

SUPPORTING INFORMATION

for

Beryllium Compounds for the Carbon–Halogen Bond Activation of Phenyl Halides: The Role of Non-Innocent Ligands

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Table S1. Relative energies (in kcal/mol) calculated at the ω B97X-D/def2-SVPP level.

Multiplicity	NtBuNtBuBe	NNBe	NPBe	NSBe	NOBe	(CAAC) ₂ Be
S _{BS}	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	8.7
T	19.4	14.9	27.5	28.8	19.8	5.5

S_{BS} = Singlet Broken Symmetry; S = Singlet; T = Triplet

Figure S1. Optimized geometries calculated at the ω B97X-D/def2-SVPP level.

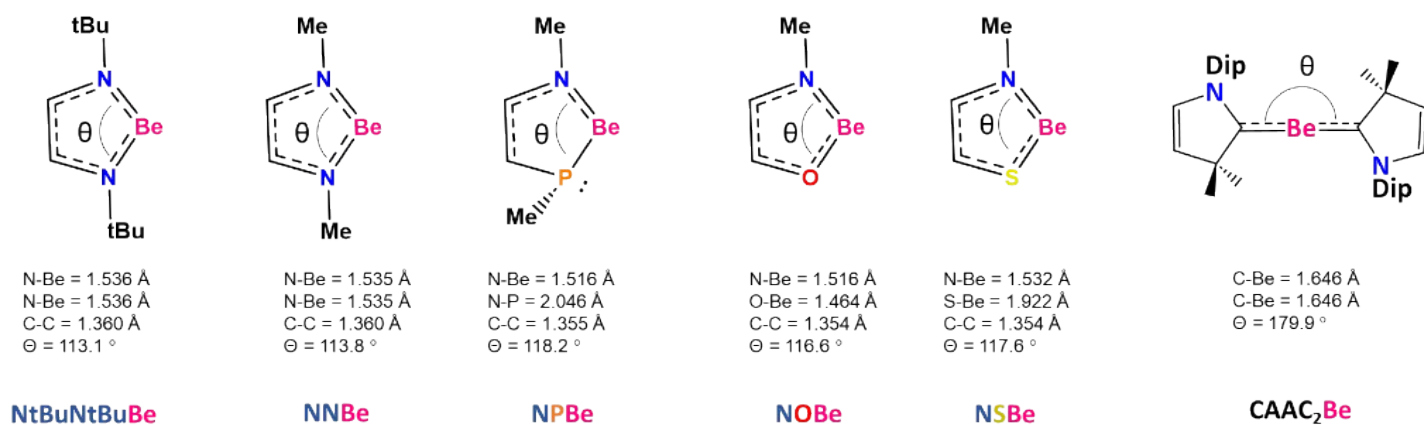
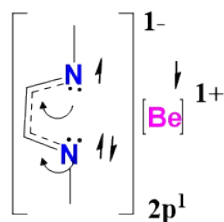


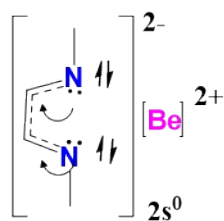
Table S2. (a) NICS (in ppm) calculated at the B3PW91/6-311+G**// ω B97X-D/def2-SVPP level. $n = 5$ for the five-membered rings and 6 for the six-membered ring (benzene). Values for intermediates and products are given only for X = Cl.

Compound	NICS(0)	NICS(1) _{zz}	NICS(-1) _{zz}	MCI	(MCI) ^{1/n}
NtBuNtBuBe	-9.2	-9.6	-9.6	0.0322	0.5030
NNBe	-8.7	-9.9	-9.9	0.0330	0.5055
NOBe	-6.3	-8.2	-8.2	0.0322	0.5030
NPBe	-2.9	1.4	-0.5	0.0242	0.4751
NSBe	-8.0	-7.6	-7.6	0.0318	0.5017
Benzene	-8.3	-29.4	-29.4	0.0415	0.5884
1.3a	1.4	-5.3	-	0.0180	0.4479
2.3a	1.7	-5.6	-	0.0178	0.4468
4.3c	1.4	-8.2	-	0.0187	0.4512
5.3c	-1.1	-11.3	-	0.0213	0.4631
1.5a	-2.6	2.4	-	-0.0091	-0.3903
2.5a	-1.6	-2.3	-	-0.0128	-0.4184
3.4a	-0.2	6.2	-	-0.0152	-0.4331
3.4b	-1.4	0.6	-	0.0166	0.4406
4.5a	-2.0	0.3	-	0.0159	0.4368
4.5b	-4.9	-3.1	-	0.0214	0.4634
5.5a	-2.4	-1.6	-	0.0166	0.4408
5.5b	-2.9	0.0	-	-0.0125	-0.4160

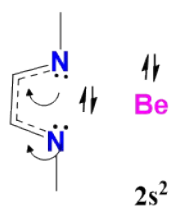
Figure S2. Energy Decomposition Analysis (EDA) calculated at the BLYP-D3(BJ)/TZ2P// ω B97X-D/def2-SVPP level of theory. All energies are in kcal/mol.



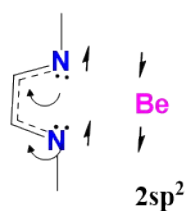
conf Be	ΔE_{Int}	ΔE_{Pauli}	ΔV_{elst}	ΔE_{orb}	ΔE_{dis}
Be ¹⁺	-400.0	674.3	-330.5	-740.7	-3.2



conf Be	ΔE_{Int}	ΔE_{Pauli}	ΔV_{elst}	ΔE_{orb}	ΔE_{dis}
Be ²⁺	-848.6	97.3	-604.9	-337.8	-3.2

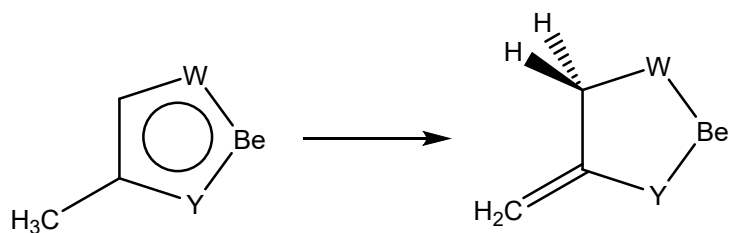


conf Be	ΔE_{Int}	ΔE_{Pauli}	ΔV_{elst}	ΔE_{orb}	ΔE_{dis}
Be ^{0(s)}	-116.8	516.2	-284.5	-345.3	-3.2



conf Be	ΔE_{Int}	ΔE_{Pauli}	ΔV_{elst}	ΔE_{orb}	ΔE_{dis}
Be ^{0(t)}	-210.2	858.2	-252.0	-813.2	-3.2

Figure S3. Isomerization Stabilization Energies (ISEs) calculated at ω B97X-D/def2-TZVP(SMD:toluene)// ω B97X-D/def2-SVPP level of theory. ISE based on Gibbs energies.



Ring	ISE (kcal/mol)
NNBe	3.8
NPBe	8.4
NOBe	5.7
NSBe	11.9

Figure S4. IBO analysis along the intrinsic reaction coordinate using the PBE/def2-SVPP// ω B97X-D/def2-SVPP method. (a) and (b) for the **NNBe**. EOS black for ligand and red for Be and F.

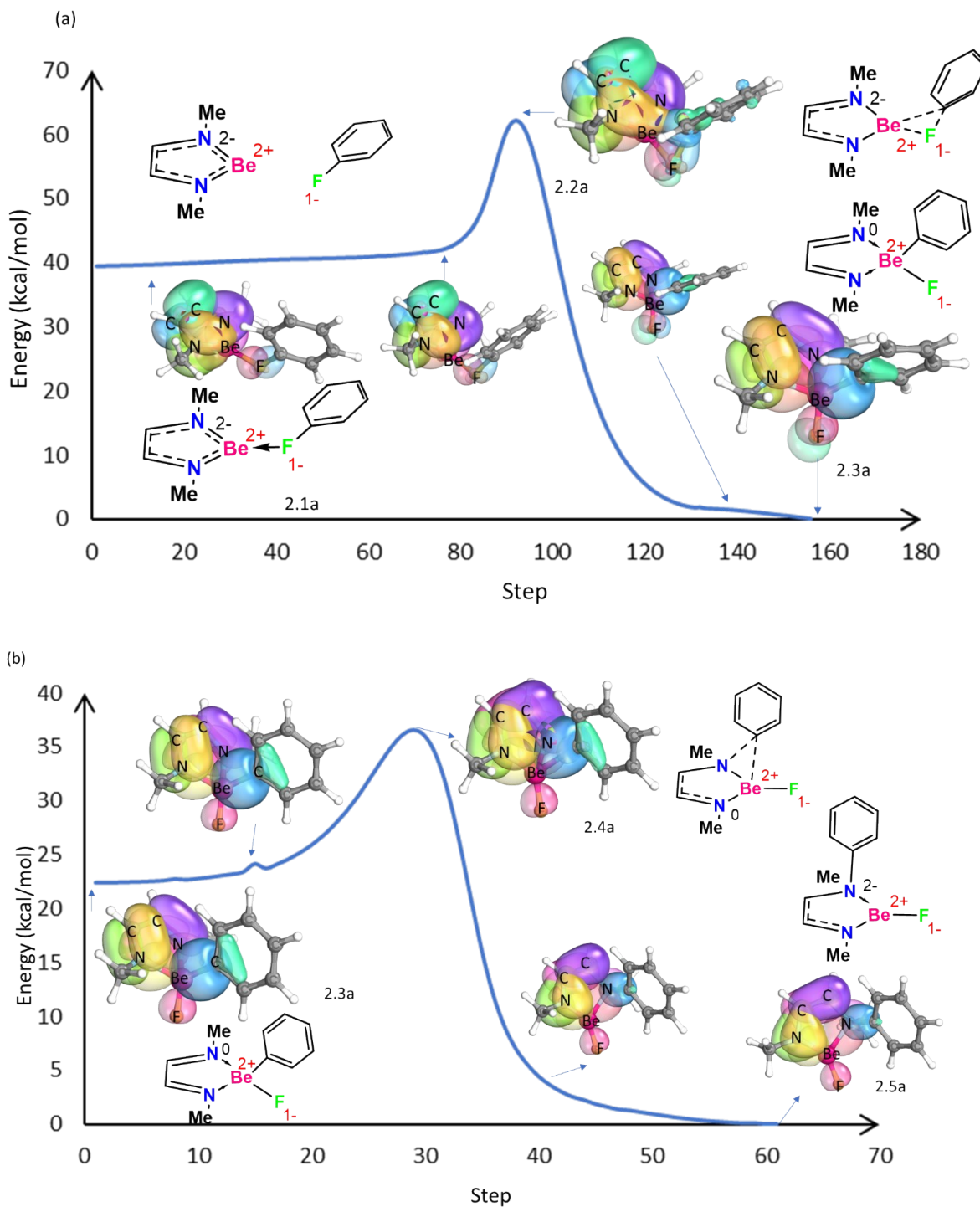
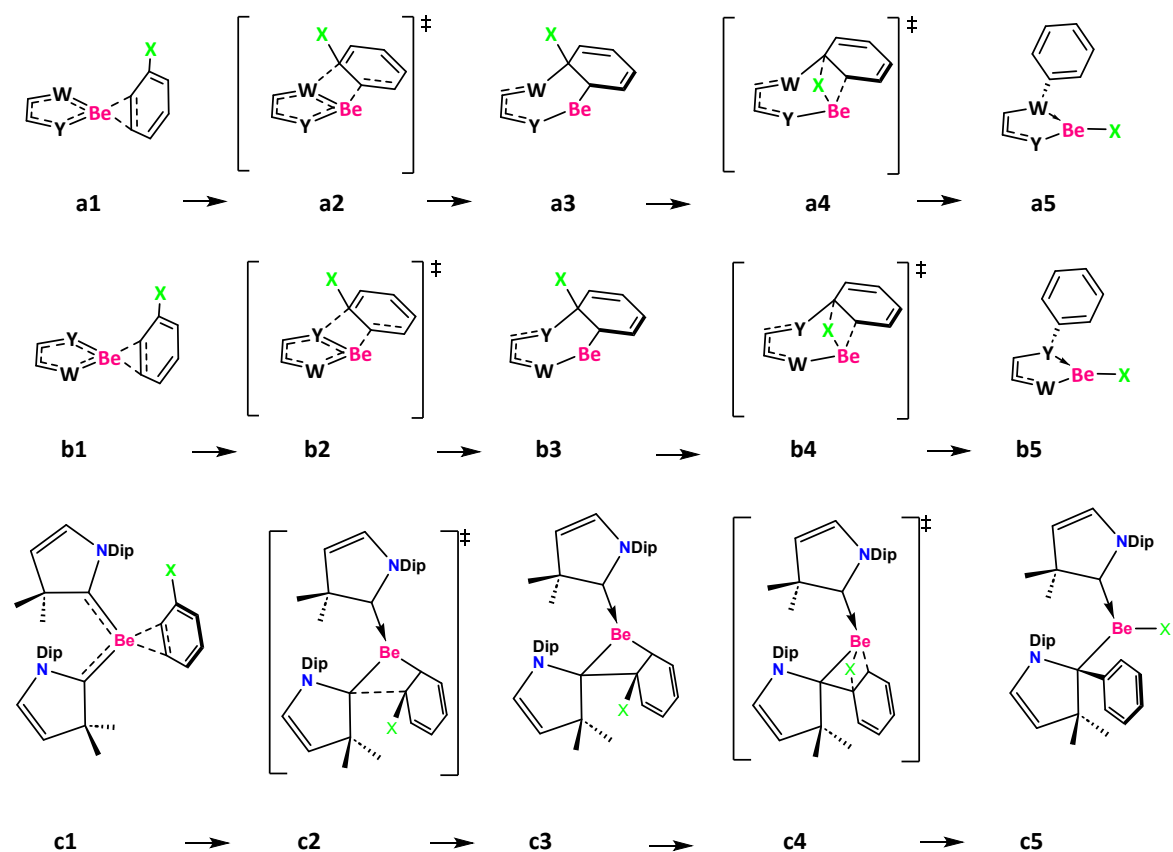


Table S3. Ph–X bonding energies calculated at ω B97X-D/def2-SVPP level.

Homolytic dissociation	
Molecule	BE (kcal/mol)
PhF	131.7
PhCl	97.4
PhBr	84.8
PhI	70.9

Heterolytic dissociation (Ph ⁺ + X ⁻)	
Molecule	BE (kcal/mol)
PhF	314.2
PhCl	254.8
PhBr	235.2
PhI	219.0

Figure S5. Reactions mechanism for Ph–X bond activation calculated at ω B97X-D/def2-TZVP(SMD:toluene)// ω B97X-D/def2-SVPP level of theory. **a5**, **b5**, and **c5** point out the product. TS were not calculated due to the high cost to get intermediates **a3**, **b3**, **c3**, and products.



Reaction	a1	a2	a3	a4	Reaction	a1	a2	a3	a4
NtBuNtBuBe+FPh	16.6	49.5	45.9	57.6	NNBe+FPh	-1.6	30.6	27.0	-
NtBuNtBuBe+ClPh	18.1	54.9	52.0	-	NNBe+ClPh	-1.7	33.4	31.5	-
NtBuNtBuBe+BrPh	17.1	55.3	52.3	-	NNBe+BrPh	-1.4	34.2	31.5	-
NtBuNtBuBe+IPh	16.4	53.3	50.3	-	NNBe+IPh	-2.2	33.2	31.0	-
Reaction	a1	a2	a3	a4	Reaction	a1	a2	a3	a4
NPBe+FPh	0.1	-	32.5	-	NOBe+FPh	-3.9	-	25.7	-
NPBe+ClPh	-1.7	-	28.8	-	NOBe+ClPh	-4.2	-	30.3	-
NPBe+BrPh	-0.7	-	27.3	-	NOBe+BrPh	-3.8	-	24.4	-
NPBe+IPh	-1.8	-	25.5	-	NOBe+IPh	-3.9	-	23.4	-
Reaction	a1	a2	a3	a4	Reaction	b1	b2	b3	b4
NSBe+FPh	-2.8	-	32.0	-	NPBe+FPh	0.1	-	12.7	-
NSBe+ClPh	-2.9	-	36.9	-	NPBe+ClPh	-1.7	-	16.1	-

NSBe+BrPh	-2.6	-	37.0	-	NPBe+BrPh	-0.7	-	13.7	-
NSBe+IPh	-3.2	-	36.9	-	NPBe+IPh	-1.8	-	12.3	-
Reaction	b1	b2	b3	b4	Reaction	b1	b2	b3	b4
NOBe+FPh	-3.9	-	36.4	-	NSBe+FPh	-2.8	-	---	-
NOBe+ClPh	-4.2	-	40.9	-	NSBe+ClPh	-2.9	-	34.7	-
NOBe+BrPh	-3.8	-	41.1	-	NSBe+BrPh	-2.6	-	33.3	-
NOBe+IPh	-3.9	-	41.1	-	NSBe+IPh	-3.2	-	32.4	-
Reaction	c1	c2	c3	c4					
CAAC ₂ Be+FPh	49.4	-	35.0	-					
CAAC ₂ Be+ClPh	49.7	-	41.0	-					
CAAC ₂ Be+BrPh	48.7	-	41.2	-					
CAAC ₂ Be+IPh	49.4	-	---	-					

Figure S6. HOMO, LUMO and GAP_{HL} calculated at ω B97X-D/ def2-SVPP level of theory. $(CAAC)_2Be(113^\circ)$ refers to the distorted $CAAC_2Be$ complex with a $\angle CBeC$ angle of 113° . Isosurface values of 0.03 a.u.

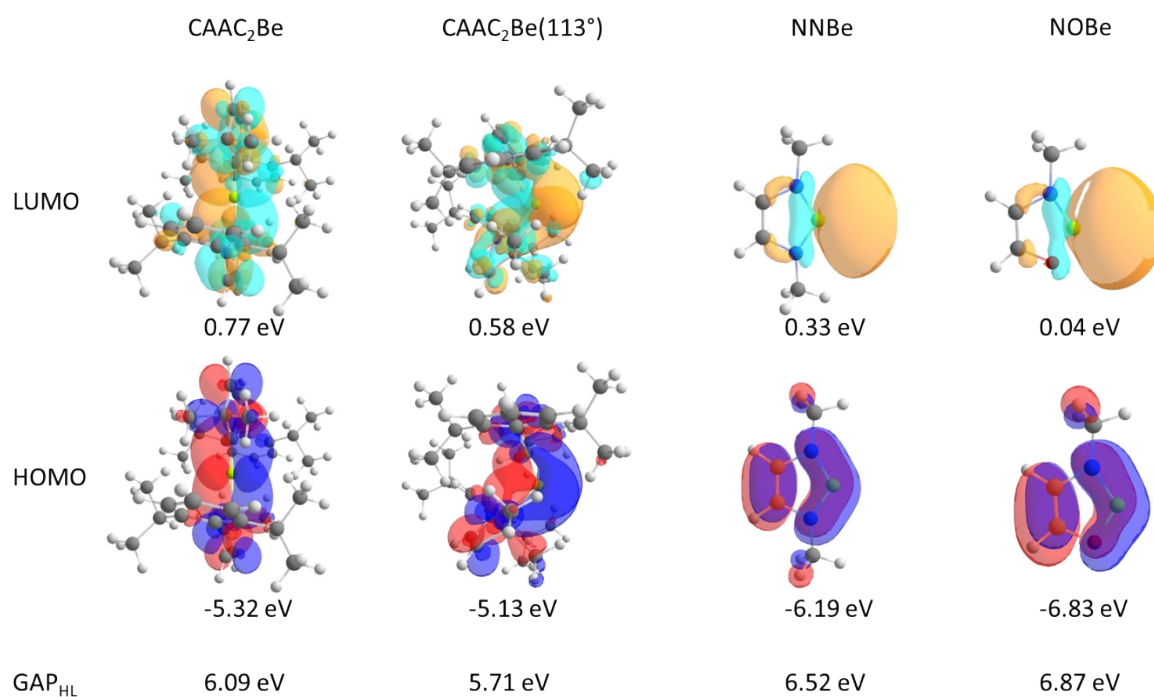


Figure S7. Reaction mechanism for the Ph–F bond activation using **NNBe**. In red, the Gibbs energy profile calculated at ω B97X-D/def2-TZVP(SMD:toluene)// ω B97X-D/def2-SVPP level of theory and in blue with the ω B97X-D/def2-TZVPP(SMD:toluene)// ω B97X-D/def2-TZVPP method.

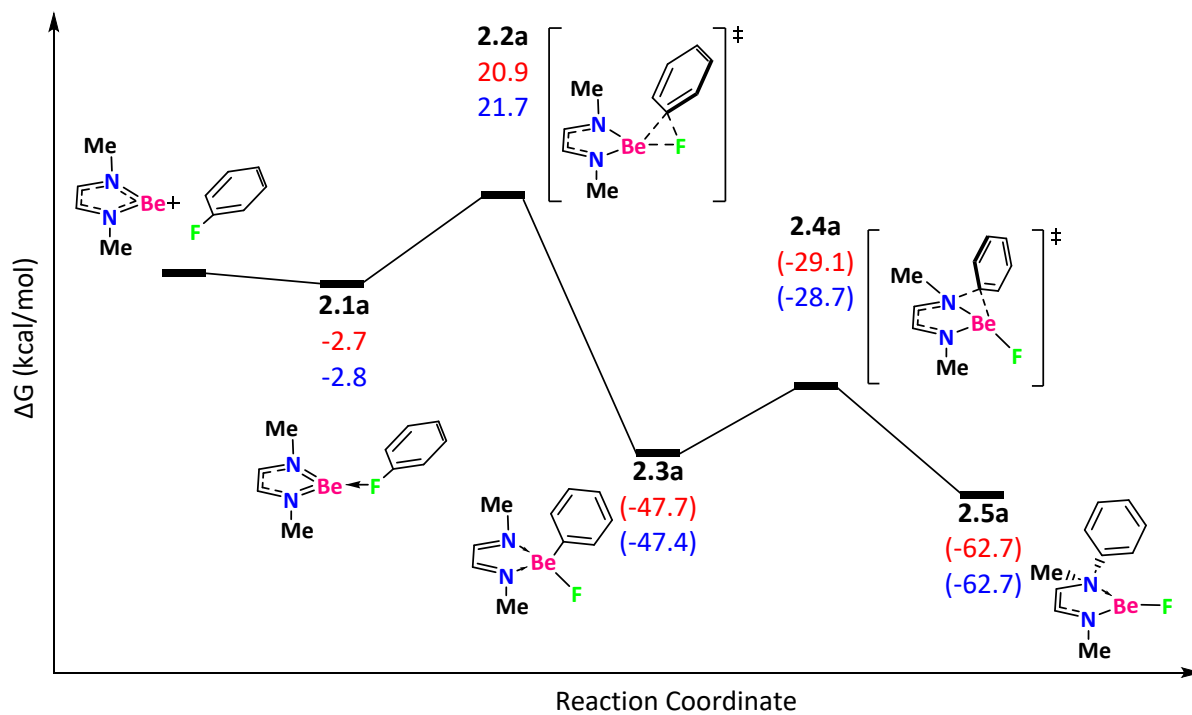


Table S4. Isomerization stabilization energies (ISEs, kcal/mol) and Gibbs energy barriers for the oxidative addition for different five-membered rings and halogens.

Ring	ISE	Halogen	Step	ΔG^\ddagger
NNBe	3.8	Cl	2.2a	20.6
		Br		17.2
		I		15.6
NPBe	8.4	-	-	-
NOBe	5.7	Cl	4.2c	24.0
		Br		20.8
		I		18.5
NSBe	11.9	Cl	5.2c	30.6
		Br		26.6
		I		25.1

Table S5. Cartesian coordinates (xyz format) of the optimized geometries for all the compounds involved in the reaction mechanisms calculated at the ω B97X-D/def2-SVPP level.

NNBe+FPha1

C	-2.15874	1.65194	-0.27139
C	-2.92499	0.52110	-0.20408
H	-2.54594	2.66105	-0.44650
H	-4.01285	0.49441	-0.32107
Be	-0.71050	-0.12993	0.11606
C	-2.88037	-1.89377	0.11652
H	-3.62393	-1.91376	0.93931
H	-3.41746	-2.15031	-0.81940
H	-2.15599	-2.70536	0.31011
C	0.13112	2.51234	-0.12163
H	-0.36658	3.47721	-0.33217
H	0.66549	2.61408	0.84640
H	0.91249	2.36124	-0.89501
N	-0.80544	1.42970	-0.09878
N	-2.19760	-0.63411	0.02694
C	1.82806	-0.63679	-0.85969
C	2.64690	0.24153	-0.18556
C	0.81367	-1.36996	-0.20621
H	3.41487	0.78949	-0.73540
H	0.29370	-2.16081	-0.75220
C	2.47199	0.40785	1.20454
C	0.65520	-1.19462	1.18971
H	3.12245	1.10067	1.74435
H	-0.03684	-1.83566	1.74145
C	1.49216	-0.29223	1.88363
H	1.36152	-0.16036	2.95984
F	1.97804	-0.81174	-2.16403

NNBe+IPha1

C	2.93159	-0.52904	1.71508
C	3.38995	-1.33943	0.71322
H	3.29808	-0.54056	2.74689
H	4.17531	-2.09306	0.82750
Be	1.72741	0.01100	-0.20210
C	3.14370	-1.92704	-1.63781
H	4.21440	-1.80138	-1.89868
H	2.96873	-3.00971	-1.47283
H	2.55396	-1.63244	-2.52456
C	1.34065	1.25362	2.25834
H	1.77738	1.14201	3.26825
H	1.48090	2.30953	1.94551

H	0.24531	1.09590	2.34662
N	1.93155	0.34160	1.32617
N	2.76232	-1.13341	-0.50375
C	-0.96942	0.64561	-0.45688
C	-1.04550	1.94654	-0.00006
C	0.07963	0.23898	-1.32062
H	-1.85435	2.25447	0.66642
H	0.06011	-0.75012	-1.78445
C	-0.06738	2.88758	-0.39429
C	1.05271	1.19016	-1.70796
H	-0.13878	3.91480	-0.02746
H	1.79714	0.92667	-2.46380
C	0.96689	2.51792	-1.23003
H	1.72082	3.24681	-1.53634
I	-2.39628	-0.77120	0.13820

NNBe+BePha1

C	2.68931	-0.02887	1.68546
C	3.26182	-0.83974	0.74405
H	3.08539	0.13735	2.69264
H	4.18345	-1.41186	0.88858
Be	1.33719	0.06395	-0.20758
C	3.05922	-1.69932	-1.52650
H	4.05152	-1.36101	-1.88940
H	3.15893	-2.76573	-1.23955
H	2.36479	-1.65722	-2.38487
C	0.80026	1.46786	2.13390
H	1.28309	1.55452	3.12502
H	0.72005	2.48963	1.70724
H	-0.23926	1.11403	2.29561
N	1.52662	0.58923	1.26768
N	2.56367	-0.88857	-0.45025
C	-1.43157	0.20525	-0.40117
C	-1.72168	1.51507	-0.07860
C	-0.35309	-0.11674	-1.26324
H	-2.55420	1.74420	0.58994
H	-0.22373	-1.14217	-1.61731
C	-0.93237	2.55718	-0.61420
C	0.42709	0.93719	-1.79435
H	-1.16860	3.59259	-0.35587
H	1.18433	0.72176	-2.55248
C	0.12671	2.27598	-1.45410
H	0.73531	3.08276	-1.86906
Br	-2.46046	-1.19721	0.31801

NNBe+BrPha1

C	-2.35333	1.17802	-1.13931
C	-3.05397	0.11466	-0.63994
H	-2.75593	1.92470	-1.83171
H	-4.09904	-0.11126	-0.87341
Be	-0.90603	0.00280	0.25450
C	-2.92905	-1.84994	0.79456
H	-3.81584	-1.59885	1.41178
H	-3.25778	-2.57935	0.02645
H	-2.20997	-2.37075	1.45209
C	-0.17312	2.29884	-1.13520
H	-0.68400	2.99195	-1.82913
H	0.21019	2.89690	-0.28214
H	0.71843	1.89453	-1.65854
N	-1.04639	1.25241	-0.69698
N	-2.31825	-0.68629	0.21671
C	1.77947	-0.57446	-0.09288
C	2.42145	0.61449	0.18694
C	0.72403	-1.05059	0.72377
H	3.23004	0.96062	-0.45975
H	0.32938	-2.05658	0.56479
C	2.02000	1.37414	1.30750
C	0.33139	-0.27815	1.84168
H	2.53245	2.31472	1.52491
H	-0.39758	-0.68077	2.54978
C	0.98998	0.94173	2.11948
H	0.68132	1.53116	2.98598
Cl	2.24434	-1.51198	-1.47275

NNBe+BrPha3

C	-1.50227	0.14395	1.50690
C	-2.59893	-0.18345	0.78401
H	-1.48225	0.74516	2.41800
H	-3.59699	0.19082	1.04549
Be	-0.89997	-1.21172	-0.47870
C	-3.61059	-1.25773	-1.14444
H	-4.41676	-1.76407	-0.57768
H	-4.03640	-0.33377	-1.58366
H	-3.32990	-1.92082	-1.97843
C	0.28608	-1.41358	2.01454
H	-0.51727	-2.05917	2.40276
H	1.05928	-2.04386	1.55031
H	0.73875	-0.85846	2.85480
N	-0.31049	-0.50773	1.02258
N	-2.45293	-0.99196	-0.32477

C	0.72959	0.15762	0.06610
C	2.08751	0.25967	0.68166
C	0.63466	-0.75151	-1.19059
H	2.25192	1.05036	1.41934
H	0.40424	-0.19789	-2.11785
C	3.06943	-0.60029	0.34894
C	1.77186	-1.65893	-1.40225
H	4.04350	-0.50322	0.84013
H	1.68908	-2.36242	-2.23938
C	2.90027	-1.63354	-0.65963
H	3.71883	-2.33108	-0.85415
Br	0.10892	1.98171	-0.34803

NNBe+IPha3

C	-1.56207	-0.17520	1.52184
C	-2.66401	-0.38857	0.76440
H	-1.52325	0.36535	2.46969
H	-3.63884	0.04054	1.02882
Be	-1.01166	-1.45814	-0.52061
C	-3.70183	-1.27972	-1.24249
H	-4.55368	-1.76438	-0.72601
H	-4.05391	-0.30384	-1.63171
H	-3.44440	-1.90755	-2.11069
C	0.10382	-1.86776	1.98839
H	-0.75221	-2.46982	2.33156
H	0.84162	-2.53061	1.51273
H	0.57392	-1.38238	2.86158
N	-0.40520	-0.87903	1.02596
N	-2.55001	-1.14447	-0.38345
C	0.70245	-0.24317	0.12500
C	2.05383	-0.32355	0.75486
C	0.54519	-1.03575	-1.20178
H	2.27395	0.35571	1.58364
H	0.31834	-0.40720	-2.08033
C	2.97608	-1.21127	0.33230
C	1.62185	-1.98360	-1.51762
H	3.94547	-1.24273	0.84103
H	1.49248	-2.58421	-2.42592
C	2.74905	-2.11136	-0.78425
H	3.52233	-2.83340	-1.05762
I	0.24123	1.89398	-0.17841

NNBe+ClPha3

C	1.47290	-1.11875	1.04204
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C	2.57187	-0.47509	0.58405
H	1.45091	-2.08933	1.54126
H	3.57211	-0.92268	0.64642
Be	0.87211	1.02840	-0.04240
C	3.58961	1.40669	-0.56337
H	4.38056	1.58392	0.19203
H	4.03532	0.81196	-1.38536
H	3.30939	2.38713	-0.98090
C	-0.35464	-0.03061	2.21075
H	0.42707	0.34483	2.88961
H	-1.13195	0.74027	2.09885
H	-0.81123	-0.93335	2.65317
N	0.27834	-0.32127	0.91783
N	2.42656	0.77012	0.00603
C	-0.73054	-0.45285	-0.27027
C	-2.08978	-0.88724	0.17394
C	-0.65582	0.96576	-0.90138
H	-2.23632	-1.95163	0.37867
H	-0.43422	0.94337	-1.98326
C	-3.08804	0.00460	0.31998
C	-1.80970	1.83502	-0.62526
H	-4.06424	-0.34753	0.67037
H	-1.74399	2.86802	-0.98731
C	-2.93484	1.41359	-0.00676
H	-3.76634	2.09861	0.17746
Cl	-0.07270	-1.69152	-1.41123

NNBe+FPha3

C	-1.45300	-1.56174	-0.05018
C	-2.55454	-0.77781	0.00635
H	-1.42029	-2.64429	0.08793
H	-3.54579	-1.18838	0.23784
Be	-0.87596	0.83125	-0.36029
C	-3.59237	1.41565	-0.08304
H	-4.38523	1.14861	-0.80957
H	-4.03438	1.36127	0.93184
H	-3.32008	2.46731	-0.26788
C	0.36471	-1.30639	-1.65232
H	-0.41079	-1.37717	-2.43116
H	1.14341	-0.60268	-1.98461
H	0.82520	-2.30038	-1.51109
N	-0.27119	-0.82451	-0.42314
N	-2.42495	0.57894	-0.21820
C	0.70994	-0.28147	0.65810
C	2.06772	-0.89069	0.57458

C	0.64418	1.24362	0.41349
H	2.19106	-1.88359	1.01811
H	0.41056	1.79167	1.34586
C	3.08164	-0.23556	-0.02181
C	1.81300	1.81978	-0.26701
H	4.06286	-0.71720	-0.09103
H	1.76291	2.88391	-0.52622
C	2.93818	1.11900	-0.53564
H	3.78258	1.58557	-1.04949
F	0.13312	-0.59966	1.85832

NNBe+IPha2

C	-1.32149	-1.04199	1.64825
C	-2.28665	-1.35078	0.73765
H	-1.48977	-0.72196	2.67890
H	-3.35877	-1.27111	0.95495
Be	-0.28240	-1.68873	-0.44134
C	-2.83453	-1.92990	-1.55394
H	-3.62053	-2.66161	-1.28190
H	-3.33560	-0.97728	-1.81781
H	-2.33638	-2.30650	-2.46199
C	0.96062	-1.68894	2.10595
H	0.58158	-2.60932	2.58134
H	1.91278	-1.92415	1.61163
H	1.14787	-0.93793	2.89591
N	-0.02104	-1.22478	1.14196
N	-1.86412	-1.75948	-0.50124
C	0.80183	0.08398	-0.00654
C	2.04879	0.47011	0.65008
C	0.94649	-0.71537	-1.26337
H	1.99821	1.16185	1.49490
H	0.31314	-0.40396	-2.10940
C	3.24947	-0.00043	0.22269
C	2.27305	-1.15853	-1.64395
H	4.15287	0.31789	0.75366
H	2.35845	-1.72849	-2.57577
C	3.38291	-0.86723	-0.91744
H	4.37018	-1.22342	-1.22012
I	-0.59795	1.73821	-0.07736

NNBe+ClPha2

C	-1.57183	-1.56521	-0.46028
C	-2.59207	-0.67210	-0.33088
H	-1.65281	-2.65008	-0.36109

H	-3.61926	-0.96949	-0.08671
Be	-0.72513	0.67612	-0.79161
C	-3.28567	1.65470	-0.24652
H	-4.15214	1.57309	-0.93277
H	-3.67102	1.59877	0.79092
H	-2.85135	2.65846	-0.38537
C	0.53406	-1.71007	-1.64714
H	-0.01422	-2.00001	-2.55982
H	1.40125	-1.10510	-1.94701
H	0.90058	-2.62932	-1.15286
N	-0.35071	-0.94770	-0.78745
N	-2.28275	0.65352	-0.50803
C	0.70881	-0.07422	0.59540
C	2.00005	-0.75238	0.60206
C	0.68670	1.32413	0.06893
H	2.07182	-1.70593	1.13100
H	0.15442	2.05460	0.69913
C	3.07800	-0.20638	-0.01672
C	1.89392	1.81885	-0.56198
H	4.02783	-0.75073	0.00620
H	1.87085	2.84483	-0.94546
C	3.02976	1.07953	-0.66273
H	3.92059	1.47445	-1.15617
Cl	-0.23189	-0.37764	2.06435

NNBr+BrPha2

C	-1.52711	-0.39031	1.66556
C	-2.53466	-0.59028	0.77092
H	-1.63485	0.02035	2.67205
H	-3.57888	-0.32674	0.97897
Be	-0.61941	-1.32501	-0.37252
C	-3.18527	-1.23113	-1.47882
H	-4.04991	-1.85517	-1.17700
H	-3.57443	-0.23701	-1.77621
H	-2.74280	-1.69582	-2.37501
C	0.62689	-1.37197	2.16799
H	0.11100	-2.18406	2.70822
H	1.51932	-1.79451	1.68624
H	0.94967	-0.61185	2.90370
N	-0.27798	-0.81775	1.17835
N	-2.19103	-1.13717	-0.43969
C	0.74436	0.28266	-0.05263
C	2.03148	0.52042	0.59297
C	0.75575	-0.61843	-1.24492
H	2.08231	1.28723	1.36994

H	0.19190	-0.25700	-2.11971
C	3.13876	-0.17651	0.22875
C	1.99217	-1.30513	-1.56027
H	4.08174	0.03305	0.74452
H	1.98884	-1.95588	-2.44175
C	3.12918	-1.14727	-0.83356
H	4.04423	-1.68771	-1.08590
Br	-0.30448	1.89764	-0.20870

NNBe+FPha2

C	1.59081	1.63247	-0.01791
C	2.60444	0.72758	0.03828
H	1.66378	2.69496	0.22629
H	3.61870	0.97936	0.37074
Be	0.76829	-0.52511	-0.72387
C	3.28213	-1.59818	-0.15188
H	4.23024	-1.38754	-0.68587
H	3.52726	-1.75022	0.91869
H	2.89348	-2.55352	-0.54203
C	-0.50223	1.95008	-1.20956
H	0.03975	2.40225	-2.05838
H	-1.35794	1.38885	-1.61267
H	-0.89107	2.76646	-0.57124
N	0.38591	1.06877	-0.48070
N	2.30255	-0.55999	-0.34530
C	-0.66699	-0.03819	0.76923
C	-1.93810	0.63908	0.92309
C	-0.65206	-1.31952	0.02917
H	-1.97725	1.48254	1.61713
H	-0.09193	-2.13214	0.51999
C	-3.02865	0.21741	0.22967
C	-1.86422	-1.69735	-0.66171
H	-3.97568	0.75217	0.35586
H	-1.85889	-2.64830	-1.20493
C	-2.99403	-0.93751	-0.62680
H	-3.89218	-1.23569	-1.17220
F	0.13253	0.03606	1.84296

NPBe+FPhab1

C	1.86441	1.88627	-0.27375
C	2.88723	1.09269	0.12146
H	2.03239	2.92682	-0.59156
H	3.90599	1.49452	0.13880
Be	0.53971	-0.03257	0.23674

C	3.03997	-1.73469	-0.53040
H	2.73178	-1.42590	-1.54432
H	4.14056	-1.81836	-0.51634
H	2.63540	-2.74304	-0.32532
C	-0.47689	2.32225	-0.80277
H	-0.08701	3.34776	-0.93718
H	-0.86674	1.98565	-1.78597
H	-1.34420	2.39102	-0.11832
N	0.53860	1.44293	-0.28506
P	2.46552	-0.55199	0.81520
C	-2.30205	-0.17209	0.86191
C	-1.23560	-1.07640	0.92552
C	-2.93147	0.13099	-0.33639
H	-0.81194	-1.34552	1.89748
H	-3.75649	0.84641	-0.34146
C	-0.80387	-1.69506	-0.26366
C	-2.47519	-0.47173	-1.51093
H	-0.01837	-2.45408	-0.22213
H	-2.95807	-0.22696	-2.46047
C	-1.41292	-1.37258	-1.48399
H	-1.06181	-1.84200	-2.40536
F	-2.70836	0.41281	1.97674

NPBe+ClPhab1

C	-3.07144	-0.05038	-0.32457
C	-2.85426	1.13105	0.29730
H	-4.06178	-0.32612	-0.71821
H	-3.67980	1.84074	0.41910
Be	-0.75578	-0.40414	0.15551
C	-0.44888	2.68699	-0.10898
H	-0.58949	2.44133	-1.17506
H	-0.89260	3.68033	0.07913
H	0.63484	2.76557	0.09397
C	-2.37036	-2.20782	-1.18919
H	-3.10410	-2.82973	-0.63667
H	-2.79016	-2.02040	-2.19814
H	-1.46241	-2.82203	-1.32683
N	-2.04656	-0.98840	-0.49591
P	-1.19984	1.41571	1.05482
C	1.91872	-0.17362	-0.42783
C	1.08550	-1.30409	-0.49049
C	2.41982	0.27515	0.79097
H	0.75497	-1.68249	-1.46126
H	3.06287	1.15693	0.82037
C	0.75156	-1.97461	0.69886

C	2.07515	-0.39927	1.96372
H	0.12926	-2.87249	0.65388
H	2.45361	-0.03213	2.92091
C	1.23930	-1.51168	1.92781
H	0.96173	-2.02412	2.85127
Cl	2.32112	0.65847	-1.88946

NPBe+BrPhab1

C	3.27718	-0.59472	-0.69005
C	3.10328	-1.30031	0.45069
H	4.15663	-0.74103	-1.33562
H	3.85436	-2.03884	0.75136
Be	1.21652	0.42382	-0.03535
C	0.52585	-2.31571	1.28323
H	0.37775	-2.58133	0.22287
H	0.91758	-3.20234	1.81183
H	-0.45760	-2.07572	1.72733
C	2.60232	1.03728	-2.35453
H	3.55286	1.60852	-2.34445
H	2.64989	0.33176	-3.20884
H	1.79432	1.75792	-2.57449
N	2.34956	0.36846	-1.10501
P	1.68269	-0.85521	1.53465
C	-1.54822	0.51269	0.01328
C	-0.64090	1.29794	-0.71920
C	-1.77169	0.76104	1.36485
H	-0.51585	1.13479	-1.79286
H	-2.47504	0.14180	1.92545
C	0.04972	2.33431	-0.06773
C	-1.07583	1.79268	1.99950
H	0.73202	2.96857	-0.64024
H	-1.23996	1.97106	3.06495
C	-0.16297	2.57276	1.29658
H	0.38874	3.36817	1.80222
Br	-2.46976	-0.87650	-0.85750

NPBe+IPhab1

C	-3.45091	-1.15457	0.63291
C	-3.31815	-1.45649	-0.67889
H	-4.23000	-1.61511	1.25950
H	-4.00062	-2.17842	-1.14066
Be	-1.61243	0.30930	0.18968
C	-0.74350	-1.78192	-1.95819
H	-0.46638	-2.34286	-1.04943

H	-1.06965	-2.50460	-2.72656
H	0.15729	-1.27195	-2.34640
C	-2.81663	0.00857	2.66593
H	-3.81178	0.45093	2.87652
H	-2.73210	-0.91806	3.26900
H	-2.05962	0.71512	3.05114
N	-2.60695	-0.23147	1.26195
P	-2.08876	-0.50284	-1.66347
C	1.09707	0.87079	-0.01772
C	0.17722	1.24393	0.97938
C	1.11514	1.53744	-1.24123
H	0.19889	0.76233	1.96083
H	1.82758	1.24755	-2.01676
C	-0.73033	2.28709	0.72642
C	0.20446	2.56993	-1.48159
H	-1.42400	2.60019	1.51151
H	0.21185	3.07359	-2.45131
C	-0.72063	2.94244	-0.51231
H	-1.44063	3.73896	-0.71191
I	2.45258	-0.68368	0.36200

NPBe+IPha3

C	1.13990	-1.55023	0.01550
C	2.44717	-1.52957	0.33255
H	0.40579	-2.27352	0.38814
H	2.81196	-2.29288	1.03253
Be	1.80677	0.67245	-0.18762
C	4.60053	0.11800	1.18754
H	3.97227	0.38963	2.05194
H	5.24462	-0.73358	1.46779
H	5.26274	0.97080	0.96023
C	0.46852	-0.98050	-2.25669
H	1.29930	-1.65910	-2.49630
H	-0.49143	-1.51869	-2.35849
H	0.49743	-0.13101	-2.95490
N	0.64917	-0.51222	-0.88041
P	3.63350	-0.28683	-0.36170
C	-0.33794	0.44262	-0.32632
C	-0.91165	1.36382	-1.32439
C	0.37541	1.15778	0.78113
H	-1.30857	0.94702	-2.25250
H	0.55471	0.54033	1.67541
C	-1.11321	2.67665	-1.04330
C	-0.01240	2.52329	1.08455
H	-1.61906	3.29542	-1.79108

H	0.31359	2.94604	2.04002
C	-0.71794	3.27543	0.20393
H	-0.96962	4.31728	0.41356
I	-2.22411	-0.84120	0.41954

NPBe+BrPha3

C	-1.03487	-1.52921	-0.16639
C	-2.34019	-1.28665	-0.38795
H	-0.44465	-2.31564	-0.64868
H	-2.85919	-1.92398	-1.11604
Be	-1.32970	0.73460	0.20515
C	-4.28493	0.69832	-0.96349
H	-3.69052	0.94097	-1.85992
H	-5.06030	-0.03773	-1.23840
H	-4.80288	1.61535	-0.63465
C	-0.17395	-1.24920	2.09318
H	-1.10913	-1.76595	2.35210
H	0.66098	-1.97306	2.09298
H	0.01083	-0.46414	2.84104
N	-0.33921	-0.65353	0.76500
P	-3.27308	0.06093	0.47469
C	0.78677	0.14607	0.20219
C	1.55834	0.87787	1.23971
C	0.11745	1.07958	-0.78187
H	1.96162	0.30559	2.07827
H	-0.14969	0.58797	-1.73097
C	1.91524	2.17433	1.08124
C	0.67663	2.41292	-0.96248
H	2.55241	2.63215	1.84485
H	0.35714	2.97990	-1.84298
C	1.52230	2.96393	-0.06087
H	1.90119	3.98180	-0.17615
Br	2.14299	-1.18768	-0.65763

NPBe+ClPha3

C	-1.01880	-1.49769	-0.48006
C	-2.26671	-0.99331	-0.51915
H	-0.63021	-2.27329	-1.14770
H	-2.95039	-1.38716	-1.28292
Be	-0.84570	0.67401	0.26615
C	-3.83277	1.37107	-0.56026
H	-3.27741	1.64178	-1.47356
H	-4.76418	0.85365	-0.84918
H	-4.12009	2.30251	-0.04326

C	0.04718	-1.77613	1.69033
H	-0.95040	-2.14066	1.97498
H	0.70908	-2.63621	1.48307
H	0.45421	-1.18386	2.52297
N	-0.09851	-0.93759	0.49789
P	-2.85609	0.32246	0.64243
C	1.12849	-0.28527	-0.06678
C	2.12002	0.07737	0.98702
C	0.57122	0.93880	-0.77834
H	2.49073	-0.72533	1.62912
H	0.17930	0.70259	-1.78075
C	2.68382	1.30444	1.05201
C	1.34327	2.17704	-0.74092
H	3.46076	1.47663	1.80429
H	1.05921	2.96634	-1.44486
C	2.33545	2.38252	0.15448
H	2.87070	3.33286	0.21134
Cl	1.98326	-1.53486	-1.18940

NPBe+FPha3

C	-1.13980	1.59989	-0.22691
C	-2.34560	1.15944	0.15971
Be	-0.61202	-0.89799	0.22530
N	-0.09471	0.63527	-0.47774
C	0.28149	0.57806	-1.89644
H	0.99617	-0.24327	-2.06455
H	-0.63016	0.39123	-2.48572
H	0.74486	1.52118	-2.23483
H	-0.90422	2.65331	-0.42572
H	-3.14865	1.90089	0.26720
P	-2.65100	-0.60333	0.64157
C	-3.65339	-1.19225	-0.82984
H	-3.17543	-1.00755	-1.80660
H	-3.82204	-2.27769	-0.72155
H	-4.64264	-0.70273	-0.82702
C	1.09828	0.51404	0.51694
C	1.02743	-0.97634	0.88688
C	2.39274	0.98594	-0.04653
H	0.90777	-1.12592	1.97610
H	2.55859	2.06732	-0.07289
C	2.09146	-1.82252	0.33330
C	3.31072	0.10529	-0.49183
H	2.02988	-2.89718	0.54004
H	4.24649	0.48225	-0.91833
C	3.13393	-1.33346	-0.37776

H	3.89839	-1.99928	-0.78580
F	0.73705	1.30267	1.57933
NPBe+BrPhb3			
C	1.75470	-1.48630	-0.24512
C	2.87827	-0.78491	-0.57460
H	1.58963	-2.45737	-0.72473
H	3.63974	-1.24898	-1.22247
Be	1.70525	1.14151	0.01936
C	4.46522	1.01689	-0.21557
H	5.04210	0.64616	0.65240
H	4.99850	0.70776	-1.13526
H	4.47066	2.11802	-0.17754
C	-0.21003	-2.47885	1.55588
H	0.53236	-3.15915	2.00546
H	-0.98291	-2.26302	2.31186
H	-0.68471	-2.96343	0.68638
P	0.64673	-0.92727	1.06908
N	3.10614	0.52374	-0.21208
C	-0.67705	0.15435	0.26913
C	-1.56915	0.71817	1.33031
C	0.07236	1.24604	-0.51379
H	-1.95411	0.02768	2.08837
H	0.27312	0.87076	-1.53737
C	-1.95579	2.00775	1.33696
C	-0.59521	2.56796	-0.58360
H	-2.63594	2.35650	2.12068
H	-0.27873	3.25468	-1.37708
C	-1.53071	2.94640	0.30660
H	-1.98359	3.94045	0.26518
Br	-1.88819	-0.90281	-0.98806

NPBe+IPhb3

C	1.81396	-1.64055	-0.14217
C	2.98177	-1.13463	-0.63971
H	1.47045	-2.61623	-0.50290
H	3.60487	-1.75652	-1.30275
Be	2.15203	0.98409	-0.08820
C	4.82014	0.44969	-0.62132
H	5.43983	0.10327	0.22711
H	5.20510	-0.03101	-1.54100
H	4.96760	1.53677	-0.72434
C	-0.02647	-2.15138	1.98116
H	0.67731	-2.84970	2.46373
H	-0.69066	-1.73692	2.75733
H	-0.63851	-2.69114	1.23879

P	0.94668	-0.80567	1.19848
N	3.41877	0.15094	-0.42666
C	-0.29137	0.39230	0.44182
C	-0.95799	1.18067	1.51631
C	0.50640	1.27503	-0.52482
H	-1.33081	0.64070	2.39327
H	0.58529	0.77156	-1.50854
C	-1.16768	2.50843	1.40993
C	0.00662	2.65778	-0.69786
H	-1.68741	3.03251	2.21837
H	0.30935	3.19991	-1.60080
C	-0.76396	3.25788	0.22990
H	-1.09231	4.29366	0.11047
I	-1.98280	-0.67125	-0.69030

NPBe+ClPhb3

C	1.75094	1.29335	0.42659
C	2.76016	0.38121	0.52482
H	1.81128	2.19940	1.03989
H	3.65600	0.61902	1.12176
Be	1.20818	-1.23171	-0.10704
C	3.95361	-1.57681	-0.27621
H	4.46587	-1.18428	-1.17454
H	4.64877	-1.47976	0.58012
H	3.76606	-2.65040	-0.43753
C	-0.19254	2.85339	-0.92971
H	0.61976	3.49294	-1.31308
H	-1.03157	2.89869	-1.64354
H	-0.53482	3.22501	0.05024
P	0.43151	1.12725	-0.80286
N	2.71086	-0.88513	-0.01879
C	-0.97672	0.17670	0.03114
C	-2.06050	-0.07132	-0.97714
C	-0.36355	-1.12944	0.57446
H	-2.39427	0.78120	-1.57847
H	-0.02782	-0.93888	1.61412
C	-2.66549	-1.26530	-1.10807
C	-1.24380	-2.32410	0.54084
H	-3.47188	-1.37710	-1.84022
H	-0.97834	-3.16593	1.19103
C	-2.30852	-2.40924	-0.27672
H	-2.91866	-3.31545	-0.31956
Cl	-1.75373	1.14935	1.41954

NPBe+FPhb3

C	-2.30363	0.43386	0.78410
C	-1.32632	1.37177	0.79681
Be	-1.04965	-0.96169	-0.74982
N	-2.40041	-0.61563	-0.12091
C	-3.70165	-1.23390	-0.27701
H	-3.61600	-2.16520	-0.86051
H	-4.14045	-1.49486	0.70534
H	-4.41435	-0.57069	-0.80244
H	-3.07219	0.44579	1.57267
H	-1.30721	2.06340	1.64698
P	-0.10987	1.62304	-0.53552
C	0.85209	3.04195	0.14567
H	1.19874	2.86850	1.17889
H	1.72742	3.21204	-0.49992
H	0.21982	3.94563	0.12831
C	1.14185	0.19284	-0.30044
C	0.62460	-1.00989	-1.08945
C	1.43202	-0.17382	1.12454
H	0.73080	-0.79929	-2.16922
H	1.51102	0.63369	1.85933
C	1.19406	-2.32680	-0.70549
C	1.69570	-1.44470	1.48926
H	1.16489	-3.13831	-1.44166
H	1.96052	-1.65860	2.53041
C	1.66631	-2.54683	0.53799
H	2.02829	-3.53216	0.84371
F	2.33422	0.68596	-0.87215

NOBe+FPhab1

C	1.98822	1.79963	-0.57213
C	2.83780	0.81089	-0.19681
H	2.25924	2.80911	-0.89453
H	3.92936	0.88453	-0.16714
Be	0.68808	0.04390	-0.03998
C	2.93437	-1.50655	0.59775
H	3.53771	-1.29906	1.50557
H	2.25687	-2.34429	0.84364
H	3.63302	-1.86782	-0.18507
N	2.17405	-0.36743	0.17312
O	0.67477	1.48190	-0.52479
C	-1.85325	0.12211	0.90374
C	-2.58339	0.56565	-0.18370
C	-0.90085	-0.90574	0.78644
H	-3.29709	1.38129	-0.05190
H	-0.41773	-1.29624	1.68607

C	-2.37959	-0.03814	-1.43050
C	-0.70935	-1.50130	-0.47845
H	-2.95124	0.31420	-2.29273
H	-0.01589	-2.34042	-0.57775
C	-1.44988	-1.05840	-1.58618
H	-1.28862	-1.51776	-2.56346
F	-2.03544	0.67654	2.08919

NOBe+ClPhab1

C	2.19989	0.00587	1.87814
C	2.99298	-0.33328	0.83100
H	2.48346	0.03028	2.93430
H	4.04364	-0.63244	0.89705
Be	0.90676	0.18437	0.04774
C	3.03137	-0.59705	-1.60582
H	3.44249	-1.62727	-1.59029
H	2.34974	-0.53219	-2.47322
H	3.87908	0.09178	-1.80238
N	2.32621	-0.27119	-0.40060
O	0.92980	0.33880	1.55665
C	-1.77030	-0.37268	-0.17089
C	-2.33986	0.65511	0.56413
C	-0.75623	-0.11009	-1.11552
H	-3.11102	0.42900	1.30279
H	-0.37853	-0.91761	-1.74748
C	-1.90654	1.97304	0.36206
C	-0.33062	1.21948	-1.30634
H	-2.35350	2.77713	0.95190
H	0.41067	1.44178	-2.07859
C	-0.91032	2.25992	-0.55864
H	-0.56807	3.28650	-0.70540
Cl	-2.28289	-2.00579	0.07074

NOBe+BrPhab1

C	2.60654	-0.22865	1.85810
C	3.21708	-0.87916	0.83606
H	2.91211	-0.22559	2.90836
H	4.11253	-1.50276	0.91989
Be	1.39965	0.24546	0.02208
C	3.08960	-1.32419	-1.57080
H	3.05695	-2.43065	-1.49313
H	2.48638	-1.04094	-2.45243
H	4.14008	-1.04148	-1.78866
N	2.58066	-0.67740	-0.39660

O	1.51010	0.48413	1.51582
C	-1.36071	0.34595	-0.19718
C	-1.65454	1.49838	0.51435
C	-0.30891	0.32858	-1.13671
H	-2.46131	1.49640	1.25005
H	-0.13363	-0.56039	-1.74771
C	-0.89844	2.65996	0.29759
C	0.44075	1.50284	-1.34680
H	-1.12930	3.56105	0.87117
H	1.21263	1.51744	-2.12116
C	0.14046	2.66928	-0.61958
H	0.73119	3.57370	-0.77985
Br	-2.35151	-1.22565	0.09099

NOBe+IPhab1

C	2.79185	-0.75543	1.88324
C	3.41330	-1.32627	0.82104
H	3.00936	-0.92895	2.94100
H	4.23287	-2.04960	0.87328
Be	1.78264	0.08639	0.05832
C	3.44451	-1.41491	-1.62815
H	3.31628	-2.51313	-1.72087
H	2.94064	-0.95480	-2.49743
H	4.52880	-1.20157	-1.72827
N	2.89444	-0.89811	-0.40914
O	1.79981	0.10960	1.57529
C	-0.88373	0.75664	-0.19942
C	-0.95371	1.89906	0.58434
C	0.16872	0.59080	-1.12562
H	-1.75945	2.02101	1.31153
H	0.18614	-0.26973	-1.79983
C	0.02358	2.89799	0.45430
C	1.14482	1.59997	-1.24533
H	-0.03754	3.78865	1.08475
H	1.92617	1.50638	-2.00460
C	1.06642	2.75522	-0.44653
H	1.83106	3.52959	-0.53902
I	-2.32564	-0.75249	-0.00905

NOBe+FPha3

C	2.92460	0.16972	-0.02520
C	2.09591	-0.89453	0.00603
H	3.99447	0.11149	0.20849
H	2.37195	-1.92145	0.25510

Be	0.93233	1.19844	-0.44111
C	0.27946	-1.32557	-1.56600
H	0.10320	-2.38655	-1.31609
H	-0.65629	-0.89335	-1.95152
H	1.05120	-1.26594	-2.34907
N	0.75155	-0.56319	-0.40666
O	2.44507	1.37610	-0.34327
C	-0.32873	-0.21895	0.66512
C	-0.60612	1.27640	0.37723
C	-1.51561	-1.11824	0.60468
H	-0.49970	1.89351	1.28907
H	-1.41533	-2.09774	1.08210
C	-1.87348	1.55337	-0.31864
C	-2.64866	-0.72525	-0.00653
H	-2.06123	2.59287	-0.61165
H	-3.49772	-1.41548	-0.05229
C	-2.81024	0.60997	-0.56327
H	-3.73503	0.85905	-1.08976
F	0.29899	-0.36647	1.87249

NOBe+FPPh3

C	2.53456	-0.79303	-0.40739
C	1.42329	-1.53852	-0.58224
H	3.54158	-1.22409	-0.44381
H	1.31757	-2.59758	-0.80805
Be	0.81524	0.79854	-0.18244
C	3.53145	1.37072	0.08172
H	4.27076	1.34588	-0.74270
H	3.23308	2.42207	0.22247
H	4.04701	1.04525	1.00702
O	0.28314	-0.73001	-0.63787
N	2.36741	0.56823	-0.20631
C	-0.82106	-0.56336	0.44366
C	-0.72313	0.93150	0.68223
C	-2.08061	-1.07885	-0.12480
H	-0.47596	1.15858	1.73402
H	-2.20871	-2.16458	-0.14838
C	-1.82023	1.74565	0.14978
C	-3.00864	-0.22613	-0.60656
H	-1.76393	2.82764	0.31321
H	-3.92161	-0.63495	-1.05210
C	-2.87250	1.21548	-0.51410
H	-3.65761	1.85331	-0.92717
F	-0.38431	-1.30488	1.48761

NOBe+ClPha3

C	2.88470	-0.49095	-0.06156
C	2.08798	0.08333	0.86349
H	3.97027	-0.34175	-0.10287
H	2.40982	0.74085	1.67381
Be	0.84136	-1.16443	-0.81283
C	0.20638	-1.00596	1.94789
H	0.06710	-0.29861	2.78384
H	-0.75271	-1.50220	1.73948
H	0.94779	-1.76518	2.24070
N	0.70908	-0.33119	0.74408
O	2.35120	-1.27621	-1.00182
C	-0.35915	0.51225	-0.03187
C	-0.65700	-0.39585	-1.25867
C	-1.54319	0.84726	0.81619
H	-0.51039	0.11871	-2.22469
H	-1.43108	1.66709	1.53139
C	-1.95083	-1.09673	-1.22603
C	-2.69867	0.16586	0.70163
H	-2.14638	-1.80197	-2.04240
H	-3.53582	0.43323	1.35513
C	-2.89528	-0.88472	-0.28436
H	-3.84064	-1.43261	-0.30072
Cl	0.42552	2.05655	-0.55273

NOBe+ClPhb3

C	2.55571	-0.45201	-0.76819
C	1.43822	-1.08797	-1.18133
H	3.55973	-0.84830	-0.95860
H	1.32642	-2.00243	-1.75993
Be	0.84814	0.97475	-0.00272
C	3.56999	1.40664	0.42723
H	4.29216	1.68483	-0.36514
H	3.27532	2.33477	0.94279
H	4.10313	0.77272	1.16287
O	0.30644	-0.30598	-0.94445
N	2.39907	0.75465	-0.10778
C	-0.82158	-0.47995	0.12128
C	-0.70548	0.86046	0.83344
C	-2.07172	-0.73864	-0.62125
H	-0.47573	0.75978	1.90683
H	-2.22558	-1.74555	-1.01775
C	-1.76998	1.83297	0.56569
C	-2.96695	0.25165	-0.81989
H	-1.69337	2.80175	1.07215

H	-3.86722	0.03490	-1.40451
C	-2.81337	1.57785	-0.25466
H	-3.57478	2.33584	-0.45322
Cl	-0.34392	-1.87577	1.14009

NOBe+BrPha3

C	-2.99111	0.42431	-0.61648
C	-2.17041	-0.50606	-0.08096
H	-3.88442	0.15829	-1.19513
H	-2.30575	-1.58716	-0.14800
Be	-1.24325	1.62623	-0.10230
C	-1.25947	-0.37962	2.14655
H	-0.93438	-1.42764	2.28144
H	-0.67995	0.27465	2.81372
H	-2.32466	-0.29413	2.40394
N	-1.10094	0.03538	0.74921
O	-2.72088	1.72546	-0.48872
C	0.29754	0.07132	0.20048
C	0.25688	1.14448	-0.87458
C	1.32388	0.36261	1.23964
H	-0.17628	0.77302	-1.82005
H	1.35396	-0.28177	2.12138
C	1.44000	1.97204	-1.08215
C	2.31314	1.26356	1.04054
H	1.49052	2.55497	-2.00762
H	3.08214	1.36556	1.81333
C	2.42279	2.06231	-0.15858
H	3.28348	2.72018	-0.29778
Br	0.73550	-1.80863	-0.50793

NOBe+Brphb3

C	2.64848	0.09112	0.90593
C	1.50805	0.52781	1.48339
H	3.63065	0.50200	1.16627
H	1.35828	1.26156	2.27242
Be	1.01074	-1.23094	-0.14657
C	3.73890	-1.34962	-0.72074
H	4.50193	-1.75983	-0.03060
H	3.48646	-2.14334	-1.44189
H	4.20614	-0.52066	-1.28788
O	0.42350	-0.25748	1.08818
N	2.54687	-0.92891	-0.02385
C	-0.77135	0.06051	0.14557
C	-0.57327	-1.01984	-0.90688

C	-1.99415	-0.02804	0.96833
H	-0.35740	-0.61977	-1.91108
H	-2.20010	0.79056	1.66283
C	-1.55911	-2.10427	-0.93048
C	-2.80875	-1.10129	0.87945
H	-1.43048	-2.87242	-1.70152
H	-3.68881	-1.14381	1.52988
C	-2.59266	-2.18049	-0.06310
H	-3.29561	-3.01632	-0.09117
Br	-0.48706	1.87522	-0.53395

NOBe+IPha3

C	-2.80261	-1.51310	-0.71426
C	-1.62617	-1.65474	-0.06497
H	-3.25219	-2.32360	-1.30081
H	-1.02284	-2.56422	-0.03080
Be	-2.32021	0.56542	-0.23432
C	-1.21097	-0.87098	2.17784
H	-0.27288	-1.40428	2.41963
H	-1.29780	0.02622	2.80775
H	-2.06631	-1.53046	2.38094
N	-1.24624	-0.51184	0.75667
O	-3.45581	-0.34878	-0.69485
C	-0.19558	0.43212	0.26825
C	-0.80474	1.13412	-0.92206
C	0.27156	1.38648	1.30005
H	-0.83722	0.50178	-1.82658
H	0.59789	0.99074	2.26420
C	-0.40648	2.50575	-1.20195
C	0.47549	2.69735	1.02249
H	-0.63920	2.91008	-2.19213
H	0.90170	3.33232	1.80577
C	0.19286	3.27870	-0.26631
H	0.44892	4.32215	-0.46251
I	1.69303	-0.84007	-0.26907

NOBe+IPhb3

C	-2.74970	-0.31758	0.92235
C	-1.56287	-0.43016	1.55978
H	-3.62218	-0.92027	1.19995
H	-1.28703	-1.03337	2.42221
Be	-1.41459	1.25460	-0.20767
C	-4.07339	0.69478	-0.84755
H	-4.93945	0.96023	-0.21028

H	-3.98412	1.47392	-1.62141
H	-4.30847	-0.25857	-1.35997
O	-0.67254	0.54872	1.11882
N	-2.84631	0.61819	-0.09097
C	0.60500	0.45676	0.23410
C	0.19805	1.34467	-0.92963
C	1.72385	0.93617	1.06785
H	0.08600	0.81201	-1.88800
H	2.07600	0.28691	1.87384
C	0.91092	2.61580	-1.07886
C	2.27822	2.15026	0.85636
H	0.63761	3.23729	-1.93920
H	3.08873	2.47477	1.51741
C	1.86896	3.02848	-0.21961
H	2.36523	3.99362	-0.34484
I	0.86144	-1.65353	-0.31173

NSBe+FPhab1

C	2.61347	-1.49246	-0.00772
C	2.98463	-0.19211	0.05681
H	3.32640	-2.31947	-0.00513
H	4.03786	0.11168	0.11518
Be	0.61577	0.08420	-0.03281
C	2.42631	2.16720	0.13504
H	2.98893	2.37992	1.06603
H	3.06972	2.46386	-0.71772
H	1.54802	2.83771	0.12873
N	2.00570	0.79246	0.05273
S	0.88317	-1.85570	-0.08802
C	-1.97304	0.19473	0.92419
C	-2.70685	-0.61300	0.07198
C	-1.08231	1.16631	0.43641
H	-3.37442	-1.36805	0.49206
H	-0.59984	1.85009	1.14071
C	-2.56497	-0.44392	-1.30952
C	-0.95657	1.32261	-0.95850
H	-3.13866	-1.08352	-1.98503
H	-0.30873	2.10802	-1.35672
C	-1.69493	0.50833	-1.82870
H	-1.58059	0.62560	-2.90803
F	-2.09742	0.05502	2.23117

NSBe+ClPhab1

C	-2.81748	0.68135	1.28269
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C	-3.10735	-0.28967	0.38502
H	-3.53615	1.05310	2.01596
H	-4.09354	-0.76938	0.34092
Be	-0.83963	0.13670	-0.22136
C	-2.45742	-1.74276	-1.44507
H	-2.69186	-2.70044	-0.93831
H	-3.32633	-1.48114	-2.08139
H	-1.60640	-1.93362	-2.12334
N	-2.12905	-0.69507	-0.51333
S	-1.19046	1.37649	1.25361
C	1.91940	-0.43901	0.09051
C	2.48348	0.82284	0.21021
C	0.97387	-0.71129	-0.91785
H	3.20587	1.01975	1.00471
H	0.60073	-1.73028	-1.04767
C	2.10686	1.83618	-0.68062
C	0.60751	0.31481	-1.80736
H	2.54673	2.83077	-0.57255
H	-0.08015	0.09635	-2.62959
C	1.17439	1.59437	-1.67970
H	0.87485	2.38984	-2.36512
Cl	2.35976	-1.69888	1.18766

NOBe+BrPhab1

C	3.07887	-0.57132	-1.51875
C	3.33653	-0.96517	-0.24932
H	3.72925	-0.80890	-2.36311
H	4.22682	-1.55233	0.01068
Be	1.28527	0.19900	0.11181
C	2.74471	-1.04942	2.10151
H	2.81489	-2.15244	2.18431
H	3.69725	-0.62649	2.47966
H	1.94793	-0.72333	2.79397
N	2.44808	-0.61896	0.75987
S	1.60836	0.36817	-1.81199
C	-1.53857	0.32227	0.22400
C	-1.83083	1.48446	-0.47559
C	-0.52198	0.30957	1.20038
H	-2.61286	1.48150	-1.23762
H	-0.35327	-0.58835	1.80105
C	-1.10779	2.65509	-0.20914
C	0.19500	1.49224	1.45822
H	-1.33761	3.56345	-0.77180
H	0.94462	1.50691	2.25434
C	-0.09904	2.66558	0.74312

H	0.46843	3.57744	0.94071
Br	-2.48795	-1.25975	-0.12895
NSBe+IPhab1			
C	3.25998	-1.06008	-1.50701
C	3.52472	-1.35315	-0.21207
H	3.82490	-1.47662	-2.34343
H	4.33393	-2.03521	0.07899
Be	1.68396	0.13459	0.09336
C	3.04379	-1.11418	2.15330
H	2.91055	-2.19535	2.35777
H	4.08121	-0.84677	2.43824
H	2.36784	-0.56952	2.83660
N	2.74901	-0.77607	0.78482
S	1.92384	0.04865	-1.84831
C	-1.07093	0.75902	0.22815
C	-1.16426	1.89641	-0.56348
C	-0.04846	0.64874	1.19398
H	-1.94919	1.97987	-1.31850
H	-0.01723	-0.20933	1.87156
C	-0.23776	2.93696	-0.40502
C	0.87405	1.70041	1.34401
H	-0.31482	3.82093	-1.04320
H	1.63297	1.64665	2.12960
C	0.77816	2.84475	0.53425
H	1.50598	3.65105	0.64750
I	-2.43193	-0.81515	-0.01030

NSBe+FPha3

C	2.75600	-0.62901	-0.05247
C	1.63279	-1.35273	0.06610
H	3.71200	-1.11498	-0.27318
H	1.59025	-2.44218	-0.03391
Be	0.80088	1.06359	0.24408
C	-0.08802	-1.03494	1.74272
H	-0.45624	-2.07520	1.73279
H	0.72607	-0.94300	2.47887
H	-0.91625	-0.37118	2.03649
N	0.43726	-0.63740	0.42837
S	2.77819	1.13484	0.12300
C	-0.65736	-0.33831	-0.64393
C	-0.77208	1.19503	-0.53226
C	-1.91613	-1.10459	-0.43329
H	-0.60153	1.68460	-1.50950
H	-1.92267	-2.14820	-0.76274
C	-1.99274	1.69376	0.11718

C	-2.98990	-0.51968	0.13203
H	-2.07070	2.77677	0.26598
H	-3.89785	-1.11105	0.29105
C	-3.01327	0.88981	0.49306
H	-3.90058	1.29901	0.98231
F	-0.08152	-0.70006	-1.83176

NSBe+ClPha3

C	2.77230	-0.26677	0.51578
C	1.65180	-0.74854	1.07463
H	3.74108	-0.73638	0.71520
H	1.62450	-1.60035	1.76163
Be	0.79101	1.09811	-0.47836
C	-0.08235	0.62568	2.04137
H	-0.44830	-0.12229	2.76501
H	0.73942	1.20148	2.49546
H	-0.90743	1.31009	1.79102
N	0.43904	-0.01487	0.82065
S	2.76957	1.12527	-0.58021
C	-0.68033	-0.52527	-0.14674
C	-0.78924	0.67435	-1.12225
C	-1.93746	-0.89730	0.56691
H	-0.63428	0.38796	-2.17749
H	-1.96293	-1.86573	1.07454
C	-1.99466	1.50356	-0.97480
C	-2.99620	-0.06425	0.58011
H	-2.05849	2.39440	-1.61042
H	-3.89526	-0.36262	1.12976
C	-3.01309	1.19856	-0.14067
H	-3.88873	1.84730	-0.06011
Cl	-0.02615	-1.98510	-0.98814

NSBe+ClPhb3

C	2.35472	-0.93238	0.61823
C	1.33619	-1.82076	0.81248
Be	0.92763	0.03580	-1.08650
N	2.32921	0.01324	-0.35790
C	3.43902	0.94114	-0.45111
H	3.23273	1.68840	-1.23353
H	3.59544	1.48780	0.49772
H	4.38423	0.43090	-0.71633
H	3.22980	-0.96123	1.28363
H	1.34366	-2.57994	1.59490
S	0.02193	-1.80568	-0.34951

C	-1.05389	-0.19768	-0.04468
C	-0.65560	0.75231	-1.16581
C	-0.84283	0.35922	1.31288
H	-1.13916	0.47633	-2.11603
H	-0.89994	-0.33409	2.15602
C	-0.70082	2.18748	-0.85552
C	-0.68685	1.68680	1.50674
H	-0.68834	2.88886	-1.69696
H	-0.58882	2.05784	2.53234
C	-0.67649	2.64389	0.41636
H	-0.64270	3.71343	0.63692
Cl	-2.78079	-0.81961	-0.19957

NSBe+BrPha3

C	-2.79028	-0.25209	0.60226
C	-1.67422	0.02990	1.29179
H	-3.76051	0.13231	0.93366
H	-1.65418	0.62077	2.21315
Be	-0.80064	-1.23734	-0.75545
C	0.03928	-1.59192	1.79308
H	0.39887	-1.11657	2.72133
H	-0.79293	-2.27337	2.02993
H	0.86437	-2.16970	1.34924
N	-0.45850	-0.59023	0.83177
S	-2.77808	-1.22891	-0.87521
C	0.68490	0.17813	0.08981
C	0.78199	-0.63706	-1.22499
C	1.93969	0.26010	0.89390
H	0.61673	-0.03134	-2.13321
H	1.97493	0.98746	1.70992
C	1.98102	-1.47498	-1.37032
C	2.99155	-0.53730	0.62185
H	2.03534	-2.09966	-2.26957
H	3.88752	-0.45664	1.24649
C	3.00326	-1.47658	-0.48711
H	3.87424	-2.11992	-0.63328
Br	0.04782	2.00803	-0.26362

NSBe+BrPhb3

C	2.69337	-1.16891	0.60314
C	1.56352	-1.90477	0.81803
Be	1.38753	0.00750	-1.06420
N	2.78532	-0.22498	-0.37121
C	4.02457	0.51595	-0.50295

H	3.91663	1.28250	-1.28659
H	4.29246	1.03608	0.43580
H	4.86887	-0.13863	-0.79013
H	3.56842	-1.32472	1.25055
H	1.48096	-2.65801	1.60204
S	0.24191	-1.71384	-0.32161
C	-0.59076	0.00492	-0.00509
C	-0.11188	0.89242	-1.14145
C	-0.28243	0.54773	1.33740
H	-0.61036	0.64315	-2.09176
H	-0.35836	-0.13096	2.19103
C	-0.04372	2.33138	-0.85738
C	-0.01641	1.86156	1.51094
H	0.00537	3.01823	-1.70918
H	0.14803	2.23335	2.52754
C	0.03148	2.80178	0.40789
H	0.14511	3.86899	0.61234
Br	-2.57090	-0.40446	-0.10754

NSBe+IPha3

C	-2.82204	-0.53636	0.58405
C	-1.70757	-0.32105	1.30012
H	-3.78439	-0.13739	0.92105
H	-1.68459	0.21859	2.25245
Be	-0.84251	-1.51704	-0.79068
C	-0.05443	-2.01508	1.74756
H	0.30763	-1.59573	2.70143
H	-0.91392	-2.67594	1.94187
H	0.75643	-2.60089	1.28852
N	-0.50315	-0.95250	0.82660
S	-2.81739	-1.44247	-0.93694
C	0.67768	-0.19379	0.13564
C	0.75292	-0.92832	-1.22686
C	1.92630	-0.22429	0.95145
H	0.58022	-0.27818	-2.10204
H	1.97843	0.41508	1.83766
C	1.93555	-1.77321	-1.44268
C	2.96130	-1.02144	0.61721
H	1.97454	-2.32641	-2.38830
H	3.85083	-1.02030	1.25628
C	2.96015	-1.86233	-0.56688
H	3.81921	-2.50722	-0.76692
I	0.10013	1.91658	-0.13532

NSBe+IPhb3

C	3.05281	-1.26830	0.59299
C	1.88761	-1.94996	0.79690
Be	1.80900	0.00347	-1.05148
N	3.19183	-0.31290	-0.36481
C	4.47106	0.35799	-0.49315
H	4.40689	1.13240	-1.27370
H	4.76763	0.85799	0.44788
H	5.27645	-0.34243	-0.78304
H	3.91940	-1.48013	1.23590
H	1.76731	-2.71053	1.56896
S	0.57509	-1.67632	-0.33729
C	-0.15098	0.07158	-0.00280
C	0.33742	0.94040	-1.14280
C	0.20002	0.60176	1.32882
H	-0.14769	0.69213	-2.09997
H	0.14531	-0.07754	2.18368
C	0.42173	2.37836	-0.86854
C	0.48509	1.91387	1.49959
H	0.46512	3.06275	-1.72236
H	0.68149	2.28188	2.51164
C	0.51311	2.85153	0.39611
H	0.63464	3.91875	0.59603
I	-2.41517	-0.25889	-0.05946

CAAC2Be+FPhc1

C	0.68549	-0.20224	1.42082
C	0.33976	-0.55412	2.86498
C	1.09658	-1.83324	3.12002
C	1.86957	-2.07123	2.06170
N	1.63672	-1.07512	1.06578
C	0.93846	0.52875	3.80581
C	-1.17045	-0.64570	3.10338
C	2.56570	-0.96342	-0.04196
C	3.63244	-0.04414	0.08554
C	4.52135	0.07410	-0.98320
C	4.41297	-0.73588	-2.10898
C	3.42304	-1.70474	-2.16470
C	2.48227	-1.83778	-1.13669
C	3.91789	0.69590	1.38220
C	1.47080	-2.96531	-1.20360
C	0.71161	-3.02108	-2.53274
C	2.15621	-4.31012	-0.92069
C	4.60452	2.05090	1.19571
C	4.75455	-0.19282	2.31718
H	4.58985	2.60535	2.14986

H	4.09393	2.66036	0.43582
H	5.66431	1.93634	0.90568
H	2.95495	0.88629	1.87013
H	4.25872	-1.15258	2.53542
H	4.92880	0.32198	3.27874
H	5.73763	-0.41265	1.86377
H	5.33081	0.80447	-0.92697
H	5.125703	-0.62871	-2.93139
H	3.373184	-2.37322	-3.02836
H	0.735292	-2.78883	-0.40804
H	1.385909	-3.22664	-3.38216
H	0.180488	-2.07791	-2.73825
H	-0.03595	-3.83263	-2.5097
H	1.419251	-5.13235	-0.92147
H	2.667139	-4.31145	0.05683
H	2.913789	-4.53447	-1.69241
H	-1.62306	-1.46585	2.52805
H	-1.65294	0.293665	2.786469
H	-1.3769	-0.8186	4.174188
H	0.458066	1.503596	3.640293
H	2.024418	0.642442	3.66175
H	0.763652	0.225735	4.852453
H	2.605054	-2.85137	1.867093
H	1.073844	-2.40105	4.050882
Be	0.028402	1.132345	0.380711
C	-0.82492	0.610923	-1.08026
C	-0.54679	0.973644	-2.5356
C	-1.44306	0.047135	-3.31781
C	-2.23066	-0.59357	-2.45577
N	-1.86871	-0.24133	-1.1237
C	-1.05901	2.411992	-2.81458
C	0.941393	0.889021	-2.89133
C	-2.74939	-0.64532	-0.05153
C	-3.62262	0.318174	0.50898
C	-4.51492	-0.11045	1.493994
C	-4.60005	-1.44636	1.87444
C	-3.7855	-2.38451	1.262696
C	-2.84506	-2.004	0.298109
C	-3.68556	1.751446	0.002187
C	-1.98994	-3.08272	-0.33922
C	-1.22955	-3.90371	0.709028
C	-2.82718	-4.00321	-1.23727
C	-4.29662	2.731219	1.005211
C	-4.47527	1.81263	-1.31528
H	-4.17432	3.760331	0.629616
H	-3.8017	2.668242	1.988971

H	-5.37928	2.562615	1.147061
H	-2.65338	2.088154	-0.18
H	-4.04355	1.165919	-2.09597
H	-4.48365	2.845522	-1.70525
H	-5.52277	1.498484	-1.15472
H	-5.18698	0.61084	1.961409
H	-5.32117	-1.7542	2.636764
H	-3.87427	-3.43802	1.541542
H	-1.24919	-2.57989	-0.97425
H	-1.91758	-4.47129	1.359374
H	-0.60626	-3.26259	1.354388
H	-0.56899	-4.63757	0.216672
H	-2.18212	-4.74584	-1.73917
H	-3.36453	-3.43861	-2.01733
H	-3.58044	-4.55569	-0.64791
H	1.3309	-0.13116	-2.76584
H	1.525171	1.553743	-2.23482
H	1.098113	1.194844	-3.94112
H	-1.02319	2.599065	-3.9023
H	-0.42098	3.143957	-2.30097
H	-2.09601	2.553519	-2.47158
H	-3.06572	-1.27529	-2.61433
H	-1.50771	0.013248	-4.40598
C	0.515851	4.546973	-0.81458
C	-0.75506	4.725044	-0.12759
C	-1.12493	3.863491	0.849856
C	-0.33593	2.694485	1.233488
C	1.057049	2.598495	0.643052
C	1.342877	3.565989	-0.38836
H	0.829435	5.21325	-1.62185
H	-1.38001	5.586624	-0.38227
H	-2.03124	4.076154	1.424774
H	-0.40976	2.487973	2.309296
H	1.89674	2.467005	1.33706
F	2.567933	3.467399	-0.96083

CAAC2Be+ClPhc1

C	0.52812	-0.45979	1.44609
C	0.02681	-0.85509	2.83109
C	0.51325	-2.27146	3.00536
C	1.31194	-2.55876	1.97915
N	1.33497	-1.45339	1.07367
C	0.78580	0.00954	3.88006
C	-1.47777	-0.65667	3.01682
C	2.32410	-1.41529	0.01550

C	3.51549	-0.69230	0.25411
C	4.44916	-0.62746	-0.78009
C	4.25050	-1.30556	-1.97878
C	3.12373	-2.09607	-2.14547
C	2.14018	-2.17010	-1.15274
C	3.85316	-0.11096	1.62007
C	0.97917	-3.13282	-1.32509
C	0.25421	-2.99501	-2.66704
C	1.46735	-4.57625	-1.12904
C	4.84022	1.05767	1.58609
C	4.39488	-1.21233	2.54662
H	4.88458	1.52981	2.58248
H	4.53826	1.82453	0.85691
H	5.86387	0.72179	1.34126
H	2.92121	0.27188	2.05561
H	3.67826	-2.03707	2.68687
H	4.62027	-0.79277	3.54307
H	5.32788	-1.63776	2.13572
H	5.36106	-0.04387	-0.64362
H	4.997138	-1.23797	-2.77475
H	2.999835	-2.66585	-3.07027
H	0.250924	-2.91378	-0.53274
H	0.925321	-3.19848	-3.51939
H	-0.17366	-1.98894	-2.80174
H	-0.57317	-3.72346	-2.72497
H	0.624078	-5.28726	-1.18133
H	1.967182	-4.71113	-0.15511
H	2.193128	-4.85389	-1.91373
H	-2.05848	-1.3213	2.362252
H	-1.7458	0.383552	2.769908
H	-1.76145	-0.86625	4.063019
H	0.534315	1.073653	3.768296
H	1.877486	-0.1074	3.794686
H	0.486182	-0.31805	4.890244
H	1.90838	-3.44199	1.753218
H	0.313975	-2.90199	3.872569
Be	0.146907	1.032798	0.441305
C	-0.79147	0.710519	-1.03722
C	-0.43261	1.108538	-2.46771
C	-1.46647	0.410769	-3.31271
C	-2.3578	-0.15021	-2.49866
N	-1.95711	0.043774	-1.14495
C	-0.67248	2.630989	-2.64684
C	1.016312	0.77366	-2.83803
C	-2.91232	-0.29392	-0.11626
C	-3.62801	0.74961	0.516727

C	-4.60846	0.391831	1.445226
C	-4.92292	-0.93914	1.702133
C	-4.25269	-1.94445	1.024179
C	-3.23416	-1.64397	0.112355
C	-3.42938	2.21213	0.146569
C	-2.53562	-2.79107	-0.59395
C	-1.9557	-3.8017	0.402918
C	-3.46913	-3.49434	-1.58804
C	-3.88553	3.186409	1.233337
C	-4.16258	2.52965	-1.16672
H	-3.58652	4.210171	0.954739
H	-3.42387	2.953468	2.207891
H	-4.98335	3.190407	1.358152
H	-2.35034	2.379124	0.00552
H	-3.82755	1.891844	-2.00066
H	-3.98281	3.579851	-1.4557
H	-5.25215	2.387554	-1.04656
H	-5.16365	1.172412	1.967699
H	-5.70605	-1.18772	2.423839
H	-4.51564	-2.9892	1.211034
H	-1.69893	-2.36647	-1.16359
H	-2.75149	-4.31711	0.968689
H	-1.28508	-3.31411	1.129859
H	-1.37854	-4.57793	-0.12833
H	-2.93019	-4.29391	-2.12653
H	-3.8733	-2.79462	-2.33805
H	-4.3268	-3.95724	-1.06842
H	1.201171	-0.30938	-2.81318
H	1.709487	1.249269	-2.12681
H	1.239419	1.141908	-3.85523
H	-0.61331	2.878656	-3.72127
H	0.093904	3.199371	-2.10352
H	-1.66143	2.938793	-2.27139
H	-3.29542	-0.66583	-2.70291
H	-1.52097	0.46514	-4.40053
C	1.086101	4.457769	-0.52061
C	-0.13242	4.734312	0.224998
C	-0.57129	3.849028	1.151577
C	0.059484	2.558486	1.39708
C	1.401218	2.304928	0.710447
C	1.792378	3.33957	-0.22931
H	1.450886	5.166029	-1.26825
H	-0.64123	5.690992	0.07237
H	-1.41305	4.130724	1.792889
H	0.02161	2.291432	2.461845
H	2.233947	1.994089	1.353845

Cl	3.338178	3.112835	-1.0628
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CAAC2Be+BrPhc1

C	0.11471	-0.77199	1.48125
C	-0.56701	-1.08040	2.81025
C	-0.51236	-2.58395	2.90789
C	0.24351	-3.03148	1.90695
N	0.63416	-1.93144	1.08200
C	0.34214	-0.53518	3.95155
C	-1.95931	-0.46277	2.94448
C	1.65567	-2.11638	0.07227
C	2.97813	-1.73431	0.39548
C	3.95015	-1.87910	-0.59455
C	3.64743	-2.44498	-1.82963
C	2.36611	-2.91142	-2.08040
C	1.34492	-2.75775	-1.13604
C	3.37550	-1.30672	1.80211
C	-0.01776	-3.37016	-1.40697
C	-0.60817	-2.98576	-2.76712
C	0.06117	-4.89887	-1.27579
C	4.65278	-0.46875	1.87527
C	3.51966	-2.54035	2.70887
H	4.76613	-0.06054	2.89414
H	4.62692	0.37742	1.17144
H	5.55319	-1.07356	1.66517
H	2.56298	-0.68346	2.19859
H	2.59244	-3.13214	2.76989
H	3.78451	-2.22989	3.73520
H	4.32128	-3.20241	2.33547
H	4.97312	-1.55560	-0.39550
H	4.427282	-2.54632	-2.58941
H	2.150044	-3.40094	-3.03376
H	-0.70494	-3.00124	-0.63363
H	0.029121	-3.32554	-3.60188
H	-0.74372	-1.89707	-2.86437
H	-1.59595	-3.4609	-2.89819
H	-0.93638	-5.35596	-1.39983
H	0.459236	-5.20726	-0.29445
H	0.726179	-5.32319	-2.04878
H	-2.66752	-0.89836	2.225933
H	-1.89929	0.620294	2.748906
H	-2.35332	-0.62888	3.962246
H	0.410138	0.561033	3.910557
H	1.358102	-0.95724	3.903027
H	-0.10064	-0.82297	4.920276

H	0.586814	-4.03372	1.653057
H	-0.93706	-3.17659	3.718851
Be	0.195495	0.824352	0.561135
C	-0.73179	0.818362	-0.97228
C	-0.1873	1.147051	-2.35987
C	-1.31359	0.787002	-3.29189
C	-2.37407	0.464008	-2.55499
N	-2.02127	0.497019	-1.17336
C	0.001384	2.683763	-2.47235
C	1.138523	0.442626	-2.66476
C	-3.09305	0.384444	-0.21234
C	-3.54195	1.553272	0.445495
C	-4.63758	1.431975	1.303542
C	-5.30714	0.223444	1.468862
C	-4.88638	-0.8954	0.768217
C	-3.77257	-0.8396	-0.07767
C	-2.93465	2.922319	0.176063
C	-3.35993	-2.10045	-0.81499
C	-3.12664	-3.26899	0.149926
C	-4.38508	-2.49035	-1.888
C	-3.18945	3.935734	1.292704
C	-3.46078	3.484462	-1.15438
H	-2.5977	4.845581	1.100785
H	-2.89055	3.53927	2.277705
H	-4.25038	4.239912	1.345892
H	-1.84301	2.796971	0.105356
H	-3.25112	2.817029	-2.00579
H	-2.98458	4.457357	-1.36738
H	-4.55402	3.639922	-1.10514
H	-4.99816	2.309797	1.841796
H	-6.17054	0.163289	2.137489
H	-5.42616	-1.83907	0.88538
H	-2.40822	-1.89084	-1.32077
H	-4.06144	-3.57533	0.650914
H	-2.3936	-3.00797	0.930766
H	-2.74649	-4.14923	-0.39641
H	-4.04688	-3.38625	-2.43784
H	-4.54245	-1.68299	-2.62212
H	-5.36452	-2.72313	-1.43384
H	1.014755	-0.64784	-2.72413
H	1.867152	0.656366	-1.86702
H	1.545674	0.800452	-3.62702
H	0.192217	2.94348	-3.52825
H	0.854886	3.006082	-1.86191
H	-0.89214	3.232022	-2.13351
H	-3.40153	0.230428	-2.83128

H	-1.27949	0.888897	-4.37709
C	1.951185	3.9876	-0.13168
C	0.805394	4.485302	0.61486
C	0.155425	3.663592	1.473109
C	0.457184	2.247291	1.622608
C	1.719507	1.725816	0.91848
C	2.3719	2.717814	0.07941
H	2.492584	4.651992	-0.80937
H	0.538046	5.543131	0.530491
H	-0.60896	4.087397	2.133187
H	0.346442	1.926541	2.667433
H	2.43755	1.182735	1.546025
Br	3.989905	2.180511	-0.80759

CAAC2Be+IPhc1

C	0.31047	0.91962	1.49667
C	1.10996	1.13574	2.77949
C	1.33684	2.62544	2.82158
C	0.62808	3.17586	1.83812
N	0.00037	2.14344	1.07480
C	0.19030	0.79935	3.99001
C	2.37602	0.28173	2.86503
C	-1.01061	2.48738	0.09797
C	-2.36534	2.36433	0.48271
C	-3.33495	2.65795	-0.47612
C	-2.98433	3.12646	-1.73943
C	-1.65082	3.34380	-2.05182
C	-0.63625	3.02866	-1.14095
C	-2.76980	2.05785	1.91866
C	0.80542	3.36458	-1.48055
C	1.25851	2.84597	-2.84891
C	1.02592	4.88246	-1.39196
C	-4.17774	1.48318	2.07702
C	-2.63928	3.32289	2.78394
H	-4.31920	1.13941	3.11581
H	-4.34889	0.62446	1.41028
H	-4.95528	2.24189	1.87599
H	-2.07142	1.30279	2.30420
H	-1.61984	3.74007	2.77758
H	-2.89961	3.09567	3.83295
H	-3.32925	4.10683	2.42388
H	-4.39054	2.52964	-0.23056
H	-3.76294	3.349057	-2.47411
H	-1.38917	3.75996	-3.02844
H	1.442326	2.887604	-0.72317

H	0.67309	3.291459	-3.67189
H	1.172151	1.750546	-2.92364
H	2.315894	3.111867	-3.02091
H	2.087565	5.133763	-1.56254
H	0.733539	5.285256	-0.40774
H	0.426498	5.409715	-2.15508
H	3.111599	0.570302	2.101759
H	2.116764	-0.77754	2.705325
H	2.845449	0.397511	3.857547
H	-0.03437	-0.27573	4.024011
H	-0.75727	1.35979	3.957119
H	0.717493	1.075168	4.919162
H	0.463129	4.216205	1.560891
H	1.904567	3.152283	3.5893
Be	-0.10297	-0.67231	0.651737
C	0.751081	-0.8813	-0.92198
C	0.088148	-1.12068	-2.27522
C	1.215162	-1.00141	-3.26561
C	2.351643	-0.87227	-2.5852
N	2.064477	-0.81357	-1.18844
C	-0.39801	-2.59385	-2.33584
C	-1.08922	-0.17835	-2.54216
C	3.185891	-0.88326	-0.28104
C	3.440708	-2.0999	0.39295
C	4.583618	-2.16683	1.193531
C	5.47537	-1.10281	1.287337
C	5.23481	0.059071	0.571554
C	4.087893	0.193774	-0.21924
C	2.572719	-3.33485	0.199099
C	3.881579	1.491981	-0.97906
C	3.904587	2.706922	-0.04417
C	4.917102	1.660232	-2.09898
C	2.706825	-4.35954	1.326519
C	2.895244	-4.01051	-1.14334
H	1.93489	-5.13694	1.204983
H	2.564521	-3.89645	2.317404
H	3.689433	-4.86488	1.314913
H	1.520846	-3.00886	0.190588
H	2.764592	-3.33048	-2.0004
H	2.228112	-4.87606	-1.29901
H	3.938995	-4.37418	-1.15483
H	4.800485	-3.08487	1.741892
H	6.369826	-1.19114	1.910381
H	5.94926	0.884774	0.62957
H	2.888215	1.449545	-1.44534
H	4.896287	2.842852	0.421454

H	3.161721	2.609705	0.764405
H	3.678978	3.629374	-0.60649
H	4.717211	2.581266	-2.67443
H	4.905401	0.811855	-2.80308
H	5.938421	1.737061	-1.68575
H	-0.75825	0.863098	-2.65657
H	-1.7948	-0.21714	-1.69727
H	-1.61638	-0.47956	-3.46439
H	-0.69053	-2.83042	-3.37362
H	-1.26273	-2.7342	-1.6753
H	0.389526	-3.29867	-2.02527
H	3.390221	-0.84117	-2.9123
H	1.108959	-1.11257	-4.34513
C	-2.3329	-3.56399	0.181893
C	-1.24706	-4.18143	0.929698
C	-0.46991	-3.4163	1.732702
C	-0.556	-1.96638	1.799112
C	-1.74537	-1.2962	1.07834
C	-2.56411	-2.23656	0.324479
H	-2.98035	-4.19017	-0.437
H	-1.13623	-5.26993	0.901597
H	0.239937	-3.9086	2.406531
H	-0.38569	-1.60581	2.822464
H	-2.35462	-0.61789	1.690227
I	-4.31026	-1.47416	-0.64548

CAAC2Be+FPhc3

C	1.35192	-0.18662	1.40999
C	1.07945	-0.63509	2.82837
C	2.26648	-1.50979	3.14400
C	3.13302	-1.41909	2.13471
N	2.56234	-0.60520	1.10522
C	1.18335	0.62965	3.73025
C	-0.30410	-1.27145	3.00638
C	3.29258	-0.23290	-0.08279
C	3.67231	1.11899	-0.24005
C	4.33611	1.45895	-1.42084
C	4.64733	0.49977	-2.37941
C	4.29721	-0.82660	-2.17660
C	3.59803	-1.22168	-1.03165
C	3.45646	2.15989	0.85473
C	3.20324	-2.68124	-0.86812
C	2.52438	-3.23109	-2.12774
C	4.41922	-3.54143	-0.49454
C	3.53701	3.60479	0.35941

C	4.45840	1.93435	1.99836
H	3.27655	4.28999	1.18311
H	2.82746	3.79240	-0.46362
H	4.55455	3.87397	0.02548
H	2.43811	2.03377	1.25499
H	4.37724	0.92448	2.43539
H	4.28676	2.66495	2.80810
H	5.49401	2.06275	1.63625
H	4.62636	2.49512	-1.59864
H	5.171211	0.793578	-3.29299
H	4.552737	-1.5699	-2.93541
H	2.46964	-2.75096	-0.04876
H	3.222986	-3.28054	-2.98033
H	1.668179	-2.60403	-2.42172
H	2.158956	-4.25661	-1.94987
H	4.114083	-4.5881	-0.32212
H	4.92192	-3.17822	0.417487
H	5.166668	-3.53463	-1.30741
H	-0.4034	-2.19996	2.42954
H	-1.09473	-0.58294	2.662067
H	-0.47779	-1.5012	4.071308
H	0.355517	1.322006	3.520619
H	2.13714	1.160969	3.578571
H	1.121143	0.319515	4.786608
H	4.13194	-1.82937	1.995816
H	2.416384	-2.04382	4.082672
Be	0.242096	0.78842	0.462277
C	-1.08605	0.731276	-0.69779
C	-0.52758	1.078447	-2.13082
C	-1.77156	0.887649	-2.98986
C	-2.60258	0.066004	-2.33083
N	-2.16262	-0.22037	-1.04504
C	0.17664	2.425786	-2.31251
C	0.485009	-0.00665	-2.55719
C	-2.84889	-1.09983	-0.16639
C	-4.16428	-0.81722	0.272074
C	-4.77956	-1.69162	1.17386
C	-4.12925	-2.82394	1.644017
C	-2.86316	-3.13428	1.158038
C	-2.22211	-2.30782	0.231414
C	-4.96182	0.373782	-0.23623
C	-0.94696	-2.77644	-0.45917
C	-0.22099	-3.92848	0.242013
C	-1.29501	-3.21546	-1.89248
C	-5.53008	1.24925	0.885887
C	-6.08143	-0.09412	-1.17806

H	-6.01664	2.142798	0.455396
H	-4.72738	1.586223	1.557947
H	-6.29224	0.714128	1.480676
H	-4.28073	1.003539	-0.8216
H	-5.68902	-0.7127	-2.00359
H	-6.60621	0.772393	-1.61864
H	-6.82813	-0.70254	-0.6363
H	-5.79259	-1.47267	1.524786
H	-4.61929	-3.48356	2.366374
H	-2.38308	-4.05667	1.49277
H	-0.25425	-1.91885	-0.51386
H	-0.82507	-4.85262	0.243783
H	0.045725	-3.69929	1.28723
H	0.712589	-4.16194	-0.2937
H	-0.39366	-3.54843	-2.43552
H	-1.75658	-2.39972	-2.46896
H	-2.00697	-4.05993	-1.86344
H	0.062718	-1.01248	-2.41758
H	1.421218	0.068925	-1.97304
H	0.746859	0.106139	-3.62501
H	0.558347	2.493696	-3.3474
H	1.043628	2.522856	-1.63402
H	-0.48663	3.281235	-2.14129
H	-3.51721	-0.40559	-2.69837
H	-1.88006	1.22411	-4.02185
C	-2.39992	3.069713	-0.48068
C	-1.95846	4.341476	-0.45973
C	-0.69798	4.725458	0.168773
C	0.032256	3.806603	0.835677
C	-0.35864	2.392967	0.918606
C	-1.61902	1.955816	0.146039
H	-3.35326	2.819072	-0.95377
H	-2.55942	5.125389	-0.93364
H	-0.38383	5.772736	0.129028
H	0.92100	4.125266	1.393724
H	-0.5524	2.166094	1.98811
F	-2.47483	1.358658	1.118823

CAAC2Be+ClPhc3

C	1.42728	-0.21308	1.37137
C	1.12164	-0.62837	2.79633
C	2.34074	-1.42132	3.19053
C	3.21927	-1.37292	2.19032
N	2.64783	-0.62943	1.10932
C	1.04476	0.65351	3.66773

C	-0.19818	-1.40405	2.91713
C	3.40744	-0.32400	-0.07989
C	3.90335	0.98782	-0.23979
C	4.63989	1.25036	-1.39742
C	4.89360	0.25450	-2.33512
C	4.40430	-1.02924	-2.14127
C	3.63871	-1.34653	-1.01503
C	3.69850	2.06963	0.81635
C	3.08979	-2.75551	-0.84735
C	2.48148	-3.29419	-2.14741
C	4.17014	-3.71794	-0.33204
C	3.89753	3.48885	0.28078
C	4.61591	1.83353	2.02630
H	3.61676	4.21870	1.05833
H	3.26889	3.68336	-0.60402
H	4.95202	3.68728	0.01962
H	2.65121	2.01025	1.15522
H	4.44817	0.85213	2.49950
H	4.44096	2.60691	2.79453
H	5.67715	1.88734	1.72445
H	5.03195	2.25268	-1.57460
H	5.476105	0.487308	-3.23075
H	4.607288	-1.79728	-2.89095
H	2.281157	-2.71808	-0.09885
H	3.251241	-3.46605	-2.9191
H	1.732031	-2.59889	-2.55639
H	1.989718	-4.26434	-1.96527
H	3.741326	-4.72133	-0.16524
H	4.615692	-3.37823	0.617019
H	4.987689	-3.81418	-1.06847
H	-0.15604	-2.35314	2.367304
H	-1.03527	-0.81167	2.512865
H	-0.40091	-1.62523	3.978913
H	0.119107	1.206458	3.445967
H	1.911081	1.315546	3.501266
H	1.025828	0.363317	4.731496
H	4.229551	-1.76561	2.087563
H	2.481963	-1.90397	4.157979
Be	0.375282	0.761876	0.352156
C	-1.02746	0.725263	-0.70643
C	-0.468	1.015575	-2.1723
C	-1.71129	0.824415	-3.02245
C	-2.57996	0.078399	-2.3296
N	-2.16862	-0.16653	-1.02543
C	0.256089	2.333551	-2.45977
C	0.524926	-0.10676	-2.54393

C	-2.87731	-1.06771	-0.18199
C	-4.21512	-0.79532	0.201061
C	-4.86196	-1.67427	1.074509
C	-4.22542	-2.80291	1.571153
C	-2.94624	-3.11378	1.123748
C	-2.27514	-2.28905	0.216068
C	-5.0071	0.38555	-0.3452
C	-1.00545	-2.7878	-0.46468
C	-0.35566	-4.00842	0.195621
C	-1.342	-3.16062	-1.9204
C	-5.74886	1.190952	0.728718
C	-6.00653	-0.09255	-1.41136
H	-6.20565	2.087492	0.272963
H	-5.06198	1.523735	1.520838
H	-6.56599	0.608932	1.190821
H	-4.29411	1.068422	-0.82717
H	-5.52055	-0.68201	-2.20682
H	-6.51281	0.768024	-1.88397
H	-6.78248	-0.73514	-0.95738
H	-5.88912	-1.46173	1.384387
H	-4.73874	-3.46228	2.27726
H	-2.48128	-4.04016	1.46777
H	-0.26938	-1.96467	-0.47116
H	-1.00304	-4.89971	0.123751
H	-0.11849	-3.8551	1.260395
H	0.585258	-4.256	-0.32114
H	-0.44396	-3.51638	-2.45436
H	-1.75509	-2.30952	-2.48155
H	-2.09014	-3.97349	-1.93191
H	0.092964	-1.09655	-2.34589
H	1.467379	-0.0106	-1.9704
H	0.784488	-0.05784	-3.61728
H	0.570324	2.328138	-3.51953
H	1.165003	2.449029	-1.84534
H	-0.37919	3.21247	-2.30618
H	-3.51017	-0.36829	-2.68428
H	-1.80917	1.131517	-4.06442
C	-2.23561	3.105039	-0.52113
C	-1.77697	4.366059	-0.63917
C	-0.45305	4.764274	-0.17662
C	0.349047	3.867432	0.435695
C	-0.04173	2.471378	0.676736
C	-1.40987	2.030233	0.103783
H	-3.22936	2.835933	-0.88906
H	-2.41015	5.120741	-1.11805
H	-0.1345	5.802048	-0.31012

H	1.303838	4.202888	0.855748
H	-0.04054	2.361888	1.776644
Cl	-2.39156	1.448183	1.622333

CAAC2Be+BrPhc3

C	-1.60560	0.15042	1.36766
C	-1.32957	0.47330	2.82271
C	-2.61412	1.11241	3.28244
C	-3.48566	1.08514	2.27569
N	-2.85475	0.49265	1.13648
C	-1.09670	-0.84446	3.60345
C	-0.10511	1.38998	2.97434
C	-3.57745	0.26834	-0.09185
C	-3.97566	-1.04781	-0.40824
C	-4.65421	-1.22862	-1.61565
C	-4.95229	-0.15316	-2.44684
C	-4.56908	1.13267	-2.09292
C	-3.85960	1.37245	-0.91226
C	-3.73026	-2.21976	0.53716
C	-3.42146	2.78878	-0.56841
C	-2.77095	3.49291	-1.76428
C	-4.59946	3.61641	-0.03417
C	-3.82953	-3.58556	-0.14475
C	-4.68980	-2.16344	1.73658
H	-3.54749	-4.37554	0.57079
H	-3.14933	-3.66031	-1.00940
H	-4.85869	-3.80674	-0.47846
H	-2.69786	-2.13445	0.91397
H	-4.59760	-1.22494	2.30724
H	-4.48113	-2.99548	2.43135
H	-5.73764	-2.25446	1.39929
H	-4.96364	-2.22992	-1.91794
H	-5.48714	-0.32411	-3.385
H	-4.80934	1.964932	-2.75862
H	-2.65839	2.729974	0.225818
H	-3.49772	3.681433	-2.57295
H	-1.94444	2.893382	-2.17626
H	-2.36853	4.472833	-1.45728
H	-4.26107	4.626537	0.254875
H	-5.06907	3.150726	0.848023
H	-5.38057	3.727175	-0.80717
H	-0.28081	2.359819	2.489643
H	0.787917	0.928039	2.519808
H	0.095037	1.566396	4.044847
H	-0.11574	-1.27302	3.345628

H	-1.88433	-1.58796	3.393632
H	-1.10155	-0.62685	4.684545
H	-4.52332	1.406164	2.198179
H	-2.79183	1.494617	4.288005
Be	-0.48414	-0.66993	0.279501
C	0.899676	-0.54362	-0.80238
C	0.263002	-0.78087	-2.25422
C	1.454327	-0.54156	-3.16075
C	2.348195	0.19142	-2.48747
N	2.012464	0.375121	-1.15197
C	-0.46955	-2.09073	-2.55881
C	-0.75266	0.350085	-2.5245
C	2.775594	1.236474	-0.31442
C	4.146352	0.974195	-0.06215
C	4.844495	1.809957	0.814454
C	4.227051	2.883254	1.440277
C	2.909155	3.190719	1.120052
C	2.183957	2.412797	0.21337
C	4.91825	-0.14649	-0.74797
C	0.860743	2.928735	-0.33916
C	0.243662	4.091924	0.445036
C	1.087256	3.405063	-1.78609
C	5.778058	-0.9923	0.200073
C	5.808373	0.426444	-1.86383
H	6.205828	-1.84922	-0.35013
H	5.182602	-1.38674	1.037089
H	6.625224	-0.41632	0.612958
H	4.185162	-0.82375	-1.20805
H	5.242906	1.05328	-2.57326
H	6.291774	-0.38753	-2.43318
H	6.6057	1.060117	-1.43519
H	5.897751	1.604247	1.025197
H	4.783349	3.506187	2.146885
H	2.457379	4.082437	1.55989
H	0.13735	2.094585	-0.34832
H	0.834251	5.017176	0.325541
H	0.158632	3.894672	1.524634
H	-0.7683	4.303791	0.062068
H	0.151737	3.79169	-2.22662
H	1.462144	2.600921	-2.43628
H	1.829589	4.223203	-1.79408
H	-0.31593	1.333296	-2.30424
H	-1.66459	0.222529	-1.91109
H	-1.06619	0.346551	-3.58435
H	-0.82872	-2.04701	-3.60322
H	-1.35111	-2.2301	-1.91053

H	0.172048	-2.97367	-2.46335
H	3.246237	0.671359	-2.87793
H	1.495258	-0.7994	-4.21969
C	2.15093	-2.89436	-0.80957
C	1.73307	-4.16903	-0.95343
C	0.460647	-4.63797	-0.42561
C	-0.34067	-3.79045	0.257599
C	0.001743	-2.38697	0.502642
C	1.328293	-1.88621	-0.09337
H	3.104618	-2.56975	-1.23356
H	2.360486	-4.87506	-1.50794
H	0.179979	-5.6855	-0.56633
H	-1.25289	-4.17672	0.726019
H	-0.00112	-2.28059	1.600864
Br	2.45243	-1.35116	1.600616

CAAC2Be

C	-0.77636	-0.00012	1.45163
C	-0.30183	0.00007	2.90716
C	-1.61179	0.00008	3.67900
C	-2.63660	-0.00006	2.81082
N	-2.16003	-0.00015	1.50362
C	0.53502	-1.25470	3.22548
C	0.53494	1.25494	3.22522
C	-2.95178	-0.00030	0.32420
C	-3.30248	-1.23226	-0.26070
C	-4.02441	-1.20735	-1.45779
C	-4.37975	-0.00059	-2.05338
C	-4.02524	1.20632	-1.45758
C	-3.30333	1.23152	-0.26049
C	-2.92201	-2.55344	0.38921
C	-2.92368	2.55286	0.38961
C	-1.97606	3.37231	-0.49363
C	-4.17092	3.35662	0.77882
C	-1.97438	-3.37254	-0.49432
C	-4.16884	-3.35766	0.77882
H	-1.05720	-2.80274	-0.71915
H	-2.44763	-3.65026	-1.45357
H	-1.68011	-4.30433	0.02021
H	-2.37763	-2.32088	1.31693
H	-4.83254	-2.76752	1.43402
H	-3.88169	-4.27646	1.31976
H	-4.75206	-3.65994	-0.10954
H	-4.30957	-2.14859	-1.93752
H	-4.93861	-0.0007	-2.99365

H	-4.31108	2.147435	-1.93716
H	-2.37953	2.32053	1.317515
H	-2.44907	3.649696	-1.45308
H	-1.05853	2.802926	-0.71802
H	-1.68241	4.304291	0.020925
H	-3.88426	4.275492	1.319899
H	-4.83464	2.766233	1.433769
H	-4.75396	3.658781	-0.1097
H	-0.02853	2.173311	2.987891
H	1.467915	1.256159	2.633702
H	0.806975	1.281934	4.296838
H	1.467967	-1.256	2.633909
H	-0.02842	-2.17315	2.988352
H	0.807093	-1.28147	4.297083
H	-3.71359	-0.00011	2.98809
H	-1.68719	0.00015	4.767246
Be	-1.4E-05	-0.00028	-7.6E-05
C	0.776421	-4.4E-05	-1.45173
C	0.301966	0.000228	-2.90729
C	1.611982	0.00085	-3.67905
C	2.636739	0.000525	-2.81082
N	2.160091	-7.8E-05	-1.50364
C	-0.53441	-1.25478	-3.22587
C	-0.53521	1.254873	-3.22515
C	2.951732	0.000151	-0.32416
C	3.30295	-1.23166	0.260744
C	4.024705	-1.20645	1.457934
C	4.379435	0.000461	2.053582
C	4.024449	1.207216	1.457762
C	3.302637	1.232122	0.260603
C	2.923142	-2.55298	-0.38928
C	2.922577	2.553315	-0.38954
C	1.97491	3.372657	0.493748
C	4.169611	3.357301	-0.77897
C	1.975358	-3.37228	0.49391
C	4.17032	-3.3569	-0.77837
H	1.057901	-2.80274	0.71826
H	2.448252	-3.64977	1.453388
H	1.681586	-4.30421	-0.02066
H	2.37907	-2.32061	-1.31722
H	4.834129	-2.76664	-1.43334
H	3.883605	-4.2758	-1.31937
H	4.753283	-3.65901	0.11022
H	4.310265	-2.14757	1.937681
H	4.938195	0.000586	2.993916
H	4.309814	2.148458	1.937376

H	2.378363	2.320791	-1.31736
H	2.447957	3.650178	1.453141
H	1.05749	2.80313	0.718267
H	1.681056	4.304554	-0.02084
H	3.882705	4.276072	-1.32008
H	4.833353	2.766979	-1.43396
H	4.752704	3.659624	0.109453
H	0.027899	2.173394	-2.9875
H	-1.46826	1.255609	-2.63375
H	-0.80712	1.282066	-4.29679
H	-0.80659	-1.28135	-4.29746
H	-1.4673	-1.25662	-2.6342
H	0.029418	-2.17306	-2.98905
H	3.713741	0.000678	-2.98802
H	1.687445	0.001291	-4.7673

NtBuNtBuBe

C	0.68018	-1.28098	-0.00015
C	-0.68018	-1.28098	-0.00011
H	1.28520	-2.19096	-0.00002
H	-1.28519	-2.19096	0.00004
Be	0.00001	0.83961	-0.00050
N	1.28192	-0.00765	-0.00041
N	-1.28192	-0.00764	-0.00031
C	-2.72399	0.17164	0.00001
C	-3.35030	-0.45146	-1.25914
C	-3.34949	-0.45032	1.26013
C	-2.98972	1.68160	-0.00060
H	-2.90225	-0.00980	-2.16588
H	-3.17546	-1.54033	-1.29353
H	-4.44149	-0.28281	-1.28594
H	-2.90099	-0.00770	2.16617
H	-4.44069	-0.28185	1.28742
H	-3.17440	-1.53912	1.29547
H	-4.07092	1.90206	-0.00027
H	-2.54820	2.15139	0.89831
H	-2.54889	2.15057	-0.90028
C	2.72400	0.17164	0.00001
C	3.35039	-0.45162	-1.25901
C	2.98971	1.68160	-0.00076
C	3.34938	-0.45017	1.26025
H	3.17563	-1.54050	-1.29324
H	2.90235	-0.01013	-2.16584
H	4.44157	-0.28290	-1.28580
H	2.548048	2.151509	0.89802

H	4.070914	1.902064	-0.00026
H	2.549039	2.150457	-0.90057
H	4.440601	-0.28177	1.287562
H	2.900881	-0.00739	2.166212
H	3.174213	-1.53895	1.295753

NNBe

C	-0.68010	0.98667	-0.00001
C	0.68009	0.98669	-0.00001
H	-1.30050	1.88743	0.00015
H	1.30041	1.88751	0.00009
Be	0.00002	-1.12403	0.00012
C	2.71868	-0.38386	-0.00002
H	3.16854	0.09256	-0.89389
H	3.16857	0.09241	0.89391
H	3.02692	-1.44256	-0.00012
C	-2.71868	-0.38384	-0.00002
H	-3.16851	0.09250	-0.89395
H	-3.02699	-1.44252	0.00001
H	-3.16854	0.09255	0.89387
N	-1.28544	-0.28560	-0.00002
N	1.28545	-0.28551	-0.00001

NPBe

C	0.99583	0.96702	0.19630
C	-0.32133	1.23240	0.02247
H	1.70122	1.74361	0.52565
H	-0.69247	2.24522	0.21269
Be	0.29914	-1.09667	-0.46024
C	-2.46991	-0.53422	0.83699
H	-1.86700	-0.67625	1.74844
H	-3.21563	0.25559	1.03196
H	-3.02038	-1.46606	0.62057
C	2.95607	-0.49837	0.17177
H	3.56156	0.14091	-0.49982
H	3.25619	-0.27297	1.21377
H	3.22884	-1.54659	-0.03212
N	1.54192	-0.30942	-0.03276
P	-1.46042	-0.05812	-0.67440

NOBe

	-		
C	1.39725	0.65952	0.00008
C	-	0.91440	-

	0.06699		0.00015
	-		
H	2.20638	1.39243	0.00018
			-
H	0.38411	1.91071	0.00015
	-	-	-
Be	0.38521	1.25674	0.00016
			-
C	2.18354	0.09039	0.00029
			-
H	2.54299	0.45618	0.89386
H	2.54274	0.45619	0.89453
			-
H	2.66832	1.08015	0.00036
			-
N	0.75469	0.24040	0.00006
	-	-	-
O	1.74870	0.66585	0.00027

NSBe

C	-0.85915	1.07335	-0.00007
C	0.49255	0.99098	0.00005
H	-1.39759	2.02269	-0.00011
H	1.12369	1.88820	0.00012
Be	-0.07860	-1.20827	-0.00002
C	2.56431	-0.30745	0.00024
H	2.99335	0.18300	-0.89451
H	2.99318	0.18296	0.89509
H	2.90573	-1.35525	0.00025
N	1.12300	-0.25738	0.00010
S	-1.83445	-0.42676	-0.00017

FPh

C	0.93748	-0.00001	0.00054
C	0.26172	1.21510	-0.00016
C	0.26171	-1.21503	-0.00013
H	0.83252	2.14683	0.00006
H	0.83250	-2.14676	-0.00048
C	-1.13297	1.20710	-0.00022
C	-1.13292	-1.20709	-0.00006
H	-1.67572	2.15665	0.00040
H	-1.67557	-2.15668	0.00028
C	-1.83350	-0.00005	0.00006
H	-2.92675	-0.00005	0.00029
F	2.27155	-0.00001	-0.00007

CIPh

C	-0.51070	-0.00004	-0.00005
C	0.17518	1.21388	0.00017
C	0.17525	-1.21392	0.00011
H	-0.38163	2.15356	0.00043
H	-0.38183	-2.15346	0.00042
C	1.56972	1.20644	0.00006
C	1.56974	-1.20642	0.00014
H	2.11112	2.15673	0.00024
H	2.11148	-2.15653	0.00020
C	2.27003	0.00002	-0.00027
H	3.36340	0.00001	-0.00076
Cl	-2.25399	0.00000	-0.00009

BrPh

C	0.09190	0.00021	0.00021
C	0.77824	1.21387	0.00010
C	0.77826	-1.21389	0.00017
H	0.22786	2.15771	0.00055
H	0.22708	-2.15728	0.00041
C	2.17334	1.20629	-0.00015
C	2.17303	-1.20648	-0.00003
H	2.71430	2.15685	0.00033
H	2.71460	-2.15670	-0.00016
C	2.87312	0.00000	-0.00008
H	3.96653	-0.00034	-0.00047
	-		
Br	1.80165	-0.00001	-0.00006

IPh

C	0.55583	-0.00017	-0.00055
C	1.24602	-1.21305	-0.00065
C	1.24585	1.21298	-0.00062
H	0.70397	-2.16201	-0.00023
H	0.70314	2.16157	-0.00134
C	2.64143	-1.20595	-0.00013
C	2.64096	1.20613	0.00019
H	3.18208	-2.15686	0.00042
H	3.18202	2.15681	0.00037
C	3.34117	0.00013	0.00055
H	4.43472	0.00047	0.00178
I	-1.55158	-0.00001	0.00012

1.1Fa

C	2.49273	0.56901	-0.75572
C	1.82030	1.74770	-0.76541
H	3.44917	0.41125	-1.26079
H	2.17336	2.64349	-1.28305
Be	0.62118	0.29629	0.55042
C	-0.21574	2.93166	0.02280
C	2.50211	-1.75641	0.11886
N	1.87679	-0.44903	-0.00879
N	0.62787	1.74775	-0.02549
C	-1.78164	-0.97570	0.53183
C	-1.54824	-1.27468	-0.79665
C	-2.99606	-1.11848	1.17262
H	-0.55348	-1.13043	-1.23046
H	-3.10166	-0.85487	2.22664
C	-2.63123	-1.75489	-1.53459
C	-4.06220	-1.60206	0.41296
H	-2.48944	-2.00009	-2.59011
H	-5.04144	-1.72863	0.88184
C	-3.88085	-1.91746	-0.93465
H	-4.72230	-2.29208	-1.52293
F	-0.72403	-0.48022	1.29199
C	-1.45945	2.59730	0.85539
H	-2.04593	1.79273	0.37569
H	-1.17202	2.26973	1.87116
H	-2.11741	3.47786	0.95526
C	-0.66940	3.33901	-1.39110
H	0.19117	3.61395	-2.02424
H	-1.18969	2.495697	-1.87831
H	-1.35535	4.204544	-1.35733
C	0.526508	4.103887	0.689802
H	0.833401	3.824554	1.712641
H	1.438063	4.368693	0.127289
H	-0.11136	5.004617	0.74505
C	1.603142	-2.63511	0.997408
H	0.610265	-2.77477	0.53287
H	2.048497	-3.63438	1.143315
H	1.462713	-2.17509	1.992103
C	2.654885	-2.42819	-1.25847
H	3.288351	-1.82314	-1.92895
H	3.115265	-3.42837	-1.16719
H	1.668117	-2.54259	-1.7414
C	3.88237	-1.63752	0.791265
H	3.779513	-1.15537	1.778739
H	4.349649	-2.62948	0.928017
H	4.568175	-1.02049	0.186419

1.2aF

C	1.46813	0.81927	-1.32054
C	0.19368	1.34006	-1.37221
H	2.11454	0.74788	-2.20101
H	-0.26494	1.71714	-2.28957
Be	0.54458	0.52605	0.79649
C	-1.71560	2.08604	-0.00789
C	3.18092	-0.21847	0.12909
N	1.87237	0.39354	-0.08280
N	-0.46203	1.34635	-0.16376
C	-1.01692	-1.16989	0.47104
C	-0.52291	-1.68020	-0.70339
C	-2.16811	-1.57264	1.11564
H	0.36549	-1.28225	-1.20717
H	-2.46294	-1.16291	2.08254
C	-1.31630	-2.65556	-1.32445
C	-2.94230	-2.53111	0.45943
H	-0.98186	-3.07168	-2.27988
H	-3.87929	-2.86201	0.91660
C	-2.51592	-3.07676	-0.75500
H	-3.12046	-3.83849	-1.25394
F	0.00517	-0.52430	1.81906
C	-2.11136	2.04492	1.47176
H	-2.29537	1.01437	1.80974
H	-1.30650	2.47261	2.09601
H	-3.03036	2.62982	1.64704
C	-2.83517	1.47817	-0.86983
H	-2.57301	1.50947	-1.94138
H	-3.01672	0.425753	-0.5972
H	-3.77678	2.039935	-0.73849
C	-1.49975	3.557842	-0.40659
H	-0.67152	3.994546	0.177434
H	-1.2493	3.657115	-1.476
H	-2.41413	4.147585	-0.21789
C	3.343672	-0.44623	1.636161
H	2.556086	-1.11907	2.017018
H	4.323975	-0.89925	1.863582
H	3.272826	0.513551	2.178785
C	3.268838	-1.57191	-0.59845
H	3.117011	-1.44779	-1.68546
H	4.256123	-2.04362	-0.44736
H	2.494074	-2.26117	-0.22012
C	4.302229	0.712851	-0.3603
H	4.22634	1.694257	0.138536
H	5.294231	0.280648	-0.14057
H	4.246534	0.880448	-1.44968

1.3aF

C	-0.73964	-1.61272	-1.29835
C	0.73968	-1.61272	-1.29834
H	-1.28582	-2.02671	-2.15634
H	1.28588	-2.02671	-2.15633
Be	0.00004	-0.28290	0.78482
C	2.73772	-1.08719	-0.01446
C	-2.73769	-1.08725	-0.01446
N	-1.29037	-1.11802	-0.26416
N	1.29040	-1.11800	-0.26416
C	0.00001	1.41157	0.23597
C	-0.00001	1.83040	-1.10301
C	-0.00001	2.43271	1.20286
H	0.00001	1.08072	-1.91030
H	-0.00001	2.15988	2.26570
C	-0.00004	3.17808	-1.47254
C	-0.00005	3.78703	0.85711
H	-0.00006	3.46137	-2.53097
H	-0.00007	4.55365	1.63941
C	-0.00007	4.16534	-0.48607
H	-0.00010	5.22451	-0.76317
F	0.00003	-0.69882	2.21087
C	3.11201	0.35226	0.36560
H	2.88190	1.05249	-0.45386
H	2.55095	0.68321	1.25341
H	4.19162	0.40204	0.58777
C	3.56685	-1.54614	-1.21589
H	3.36605	-2.59878	-1.48269
H	3.385708	-0.91071	-2.10084
H	4.638048	-1.47148	-0.96708
C	2.959056	-2.02097	1.187219
H	2.313464	-1.71771	2.027516
H	2.716236	-3.06458	0.921002
H	4.015263	-1.97703	1.503536
C	-3.11201	0.352157	0.365736
H	-2.88154	1.052521	-0.45351
H	-4.1917	0.401982	0.587519
H	-2.55125	0.682888	1.253813
C	-3.56684	-1.54608	-1.21592
H	-3.36609	-2.59872	-1.48277
H	-4.63804	-1.47138	-0.96711
H	-3.38567	-0.91062	-2.10083
C	-2.95904	-2.02113	1.187137
H	-2.31352	-1.71789	2.027494
H	-4.01527	-1.97729	1.503396
H	-2.71613	-3.0647	0.920848

1.4aF

C	-0.29322	-1.31586	-1.44548
C	1.09222	-1.09688	-1.41318
H	-0.84797	-1.49531	-2.36830
H	1.70572	-1.18214	-2.31652
Be	0.31453	-0.61855	0.83549
C	2.97378	-0.32717	-0.00017
C	-2.29399	-1.48072	-0.03474
N	-0.88937	-1.05699	-0.26136
N	1.57644	-0.69498	-0.25598
C	-0.72430	0.99183	0.03376
C	-0.65199	1.58386	-1.21028
C	-0.99133	1.74842	1.17352
H	-0.45787	0.95768	-2.09459
H	-1.03438	1.28400	2.16249
C	-0.81330	2.96343	-1.34181
C	-1.15387	3.13230	1.04393
H	-0.75093	3.43376	-2.32810
H	-1.34403	3.73724	1.93599
C	-1.06691	3.73953	-0.20850
H	-1.20339	4.82055	-0.30476
F	0.34015	-0.70318	2.29266
C	2.95382	1.08276	0.61164
H	2.51051	1.80435	-0.09610
H	2.34931	1.09526	1.53466
H	3.97713	1.41314	0.86171
C	3.83339	-0.32599	-1.26692
H	3.89279	-1.32824	-1.72633
H	3.449245	0.386108	-2.01853
H	4.861877	-0.02	-1.01223
C	3.535341	-1.33559	1.013611
H	2.914142	-1.35	1.924693
H	3.538692	-2.35154	0.581593
H	4.570361	-1.07221	1.294024
C	-2.80278	-0.95193	1.309823
H	-3.02194	0.125498	1.262691
H	-3.73785	-1.4742	1.572924
H	-2.06445	-1.12888	2.109179
C	-3.22642	-1.00892	-1.15618
H	-2.99505	-1.48071	-2.1259
H	-4.26794	-1.27226	-0.90518
H	-3.1667	0.086462	-1.2736
C	-2.25069	-3.01785	0.028826
H	-1.57189	-3.34568	0.834364
H	-3.25913	-3.41532	0.235351
H	-1.8937	-3.44839	-0.92124

1.5aF

C	-0.09016	0.50921	-1.55042
C	-1.36868	0.08020	-1.46375
H	0.42002	0.75363	-2.48000
H	-1.97052	-0.03740	-2.37334
Be	-0.77694	0.14693	0.83796
C	-3.27467	-0.67746	-0.10623
C	1.11137	1.98758	0.07835
N	0.61286	0.57812	-0.26931
N	-1.89862	-0.19471	-0.23777
C	1.64595	-0.45808	-0.16994
C	2.47520	-0.76505	-1.25434
C	1.80150	-1.16614	1.02546
H	2.35709	-0.24270	-2.20452
H	1.15843	-0.93745	1.87886
C	3.45037	-1.75296	-1.13821
C	2.77600	-2.15800	1.13563
H	4.08953	-1.98047	-1.99612
H	2.87970	-2.70248	2.07822
C	3.60634	-2.45369	0.05757
H	4.36932	-3.23224	0.14410
F	-0.65361	0.21129	2.28256
C	1.89536	1.95975	1.39437
H	2.13311	2.99743	1.68345
H	1.30381	1.50377	2.20362
H	2.84681	1.41274	1.29412
C	-0.12831	2.87471	0.24452
H	-0.71595	2.57801	1.13170
H	0.181494	3.922253	0.394449
H	-0.77489	2.829488	-0.64737
C	2.009948	2.54576	-1.03009
H	2.38415	3.537639	-0.72571
H	2.887766	1.900676	-1.20111
H	1.466596	2.672715	-1.98049
C	-3.54751	-0.90254	1.384637
H	-2.84222	-1.64085	1.803649
H	-3.42663	0.035335	1.952884
H	-4.57447	-1.27552	1.540007
C	-3.45185	-2.00958	-0.85423
H	-2.73061	-2.75511	-0.47726
H	-4.47243	-2.40829	-0.71677
H	-3.28317	-1.89231	-1.9392
C	-4.2668	0.366499	-0.6465
H	-5.30962	0.030605	-0.50824
H	-4.13516	1.325632	-0.11621
H	-4.11589	0.550319	-1.72492

1.1aCl

C	-2.10626	1.12608	1.06175
C	-1.07814	2.01070	1.02430
H	-2.94477	1.20271	1.75840
H	-0.99768	2.86717	1.69859
Be	-0.72564	0.49928	-0.66782
C	1.06165	2.61321	-0.05233
C	-3.10806	-0.88310	0.02655
N	-2.03869	0.10530	0.10142
N	-0.12619	1.77099	0.02531
C	1.53561	-1.47174	-0.53783
C	1.04613	-1.55273	0.75941
C	2.84619	-1.78121	-0.87698
H	0.01105	-1.27371	0.98301
H	3.19281	-1.69235	-1.90885
C	1.92434	-1.96750	1.75998
C	3.70637	-2.19450	0.14081
H	1.56314	-2.03432	2.78950
H	4.74470	-2.43800	-0.09957
C	3.24800	-2.28656	1.45508
H	3.92959	-2.60516	2.24812
Cl	0.45307	-0.91315	-1.83608
C	1.91727	2.16573	-1.24273
H	2.31499	1.14810	-1.08667
H	1.32587	2.17701	-2.17594
H	2.77906	2.84233	-1.37555
C	1.90151	2.47440	1.23118
H	1.33751	2.81523	2.11619
H	2.171562	1.415506	1.391518
H	2.830653	3.06933	1.169385
C	0.67249	4.087406	-0.26826
H	0.080955	4.189756	-1.19445
H	0.062174	4.47293	0.565423
H	1.570133	4.726117	-0.35034
C	-2.77278	-1.8934	-1.07508
H	-1.83749	-2.43361	-0.84654
H	-3.57821	-2.64071	-1.17934
H	-2.6522	-1.38524	-2.04901
C	-3.24266	-1.64451	1.35888
H	-3.4937	-0.96359	2.189254
H	-4.03528	-2.41146	1.299818
H	-2.29271	-2.14846	1.610735
C	-4.44701	-0.20558	-0.31919
H	-4.35986	0.331502	-1.2794
H	-5.26095	-0.94821	-0.40155
H	-4.73464	0.529318	0.451452

1.2acl

C	-0.68708	-1.67443	-1.38248
C	0.68999	-1.67324	-1.38257
H	-1.27913	-2.08168	-2.20656
H	1.28264	-2.07958	-2.20666
Be	0.00066	-0.49791	0.51902
C	2.71117	-1.25210	-0.07960
C	-2.70887	-1.25616	-0.07957
N	-1.26085	-1.12519	-0.27185
N	1.26300	-1.12298	-0.27205
C	-0.00156	1.64315	0.41088
C	-1.21772	2.24291	0.07863
C	1.21341	2.24472	0.07751
H	-2.16251	1.81675	0.41339
H	2.15915	1.82000	0.41141
C	-1.20825	3.38205	-0.72306
C	1.20153	3.38386	-0.72414
H	-2.16192	3.82919	-1.01870
H	2.15427	3.83239	-1.02067
C	-0.00398	3.95226	-1.13949
H	-0.00493	4.84937	-1.76403
Cl	-0.00014	0.65388	2.24274
C	3.07967	-0.75611	1.32306
H	2.84290	0.30907	1.46855
H	2.52873	-1.32582	2.09089
H	4.16017	-0.88883	1.50316
C	3.47780	-0.44678	-1.14392
H	3.26955	-0.83043	-2.15729
H	3.185277	0.615834	-1.12648
H	4.56713	-0.51269	-0.97546
C	3.121858	-2.7351	-0.16601
H	2.545888	-3.33193	0.561806
H	2.940228	-3.15605	-1.16861
H	4.197206	-2.85202	0.055479
C	-3.07806	-0.76128	1.323295
H	-2.84217	0.303966	1.469539
H	-4.15848	-0.89499	1.503116
H	-2.52674	-1.33099	2.090866
C	-3.47622	-0.45137	-1.14375
H	-3.26829	-0.83536	-2.15706
H	-4.56547	-0.51754	-0.97485
H	-3.18387	0.611314	-1.12695
C	-3.11785	-2.7396	-0.1666
H	-2.54122	-3.33609	0.560979
H	-4.19307	-2.8578	0.054842
H	-2.93577	-3.15995	-1.16936

1.3acl

C	-0.73742	-1.47604	-1.53665
C	0.73770	-1.47591	-1.53665
H	-1.28832	-1.83613	-2.41466
H	1.28866	-1.83592	-2.41466
Be	0.00003	-0.29378	0.58409
C	2.74210	-1.00614	-0.24664
C	-2.74191	-1.00657	-0.24665
N	-1.28613	-1.03322	-0.47539
N	1.28633	-1.03300	-0.47539
C	-0.00014	1.43925	0.18620
C	-0.00019	1.93240	-1.12725
C	-0.00024	2.40076	1.21116
H	-0.00012	1.23074	-1.97654
H	-0.00021	2.06530	2.25526
C	-0.00031	3.29879	-1.41929
C	-0.00036	3.77188	0.94141
H	-0.00034	3.64220	-2.45961
H	-0.00043	4.49239	1.76631
C	-0.00040	4.22725	-0.37773
H	-0.00050	5.30054	-0.59304
Cl	0.00008	-0.94028	2.45594
C	3.08452	0.32205	0.44008
H	2.83629	1.17940	-0.20621
H	2.52163	0.43190	1.38051
H	4.16354	0.34575	0.66856
C	3.54599	-1.14780	-1.54206
H	3.41148	-2.13454	-2.01889
H	3.278775	-0.359	-2.26723
H	4.619244	-1.04394	-1.31411
C	3.035683	-2.18008	0.702999
H	2.432743	-2.09164	1.621246
H	2.799534	-3.1433	0.217664
H	4.105988	-2.17774	0.971112
C	-3.08449	0.321586	0.44004
H	-2.83642	1.17895	-0.20629
H	-4.16351	0.345135	0.668566
H	-2.52157	0.431552	1.380439
C	-3.54579	-1.14837	-1.54205
H	-3.41116	-2.13511	-2.01886
H	-4.61905	-1.04464	-1.3141
H	-3.27868	-0.35956	-2.26725
C	-3.03532	-2.18053	0.703025
H	-2.43237	-2.09199	1.621261
H	-4.10562	-2.17832	0.971157
H	-2.79905	-3.14373	0.217711

1.4acl

C	-1.08130	-0.79491	-1.68666
C	0.29251	-1.05843	-1.72013
H	-1.67664	-0.76044	-2.60501
H	0.85803	-1.15602	-2.64764
Be	-0.34097	-0.61696	0.59961
C	2.25983	-1.49556	-0.32884
C	-2.98297	-0.12879	-0.25505
N	-1.58283	-0.50676	-0.50056
N	0.88053	-0.96076	-0.50274
C	0.82167	1.01933	0.02281
C	0.75992	1.75391	-1.14500
C	1.15527	1.63119	1.23106
H	0.52605	1.24313	-2.09067
H	1.20123	1.06282	2.16343
C	0.98713	3.12974	-1.12520
C	1.38043	3.01190	1.25352
H	0.93314	3.70813	-2.05269
H	1.61703	3.50091	2.20337
C	1.29794	3.76127	0.08079
H	1.48374	4.83894	0.10424
Cl	-0.47538	-1.08235	2.47171
C	2.84911	-1.09010	1.02445
H	3.13433	-0.02725	1.03932
H	2.13843	-1.28300	1.84384
H	3.75985	-1.68429	1.20817
C	3.19821	-1.02019	-1.44474
H	2.93752	-1.44126	-2.42984
H	3.188726	0.081238	-1.51542
H	4.228763	-1.34051	-1.21735
C	2.103701	-3.02607	-0.35724
H	1.429579	-3.35326	0.452378
H	1.684728	-3.36733	-1.31822
H	3.086534	-3.50669	-0.21331
C	-2.95734	1.129913	0.625671
H	-2.44187	1.955398	0.104735
H	-3.98454	1.451866	0.870053
H	-2.42261	0.931428	1.569746
C	-3.74796	0.173209	-1.54758
H	-3.84615	-0.71826	-2.19132
H	-4.76842	0.508521	-1.29809
H	-3.2618	0.978208	-2.12668
C	-3.66137	-1.28688	0.492135
H	-3.12427	-1.5088	1.428705
H	-4.70795	-1.03192	0.734994
H	-3.66066	-2.19842	-0.13107

1.5acl

C	-0.00145	0.28100	-1.72053
C	-1.27906	-0.13834	-1.62418
H	0.53257	0.41353	-2.65837
H	-1.84695	-0.36502	-2.53421
Be	-0.78013	0.24228	0.66242
C	-3.24345	-0.74314	-0.29529
C	1.21841	1.94665	-0.31615
N	0.67067	0.51051	-0.43911
N	-1.85603	-0.26954	-0.39246
C	1.68964	-0.52240	-0.19328
C	2.48257	-1.01871	-1.23440
C	1.87599	-1.02989	1.09528
H	2.34567	-0.65788	-2.25381
H	1.26904	-0.65857	1.92362
C	3.44893	-1.99061	-0.98670
C	2.83971	-2.00874	1.33842
H	4.05875	-2.36333	-1.81449
H	2.96287	-2.39519	2.35389
C	3.63307	-2.49161	0.30143
H	4.38797	-3.25916	0.49289
Cl	-0.83469	0.65075	2.54053
C	2.01082	2.10674	0.98439
H	2.27624	3.17078	1.10271
H	1.41592	1.80647	1.86063
H	2.94773	1.52657	0.96948
C	0.01027	2.88999	-0.30384
H	-0.57918	2.77086	0.62170
H	0.357757	3.935779	-0.3417
H	-0.64198	2.712189	-1.17496
C	2.135261	2.290223	-1.4966
H	2.57094	3.289405	-1.3296
H	2.972086	1.576956	-1.58118
H	1.592558	2.323818	-2.45477
C	-3.62127	-0.86134	1.183672
H	-2.94665	-1.55882	1.708903
H	-3.55503	0.114661	1.691279
H	-4.65416	-1.237	1.283622
C	-3.38353	-2.12893	-0.9489
H	-2.68426	-2.84227	-0.47959
H	-4.4105	-2.5158	-0.82859
H	-3.1659	-2.10041	-2.0308
C	-4.19567	0.259127	-0.97047
H	-5.24611	-0.06662	-0.87191
H	-4.09311	1.252972	-0.5014
H	-3.97996	0.367148	-2.04807

1.1aBr

C	-1.93123	1.38500	1.21678
C	-0.81496	2.14126	1.05880
H	-2.68509	1.57519	1.98482
H	-0.56902	2.98986	1.70194
Be	-0.79525	0.55776	-0.60582
C	1.25038	2.49436	-0.24964
C	-3.28652	-0.46583	0.29417
N	-2.07580	0.34716	0.28432
N	-0.00175	1.78058	-0.02137
C	1.42861	-1.46740	-0.10443
C	0.87237	-1.33725	1.16315
C	2.77947	-1.71706	-0.31330
H	-0.18837	-1.09736	1.28818
H	3.18833	-1.80150	-1.32292
C	1.71677	-1.46804	2.26445
C	3.60695	-1.84168	0.80396
H	1.29964	-1.35691	3.26854
H	4.67439	-2.03027	0.66153
C	3.07822	-1.71700	2.08820
H	3.73430	-1.80677	2.95809
Br	0.29718	-1.22622	-1.63860
C	1.87341	2.00162	-1.56046
H	2.17398	0.94328	-1.48528
H	1.15574	2.10498	-2.39420
H	2.77648	2.58629	-1.80747
C	2.24019	2.22531	0.89956
H	1.82589	2.56678	1.86392
H	2.442339	1.143165	0.984813
H	3.19901	2.749313	0.734552
C	1.002189	4.008779	-0.38048
H	0.27897	4.205232	-1.19079
H	0.592346	4.43934	0.548336
H	1.942215	4.542191	-0.608
C	-3.16894	-1.54331	-0.78845
H	-2.33245	-2.23086	-0.57517
H	-4.09443	-2.14182	-0.84578
H	-3.00174	-1.08331	-1.78004
C	-3.46982	-1.16379	1.654799
H	-3.58153	-0.43236	2.472741
H	-4.36866	-1.80583	1.652785
H	-2.59372	-1.79631	1.883537
C	-4.51974	0.404724	-0.01139
H	-4.39913	0.897095	-0.99179
H	-5.44403	-0.20063	-0.03025
H	-4.64703	1.195599	0.747146

1.2aBr

C	-0.68677	-1.88387	-1.46293
C	0.68865	-1.88320	-1.46295
H	-1.27685	-2.37115	-2.24363
H	1.27918	-2.36994	-2.24364
Be	0.00030	-0.53899	0.32130
C	2.71712	-1.34222	-0.22429
C	-2.71572	-1.34468	-0.22422
N	-1.26461	-1.23268	-0.40917
N	1.26591	-1.23142	-0.40922
C	-0.00093	1.59690	0.05353
C	-1.21509	2.14415	-0.37018
C	1.21259	2.14478	-0.37119
H	-2.16164	1.77178	0.02031
H	2.15966	1.77286	0.01846
C	-1.20662	3.15370	-1.32939
C	1.20279	3.15433	-1.33039
H	-2.16003	3.55203	-1.68905
H	2.15569	3.55312	-1.69085
C	-0.00225	3.65645	-1.82443
H	-0.00276	4.45055	-2.57542
Br	-0.00017	0.80775	2.09824
C	3.10931	-0.72099	1.12033
H	2.88259	0.35545	1.16766
H	2.56780	-1.21197	1.94701
H	4.19192	-0.84335	1.29539
C	3.46644	-0.63377	-1.36734
H	3.24610	-1.10686	-2.33942
H	3.169591	0.425225	-1.44102
H	4.558252	-0.68108	-1.20875
C	3.131537	-2.82634	-0.18248
H	2.573085	-3.35449	0.609424
H	2.932245	-3.33892	-1.13793
H	4.21154	-2.91996	0.027173
C	-3.10823	-0.72441	1.120753
H	-2.88179	0.352056	1.16876
H	-4.19081	-0.84722	1.295685
H	-2.5666	-1.21571	1.94716
C	-3.46559	-0.63622	-1.36689
H	-3.24475	-1.10858	-2.33921
H	-4.55737	-0.68459	-1.2084
H	-3.16967	0.423076	-1.43994
C	-3.12909	-2.82911	-0.1831
H	-2.57003	-3.35732	0.608335
H	-4.20896	-2.92356	0.026851
H	-2.92979	-3.34104	-1.13889

1.3aBr

C	0.73686	-1.01549	2.03300
C	-0.73688	-1.01546	2.03301
H	1.28695	-1.21642	2.96069
H	-1.28698	-1.21638	2.96070
Be	-0.00001	-0.23791	-0.26097
C	-2.74846	-0.77250	0.69826
C	2.74844	-0.77258	0.69825
N	1.28801	-0.76353	0.91162
N	-1.28803	-0.76349	0.91163
C	0.00003	1.53728	-0.21693
C	0.00004	2.26777	0.98151
C	0.00004	2.29046	-1.40336
H	0.00004	1.73875	1.94747
H	0.00002	1.76833	-2.36758
C	0.00007	3.66468	1.01283
C	0.00006	3.68794	-1.39442
H	0.00008	4.19596	1.97075
H	0.00007	4.24026	-2.34020
C	0.00008	4.38189	-0.18402
H	0.00009	5.47652	-0.17260
Br	-0.00003	-1.32353	-2.11158
C	-3.09574	0.39044	-0.23918
H	-2.84557	1.35993	0.22082
H	-2.54080	0.30987	-1.18748
H	-4.17628	0.36754	-0.46031
C	-3.53318	-0.63796	2.00691
H	-3.40620	-1.51083	2.67078
H	-3.24432	0.276379	2.554811
H	-4.60816	-0.56417	1.775625
C	-3.06846	-2.11415	0.017677
H	-2.50264	-2.21753	-0.92217
H	-2.8088	-2.95904	0.679371
H	-4.148	-2.16426	-0.20449
C	3.095748	0.390351	-0.23919
H	2.845592	1.359843	0.2208
H	4.176284	0.367425	-0.46032
H	2.540808	0.30978	-1.18749
C	3.533155	-0.63806	2.006898
H	3.406157	-1.51093	2.670767
H	4.608145	-0.5643	1.775615
H	3.244322	0.27629	2.554797
C	3.068404	-2.11424	0.017671
H	2.502589	-2.21761	-0.92218
H	4.147948	-2.16438	-0.20449
H	2.808719	-2.95913	0.679366

1.4aBr

C	0.92987	0.17876	2.11258
C	-0.42179	-0.17271	2.18110
H	1.45340	0.59258	2.98040
H	-1.04383	0.02274	3.05527
Be	0.34441	-0.54194	-0.10786
C	-2.25556	-1.25467	0.97726
C	2.88731	0.45296	0.63392
N	1.49783	0.06354	0.92650
N	-0.92937	-0.57401	0.98960
C	-0.97449	1.07547	-0.22242
C	-1.01412	2.18963	0.59347
C	-1.29974	1.17522	-1.57535
H	-0.79014	2.08101	1.66473
H	-1.27295	0.30418	-2.23475
C	-1.33135	3.44045	0.06529
C	-1.61632	2.42972	-2.10792
H	-1.35506	4.32066	0.71522
H	-1.84619	2.51685	-3.17413
C	-1.63194	3.56078	-1.29311
H	-1.88723	4.53706	-1.71497
Br	0.67835	-1.75402	-1.77942
C	-2.80003	-1.40984	-0.44473
H	-3.17144	-0.45379	-0.84411
H	-2.03500	-1.81224	-1.12751
H	-3.64624	-2.11663	-0.42345
C	-3.28953	-0.49846	1.82121
H	-3.06686	-0.52780	2.90051
H	-3.35638	0.555361	1.499748
H	-4.2805	-0.96223	1.682884
C	-1.99275	-2.65542	1.557667
H	-1.26164	-3.19502	0.932058
H	-1.59502	-2.59324	2.583998
H	-2.93199	-3.23411	1.580155
C	2.853821	1.314303	-0.63756
H	2.257438	2.227663	-0.4691
H	3.876273	1.60881	-0.93138
H	2.400941	0.757044	-1.4749
C	3.526168	1.258541	1.770229
H	3.631103	0.665382	2.695336
H	4.539474	1.571549	1.468244
H	2.947346	2.171282	1.997664
C	3.700535	-0.82735	0.391114
H	3.265465	-1.41325	-0.43452
H	4.745936	-0.57914	0.136658
H	3.703375	-1.45732	1.297964

1.5aBr

C	0.24219	1.46225	1.36256
C	-1.02865	1.73340	1.00785
H	0.84459	2.09115	2.01347
H	-1.51727	2.63702	1.38983
Be	-0.72321	-0.35574	-0.07207
C	-3.08172	1.20262	-0.20489
C	1.32849	-0.73243	1.82934
N	0.81057	0.25383	0.76134
N	-1.70055	0.87534	0.18148
C	1.82878	0.60582	-0.24283
C	2.69214	1.69053	-0.04893
C	1.94491	-0.14357	-1.41608
H	2.61363	2.30641	0.84681
H	1.28545	-0.99614	-1.58998
C	3.65549	2.00795	-1.00346
C	2.90509	0.18186	-2.37403
H	4.32088	2.85848	-0.83046
H	2.97060	-0.41583	-3.28729
C	3.76721	1.25599	-2.17231
H	4.51943	1.51162	-2.92346
Br	-0.98373	-2.23032	-0.93112
C	2.03756	-1.91695	1.16768
H	2.28886	-2.65360	1.94908
H	1.39476	-2.41658	0.42695
H	2.97687	-1.61137	0.67939
C	0.10999	-1.22704	2.61630
H	-0.54703	-1.85449	1.98920
H	0.444636	-1.8466	3.464795
H	-0.47352	-0.38145	3.016833
C	2.314243	-0.04546	2.783443
H	2.716723	-0.79974	3.479898
H	3.169703	0.391518	2.241977
H	1.833453	0.737976	3.390565
C	-3.59975	0.135893	-1.1724
H	-2.9602	0.070692	-2.06923
H	-3.61835	-0.85914	-0.69897
H	-4.62519	0.3852	-1.49532
C	-3.12748	2.566447	-0.91661
H	-2.46411	2.557102	-1.79867
H	-4.15357	2.795431	-1.2534
H	-2.80485	3.390397	-0.25674
C	-3.98826	1.223573	1.038252
H	-5.03593	1.432818	0.759371
H	-3.95211	0.245986	1.54921
H	-3.67568	1.997769	1.760769

1.1al

C	-1.94986	1.69231	1.07720
C	-0.84100	2.40233	0.74710
H	-2.66627	2.01329	1.83732
H	-0.56921	3.34500	1.22835
Be	-0.88460	0.55187	-0.61582
C	1.13946	2.55833	-0.70727
C	-3.36269	-0.25412	0.53301
N	-2.13678	0.51411	0.34194
N	-0.07128	1.85917	-0.28589
C	1.51757	-1.26094	0.44088
C	0.90853	-0.79249	1.60222
C	2.89009	-1.47412	0.35493
H	-0.16736	-0.59274	1.63592
H	3.35229	-1.83058	-0.56894
C	1.71139	-0.53543	2.71278
C	3.67657	-1.20815	1.47770
H	1.24751	-0.15462	3.62625
H	4.75758	-1.36389	1.42362
C	3.09018	-0.73955	2.65248
H	3.71305	-0.52407	3.52490
I	0.31498	-1.56664	-1.28539
C	1.76588	1.82063	-1.89505
H	2.14491	0.82932	-1.59464
H	1.02655	1.68542	-2.70526
H	2.61883	2.39212	-2.29980
C	2.16905	2.59874	0.43781
H	1.76637	3.12757	1.31855
H	2.431254	1.573406	0.7518
H	3.093207	3.116386	0.123352
C	0.803597	3.992292	-1.15948
H	0.060758	3.966416	-1.97537
H	0.378005	4.590363	-0.33663
H	1.707737	4.51426	-1.52024
C	-3.33523	-1.48374	-0.3802
H	-2.51953	-2.17055	-0.097
H	-4.28548	-2.04053	-0.31073
H	-3.19352	-1.18422	-1.43527
C	-3.48457	-0.73866	1.989788
H	-3.52528	0.107361	2.696418
H	-4.40026	-1.33953	2.13249
H	-2.61434	-1.36324	2.259165
C	-4.59123	0.598691	0.16365
H	-4.51179	0.938084	-0.88362
H	-5.52747	0.023699	0.279676
H	-4.66303	1.495749	0.801221

1.2al

C	-0.68540	2.35229	1.16427
C	0.68592	2.35212	1.16433
H	-1.27426	3.03455	1.78229
H	1.27490	3.03426	1.78238
Be	0.00013	0.59179	-0.20263
C	2.72707	1.50236	0.14767
C	-2.72666	1.50307	0.14746
N	-1.27120	1.43940	0.32423
N	1.27157	1.43910	0.32432
C	-0.00023	-1.47478	0.49484
C	-1.21193	-1.86697	1.07413
C	1.21123	-1.86704	1.07458
H	-2.16232	-1.62713	0.59729
H	2.16181	-1.62725	0.59811
C	-1.20521	-2.54438	2.29075
C	1.20401	-2.54445	2.29120
H	-2.15866	-2.81443	2.75399
H	2.15727	-2.81454	2.75480
C	-0.00073	-2.87720	2.91166
H	-0.00093	-3.41023	3.86607
I	-0.00002	-1.25282	-1.84364
C	3.15250	0.57642	-0.99585
H	2.91785	-0.47949	-0.78936
H	2.64268	0.85700	-1.93304
H	4.24133	0.64891	-1.15965
C	3.44573	1.08887	1.44526
H	3.19108	1.77238	2.27307
H	3.149783	0.072478	1.753599
H	4.54199	1.109622	1.312632
C	3.156597	2.930705	-0.24374
H	2.614079	3.254879	-1.14841
H	2.950769	3.661838	0.554913
H	4.240274	2.963385	-0.45297
C	-3.15227	0.577282	-0.99612
H	-2.91815	-0.47872	-0.78953
H	-4.24102	0.650278	-1.16016
H	-2.64212	0.857622	-1.93321
C	-3.4455	1.08971	1.445001
H	-3.19117	1.773465	2.272698
H	-4.54174	1.110183	1.312152
H	-3.14936	0.073458	1.753615
C	-3.15576	2.931556	-0.24388
H	-2.61309	3.255634	-1.14849
H	-4.23941	2.964585	-0.45318
H	-2.94976	3.662574	0.554831

1.3al

C	0.74239	-0.07049	2.42798
C	-0.72868	-0.10425	2.43058
H	1.29061	0.03499	3.37220
H	-1.27816	-0.02299	3.37649
Be	0.00196	-0.07614	0.01178
C	-2.74800	-0.29474	1.10558
C	2.76390	-0.16849	1.09657
N	1.29668	-0.15396	1.28229
N	-1.28249	-0.21364	1.28686
C	-0.03822	1.59625	-0.57018
C	-0.05775	2.68218	0.32023
C	-0.05356	1.91517	-1.93848
H	-0.04677	2.50159	1.40629
H	-0.03935	1.10601	-2.67795
C	-0.09110	4.01039	-0.11164
C	-0.08714	3.23685	-2.39120
H	-0.10540	4.82775	0.61732
H	-0.09892	3.44518	-3.46631
C	-0.10619	4.29154	-1.47813
H	-0.13294	5.32790	-1.82961
I	0.04268	-1.93191	-1.48709
C	-3.10453	0.41107	-0.20756
H	-2.85713	1.48383	-0.16206
H	-2.55592	-0.03000	-1.05511
H	-4.18581	0.30112	-0.39578
C	-3.51132	0.35817	2.26351
H	-3.39469	-0.18749	3.21583
H	-3.19447	1.406043	2.407709
H	-4.58777	0.360914	2.027114
C	-3.0892	-1.7914	1.016319
H	-2.53533	-2.26887	0.19191
H	-2.83273	-2.30788	1.957971
H	-4.17103	-1.91131	0.836626
C	3.084653	0.546311	-0.22087
H	2.791311	1.607543	-0.17893
H	4.169114	0.482978	-0.41224
H	2.553616	0.077832	-1.0649
C	3.499445	0.524577	2.249307
H	3.415402	-0.02422	3.203257
H	4.5731	0.582061	2.007446
H	3.129683	1.555076	2.392955
C	3.172718	-1.64854	1.013374
H	2.639334	-2.15431	0.192277
H	4.258499	-1.72036	0.831797
H	2.941908	-2.17177	1.957958

1.4al

C	0.34120	1.37794	2.04255
C	-0.86338	0.68235	2.16338
H	0.59307	2.19469	2.72630
H	-1.64127	0.96487	2.87280
Be	0.32585	-0.18654	0.22016
C	-2.14937	-1.23274	1.35577
C	2.35291	1.75390	0.67070
N	1.10096	1.05410	1.01107
N	-1.06028	-0.22759	1.17531
C	-1.33580	0.81804	-0.55309
C	-1.76513	2.08740	-0.21509
C	-1.47679	0.34636	-1.85852
H	-1.67879	2.42508	0.82801
H	-1.14771	-0.65569	-2.14355
C	-2.29564	2.93524	-1.18603
C	-2.00818	1.19607	-2.83495
H	-2.62666	3.94229	-0.91442
H	-2.09792	0.83732	-3.86470
C	-2.41511	2.48715	-2.50346
H	-2.83569	3.14416	-3.27013
I	1.35394	-1.93666	-0.90393
C	-2.45729	-1.98618	0.06003
H	-3.00923	-1.35618	-0.65357
H	-1.54036	-2.36062	-0.42092
H	-3.09187	-2.85515	0.30166
C	-3.44461	-0.57989	1.85632
H	-3.36327	-0.19774	2.88694
H	-3.74242	0.24931	1.191034
H	-4.25339	-1.32923	1.851944
C	-1.6027	-2.23218	2.38993
H	-0.68081	-2.70564	2.011871
H	-1.37228	-1.7306	3.344268
H	-2.35116	-3.02023	2.580571
C	2.325107	2.017013	-0.84218
H	1.462607	2.652642	-1.10804
H	3.25092	2.525332	-1.16242
H	2.241942	1.071492	-1.40361
C	2.494799	3.092931	1.40446
H	2.604161	2.963648	2.495168
H	3.402632	3.606451	1.047078
H	1.633548	3.755834	1.20835
C	3.533845	0.842925	1.036985
H	3.462678	-0.12167	0.50911
H	4.490245	1.323051	0.765482
H	3.540905	0.642252	2.122673

1.5al

C	0.68572	1.80735	1.22215
C	-0.54168	2.22610	0.86305
H	1.39953	2.40986	1.77807
H	-0.86897	3.23643	1.13317
Be	-0.62462	-0.01735	0.10559
C	-2.67159	1.91818	-0.28121
C	1.55674	-0.40849	1.93157
N	1.04444	0.46260	0.76545
N	-1.37352	1.38817	0.17009
C	1.99233	0.53485	-0.36175
C	2.93081	1.56903	-0.45312
C	1.96230	-0.43458	-1.36756
H	2.96353	2.35111	0.30482
H	1.24051	-1.25165	-1.32302
C	3.82454	1.62185	-1.52026
C	2.85287	-0.37478	-2.43900
H	4.55153	2.43734	-1.56961
H	2.80319	-1.14236	-3.21591
C	3.79080	0.65071	-2.51987
H	4.49003	0.69746	-3.35918
I	-1.34372	-2.14621	-0.42448
C	2.04766	-1.76812	1.42689
H	2.28952	-2.39539	2.30116
H	1.27864	-2.29432	0.84175
H	2.96133	-1.67587	0.81812
C	0.38677	-0.60530	2.90023
H	-0.41144	-1.21887	2.44818
H	0.739626	-1.13288	3.801842
H	-0.03956	0.362355	3.212711
C	2.721408	0.280968	2.65629
H	3.135878	-0.41729	3.40215
H	3.535679	0.540935	1.95934
H	2.406951	1.18744	3.197039
C	-3.41102	0.846379	-1.08408
H	-2.8065	0.505984	-1.9423
H	-3.64445	-0.03369	-0.46327
H	-4.3596	1.255882	-1.47203
C	-2.45218	3.138357	-1.19381
H	-1.82135	2.858938	-2.05533
H	-3.41577	3.518649	-1.57562
H	-1.95561	3.970309	-0.66491
C	-3.53706	2.309478	0.929326
H	-4.52681	2.673019	0.601778

H	-3.68589	1.435834	1.586955
H	-3.07117	3.112087	1.527312

2.1aF

C	-2.96991	1.11650	0.30377
C	-3.30140	-0.17025	0.58564
H	-3.58769	1.99012	0.53323
H	-4.22499	-0.48590	1.08068
Be	-1.26666	-0.21891	-0.48186
C	-2.59627	-2.50774	0.44319
H	-2.72254	-2.71588	1.52596
H	-3.50576	-2.88321	-0.07036
H	-1.74667	-3.11717	0.08938
C	-1.30709	2.57431	-0.74591
H	-1.98028	3.02372	-1.50535
H	-1.25492	3.28758	0.10396
H	-0.29968	2.52527	-1.19710
N	-1.73063	1.26501	-0.33822
N	-2.35097	-1.11785	0.18013
C	1.49342	-0.35631	-0.40921
C	2.62503	-0.99596	-0.87623
C	1.47521	0.57254	0.61284
H	2.55741	-1.72147	-1.68925
H	0.53134	1.03532	0.92039
C	3.83585	-0.67418	-0.26188
C	2.69974	0.87544	1.21108
H	4.75499	-1.15874	-0.60120
H	2.72884	1.60541	2.02396
C	3.87315	0.25696	0.77755
H	4.82574	0.50139	1.25426
F	0.28840	-0.68764	-1.03106

2.2aF

C	2.37695	0.74387	-1.04436
C	2.42762	-0.63582	-1.03472
H	2.81270	1.37413	-1.82628
H	2.91224	-1.24250	-1.80654
Be	1.08823	0.01737	0.78663
C	1.66066	-2.63303	0.11252
H	0.86904	-3.02417	-0.56386
H	2.60409	-3.14516	-0.15423
H	1.39707	-2.92689	1.14226
C	1.46343	2.69508	0.07207
H	2.34896	3.27083	-0.25590

H	0.60994	3.00455	-0.57068
H	1.22959	2.99613	1.10704
N	1.69592	1.28096	0.00772
N	1.78493	-1.20642	0.02331
C	-0.95377	-0.02080	0.48051
C	-1.60019	1.19043	0.26941
C	-1.51656	-1.25598	0.18425
H	-1.16361	2.13523	0.59749
H	-1.01399	-2.19050	0.43934
C	-2.81527	1.15684	-0.41449
C	-2.73315	-1.25658	-0.49817
H	-3.32622	2.09924	-0.63324
H	-3.17905	-2.21359	-0.78513
C	-3.38143	-0.05834	-0.80715
H	-4.33858	-0.07279	-1.33438
F	-0.00566	-0.02331	1.92902

2.3aF

C	2.24944	0.73984	-1.10299
C	2.24950	-0.73986	-1.10291
H	2.71481	1.31103	-1.92107
H	2.71492	-1.31110	-1.92093
Be	0.76810	0.00004	0.90931
C	1.48177	-2.69634	0.03321
H	1.97533	-3.27515	-0.76810
H	1.88678	-2.98525	1.01693
H	0.40022	-2.91157	0.04460
C	1.48160	2.69639	0.03295
H	1.97506	3.27515	-0.76847
H	0.40004	2.91154	0.04439
H	1.88666	2.98544	1.01660
N	1.64339	1.27666	-0.12335
N	1.64346	-1.27661	-0.12322
C	-0.89397	-0.00001	0.28412
C	-1.96092	0.00010	1.20196
C	-1.24927	-0.00015	-1.07465
H	-1.74032	0.00021	2.27621
H	-0.46261	-0.00024	-1.84615
C	-3.29680	0.00007	0.79084
C	-2.57785	-0.00018	-1.50787
H	-4.09974	0.00016	1.53579
H	-2.81038	-0.00030	-2.57852
C	-3.61003	-0.00007	-0.56892
H	-4.65475	-0.00010	-0.89652
F	1.16588	0.00011	2.32661

2.4aF

C	1.52292	0.58350	-1.55073
C	2.13690	-0.60039	-1.10121
H	1.38351	0.84508	-2.60381
H	2.64569	-1.29942	-1.77859
Be	1.09413	0.36779	0.89029
C	2.52023	-2.06091	0.78261
H	3.10255	-2.66226	0.06142
H	3.16983	-1.79972	1.63511
H	1.69355	-2.68084	1.17099
C	0.31388	2.53780	-0.79812
H	-0.30303	2.54792	-1.71411
H	-0.30724	2.82824	0.06037
H	1.13122	3.27138	-0.90275
N	0.90223	1.23577	-0.55586
N	1.99293	-0.86086	0.18000
C	-0.73784	0.10125	0.03853
C	-1.65195	0.50468	1.00906
C	-1.11617	-0.72632	-1.00028
H	-1.34585	1.15989	1.83092
H	-0.38585	-0.98187	-1.78399
C	-2.96369	0.02092	0.94387
C	-2.41913	-1.22059	-1.05959
H	-3.68884	0.31889	1.70746
H	-2.71952	-1.88953	-1.87209
C	-3.34557	-0.84075	-0.08438
H	-4.37330	-1.21232	-0.13397
F	1.08857	0.85155	2.25716

2.5aF

C	1.07457	-1.33024	0.92636
C	2.16036	-1.33109	0.11849
H	0.75442	-2.13487	1.59042
H	2.81373	-2.21051	0.04299
Be	1.40189	0.91826	-0.19170
C	3.58440	-0.20216	-1.48870
H	4.53481	-0.41036	-0.95775
H	3.48443	-0.94407	-2.30573
H	3.67813	0.79169	-1.95457
C	0.30783	0.54724	2.25134
H	1.34261	0.63401	2.61729
H	-0.13881	1.55091	2.19970
H	-0.27676	-0.07967	2.94836

N	0.34094	-0.07260	0.90722
N	2.44679	-0.20955	-0.60152
C	-0.98588	-0.12716	0.29519
C	-1.58105	-1.34101	-0.04975
C	-1.65937	1.07210	0.03246
H	-1.04989	-2.27725	0.12541
H	-1.17882	2.02831	0.25139
C	-2.84674	-1.35530	-0.63760
C	-2.92299	1.04830	-0.55114
H	-3.30269	-2.31320	-0.90351
H	-3.43441	1.99277	-0.75660
C	-3.52545	-0.16483	-0.88507
H	-4.51637	-0.18024	-1.34693
F	1.17043	2.32883	-0.33255

2.1aCl

C	2.99331	1.16044	-0.48213
C	3.23876	-0.09331	-0.94880
H	3.56843	2.05376	-0.74431
H	4.03950	-0.35732	-1.64654
Be	1.45445	-0.25210	0.49884
C	2.51876	-2.42984	-0.90565
H	2.39654	-2.52445	-2.00430
H	3.50946	-2.85662	-0.64668
H	1.75289	-3.06917	-0.43398
C	1.58184	2.50167	1.00316
H	2.38393	2.88175	1.66870
H	1.38628	3.28836	0.24460
H	0.66975	2.40107	1.61784
N	1.91324	1.23879	0.40546
N	2.37191	-1.07359	-0.45592
C	-1.65665	-0.29507	0.41849
C	-2.91297	-0.86101	0.59631
C	-1.38972	0.68277	-0.52948
H	-3.07942	-1.63013	1.35389
H	-0.37876	1.09464	-0.63447
C	-3.95149	-0.42017	-0.22379
C	-2.44417	1.10620	-1.33941
H	-4.94845	-0.85284	-0.10474
H	-2.25853	1.87316	-2.09598
C	-3.71870	0.55949	-1.18950
H	-4.53648	0.89792	-1.83118
Cl	-0.34546	-0.87148	1.48352

2.2aCl

C	-2.41734	-0.68968	-1.25091
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C	-2.41667	0.69056	-1.25117
H	-2.92367	-1.30915	-1.99835
H	-2.92240	1.31024	-1.99884
Be	-1.07301	0.00008	0.54266
C	-1.52737	2.66499	-0.14891
H	-0.67350	2.99435	-0.78175
H	-2.42253	3.22014	-0.48684
H	-1.31191	2.97262	0.88833
C	-1.52965	-2.66457	-0.14806
H	-2.42551	-3.21909	-0.48517
H	-0.67645	-2.99498	-0.78125
H	-1.31385	-2.97190	0.88919
N	-1.72287	-1.24551	-0.21523
N	-1.72182	1.24608	-0.21559
C	1.00325	0.00002	0.44331
C	1.58287	1.22111	0.08458
C	1.58184	-1.22166	0.08489
H	1.16258	2.16504	0.43770
H	1.16071	-2.16514	0.43823
C	2.68401	1.20690	-0.76729
C	2.68296	-1.20862	-0.76702
H	3.11994	2.15753	-1.08862
H	3.11806	-2.15970	-1.08814
C	3.23343	-0.00114	-1.20420
H	4.10249	-0.00160	-1.86712
Cl	0.06746	0.00058	2.25391

2.3aCl

C	2.03706	-1.56613	-0.73829
C	2.03676	-1.56513	0.74095
H	2.49133	-2.38406	-1.31702
H	2.49073	-2.38233	1.32094
Be	0.70942	0.50742	-0.00048
C	1.32406	-0.35752	2.68343
H	1.80504	-1.15540	3.27618
H	1.76202	0.62345	2.93048
H	0.24669	-0.30725	2.91286
C	1.32506	-0.36111	-2.68267
H	1.80626	-1.15980	-3.27414
H	0.24778	-0.31117	-2.91257
H	1.76312	0.61952	-2.93086
N	1.46250	-0.56116	-1.26525
N	1.46204	-0.55943	1.26635
C	-1.02178	0.17837	-0.00031
C	-1.96331	1.22379	-0.00050

C	-1.54472	-1.12683	0.00005
H	-1.60717	2.26081	-0.00083
H	-0.85971	-1.98915	0.00022
C	-3.33978	0.98275	-0.00036
C	-2.91704	-1.38861	0.00022
H	-4.04331	1.82219	-0.00055
H	-3.28360	-2.42101	0.00049
C	-3.82217	-0.32674	0.00001
H	-4.89986	-0.51921	0.00012
Cl	1.53449	2.29181	-0.00155

2.4aCl

C	-1.11783	-1.45768	1.40967
C	-1.75097	-1.81635	0.20779
H	-0.82072	-2.16298	2.19079
H	-2.12098	-2.83126	0.01018
Be	-1.10789	0.51089	-0.08442
C	-2.40766	-1.08164	-2.00157
H	-2.86624	-2.08350	-2.08145
H	-3.18009	-0.31770	-2.19120
H	-1.63924	-0.98200	-2.78782
C	-0.18757	0.42552	2.61183
H	0.57745	-0.21026	3.09076
H	0.24551	1.40866	2.38363
H	-1.03085	0.56819	3.30802
N	-0.70432	-0.17682	1.39777
N	-1.81474	-0.86706	-0.70340
C	0.86657	0.00069	0.09027
C	1.62682	1.16001	-0.05328
C	1.42291	-1.24558	-0.13016
H	1.18842	2.14716	0.12241
H	0.82519	-2.14969	0.06104
C	2.95387	1.05097	-0.48316
C	2.74128	-1.35557	-0.57031
H	3.55257	1.95708	-0.61694
H	3.17840	-2.34076	-0.75957
C	3.50905	-0.20102	-0.74508
H	4.54895	-0.28116	-1.07485
Cl	-1.54896	2.33328	-0.48200

2.5aCl

C	0.79400	-1.54898	1.09768
C	1.93776	-1.67923	0.39047
H	0.30166	-2.30142	1.71517

H	2.51148	-2.61492	0.39329
Be	1.35993	0.58909	-0.14000
C	3.59441	-0.72052	-1.10922
H	4.46994	-0.94625	-0.46903
H	3.53328	-1.50504	-1.88925
H	3.79070	0.23761	-1.61553
C	0.24991	0.50344	2.26847
H	1.29193	0.47269	2.62195
H	-0.04710	1.55402	2.12588
H	-0.39606	0.02451	3.02560
N	0.19122	-0.22053	0.98465
N	2.37318	-0.61266	-0.34682
C	-1.11455	-0.24428	0.34154
C	-1.22348	-0.90715	-0.88776
C	-2.23443	0.38310	0.88467
H	-0.34269	-1.39598	-1.31385
H	-2.18105	0.91333	1.83577
C	-2.43918	-0.94220	-1.55920
C	-3.45471	0.33969	0.20458
H	-2.50747	-1.45891	-2.52042
H	-4.32637	0.83344	0.64311
C	-3.56499	-0.32005	-1.01423
H	-4.52184	-0.34893	-1.54208
Cl	1.16263	2.40170	-0.62456

2.1aBr

C	-3.04117	1.49893	0.10318
C	-3.34112	0.52793	1.00848
H	-3.57721	2.44674	-0.00497
H	-4.15436	0.58166	1.73899
Be	-1.55526	-0.23936	-0.23278
C	-2.71657	-1.66981	1.87723
H	-2.62982	-1.33216	2.93024
H	-3.71186	-2.14653	1.76388
H	-1.95627	-2.45412	1.71972
C	-1.56099	2.12021	-1.74498
H	-2.34969	2.27543	-2.50942
H	-1.30776	3.11784	-1.32898
H	-0.66613	1.74344	-2.27119
N	-1.95873	1.18961	-0.72599
N	-2.51430	-0.59540	0.94503
C	1.67644	-0.21813	-0.07627
C	2.96017	-0.74672	0.00454
C	1.34640	1.04072	0.40834
H	3.18712	-1.74203	-0.38536

H	0.31938	1.41790	0.32885
C	3.95477	0.02795	0.60200
C	2.35703	1.79722	1.00340
H	4.97011	-0.37033	0.67948
H	2.11864	2.78969	1.39503
C	3.65499	1.29580	1.10073
H	4.43886	1.89639	1.56988
Br	0.31747	-1.29916	-0.91281

2.2aBr

C	2.49686	-1.58646	-0.57779
C	2.51479	-1.46294	0.79485
H	3.04903	-2.34706	-1.13946
H	3.08522	-2.11134	1.46792
Be	1.06059	0.17989	-0.02675
C	1.57970	-0.24661	2.68195
H	0.76019	-0.88492	3.08065
H	2.49682	-0.49481	3.24894
H	1.32281	0.80327	2.90415
C	1.50945	-0.72724	-2.62705
H	2.40296	-1.10136	-3.16132
H	0.66407	-1.40555	-2.87916
H	1.26890	0.26934	-3.03537
N	1.72693	-0.65014	-1.21223
N	1.75802	-0.42753	1.27105
C	-1.02717	0.10810	-0.00042
C	-1.56829	-0.20482	1.25257
C	-1.59193	-0.39111	-1.18040
H	-1.16197	0.24091	2.16311
H	-1.20424	-0.08850	-2.15561
C	-2.60672	-1.12907	1.32094
C	-2.62988	-1.31358	-1.08751
H	-3.00836	-1.40736	2.29974
H	-3.04963	-1.73724	-2.00465
C	-3.13687	-1.69268	0.15774
H	-3.95634	-2.41327	0.22053
Br	-0.12989	2.03944	-0.16353

2.3aBr

C	1.33073	2.29218	0.73953
C	1.33091	2.29228	-0.73902
H	1.62398	3.17917	1.32024
H	1.62420	3.17939	-1.31954
Be	0.46199	-0.00267	-0.00004

C	0.86958	0.96986	-2.68276
H	1.20141	1.84232	-3.27243
H	1.47938	0.08465	-2.92778
H	-0.17993	0.72683	-2.91842
C	0.86946	0.96929	2.68297
H	1.20119	1.84165	3.27283
H	-0.18004	0.72612	2.91852
H	1.47932	0.08407	2.92782
N	0.96133	1.19365	1.26486
N	0.96144	1.19390	-1.26461
C	-1.28851	-0.13711	-0.00008
C	-1.93987	-1.38395	0.00002
C	-2.11979	0.99777	-0.00015
H	-1.33726	-2.30005	0.00008
H	-1.67079	2.00281	-0.00023
C	-3.33293	-1.49353	0.00004
C	-3.51402	0.90877	-0.00014
H	-3.80491	-2.48173	0.00012
H	-4.12596	1.81751	-0.00020
C	-4.12581	-0.34515	-0.00003
H	-5.21749	-0.42744	-0.00002
Br	1.83203	-1.63999	-0.00014

2.4aBr

C	0.02713	2.16279	1.28529
C	0.56052	2.61676	0.06786
H	-0.56289	2.77467	1.97326
H	0.53822	3.67231	-0.23452
Be	0.85320	0.20662	0.02635
C	1.59183	1.97622	-2.02558
H	1.71040	3.06348	-2.18005
H	2.57515	1.48916	-2.13192
H	0.93342	1.57720	-2.81712
C	-0.19024	0.19442	2.67886
H	-1.17008	0.52354	3.06656
H	-0.19026	-0.89722	2.55900
H	0.59761	0.46573	3.40097
N	0.12754	0.82601	1.41207
N	1.03839	1.67930	-0.72578
C	-1.17189	-0.06881	0.10565
C	-1.45317	-1.43375	0.12360
C	-2.12134	0.84510	-0.31434
H	-0.70802	-2.16033	0.46140
H	-1.90864	1.92232	-0.24718
C	-2.69242	-1.87821	-0.34975

C	-3.35114	0.40323	-0.80027
H	-2.91334	-2.94987	-0.35643
H	-4.09486	1.12516	-1.15113
C	-3.63657	-0.96456	-0.81660
H	-4.60492	-1.31734	-1.18333
Br	2.08136	-1.45062	-0.16563

2.5aBr

C	-0.26332	2.19474	0.86829
C	-1.38505	2.39903	0.14397
H	0.35952	2.94396	1.35889
H	-1.79752	3.40467	-0.00807
Be	-1.20751	0.01177	-0.00208
C	-3.20263	1.50447	-1.20109
H	-4.00711	2.00665	-0.62883
H	-3.01024	2.10236	-2.11383
H	-3.58540	0.52278	-1.52184
C	-0.02511	0.30789	2.36829
H	-1.01614	0.61645	2.73390
H	0.03960	-0.79032	2.40717
H	0.75173	0.75601	3.01328
N	0.10693	0.78395	0.97719
N	-2.00853	1.31494	-0.41156
C	1.37215	0.46415	0.32885
C	1.62321	1.01454	-0.93423
C	2.30621	-0.40206	0.89722
H	0.89179	1.69400	-1.37902
H	2.13685	-0.85764	1.87279
C	2.79532	0.70329	-1.61349
C	3.48279	-0.70677	0.20865
H	2.97487	1.14006	-2.59976
H	4.20606	-1.38727	0.66662
C	3.73470	-0.15851	-1.04448
H	4.65710	-0.40171	-1.57846
Br	-1.34541	-2.01182	-0.18017

2.1al

C	-3.03761	1.76523	-0.29308
C	-3.42190	1.08421	0.82234
H	-3.49555	2.69122	-0.65405
H	-4.23577	1.38483	1.48967
Be	-1.68325	-0.10672	-0.12640
C	-2.98951	-0.86120	2.23508
H	-2.93867	-0.26655	3.16968

H	-4.00098	-1.31390	2.18543
H	-2.26298	-1.68655	2.33000
C	-1.48976	1.78443	-2.18715
H	-2.26698	1.84212	-2.97589
H	-1.11762	2.81661	-2.01731
H	-0.65067	1.19454	-2.59622
N	-1.97838	1.17299	-0.98271
N	-2.68430	-0.07112	1.07410
C	1.72302	0.01533	0.10689
C	3.04574	-0.37313	0.30421
C	1.30430	1.33292	0.25506
H	3.35791	-1.41395	0.18372
H	0.25463	1.60876	0.09258
C	3.97781	0.60045	0.66588
C	2.25196	2.29101	0.61907
H	5.02038	0.31226	0.82673
H	1.93774	3.33097	0.74273
C	3.58312	1.92914	0.82384
H	4.31830	2.68620	1.10947
I	0.29753	-1.46949	-0.45535

2.2a1

C	-2.95910	1.11530	-0.68606
C	-2.95943	1.11396	0.68650
H	-3.72075	1.59683	-1.30800
H	-3.72143	1.59418	1.30903
Be	-1.07258	-0.07348	-0.00051
C	-1.71493	0.43073	2.66857
H	-1.12294	1.31466	2.99638
H	-2.67309	0.45366	3.22205
H	-1.16946	-0.47262	2.99368
C	-1.71344	0.43636	-2.66887
H	-2.67125	0.46161	-3.22285
H	-1.12041	1.32052	-2.99416
H	-1.16868	-0.46672	-2.99591
N	-1.91655	0.41414	-1.25036
N	-1.91710	0.41175	1.24988
C	1.00421	0.40156	0.00033
C	1.37716	0.98306	1.21942
C	1.37845	0.98410	-1.21786
H	1.12169	0.50399	2.16738
H	1.12403	0.50583	-2.16650
C	2.03990	2.20676	1.20994
C	2.04120	2.20779	-1.20663
H	2.30082	2.68023	2.16074

H	2.30318	2.68204	-2.15676
C	2.36896	2.82550	0.00209
H	2.89278	3.78499	0.00279
I	0.63346	-1.84296	-0.00089

2.3al

C	-0.49368	2.71268	-0.73783
C	-0.49367	2.71265	0.73796
H	-0.61990	3.63746	-1.31895
H	-0.61986	3.63740	1.31913
Be	-0.09061	0.30336	0.00000
C	-0.28735	1.33172	2.68397
H	-0.42810	2.25888	3.26598
H	-1.06851	0.59671	2.93842
H	0.68896	0.87658	2.91914
C	-0.28740	1.33185	-2.68391
H	-0.42817	2.25904	-3.26588
H	0.68893	0.87675	-2.91913
H	-1.06854	0.59684	-2.93839
N	-0.33648	1.56281	-1.26333
N	-0.33647	1.56275	1.26340
C	1.57248	-0.24575	-0.00002
C	1.93445	-1.60505	0.00001
C	2.63311	0.67957	-0.00005
H	1.14723	-2.36792	0.00004
H	2.41716	1.75880	-0.00008
C	3.26980	-2.01676	0.00002
C	3.97372	0.28702	-0.00006
H	3.51232	-3.08474	0.00004
H	4.76967	1.03940	-0.00008
C	4.29520	-1.07061	-0.00002
H	5.34237	-1.38999	-0.00002
I	-1.99925	-1.10361	-0.00002

2.4al

C	-0.95620	2.23571	1.26261
C	-0.52520	2.81058	0.05719
H	-1.70004	2.67340	1.93391
H	-0.80916	3.82499	-0.25308
Be	0.38511	0.56429	0.04608
C	0.70930	2.46854	-1.99590
H	0.51990	3.54407	-2.16078
H	1.79469	2.28250	-2.05252
H	0.22937	1.89702	-2.80953

C	-0.66681	0.29629	2.68209
H	-1.69870	0.38032	3.06499
H	-0.39887	-0.76353	2.57826
H	0.02936	0.76130	3.39965
N	-0.50983	0.97163	1.40706
N	0.20435	2.02976	-0.71615
C	-1.49248	-0.24491	0.10170
C	-1.42412	-1.63603	0.16557
C	-2.62708	0.38625	-0.37702
H	-0.53563	-2.14342	0.55337
H	-2.69593	1.48336	-0.34219
C	-2.49483	-2.39264	-0.32184
C	-3.68837	-0.36599	-0.87785
H	-2.43947	-3.48492	-0.29089
H	-4.57694	0.13354	-1.27542
C	-3.62063	-1.76145	-0.84886
H	-4.45687	-2.35756	-1.22528
I	2.22745	-0.79766	-0.09863

2.5al

C	0.68002	2.48744	0.74021
C	-0.36429	2.96831	0.03221
H	1.51394	3.04800	1.16462
H	-0.47433	4.04003	-0.17647
Be	-0.88274	0.62867	0.03435
C	-2.43260	2.56847	-1.18481
H	-3.06986	3.24692	-0.58448
H	-2.12539	3.11020	-2.10071
H	-3.05507	1.71436	-1.49487
C	0.41313	0.71569	2.36558
H	-0.44562	1.30780	2.71630
H	0.17955	-0.35303	2.48800
H	1.30208	0.97995	2.96565
N	0.62831	1.03843	0.94054
N	-1.29810	2.08205	-0.43487
C	1.73090	0.32839	0.30300
C	2.06653	0.67732	-1.01104
C	2.41779	-0.70700	0.93583
H	1.52925	1.49130	-1.50508
H	2.17538	-1.00913	1.95463
C	3.07695	-0.00403	-1.67950
C	3.43469	-1.38349	0.25767
H	3.32328	0.27551	-2.70755
H	3.96460	-2.19431	0.76536
C	3.76909	-1.03891	-1.04739

H	4.56393	-1.57412	-1.57369
I	-1.69652	-1.47386	-0.07282

3.1aF

C	-2.58455	1.31548	-0.72932
C	-2.95852	0.07592	-1.12158
H	-3.09625	2.21853	-1.09557
H	-3.79249	-0.04426	-1.82155
Be	-0.95596	0.11262	0.52187
C	-3.07021	-2.20915	0.65555
H	-3.52982	-1.51635	1.38023
H	-3.87918	-2.73108	0.11513
H	-2.49563	-2.97322	1.20895
C	-1.19162	2.87059	0.51910
H	-0.80309	3.45653	-0.34008
H	-2.06260	3.42236	0.92629
H	-0.41471	2.87491	1.30367
N	-1.52256	1.51589	0.16024
P	-1.93494	-1.35561	-0.57630
C	1.70348	-0.07627	0.65158
C	2.23538	-1.34094	0.49987
C	2.22437	1.07524	0.09554
H	1.74905	-2.20727	0.95191
H	1.73184	2.03823	0.24462
C	3.39826	-1.44906	-0.26369
C	3.38761	0.94031	-0.66373
H	3.85267	-2.43184	-0.41231
H	3.83402	1.82588	-1.12288
C	3.97225	-0.31459	-0.83978
H	4.88205	-0.41069	-1.43758
F	0.53681	0.04728	1.41260

3.2aF

C	2.66412	0.26330	0.89885
C	1.99666	1.45079	0.86314
H	3.44579	0.06033	1.64554
H	2.17955	2.22640	1.61275
Be	1.09359	-0.39077	-0.86261
C	-0.60236	2.45757	0.17466
H	-1.05131	1.81850	0.95577
H	-0.33487	3.43108	0.62150
H	-1.34840	2.64095	-0.61517
C	3.15232	-1.94936	0.03676
H	4.20902	-1.76584	-0.23879

H	3.14387	-2.42463	1.03826
H	2.74300	-2.68059	-0.67961
N	2.36081	-0.74041	0.00759
P	0.91403	1.69279	-0.55255
C	-0.98356	-0.58889	-0.43159
C	-1.05583	-1.13075	0.84452
C	-2.06781	-0.08022	-1.13050
H	-0.17911	-1.55515	1.33789
H	-1.95681	0.27722	-2.15652
C	-2.29221	-1.04661	1.49176
C	-3.28462	-0.01584	-0.45515
H	-2.37719	-1.42968	2.51299
H	-4.15376	0.40784	-0.96665
C	-3.40294	-0.49463	0.85307
H	-4.36431	-0.44483	1.36989
F	0.07684	-1.37775	-1.51392

3.3aF

C	2.45150	-0.10941	0.52299
C	2.02824	1.17423	0.43462
H	3.37511	-0.31992	1.08583
H	2.59547	1.95117	0.95708
Be	0.31091	-1.37719	-0.39771
C	0.18621	3.28358	0.13307
H	-0.00239	3.16415	1.21348
H	0.98871	4.02717	-0.01393
H	-0.72547	3.66651	-0.35504
C	2.65569	-2.40108	-0.12155
H	3.15154	-2.64372	0.83908
H	2.03842	-3.26784	-0.40921
H	3.44159	-2.28192	-0.89158
N	1.82396	-1.20925	-0.00454
P	0.69496	1.68951	-0.67049
C	-0.72364	0.63019	-0.10049
C	-0.77744	-0.00005	1.15949
C	-1.82664	0.48986	-0.96543
C	-1.90028	-0.74911	1.53254
C	-2.95018	-0.23135	-0.57968
C	-2.98605	-0.85705	0.66904
H	0.06135	0.12381	1.85357
H	-1.78676	0.95089	-1.95774
H	-1.92038	-1.24513	2.50674
H	-3.79645	-0.32819	-1.26494
H	-3.85984	-1.44630	0.96036
F	-0.54901	-2.34430	-0.99460

3.4aF

C	2.29392	-1.42948	0.07783
C	1.13046	-1.46824	0.80890
H	2.89806	-2.34670	-0.00813
H	0.80299	-2.37723	1.31794
Be	1.90009	1.03718	-0.39019
C	0.00000	0.58567	2.59128
H	-0.59999	-0.18118	3.10856
H	0.97016	0.69786	3.10236
H	-0.53506	1.54897	2.62808
C	4.00702	-0.43922	-1.28941
H	4.85781	-0.71168	-0.63486
H	3.94379	-1.19081	-2.09991
H	4.24206	0.53150	-1.75385
N	2.76314	-0.32806	-0.55119
P	0.30522	0.09723	0.84925
C	-1.37097	-0.03858	0.13356
C	-1.90572	-1.26811	-0.26405
C	-2.12515	1.12910	-0.04823
H	-1.31292	-2.18013	-0.14760
H	-1.70624	2.10247	0.22949
C	-3.18448	-1.33168	-0.81870
C	-3.40334	1.06334	-0.59847
H	-3.59528	-2.29742	-1.12683
H	-3.98186	1.98081	-0.73859
C	-3.93566	-0.16842	-0.98272
H	-4.93667	-0.22008	-1.42050
F	2.04399	2.39184	-0.82620

3.2b

C	-0.91997	0.93629	1.41139
C	-2.02780	0.16009	1.38411
H	-0.40577	1.20577	2.34522
H	-2.42032	-0.24357	2.32563
Be	-1.16162	0.62186	-0.98271
C	-2.98994	-1.89286	-0.42576
H	-1.99601	-2.37092	-0.40121
H	-3.62234	-2.36071	0.34865
H	-3.45074	-2.11074	-1.40452
C	0.38815	2.62160	0.26032
H	-0.23538	3.44357	0.65763
H	1.29139	2.53149	0.89687
H	0.71506	2.91065	-0.75181

N	-0.35076	1.38252	0.20982
P	-2.96893	-0.03418	-0.19421
C	1.13500	-0.06177	-0.49447
C	2.34022	0.53059	-0.82102
C	1.00535	-1.20693	0.27005
H	2.38959	1.38775	-1.49407
H	0.02545	-1.64673	0.47265
C	3.49049	-0.01614	-0.24500
C	2.17262	-1.72833	0.82820
H	4.45890	0.44278	-0.46436
H	2.10128	-2.61536	1.46430
C	3.41392	-1.13692	0.58146
H	4.32089	-1.56057	1.01928
F	0.04617	0.01117	-1.79274

3.4b

C	-0.75259	0.10444	-1.63445
C	-1.85259	-0.61735	-1.38723
H	-0.31633	0.26325	-2.62903
H	-2.37537	-1.05520	-2.24793
Be	-1.05798	0.51088	0.97092
C	-4.09492	-0.35947	0.39425
H	-4.45419	-0.45333	1.43323
H	-4.18344	0.69725	0.09248
H	-4.75910	-0.96869	-0.24315
C	-0.03278	2.22941	-0.77812
H	0.57108	2.48496	-1.66763
H	-1.07127	2.55263	-0.94663
H	0.35514	2.74830	0.11015
N	-0.04982	0.77370	-0.54236
P	-2.34881	-1.02162	0.32843
C	1.24912	0.17696	-0.25849
C	1.30999	-1.20781	-0.05221
C	2.41253	0.94037	-0.14438
H	0.40534	-1.81606	-0.13837
H	2.39753	2.02011	-0.29297
C	2.52193	-1.81437	0.26171
C	3.62370	0.32132	0.16926
H	2.55201	-2.89536	0.42257
H	4.52725	0.93131	0.25475
C	3.68644	-1.05384	0.37277
H	4.63760	-1.53285	0.61922
F	-0.76650	1.39672	2.06234

2.1aCl

C	3.40817	0.62812	0.18137
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C	2.71788	1.77445	-0.02428
H	4.48498	0.63501	0.41049
H	3.23747	2.73718	0.02992
Be	1.31017	-0.38123	-0.26433
C	0.00296	2.14649	0.96028
H	0.36112	1.65976	1.88336
H	0.06896	3.23976	1.09959
H	-1.06309	1.89385	0.81430
C	3.60914	-1.78816	0.37625
H	4.41420	-1.92339	-0.37430
H	4.08986	-1.73896	1.37398
H	2.98761	-2.69993	0.35723
N	2.79638	-0.62871	0.10682
P	0.96495	1.63870	-0.57554
C	-1.62670	-0.96664	-0.16728
C	-2.26047	-0.98281	1.06760
C	-2.04664	-0.17478	-1.22781
H	-1.88872	-1.61167	1.87909
H	-1.50360	-0.16901	-2.17448
C	-3.37535	-0.16233	1.24123
C	-3.16097	0.63939	-1.03077
H	-3.88877	-0.15292	2.20613
H	-3.50261	1.28257	-1.84561
C	-3.82338	0.64640	0.19712
H	-4.69171	1.29384	0.34377
Cl	-0.18019	-1.98009	-0.38253

2.2aCl

C	2.56758	0.43049	1.09549
C	2.09341	1.67061	0.77315
H	3.27871	0.27856	1.92085
H	2.35913	2.54861	1.36991
Be	1.01872	-0.33796	-0.65615
C	-0.33279	2.76800	-0.34169
H	-0.92831	2.30483	0.46439
H	-0.02210	3.77793	-0.02149
H	-0.96577	2.87711	-1.23762
C	2.74034	-1.95281	0.74414
H	3.83227	-1.97703	0.56229
H	2.57247	-2.20536	1.81121
H	2.28316	-2.75054	0.13675
N	2.15531	-0.67793	0.39956
P	1.15409	1.75049	-0.75015
C	-1.02829	-0.57817	-0.26829
C	-1.12799	-1.05933	1.04015

C	-2.07121	0.11577	-0.88639
H	-0.32172	-1.64046	1.49084
H	-1.98936	0.42559	-1.93079
C	-2.26822	-0.72884	1.77378
C	-3.20005	0.42226	-0.13293
H	-2.34216	-1.06423	2.81242
H	-4.01165	0.98889	-0.59873
C	-3.30434	0.00651	1.19744
H	-4.19812	0.24614	1.77901
Cl	-0.02533	-1.79630	-1.61460

2.4aCl

C	1.94554	-1.88894	-0.21842
C	0.76145	-1.96864	0.47307
H	2.45503	-2.81958	-0.51377
H	0.32100	-2.92735	0.75412
Be	1.81855	0.63600	-0.09064
C	-0.17909	-0.23703	2.67263
H	-0.89076	-1.01045	3.00530
H	0.78068	-0.36991	3.19791
H	-0.58535	0.75812	2.91761
C	3.79021	-0.79970	-1.31436
H	4.56606	-1.37553	-0.77394
H	3.64684	-1.26427	-2.30894
H	4.18005	0.21775	-1.47389
N	2.54925	-0.72576	-0.56521
P	0.11410	-0.36842	0.86802
C	-1.53747	-0.12958	0.12764
C	-2.18878	-1.15781	-0.56095
C	-2.15100	1.12655	0.23121
H	-1.70327	-2.13251	-0.66581
H	-1.63811	1.95045	0.73940
C	-3.44675	-0.93842	-1.12309
C	-3.40898	1.34181	-0.32726
H	-3.94994	-1.74836	-1.65903
H	-3.87997	2.32514	-0.24236
C	-4.05960	0.30813	-1.00301
H	-5.04515	0.47863	-1.44570
Cl	2.22114	2.47307	-0.23394

2.3bCl

C	-0.91296	0.65479	1.61872
C	-2.08346	-0.00566	1.54494
H	-0.34604	0.80042	2.54727

H	-2.49168	-0.45277	2.46093
Be	-1.25810	0.57634	-0.86400
C	-3.22380	-1.84734	-0.35626
H	-3.71028	-1.97278	-1.33860
H	-2.26165	-2.38589	-0.37701
H	-3.87714	-2.31542	0.40025
C	0.09243	2.56542	0.51113
H	0.89607	2.68028	1.26093
H	0.46371	2.90641	-0.46835
H	-0.75997	3.20294	0.80346
N	-0.35070	1.18235	0.41995
P	-3.06375	-0.01377	-0.01955
C	1.18697	0.10722	-0.12565
C	2.40443	0.78086	-0.20961
C	1.11044	-1.18256	0.40102
H	2.46144	1.80616	-0.57985
H	0.14045	-1.66573	0.54762
C	3.57405	0.08647	0.10596
C	2.29117	-1.85428	0.70804
H	4.53403	0.60038	-0.00237
H	2.23043	-2.87757	1.09072
C	3.53161	-1.23189	0.55657
H	4.45389	-1.76333	0.80333
Cl	0.22853	0.15432	-2.05105

3.4b

C	0.66547	-1.19852	1.41987
C	1.75980	-1.64143	0.79029
H	0.19609	-1.68521	2.28415
H	2.24539	-2.54138	1.19007
Be	1.03086	0.72759	-0.35542
C	4.04568	-0.36281	-0.41835
H	4.40015	0.24899	-1.26528
H	4.14229	0.23420	0.50333
H	4.70540	-1.24452	-0.34397
C	0.00771	0.99753	2.11173
H	-0.63325	0.63621	2.93565
H	1.04221	1.09283	2.47439
H	-0.33323	1.98337	1.76476
N	0.01150	0.03832	0.98789
P	2.29314	-0.89026	-0.79228
C	-1.29626	-0.20236	0.38161
C	-1.39426	-1.18212	-0.61490
C	-2.42442	0.54344	0.72716
H	-0.51656	-1.77010	-0.89660

H	-2.37911	1.32006	1.49010
C	-2.61032	-1.40985	-1.25169
C	-3.63946	0.30524	0.08336
H	-2.66975	-2.17614	-2.02910
H	-4.51529	0.89706	0.36349
C	-3.74028	-0.66913	-0.90509
H	-4.69453	-0.84910	-1.40699
Cl	0.71572	2.52642	-0.85985

3.1aBr

C	3.47397	0.94084	0.15198
C	2.75671	2.06180	-0.09599
H	4.55538	0.97999	0.35448
H	3.25860	3.03535	-0.10461
Be	1.38391	-0.13140	-0.18783
C	0.05569	2.44439	0.92354
H	0.43633	2.01278	1.86480
H	0.11026	3.54440	1.00188
H	-1.00927	2.17130	0.81081
C	3.72772	-1.45631	0.46787
H	4.52554	-1.60816	-0.28724
H	4.22026	-1.35145	1.45558
H	3.12754	-2.38229	0.49925
N	2.88516	-0.32905	0.15752
P	0.99607	1.86459	-0.59937
C	-1.68280	-0.67718	-0.07574
C	-2.36208	-0.60632	1.13447
C	-2.02505	0.09535	-1.17941
H	-2.05881	-1.21794	1.98710
H	-1.45443	0.03820	-2.10820
C	-3.43368	0.28141	1.23663
C	-3.09720	0.97806	-1.05466
H	-3.97679	0.35884	2.18216
H	-3.37320	1.60563	-1.90586
C	-3.79920	1.07146	0.14713
H	-4.63260	1.77300	0.23770
Br	-0.17389	-1.85430	-0.20810

3.2aBr

C	2.65044	0.69383	1.17018
C	2.43710	1.81786	0.42012
H	3.32883	0.69678	2.03598
H	2.89717	2.77169	0.69618
Be	0.95835	-0.30392	-0.31364

C	0.27202	2.90635	-1.17720
H	-0.47669	2.81312	-0.37006
H	0.76766	3.88890	-1.09122
H	-0.24664	2.87280	-2.14978
C	2.28511	-1.63526	1.68859
H	3.36973	-1.81653	1.81058
H	1.84757	-1.52734	2.70407
H	1.84530	-2.53632	1.23119
N	2.01439	-0.48164	0.86486
P	1.52377	1.55027	-1.09502
C	-1.07516	-0.19488	0.05791
C	-1.27041	-0.35995	1.43492
C	-1.95793	0.56785	-0.71622
H	-0.61092	-1.00047	2.02404
H	-1.82469	0.64156	-1.79808
C	-2.30273	0.34561	2.05109
C	-2.98708	1.25382	-0.07891
H	-2.43669	0.25108	3.13257
H	-3.66055	1.87526	-0.67642
C	-3.16267	1.15145	1.30359
H	-3.97816	1.68830	1.79502
Br	-0.31271	-1.95902	-0.98979

3.4aBr

C	1.14478	2.54815	0.31382
C	-0.04421	2.42453	-0.36187
H	1.45914	3.54323	0.66569
H	-0.67862	3.28703	-0.57567
Be	1.52952	0.06538	0.03323
C	-0.63900	0.66755	-2.66429
H	-1.50681	1.28595	-2.94718
H	0.26013	1.03576	-3.18456
H	-0.82366	-0.37653	-2.96622
C	3.20813	1.79982	1.30389
H	3.87549	2.47379	0.73296
H	3.01066	2.26317	2.28935
H	3.75295	0.85899	1.47911
N	1.98083	1.51350	0.58298
P	-0.35203	0.75176	-0.85626
C	-1.89805	0.11612	-0.12510
C	-2.75946	0.93564	0.61120
C	-2.20702	-1.24178	-0.28551
H	-2.51114	1.99052	0.76056
H	-1.52387	-1.90116	-0.83179
C	-3.92623	0.40695	1.16451

C	-3.37503	-1.76573	0.26377
H	-4.59435	1.05329	1.74077
H	-3.60684	-2.82661	0.13484
C	-4.23704	-0.94086	0.98825
H	-5.15104	-1.35384	1.42454
Br	2.33524	-1.80481	0.07588

3.2bBr

C	-0.85186	-1.52671	1.49122
C	-1.90907	-1.84597	0.70320
H	-0.29441	-2.27512	2.07180
H	-2.21749	-2.89472	0.61799
Be	-1.27102	0.68320	0.50085
C	-3.00270	-0.79499	-1.80156
H	-3.55023	0.04007	-2.27101
H	-2.01957	-0.87793	-2.29625
H	-3.57099	-1.71947	-2.00268
C	0.39145	0.17345	2.68541
H	1.27313	-0.48662	2.80710
H	0.74793	1.20956	2.56258
H	-0.20070	0.12968	3.61886
N	-0.40345	-0.20939	1.54532
P	-2.93177	-0.47684	0.03669
C	1.18023	0.01618	-0.13761
C	2.43527	0.21442	0.41125
C	0.88080	-0.96486	-1.06457
H	2.64243	1.02905	1.10691
H	-0.12265	-1.08894	-1.47665
C	3.44144	-0.68220	0.03894
C	1.91049	-1.83937	-1.42119
H	4.44037	-0.55848	0.46788
H	1.69585	-2.63615	-2.13938
C	3.18595	-1.70673	-0.87226
H	3.98278	-2.39602	-1.16232
Br	0.08876	2.06147	-0.44207

3.4b

C	-0.59532	-2.00601	0.98347
C	-1.82782	-2.14250	0.48163
H	0.01879	-2.82434	1.37941
H	-2.25462	-3.15363	0.44997
Be	-1.06675	0.46723	0.15164
C	-3.17939	-0.98896	-1.78342
H	-3.63389	-0.07395	-2.19984

H	-2.28572	-1.23237	-2.38184
H	-3.91424	-1.80538	-1.89092
C	0.09747	-0.20524	2.43552
H	0.76190	-0.84306	3.04496
H	0.44817	0.83782	2.46040
H	-0.92067	-0.24808	2.85137
N	0.03777	-0.68577	1.03762
P	-2.81912	-0.67273	0.02344
C	1.31528	-0.69324	0.33291
C	2.47801	-0.14910	0.87676
C	1.34172	-1.23326	-0.95830
H	2.48654	0.29163	1.87349
H	0.43013	-1.65949	-1.38578
C	3.65827	-0.15082	0.13129
C	2.52199	-1.22991	-1.69393
H	4.56321	0.28122	0.56710
H	2.52729	-1.65294	-2.70203
C	3.68825	-0.68942	-1.15143
H	4.61610	-0.68525	-1.72944
Br	-0.38698	2.36345	-0.18529

3.1al

C	3.56519	1.21582	0.14380
C	2.82439	2.31325	-0.13648
H	4.64658	1.28331	0.33863
H	3.30621	3.29608	-0.17889
Be	1.49273	0.08899	-0.14667
C	0.13138	2.69527	0.88960
H	0.52407	2.30161	1.84232
H	0.17993	3.79780	0.92503
H	-0.93258	2.41158	0.79745
C	3.86955	-1.16170	0.54028
H	4.66786	-1.32304	-0.21235
H	4.36321	-1.01242	1.52176
H	3.29025	-2.09921	0.60734
N	3.00153	-0.06455	0.19497
P	1.06412	2.06687	-0.61788
C	-1.77803	-0.38635	-0.04186
C	-2.49832	-0.28373	1.14493
C	-2.03778	0.42618	-1.14206
H	-2.27081	-0.92047	2.00307
H	-1.44438	0.35381	-2.05570
C	-3.51597	0.66763	1.22552
C	-3.05749	1.37261	-1.04044
H	-4.08546	0.76573	2.15365

H	-3.26327	2.02775	-1.89087
C	-3.79457	1.49358	0.13718
H	-4.58650	2.24366	0.20978
I	-0.18092	-1.77639	-0.14894

3.2al

C	2.92581	-0.82610	1.06123
C	3.38904	0.01076	0.08438
H	3.58299	-1.20142	1.85979
H	4.41899	0.38078	0.11088
Be	0.76288	-0.52578	-0.07228
C	2.20364	2.13162	-1.51497
H	1.74462	2.63800	-0.64722
H	3.22143	2.53233	-1.66348
H	1.61446	2.36841	-2.41693
C	1.20275	-2.19148	2.07136
H	1.36513	-3.23174	1.72471
H	1.75388	-2.06411	3.02278
H	0.12551	-2.08952	2.28982
N	1.60939	-1.21520	1.09043
P	2.25675	0.29446	-1.27783
C	-0.79574	0.74873	0.19581
C	-0.96007	0.96865	1.57173
C	-1.01132	1.78899	-0.72166
H	-0.83977	0.15185	2.28719
H	-0.92783	1.60344	-1.79554
C	-1.23523	2.25713	2.02614
C	-1.29595	3.06520	-0.24963
H	-1.32628	2.43493	3.10146
H	-1.43393	3.88020	-0.96609
C	-1.40517	3.30659	1.12284
H	-1.63320	4.31192	1.48666
I	-1.47059	-1.37892	-0.57460

3.4al

C	-0.25346	2.94224	-0.39165
C	0.88760	2.60689	0.29246
H	-0.36359	3.96611	-0.78141
H	1.68064	3.33319	0.48078
Be	-1.12398	0.60194	-0.02212
C	1.14418	0.83017	2.64502
H	2.12257	1.26879	2.90136
H	0.34518	1.38418	3.16433
H	1.12154	-0.22253	2.97215

C	-2.41695	2.58465	-1.38545
H	-2.86415	3.48330	-0.91932
H	-2.13716	2.83812	-2.42598
H	-3.19552	1.80725	-1.42959
N	-1.28476	2.08720	-0.62434
P	0.85560	0.92100	0.83879
C	2.21987	-0.04670	0.11268
C	3.32808	0.56319	-0.48448
C	2.13796	-1.44533	0.15248
H	3.38638	1.65410	-0.54237
H	1.25826	-1.93173	0.58811
C	4.35193	-0.21795	-1.02018
C	3.16421	-2.22285	-0.38051
H	5.21572	0.26421	-1.48664
H	3.09075	-3.31348	-0.34920
C	4.27291	-1.60952	-0.96522
H	5.07577	-2.22011	-1.38824
I	-2.39810	-1.26516	-0.00675

3.2bl

C	-0.80990	-1.93113	0.95434
C	-2.01079	-2.06800	0.36015
H	-0.15713	-2.78410	1.18719
H	-2.35289	-3.07393	0.08618
Be	-1.43306	0.41215	0.69876
C	-3.32227	-0.42977	-1.65295
H	-3.86864	0.50720	-1.85632
H	-2.36307	-0.39888	-2.19627
H	-3.92569	-1.26072	-2.05680
C	0.32162	-0.54543	2.56105
H	1.17827	-1.24029	2.64042
H	0.69584	0.47927	2.72992
H	-0.40251	-0.78531	3.35969
N	-0.29774	-0.64122	1.24888
P	-3.15316	-0.61753	0.20364
C	1.07905	-0.16606	-0.05370
C	2.36898	-0.26530	0.52623
C	0.83544	-0.94303	-1.22004
H	2.66589	0.41185	1.33096
H	-0.09994	-0.82064	-1.77274
C	3.26464	-1.24298	0.09428
C	1.74625	-1.90447	-1.63107
H	4.23538	-1.31369	0.59574
H	1.49767	-2.51269	-2.50664
C	2.96481	-2.08853	-0.97079

H	3.68102	-2.83984	-1.31121
I	0.29627	1.83477	-0.16277

3.4bl

C	-0.24972	-2.48205	0.83262
C	-1.46784	-2.72823	0.33792
H	0.47113	-3.24580	1.14902
H	-1.76558	-3.77879	0.22275
Be	-1.03636	-0.03272	0.21574
C	-3.03660	-1.56721	-1.78256
H	-3.64667	-0.70229	-2.09400
H	-2.14612	-1.61192	-2.43126
H	-3.64016	-2.47739	-1.94153
C	0.23099	-0.74030	2.43233
H	0.96605	-1.35231	2.98399
H	0.46554	0.32850	2.55122
H	-0.77324	-0.93105	2.84035
N	0.21530	-1.10046	0.99654
P	-2.64478	-1.35983	0.03246
C	1.48094	-0.89675	0.29751
C	2.57872	-0.27982	0.89498
C	1.55682	-1.30554	-1.03908
H	2.54531	0.05994	1.93003
H	0.69520	-1.78900	-1.50769
C	3.74485	-0.07426	0.15574
C	2.72219	-1.09544	-1.76819
H	4.59917	0.41347	0.63290
H	2.76691	-1.41419	-2.81306
C	3.82359	-0.47924	-1.17316
H	4.73937	-0.31257	-1.74622
I	-0.59001	2.16864	-0.06096

4.1aF

C	2.67250	1.73779	-0.05443
C	3.47570	0.66425	0.12665
H	2.96607	2.79036	-0.06005
H	4.55616	0.70441	0.29647
Be	1.35481	-0.07305	-0.19048
C	3.53109	-1.78550	0.26688
H	4.03004	-1.82745	1.25705
H	2.84865	-2.65050	0.20757
H	4.31603	-1.93177	-0.50372
N	2.79675	-0.56699	0.07626
O	1.35558	1.44450	-0.25496

C	-1.40880	-0.43171	-0.13749
C	-2.40072	-1.39245	-0.13474
C	-1.60727	0.92461	0.02599
H	-2.15623	-2.44735	-0.27347
H	-0.75719	1.61598	0.00823
C	-3.71013	-0.94831	0.05216
C	-2.92877	1.33824	0.21219
H	-4.52683	-1.67460	0.06219
H	-3.13597	2.40281	0.34792
C	-3.97219	0.41188	0.22562
H	-5.00031	0.75259	0.37228
F	-0.09890	-0.90469	-0.32707

4.2aF

C	2.17290	-1.37951	-0.71264
C	1.94075	-1.14375	0.66190
H	2.54982	-2.33388	-1.11115
H	2.00011	-1.90409	1.44697
Be	1.18831	0.81946	-0.66972
C	1.16010	0.55837	2.18778
H	0.60780	-0.18389	2.78939
H	2.12253	0.78218	2.67943
H	0.57620	1.48636	2.12255
N	1.44551	0.07437	0.85388
O	1.85932	-0.45548	-1.51009
C	-0.55263	0.11579	-0.08600
C	-1.44825	1.18243	-0.01369
C	-0.99976	-1.18988	-0.11177
H	-1.08848	2.21612	0.01095
H	-0.27567	-2.02130	-0.10582
C	-2.82069	0.91287	-0.02503
C	-2.36864	-1.46214	-0.13637
H	-3.53600	1.74037	0.00981
H	-2.72644	-2.49551	-0.17650
C	-3.27904	-0.40399	-0.08884
H	-4.35369	-0.60836	-0.09083
F	1.28322	2.22514	-0.98271

4.5aF

C	2.38954	-1.34586	-0.62936
C	1.47329	-1.44017	0.35540
H	3.00817	-2.19393	-0.95103
H	1.25592	-2.32181	0.96139
Be	1.70276	0.87339	-0.55575

C	1.00637	0.28644	1.99963
H	2.09072	0.32823	2.18596
H	0.58075	1.29200	2.13064
H	0.53703	-0.40879	2.71823
N	0.78678	-0.18278	0.61165
O	2.57711	-0.19474	-1.24574
C	-0.62938	-0.14891	0.24529
C	-1.26622	1.09373	0.15223
C	-1.34492	-1.31631	-0.02127
H	-0.69730	2.01237	0.31581
H	-0.84985	-2.28712	0.02235
C	-2.61483	1.15983	-0.18773
C	-2.69556	-1.24008	-0.36406
H	-3.10015	2.13652	-0.26542
H	-3.24702	-2.16110	-0.57288
C	-3.33655	-0.00624	-0.44377
H	-4.39467	0.04905	-0.71356
F	1.55450	2.29375	-0.50693

4.2bF

C	1.43912	-0.99948	-1.51450
C	2.18383	-1.16836	-0.33674
H	1.24039	-1.77020	-2.26466
H	2.77151	-2.06800	-0.11357
Be	1.10244	1.00449	-0.16053
C	2.69151	-0.20027	1.82212
H	3.40881	-1.03463	1.91466
H	3.22035	0.74930	2.00674
H	1.92003	-0.31138	2.60478
N	2.07157	-0.16916	0.51888
O	0.78908	0.12604	-1.56208
C	-0.76298	0.10920	-0.30379
C	-1.67224	1.15469	-0.26340
C	-1.08442	-1.19018	0.00436
H	-1.38607	2.17164	-0.54521
H	-0.33923	-1.98998	-0.13720
C	-2.96154	0.86548	0.19978
C	-2.36688	-1.46820	0.47942
H	-3.70287	1.66771	0.26420
H	-2.64284	-2.49087	0.75398
C	-3.30396	-0.43499	0.57403
H	-4.31693	-0.65050	0.92550
F	1.06987	2.43082	0.01441

4.5bF

C	1.01383	-1.46142	-0.56780
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C	2.32753	-1.30886	-0.30895
H	0.45959	-2.28050	-1.01884
H	3.03615	-2.13490	-0.43761
Be	1.53737	0.94288	0.08225
C	4.14060	0.11342	0.44782
H	4.82669	-0.20270	-0.36227
H	4.32914	1.18115	0.64258
H	4.41658	-0.44538	1.36406
N	2.75427	-0.07189	0.08811
O	0.33630	-0.22649	-0.41280
C	-1.02940	-0.17043	-0.18249
C	-1.68241	1.01066	-0.52844
C	-1.71240	-1.24002	0.38976
H	-1.11102	1.83747	-0.95485
H	-1.17747	-2.14628	0.68118
C	-3.05182	1.11348	-0.29985
C	-3.08696	-1.12256	0.60264
H	-3.56986	2.03920	-0.56480
H	-3.63032	-1.95844	1.05205
C	-3.76016	0.04815	0.25968
H	-4.83604	0.13468	0.43245
F	1.13154	2.29164	0.29427

4.2c

C	-2.01379	-1.61844	-0.86589
C	-2.59562	-0.39495	-0.99806
H	-2.19565	-2.49753	-1.49148
H	-3.33726	-0.12293	-1.75596
Be	-1.03090	-0.29929	0.71438
C	-2.58457	1.88894	-0.11720
H	-2.14682	2.44387	-0.97665
H	-3.68620	1.97114	-0.20565
H	-2.29192	2.42046	0.80514
N	-2.14698	0.52539	-0.05731
O	-1.11726	-1.72090	0.12900
C	0.99954	0.07699	0.66221
C	1.26044	1.33108	0.16069
C	1.74747	-1.07012	0.53661
H	0.63214	2.19295	0.38845
H	1.46302	-2.00228	1.02465
C	2.35395	1.39456	-0.70776
C	2.83091	-0.95862	-0.33579
H	2.59758	2.34771	-1.18445
H	3.44632	-1.84120	-0.52958
C	3.12915	0.25972	-0.95506

H	3.98473	0.32631	-1.63147
F	-0.12670	0.06589	1.97669

4.3cF

C	2.23127	-1.13639	-1.17780
C	2.33792	-1.12302	0.30873
H	2.63274	-1.98255	-1.76730
H	2.79699	-1.94837	0.87320
Be	0.85929	0.93370	-0.40941
C	1.72563	0.13427	2.24838
H	2.21331	-0.65862	2.84158
H	2.17935	1.11570	2.46374
H	0.65493	0.20238	2.50485
N	1.81048	-0.09292	0.83186
O	1.67027	-0.20382	-1.71505
C	-0.77492	0.29685	-0.21796
C	-1.83511	1.21684	-0.11922
C	-1.12058	-1.05958	-0.12849
H	-1.62251	2.29028	-0.18638
H	-0.33948	-1.83476	-0.19807
C	-3.15904	0.80566	0.05724
C	-2.43724	-1.49253	0.04553
H	-3.95858	1.55062	0.12735
H	-2.66389	-2.56221	0.10743
C	-3.46424	-0.55298	0.14065
H	-4.49978	-0.87985	0.27838
F	1.34578	2.30211	-0.49468

4.4cF

C	2.17290	-1.37951	-0.71264
C	1.94075	-1.14375	0.66190
H	2.54982	-2.33388	-1.11115
H	2.00011	-1.90409	1.44697
Be	1.18831	0.81946	-0.66972
C	1.16010	0.55837	2.18778
H	0.60780	-0.18389	2.78939
H	2.12253	0.78218	2.67943
H	0.57620	1.48636	2.12255
N	1.44551	0.07437	0.85388
O	1.85932	-0.45548	-1.51009
C	-0.55263	0.11579	-0.08600
C	-1.44825	1.18243	-0.01369
C	-0.99976	-1.18988	-0.11177
H	-1.08848	2.21612	0.01095

H	-0.27567	-2.02130	-0.10582
C	-2.82069	0.91287	-0.02503
C	-2.36864	-1.46214	-0.13637
H	-3.53600	1.74037	0.00981
H	-2.72644	-2.49551	-0.17650
C	-3.27904	-0.40399	-0.08884
H	-4.35369	-0.60836	-0.09083
F	1.28322	2.22514	-0.98271

4.4dF

C	1.43912	-0.99948	-1.51450
C	2.18383	-1.16836	-0.33674
H	1.24039	-1.77020	-2.26466
H	2.77151	-2.06800	-0.11357
Be	1.10244	1.00449	-0.16053
C	2.69151	-0.20027	1.82212
H	3.40881	-1.03463	1.91466
H	3.22035	0.74930	2.00674
H	1.92003	-0.31138	2.60478
N	2.07157	-0.16916	0.51888
O	0.78908	0.12604	-1.56208
C	-0.76298	0.10920	-0.30379
C	-1.67224	1.15469	-0.26340
C	-1.08442	-1.19018	0.00436
H	-1.38607	2.17164	-0.54521
H	-0.33923	-1.98998	-0.13720
C	-2.96154	0.86548	0.19978
C	-2.36688	-1.46820	0.47942
H	-3.70287	1.66771	0.26420
H	-2.64284	-2.49087	0.75398
C	-3.30396	-0.43499	0.57403
H	-4.31693	-0.65050	0.92550
F	1.06987	2.43082	0.01441

4.1aCl

C	2.68091	1.83017	-0.25493
C	3.46027	0.88825	0.32541
H	2.91164	2.88986	-0.38863
H	4.45362	1.06058	0.75111
Be	1.53896	-0.10060	-0.37472
C	3.58792	-1.47960	0.95761
H	3.79240	-1.29233	2.03158
H	2.99016	-2.40467	0.89328
H	4.56157	-1.68061	0.46587

N	2.87938	-0.39258	0.34229
O	1.48507	1.37749	-0.72552
C	-1.58269	-0.45429	-0.22876
C	-2.72245	-1.20509	0.03321
C	-1.52456	0.92613	-0.09521
H	-2.72080	-2.29073	-0.08685
H	-0.59908	1.47413	-0.30951
C	-3.86645	-0.52834	0.45492
C	-2.68328	1.57692	0.33311
H	-4.77689	-1.09469	0.66836
H	-2.66580	2.66351	0.45201
C	-3.84702	0.85868	0.60605
H	-4.74670	1.38240	0.93974
Cl	-0.14165	-1.35611	-0.78226

4.2aCl

C	-2.59153	1.34890	-0.30441
C	-1.83302	0.75452	-1.25796
H	-3.19148	2.25159	-0.47231
H	-1.70897	1.08136	-2.29225
Be	-1.61499	-0.34583	0.88060
C	-1.17968	-1.57984	-1.62215
H	-0.57868	-1.40945	-2.53300
H	-0.77759	-2.44522	-1.07366
H	-2.21842	-1.80552	-1.91637
N	-1.18734	-0.41128	-0.75897
O	-2.61557	0.82481	0.91700
C	0.60194	-0.09365	-0.16844
C	0.84521	1.23527	0.14739
C	1.59628	-0.94004	-0.64188
H	0.02424	1.91907	0.38221
H	1.37810	-1.95359	-0.98110
C	2.17102	1.66344	0.20847
C	2.91543	-0.48974	-0.57759
H	2.38436	2.69394	0.50712
H	3.71923	-1.16200	-0.89206
C	3.21177	0.80124	-0.13817
H	4.24871	1.14416	-0.09651
Cl	-0.11812	-1.10890	1.76181

4.5aCl

C	-1.95727	-1.97976	-0.52103
C	-1.01688	-1.89549	0.43933
H	-2.42152	-2.92661	-0.82479

H	-0.60700	-2.71484	1.03336
Be	-1.66383	0.32909	-0.49173
C	-0.87579	-0.11733	2.07094
H	-0.23414	-0.66729	2.78144
H	-0.73030	0.96419	2.19745
H	-1.93200	-0.35305	2.27046
N	-0.56826	-0.52966	0.67988
O	-2.36165	-0.88346	-1.13769
C	0.81833	-0.25599	0.29508
C	1.59252	-1.23515	-0.33025
C	1.36228	1.01551	0.51334
H	1.16878	-2.22032	-0.52887
H	0.76019	1.81168	0.95360
C	2.90337	-0.95095	-0.71416
C	2.67190	1.28890	0.12830
H	3.49703	-1.72912	-1.20193
H	3.08061	2.28830	0.30051
C	3.45195	0.30727	-0.48241
H	4.47976	0.52657	-0.78352
Cl	-1.83750	2.20102	-0.48726

4.5bCl

C	1.22698	-1.51430	-0.99057
C	2.39702	-1.35720	-0.32477
H	0.81373	-2.40220	-1.46638
H	3.10257	-2.17968	-0.15848
Be	1.45422	0.78159	-0.32798
C	3.87696	0.13880	0.90511
H	4.79583	-0.21279	0.39701
H	3.99797	1.21630	1.09870
H	3.81674	-0.37079	1.88726
N	2.69885	-0.07961	0.10184
O	0.57925	-0.30787	-1.17810
C	-0.96257	-0.00683	-0.26730
C	-2.03287	0.27336	-1.09475
C	-1.04459	-0.69930	0.92392
H	-1.88026	0.71850	-2.07908
H	-0.14396	-1.00956	1.46063
C	-3.30206	0.02032	-0.57312
C	-2.32810	-0.93821	1.42043
H	-4.18162	0.27157	-1.17317
H	-2.43946	-1.43872	2.38659
C	-3.45516	-0.56857	0.68498
H	-4.45503	-0.76638	1.07909
Cl	0.05747	1.99878	0.14636

4.5bCl

C	0.79610	-1.78673	-0.52080
C	2.12438	-1.72605	-0.30846
H	0.14756	-2.58047	-0.88251
H	2.76531	-2.60846	-0.41193
Be	1.50342	0.58570	0.01959
C	4.06097	-0.39174	0.30164
H	4.68513	-0.71998	-0.55238
H	4.30674	0.66176	0.50820
H	4.35677	-0.98451	1.18939
N	2.64909	-0.50376	0.01633
O	0.22123	-0.49399	-0.39776
C	-1.14492	-0.34628	-0.18638
C	-1.78368	0.71732	-0.81522
C	-1.83078	-1.22594	0.64561
H	-1.20943	1.39285	-1.45197
H	-1.29793	-2.04199	1.13983
C	-3.14761	0.90187	-0.59975
C	-3.19863	-1.03442	0.84121
H	-3.65803	1.73872	-1.08405
H	-3.74890	-1.71865	1.49286
C	-3.85879	0.02662	0.22226
H	-4.92969	0.17470	0.38400
Cl	1.18548	2.41257	0.30455

4.2cCl

C	2.27600	-0.45599	1.66019
C	2.27590	-1.33073	0.59653
H	2.64943	-0.67259	2.66683
H	2.61788	-2.36974	0.62956
Be	1.25798	0.66426	-0.05062
C	1.53621	-1.56292	-1.71001
H	0.54937	-2.07374	-1.64979
H	1.53248	-0.93126	-2.61352
H	2.30965	-2.34227	-1.83667
N	1.77544	-0.76488	-0.54513
O	1.77854	0.73868	1.41261
C	-0.79183	0.42876	-0.12403
C	-1.43200	-0.31242	-1.11385
C	-1.30695	0.57921	1.16301
H	-1.04756	-0.33936	-2.13558
H	-0.80457	1.20347	1.90328
C	-2.57657	-1.02622	-0.76060

C	-2.45496	-0.14503	1.48650
H	-3.07861	-1.63694	-1.51686
H	-2.85556	-0.07389	2.50208
C	-3.08748	-0.94935	0.53650
H	-3.99112	-1.50383	0.80286
Cl	0.22355	2.12799	-0.96707

4.3cCl

C	-1.93768	-1.55723	-1.25880
C	-2.04036	-1.69724	0.21892
H	-2.27804	-2.35705	-1.94151
H	-2.45288	-2.59134	0.70749
Be	-0.81065	0.52526	-0.30723
C	-1.52510	-0.54616	2.25895
H	-0.46234	-0.44055	2.53494
H	-2.03011	0.39669	2.52647
H	-1.97996	-1.40151	2.78662
N	-1.58276	-0.67990	0.82901
O	-1.45159	-0.52827	-1.68825
C	0.91149	0.19492	-0.18261
C	1.81912	1.25584	-0.01200
C	1.45955	-1.09719	-0.21311
H	1.44103	2.28420	0.01850
H	0.80269	-1.97239	-0.34371
C	3.19291	1.03754	0.11888
C	2.82990	-1.33525	-0.08619
H	3.87197	1.88678	0.24835
H	3.21933	-2.35830	-0.12013
C	3.70330	-0.26037	0.08185
H	4.77901	-0.43453	0.18423
Cl	-1.73264	2.22960	-0.18970

4.4cCl

C	-1.67769	-1.92720	-0.85511
C	-1.38775	-1.88546	0.52432
H	-1.87666	-2.85631	-1.40957
H	-1.22239	-2.75951	1.16128
Be	-1.21662	0.38468	-0.43894
C	-0.92088	-0.32762	2.31538
H	-0.18351	-1.01242	2.76777
H	-0.57156	0.70915	2.40949
H	-1.88323	-0.42275	2.84672
N	-1.15772	-0.63327	0.91976
O	-1.64269	-0.82832	-1.47843

C	0.68797	0.03546	-0.02576
C	1.39086	-1.09719	-0.38822
C	1.35199	1.21836	0.29974
H	0.85887	-2.04530	-0.56705
H	0.79522	2.11302	0.59503
C	2.77976	-1.04966	-0.51706
C	2.74466	1.26494	0.18497
H	3.33533	-1.94017	-0.82599
H	3.27384	2.19497	0.41361
C	3.45592	0.13704	-0.22640
H	4.54578	0.17876	-0.30997
Cl	-1.85346	2.18525	-0.45927

4.4dCl

C	1.07727	-1.45943	-1.53152
C	1.83943	-1.73681	-0.38779
H	0.73424	-2.18730	-2.27157
H	2.31265	-2.70778	-0.19442
Be	1.09221	0.55774	-0.17111
C	2.60054	-0.84216	1.73314
H	3.13241	-1.80517	1.82574
H	3.32631	-0.01788	1.83165
H	1.88040	-0.75588	2.56534
N	1.90707	-0.73502	0.47134
O	0.60284	-0.24513	-1.55973
C	-0.89827	-0.01281	-0.30090
C	-1.68880	1.12516	-0.36417
C	-1.36862	-1.23758	0.11355
H	-1.29489	2.07361	-0.73841
H	-0.72747	-2.12994	0.03869
C	-2.99854	1.02647	0.11856
C	-2.66995	-1.32419	0.60867
H	-3.64391	1.90994	0.10449
H	-3.05794	-2.27991	0.97363
C	-3.48280	-0.18669	0.60986
H	-4.51038	-0.25414	0.97801
Cl	1.46153	2.40693	0.06785

4.1aBr

C	2.69941	2.03353	-0.41814
C	3.49901	1.20551	0.29400
H	2.90245	3.07079	-0.69592
H	4.48318	1.46458	0.69646
Be	1.60893	0.07340	-0.26814

C	3.68457	-1.04288	1.25663
H	3.88210	-0.69499	2.29112
H	3.10833	-1.98100	1.32993
H	4.66370	-1.29144	0.79865
N	2.95251	-0.07459	0.48946
O	1.52219	1.48537	-0.82703
C	-1.62723	-0.24822	-0.05805
C	-2.78828	-0.89643	0.35050
C	-1.52175	1.13334	-0.16079
H	-2.83467	-1.98575	0.42332
H	-0.58530	1.60934	-0.47659
C	-3.89795	-0.11486	0.67223
C	-2.64676	1.89166	0.17021
H	-4.82076	-0.60242	0.99782
H	-2.58819	2.98108	0.09951
C	-3.82781	1.27563	0.58228
H	-4.70080	1.88254	0.83727
Br	-0.12086	-1.35803	-0.51920

4.2aBr

C	-2.53993	-1.50477	-0.85112
C	-1.77083	-1.85683	0.20786
H	-3.11838	-2.21439	-1.45495
H	-1.61398	-2.86470	0.59694
Be	-1.64410	0.51718	-0.24983
C	-1.16088	-0.67251	2.26375
H	-0.54146	-1.47916	2.69442
H	-0.78203	0.30401	2.60305
H	-2.19732	-0.78859	2.62247
N	-1.16539	-0.71966	0.81156
O	-2.60563	-0.22308	-1.19723
C	0.62610	-0.41533	0.20361
C	1.61719	-0.29595	1.16981
C	0.87455	-0.95213	-1.05202
H	1.39532	0.02653	2.18803
H	0.05733	-1.17759	-1.74338
C	2.93845	-0.49917	0.77141
C	2.20247	-1.14326	-1.43229
H	3.73981	-0.35241	1.50161
H	2.42042	-1.51036	-2.43936
C	3.23980	-0.90162	-0.53079
H	4.27872	-1.06223	-0.82960
Br	-0.12060	1.86634	-0.15269

4.5aBr

C	1.01807	2.68763	-0.62152
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C	0.04150	2.43994	0.27091
H	1.21189	3.68181	-1.04283
H	-0.68066	3.14771	0.68186
Be	1.37578	0.39882	-0.31662
C	0.36255	0.89544	2.11687
H	-0.41518	1.32556	2.77230
H	0.51765	-0.16746	2.35724
H	1.30659	1.43644	2.28205
N	-0.00049	1.04236	0.69394
O	1.79154	1.69476	-1.03309
C	-1.21883	0.35191	0.28780
C	-1.63193	0.47938	-1.04413
C	-1.95140	-0.45293	1.15952
H	-1.06152	1.11133	-1.73064
H	-1.65442	-0.58117	2.20037
C	-2.76356	-0.19067	-1.49400
C	-3.08978	-1.11946	0.69977
H	-3.06925	-0.08388	-2.53827
H	-3.65596	-1.74676	1.39377
C	-3.50166	-0.99350	-0.62264
H	-4.39190	-1.51973	-0.97671
Br	1.95631	-1.53257	-0.14974

4.2bBr

C	-1.19187	-1.89092	-0.98579
C	-2.35545	-1.75916	-0.30046
H	-0.75908	-2.77854	-1.44521
H	-3.03259	-2.59885	-0.10484
Be	-1.47990	0.40665	-0.37645
C	-3.86303	-0.27561	0.91248
H	-3.79060	-0.77924	1.89674
H	-3.99637	0.80131	1.10083
H	-4.77968	-0.64237	0.41110
N	-2.68605	-0.48283	0.10452
O	-0.58185	-0.67663	-1.20352
C	0.99408	-0.32063	-0.26370
C	1.05237	-0.97678	0.94829
C	2.06883	-0.10062	-1.10248
H	0.14450	-1.24424	1.49583
H	1.93051	0.31772	-2.10059
C	2.32918	-1.23829	1.45220
C	3.33022	-0.37620	-0.57244
H	2.42610	-1.71007	2.43427
H	4.21638	-0.17119	-1.18020
C	3.46592	-0.92681	0.70497

H	4.45962	-1.14154	1.10569
Br	-0.06924	1.83724	0.05801

4.5bBr

C	-0.26265	2.27969	-0.49529
C	-1.58295	2.42197	-0.27572
H	0.50629	2.97758	-0.81648
H	-2.07571	3.39866	-0.33205
Be	-1.33640	0.02881	-0.06599
C	-3.70588	1.38618	0.29056
H	-4.26484	1.88951	-0.52209
H	-4.12830	0.37614	0.41024
H	-3.89428	1.94084	1.23050
N	-2.29581	1.28296	-0.00831
O	0.09995	0.90759	-0.43847
C	1.42482	0.54874	-0.20528
C	1.94204	-0.52746	-0.91750
C	2.18385	1.24491	0.72998
H	1.31166	-1.05535	-1.63573
H	1.74059	2.07636	1.28354
C	3.26006	-0.91393	-0.68111
C	3.50462	0.85337	0.94626
H	3.67686	-1.76228	-1.23046
H	4.11202	1.39293	1.67804
C	4.04439	-0.22407	0.24417
H	5.07918	-0.52915	0.42056
Br	-1.32276	-1.98509	0.15793

4.2cBr

C	-2.25487	-1.49194	-1.46230
C	-2.38874	-1.83315	-0.13313
H	-2.64217	-2.06376	-2.31239
H	-2.88019	-2.73601	0.24295
Be	-1.12631	0.12157	-0.29954
C	-1.71798	-1.15504	2.10958
H	-0.77996	-1.70171	2.35330
H	-1.70128	-0.20122	2.66277
H	-2.56417	-1.75783	2.48674
N	-1.82195	-0.91197	0.70192
O	-1.59777	-0.37527	-1.69616
C	0.87730	0.09118	-0.04568
C	1.42138	-0.31855	1.17347
C	1.51904	-0.15970	-1.26245
H	0.94648	-0.04780	2.11929

H	1.09891	0.20712	-2.20103
C	2.57825	-1.09590	1.15971
C	2.67366	-0.93916	-1.25060
H	2.99761	-1.44771	2.10699
H	3.16354	-1.17747	-2.19920
C	3.20367	-1.41226	-0.04753
H	4.11628	-2.01428	-0.05033
Br	-0.20527	2.04936	0.09139

4.3cBr

C	1.12381	2.24655	-1.31320
C	1.17872	2.46969	0.15601
H	1.28071	3.07032	-2.03285
H	1.37581	3.45236	0.60703
Be	0.52479	0.00249	-0.26637
C	0.93307	1.31942	2.24577
H	-0.07418	0.97628	2.53637
H	1.64873	0.53756	2.54965
H	1.16981	2.28101	2.73141
N	0.96178	1.40062	0.81035
O	0.89119	1.11444	-1.69382
C	-1.21691	-0.15967	-0.16165
C	-1.81041	-1.42397	0.00353
C	-2.08984	0.93986	-0.20740
H	-1.17205	-2.31410	0.04439
H	-1.68809	1.95723	-0.33798
C	-3.19416	-1.58031	0.11549
C	-3.47545	0.80312	-0.09787
H	-3.62346	-2.57971	0.24166
H	-4.12326	1.68517	-0.14065
C	-4.03187	-0.46561	0.06593
H	-5.11618	-0.58550	0.15473
Br	1.99598	-1.48871	-0.06428

4.4cBr

C	0.37905	2.61343	-0.90723
C	0.05555	2.52974	0.46151
H	0.22295	3.51435	-1.51871
H	-0.47651	3.29525	1.03397
Be	0.85937	0.33985	-0.34649
C	0.17135	1.00926	2.34321
H	0.27998	-0.07240	2.49806
H	0.98314	1.52234	2.88665
H	-0.80277	1.34862	2.73449

N	0.32583	1.31202	0.93529
O	0.82086	1.56180	-1.45430
C	-1.04416	-0.08962	-0.00090
C	-1.21241	-1.40898	0.42037
C	-2.11033	0.63949	-0.49240
H	-0.37221	-1.98397	0.82128
H	-1.98413	1.70430	-0.74408
C	-2.46411	-2.01269	0.26826
C	-3.35678	0.03483	-0.65943
H	-2.60081	-3.05497	0.57173
H	-4.19486	0.60441	-1.07179
C	-3.53113	-1.29623	-0.27503
H	-4.50899	-1.77317	-0.38776
Br	2.28134	-1.15023	-0.20859

4.4dBr

C	0.08212	2.07305	-1.50748
C	0.72996	2.58204	-0.37350
H	-0.51426	2.64358	-2.22413
H	0.84286	3.65394	-0.16817
Be	0.84138	0.17143	-0.20042
C	1.83448	1.97559	1.69915
H	1.21500	1.65217	2.55376
H	2.79334	1.43443	1.75829
H	2.02387	3.05929	1.79090
N	1.17024	1.65374	0.45799
O	0.06994	0.76907	-1.55845
C	-1.22372	-0.01110	-0.29826
C	-1.56914	-1.35065	-0.40190
C	-2.08744	0.95765	0.15968
H	-0.87635	-2.08918	-0.81371
H	-1.80267	2.02027	0.10983
C	-2.82220	-1.73311	0.08923
C	-3.32891	0.56645	0.66182
H	-3.11714	-2.78569	0.04444
H	-4.02195	1.31427	1.05863
C	-3.69220	-0.78301	0.62600
H	-4.67248	-1.09192	0.99965
Br	1.95644	-1.53963	0.02930

4.1al

C	2.71036	2.19654	-0.65113
C	3.50749	1.53472	0.22061
H	2.87736	3.18957	-1.07609

H	4.45041	1.91186	0.62885
Be	1.71530	0.21495	-0.25985
C	3.74860	-0.52723	1.52611
H	3.87375	-0.01169	2.50004
H	3.21055	-1.47086	1.72062
H	4.76149	-0.79362	1.16081
N	3.01749	0.26887	0.58095
O	1.59155	1.52324	-1.03236
C	-1.69317	-0.01075	0.03683
C	-2.89928	-0.51467	0.51840
C	-1.48972	1.34281	-0.21254
H	-3.03757	-1.58187	0.70950
H	-0.52782	1.71600	-0.58654
C	-3.94180	0.38052	0.76012
C	-2.54788	2.21865	0.04069
H	-4.89475	0.00264	1.14096
H	-2.40627	3.28670	-0.14528
C	-3.76684	1.74379	0.52296
H	-4.58646	2.44098	0.71700
I	-0.11704	-1.39252	-0.34171

4.2aI

C	-2.41320	-1.96718	-0.89750
C	-1.67215	-2.27640	0.19552
H	-2.92891	-2.70659	-1.52200
H	-1.47636	-3.27373	0.59390
Be	-1.66835	0.10870	-0.24445
C	-1.13028	-1.08217	2.26403
H	-0.48378	-1.87626	2.67771
H	-0.77709	-0.09868	2.61152
H	-2.15902	-1.23202	2.63270
N	-1.14908	-1.11135	0.81269
O	-2.52802	-0.69172	-1.24735
C	0.66951	-0.71323	0.20152
C	0.92873	-1.19782	-1.07169
C	1.65112	-0.61364	1.17833
H	0.12011	-1.41596	-1.77545
H	1.41893	-0.33765	2.20802
C	2.26227	-1.33811	-1.45603
C	2.97775	-0.76741	0.77652
H	2.49221	-1.65588	-2.47704
H	3.77409	-0.63164	1.51416
C	3.29036	-1.10534	-0.54180
H	4.33359	-1.22586	-0.84454
I	-0.16523	1.76793	-0.08009

4.5aI

C	-0.17683	3.04272	-0.66365
C	-1.05403	2.53103	0.21915
H	-0.27989	4.04080	-1.10696
H	-1.96289	2.99742	0.60323
Be	0.83889	0.97175	-0.29379
C	-0.33449	1.20204	2.11540
H	-1.22573	1.39761	2.73736
H	0.12364	0.24226	2.39895
H	0.39917	2.00577	2.27965
N	-0.68471	1.19409	0.68071
O	0.86830	2.31914	-1.03701
C	-1.63473	0.16171	0.27877
C	-2.05883	0.14170	-1.05548
C	-2.09108	-0.81814	1.15982
H	-1.70653	0.90887	-1.75053
H	-1.77412	-0.83773	2.20250
C	-2.92893	-0.84778	-1.49861
C	-2.96844	-1.80607	0.70665
H	-3.24676	-0.85259	-2.54476
H	-3.31867	-2.56793	1.40845
C	-3.39125	-1.82722	-0.61811
H	-4.07636	-2.60431	-0.96682
I	2.10171	-0.87187	-0.08337

4.2bI

C	-1.14417	-2.21640	-1.02321
C	-2.29868	-2.13345	-0.31351
H	-0.68650	-3.08602	-1.49311
H	-2.94242	-2.99821	-0.11434
Be	-1.50689	0.06602	-0.40392
C	-3.82887	-0.71159	0.94467
H	-3.71833	-1.21805	1.92375
H	-3.99360	0.35930	1.14186
H	-4.74231	-1.10689	0.45962
N	-2.66249	-0.87419	0.11121
O	-0.57474	-0.98463	-1.23250
C	1.00744	-0.61130	-0.26166
C	1.04016	-1.25601	0.95838
C	2.09351	-0.44730	-1.10051
H	0.12359	-1.48916	1.50711
H	1.97535	-0.04479	-2.10780
C	2.30574	-1.54468	1.47553

C	3.34316	-0.74901	-0.55821
H	2.38283	-2.00202	2.46613
H	4.23822	-0.58270	-1.16463
C	3.45546	-1.27785	0.73098
H	4.44021	-1.51301	1.14220
I	-0.06899	1.75659	0.03437

4.5bl

C	0.48472	2.59975	-0.42658
C	-0.78388	3.00668	-0.23567
H	1.39623	3.12849	-0.69287
H	-1.06082	4.06615	-0.26405
Be	-1.03788	0.61032	-0.10486
C	-3.09362	2.41236	0.23620
H	-3.50694	3.05691	-0.56334
H	-3.71812	1.50699	0.29281
H	-3.19582	2.95111	1.19826
N	-1.72536	2.03155	-0.03217
O	0.55140	1.17965	-0.41042
C	1.77365	0.54624	-0.19445
C	2.10045	-0.53285	-1.00687
C	2.61342	0.98283	0.82467
H	1.40928	-0.84994	-1.79045
H	2.31650	1.82577	1.45391
C	3.30765	-1.19385	-0.78634
C	3.82313	0.31909	1.02515
H	3.57450	-2.04799	-1.41447
H	4.49366	0.65126	1.82234
C	4.17131	-0.76827	0.22349
H	5.11899	-1.28767	0.38813
I	-1.53567	-1.57231	0.10453

4.2cl

C	-2.24774	-1.94266	-1.47340
C	-2.46988	-2.18525	-0.13793
H	-2.70348	-2.48291	-2.30970
H	-3.12750	-2.96321	0.26329
Be	-0.93731	-0.44740	-0.35142
C	-1.78545	-1.47904	2.10161
H	-0.91584	-2.07712	2.45197
H	-1.72986	-0.49371	2.59610
H	-2.70229	-1.98414	2.45699
N	-1.77582	-1.32787	0.67646
O	-1.40550	-0.95717	-1.73852

C	0.98914	-0.14758	-0.04422
C	1.49380	-0.58210	1.19004
C	1.71006	-0.36051	-1.22876
H	0.95422	-0.37195	2.11719
H	1.32427	0.00629	-2.18321
C	2.67794	-1.31325	1.22125
C	2.89033	-1.09631	-1.17910
H	3.06006	-1.67784	2.17922
H	3.43516	-1.29731	-2.10588
C	3.37662	-1.57410	0.04042
H	4.31079	-2.14143	0.07204
I	-0.26963	1.85491	0.03964

4.3cl

C	0.42366	2.58735	-1.31739
C	0.41338	2.82808	0.14671
H	0.51842	3.41086	-2.04698
H	0.49394	3.82847	0.59360
Be	0.10846	0.30380	-0.27373
C	0.25168	1.67469	2.24295
H	-0.71621	1.22073	2.51468
H	1.04583	0.98570	2.57557
H	0.36528	2.66284	2.71929
N	0.30630	1.74365	0.80655
O	0.32498	1.42950	-1.68548
C	-1.55298	-0.22311	-0.17069
C	-1.89657	-1.57561	0.00413
C	-2.61933	0.69139	-0.22872
H	-1.10262	-2.32941	0.05550
H	-2.41802	1.76479	-0.36736
C	-3.22602	-1.99077	0.11394
C	-3.95398	0.29401	-0.12268
H	-3.45663	-3.05245	0.24952
H	-4.75695	1.03665	-0.17624
C	-4.25964	-1.05593	0.05114
H	-5.30207	-1.37844	0.13738
I	2.05038	-0.98844	-0.03091

4.4cl

C	-0.54941	2.75321	-0.90802
C	-0.88330	2.60538	0.45068
H	-0.86441	3.60478	-1.52861
H	-1.56933	3.24850	1.00924
Be	0.37031	0.63168	-0.32370

C	-0.49692	1.15376	2.34971
H	-0.16499	0.12173	2.52458
H	0.17540	1.83340	2.90028
H	-1.52914	1.28342	2.71649
N	-0.38152	1.46695	0.93971
O	0.11081	1.81125	-1.43909
C	-1.40990	-0.18619	0.00411
C	-1.33510	-1.49791	0.47390
C	-2.57770	0.30161	-0.55235
H	-0.41882	-1.88502	0.92982
H	-2.65534	1.36136	-0.84059
C	-2.43693	-2.34130	0.30458
C	-3.67271	-0.54303	-0.73802
H	-2.37899	-3.37815	0.64896
H	-4.58751	-0.16289	-1.20203
C	-3.59939	-1.86852	-0.30525
H	-4.45943	-2.53250	-0.43085
I	2.27403	-0.62344	-0.13158

4.4dl

C	0.90534	2.17493	1.51190
C	0.39957	2.85054	0.39412
H	1.64958	2.55136	2.21822
H	0.58132	3.91392	0.19425
Be	-0.37234	0.56702	0.21518
C	-0.87278	2.59467	-1.65451
H	-0.40363	2.10363	-2.52466
H	-1.95093	2.36453	-1.68292
H	-0.73307	3.68576	-1.74682
N	-0.29720	2.08645	-0.43081
O	0.55506	0.91743	1.56222
C	1.55359	-0.19237	0.29419
C	1.54878	-1.56930	0.46461
C	2.62283	0.49734	-0.23375
H	0.70906	-2.08292	0.93971
H	2.62687	1.59782	-0.23274
C	2.64213	-2.28590	-0.03304
C	3.70125	-0.22547	-0.74390
H	2.65965	-3.37519	0.06614
H	4.54745	0.29767	-1.19888
C	3.70583	-1.61981	-0.64336
H	4.55938	-2.18879	-1.02215
I	-2.11992	-0.87600	-0.02812

5.1aF

C	3.27654	-1.26787	0.00846
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C	3.51026	0.03841	0.27245
H	4.04585	-2.04048	0.05809
H	4.50482	0.40319	0.56030
Be	1.20623	0.16654	-0.26375
C	2.74671	2.34011	0.47101
H	3.48125	2.77927	-0.23346
H	1.81973	2.93298	0.39296
H	3.14287	2.47915	1.49661
N	2.47024	0.95559	0.17837
S	1.62870	-1.73602	-0.46150
C	-1.60998	0.42360	-0.15454
C	-1.75076	-0.80147	0.46549
C	-2.65310	1.24311	-0.53918
H	-0.87477	-1.40093	0.73350
H	-2.45807	2.20041	-1.02642
C	-3.05577	-1.23191	0.71478
C	-3.94609	0.78898	-0.27744
H	-3.21187	-2.19822	1.20088
H	-4.80045	1.40641	-0.56676
C	-4.14644	-0.44369	0.34652
H	-5.16254	-0.79337	0.54565
F	-0.32119	0.90189	-0.42402

5.2aF

C	-2.32214	-0.58307	-1.16020
C	-1.43161	0.39846	-1.43481
H	-2.78071	-1.18495	-1.94948
H	-1.13112	0.65186	-2.45844
Be	-1.39360	0.40615	0.99437
C	-0.32597	2.40767	-0.65734
H	-1.07918	3.05025	-1.14842
H	-0.02282	2.90531	0.27757
H	0.56186	2.34629	-1.31795
N	-0.87040	1.10134	-0.37045
S	-2.79054	-0.91533	0.51572
C	0.90174	0.04987	0.48455
C	0.88645	-1.24250	-0.00144
C	2.01048	0.86477	0.57106
H	-0.02691	-1.84203	-0.01640
H	1.96443	1.84955	1.03684
C	2.09218	-1.71454	-0.52566
C	3.19699	0.35818	0.03219
H	2.11907	-2.72288	-0.94853
H	4.09707	0.97907	0.06358
C	3.24218	-0.92278	-0.51783

H	4.17713	-1.31093	-0.92905
F	-0.11829	0.32148	1.89014

5.5aF

C	2.22703	-1.44801	0.12482
C	1.22551	-1.17934	0.97340
H	2.78866	-2.38246	0.23044
H	0.92395	-1.83545	1.79656
Be	1.37957	0.98557	-0.46361
C	0.55978	0.84768	2.08199
H	1.61837	0.97526	2.35592
H	0.10998	1.83966	1.93962
H	0.02945	0.31051	2.88796
N	0.49999	0.06921	0.81956
S	2.69567	-0.35549	-1.16297
C	-0.87292	-0.08512	0.32299
C	-1.62719	1.06244	0.05086
C	-1.42117	-1.34570	0.08324
H	-1.19000	2.05421	0.18253
H	-0.83302	-2.24668	0.26113
C	-2.92617	0.94022	-0.43458
C	-2.72327	-1.45687	-0.40576
H	-3.50198	1.84466	-0.64890
H	-3.14194	-2.45013	-0.58980
C	-3.48309	-0.31837	-0.66049
H	-4.50194	-0.41031	-1.04615
F	1.08871	2.38446	-0.60701

5.2bF

C	1.72419	1.08891	-1.38747
C	2.44981	-0.01643	-1.05153
H	1.75088	1.54278	-2.37931
H	3.10693	-0.50572	-1.78356
Be	1.26410	0.24950	1.01405
C	3.11591	-1.74220	0.51817
H	4.20516	-1.59239	0.38949
H	2.94225	-2.03095	1.56736
H	2.81545	-2.60024	-0.11598
N	2.36487	-0.54644	0.21121
S	0.74398	1.82060	-0.13159
C	-1.06258	0.00158	0.45077
C	-2.20338	0.62340	0.90757
C	-0.98812	-0.98897	-0.50261
H	-2.17190	1.37189	1.70048

H	-0.03929	-1.43906	-0.80358
C	-3.38830	0.26567	0.26233
C	-2.19985	-1.32299	-1.11920
H	-4.32026	0.75276	0.56321
H	-2.19431	-2.08221	-1.90649
C	-3.39137	-0.70304	-0.74527
H	-4.32836	-0.97825	-1.23527
F	0.04237	-0.21964	1.84198

5.5bF

C	1.35672	-1.48296	-1.03409
C	2.27043	-1.21071	-0.05630
H	1.27053	-2.43812	-1.55137
H	2.95923	-2.00534	0.26635
Be	1.41211	1.14742	-0.02791
C	3.36116	0.17248	1.58775
H	4.37920	-0.10225	1.25236
H	3.38567	1.23025	1.89394
H	3.11782	-0.42867	2.48464
N	2.37763	-0.00118	0.53454
S	0.37114	-0.12337	-1.53915
C	-1.11398	-0.17593	-0.50486
C	-2.04766	0.84743	-0.68405
C	-1.32823	-1.17835	0.43814
H	-1.86664	1.63742	-1.41913
H	-0.58197	-1.96685	0.56953
C	-3.20658	0.85978	0.08926
C	-2.49318	-1.15733	1.20563
H	-3.93731	1.66175	-0.04777
H	-2.66332	-1.94344	1.94695
C	-3.43368	-0.14255	1.03349
H	-4.34505	-0.13017	1.63764
F	1.09574	2.52075	0.16814

5.1aCl

C	3.30745	-1.04342	0.54230
C	3.14026	0.20182	1.04646
H	4.08776	-1.72874	0.87881
H	3.78700	0.59874	1.83960
Be	1.40418	0.20667	-0.56807
C	1.95013	2.32227	1.12408
H	2.84218	2.96424	0.98310
H	1.09770	2.83074	0.64305
H	1.73908	2.27478	2.21075

N	2.12670	1.01148	0.54928
S	2.21089	-1.56681	-0.74953
C	-1.70216	0.18973	-0.48278
C	-1.51016	-1.03388	0.14386
C	-2.86576	0.93820	-0.35669
H	-0.57201	-1.58692	0.02691
H	-2.97465	1.89758	-0.86709
C	-2.54503	-1.52161	0.94254
C	-3.88743	0.42697	0.44367
H	-2.41597	-2.48092	1.45028
H	-4.81358	0.99606	0.55962
C	-3.72805	-0.79817	1.09181
H	-4.53192	-1.19016	1.72033
Cl	-0.41641	0.85266	-1.52923

5.2aCl

C	2.17649	-1.53961	0.55955
C	1.36361	-0.93570	1.46364
H	2.54871	-2.55737	0.70365
H	1.02878	-1.43182	2.38214
Be	1.47651	0.79531	-0.24840
C	0.34832	1.10410	2.28089
H	1.07241	1.23756	3.10592
H	0.05884	2.10623	1.92633
H	-0.55155	0.60314	2.68949
N	0.93781	0.35399	1.20062
S	2.68648	-0.65024	-0.87459
C	-0.94281	0.27705	-0.27053
C	-2.04226	0.81348	0.36882
C	-0.89696	-0.95021	-0.90127
H	-2.03389	1.81369	0.80283
H	0.00197	-1.32291	-1.39572
C	-3.18338	0.00772	0.42700
C	-2.06270	-1.72135	-0.82871
H	-4.07285	0.39301	0.93398
H	-2.06209	-2.70877	-1.29931
C	-3.19774	-1.25423	-0.16758
H	-4.09955	-1.86997	-0.12379
Cl	0.19291	1.98084	-1.21962

5.5aCl

C	2.05233	-1.82757	0.20132
C	0.96417	-1.57705	0.93929
H	2.52529	-2.81422	0.24415

H	0.47483	-2.29728	1.60245
Be	1.36361	0.69347	-0.29388
C	0.52845	0.43192	2.18956
H	1.59653	0.40873	2.45526
H	0.20436	1.48021	2.10853
H	-0.04949	-0.09025	2.97186
N	0.37743	-0.24255	0.88125
S	2.75783	-0.62248	-0.86290
C	-0.98435	-0.27404	0.34889
C	-2.05966	0.32753	0.99935
C	-1.18093	-0.90844	-0.88347
H	-1.93349	0.83683	1.95482
H	-0.33315	-1.37290	-1.39581
C	-3.32893	0.28750	0.41744
C	-2.44745	-0.94095	-1.45546
H	-4.16721	0.76319	0.93382
H	-2.58759	-1.43419	-2.42094
C	-3.52931	-0.34359	-0.80593
H	-4.52444	-0.36774	-1.25752
Cl	0.96981	2.51291	-0.59349

5.2bCl

C	1.72117	-1.87670	0.21241
C	2.50716	-0.89735	0.76973
H	1.71192	-2.91158	0.55535
H	3.19870	-1.14527	1.58762
Be	1.28943	0.56902	-0.74237
C	3.27439	1.38679	0.98102
H	4.35052	1.17154	0.84518
H	3.06943	2.37126	0.53275
H	3.07007	1.46450	2.06544
N	2.44012	0.38534	0.34630
S	0.73308	-1.39288	-1.12521
C	-1.00141	-0.16870	-0.21567
C	-2.19328	-0.35753	-0.91180
C	-0.95539	-0.06468	1.16623
H	-2.19538	-0.56135	-1.98531
H	-0.00381	-0.07612	1.70700
C	-3.38457	-0.20157	-0.20860
C	-2.16519	0.09895	1.84946
H	-4.33342	-0.30076	-0.74464
H	-2.14637	0.24151	2.93432
C	-3.37871	0.04860	1.16798
H	-4.32133	0.16522	1.70878
Cl	-0.17137	1.71099	-1.14837

5.5bCl

C	1.09168	-1.91546	-0.92922
C	2.06111	-1.67735	0.00148
H	0.89347	-2.88478	-1.38575
H	2.67541	-2.51610	0.36032
Be	1.44300	0.74329	-0.11958
C	3.34375	-0.30638	1.51416
H	4.31610	-0.70367	1.16674
H	3.48209	0.76035	1.74894
H	3.07227	-0.82492	2.45308
N	2.31267	-0.44567	0.50124
S	0.24721	-0.48778	-1.50226
C	-1.24042	-0.34098	-0.48240
C	-2.06514	0.75896	-0.72787
C	-1.56073	-1.26841	0.50588
H	-1.79828	1.48981	-1.49673
H	-0.89805	-2.11874	0.68910
C	-3.22431	0.92558	0.02651
C	-2.72637	-1.09291	1.25266
H	-3.86906	1.78859	-0.16109
H	-2.98244	-1.82001	2.02846
C	-3.55937	-0.00039	1.01530
H	-4.47153	0.13233	1.60336
Cl	1.23192	2.59718	0.05531

5.2cCl

C	-1.65883	-1.90237	-0.88363
C	-1.99874	-1.59099	0.49409
H	-1.72609	-2.94402	-1.21964
H	-2.46550	-2.35492	1.13357
Be	-0.76805	0.63736	-0.07650
C	-1.92437	-0.06300	2.32942
H	-2.49447	-0.83316	2.87645
H	-0.94897	0.09987	2.81964
H	-2.46449	0.89756	2.33858
N	-1.67998	-0.43487	0.95501
S	-1.06448	-0.72669	-1.84567
C	0.96797	0.15517	-0.02016
C	1.90633	1.14468	-0.36005
C	1.46032	-1.06734	0.45141
H	1.55991	2.11120	-0.74189
H	0.76640	-1.88767	0.68894
C	3.27610	0.93049	-0.18947

C	2.82600	-1.29208	0.63175
H	3.98735	1.72117	-0.44872
H	3.18072	-2.25395	1.01598
C	3.73922	-0.28696	0.31023
H	4.81225	-0.45635	0.44209
Cl	-1.40632	2.46213	-0.13734

5.4cCl

C	-1.58625	-1.91580	-0.91049
C	-1.99568	-1.60919	0.44478
H	-1.59501	-2.95996	-1.24410
H	-2.47738	-2.37958	1.06510
Be	-0.78971	0.63363	-0.07602
C	-2.03852	-0.07679	2.27973
H	-2.61732	-0.85939	2.79938
H	-1.09435	0.10983	2.81984
H	-2.60194	0.87019	2.26039
N	-1.71741	-0.44574	0.91990
S	-0.97543	-0.72010	-1.84245
C	0.95631	0.14220	-0.02662
C	1.44872	-1.06758	0.47391
C	1.88795	1.13682	-0.36791
H	0.75719	-1.89215	0.70352
H	1.53819	2.09152	-0.77513
C	2.81181	-1.27151	0.69162
C	3.25551	0.94170	-0.16099
H	3.16906	-2.22210	1.10043
H	3.96368	1.73539	-0.41912
C	3.72004	-0.26055	0.37303
H	4.79163	-0.41511	0.53168
Cl	-1.40032	2.46546	-0.13414

5.4dCl

C	-1.77751	-2.01967	-0.09622
C	-1.31030	-1.53789	1.13091
H	-2.01499	-3.08241	-0.21594
H	-1.11419	-2.20088	1.98173
Be	-1.08449	0.57992	-0.27188
C	-0.58612	0.33665	2.45468
H	0.12789	-0.30618	2.99698
H	-0.13843	1.32424	2.28097
H	-1.49665	0.47020	3.06343
N	-0.98006	-0.24755	1.18493
S	-1.87536	-0.98153	-1.41295

C	0.84399	0.02960	-0.04056
C	1.62041	1.18695	-0.03996
C	1.42278	-1.22086	-0.14672
H	1.16395	2.17618	0.05895
H	0.80602	-2.12893	-0.08018
C	3.00421	1.06782	-0.21738
C	2.80040	-1.33631	-0.33313
H	3.62040	1.97195	-0.23931
H	3.25756	-2.32458	-0.43974
C	3.59270	-0.18621	-0.36809
H	4.67472	-0.27222	-0.50217
Cl	-1.49091	2.44529	-0.44504

5.1aBr

C	-3.39116	1.42808	0.09771
C	-3.31261	0.49492	1.07605
H	-4.14546	2.21693	0.07870
H	-4.01129	0.48112	1.92258
Be	-1.50863	-0.23179	-0.28640
C	-2.24809	-1.44404	2.08418
H	-3.17529	-2.04405	2.17281
H	-1.41699	-2.14515	1.89881
H	-2.06521	-0.96281	3.06532
N	-2.32616	-0.47995	1.01409
S	-2.21769	1.33306	-1.22662
C	1.73011	-0.14446	-0.14918
C	1.48346	1.22239	-0.12905
C	2.91746	-0.70620	0.30783
H	0.53269	1.63358	-0.48624
H	3.07959	-1.78634	0.28005
C	2.47935	2.05726	0.37978
C	3.89980	0.14880	0.80806
H	2.30338	3.13574	0.40942
H	4.83987	-0.27226	1.17468
C	3.68196	1.52606	0.84510
H	4.45490	2.19027	1.24071
Br	0.39894	-1.34246	-0.85734

5.2aBr

C	2.48976	-1.71747	-0.19334
C	1.54447	-1.75097	0.76558
H	3.03624	-2.62417	-0.47278
H	1.26632	-2.65152	1.32258
Be	1.42137	0.65309	-0.02230

C	0.70449	-0.26342	2.49216
H	1.69100	-0.23898	2.98557
H	0.22437	0.71860	2.62351
H	0.08736	-1.04656	2.96736
N	0.89954	-0.52636	1.07372
S	2.88981	-0.22650	-1.04435
C	-0.86317	-0.42181	0.21568
C	-1.96316	-0.28895	1.04625
C	-0.90252	-1.06148	-1.01173
H	-1.88798	0.13504	2.04849
H	0.01056	-1.26455	-1.57802
C	-3.20744	-0.62753	0.51153
C	-2.15878	-1.38650	-1.52525
H	-4.10366	-0.48082	1.12133
H	-2.22614	-1.84402	-2.51636
C	-3.31302	-1.15844	-0.77505
H	-4.29292	-1.42164	-1.18104
Br	-0.17166	1.92783	-0.20551

5.5aBr

C	-1.36111	2.62615	-0.04815
C	-0.32146	2.25040	0.70578
H	-1.59495	3.68942	-0.16561
H	0.35195	2.93286	1.23364
Be	-1.28089	-0.03172	-0.13762
C	-0.28967	0.42319	2.26773
H	-1.31308	0.72725	2.53604
H	-0.20602	-0.66958	2.36559
H	0.42524	0.92392	2.94359
N	-0.05473	0.82419	0.86235
S	-2.37585	1.46206	-0.88525
C	1.25524	0.45999	0.32161
C	2.19036	-0.27257	1.04966
C	1.54036	0.84110	-0.99482
H	1.99177	-0.59146	2.07285
H	0.80318	1.41171	-1.56732
C	3.40853	-0.61804	0.45991
C	2.75429	0.48980	-1.57388
H	4.13493	-1.19504	1.03863
H	2.96222	0.78677	-2.60523
C	3.69618	-0.24131	-0.84782
H	4.64956	-0.51882	-1.30483
Br	-1.31202	-2.06528	-0.16885

5.2bBr

C	1.86080	-2.01680	-0.67638
C	2.60413	-1.37985	0.28998
H	1.90493	-3.08999	-0.86340
H	3.31938	-1.95039	0.89955
Be	1.29062	0.57526	-0.35794
C	3.25057	0.56595	1.57041
H	4.33106	0.54297	1.33610
H	2.94917	1.61958	1.67527
H	3.09751	0.07463	2.54945
N	2.45926	-0.05944	0.52816
S	0.82825	-1.00736	-1.62535
C	-0.94118	-0.45407	-0.24737
C	-2.14041	-0.36337	-0.95079
C	-0.86652	-0.98825	1.02922
H	-2.16049	-0.07204	-2.00384
H	0.09577	-1.21827	1.49696
C	-3.32007	-0.56725	-0.24131
C	-2.06427	-1.17511	1.72780
H	-4.27803	-0.44791	-0.75639
H	-2.02757	-1.53096	2.76196
C	-3.28918	-0.94625	1.10590
H	-4.22276	-1.10580	1.65157
Br	-0.26290	1.86745	-0.19005

5.5bBr

C	-0.26374	2.49404	-0.91917
C	-1.26789	2.51334	0.00399
H	0.19284	3.37981	-1.35999
H	-1.63746	3.48081	0.37427
Be	-1.31857	0.01835	-0.14687
C	-2.87276	1.51661	1.50306
H	-3.69300	2.18194	1.17429
H	-3.30641	0.52624	1.71122
H	-2.46429	1.91187	2.45237
N	-1.84464	1.38685	0.48539
S	0.17429	0.89807	-1.50563
C	1.56706	0.35618	-0.48463
C	2.10815	-0.89978	-0.76704
C	2.07847	1.13976	0.54672
H	1.69245	-1.51352	-1.57155
H	1.63737	2.11810	0.75582
C	3.17414	-1.37073	-0.00342
C	3.14805	0.65896	1.30238
H	3.59690	-2.35585	-0.21884
H	3.55186	1.27144	2.11353

C	3.69746	-0.59321	1.03047
H	4.53423	-0.96668	1.62697
Br	-1.62629	-1.97359	0.02708

5.2cBr

C	2.81140	-1.63490	-0.54316
C	2.65977	-1.30542	0.78707
H	3.52150	-2.39675	-0.87419
H	3.25312	-1.79180	1.57223
Be	0.92219	0.12861	-0.16740
C	1.55355	-0.02814	2.50874
H	2.49394	-0.09883	3.08423
H	1.17363	1.00272	2.59860
H	0.81447	-0.70676	2.98427
N	1.75148	-0.36330	1.12223
S	1.82680	-0.81801	-1.69454
C	-1.07470	-0.06602	-0.04959
C	-1.72154	-0.49429	-1.21327
C	-1.61462	-0.30413	1.21452
H	-1.31921	-0.25129	-2.19886
H	-1.15215	0.10977	2.11290
C	-2.85981	-1.28534	-1.08927
C	-2.75771	-1.09799	1.31760
H	-3.34658	-1.66418	-1.99259
H	-3.17057	-1.31446	2.30726
C	-3.37823	-1.59456	0.17194
H	-4.28004	-2.20657	0.25804
Br	-0.13928	2.03713	-0.24436

5.3cBr

C	0.77190	2.61585	-0.88900
C	1.07117	2.43815	0.52604
H	0.61331	3.63368	-1.26611
H	1.26055	3.31535	1.16239
Be	0.56361	-0.06219	-0.04511
C	1.29070	0.98604	2.40814
H	1.56524	1.89817	2.96465
H	0.37052	0.54823	2.83197
H	2.08669	0.22769	2.48798
N	1.05695	1.24935	1.00711
S	0.59238	1.31071	-1.84541
C	-1.21754	-0.18425	-0.01258
C	-1.79672	-1.43165	-0.30488
C	-2.08413	0.85121	0.36363

H	-1.15633	-2.26720	-0.60861
H	-1.68676	1.85613	0.57076
C	-3.17344	-1.63858	-0.19086
C	-3.46135	0.65757	0.48447
H	-3.59663	-2.62360	-0.41234
H	-4.10977	1.48514	0.79012
C	-4.00953	-0.59504	0.20689
H	-5.08831	-0.75583	0.29595
Br	1.89326	-1.68519	-0.04888

5.4cBr

C	0.47517	2.60135	-0.97518
C	0.97238	2.51244	0.37996
H	0.11367	3.56535	-1.35062
H	1.16073	3.42642	0.96237
Be	0.63032	-0.01713	-0.04930
C	1.56412	1.16860	2.26783
H	1.81669	2.12842	2.74966
H	0.76075	0.66716	2.83432
H	2.43813	0.49694	2.26843
N	1.12046	1.34378	0.90301
S	0.31657	1.22429	-1.84483
C	-1.18407	-0.17127	-0.01739
C	-1.71201	-1.43493	-0.32997
C	-2.06618	0.80779	0.45148
H	-1.05278	-2.22026	-0.71482
H	-1.70390	1.82765	0.64930
C	-3.06308	-1.71918	-0.11885
C	-3.41586	0.53274	0.67287
H	-3.45177	-2.71567	-0.35098
H	-4.08180	1.31239	1.05595
C	-3.91666	-0.73845	0.38689
H	-4.97624	-0.95949	0.54730
Br	1.93212	-1.65172	-0.04467

5.4dBr

C	0.32073	2.84106	-0.16341
C	0.03573	2.26338	1.07764
H	0.07910	3.89322	-0.35008
H	-0.48470	2.81062	1.87229
Be	0.86157	0.20366	-0.17361
C	0.13828	0.33256	2.51088
H	-0.84199	0.57270	2.95606
H	0.24142	-0.75530	2.40136

H	0.94209	0.69228	3.17553
N	0.31001	0.96551	1.21455
S	0.95511	1.89074	-1.39502
C	-1.12048	-0.16669	-0.03447
C	-1.31879	-1.54155	0.07700
C	-2.17773	0.68943	-0.28214
H	-0.48877	-2.22054	0.29285
H	-2.02340	1.77767	-0.29820
C	-2.60260	-2.05715	-0.13732
C	-3.45394	0.17269	-0.50614
H	-2.76339	-3.13736	-0.07040
H	-4.28586	0.84856	-0.72553
C	-3.66560	-1.20609	-0.43286
H	-4.66697	-1.61570	-0.59328
Br	2.18459	-1.39020	-0.19437

5.1al

C	-3.48049	1.68099	-0.19170
C	-3.50805	0.91012	0.92204
H	-4.19514	2.48364	-0.38421
H	-4.26031	1.05370	1.70863
Be	-1.64807	-0.08129	-0.17849
C	-2.60087	-0.87617	2.29441
H	-3.55873	-1.42056	2.41063
H	-1.79266	-1.62664	2.28289
H	-2.45948	-0.25035	3.19764
N	-2.56451	-0.09413	1.08268
S	-2.22992	1.33946	-1.39631
C	1.79990	0.08622	0.01008
C	1.48776	1.42258	-0.21643
C	3.02460	-0.31558	0.53853
H	0.51451	1.72091	-0.62267
H	3.25071	-1.37044	0.71422
C	2.44563	2.38644	0.10351
C	3.96813	0.66445	0.84855
H	2.21451	3.44144	-0.06641
H	4.93341	0.36590	1.26665
C	3.68048	2.01186	0.63189
H	4.42348	2.77476	0.87904
I	0.38207	-1.42349	-0.48218

5.2al

C	2.73077	-1.74273	-0.29880
C	1.75873	-1.94175	0.60896

H	3.36408	-2.57216	-0.63022
H	1.53839	-2.90734	1.07487
Be	1.47143	0.51577	0.03659
C	0.84333	-0.65926	2.44935
H	1.84390	-0.55784	2.90228
H	0.26383	0.25003	2.67308
H	0.34128	-1.54014	2.88639
N	1.00091	-0.80122	1.00547
S	3.03270	-0.15335	-1.00190
C	-0.72612	-0.81972	0.21146
C	-0.72755	-1.33731	-1.07744
C	-1.81549	-0.92917	1.06470
H	0.18748	-1.37389	-1.67517
H	-1.76417	-0.62664	2.11162
C	-1.95151	-1.73089	-1.61470
C	-3.02987	-1.32912	0.50683
H	-1.99154	-2.07899	-2.65070
H	-3.92160	-1.35522	1.13988
C	-3.10923	-1.70740	-0.83450
H	-4.06528	-2.02183	-1.26050
I	-0.39717	1.77296	-0.07209

5.5al

C	0.18023	3.19051	-0.11719
C	0.98678	2.43166	0.63327
H	0.41347	4.24888	-0.27344
H	1.90281	2.77959	1.12083
Be	-0.87341	0.74955	-0.10263
C	0.29447	0.82783	2.27887
H	-0.47689	1.56382	2.55192
H	-0.11046	-0.18350	2.43274
H	1.18514	0.98322	2.91221
N	0.62723	1.03324	0.85002
S	-1.25979	2.54264	-0.88735
C	1.64173	0.12417	0.31312
C	2.15130	-0.94433	1.04809
C	2.06637	0.32898	-1.00481
H	1.83090	-1.13484	2.07213
H	1.66188	1.16447	-1.58319
C	3.08536	-1.80241	0.46394
C	2.99531	-0.53230	-1.57793
H	3.47741	-2.63950	1.04779
H	3.31470	-0.36543	-2.61003
C	3.51100	-1.60244	-0.84522
H	4.23962	-2.28043	-1.29726

I	-1.88027	-1.26754	-0.09186
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5.2bl

C	2.12465	-2.11324	-0.69576
C	2.82694	-1.41895	0.26178
H	2.26276	-3.17561	-0.89749
H	3.60312	-1.92906	0.85032
Be	1.35140	0.43775	-0.35597
C	3.32886	0.56755	1.54722
H	4.38740	0.70648	1.25901
H	2.88980	1.56296	1.71652
H	3.29916	0.01933	2.50700
N	2.57332	-0.11887	0.51606
S	0.99154	-1.18846	-1.61821
C	-0.80557	-0.88159	-0.26315
C	-0.67441	-1.39212	1.01884
C	-2.00965	-0.92080	-0.96318
H	0.30860	-1.53469	1.47858
H	-2.05972	-0.66503	-2.02441
C	-1.84626	-1.64895	1.73626
C	-3.16476	-1.19343	-0.23716
H	-1.77551	-1.97428	2.77844
H	-4.13361	-1.16704	-0.74454
C	-3.09076	-1.52406	1.12123
H	-4.00453	-1.73586	1.68270
I	-0.45651	1.71968	-0.11434

5.5bl

C	0.94155	2.67075	-0.89345
C	-0.01356	3.02845	0.01184
H	1.68512	3.34773	-1.31336
H	-0.03397	4.06092	0.38987
Be	-0.91037	0.70515	-0.17672
C	-1.89482	2.63642	1.46916
H	-2.43765	3.53816	1.12928
H	-2.63966	1.85031	1.66795
H	-1.39208	2.87252	2.42591
N	-0.95402	2.16562	0.46744
S	0.81190	1.02746	-1.49954
C	1.92211	0.02742	-0.47805
C	2.05225	-1.32033	-0.81824
C	2.60582	0.56065	0.61156
H	1.50569	-1.73194	-1.67174
H	2.48686	1.61828	0.86242

C	2.87726	-2.14026	-0.05107
C	3.43225	-0.26900	1.36945
H	2.97776	-3.19758	-0.31086
H	3.96966	0.14566	2.22693
C	3.56931	-1.61734	1.04189
H	4.21549	-2.26400	1.64168
I	-1.99926	-1.24754	0.01511

5.2cl

C	3.03295	-1.66005	-0.67322
C	2.86050	-1.46742	0.67953
H	3.88340	-2.21492	-1.07664
H	3.57538	-1.86452	1.41214
Be	0.85993	-0.31841	-0.13026
C	1.57735	-0.57550	2.52155
H	2.51478	-0.69417	3.09332
H	1.18333	0.43566	2.72066
H	0.84421	-1.30858	2.91750
N	1.78751	-0.76463	1.10877
S	1.85502	-0.99364	-1.74062
C	-1.07973	-0.38904	-0.03597
C	-1.62771	-0.75735	1.20064
C	-1.72198	-0.75608	-1.22958
H	-1.17537	-0.41459	2.13446
H	-1.32409	-0.42934	-2.19395
C	-2.74965	-1.58334	1.23722
C	-2.84122	-1.57967	-1.17908
H	-3.15790	-1.89440	2.20323
H	-3.31770	-1.89629	-2.11123
C	-3.35542	-1.99973	0.05138
H	-4.24158	-2.63962	0.08408
I	-0.16958	1.88781	-0.07564

5.3cl

C	1.37190	2.61635	-0.86899
C	1.02718	2.62567	0.54663
H	2.00255	3.42231	-1.26288
H	1.31875	3.47684	1.17913
Be	-0.00564	0.27367	-0.04182
C	0.07984	1.50242	2.43095
H	0.39285	2.39141	3.00416
H	-1.01131	1.35974	2.50508
H	0.56165	0.59812	2.84057
N	0.42839	1.60109	1.03241

S	0.90557	1.36147	-1.79609
C	-1.69409	-0.09522	-0.09579
C	-2.18319	-1.40986	-0.20673
C	-2.66226	0.92517	-0.01363
H	-1.47196	-2.24159	-0.27141
H	-2.34368	1.97427	0.06956
C	-3.55045	-1.69294	-0.23151
C	-4.03313	0.65981	-0.03793
H	-3.89351	-2.72919	-0.31761
H	-4.75553	1.48037	0.02596
C	-4.48109	-0.65697	-0.14658
H	-5.55371	-0.87442	-0.16641
I	1.77435	-1.31680	0.10968

5.4cl

C	0.74781	2.73430	-1.05546
C	0.21825	2.87322	0.27601
H	1.41194	3.50664	-1.45777
H	0.31475	3.82689	0.81525
Be	-0.25631	0.36475	-0.04598
C	-0.80823	1.89289	2.20071
H	-0.72201	2.90498	2.63152
H	-1.86185	1.56885	2.20235
H	-0.23979	1.17782	2.81952
N	-0.30347	1.83594	0.84552
S	0.48585	1.32159	-1.84855
C	1.43659	-0.35216	-0.02462
C	1.56810	-1.70457	-0.37899
C	2.55046	0.29936	0.51577
H	0.72382	-2.23716	-0.82883
H	2.50633	1.37521	0.73808
C	2.75549	-2.39520	-0.12802
C	3.73723	-0.38426	0.77801
H	2.83396	-3.45447	-0.39129
H	4.58888	0.14080	1.22153
C	3.83897	-1.73904	0.45622
H	4.77115	-2.27907	0.64741
I	-2.17395	-0.93083	-0.00743

5.4dl

C	0.83354	2.94338	-0.18077
C	0.99358	2.31498	1.05662
H	1.33371	3.89706	-0.38261
H	1.66173	2.70802	1.83147

Be	-0.38527	0.55114	-0.14827
C	0.40651	0.50250	2.52620
H	-0.25857	1.07784	3.19236
H	0.01290	-0.51952	2.44437
H	1.42396	0.47965	2.95153
N	0.38508	1.13682	1.21853
S	-0.06522	2.19078	-1.38607
C	1.42090	-0.35352	-0.02164
C	1.26390	-1.73008	0.13285
C	2.65335	0.19204	-0.33338
H	0.29930	-2.16967	0.40204
H	2.78631	1.28197	-0.37833
C	2.36079	-2.56551	-0.10900
C	3.74209	-0.64274	-0.58439
H	2.23892	-3.64828	-0.01034
H	4.71039	-0.21070	-0.85355
C	3.59349	-2.02698	-0.47191
H	4.44720	-2.68584	-0.65433
I	-2.30897	-0.70245	-0.12056

6.1aF

C	1.03926	0.05972	1.43381
C	0.76746	-0.22245	2.92150
C	2.10872	-0.69411	3.43458
C	2.99812	-0.60550	2.44368
N	2.37009	-0.16612	1.25996
C	0.36468	1.03780	3.71869
C	-0.33616	-1.28356	3.07062
C	3.10846	-0.05963	0.04163
C	3.34413	1.21518	-0.52260
C	4.11061	1.27463	-1.68812
C	4.65116	0.12510	-2.26026
C	4.41761	-1.11397	-1.68225
C	3.62758	-1.23578	-0.53287
C	2.80766	2.47973	0.13592
C	3.37096	-2.62096	0.04842
C	2.78928	-3.58627	-0.99154
C	4.65022	-3.20666	0.66331
C	2.81687	3.71353	-0.76712
C	3.54796	2.79067	1.44556
H	2.27062	4.53193	-0.26919
H	2.31438	3.52869	-1.73085
H	3.84275	4.07039	-0.97112
H	1.75502	2.27935	0.38706
H	3.48154	1.96550	2.17277

H	3.11177	3.68835	1.91853
H	4.61714	2.99255	1.25223
H	4.30461	2.24010	-2.15882
H	5.258295	0.201178	-3.16681
H	4.844108	-2.0098	-2.14229
H	2.620611	-2.52651	0.848891
H	3.477759	-3.74338	-1.83993
H	1.834455	-3.21089	-1.3921
H	2.608022	-4.57219	-0.52976
H	4.440792	-4.17783	1.144884
H	5.084096	-2.53677	1.424074
H	5.420331	-3.37176	-0.11139
H	-0.05368	-2.21468	2.556518
H	-1.28401	-0.92581	2.633988
H	-0.5109	-1.51245	4.137362
H	-0.60647	1.425432	3.375147
H	1.12646	1.829702	3.620164
H	0.282543	0.782848	4.790591
H	4.071301	-0.79539	2.432854
H	2.312205	-0.97881	4.467393
Be	-0.15611	0.414063	0.312372
C	-0.75546	-0.10271	-1.16118
C	-0.23131	0.086455	-2.58563
C	-1.44518	-0.21942	-3.43963
C	-2.4282	-0.65157	-2.64534
N	-2.01195	-0.62235	-1.29634
C	0.328925	1.497184	-2.80754
C	0.874024	-0.94804	-2.89368
C	-2.75467	-1.26103	-0.24855
C	-3.94779	-0.67914	0.217951
C	-4.63229	-1.31131	1.262811
C	-4.15762	-2.48833	1.8202
C	-3.00024	-3.07618	1.315618
C	-2.28191	-2.49325	0.270903
C	-4.54877	0.570065	-0.4033
C	-1.07177	-3.20844	-0.32231
C	-0.50748	-4.32164	0.563672
C	-1.3997	-3.79481	-1.70467
C	-4.80555	1.677275	0.624889
C	-5.82843	0.225739	-1.17897
H	-5.12629	2.602517	0.115261
H	-3.89195	1.902732	1.195905
H	-5.60249	1.393916	1.335681
H	-3.82583	0.960284	-1.1323
H	-5.6439	-0.54639	-1.9461
H	-6.22768	1.123072	-1.68367

H	-6.61297	-0.15838	-0.5028
H	-5.55599	-0.8674	1.64508
H	-4.69763	-2.96464	2.643564
H	-2.65798	-4.01629	1.751134
H	-0.27625	-2.45304	-0.44411
H	-1.20487	-5.17398	0.645994
H	-0.27333	-3.97135	1.581702
H	0.423714	-4.70819	0.119538
H	-0.50516	-4.28066	-2.13379
H	-1.73593	-3.02897	-2.42006
H	-2.19386	-4.55861	-1.62077
H	0.503878	-1.97581	-2.7483
H	1.742193	-0.78703	-2.23626
H	1.206848	-0.84688	-3.94253
H	0.716626	1.601064	-3.83696
H	1.157718	1.675985	-2.10411
H	-0.43197	2.27373	-2.63767
H	-3.42663	-1.02019	-2.88445
H	-1.46818	-0.16225	-4.52844
C	-0.30541	3.357724	1.225265
C	-0.35546	4.711597	0.909289
C	-1.12143	5.182697	-0.15864
C	-1.86877	4.257954	-0.8975
C	-1.83859	2.90377	-0.59839
C	-1.00156	2.419499	0.430431
H	0.318266	3.02406	2.051509
H	0.227194	5.410965	1.517909
H	-1.15099	6.247897	-0.4006
H	-2.49021	4.597849	-1.73234
H	-2.41671	2.205062	-1.2027
F	-1.55393	1.22166	1.181963

6.2aF

C	1.11420	-0.10052	1.42032
C	1.01800	0.02445	2.93995
C	2.31368	-0.54835	3.44559
C	3.00833	-0.98357	2.40010
N	2.27645	-0.69754	1.19965
C	0.80985	1.47613	3.40493
C	-0.14876	-0.87475	3.41669
C	2.84776	-1.15209	-0.04274
C	3.97279	-0.47929	-0.55819
C	4.57900	-1.01265	-1.70146
C	4.10467	-2.17607	-2.29074
C	3.00091	-2.82832	-1.75261

C	2.34299	-2.33283	-0.62475
C	4.57160	0.76603	0.08640
C	1.13555	-3.06443	-0.04673
C	0.42865	-3.95982	-1.06840
C	1.53291	-3.89075	1.18609
C	4.97443	1.82820	-0.94722
C	5.80033	0.41904	0.94303
H	5.15230	2.79144	-0.44073
H	4.19472	1.98673	-1.70905
H	5.90797	1.55289	-1.46921
H	3.80721	1.21277	0.74214
H	5.56285	-0.27068	1.76677
H	6.22195	1.33680	1.38850
H	6.58543	-0.05084	0.32391
H	5.44813	-0.51027	-2.13291
H	4.597969	-2.58108	-3.17874
H	2.639352	-3.73671	-2.23657
H	0.409724	-2.2969	0.274506
H	1.058916	-4.81188	-1.37735
H	0.131352	-3.40234	-1.97321
H	-0.48387	-4.3871	-0.6255
H	0.649018	-4.39357	1.613956
H	1.974951	-3.26661	1.979009
H	2.270567	-4.66503	0.909169
H	0.030084	-1.92896	3.141106
H	-1.0837	-0.52013	2.956877
H	-0.22693	-0.8191	4.516619
H	-0.16012	1.841684	3.039319
H	1.601527	2.136622	3.015778
H	0.827052	1.509838	4.508735
H	3.955061	-1.51595	2.325495
H	2.593708	-0.62745	4.496499
Be	-0.25178	0.838114	0.467356
C	-0.99749	0.19704	-1.14764
C	-0.5138	0.280308	-2.58866
C	-1.60808	-0.38154	-3.38502
C	-2.6141	-0.64346	-2.55421
N	-2.23493	-0.26378	-1.22708
C	-0.50548	1.78711	-2.9736
C	0.868409	-0.32358	-2.82686
C	-3.25587	-0.32267	-0.20424
C	-3.95087	0.85986	0.111682
C	-5.03591	0.750814	0.980187
C	-5.41183	-0.47691	1.520282
C	-4.68832	-1.61974	1.213175
C	-3.58926	-1.56311	0.347615

C	-3.5439	2.207984	-0.46286
C	-2.79682	-2.82483	0.05171
C	-2.294	-3.46887	1.348346
C	-3.60503	-3.81845	-0.79133
C	-3.82469	3.372268	0.488872
C	-4.20358	2.449822	-1.82806
H	-3.32987	4.284282	0.113674
H	-3.42677	3.155136	1.493459
H	-4.9041	3.59306	0.574258
H	-2.45256	2.191712	-0.60015
H	-3.96071	1.653808	-2.5527
H	-3.86251	3.409148	-2.25619
H	-5.30345	2.491218	-1.72791
H	-5.59753	1.646433	1.254524
H	-6.26848	-0.53589	2.197827
H	-4.97922	-2.57668	1.655922
H	-1.90925	-2.53653	-0.53315
H	-3.12894	-3.78549	1.996972
H	-1.67267	-2.76012	1.918348
H	-1.69307	-4.36898	1.13229
H	-2.99678	-4.70652	-1.04029
H	-3.94209	-3.36227	-1.7377
H	-4.50202	-4.16401	-0.24728
H	0.866667	-1.40772	-2.64568
H	1.61579	0.1344	-2.16042
H	1.179011	-0.15196	-3.87211
H	-0.28032	1.878045	-4.05027
H	0.253643	2.331259	-2.39479
H	-1.48442	2.2563	-2.78437
H	-3.60942	-1.05584	-2.71874
H	-1.59189	-0.53696	-4.46428
C	1.687051	2.731474	-0.46658
C	2.197056	4.021963	-0.63991
C	1.505896	5.113975	-0.11412
C	0.314855	4.891534	0.579757
C	-0.16993	3.590945	0.740769
C	0.49152	2.463744	0.218826
H	2.240634	1.892604	-0.90595
H	3.133136	4.179806	-1.1868
H	1.893715	6.129779	-0.24299
H	-0.23621	5.74021	1.00072
H	-1.1005	3.439712	1.299925
F	-1.45277	0.890906	1.442334

6.3aF

C	1.44537	0.10644	1.45820
C	1.48182	0.45892	2.94033
C	2.94887	0.53710	3.25954
C	3.63072	0.19608	2.17059
N	2.70712	-0.04999	1.10198
C	0.72694	1.76207	3.25499
C	0.87624	-0.72347	3.74371
C	3.23827	-0.47756	-0.16794
C	4.00932	0.43589	-0.91138
C	4.58361	-0.01907	-2.10269
C	4.40528	-1.32708	-2.52922
C	3.65281	-2.21380	-1.76560
C	3.05570	-1.81847	-0.56616
C	4.26573	1.87254	-0.46886
C	2.26498	-2.81199	0.28177
C	1.83658	-4.06606	-0.48392
C	3.05700	-3.22337	1.53300
C	3.96504	2.89769	-1.57241
C	5.71404	2.04839	0.01427
H	4.02347	3.91869	-1.15755
H	2.96157	2.76341	-2.00533
H	4.69922	2.83511	-2.39424
H	3.59818	2.09955	0.37726
H	5.97517	1.34702	0.82300
H	5.87111	3.07386	0.39121
H	6.42564	1.87815	-0.81292
H	5.18207	0.66635	-2.70845
H	4.858768	-1.66478	-3.46514
H	3.523689	-3.23615	-2.12291
H	1.343032	-2.3028	0.611406
H	2.70296	-4.68525	-0.77615
H	1.258039	-3.82235	-1.38999
H	1.19828	-4.69299	0.159367
H	2.447039	-3.89226	2.164688
H	3.351687	-2.36066	2.151657
H	3.97657	-3.76447	1.246717
H	1.37642	-1.67464	3.492475
H	-0.19366	-0.80623	3.508204
H	1.016462	-0.53357	4.821779
H	-0.33791	1.64389	3.005214
H	1.129387	2.611018	2.678564
H	0.823948	1.986108	4.331523
H	4.695198	0.058894	1.989814
H	3.361786	0.770649	4.241256
Be	-0.2309	0.081775	0.667506
C	-0.86555	-0.00494	-0.92648

C	-0.27983	0.039957	-2.35814
C	-1.4842	0.305492	-3.2312
C	-2.57215	0.122429	-2.48823
N	-2.23349	-0.1311	-1.13956
C	0.88318	0.974087	-2.66258
C	0.180078	-1.40934	-2.65393
C	-3.25058	-0.63871	-0.25836
C	-4.44479	0.100448	-0.07997
C	-5.46667	-0.45322	0.699812
C	-5.33006	-1.69523	1.300339
C	-4.15379	-2.40971	1.115122
C	-3.10584	-1.91203	0.339249
C	-4.71046	1.472254	-0.69905
C	-1.89442	-2.8085	0.124174
C	-1.3776	-3.4179	1.431616
C	-2.20673	-3.88575	-0.92216
C	-5.14278	2.509033	0.350703
C	-5.78077	1.396959	-1.79966
H	-5.12506	3.521998	-0.08827
H	-4.48163	2.503879	1.232043
H	-6.1704	2.321615	0.70818
H	-3.77872	1.84188	-1.15245
H	-5.52711	0.668358	-2.58748
H	-5.91415	2.383345	-2.27843
H	-6.75455	1.091452	-1.37757
H	-6.39529	0.107224	0.840835
H	-6.13966	-2.10859	1.908641
H	-4.05267	-3.39422	1.579252
H	-1.08034	-2.18951	-0.27103
H	-2.08469	-4.14705	1.865435
H	-1.19306	-2.61964	2.167242
H	-0.43246	-3.95813	1.25231
H	-1.30594	-4.48601	-1.1456
H	-2.56019	-3.43336	-1.86533
H	-2.99526	-4.57351	-0.56572
H	-0.63177	-2.13386	-2.4828
H	1.032183	-1.66854	-2.00958
H	0.501561	-1.49864	-3.70693
H	1.233859	0.791621	-3.69406
H	1.729761	0.778485	-1.98869
H	0.588582	2.030372	-2.58087
H	-3.61703	0.096487	-2.78966
H	-1.44766	0.496868	-4.3039
C	-1.702	2.468601	0.532098
C	-1.79997	3.836643	0.788549
C	-0.70054	4.667515	0.56385

C	0.494257	4.112202	0.105772
C	0.56933	2.740022	-0.14351
C	-0.52871	1.891554	0.042167
H	-2.54247	1.811938	0.764336
H	-2.73306	4.257438	1.176895
H	-0.77165	5.741898	0.759878
H	1.373798	4.746384	-0.04967
H	1.526417	2.322571	-0.45908
F	-1.20417	-0.26616	1.780383

6.4aF

C	1.12051	0.66931	1.27351
C	1.13669	0.95138	2.85647
C	2.63291	1.05324	3.12409
C	3.30907	0.47344	2.12589
N	2.49828	0.11201	1.05659
C	0.38042	2.21735	3.28452
C	0.59352	-0.20517	3.71890
C	2.92344	-0.82601	0.07485
C	3.88946	-0.46510	-0.90019
C	4.23071	-1.38526	-1.89868
C	3.69016	-2.66246	-1.92808
C	2.82667	-3.05129	-0.91081
C	2.44666	-2.16362	0.09958
C	4.66174	0.84596	-0.86746
C	1.64510	-2.68869	1.27605
C	0.65112	-3.79358	0.91941
C	2.60252	-3.14372	2.38660
C	4.43482	1.71263	-2.11020
C	6.15759	0.58876	-0.63376
H	4.99538	2.66055	-2.02362
H	3.36937	1.96470	-2.23238
H	4.77768	1.20497	-3.02972
H	4.31005	1.41697	-0.00362
H	6.31930	-0.02476	0.26944
H	6.69387	1.54491	-0.49946
H	6.62237	0.06045	-1.48507
H	4.95671	-1.09496	-2.66421
H	3.96938	-3.3657	-2.71791
H	2.446994	-4.0758	-0.89587
H	1.056983	-1.86463	1.690745
H	1.149487	-4.754	0.695355
H	0.036308	-3.51156	0.047842
H	-0.03496	-3.96166	1.765047
H	2.033143	-3.50113	3.262909

H	3.248597	-2.31362	2.718508
H	3.250466	-3.96699	2.034216
H	1.106915	-1.15192	3.49805
H	-0.48662	-0.35801	3.56624
H	0.775044	0.019606	4.785993
H	-0.69694	2.142178	3.049921
H	0.774389	3.131545	2.814666
H	0.47041	2.337295	4.379096
H	4.380452	0.257986	2.074597
H	3.063067	1.418461	4.05834
Be	-0.27826	-0.31503	0.678871
C	-1.00989	-0.14422	-1.02403
C	-0.36472	-0.07509	-2.39084
C	-1.51299	0.213852	-3.31779
C	-2.63778	0.182833	-2.60566
N	-2.31038	-0.05573	-1.23317
C	0.800042	0.911164	-2.50635
C	0.147793	-1.51394	-2.68024
C	-3.38111	-0.26804	-0.28263
C	-4.13277	0.832414	0.155193
C	-5.21255	0.580777	1.010075
C	-5.52687	-0.71128	1.403867
C	-4.76807	-1.78445	0.946179
C	-3.68286	-1.59273	0.091593
C	-3.85096	2.261501	-0.28412
C	-2.89851	-2.78161	-0.44215
C	-2.8747	-3.97051	0.518792
C	-3.4216	-3.20559	-1.82237
C	-3.73083	3.215047	0.912017
C	-4.92318	2.758578	-1.26443
H	-3.44225	4.224628	0.573483
H	-2.9748	2.868643	1.636017
H	-4.69082	3.314957	1.446913
H	-2.88834	2.273384	-0.81911
H	-5.00684	2.101814	-2.1466
H	-4.68061	3.77544	-1.61957
H	-5.91511	2.795421	-0.7805
H	-5.82068	1.414335	1.371039
H	-6.37123	-0.88821	2.075953
H	-5.02802	-2.79414	1.269234
H	-1.85396	-2.45961	-0.55382
H	-3.86132	-4.46011	0.6011
H	-2.54715	-3.65167	1.521346
H	-2.16452	-4.73105	0.152372
H	-2.82377	-4.0451	-2.21925
H	-3.37286	-2.3829	-2.55619

H	-4.47348	-3.53682	-1.75595
H	-0.66409	-2.2577	-2.61141
H	0.944277	-1.78491	-1.97207
H	0.56639	-1.54962	-3.69993
H	1.240331	0.840728	-3.51611
H	1.576987	0.653151	-1.77249
H	0.481228	1.949311	-2.32559
H	-3.6852	0.283215	-2.88714
H	-1.42343	0.357937	-4.39471
C	2.067442	2.838357	0.211482
C	1.8928	4.051273	-0.45226
C	0.613941	4.504364	-0.77262
C	-0.48305	3.735806	-0.38758
C	-0.29099	2.520674	0.268221
C	0.986874	2.020546	0.561216
H	3.071707	2.529781	0.489215
H	2.76943	4.652281	-0.71392
H	0.472036	5.453599	-1.29701
H	-1.49593	4.08559	-0.60456
H	-1.17081	1.948543	0.581171
F	-1.15429	-1.17455	1.496888

6.1aCl

C	1.256415	-0.072178	1.440513
C	1.158473	-0.395046	2.952817
C	2.565083	-0.808059	3.321054
C	3.339306	-0.683896	2.244509
N	2.577664	-0.258230	1.139064
C	0.791650	0.809453	3.847135
C	0.169353	-1.552378	3.180129
C	3.212789	-0.176115	-0.135147
C	3.441277	1.085198	-0.727178
C	4.122225	1.107904	-1.946513
C	4.584335	-0.064442	-2.541814
C	4.363685	-1.290816	-1.931092
C	3.664161	-1.374099	-0.721958
C	2.979922	2.369911	-0.046968
C	3.410410	-2.741291	-0.096520
C	2.525960	-3.625105	-0.984266
C	4.728008	-3.446539	0.250822
C	3.004887	3.599911	-0.955985
C	3.785551	2.664751	1.227948
H	2.521344	4.445378	-0.439821
H	2.455591	3.438501	-1.897948
H	4.038170	3.903740	-1.203849

H	1.931709	2.211332	0.257491
H	3.714853	1.853911	1.969755
H	3.402990	3.584933	1.703695
H	4.852944	2.822429	0.989455
H	4.308759	2.061093	-2.444500
H	5.120999	-0.015127	-3.493564
H	4.725379	-2.204910	-2.411066
H	2.858753	-2.596723	0.843354
H	2.973774	-3.788394	-1.980784
H	1.534869	-3.167400	-1.126592
H	2.381951	-4.613306	-0.512552
H	4.530303	-4.395162	0.779738
H	5.362450	-2.819083	0.900181
H	5.310562	-3.684578	-0.656865
H	0.508578	-2.447575	2.635020
H	-0.842157	-1.291934	2.825691
H	0.107638	-1.803096	4.254828
H	-0.228917	1.168596	3.655390
H	1.503412	1.638581	3.694861
H	0.858526	0.504878	4.907126
H	4.409481	-0.846254	2.112329
H	2.880520	-1.094424	4.324743
Be	-0.039723	0.264863	0.403018
C	-0.760992	-0.130353	-1.073768
C	-0.197565	0.078678	-2.487573
C	-1.388423	-0.160000	-3.384378
C	-2.412422	-0.556808	-2.629708
N	-2.045170	-0.562817	-1.263817
C	0.396754	1.481604	-2.660687
C	0.872998	-0.981339	-2.814409
C	-2.933632	-1.134678	-0.294858
C	-4.165395	-0.501085	-0.033309
C	-5.017559	-1.074607	0.915781
C	-4.667046	-2.237226	1.585214
C	-3.465371	-2.872926	1.283976
C	-2.585436	-2.357348	0.329295
C	-4.629735	0.751746	-0.764580
C	-1.344551	-3.143804	-0.082006
C	-0.960659	-4.264372	0.887182
C	-1.519695	-3.738646	-1.488777
C	-5.021131	1.892414	0.183162
C	-5.792336	0.423040	-1.713655
H	-5.252342	2.803014	-0.396965
H	-4.205350	2.130134	0.882935
H	-5.919428	1.639376	0.774002
H	-3.796601	1.116864	-1.382768

H	-5.531238	-0.379479	-2.424426
H	-6.081053	1.315901	-2.295871
H	-6.679937	0.086446	-1.148997
H	-5.974396	-0.593827	1.138221
H	-5.339656	-2.664754	2.334264
H	-3.224685	-3.807168	1.794102
H	-0.499705	-2.434132	-0.111903
H	-1.676617	-5.104783	0.846918
H	-0.903833	-3.914681	1.930009
H	0.030098	-4.664666	0.611237
H	-0.603824	-4.276600	-1.792291
H	-1.722140	-2.969995	-2.250705
H	-2.356722	-4.459972	-1.499940
H	0.462059	-1.998325	-2.709434
H	1.733596	-0.878082	-2.140551
H	1.226558	-0.855984	-3.853699
H	0.837244	1.592945	-3.667791
H	1.189036	1.640224	-1.915171
H	-0.361376	2.266208	-2.519068
H	-3.413599	-0.885081	-2.907872
H	-1.368469	-0.089964	-4.472362
C	-0.038896	3.275126	1.444880
C	0.143070	4.594845	1.048704
C	-0.523087	5.119196	-0.061668
C	-1.409601	4.289850	-0.757002
C	-1.611353	2.971583	-0.373276
C	-0.877200	2.416681	0.698193
H	0.501874	2.894480	2.309518
H	0.825525	5.225570	1.627853
H	-0.372720	6.158029	-0.365612
H	-1.959832	4.677190	-1.620497
H	-2.303792	2.342220	-0.934401
Cl	-1.836182	1.095232	1.701826

6.2aCl

C	1.330265	-0.068468	1.452949
C	1.470241	0.102513	2.973798
C	2.890981	-0.287627	3.267387
C	3.447508	-0.708249	2.139662
N	2.502473	-0.566808	1.068842
C	1.161110	1.525674	3.469347
C	0.566899	-0.944429	3.679720
C	2.964546	-1.034296	-0.217400
C	4.006131	-0.330688	-0.853307
C	4.527591	-0.862819	-2.037596

C	4.058966	-2.060947	-2.554588
C	3.053501	-2.754523	-1.890595
C	2.484407	-2.264232	-0.712166
C	4.619727	0.954082	-0.309161
C	1.412513	-3.066897	0.014360
C	0.700352	-4.067379	-0.898249
C	2.009442	-3.797737	1.226772
C	4.642837	2.073879	-1.360165
C	6.041885	0.710931	0.219316
H	4.920047	3.029300	-0.883271
H	3.661668	2.209590	-1.842630
H	5.386005	1.871774	-2.151285
H	4.007174	1.304031	0.535335
H	6.069162	-0.059343	1.006683
H	6.454221	1.642297	0.644628
H	6.714973	0.382164	-0.592203
H	5.328842	-0.331430	-2.557964
H	4.484256	-2.465464	-3.477294
H	2.703546	-3.697609	-2.311531
H	0.652810	-2.356403	0.383074
H	1.375850	-4.874260	-1.231191
H	0.274492	-3.579038	-1.791767
H	-0.123129	-4.551265	-0.352912
H	1.221116	-4.343145	1.773934
H	2.488371	-3.104994	1.937281
H	2.769788	-4.529147	0.899090
H	0.765766	-1.961542	3.299199
H	-0.491402	-0.697734	3.515671
H	0.784529	-0.932724	4.761797
H	0.111222	1.780002	3.266093
H	1.803062	2.266762	2.967048
H	1.343782	1.573265	4.557548
H	4.424433	-1.137125	1.924318
H	3.342929	-0.278843	4.259442
Be	-0.231468	0.743818	0.625774
C	-0.969384	0.206507	-1.038051
C	-0.409456	0.491707	-2.432615
C	-1.351135	-0.221987	-3.363110
C	-2.377740	-0.662362	-2.641834
N	-2.147290	-0.359718	-1.261304
C	-0.589767	2.017736	-2.697873
C	1.055572	0.127322	-2.638226
C	-3.279040	-0.582142	-0.382661
C	-4.179355	0.484198	-0.194120
C	-5.363237	0.212435	0.490227
C	-5.633033	-1.058002	0.991136

C	-4.704346	-2.075614	0.830532
C	-3.508805	-1.858397	0.137165
C	-3.870142	1.895275	-0.670172
C	-2.476829	-2.967392	0.059810
C	-1.889313	-3.203338	1.458359
C	-3.048535	-4.249614	-0.554750
C	-4.347648	2.968618	0.312147
C	-4.429907	2.150471	-2.076071
H	-3.918701	3.945325	0.028940
H	-4.014973	2.730256	1.335784
H	-5.446898	3.079186	0.311310
H	-2.774763	1.994044	-0.705938
H	-4.037159	1.430193	-2.813829
H	-4.164527	3.165911	-2.420217
H	-5.531846	2.066637	-2.076100
H	-6.085525	1.014930	0.656433
H	-6.566567	-1.246535	1.528780
H	-4.904725	-3.059891	1.263147
H	-1.655818	-2.624510	-0.589963
H	-2.672328	-3.529097	2.165549
H	-1.452260	-2.269962	1.849841
H	-1.112539	-3.986775	1.439135
H	-2.264774	-5.020044	-0.657754
H	-3.471262	-4.058613	-1.556479
H	-3.849579	-4.678459	0.072079
H	1.227078	-0.951201	-2.515441
H	1.685408	0.668341	-1.917627
H	1.371677	0.412769	-3.656552
H	-0.330540	2.219556	-3.751392
H	0.067852	2.607120	-2.043617
H	-1.629009	2.340318	-2.531739
H	-3.302766	-1.168861	-2.916097
H	-1.235335	-0.279568	-4.445804
C	1.515175	2.886862	0.017036
C	1.849450	4.228812	-0.188543
C	0.904919	5.221320	0.071589
C	-0.353195	4.848228	0.549854
C	-0.657564	3.500385	0.753984
C	0.257439	2.467213	0.477675
H	2.270016	2.127382	-0.204786
H	2.845659	4.501003	-0.554891
H	1.147718	6.276657	-0.089180
H	-1.101752	5.617471	0.770554
H	-1.643374	3.237755	1.152849
Cl	-1.804733	0.594574	1.993448

6.3aCl

C	-1.583398	-0.293221	1.447654
C	-1.729555	-0.908705	2.843673
C	-3.204216	-1.166366	2.974045
C	-3.814697	-0.630515	1.923622
N	-2.825549	-0.125954	1.019034
C	-0.855515	-2.144461	3.094343
C	-1.424116	0.187757	3.910102
C	-3.285435	0.538861	-0.173347
C	-4.032520	-0.198649	-1.113179
C	-4.520767	0.487522	-2.229536
C	-4.292363	1.846750	-2.394384
C	-3.580645	2.556629	-1.432749
C	-3.063825	1.925550	-0.299075
C	-4.375352	-1.678424	-0.950673
C	-2.354113	2.726074	0.787802
C	-1.739011	4.037008	0.296148
C	-3.321900	2.994701	1.950950
C	-3.998955	-2.535337	-2.167714
C	-5.873764	-1.850158	-0.650549
H	-4.246673	-3.591790	-1.966021
H	-2.925459	-2.481314	-2.400095
H	-4.557363	-2.232689	-3.070295
H	-3.811379	-2.077485	-0.093350
H	-6.203659	-1.246712	0.211300
H	-6.103616	-2.907947	-0.434931
H	-6.483354	-1.541581	-1.518098
H	-5.095068	-0.055494	-2.984868
H	-4.680334	2.362730	-3.276869
H	-3.417349	3.626028	-1.576383
H	-1.518548	2.120349	1.171833
H	-2.505060	4.769961	-0.012429
H	-1.048682	3.871984	-0.548123
H	-1.162486	4.495524	1.116153
H	-2.800618	3.514472	2.773467
H	-3.749332	2.063097	2.359137
H	-4.160201	3.631779	1.616446
H	-1.995094	1.110193	3.711626
H	-0.352104	0.424349	3.905883
H	-1.719913	-0.195989	4.901441
H	0.207922	-1.876784	3.007270
H	-1.075763	-2.948998	2.375197
H	-1.045263	-2.520238	4.114813
H	-4.867332	-0.506766	1.678742
H	-3.677200	-1.615506	3.847573
Be	0.122897	-0.055653	0.697991
C	0.829784	0.061278	-0.875671

C	0.203694	0.142662	-2.303873
C	1.372628	-0.080010	-3.231829
C	2.485154	-0.005704	-2.509381
N	2.204512	0.160499	-1.137659
C	-0.963303	-0.757684	-2.676007
C	-0.259515	1.608735	-2.472966
C	3.303548	0.570155	-0.300214
C	4.412938	-0.290433	-0.138347
C	5.491748	0.148904	0.639004
C	5.495029	1.401600	1.231008
C	4.421371	2.258257	1.018570
C	3.327610	1.875180	0.242993
C	4.544706	-1.659402	-0.801798
C	2.247879	2.895794	-0.079488
C	2.005474	3.922147	1.028845
C	2.600561	3.599308	-1.399157
C	4.959501	-2.758432	0.189913
C	5.564824	-1.623099	-1.952015
H	4.809723	-3.754401	-0.262172
H	4.381708	-2.712621	1.126648
H	6.027332	-2.676594	0.458379
H	3.567775	-1.941291	-1.222631
H	5.319618	-0.865105	-2.713575
H	5.614698	-2.605294	-2.454840
H	6.573635	-1.386276	-1.569878
H	6.352069	-0.510995	0.781628
H	6.342078	1.720399	1.845402
H	4.443189	3.254339	1.465203
H	1.302634	2.351965	-0.213696
H	2.859603	4.609723	1.160823
H	1.802477	3.418083	1.988058
H	1.132980	4.546069	0.770075
H	1.803180	4.304602	-1.696565
H	2.742638	2.875099	-2.219787
H	3.539888	4.171494	-1.291288
H	0.562061	2.315633	-2.293551
H	-1.076281	1.829174	-1.771105
H	-0.631189	1.772154	-3.500185
H	-1.325056	-0.478812	-3.681704
H	-1.801373	-0.621349	-1.981916
H	-0.668857	-1.816961	-2.701714
H	3.523048	-0.010424	-2.836191
H	1.294544	-0.199998	-4.312374
C	1.615565	-2.450572	0.503395
C	1.673893	-3.830339	0.702741
C	0.583836	-4.632059	0.361951

C	-0.570762	-4.036136	-0.144086
C	-0.615111	-2.652124	-0.320777
C	0.483568	-1.829569	-0.030832
H	2.451846	-1.824463	0.819978
H	2.570564	-4.283539	1.135746
H	0.628315	-5.715394	0.510167
H	-1.447227	-4.646244	-0.387064
H	-1.553329	-2.210155	-0.657716
Cl	1.336498	0.484704	2.225891

6.4aCl

C	1.529745	-0.368851	1.531039
C	1.691800	-0.539390	3.046023
C	3.174072	-0.652550	3.247110
C	3.766144	-0.550083	2.063741
N	2.762527	-0.374245	1.058713
C	1.193727	0.722899	3.792523
C	1.010264	-1.826388	3.559238
C	3.261610	-0.199203	-0.284206
C	3.755086	1.067741	-0.637023
C	4.359742	1.188511	-1.892425
C	4.481819	0.091843	-2.735895
C	4.003863	-1.155743	-2.344506
C	3.385412	-1.334595	-1.106262
C	3.719428	2.261743	0.310998
C	2.861861	-2.699694	-0.670492
C	2.460463	-3.601933	-1.841127
C	3.871588	-3.434097	0.225209
C	3.191036	3.546714	-0.337324
C	5.114139	2.505859	0.909215
H	3.141499	4.348183	0.419478
H	2.179727	3.415440	-0.749965
H	3.855260	3.899150	-1.145594
H	3.039501	2.019053	1.143541
H	5.511774	1.611568	1.416092
H	5.077139	3.325202	1.647825
H	5.832420	2.791683	0.120497
H	4.746268	2.159107	-2.213492
H	4.957237	0.208394	-3.713628
H	4.102362	-2.001868	-3.027241
H	1.949782	-2.523398	-0.074943
H	3.341737	-3.959983	-2.401870
H	1.783470	-3.089401	-2.542829
H	1.937640	-4.493982	-1.456507
H	3.466954	-4.416180	0.525708

H	4.102904	-2.876816	1.146735
H	4.817840	-3.605469	-0.317755
H	1.378909	-2.710158	3.010097
H	-0.079566	-1.754523	3.441279
H	1.251199	-1.959959	4.627809
H	0.110762	0.849090	3.657650
H	1.712447	1.625588	3.424633
H	1.416956	0.612778	4.867383
H	4.810583	-0.583223	1.758262
H	3.655989	-0.792853	4.214877
Be	-0.190417	-0.090898	0.731242
C	-0.926604	0.563419	-0.796209
C	-0.263753	0.580893	-2.243566
C	-1.484144	0.638672	-3.153180
C	-2.538646	0.173853	-2.471015
N	-2.276827	-0.023890	-1.123744
C	0.717142	1.729872	-2.480236
C	0.464120	-0.732461	-2.559964
C	-3.145452	-0.862685	-0.357355
C	-4.410811	-0.378541	0.044409
C	-5.271928	-1.220317	0.755857
C	-4.914386	-2.522958	1.070886
C	-3.674756	-3.001441	0.664339
C	-2.785515	-2.195775	-0.047237
C	-4.849212	1.052752	-0.210366
C	-1.463496	-2.792128	-0.499340
C	-0.798729	-3.688335	0.550870
C	-1.649601	-3.539700	-1.825656
C	-4.696724	1.890952	1.064810
C	-6.261208	1.161416	-0.796055
H	-4.922472	2.953923	0.863665
H	-3.667226	1.824564	1.453350
H	-5.384219	1.534289	1.853824
H	-4.167033	1.472724	-0.955079
H	-6.365872	0.545613	-1.706646
H	-6.479412	2.210438	-1.064844
H	-7.038699	0.840497	-0.080341
H	-6.243069	-0.838789	1.084485
H	-5.598074	-3.165267	1.633743
H	-3.397719	-4.031314	0.905491
H	-0.771424	-1.959173	-0.690733
H	-1.346404	-4.634495	0.703181
H	-0.732684	-3.172857	1.523582
H	0.222117	-3.959974	0.226617
H	-0.687054	-3.930489	-2.202831
H	-2.079363	-2.876548	-2.595386

H	-2.339303	-4.392747	-1.692167
H	-0.240417	-1.570639	-2.636193
H	1.198861	-0.955370	-1.776184
H	1.002446	-0.664837	-3.523217
H	1.115820	1.670258	-3.509069
H	1.574127	1.655801	-1.793660
H	0.252128	2.719835	-2.353467
H	-3.539139	-0.058474	-2.847800
H	-1.451759	0.866319	-4.219659
C	-2.063342	2.912661	-0.811545
C	-2.127536	4.236460	-0.384120
C	-1.207452	4.732478	0.541027
C	-0.208835	3.886223	1.012993
C	-0.154304	2.565248	0.568989
C	-1.084341	2.029530	-0.332382
H	-2.768227	2.565891	-1.565767
H	-2.906472	4.893137	-0.783898
H	-1.266935	5.769626	0.883554
H	0.533840	4.249298	1.730201
H	0.669675	1.940037	0.936216
Cl	-1.535812	-0.229729	2.182383

6.1aBr

C	1.357049	-0.040028	1.402963
C	1.266411	-0.283541	2.932449
C	2.678231	-0.658001	3.321048
C	3.452018	-0.570730	2.241684
N	2.686302	-0.210443	1.116178
C	0.902925	0.974813	3.752481
C	0.297854	-1.439086	3.241067
C	3.337749	-0.168601	-0.150929
C	3.557250	1.072103	-0.787677
C	4.258813	1.058031	-1.995459
C	4.751797	-0.128764	-2.534646
C	4.543165	-1.333353	-1.877853
C	3.823110	-1.380641	-0.678976
C	3.071358	2.375960	-0.162292
C	3.581225	-2.725898	-0.002833
C	2.710987	-3.651057	-0.861957
C	4.903505	-3.403299	0.379577
C	3.096613	3.570219	-1.117660
C	3.860140	2.726291	1.109266
H	2.606336	4.432822	-0.637984
H	2.554851	3.369802	-2.056592
H	4.130298	3.869581	-1.368868

H	2.021096	2.217931	0.136962
H	3.791285	1.941151	1.878216
H	3.462643	3.658157	1.548963
H	4.927955	2.887944	0.875564
H	4.439825	1.993740	-2.527412
H	5.304755	-0.108098	-3.478103
H	4.930930	-2.258924	-2.313565
H	3.021758	-2.551996	0.927515
H	3.160737	-3.837588	-1.853498
H	1.713258	-3.212749	-1.016802
H	2.581627	-4.626352	-0.360116
H	4.710865	-4.335392	0.938871
H	5.524961	-2.747339	1.013180
H	5.497395	-3.666315	-0.513765
H	0.652785	-2.363411	2.757518
H	-0.719128	-1.223977	2.873478
H	0.243651	-1.616997	4.330554
H	-0.126402	1.309587	3.565396
H	1.599248	1.799607	3.523527
H	0.999742	0.745424	4.828875
H	4.525254	-0.719375	2.118749
H	2.994733	-0.890848	4.338064
Be	0.058850	0.206548	0.335808
C	-0.636849	-0.240843	-1.140714
C	-0.027836	-0.060152	-2.541544
C	-1.176694	-0.357883	-3.472804
C	-2.216184	-0.761000	-2.744425
N	-1.904264	-0.711212	-1.365334
C	0.539514	1.350133	-2.741377
C	1.074558	-1.105995	-2.801264
C	-2.823086	-1.278339	-0.422249
C	-4.096388	-0.692825	-0.262753
C	-4.974616	-1.260087	0.666191
C	-4.610659	-2.369312	1.415033
C	-3.367671	-2.962370	1.210994
C	-2.460890	-2.454904	0.277511
C	-4.576846	0.499456	-1.082265
C	-1.175905	-3.211658	-0.040298
C	-0.784342	-4.254314	1.008661
C	-1.280855	-3.888990	-1.416385
C	-5.087809	1.663105	-0.223248
C	-5.661259	0.063235	-2.079823
H	-5.345152	2.521354	-0.868625
H	-4.327747	1.994613	0.500908
H	-5.998429	1.386910	0.337131
H	-3.725923	0.881094	-1.665810

H	-5.324326	-0.766340	-2.724555
H	-5.951533	0.906586	-2.730929
H	-6.566910	-0.281282	-1.549727
H	-5.962722	-0.814265	0.811643
H	-5.304260	-2.789145	2.149149
H	-3.113969	-3.859016	1.779429
H	-0.357502	-2.472725	-0.083416
H	-1.460212	-5.128202	0.994262
H	-0.785831	-3.837290	2.028183
H	0.233619	-4.624481	0.796720
H	-0.337776	-4.409875	-1.660211
H	-1.483046	-3.168033	-2.224127
H	-2.093023	-4.638193	-1.415967
H	0.680381	-2.127869	-2.681060
H	1.908961	-0.966340	-2.102464
H	1.461371	-1.002451	-3.831068
H	1.018504	1.436478	-3.733252
H	1.295978	1.558032	-1.971586
H	-0.243182	2.118555	-2.660478
H	-3.193448	-1.132228	-3.050726
H	-1.115358	-0.325124	-4.560987
C	-0.038882	3.319330	1.188835
C	0.152459	4.600654	0.681621
C	-0.510195	5.030698	-0.470051
C	-1.399601	4.151319	-1.095329
C	-1.606424	2.870610	-0.600526
C	-0.882827	2.410507	0.518031
H	0.493688	3.013162	2.088634
H	0.836942	5.275430	1.206043
H	-0.354176	6.039062	-0.861672
H	-1.946662	4.467065	-1.989434
H	-2.304190	2.200767	-1.106274
Br	-1.937704	1.079257	1.697141

6.2aBr

C	1.426467	-0.034323	1.411233
C	1.573645	0.186056	2.926316
C	3.004406	-0.162868	3.221541
C	3.559238	-0.616832	2.106433
N	2.603846	-0.531748	1.038734
C	1.234456	1.611930	3.391834
C	0.711625	-0.871944	3.668934
C	3.072744	-1.035960	-0.231633
C	4.101814	-0.335608	-0.891187
C	4.623310	-0.889870	-2.064896

C	4.166976	-2.106028	-2.549300
C	3.178735	-2.798570	-1.858802
C	2.612489	-2.288880	-0.686654
C	4.704895	0.969009	-0.383707
C	1.570878	-3.097020	0.077347
C	0.903770	-4.170460	-0.784571
C	2.189822	-3.749811	1.323160
C	4.673605	2.075343	-1.447987
C	6.145294	0.757373	0.107376
H	4.974610	3.036575	-0.997760
H	3.669145	2.206648	-1.880580
H	5.375846	1.862592	-2.272987
H	4.112777	1.318394	0.474914
H	6.208512	-0.012327	0.893785
H	6.548890	1.697596	0.521468
H	6.804613	0.442105	-0.720554
H	5.413752	-0.360448	-2.603577
H	4.589735	-2.526560	-3.465947
H	2.842728	-3.758063	-2.252771
H	0.782873	-2.400350	0.412575
H	1.616005	-4.960055	-1.079779
H	0.453451	-3.746971	-1.698755
H	0.105622	-4.664889	-0.212240
H	1.416420	-4.290644	1.895697
H	2.648902	-3.012378	2.000484
H	2.970213	-4.474346	1.029286
H	0.941473	-1.891818	3.314805
H	-0.357159	-0.669666	3.514463
H	0.938691	-0.822013	4.747801
H	0.180796	1.847004	3.183911
H	1.864721	2.354394	2.877189
H	1.413420	1.684099	4.479224
H	4.542121	-1.035570	1.898318
H	3.462252	-0.108260	4.209358
Be	-0.146728	0.743461	0.540419
C	-0.840216	0.169024	-1.135248
C	-0.227774	0.468970	-2.506514
C	-1.090347	-0.295405	-3.471981
C	-2.130337	-0.773669	-2.795717
N	-1.981767	-0.447820	-1.409176
C	-0.459426	1.982919	-2.802857
C	1.261061	0.176785	-2.635801
C	-3.153600	-0.698314	-0.591569
C	-4.109587	0.332261	-0.495014
C	-5.319164	0.032369	0.129331
C	-5.563450	-1.230599	0.660517

C	-4.585983	-2.211635	0.587195
C	-3.361359	-1.966455	-0.043541
C	-3.833633	1.741511	-0.996720
C	-2.292526	-3.042898	-0.037423
C	-1.826847	-3.296360	1.403635
C	-2.774969	-4.322646	-0.730248
C	-4.403172	2.822137	-0.072613
C	-4.325654	1.938218	-2.436720
H	-3.999756	3.807076	-0.365042
H	-4.115759	2.628811	0.974085
H	-5.504360	2.887316	-0.133790
H	-2.742615	1.881931	-0.976792
H	-3.863879	1.218726	-3.133758
H	-4.083975	2.955593	-2.792333
H	-5.421592	1.808257	-2.493885
H	-6.081000	0.809160	0.226285
H	-6.516664	-1.441167	1.153486
H	-4.771787	-3.189805	1.039760
H	-1.424902	-2.664952	-0.601308
H	-2.656864	-3.665920	2.030836
H	-1.456436	-2.360938	1.855814
H	-1.025287	-4.054151	1.436620
H	-1.978640	-5.086028	-0.751633
H	-3.078774	-4.119883	-1.772078
H	-3.641663	-4.764252	-0.208087
H	1.479097	-0.892603	-2.509289
H	1.818299	0.746265	-1.878926
H	1.618281	0.486718	-3.633105
H	-0.169577	2.176907	-3.849756
H	0.153329	2.606942	-2.137296
H	-1.515026	2.268431	-2.680370
H	-3.017967	-1.323026	-3.108267
H	-0.920749	-0.357868	-4.547268
C	1.586081	2.912704	0.015911
C	1.901149	4.252487	-0.230842
C	0.907465	5.224582	-0.125495
C	-0.382115	4.834719	0.243423
C	-0.667757	3.490508	0.491428
C	0.299729	2.474501	0.369024
H	2.385480	2.172224	-0.077525
H	2.922967	4.537875	-0.505119
H	1.135751	6.277694	-0.318726
H	-1.170714	5.588909	0.343386
H	-1.683470	3.219235	0.800068
Br	-1.895149	0.607631	2.000329

6.3aBr

C	1.661139	0.335405	1.373213
C	1.819671	0.969199	2.762429
C	3.295525	1.227716	2.875526
C	3.897889	0.658628	1.838353
N	2.901944	0.145703	0.946450
C	0.940310	2.197057	3.024028
C	1.551011	-0.115574	3.853651
C	3.356358	-0.551555	-0.230043
C	4.128404	0.150282	-1.177961
C	4.607626	-0.568779	-2.277138
C	4.353876	-1.926814	-2.415259
C	3.621291	-2.601482	-1.444490
C	3.105444	-1.934864	-0.330760
C	4.518179	1.621220	-1.035447
C	2.364886	-2.699138	0.760240
C	1.683923	-3.977245	0.269663
C	3.323758	-3.007699	1.920127
C	4.184479	2.478989	-2.264165
C	6.020408	1.741689	-0.726632
H	4.512526	3.517684	-2.086688
H	3.106466	2.501179	-2.478641
H	4.704150	2.119880	-3.169054
H	3.962002	2.051937	-0.188342
H	6.327386	1.121864	0.132113
H	6.284561	2.789990	-0.504137
H	6.622900	1.417768	-1.593517
H	5.199238	-0.053630	-3.038683
H	4.738274	-2.468705	-3.283653
H	3.437282	-3.670483	-1.565088
H	1.559792	-2.056398	1.147150
H	2.411348	-4.755339	-0.021740
H	1.019851	-3.776631	-0.588068
H	1.065722	-4.393085	1.081908
H	2.783042	-3.501147	2.746245
H	3.792617	-2.093039	2.321975
H	4.132451	-3.681772	1.585143
H	2.091577	-1.051104	3.634496
H	0.477529	-0.334256	3.915733
H	1.906976	0.270930	4.823891
H	-0.123008	1.926848	2.939289
H	1.153489	3.008562	2.311530
H	1.130029	2.565409	4.047130
H	4.948637	0.516747	1.596473
H	3.775134	1.689901	3.738543
Be	-0.040555	0.093799	0.600657

C	-0.731841	0.026451	-0.984987
C	-0.061849	-0.014726	-2.397236
C	-1.199777	0.242886	-3.353692
C	-2.334374	0.149151	-2.669406
N	-2.099820	-0.066933	-1.296089
C	1.116310	0.893730	-2.704138
C	0.406124	-1.474599	-2.600013
C	-3.232768	-0.510424	-0.521558
C	-4.338620	0.353299	-0.349844
C	-5.447344	-0.114174	0.366395
C	-5.486675	-1.399169	0.882846
C	-4.420528	-2.259481	0.650058
C	-3.295624	-1.847124	-0.063821
C	-4.439295	1.753139	-0.951356
C	-2.220958	-2.864062	-0.415042
C	-2.055317	-3.983330	0.614969
C	-2.521837	-3.454993	-1.801314
C	-4.891491	2.805594	0.073732
C	-5.412419	1.775755	-2.142183
H	-4.721564	3.821131	-0.324242
H	-4.352870	2.712110	1.030155
H	-5.969604	2.715912	0.294013
H	-3.445653	2.049750	-1.319855
H	-5.141604	1.049749	-2.925733
H	-5.434329	2.779175	-2.603335
H	-6.437912	1.531482	-1.812651
H	-6.304051	0.548117	0.518530
H	-6.357428	-1.740459	1.450084
H	-4.471860	-3.280140	1.033936
H	-1.260065	-2.331146	-0.457370
H	-2.932487	-4.653470	0.651112
H	-1.883012	-3.567447	1.621662
H	-1.189049	-4.610339	0.343572
H	-1.725064	-4.154503	-2.113425
H	-2.609429	-2.669531	-2.571260
H	-3.475733	-4.012736	-1.781092
H	-0.418328	-2.186702	-2.463273
H	1.205982	-1.719404	-1.886964
H	0.801888	-1.605761	-3.622827
H	1.528569	0.627793	-3.693726
H	1.918995	0.751520	-1.971321
H	0.819932	1.952301	-2.732853
H	-3.361299	0.171490	-3.028486
H	-1.086767	0.399866	-4.426350
C	-1.566986	2.473885	0.450665
C	-1.647910	3.845686	0.692414

C	-0.568729	4.674141	0.383971
C	0.599740	4.110932	-0.126953
C	0.670192	2.733252	-0.339762
C	-0.420010	1.884748	-0.088944
H	-2.399895	1.827664	0.734921
H	-2.554769	4.271787	1.131005
H	-0.632297	5.752052	0.561461
H	1.468382	4.741627	-0.343202
H	1.622860	2.319754	-0.673416
Br	-1.350494	-0.596198	2.218314

6.4aBr

C	1.596453	-0.374759	1.466940
C	1.762008	-0.582946	2.978757
C	3.240295	-0.745229	3.170899
C	3.830864	-0.625673	1.989205
N	2.829684	-0.399049	0.991873
C	1.324641	0.686820	3.752163
C	1.046686	-1.855867	3.478127
C	3.347914	-0.201034	-0.341723
C	3.859317	1.067896	-0.661030
C	4.490538	1.206231	-1.901409
C	4.624899	0.123723	-2.760928
C	4.133612	-1.127862	-2.400308
C	3.487501	-1.323787	-1.178850
C	3.818370	2.244285	0.308597
C	2.950564	-2.694512	-0.778646
C	2.553686	-3.567501	-1.973259
C	3.945303	-3.459969	0.107962
C	3.341725	3.553435	-0.331650
C	5.198157	2.446612	0.955444
H	3.275410	4.338827	0.440518
H	2.347077	3.451855	-0.790643
H	4.046942	3.911086	-1.101950
H	3.106699	2.000992	1.113977
H	5.556888	1.537307	1.464438
H	5.156443	3.257977	1.702566
H	5.947972	2.724011	0.193594
H	4.889852	2.179611	-2.196949
H	5.121235	0.254205	-3.726406
H	4.244637	-1.963404	-3.094027
H	2.034921	-2.523991	-0.187386
H	3.438412	-3.930981	-2.524979
H	1.898526	-3.030586	-2.677065
H	2.008546	-4.456960	-1.614235

H	3.532792	-4.449655	0.370314
H	4.164441	-2.933739	1.050124
H	4.898599	-3.617895	-0.426690
H	1.394099	-2.742077	2.919283
H	-0.041995	-1.760864	3.365296
H	1.284499	-2.006597	4.545107
H	0.246709	0.864038	3.636762
H	1.876908	1.572398	3.391548
H	1.557109	0.548953	4.821824
H	4.873198	-0.674915	1.679133
H	3.720308	-0.921039	4.133720
Be	-0.119744	-0.043924	0.653396
C	-0.823876	0.590096	-0.907035
C	-0.117736	0.630785	-2.334015
C	-1.310988	0.713230	-3.276477
C	-2.383487	0.230893	-2.637380
N	-2.159103	0.000349	-1.287556
C	0.873350	1.778277	-2.529438
C	0.605694	-0.683352	-2.653473
C	-3.048000	-0.857322	-0.567813
C	-4.349039	-0.406406	-0.244747
C	-5.219906	-1.260358	0.439276
C	-4.842208	-2.545384	0.799307
C	-3.574087	-2.996782	0.456674
C	-2.673105	-2.179197	-0.226384
C	-4.831160	0.999067	-0.562353
C	-1.327521	-2.760491	-0.625861
C	-0.694296	-3.650145	0.449290
C	-1.461968	-3.514710	-1.955045
C	-4.815523	1.873271	0.697044
C	-6.200210	1.023460	-1.252031
H	-5.087947	2.916132	0.452105
H	-3.813629	1.877669	1.156688
H	-5.534717	1.496414	1.447215
H	-4.119934	1.437203	-1.268364
H	-6.210045	0.376794	-2.147232
H	-6.445977	2.052419	-1.569962
H	-7.012098	0.686034	-0.583693
H	-6.217564	-0.902323	0.709650
H	-5.534005	-3.195862	1.342329
H	-3.283313	-4.015724	0.725497
H	-0.636884	-1.921586	-0.795100
H	-1.233656	-4.604897	0.574858
H	-0.678666	-3.138653	1.426269
H	0.343524	-3.906318	0.169569
H	-0.482944	-3.891434	-2.302208

H	-1.879933	-2.861349	-2.739418
H	-2.142458	-4.377516	-1.838404
H	-0.105748	-1.511737	-2.763955
H	1.314334	-0.928122	-1.853151
H	1.171939	-0.604911	-3.599688
H	1.299502	1.727651	-3.547662
H	1.711077	1.695078	-1.821238
H	0.406975	2.767984	-2.405506
H	-3.370005	0.002173	-3.050788
H	-1.246573	0.965302	-4.335921
C	-1.997039	2.923993	-0.873660
C	-2.064613	4.243504	-0.431581
C	-1.122446	4.743558	0.467861
C	-0.097586	3.906567	0.900179
C	-0.040133	2.591438	0.442216
C	-0.992298	2.051700	-0.434552
H	-2.722869	2.574268	-1.605390
H	-2.865223	4.892615	-0.799543
H	-1.185090	5.776399	0.822537
H	0.661643	4.272860	1.598029
H	0.802704	1.972047	0.776775
Br	-1.627539	-0.102397	2.190636

6.1al

C	1.477405	0.014255	1.369273
C	1.381198	-0.119213	2.913287
C	2.795256	-0.439056	3.339274
C	3.578905	-0.399619	2.265465
N	2.818955	-0.130351	1.111142
C	1.010366	1.204806	3.618835
C	0.435158	-1.261973	3.319667
C	3.497236	-0.157097	-0.141382
C	3.714859	1.044449	-0.848631
C	4.440741	0.965151	-2.039472
C	4.962507	-0.245429	-2.491781
C	4.761385	-1.408874	-1.761989
C	4.016786	-1.391638	-0.577618
C	3.210454	2.379481	-0.308394
C	3.779124	-2.693327	0.180201
C	2.917313	-3.673947	-0.623752
C	5.101690	-3.336830	0.615547
C	3.232024	3.511081	-1.337265
C	3.994034	2.813425	0.940570
H	2.740908	4.401601	-0.913326
H	2.690937	3.250225	-2.261703

H	4.265032	3.796823	-1.606004
H	2.160460	2.231629	-0.001381
H	3.933880	2.072867	1.753004
H	3.586458	3.764408	1.327082
H	5.059985	2.973111	0.697373
H	4.620412	1.868076	-2.625674
H	5.533965	-0.275856	-3.423907
H	5.173488	-2.353465	-2.129237
H	3.212469	-2.464141	1.094009
H	3.366389	-3.910631	-1.604830
H	1.915498	-3.253018	-0.798730
H	2.797426	-4.621029	-0.068397
H	4.908119	-4.231915	1.232068
H	5.712980	-2.638116	1.212246
H	5.706365	-3.653777	-0.252683
H	0.805614	-2.215942	2.909938
H	-0.587212	-1.097667	2.943250
H	0.390255	-1.352044	4.420369
H	-0.016144	1.523916	3.396631
H	1.710071	2.005118	3.322959
H	1.094955	1.070217	4.712116
H	4.656698	-0.529429	2.162542
H	3.102933	-0.599656	4.372730
Be	0.191445	0.143104	0.261480
C	-0.484157	-0.380724	-1.202090
C	0.190720	-0.247837	-2.581167
C	-0.895269	-0.631154	-3.552692
C	-1.954726	-1.039364	-2.858576
N	-1.724332	-0.901737	-1.468846
C	0.731273	1.165063	-2.828252
C	1.327902	-1.276539	-2.739986
C	-2.693684	-1.442677	-0.560158
C	-4.003366	-0.915400	-0.555374
C	-4.929148	-1.456733	0.342210
C	-4.578680	-2.482925	1.207428
C	-3.298052	-3.025240	1.151345
C	-2.341372	-2.545809	0.253737
C	-4.473969	0.179673	-1.507956
C	-1.008474	-3.266197	0.091872
C	-0.650873	-4.195476	1.253224
C	-0.993070	-4.058301	-1.225673
C	-5.130996	1.371502	-0.799966
C	-5.439304	-0.400393	-2.554509
H	-5.389576	2.149028	-1.540005
H	-4.458871	1.818976	-0.051557
H	-6.064560	1.079202	-0.288164

H	-3.596921	0.572037	-2.044166
H	-5.009376	-1.266332	-3.085890
H	-5.705354	0.365322	-3.304159
H	-6.373430	-0.743823	-2.075741
H	-5.945661	-1.054161	0.371283
H	-5.310992	-2.878697	1.916851
H	-3.050609	-3.859788	1.809982
H	-0.215781	-2.500769	0.038833
H	-1.287217	-5.098624	1.271928
H	-0.742203	-3.691275	2.228628
H	0.394099	-4.533923	1.144206
H	-0.018644	-4.559808	-1.362914
H	-1.163945	-3.412698	-2.102295
H	-1.778191	-4.835688	-1.217090
H	0.953236	-2.301021	-2.585581
H	2.127477	-1.081382	-2.015736
H	1.756416	-1.213392	-3.756311
H	1.263182	1.209664	-3.795576
H	1.437916	1.439144	-2.032456
H	-0.074630	1.912763	-2.834773
H	-2.895660	-1.470410	-3.196222
H	-0.774386	-0.657384	-4.636007
C	-0.032145	3.367016	0.862119
C	0.197545	4.580208	0.218022
C	-0.435832	4.886520	-0.987834
C	-1.327530	3.958351	-1.531923
C	-1.566918	2.744159	-0.898720
C	-0.886255	2.409711	0.285672
H	0.473162	3.158569	1.805866
H	0.884625	5.299452	0.675780
H	-0.254259	5.842762	-1.485428
H	-1.847677	4.179891	-2.469329
H	-2.265442	2.031917	-1.344696
I	-2.147494	1.139111	1.722128

6.2al

C	-1.530482	0.029250	-1.381623
C	-1.675478	0.330223	-2.885171
C	-3.109429	0.014608	-3.199054
C	-3.668876	-0.496033	-2.111918
N	-2.714079	-0.478159	-1.040433
C	-1.325482	1.774312	-3.280612
C	-0.839346	-0.704654	-3.688349
C	-3.205724	-1.037402	0.198258
C	-4.232624	-0.352060	0.876677

C	-4.777383	-0.951739	2.016612
C	-4.345035	-2.195840	2.449601
C	-3.360164	-2.872333	1.738413
C	-2.773010	-2.318790	0.596370
C	-4.808796	0.984549	0.423779
C	-1.740940	-3.109230	-0.198404
C	-1.118170	-4.250272	0.607376
C	-2.352780	-3.672518	-1.490774
C	-4.741403	2.050879	1.525833
C	-6.256275	0.822296	-0.064944
H	-5.062067	3.026507	1.122352
H	-3.721328	2.171515	1.922906
H	-5.411182	1.805026	2.368423
H	-4.216249	1.351890	-0.426656
H	-6.341437	0.072961	-0.869202
H	-6.637455	1.782077	-0.454669
H	-6.921127	0.504205	0.757388
H	-5.566060	-0.435116	2.570182
H	-4.784420	-2.650765	3.341614
H	-3.046239	-3.855406	2.089995
H	-0.929640	-2.415271	-0.480224
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H	-1.581859	-4.200203	-2.078653
H	-2.778994	-2.886134	-2.133217
H	-3.157117	-4.391603	-1.253606
H	-1.090764	-1.736976	-3.389506
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H	-0.274596	2.003431	-3.054078
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C	1.839330	-0.967148	2.937115
N	1.787442	-0.580422	1.559331
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C	-1.492945	0.132363	2.632946
C	3.003618	-0.835103	0.809874
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C	5.469276	-1.385377	-0.318514
C	4.457127	-2.332140	-0.362899
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C	3.758506	1.538779	1.438387
C	2.113546	-3.128209	0.095674
C	1.777301	-3.391458	-1.378855
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C	4.443374	2.660052	0.650871
C	4.156749	1.598652	2.919771
H	4.067156	3.637239	1.000307
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H	5.538819	2.660812	0.793640
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H	1.206056	-2.726057	0.573408
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H	1.481044	-2.454537	-1.880005
H	0.956905	-4.123154	-1.475590
H	1.703644	-5.163660	0.790320
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H	3.416204	-4.861553	0.409794
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H	1.685388	3.202180	-0.345517
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6.3a1

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6.4al

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H	-1.395666	-1.721696	-3.547966
H	0.018134	-0.621785	-3.659174
H	-1.299241	-0.515519	-4.865134
H	-0.364747	1.984419	-3.094442
H	-2.023232	2.506173	-2.661880
H	-1.656325	1.995214	-4.337232
H	-4.920443	-0.296579	-1.782172
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H	0.615495	5.599265	0.007083
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