-0.225895	-0.253636
H	2.479423	-1.407404	0.716642
H	1.958274	1.597395	-1.183413

C	0.068319	-0.438089	0.802923
N	-1.639595	-0.998569	-0.848749
N	1.163509	1.194868	-0.684701
H	-2.535679	-0.902049	-1.329400
H	0.300909	1.729192	-0.737689
H	0.185461	-1.515465	0.963654
H	0.071180	0.022657	1.799318

7-2H-mp2

N	-1.463463	0.438492	0.002508
C	-0.632244	-0.486063	-0.422314
C	1.826619	-0.040409	0.065632
N	1.747494	-0.742690	1.181219
H	2.483583	-0.734643	1.887886
H	0.983576	-1.394211	1.342435
N	2.852310	0.744296	-0.198019
H	3.667426	0.809756	0.412546
N	-0.931486	-1.794139	-0.345477
C	-2.836973	0.072729	0.414724
H	-2.820034	-0.450918	1.375474
H	-3.412843	0.990279	0.522795
H	-3.305730	-0.540939	-0.358789
C	-1.129850	1.874391	0.109085
H	-0.061189	2.043359	0.004043
H	-1.677699	2.426642	-0.658301
H	-1.440384	2.217766	1.097311
H	-1.840237	-2.122078	-0.024639
H	-0.409823	-2.471042	-0.897727
H	2.909921	1.271172	-1.066679
C	0.734109	-0.152298	-0.978641
H	0.686702	0.766381	-1.569024
H	1.032781	-0.943345	-1.679866

8-2H-mp2

C	-1.283257	-0.299054	-0.187027
N	-2.407971	-0.772462	0.352595
C	1.282990	-0.299233	0.187423
N	2.407413	-0.773161	-0.352325
C	-0.000255	-1.081873	0.000621
N	-1.282348	0.806331	-0.939627
N	1.282733	0.806613	0.939339
C	-0.258384	1.080109	-1.958099
H	0.467185	1.813351	-1.593847
H	0.241082	0.165221	-2.271224
H	-0.761647	1.494464	-2.835795
C	-2.254094	1.901020	-0.763249
H	-3.001912	1.919926	-1.559548
H	-2.741344	1.813213	0.207095
H	-1.689441	2.836653	-0.794770
C	-3.729887	-0.557782	-0.276456
H	-4.333251	0.160816	0.282451
H	-3.600754	-0.233094	-1.307163
H	-4.238966	-1.523900	-0.276343
C	-2.443773	-1.745852	1.463717
H	-2.391719	-2.770424	1.083379
H	-1.647472	-1.563330	2.183876
H	-3.393668	-1.610462	1.982561
C	0.259355	1.081401	1.958129
H	-0.466069	1.814750	1.593807
H	-0.240349	0.166908	2.272016

H	0.763211	1.496038	2.835351
C	2.254994	1.900688	0.762022
H	3.003072	1.919647	1.558078
H	2.741905	1.812034	-0.208420
H	1.690855	2.836643	0.793166
C	3.729604	-0.558034	0.275990
H	4.332747	0.160103	-0.283748
H	3.600907	-0.232496	1.306488
H	4.238655	-1.524167	0.276442
C	2.442667	-1.747241	-1.462860
H	2.390714	-2.771576	-1.081869
H	1.646060	-1.565104	-2.182779
H	3.392342	-1.612230	-1.982206
H	0.102756	-1.759966	-0.853379
H	-0.103456	-1.759152	0.855244

1-BH3-mp2

C	0.859870	-1.111225	0.000022
C	-0.000393	-0.012401	-0.000600
C	0.734578	1.172917	0.000316
H	0.230223	2.137608	0.000961
H	1.826839	1.190275	-0.001007
H	0.464980	-2.125034	0.001673
H	1.947392	-1.006596	-0.000481
B	-1.618234	-0.063786	-0.000060
H	-1.984133	0.523535	1.004661
H	-1.985412	0.531968	-0.999298
H	-1.973049	-1.228576	-0.004637

2-BH3-mp2

H	2.687664	-0.585937	-0.001077
H	0.688578	-1.841588	0.068392
C	-0.575197	-0.007264	0.000906
N	1.789210	-0.115789	-0.016225
C	0.646570	-0.750642	0.021916
H	-1.617217	-1.900373	-0.001487
C	-1.677889	-0.809586	-0.015216
H	1.740185	0.907975	-0.084142
H	-2.675489	-0.380116	-0.043892
B	-0.483777	1.607102	0.015028
H	-1.582312	2.099260	-0.129343
H	0.022712	1.933796	1.084179
H	0.269394	1.946947	-0.899831

3-BH3-mp2

H	-2.558160	0.670981	0.414809
C	0.770624	0.207367	0.003336
N	-1.560696	0.846652	0.384574
C	-0.666113	-0.062490	-0.017148
H	2.200430	1.715469	-0.379239
C	1.147502	1.450950	-0.375870
H	-1.217911	1.707671	0.790595
H	0.455886	2.213921	-0.738804
N	-1.059433	-1.260535	-0.423849
H	-0.297918	-1.923273	-0.591740
H	-2.009750	-1.600683	-0.338946
B	1.705453	-1.060630	0.403658
H	2.871928	-0.725768	0.408985
H	1.332271	-1.498261	1.484988

H	1.524788	-1.934691	-0.455926
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4-BH3-mp2

H	0.540332	-2.094392	0.419124
H	-1.578867	2.422900	0.152567
H	-1.651394	-2.379782	-0.171776
H	-1.804397	0.823232	0.714838
H	-1.861292	-0.751017	-0.650018
C	0.024045	1.193698	-0.152670
N	-1.334470	-1.419793	-0.093549
N	-1.284289	1.453670	0.109432
C	-0.011014	-1.201073	0.129501
H	0.594199	2.061167	-0.482714
C	0.692363	-0.013542	-0.013235
B	2.342381	-0.027088	0.013888
H	2.713401	0.874925	-0.725020
H	2.701889	0.179650	1.164510
H	2.733160	-1.112880	-0.383704

4a-BH3-mp2

H	-1.144630	-1.826126	0.005434
H	3.221778	-0.719579	0.004578
H	-3.221803	-0.719501	0.004020
H	2.419062	0.840615	-0.042121
H	-2.419065	0.840685	-0.042130
C	1.158022	-0.732859	-0.007240
N	-2.370580	-0.175302	0.019296
N	2.370535	-0.175384	0.019143
C	-1.158083	-0.732821	-0.007312
H	1.144497	-1.826163	0.005621
C	-0.000011	0.033664	-0.035258
B	0.000102	1.654399	0.008589
H	0.000330	2.010272	1.179258
H	0.994776	2.087283	-0.564086
H	-0.994710	2.087413	-0.563739

5-BH3-mp2

C	1.065747	-0.177906	-0.007019
N	2.024175	0.705560	-0.321315
N	1.450938	-1.470893	0.209972
C	-1.232432	-0.697842	-0.166019
H	2.999578	0.555885	-0.097058
H	1.697355	1.660666	-0.466808
H	2.430982	-1.722720	0.159808
H	0.889847	-2.024427	0.842420
N	-2.562156	-0.466074	-0.039148
H	-3.225483	-1.078417	-0.495044
H	-2.831757	0.508096	0.080251
H	-0.982585	-1.719193	-0.463439
C	-0.276803	0.267307	0.049411
B	-0.565148	1.859141	0.264293
H	-0.120167	2.208655	1.348607
H	0.000077	2.484622	-0.635482
H	-1.761878	2.101626	0.200477

6-BH3-mp2

C	-1.204479	-0.221541	-0.011007
N	-1.320860	-1.589392	-0.167421

C	1.210919	-0.144169	0.034707
H	-2.166244	-1.893741	-0.642576
H	-0.480738	-2.039663	-0.526016
H	-2.298849	1.432963	0.277108
N	2.345650	0.528116	-0.313726
H	3.221964	0.248656	0.116241
H	2.204137	1.536826	-0.364760
H	2.347084	-1.845096	0.162189
C	-0.009001	0.516282	0.090372
N	-2.374468	0.451365	0.011483
N	1.386550	-1.519914	0.232353
H	-3.241642	-0.032989	0.208505
H	0.920792	-1.888866	1.057655
B	-0.085020	2.154434	0.081144
H	-0.301117	2.553581	-1.055561
H	-0.982742	2.533622	0.830182
H	0.959714	2.627872	0.508047

7-BH3-mp2

N	-1.752156	0.110109	0.138336
C	-0.547550	-0.392879	-0.191347
C	1.836902	-0.157359	0.107344
N	2.100769	-1.460195	0.535360
H	2.803063	-1.503533	1.270473
H	1.269785	-1.996861	0.769169
N	2.956286	0.631341	0.105969
H	3.837409	0.167536	-0.091313
N	-0.503759	-1.746057	-0.488152
C	-3.007971	-0.540162	-0.205952
H	-3.325607	-1.266130	0.554823
H	-3.777098	0.231322	-0.283132
H	-2.931287	-1.031463	-1.179021
C	-1.872735	1.321478	0.945355
H	-2.502692	1.094448	1.813925
H	-0.884647	1.639362	1.267938
H	-2.322006	2.127864	0.360908
H	-1.364021	-2.282035	-0.485415
H	0.142275	-2.008861	-1.226013
H	2.820152	1.514459	-0.384379
C	0.614701	0.402171	-0.250397
B	0.560424	1.955524	-0.798716
H	-0.519496	2.160873	-1.328474
H	0.756937	2.760773	0.106954
H	1.447051	2.068748	-1.643463

8-BH3-mp2

C	-1.183883	0.227537	0.169622
N	-2.356134	0.637289	-0.391996
C	1.177138	0.165933	-0.132734
N	2.424093	0.536403	0.294868
C	0.025945	0.944006	0.044762
N	-1.290530	-0.895086	0.958055
N	1.174254	-1.028510	-0.839155
C	-0.364563	-1.154758	2.045657
H	0.451919	-1.824802	1.743952
H	0.054614	-0.210543	2.394158
H	-0.915441	-1.629647	2.867805
C	-2.182571	-2.000373	0.642535
H	-2.952318	-2.137533	1.414194
H	-2.669541	-1.820511	-0.316859

H	-1.597612	-2.927520	0.575618
C	-3.621882	0.585272	0.325118
H	-4.350851	-0.066631	-0.173994
H	-3.453910	0.229900	1.342066
H	-4.037016	1.599316	0.372531
C	-2.388091	1.419088	-1.618222
H	-2.739616	2.436208	-1.421778
H	-1.384736	1.487808	-2.033806
H	-3.066204	0.930162	-2.331009
C	0.254650	-1.292306	-1.927219
H	-0.576109	-1.947525	-1.631910
H	-0.152622	-0.349515	-2.294272
H	0.799670	-1.785794	-2.744399
C	2.090410	-2.114820	-0.535304
H	2.826196	-2.271586	-1.337915
H	2.623081	-1.893835	0.390929
H	1.525554	-3.048991	-0.410908
C	3.557688	0.525511	-0.620606
H	4.400595	-0.040009	-0.201736
H	3.262293	0.080928	-1.571758
H	3.883657	1.557675	-0.804800
C	2.607700	1.388154	1.460045
H	2.691543	2.444141	1.185080
H	1.756049	1.282897	2.129558
H	3.521758	1.064538	1.974447
B	0.072104	2.589723	0.185181
H	0.161525	2.890386	1.373373
H	1.037959	3.016382	-0.438955
H	-0.957992	3.075363	-0.249847

3-2BH3-mp2

H	2.836675	0.544713	0.069571
C	-0.490188	0.350367	0.117452
N	1.847484	0.751719	0.142837
C	0.896605	-0.157063	0.011203
H	-2.196387	0.177663	1.371538
C	-1.307908	-0.331737	1.016035
H	1.528176	1.721880	0.199545
H	-0.944638	-1.156406	1.625052
N	1.182606	-1.446615	-0.146779
H	0.415334	-2.068085	-0.394987
H	2.130244	-1.777723	-0.289374
B	-0.730503	1.887323	-0.371454
H	-0.271709	2.042948	-1.489751
H	-1.910073	2.148758	-0.294577
B	-1.675349	-0.941309	-0.664512
H	-0.998651	-0.555718	-1.594691
H	-1.458885	-2.118884	-0.482681
H	-0.105326	2.572579	0.446058
H	-2.797187	-0.566929	-0.826421

4-2BH3-mp2

H	-1.753094	1.361083	-0.430882
H	2.604651	-1.769526	-0.101571
H	-3.158327	-0.451915	-0.511542
H	2.532940	-0.001991	-0.199454
H	-1.891554	-1.600272	-0.391965
C	0.754172	-0.896961	-0.140969
N	-2.162570	-0.635348	-0.537172
N	2.066259	-0.916124	-0.192717

C	-1.305333	0.373052	-0.354750
H	0.275931	-1.876395	-0.091198
C	0.081848	0.347858	-0.136563
B	0.943373	1.704342	-0.481642
H	1.971287	1.721059	0.190381
H	1.220810	1.649096	-1.674533
B	-0.383897	0.215476	1.746472
H	-1.349096	0.933066	1.874428
H	-0.659315	-0.953963	1.917992
H	0.262859	2.676650	-0.219847
H	0.635589	0.630628	2.216958

4a-2BH3-mp2

H	-1.183858	-1.279344	-1.239719
H	3.209728	-0.212425	-0.730023
H	-3.209746	-0.212065	-0.730190
H	2.352571	1.017111	0.192648
H	-2.352535	1.017211	0.192815
C	1.172869	-0.385005	-0.613261
N	-2.338734	0.202489	-0.423642
N	2.338723	0.202289	-0.423671
C	-1.172898	-0.384793	-0.613364
H	1.183776	-1.279747	-1.239355
C	0.000014	0.131572	-0.034632
B	0.000257	1.589845	0.693941
H	0.000505	2.427573	-0.201121
H	-0.992662	1.710742	1.396910
B	-0.000257	-1.424166	1.315369
H	-1.024571	-1.141224	1.870679
H	-0.001601	-2.447335	0.673258
H	0.993179	1.710246	1.396990
H	1.025381	-1.143232	1.869290

5-2BH3-mp2

C	1.160547	-0.080725	-0.193209
N	2.019866	0.915536	-0.350487
N	1.591461	-1.357131	-0.316058
C	-1.145225	-0.581080	-0.561424
H	3.024373	0.783223	-0.343569
H	1.639296	1.855228	-0.234807
H	2.586334	-1.540735	-0.391170
H	1.071807	-2.039114	0.232008
N	-2.419972	-0.248080	-0.676982
H	-3.117965	-0.906558	-0.997133
H	-2.709557	0.637240	-0.260009
H	-0.873266	-1.536462	-1.011609
C	-0.221857	0.254428	0.088627
B	-0.467243	-0.688948	1.690479
H	-1.498261	-0.257244	2.126307
H	-0.501627	-1.887244	1.438314
B	-0.584283	1.852945	0.252951
H	0.159690	2.353907	1.080246
H	-0.433874	2.374977	-0.850205
H	0.547764	-0.380847	2.270529
H	-1.737359	1.995625	0.624677

6-2BH3-mp2

C	1.229292	-0.180060	-0.143279
N	1.464010	-1.481794	0.223510

C	-1.216856	-0.311924	-0.213470
H	2.431172	-1.796434	0.205877
H	0.989386	-1.714531	1.099624
H	2.000077	1.474145	-0.931807
N	-2.389192	0.311194	-0.146431
H	-3.277059	-0.168073	-0.214986
H	-2.360315	1.308555	0.058134
H	-2.074858	-2.077326	-0.850132
C	-0.034570	0.467110	0.090764
N	2.214287	0.498128	-0.717707
N	-1.225846	-1.615778	-0.548733
H	3.185409	0.223584	-0.617985
H	-0.346636	-2.101680	-0.678660
B	-0.124755	2.034639	-0.480867
H	0.848883	2.655522	-0.081522
H	-0.151582	1.995038	-1.708315
H	-1.116696	2.597002	-0.048760
B	0.018313	0.456865	1.888597
H	-0.192441	-0.709321	2.221234
H	1.140067	0.812307	2.187750
H	-0.853195	1.210685	2.242330

7-2BH3-mp2

N	-1.553514	-0.487237	0.078722
C	-0.754857	0.582699	-0.040702
C	1.412754	-0.543652	-0.289405
N	1.149300	-1.088171	-1.507623
H	1.847695	-1.699987	-1.920807
H	0.749217	-0.427398	-2.169654
N	2.392400	-1.071283	0.448779
H	3.175009	-1.548205	0.013833
N	-1.327831	1.757263	-0.367507
C	-2.974007	-0.396495	-0.240734
H	-3.117693	0.224036	-1.128445
H	-3.341807	-1.400864	-0.455078
H	-3.550166	0.016317	0.597341
C	-1.099009	-1.759291	0.637055
H	-0.909200	-2.484266	-0.160892
H	-0.204431	-1.601950	1.234867
H	-1.882512	-2.138506	1.298461
H	-2.267821	1.973666	-0.056781
H	-0.666647	2.534429	-0.389135
H	2.569357	-0.571311	1.322328
C	0.674914	0.576929	0.210491
B	0.859633	0.898247	1.863556
H	0.215944	1.890442	2.135592
H	0.463331	-0.075890	2.500942
H	2.050886	1.087370	2.071024
B	1.487699	1.803810	-0.730478
H	1.182129	2.878010	-0.246608
H	2.681978	1.610866	-0.652037
H	1.086818	1.687807	-1.887169

8-2BH3-mp2

C	1.201446	-0.089448	0.093080
N	2.403328	-0.424786	-0.436116
C	-1.201432	-0.089168	-0.092943
N	-2.403469	-0.424514	0.436084
C	-0.000098	-0.888765	0.000056
N	1.233659	1.043778	0.855530

N	-1.233513	1.044165	-0.855198
C	0.245658	1.372727	1.873373
H	-0.478899	2.108773	1.503523
H	-0.261098	0.471922	2.210276
H	0.771860	1.805688	2.732178
C	2.219431	2.097201	0.641984
H	2.978104	2.124912	1.433588
H	2.711135	1.954306	-0.320920
H	1.694420	3.059573	0.638670
C	3.589212	-0.431783	0.424661
H	4.375381	0.227427	0.038158
H	3.319946	-0.142751	1.440208
H	3.966226	-1.459424	0.458999
C	2.540862	-1.324016	-1.577003
H	2.602807	-2.365006	-1.244492
H	1.696001	-1.222942	-2.251537
H	3.464403	-1.046555	-2.097733
C	-0.245524	1.373215	-1.873021
H	0.478969	2.109306	-1.503158
H	0.261295	0.472458	-2.209956
H	-0.771759	1.806159	-2.731815
C	-2.219470	2.097447	-0.641766
H	-2.978048	2.125036	-1.433465
H	-2.711269	1.954451	0.321071
H	-1.694601	3.059892	-0.638389
C	-3.589071	-0.431859	-0.425099
H	-4.375604	0.227003	-0.038752
H	-3.319592	-0.142602	-1.440525
H	-3.965669	-1.459646	-0.459708
C	-2.540937	-1.324301	1.576551
H	-2.602067	-2.365206	1.243632
H	-1.696423	-1.222951	2.251484
H	-3.464841	-1.047604	2.097035
B	0.447338	-2.029828	1.286688
H	-0.356014	-2.926859	1.317920
H	1.546258	-2.441954	0.970706
B	-0.447497	-2.029653	-1.286634
H	-1.546249	-2.442199	-0.970630
H	-0.515596	-1.417522	-2.349010
H	0.356122	-2.926440	-1.318133
H	0.515106	-1.417840	2.349160

1-Aucl

C	1.835900	-1.179397	0.009829
C	2.087232	0.134335	-0.049338
C	2.522068	1.359813	0.012454
H	1.860909	2.216318	0.042615
H	3.596909	1.537858	-0.003563
H	1.757591	-1.784568	-0.888751
H	1.748324	-1.689696	0.968827
Au	-0.104308	-0.102147	0.001276
Cl	-2.317332	0.347128	-0.003386

2-Aucl

H	2.857667	2.646197	-0.000098
H	3.696716	0.460491	-0.000159
C	1.690715	-0.484780	-0.000030
N	2.215935	1.861889	0.000038
C	2.614889	0.612740	0.000055
H	3.415048	-1.788798	0.000064

C	2.325583	-1.693924	0.000006
H	1.206045	2.036135	0.000033
H	1.772195	-2.628911	0.000243
Au	-0.310808	-0.123845	-0.000013
Cl	-2.570147	0.318896	0.000031

3-Aucl

H	-4.204841	-1.087135	0.815276
C	-1.429836	0.610550	-0.119987
N	-3.534226	-0.341111	0.679442
C	-2.390166	-0.491955	-0.001220
H	-1.312412	2.706729	-0.456438
C	-1.952106	1.834302	-0.364002
H	-3.696852	0.530892	1.163743
H	-3.017729	2.010433	-0.537328
N	-2.114620	-1.665140	-0.572253
H	-1.185933	-1.769521	-0.972538
H	-2.681706	-2.494191	-0.451444
Au	0.544862	0.124379	0.005943
Cl	2.778234	-0.435103	0.125303

4-Aucl

H	-1.554963	2.025271	-0.692290
H	-3.628820	-2.511817	-0.164103
H	-3.628814	2.511821	0.164104
H	-3.860647	-0.943249	-0.808856
H	-3.860641	0.943253	0.808861
C	-2.088876	-1.206724	0.215616
N	-3.351133	1.538805	0.165999
N	-3.351138	-1.538802	-0.165995
C	-2.088874	1.206724	-0.215617
H	-1.554965	-2.025273	0.692285
C	-1.437972	-0.000001	-0.000001
Au	0.619445	0.000000	0.000000
Cl	2.927232	0.000000	0.000002

4a-Aucl

H	0.000000	1.129352	-3.494135
H	0.000000	-3.221349	-2.468283
H	0.000000	3.221349	-2.468283
H	0.000000	-2.506297	-0.877917
H	0.000000	2.506297	-0.877917
C	0.000000	-1.160191	-2.401800
N	0.000000	2.394747	-1.888460
N	0.000000	-2.394747	-1.888460
C	0.000000	1.160191	-2.401800
H	0.000000	-1.129352	-3.494135
C	0.000000	0.000000	-1.631546
Au	0.000000	0.000000	0.411337
Cl	0.000000	0.000000	2.719667

5-Aucl

C	-2.298730	-0.839781	-0.009129
N	-1.840851	-2.054550	-0.353558
N	-3.604479	-0.779305	0.346957
C	-1.984080	1.516108	-0.118155
H	-2.326722	-2.894825	-0.092128

H	-0.852329	-2.115657	-0.553098
H	-4.245421	-1.520942	0.127784
H	-3.980337	0.059753	0.743839
N	-1.292178	2.668193	-0.081574
H	-1.723208	3.544828	-0.308470
H	-0.285273	2.623163	-0.024406
H	-3.052539	1.664033	-0.264930
C	-1.419421	0.273017	-0.022810
Au	0.613939	-0.005979	0.012608
Cl	2.902390	-0.319085	0.052541

6-AuCl

C	-1.972200	-1.219004	0.031179
N	-3.334135	-1.357157	0.256527
C	-1.972220	1.219152	-0.031247
H	-3.681747	-2.293152	0.429122
H	-3.756950	-0.656399	0.854524
H	-0.314558	-2.315213	-0.339212
N	-1.321379	2.385260	0.226538
H	-1.679991	3.268501	-0.111819
H	-0.314043	2.315379	0.337299
H	-3.681474	2.293057	-0.430902
C	-1.275149	0.000001	0.000067
N	-1.321815	-2.385253	-0.227732
N	-3.334138	1.357392	-0.255986
H	-1.679401	-3.268077	0.112872
H	-3.757778	0.655065	-0.851558
Au	0.792528	-0.000009	0.000042
Cl	3.103171	-0.000059	0.000054

7-AuCl

N	1.989688	-1.625364	0.266023
C	2.029960	-0.352142	-0.200865
C	1.348685	1.959203	0.178572
N	2.621633	2.520503	0.164070
H	2.752140	3.299093	0.801880
H	3.390517	1.860501	0.177821
N	0.371811	2.895896	0.402722
H	0.531947	3.836845	0.063458
N	3.145534	-0.026017	-0.959909
C	2.686269	-2.734090	-0.383055
H	3.676894	-2.921532	0.056734
H	2.086389	-3.640864	-0.260616
H	2.790193	-2.555147	-1.457164
C	1.177012	-1.999208	1.424689
H	0.917862	-1.111050	1.998188
H	0.251356	-2.499236	1.116553
H	1.766010	-2.679061	2.052700
H	3.843232	-0.733762	-1.149581
H	2.992815	0.617535	-1.726781
H	-0.579839	2.550807	0.309494
C	1.018708	0.606954	0.048494
Au	-0.969753	0.034221	-0.046535
Cl	-3.192560	-0.586296	-0.224926

8-AuCl

C	1.240120	1.215159	-0.131933
N	0.809243	2.408743	0.404237
C	1.240698	-1.214649	0.132249

N	0.810827	-2.408257	-0.404681
C	0.533876	0.000102	0.000188
N	2.405201	1.326873	-0.877831
N	2.405667	-1.326008	0.878390
C	2.714789	0.442636	-1.990471
H	3.442712	-0.334865	-1.718012
H	1.802744	-0.037411	-2.345475
H	3.144498	1.035098	-2.809858
C	3.457902	2.286108	-0.562320
H	3.568180	3.048659	-1.347337
H	3.240425	2.784540	0.382937
H	4.418906	1.760403	-0.471310
C	0.736140	3.622280	-0.411640
H	1.221434	4.469361	0.090763
H	1.211971	3.461608	-1.379395
H	-0.317740	3.880284	-0.587166
C	-0.062686	2.449012	1.573105
H	-1.124693	2.453463	1.293182
H	0.114862	1.581968	2.208968
H	0.163599	3.361760	2.139398
C	2.714437	-0.442288	1.991666
H	3.441845	0.335917	1.719850
H	1.801996	0.036848	2.346862
H	3.144444	-1.034997	2.810718
C	3.459107	-2.284310	0.562509
H	3.569747	-3.047282	1.347065
H	3.242192	-2.782290	-0.383115
H	4.419763	-1.757877	0.472042
C	0.737784	-3.622175	0.410640
H	1.224026	-4.468747	-0.091703
H	1.212679	-3.461620	1.378871
H	-0.316086	-3.880909	0.585154
C	-0.060063	-2.448607	-1.574320
H	-1.122312	-2.453833	-1.295341
H	0.117526	-1.581208	-2.209691
H	0.167285	-3.360997	-2.140763
Au	-1.537145	-0.000304	0.000069
Cl	-3.861454	-0.000762	-0.000056

3-2Aucl

H	-1.502171	3.964373	-0.940366
C	-0.066431	1.319605	0.594350
N	-1.264706	3.264174	-0.247962
C	-0.278125	2.379843	-0.422169
H	0.098279	1.030497	2.703833
C	-0.020140	1.740719	1.892715
H	-1.937916	3.097348	0.488925
H	-0.049790	2.794844	2.173053
N	0.505459	2.450406	-1.490429
H	1.242587	1.753743	-1.584678
H	0.346895	3.089992	-2.259209
Au	-1.336460	-0.341408	0.053744
Au	1.411413	-0.175055	0.106274
Cl	-3.193355	-1.594707	-0.396579
Cl	3.392399	-1.203719	-0.394220

4-2Aucl

H	-0.237978	1.382986	-2.121950
H	0.697355	1.504926	3.244059
H	-1.018826	3.563759	-2.044946

H	-0.537731	0.520800	2.550101
H	-0.899522	3.649205	-0.329162
C	0.490351	1.659718	1.209579
N	-0.701157	3.140523	-1.182156
N	0.106691	1.299596	2.448280
C	-0.314728	1.858616	-1.148599
H	1.202559	2.485007	1.176822
C	-0.033893	1.118001	0.014995
Au	1.720732	-0.093884	-0.035236
Au	-1.683717	-0.169116	-0.063457
Cl	-3.479452	-1.580617	0.067057
Cl	3.548913	-1.432827	-0.302169

4a-2Aucl

H	-1.191764	2.527007	1.163428
H	-0.375567	1.852175	-3.237370
H	-0.375621	1.851996	3.237448
H	0.805721	0.805016	-2.497544
H	0.805686	0.804885	2.497584
C	-0.421132	1.754862	-1.188743
N	0.063000	1.493999	2.399551
N	0.063031	1.494122	-2.399486
C	-0.421151	1.754797	1.188814
H	-1.191745	2.527070	-1.163327
C	0.110546	1.178355	0.000024
Au	-1.728025	-0.091611	-0.000005
Au	1.761763	-0.042414	0.000002
Cl	-3.501335	-1.515771	-0.000032
Cl	3.640523	-1.356296	-0.000026

5-2Aucl

C	0.263382	2.279780	-0.797091
N	1.072136	3.359845	-0.661679
N	-0.353774	2.110323	-1.972418
C	0.070026	1.930748	1.568537
H	1.205139	4.010595	-1.425973
H	1.816975	3.321451	0.019887
H	-0.036675	2.555551	-2.824021
H	-1.006136	1.334973	-2.054491
N	0.033077	1.261897	2.728715
H	-0.095142	1.739806	3.608803
H	-0.002492	0.247889	2.732739
H	0.073428	3.015195	1.687608
C	0.057040	1.352199	0.296419
Au	1.367754	-0.362702	-0.013347
Au	-1.445035	-0.172133	0.015872
Cl	-3.345527	-1.415087	-0.283467
Cl	3.142428	-1.789288	-0.246740

6-2Aucl

C	0.202876	1.926681	-1.222784
N	-0.175910	1.409676	-2.408962
C	-0.205866	1.924198	1.223919
H	0.287760	1.674588	-3.269324
H	-0.617424	0.495145	-2.389441
H	1.297383	3.479604	-0.459358
N	0.176787	1.408162	2.409181
H	-0.287349	1.669842	3.270293
H	0.623646	0.496202	2.388285

H	-1.023882	3.581350	2.148333
C	-0.000177	1.196141	0.000063
N	0.766585	3.164541	-1.259706
N	-0.775354	3.159761	1.262453
H	1.012184	3.589962	-2.144503
H	-1.312821	3.469730	0.464491
Au	1.514137	-0.325020	0.017614
Au	-1.513310	-0.326594	-0.018128
Cl	3.267325	-1.800309	0.098097
Cl	-3.265595	-1.802983	-0.097866

7-2Aucl

N	1.888443	2.521242	-0.579125
C	0.799313	1.738360	-0.754089
C	0.104469	1.381295	1.607699
N	-0.133854	2.702730	1.856708
H	-0.364569	3.000292	2.796773
H	-0.570551	3.243518	1.122335
N	0.230071	0.583918	2.692997
H	-0.295853	0.777369	3.537251
N	0.209614	1.768728	-1.977068
C	2.313782	3.474049	-1.605777
H	1.444084	3.913097	-2.101134
H	2.875698	4.278165	-1.124215
H	2.963866	3.001883	-2.356515
C	2.808272	2.350875	0.548747
H	2.719489	1.341356	0.953140
H	3.831155	2.485959	0.184873
H	2.606847	3.083708	1.338586
H	0.765698	1.898751	-2.813608
H	-0.603444	1.166005	-2.076671
H	0.431516	-0.394476	2.507207
C	0.256614	0.869741	0.278022
Au	1.170894	-1.032969	0.006131
Au	-1.708247	0.055883	-0.063994
Cl	-3.849031	-0.655302	-0.479197
Cl	2.295638	-3.022822	-0.214862

8-2Aucl

C	0.841680	1.477377	-0.906305
N	1.130919	1.107982	-2.190406
C	-0.845229	1.475508	0.906331
N	-1.133378	1.105596	2.190508
C	-0.000902	0.733491	0.000030
N	1.487250	2.620836	-0.485704
N	-1.493666	2.617256	0.485576
C	1.861759	2.859411	0.904018
H	1.152143	3.520516	1.419030
H	1.930277	1.911245	1.438046
H	2.848441	3.337925	0.922521
C	1.829983	3.713074	-1.394282
H	2.913957	3.792827	-1.554063
H	1.340568	3.570680	-2.358237
H	1.482990	4.659345	-0.959487
C	2.520410	1.127726	-2.670479
H	2.631410	1.769154	-3.553509
H	3.192390	1.469341	-1.883897
H	2.810690	0.105182	-2.940838
C	0.270097	0.256554	-3.010173
H	0.484876	-0.808418	-2.855951

H	-0.782161	0.435071	-2.792814
H	0.459151	0.505785	-4.060856
C	-1.868672	2.854750	-0.904219
H	-1.160320	3.517100	-1.419348
H	-1.935311	1.906328	-1.438030
H	-2.856286	3.331312	-0.922787
C	-1.839359	3.708667	1.394042
H	-2.923496	3.785228	1.554247
H	-1.349096	3.567970	2.357822
H	-1.495363	4.655845	0.958868
C	-2.522840	1.121755	2.670771
H	-2.635318	1.762785	3.553896
H	-3.195845	1.461754	1.884360
H	-2.810470	0.098427	2.940996
C	-0.270229	0.256401	3.010162
H	-0.481917	-0.809148	2.855673
H	0.781543	0.438010	2.793039
H	-0.460095	0.504846	4.060882
Au	1.369755	-0.872719	0.481876
Au	-1.367711	-0.875754	-0.481865
Cl	3.055507	-2.350162	1.006108
Cl	-3.049763	-2.357470	-1.006086