

Supporting Information

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General Considerations for Computational Study – Density Functional Analysis

Both B3LYP and BP86 methods were probed for the calculation of the redox couple of **1** and are listed below. Due to the decrease in calculation time and relative accuracy, BP86 was chosen for this study, and the final computed redox potentials are shifted by the difference between the experimental value and the computed value (-346 mV).

	Experimental Redox Potential (V vs Fc ^{0/+})	Computed Redox Potential (BP86) (V vs Fc ^{0/+})	Computed Redox Potential (B3LYP) (V vs Fc ^{0/+})
1	-0.255	0.091	0.276

Table S1. Comparison of redox potentials for complex **1**.

General Considerations for Computational Study – Bis-Ammine Adducts

Preliminary calculations were run on the bis-ammine adducts of **2d**, **3d**, and **4d**. A clear trend with the addition of an axial ammine ligand was not observed, with a rough variation of redox potential of ± 0.4 V.

	Complex 2d	Complex 3d	Complex 4d
Mono-ammine	-0.086	-0.805	0.737
Bis-ammine	-0.229	-0.414	0.592

Table S2. Comparison of redox potentials for mono and bis-ammine complexes.

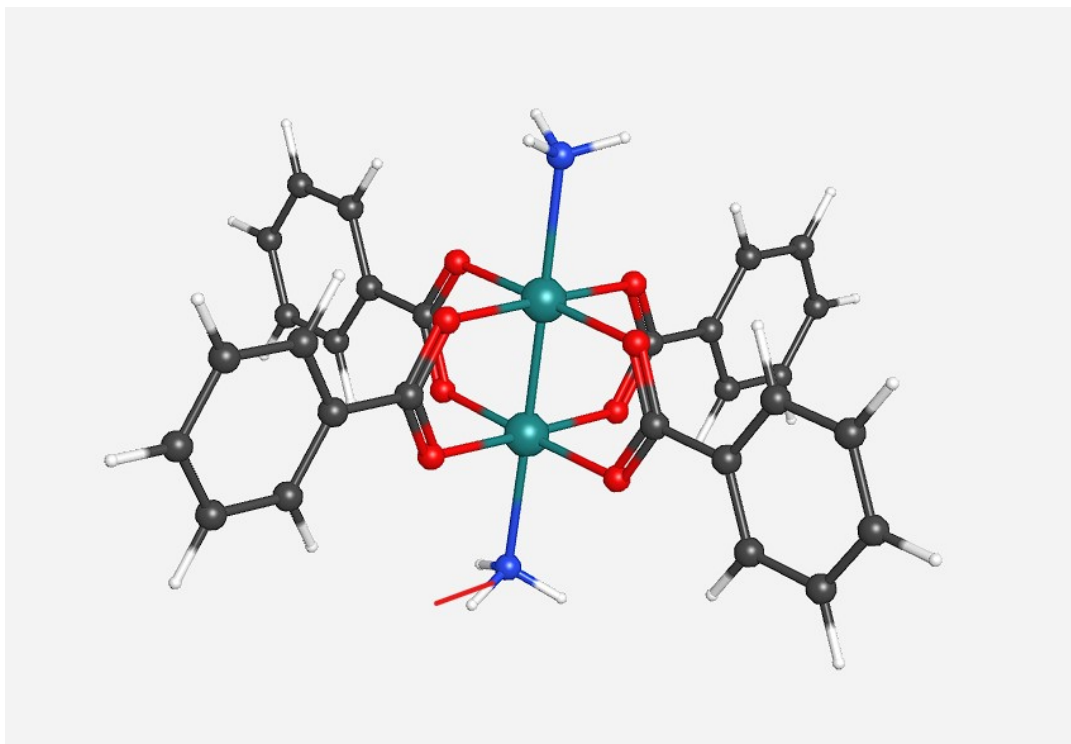


Figure S1. Bis-ammine adduct of complex **2d**.

Key Bond Lengths and Angles

2										
R	Ru ²⁺ –Ru ²⁺ (Å)	Ru ²⁺ –Ru ³⁺ (Å)	Ru ₂ ⁴⁺ –NH ₃ (Å)	Ru ₂ ⁵⁺ –NH ₃ (Å)	Ru ₂ ⁴⁺ –O (Å)	Ru ₂ ⁵⁺ –O (Å)	Ru ₂ ⁴⁺ θ ₁ (°)	Ru ₂ ⁵⁺ θ ₁ (°)	Ru ₂ ⁴⁺ θ ₂ (°)	Ru ₂ ⁵⁺ θ ₂ (°)
a	2.331	2.330	2.248	2.209	2.087	2.048	0.029	0.008	0.044	0.037
b	2.330	2.330	2.248	2.210	2.087	2.048	0.027	0.007	0.032	0.029
c	2.328	2.328	2.251	2.212	2.088	2.048	0.031	0.006	0.039	0.037
d	2.329	2.329	2.250	2.211	2.088	2.048	0.042	0.022	0.050	0.032
e	2.328	2.327	2.252	2.213	2.087	2.048	0.019	0.026	0.055	0.041
f	2.323	2.321	2.261	2.223	2.089	2.050	0.057	0.018	0.032	0.030
3										
R	Os ²⁺ –Os ²⁺ (Å)	Os ²⁺ –Os ³⁺ (Å)	Os ₂ ⁴⁺ –NH ₃ (Å)	Os ₂ ⁵⁺ –NH ₃ (Å)	Os ₂ ⁴⁺ –O (Å)	Os ₂ ⁵⁺ –O (Å)	Os ₂ ⁴⁺ θ ₁ (°)	Os ₂ ⁵⁺ θ ₁ (°)	Os ₂ ⁴⁺ θ ₂ (°)	Os ₂ ⁵⁺ θ ₂ (°)
a	2.363	2.360	2.255	2.244	2.083	2.077	0.015	0.004	0.060	0.063
b	2.363	2.360	2.255	2.244	2.083	2.077	0.016	0.003	0.046	0.052
c	2.363	2.359	2.255	2.246	2.083	2.078	0.010	0.010	0.052	0.064
d	2.362	2.359	2.256	2.245	2.083	2.078	0.036	0.020	0.042	0.015
e	2.362	2.358	2.257	2.247	2.083	2.078	0.072	0.036	0.056	0.051
f	2.361	2.354	2.259	2.254	2.083	2.079	0.056	0.056	0.036	0.022
4										
R	Rh ²⁺ –Rh ²⁺ (Å)	Rh ²⁺ –Rh ³⁺ (Å)	Rh ₂ ⁴⁺ –NH ₃ (Å)	Rh ₂ ⁵⁺ –NH ₃ (Å)	Rh ₂ ⁴⁺ –O (Å)	Rh ₂ ⁵⁺ –O (Å)	Rh ₂ ⁴⁺ θ ₁ (°)	Rh ₂ ⁵⁺ θ ₁ (°)	Rh ₂ ⁴⁺ θ ₂ (°)	Rh ₂ ⁵⁺ θ ₂ (°)
a	2.431	2.418	2.178	2.140	2.065	2.038	0.020	0.425	0.032	0.806
b	2.431	2.417	2.178	2.140	2.065	2.038	0.021	0.428	0.021	0.774
c	2.429	2.415	2.180	2.142	2.065	2.038	0.025	0.423	0.029	0.746
d	2.429	2.415	2.179	2.141	2.066	2.038	0.046	0.427	0.043	0.801
e	2.430	2.414	2.180	2.142	2.065	2.038	0.042	0.334	0.030	0.670
f	2.424	2.424	2.187	2.155	2.066	2.060	0.036	0.156	0.017	0.135
5										
R	Ir ²⁺ –Ir ²⁺ (Å)	Ir ²⁺ –Ir ³⁺ (Å)	Ir ₂ ⁴⁺ –NH ₃ (Å)	Ir ₂ ⁵⁺ –NH ₃ (Å)	Ir ₂ ⁴⁺ –O (Å)	Ir ₂ ⁵⁺ –O (Å)	Ir ₂ ⁴⁺ θ ₁ (°)	Ir ₂ ⁵⁺ θ ₁ (°)	Ir ₂ ⁴⁺ θ ₂ (°)	Ir ₂ ⁵⁺ θ ₂ (°)
a	2.465	2.421	2.173	2.145	2.061	2.037	0.028	0.187	0.034	1.053
b	2.465	2.421	2.173	2.145	2.061	2.036	0.038	0.202	0.027	1.042
c	2.464	2.421	2.174	2.147	2.062	2.036	0.026	0.230	0.034	1.121
d	2.464	2.420	2.174	2.146	2.062	2.037	0.039	0.202	0.017	1.098
e	2.463	2.421	2.174	2.147	2.062	2.036	0.026	0.221	0.030	1.071
f	2.461	2.429	2.179	2.154	2.063	2.036	0.072	0.303	0.029	1.018
6										
R	Re ²⁺ –Re ³⁺ (Å)	Re ³⁺ –Re ³⁺ (Å)	Re ₂ ⁵⁺ –NH ₃ (Å)	Re ₂ ⁶⁺ –NH ₃ (Å)	Re ₂ ⁵⁺ –O (Å)	Re ₂ ⁶⁺ –O (Å)	Re ₂ ⁵⁺ θ ₁ (°)	Re ₂ ⁶⁺ θ ₁ (°)	Re ₂ ⁵⁺ θ ₂ (°)	Re ₂ ⁶⁺ θ ₂ (°)
a	2.205	2.204	2.315	2.283	2.053	2.008	0.022	0.017	0.050	0.064
b	2.204	2.204	2.316	2.283	2.053	2.008	0.023	0.020	0.038	0.050
c	2.203	2.202	2.319	2.286	2.054	2.009	0.015	0.024	0.048	0.066
d	2.204	2.203	2.317	2.285	2.053	2.009	0.031	0.030	0.020	0.055
e	2.203	2.202	2.320	2.288	2.054	2.009	0.021	0.020	0.039	0.041
f	2.197	2.195	2.334	2.303	2.055	2.010	0.022	0.037	0.043	0.043

Table S1. Key bond lengths and angles around the dinuclear core for the optimized structures in series 2-6. For the purpose of distinguishing between the metal atoms in the table below, “M²⁺” refers to the metal atom that is not bonded to the NH₃ ligand and “M³⁺” refers to the metal atom bonded to the NH₃ ligand. It should be noted though that these assignments are artificial, since the mixed-valent species are necessarily fully delocalized due to the metal-metal bond. O–M–M–O torsion angles (θ₁) were measured by averaging the four dihedral angles of the metal center coordinated to each carboxylate. Ligand torsion angles (θ₂) were measured by averaging the four dihedral angles between the phenyl ring plane and the carboxylate plane on each benzoate ligand (see Fig. 2). R groups are organized from largest positive para-effect to largest negative para-effect (a-f).

Redox Potentials of Bimetallic Complexes Studied

Complex	Predicted $E_{1/2}$ (V vs $\text{Fc}^{0/+}$)
2	a -0.037
	b -0.028
	c -0.111
	d -0.086
	e -0.161
	f -0.506
3	a -0.766
	b -0.797
	c -0.869
	d -0.805
	e -0.823
	f -1.187
4	a 0.833
	b 0.769
	c 0.696
	d 0.737
	e 0.646
	f 0.245
5	a -1.388
	b -1.380
	c -1.457
	d -1.458
	e -1.593
	f -1.800
6	a -1.355
	b -1.366
	c -1.441
	d -1.368
	e -1.451
	f -1.872

XYZ Coordinates of DFT-Optimized Structures

BP-86 Geometry Optimized Coordinates for 4+ of **2a**

Ru	0.00282448147032	0.01242799119651	0.00983377610830
O	0.53336440682504	1.49527329733703	-1.35955384647267
C	0.53061547534671	1.21374476243085	-2.61102757759632
C	0.91454016249764	2.28544698427700	-3.57607630021912
C	1.27713933281751	3.56941238204242	-3.10992542113593
C	1.63968688599788	4.58105142426431	-4.01095202361441
C	1.63625530633428	4.29741464445378	-5.38837474232599
C	1.27931861513730	3.02823686634153	-5.87810022717136
C	0.91943519072332	2.02624586925490	-4.96530617743112
H	0.63890521491238	1.03177624466853	-5.33012493729631
H	1.28179697399529	2.82415933036626	-6.95461885161272
Br	2.12903334113658	5.67101171484989	-6.62578386420955
H	1.92075070580591	5.57528637033640	-3.64612507154839
H	1.27454644890781	3.77395066429664	-2.03349342756281
O	0.21639989345321	0.06022695743311	-3.07993602986129
Ru	-0.32129921087877	-1.45433617075841	-1.77197062388404
O	-0.85273034381552	-2.93288963819652	-0.42079280305703
C	-0.85630942970829	-2.66513300864074	0.83517326420519
O	-0.54148901671344	-1.51940158370001	1.31848217954284
C	-1.24813419256062	-3.74811028586440	1.78420729800044
C	-1.60900313665921	-5.02551521077878	1.29911444097888
C	-1.97845436039116	-6.04818976643383	2.18469909702507
C	-1.98394017647617	-5.78214028907563	3.56568753689772
C	-1.62941294532950	-4.51966040884430	4.07401461075636
C	-1.26248384380710	-3.50645925038850	3.17649405617535
H	-0.98388541614059	-2.51672139629262	3.55528527758705
H	-1.63916785174042	-4.32939685286335	5.15302256036780
Br	-2.48603260371673	-7.17093012665982	4.78226287067980
H	-2.25804878916732	-7.03741783440528	1.80545573149749
H	-1.59962247914251	-5.21582039861354	0.22006321129691
O	-2.29812054679041	-0.84246905862252	-1.87830061129852
C	-2.72702763840827	0.04459060835522	-1.05464542730574
O	-1.99736466521500	0.58506132831841	-0.14861286144902
C	-4.15358693666195	0.47039708793910	-1.15848766894156
C	-4.98818032294826	-0.07033710331270	-2.16257235114516
C	-6.32881220722959	0.32737983402608	-2.26854990902648
C	-6.83111123569811	1.27342218322517	-1.35710473490073
C	-6.02201728035021	1.82571835378415	-0.34809022259766
C	-4.68282580305674	1.41979102672534	-0.25529188367754

H	-4.03869177575294	1.84038994745111	0.52500499325357
H	-6.42954861137140	2.56097091880016	0.35469267900514
Br	-8.65867461705657	1.82333972471252	-1.49447929703595
H	-6.97249601035280	-0.09218606097487	-3.04973531794500
H	-4.58068715508871	-0.80557976974996	-2.86545019335257
O	1.66393666086002	-2.02902259114729	-1.62351396580770
C	2.40767997936601	-1.49375049453296	-0.72372854406915
O	1.99319912325958	-0.60819482375917	0.10650765828687
C	3.83284790203010	-1.92815073702980	-0.63906902213403
C	4.68393194898275	-1.39351865208311	0.35434325188782
C	6.02347647059609	-1.79935507570516	0.44210971840410
C	6.50788025848365	-2.74731444375871	-0.47692929358473
C	5.68214855891174	-3.29349272937144	-1.47581790061004
C	4.34435042597838	-2.87940924517838	-1.55045864955964
H	3.68750040325995	-3.29515411250988	-2.32276305047673
H	6.07579838829815	-4.03029292108919	-2.18486677112715
Br	8.33374915426408	-3.30853780739252	-0.36433509528008
H	6.68011759158734	-1.38456526840769	1.21502769992867
H	4.28981144198367	-0.65658848223310	1.06302229875424
N	0.33159633720937	1.40541777727157	1.74291503370149
H	1.33129344832435	1.53107320073615	1.94137373389647
H	-0.05982535077504	2.34012816292545	1.57742649088767
H	-0.10029763575303	1.04803767055461	2.60329245719899

BP-86 Geometry Optimized Coordinates for 5+ of **2a**

Ru	0.00150555433266	0.01261891198535	0.00897539107110
O	0.52248272467571	1.46781492155731	-1.33429195730116
C	0.52464459466612	1.20196926486747	-2.59381637450530
C	0.90669818301977	2.26378474945184	-3.55110185925812
C	1.26831355461152	3.54745453870277	-3.07999511758424
C	1.63162068177478	4.55595582659007	-3.98156846690542
C	1.62999875942575	4.27039616424592	-5.35963975484690
C	1.27362600854102	3.00049368876061	-5.85041867015307
C	0.91227432437844	1.99874184723869	-4.94035712008199
H	0.63262440174195	1.00503250803346	-5.30743796508996
H	1.27796562747685	2.79640278800412	-6.92667559932632
Br	2.12354497750257	5.63955825333241	-6.59361428769052
H	1.91229005753755	5.55032093519045	-3.61755752389104
H	1.26490575126358	3.75444821539360	-2.00419338249709
O	0.20423211400164	0.03721269020407	-3.04990427168152
Ru	-0.32301793920500	-1.45391897330569	-1.77255856897730
O	-0.84187631352545	-2.89928997311457	-0.44050707177315
C	-0.84889917166579	-2.64646715286107	0.82560636290341

O	-0.53110436753458	-1.49022453707035	1.29408292848456
C	-1.23482321560958	-3.72199797400974	1.76577654600458
C	-1.59470890152962	-4.99835480229132	1.27394624474239
C	-1.96118352342686	-6.02034784831288	2.15903753669192
C	-1.96457155080558	-5.75560393474954	3.54117504722783
C	-1.61031348216385	-4.49308655465891	4.05238558396143
C	-1.24585265734134	-3.47787189759602	3.15880954289747
H	-0.96791263668694	-2.48962083171038	3.54141522949071
H	-1.61875940139504	-4.30529550540944	5.13157994621778
Br	-2.46231629671228	-7.14298863989093	4.75289977392123
H	-2.24053341768508	-7.00911299723061	1.77913529874249
H	-1.58766451683139	-5.18901856411891	0.19511859069248
O	-2.26139758276398	-0.84887247154108	-1.86984287000467
C	-2.70760844718528	0.04222857692584	-1.04886439985920
O	-1.96113484462964	0.57510342842732	-0.14549376791668
C	-4.12229508483071	0.46379161373251	-1.15245502161507
C	-4.95317792211819	-0.08175833549580	-2.15859807920196
C	-6.29201016245563	0.31659679117497	-2.26392375543841
C	-6.79427518391885	1.26455766599395	-1.35310375792044
C	-5.98592393280793	1.81917618990729	-0.34335634221606
C	-4.64807131372049	1.41538373987977	-0.24778171152570
H	-4.00648534104377	1.83816026432632	0.53319363068608
H	-6.39435210973151	2.55507545359437	0.35783161183353
Br	-8.61669785627302	1.81296714421691	-1.49193047612690
H	-6.93552936984677	-0.10363397304802	-3.04454226387061
H	-4.54747873473254	-0.81770515242882	-2.86152063922160
O	1.62575267042539	-2.01223045300843	-1.62182749593381
C	2.38631499183753	-1.48478197851275	-0.72152411282595
O	1.954444881479000	-0.59665714673182	0.10424363831049
C	3.79878015249498	-1.91781945648893	-0.63748281606072
C	4.64791218911309	-1.38142729797316	0.35825982678155
C	5.98473754761107	-1.79068585222068	0.44424161395038
C	6.46675162490217	-2.74051444797325	-0.47566574711704
C	5.64012693073635	-3.28609186859227	-1.47537237291010
C	4.30431923481895	-2.87127147519982	-1.55166247697849
H	3.64872893980444	-3.28706634594672	-2.32477347042948
H	6.03271781949015	-4.02356307258414	-2.18392455819952
Br	8.28645028570256	-3.30386821156073	-0.36309377190084
H	6.64247255851584	-1.37751403828502	1.21674242238814
H	4.25775284076933	-0.64388413444526	1.06821663849650
N	0.31798838866574	1.39146463135737	1.70607946171197
H	1.31867621014313	1.52603963782740	1.89792468567151
H	-0.08555417903453	2.31998269421772	1.53031018058812
H	-0.11048011755935	1.03115449322716	2.56793739536865

BP-86 Geometry Optimized Coordinates for 4+ of **2b**

Ru	0.01070600195634	0.03917702978063	0.03900739187815
O	0.54248992790970	1.52162969790769	-1.33041624114121
C	0.54045847048020	1.24019874433829	-2.58216791845713
C	0.92599587644279	2.31091645021970	-3.54678073486292
C	1.28908144485602	3.59529384528808	-3.08109495464403
C	1.65323000551753	4.60539018523806	-3.98177927139811
C	1.65240344379413	4.32404929592521	-5.36084419776857
C	1.29441219041060	3.05295629797488	-5.84807309959140
C	0.93272156853493	2.05184956059949	-4.93638591133823
H	0.65189385000332	1.05737253284030	-5.30087403987239
H	1.30020539335017	2.85474266251350	-6.92568043535228
Cl	2.10664178898542	5.58246304727124	-6.49454806790749
H	1.93539253615389	5.60157333712362	-3.62314385280218
H	1.28508839654209	3.79981501955983	-2.00469528159069
O	0.22532026752128	0.08650164444675	-3.05067576617958
Ru	-0.31341137850333	-1.42743238978071	-1.74225853547547
O	-0.84589537241276	-2.90572611692537	-0.39116593668926
C	-0.85028268963232	-2.63808785535101	0.86507816043273
O	-0.53473992902427	-1.49213502193420	1.34802087682962
C	-1.24367609319492	-3.72017487010231	1.81357269593920
C	-1.60468913074307	-4.99801133931190	1.32871944613660
C	-1.97565984215193	-6.01931816059474	2.21377494782416
C	-1.98406398169209	-5.75577143330913	3.59639242483245
C	-1.62883645252762	-4.49132518517154	4.10247234249562
C	-1.26014297240242	-3.47883200021594	3.20624430503058
H	-0.98154030002362	-2.48905749843310	3.58486678457301
H	-1.64220909131176	-4.30707235993316	5.18248893974681
Cl	-2.44683818126910	-7.02841711822507	4.71061229528096
H	-2.25612496065077	-7.01057957801427	1.84051143594619
H	-1.59369930469396	-5.18814908698932	0.24968725153261
O	-2.29024935193423	-0.81535794777688	-1.84918165738425
C	-2.71966780723315	0.07174500692283	-1.02545897478340
O	-1.98934310024322	0.61240143728696	-0.11972310073720
C	-4.14600469678551	0.49649967356397	-1.12834233266064
C	-4.98202164092961	-0.04539144448059	-2.13110228895750
C	-6.32239117103784	0.35061579054749	-2.23489043388329
C	-6.82792773800448	1.29696262982166	-1.32378583761151
C	-6.01484795658657	1.84969677559590	-0.31660531137068
C	-4.67581657913225	1.44609486115926	-0.22515644581332
H	-4.03082304728710	1.86763635753490	0.55387727446634
H	-6.42818901615883	2.58431401185827	0.38343578124484

Cl	-8.50408882450691	1.79758109055630	-1.44621305026966
H	-6.97169846349739	-0.06662917557266	-3.01265466055575
H	-4.57429721329865	-0.78053246026400	-2.83390683768519
O	1.67174111150583	-2.00261964778083	-1.59373105111936
C	2.41619633561560	-1.46694966539626	-0.69441769813157
O	2.00110740192124	-0.58157194476792	0.13607633595154
C	3.84134018386942	-1.89970799361044	-0.61112909194435
C	4.69392154925811	-1.36346273315422	0.38061644672799
C	6.03340243356519	-1.76695157276451	0.46577357119827
C	6.52118574515239	-2.71509451966398	-0.45304920960201
C	5.69141183547536	-3.26210317233074	-1.44975989720378
C	4.35356669281752	-2.85096574287961	-1.52264941269965
H	3.69583017342717	-3.26797263829340	-2.29347358437918
H	6.09105657878402	-3.99810774265493	-2.15626624317288
Cl	8.19600567067754	-3.22525583142693	-0.35389149097973
H	6.69566016426990	-1.35411776754319	1.23493297766774
H	4.29947532203343	-0.62674498843873	1.08929093141900
N	0.33899444216824	1.43233376409617	1.77298491756082
H	1.33880037302104	1.56811404698668	1.96398895881647
H	-0.06364916785221	2.36322697794494	1.61304586164227
H	-0.08230711129848	1.06821329818889	2.63578245084192

BP-86 Geometry Optimized Coordinates for 5+ of **2b**

Ru	0.00958469074017	0.04003172674216	0.03779719368758
O	0.53168492233261	1.49484169806559	-1.30547096641637
C	0.53447216559564	1.22909541932111	-2.56531375489400
C	0.91767484268078	2.28986016207151	-3.52210623838784
C	1.27965080125050	3.57404631045428	-3.05146671431946
C	1.64411042872795	4.58114207744842	-3.95259023955386
C	1.64467046575411	4.29761231925605	-5.33228097899027
C	1.28743648017787	3.02580840892656	-5.82084737906052
C	0.92477746825762	2.02497707305325	-4.91180399863648
H	0.64496401540943	1.03120663568604	-5.27850014925238
H	1.29484028870614	2.82772740728378	-6.89818996996260
Cl	2.09881333279051	5.55188668465130	-6.46269986032947
H	1.92576118202034	5.57748847440890	-3.59485679338137
H	1.27506505713358	3.78098696476611	-1.97569566447571
O	0.21332988564717	0.06401906297668	-3.02098885157518
Ru	-0.31490218507262	-1.42632440833502	-1.74321958579395
O	-0.83483171474012	-2.87141759816439	-0.41143834304794
C	-0.84265108529875	-2.61873717893104	0.85503882387162
O	-0.52415898185023	-1.46222927673275	1.32317287591963
C	-1.22968484733662	-3.69342031277795	1.79449304757508

C	-1.58932246776464	-4.97034128191026	1.30278035043182
C	-1.95680705485532	-5.99121637694619	2.18712698933439
C	-1.96287723031075	-5.72881252396603	3.57089913971614
C	-1.60839286905903	-4.46432022460253	4.08027699743542
C	-1.24274184131307	-3.44972121346204	3.18800068993750
H	-0.96507148330751	-2.46138433528565	3.57049536741854
H	-1.62029465202928	-4.28276907298018	5.16048247130672
Cl	-2.42056631938768	-7.00033364816046	4.68039843168074
H	-2.23661332517031	-6.98211635407078	1.81323235446187
H	-1.58067306570271	-5.16073989117717	0.22395475197161
O	-2.25313338510111	-0.82107135611824	-1.84127097600508
C	-2.69999365316925	0.06998138530783	-1.02007577790019
O	-1.95283763440869	0.60314906549401	-0.11702626110570
C	-4.11437906727626	0.49007895020704	-1.12254533457565
C	-4.94674941021895	-0.05713783676582	-2.12712196253505
C	-6.28546366771845	0.33876040320202	-2.22999938721918
C	-6.79085801144687	1.28689926001298	-1.31927830618620
C	-5.97868507893283	1.84275347663619	-0.31162260763464
C	-4.64087919787412	1.44185403322315	-0.21785199271140
H	-3.99839714880694	1.86597774480757	0.56160684717256
H	-6.39310674618089	2.57790175470400	0.38678315824260
Cl	-8.46236947525199	1.78498081691150	-1.44234379632751
H	-6.93469973923899	-0.07952241143962	-3.00687826558572
H	-4.54069967279304	-0.79292090597931	-2.82996050737434
O	1.63354477434779	-1.98548602837140	-1.59226357135946
C	2.39476386521126	-1.45792936935927	-0.69210314417827
O	1.96234590257444	-0.56972840982804	0.13374430341170
C	3.80672139531724	-1.89008473771031	-0.60876642149201
C	4.65716204718440	-1.35259958648455	0.38584234596238
C	5.99358292697111	-1.76017345261681	0.46999266634530
C	6.47861433451458	-2.71045370405254	-0.44966899809258
C	5.64839181401663	-3.25655836525013	-1.44777961608181
C	4.31291119131600	-2.84385385453054	-1.52288565455597
H	3.65659116688935	-3.26048880440504	-2.29487680457010
H	6.04698235213833	-3.99342564993704	-2.15355332669335
Cl	8.14716515439965	-3.22335858401462	-0.34970751884286
H	6.65680578725856	-1.34942957680077	1.23904224044442
H	4.26671161177317	-0.61509033469126	1.09562271740124
N	0.32617063337187	1.41926496665036	1.73539628522338
H	1.32681922923605	1.55359344066079	1.92750069178204
H	-0.07708009208583	2.34785800709165	1.55948679422642
H	-0.10259450004195	1.05915100583692	2.59716413414386

BP-86 Geometry Optimized Coordinates for 4+ of **2c**

Ru	0.00395104751901	0.01177927769301	0.00885389051451
O	0.53416244638156	1.49516186582527	-1.36060848899340
C	0.53203713508624	1.21515716068454	-2.61335867902439
C	0.91560701728322	2.28572530581563	-3.57653381242859
C	1.27894028798359	3.57059795175537	-3.10974334745132
C	1.64142697280817	4.57990015835984	-4.01072297551583
C	1.63941343292024	4.30061237972062	-5.38771737110943
C	1.28193461114349	3.03245267974305	-5.87582021644184
C	0.92123849657878	2.02896401604962	-4.96746247147134
H	0.64027719851615	1.03470258027730	-5.33236478163875
H	1.29112705117915	2.84931606296944	-6.95675241843705
F	1.98495900846949	5.26097105785613	-6.25024092384282
H	1.92617905917143	5.58050329726018	-3.66462854324005
H	1.27555043475107	3.77255145887435	-2.03288190152441
O	0.21742285958753	0.06007428711691	-3.08084206979108
Ru	-0.31983251385712	-1.45406504283746	-1.77084954410327
O	-0.85152718491684	-2.93340047946203	-0.41989370694391
C	-0.85665125994076	-2.66698056829801	0.83735583233065
O	-0.54054965807356	-1.51990795329767	1.31911707013896
C	-1.25046632774287	-3.74799981932540	1.78452432710244
C	-1.61284835747111	-5.02623373364948	1.29910107460970
C	-1.98500600874679	-6.04547572041873	2.18474509934096
C	-1.99402967398395	-5.78285814052552	3.56503290315863
C	-1.63814525616480	-4.52149435685728	4.07146983452755
C	-1.26760517274793	-3.50792594054648	3.17831747081676
H	-0.98807874737879	-2.51846867725420	3.55703139645005
H	-1.65641588741610	-4.35142141999200	5.15442436761393
F	-2.34908083147987	-6.75283780665221	4.41284427107482
H	-2.26910026720698	-7.04111061303692	1.82410210821421
H	-1.60128531011032	-5.21513234605224	0.21989624097174
O	-2.29773594530281	-0.84363277293677	-1.87769526106019
C	-2.72888920689008	0.04405727465346	-1.05438451204171
O	-1.99693866773903	0.58451672079097	-0.14884803039303
C	-4.15377507375982	0.46832574403527	-1.15746776476895
C	-4.99252982852894	-0.07947466997274	-2.15600580382533
C	-6.33169362421187	0.31815263453013	-2.25874416461984
C	-6.83395167878000	1.26964614031489	-1.35505185408989
C	-6.02094800611855	1.82740673926124	-0.35403804875602
C	-4.68264936618782	1.42469070648595	-0.25947000211238
H	-4.03582130246975	1.85036771155956	0.51574143208647
H	-6.44595234666443	2.56685299156920	0.33489820292261
F	-8.11083975191651	1.65220701542805	-1.44992242863497
H	-6.99388385732442	-0.09596639008263	-3.02823221451158

H	-4.58563805195005	-0.81949149645537	-2.85409399960360
O	1.66602479290346	-2.02942263419390	-1.62340392143898
C	2.41199621740847	-1.49414459765294	-0.72408826887376
O	1.99533168485301	-0.60770381810196	0.10557401971029
C	3.83537321433439	-1.92728345970138	-0.63972950905171
C	4.69035767633692	-1.38592418313318	0.34844764226182
C	6.02822289977547	-1.79213905655140	0.43352632668607
C	6.51268624242114	-2.74573028976852	-0.47758592683719
C	5.68334760887017	-3.29699120623820	-1.46881298478801
C	4.34658638431085	-2.88564591374241	-1.54577321257208
H	3.68724505895794	-3.30623607928523	-2.31322190916766
H	6.09466394638530	-4.03823198225601	-2.16410204043228
F	7.78817043900261	-3.13675962212629	-0.39939812694883
H	6.70296788353125	-1.38322347634513	1.19485438783478
H	4.29674474547634	-0.64412886684231	1.05221403017028
N	0.33495732783320	1.40767879083381	1.74348306665234
H	1.33433065148152	1.52000875164995	1.95104276726739
H	-0.04183410582290	2.34714664888149	1.57150631122893
H	-0.10991344235636	1.05929775359682	2.60086264279964

BP-86 Geometry Optimized Coordinates for 5+ of **2c**

Ru	0.00165989191031	0.01323744094510	0.00854579110697
O	0.52262220025031	1.46879621264089	-1.33451888921809
C	0.52560817051722	1.20438857893931	-2.59555629384515
C	0.90790151843958	2.26374071910459	-3.55086916493847
C	1.27176361382601	3.54856207545201	-3.07990195565766
C	1.63583229434320	4.55356503529130	-3.98170319450425
C	1.63471107444785	4.27022402034011	-5.35897977686641
C	1.27653928734510	3.00169185966936	-5.84837178810028
C	0.91368372302956	2.00003483200984	-4.94199818662842
H	0.63253913818547	1.00649993278836	-5.30819679946822
H	1.28745386472972	2.81834092047168	-6.92892552619058
F	1.98162777741306	5.22625632725580	-6.21961897009752
H	1.92146066187279	5.55430427494306	-3.63775909157959
H	1.26808699145962	3.75397225834398	-2.00387933982770
O	0.20429909665570	0.03779294321862	-3.05004029541540
Ru	-0.32251581731038	-1.45214505534031	-1.77105568391513
O	-0.84133789163539	-2.89831747285594	-0.44023559360723
C	-0.84951859000818	-2.64716423376837	0.82758901616430
O	-0.53095254969925	-1.48930008228256	1.29470432237412
C	-1.23577571437502	-3.72086468688312	1.76502749149716
C	-1.59671244022653	-4.99826471915718	1.27212128770528
C	-1.96407929129899	-6.01762426963880	2.15639147819994

C	-1.96934817503852	-5.75608236059240	3.53787378449569
C	-1.61450142651224	-4.49505765572100	4.04890231668604
C	-1.24835985189125	-3.47908166620843	3.16007183288985
H	-0.96983466542818	-2.49110111268427	3.54280096701641
H	-1.63059471606381	-4.32889439533399	5.13217100085194
F	-2.31933834772852	-6.72579125476030	4.38183195092616
H	-2.24746634501494	-7.01294297341397	1.79530274964569
H	-1.58832406709610	-5.18658709324932	0.19298008756326
O	-2.26125930553393	-0.84882923039273	-1.86926873015515
C	-2.70999539852157	0.04312797207213	-1.04847390465665
O	-1.96123533458442	0.57600718395598	-0.14533866636242
C	-4.12220021379580	0.46268003478008	-1.15156229598952
C	-4.95702990690918	-0.09024055873462	-2.15263971776680
C	-6.29409665954303	0.30730412900137	-2.25510751543385
C	-6.79564739707462	1.26053641061898	-1.35136357588665
C	-5.98462983583668	1.82147908540641	-0.34898028938559
C	-4.64803383391221	1.42123406478405	-0.25180308063349
H	-4.00383076925745	1.84911080718093	0.52412126839457
H	-6.41136251359547	2.56123919446267	0.33803703640192
F	-8.06880395078386	1.64141477178802	-1.44723331698542
H	-6.95633277737694	-0.10717780263222	-3.02390860222352
H	-4.55144336298185	-0.83078081956687	-2.85064905117210
O	1.62604871203525	-2.01145333568629	-1.62169204346276
C	2.38904737338564	-1.48440338902884	-0.72129942118246
O	1.95501982082932	-0.59531078263618	0.10412272857417
C	3.79864649639136	-1.91664361394257	-0.63744243771239
C	4.65178461405444	-1.37406278120329	0.35376128948134
C	5.98629202581119	-1.78409860417012	0.43759696271311
C	6.46700931204760	-2.73964745904024	-0.47512406182429
C	5.63773152312541	-3.29026445068629	-1.46811539846978
C	4.30367449033657	-2.87740730695984	-1.54670690086302
H	3.64543929722865	-3.29734979868779	-2.31520257516177
H	6.04838135236483	-4.03207688989160	-2.16268542627027
F	7.73768919618332	-3.13266279205242	-0.39671149073112
H	6.66251647482135	-1.37782474583555	1.19856240764340
H	4.26213789546215	-0.63164606699693	1.05877789661772
N	0.31937225120997	1.39362508682944	1.70794943247820
H	1.32007135066117	1.52541892678494	1.90121643308403
H	-0.08131032806333	2.32320380462878	1.53170397186474
H	-0.11116289327610	1.03469258632663	2.56923102781314

BP-86 Geometry Optimized Coordinates for 4+ of **2d**

Ru	0.01056359678730	0.02805032301373	0.04561948053791
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O	0.62137042580062	1.68109604671947	-1.07186919163081
C	0.57333347489394	1.61705650793211	-2.35258138166228
C	1.01298358265509	2.80871254903106	-3.13828452553792
C	1.46910022792489	3.97098965580454	-2.47454515216272
C	1.88124768120557	5.08995368888763	-3.21489205233521
C	1.84222232468896	5.05911380073636	-4.62225181168355
C	1.38899915861706	3.90397295165372	-5.28824714783025
C	0.97585187445058	2.78299473958291	-4.55157903405075
H	0.62177492944399	1.87976763143154	-5.06155404384257
H	1.35785072432875	3.87771574533096	-6.38468534616246
H	2.16472327143883	5.93476231601515	-5.19969874574636
H	2.23378945754579	5.98894167598975	-2.69395096083498
H	1.49618062251510	3.98590783854244	-1.37899848571591
O	0.16565062830259	0.58214195558829	-2.99524239617871
Ru	-0.45380837895173	-1.09206423334432	-1.94226798602825
O	-1.05986118913378	-2.74047423654714	-0.84232630413724
C	-1.01303981634475	-2.69265220157737	0.44066402550254
O	-0.61235861029639	-1.66508900709915	1.09625932942988
C	-1.44739357664486	-3.89768727078413	1.20864321745180
C	-1.89653379506649	-5.05246125015078	0.52730957403347
C	-2.30346115664271	-6.18433399566835	1.25063265963108
C	-2.26591910973867	-6.17410191641838	2.65838485809159
C	-1.81926578023276	-5.02666476489499	3.34183829587591
C	-1.41135764133095	-3.89275069244642	2.62216589373367
H	-1.06199801569743	-2.99531120427239	3.14537578415386
H	-1.78909787521316	-5.01657829516974	4.43858199863501
H	-2.58434908645140	-7.05990171106295	3.22245787363178
H	-2.65065271463025	-7.07738080770584	0.71607435821697
H	-1.92209499155134	-5.05145625765306	-0.56839567396043
O	-2.38422119418341	-0.34153172821564	-1.88197139459339
C	-2.73407045326369	0.42131749320741	-0.90945223919763
O	-1.94672098160041	0.75383501338369	0.04757369559556
C	-4.13190668827407	0.94708676710291	-0.89227706098333
C	-5.03536236961730	0.60178048467562	-1.92376935193480
C	-6.34866307278276	1.09659403540139	-1.90543761010011
C	-6.77149206858381	1.93924676272802	-0.85926421191629
C	-5.87571403757927	2.28610327606524	0.17052301881633
C	-4.56156873052695	1.79327708681262	0.15589633018885
H	-3.85681448125238	2.05704159292438	0.95270834781272
H	-6.20311212850103	2.94242945629856	0.98657674785968
H	-7.79859744602515	2.32541688637822	-0.84661120197009
H	-7.04504769142363	0.82488301101601	-2.70863521991961
H	-4.69752480883997	-0.05497605601010	-2.73357479154200
O	1.48847497711917	-1.81536252439401	-1.95502272995259

C	2.28933304865383	-1.48861387401076	-1.00530752370284
O	1.95298030596680	-0.73117902666307	-0.02569303117387
C	3.68541621638972	-2.01807001848226	-1.04433118896356
C	4.60336341112688	-1.68376229134235	-0.02203705967364
C	5.91493064227188	-2.18206182865301	-0.06149774304639
C	6.32171962720932	-3.01710425827522	-1.11997803276767
C	5.41161319047874	-3.35276066098432	-2.14090737997793
C	4.09918764919504	-2.85656835358271	-2.10508242739239
H	3.38395362442873	-3.11181034559238	-2.89533530854478
H	5.72649036827616	-4.00298620162528	-2.96669677080920
H	7.34746643930763	-3.40597030101097	-1.14925471922309
H	6.62245945648347	-1.91892580328986	0.73478957714031
H	4.27835470585212	-1.03270902061981	0.79748913179755
N	0.43086007106969	1.09750252693125	1.97958609951282
H	0.45974702696872	0.44530777787903	2.77225119894764
H	-0.29410296764548	1.79294333598796	2.19242067776480
H	1.32873760662897	1.59543624449477	1.96925788252390

BP-86 Geometry Optimized Coordinates for 5+ of **2d**

Ru	0.01261857749148	0.02832596931938	0.04474319380599
O	0.60925926420497	1.65135175923300	-1.05141332157684
C	0.56657726442983	1.60381526989126	-2.33753861046294
C	1.00024406869241	2.78584126197745	-3.11736034533053
C	1.45443079844851	3.94749611186933	-2.44898290326069
C	1.86390949426176	5.06439979136156	-3.19130035570463
C	1.82338563574152	5.02979730183784	-4.59876752917693
C	1.37191828402768	3.87485770584567	-5.26652775326905
C	0.96051189854845	2.75373856333107	-4.53150593418619
H	0.60805553578433	1.85091242341291	-5.04273045986575
H	1.34099655159894	3.84922263598432	-6.36250460630882
H	2.14447455498503	5.90531749552487	-5.17675650708299
H	2.21548901210297	5.96447970941206	-2.67262024617685
H	1.48277778972803	3.96536621217865	-1.35378629680066
O	0.15558089114691	0.55504949777009	-2.96947517513134
Ru	-0.45155384211999	-1.09165130492062	-1.94353137463052
O	-1.04202270661547	-2.70502458822681	-0.85746825772531
C	-1.00269412938165	-2.67199910025357	0.43315414473389
O	-0.59751233613130	-1.63263971415799	1.07618340000796
C	-1.43623805143430	-3.86669144802042	1.19342164521679
C	-1.88334065720772	-5.01927219800007	0.50487307143719
C	-2.29267003365730	-6.14890963681228	1.22789429171326
C	-2.25889389451336	-6.13606555780984	2.63582221952400
C	-1.81418922797696	-4.99018548865938	3.32363375774350

C	-1.40298674524034	-3.85660568523204	2.60803299327730
H	-1.05554560000183	-2.96076889958350	3.13465947603475
H	-1.78842798178931	-4.98157530187313	4.42001553057490
H	-2.57987085767570	-7.02147966522776	3.19860344404135
H	-2.63874871247540	-7.04193706754163	0.69357432846676
H	-1.90611473802758	-5.02028685660912	-0.59061657728216
O	-2.34398304222192	-0.35320945413245	-1.87667276499146
C	-2.71138355542546	0.41373246465270	-0.90466551313437
O	-1.90862315849493	0.73799308493129	0.04844929636191
C	-4.09800140691521	0.93369012548327	-0.88820512877884
C	-4.99621451375407	0.58588020720211	-1.92486398959479
C	-6.30832747370508	1.08024449490683	-1.90585695982872
C	-6.73069481822359	1.92075605721283	-0.85763971302585
C	-5.83871330759780	2.26830820980030	0.17552788914221
C	-4.52504323140091	1.77810606610698	0.16387270721319
H	-3.82370127056019	2.04257127898888	0.96307209695755
H	-6.16906607153603	2.92281919502199	0.99119359890440
H	-7.75788222202623	2.30608425042607	-0.84588891183982
H	-7.00403589268949	0.81024206354656	-2.70956310811866
H	-4.65884340302426	-0.06898138976773	-2.73603000898902
O	1.45581141206347	-1.79576352823179	-1.95003717909719
C	2.27227797266286	-1.47745405614797	-1.00130903273020
O	1.91901735190764	-0.71532871097870	-0.02543866890703
C	3.65553566461692	-2.00542928713528	-1.03914015285818
C	4.56973325096185	-1.67129059942836	-0.01198221476150
C	5.87831404241447	-2.17349718059445	-0.05230940732886
C	6.28153956187852	-3.00825218109142	-1.11270008700418
C	5.37383791515164	-3.34197712136754	-2.13655156108644
C	4.06338856372624	-2.84393361945337	-2.10355928707530
H	3.35018902304467	-3.09766314655250	-2.89576575196587
H	5.68922430485820	-3.99187533967891	-2.96176866331530
H	7.30607291530727	-3.39972978966748	-1.14117242093616
H	6.58631893338796	-1.91412686375273	0.74413557286341
H	4.24754302122407	-1.02081567980095	0.80878080362882
N	0.43578852431129	1.08345493687224	1.94103650022048
H	0.46506470163358	0.43031906249932	2.73394748581017
H	-0.28744505347879	1.78282034143507	2.15052100964077
H	1.33750064495867	1.57550595267387	1.91843114201938

BP-86 Geometry Optimized Coordinates for 4+ of **2e**

Ru	-0.00161237326622	0.01187145812774	0.00215103631940
O	0.52933707383040	1.49686886839139	-1.36533557903405
C	0.52747493542902	1.21933190427311	-2.61904444508884

C	0.91462746191313	2.29008865489422	-3.58133093329450
C	1.28530254823059	3.57357503502894	-3.11796434591909
C	1.64874308325005	4.57691962535215	-4.02606138071985
C	1.65622414403957	4.33651275474773	-5.42062426661358
C	1.27899665590539	3.05056916241232	-5.87367524201429
C	0.91470383660865	2.04041778316826	-4.97253382984948
H	0.62390519750199	1.04933519062048	-5.33969560250040
H	1.26957114557799	2.84045580792958	-6.95155648169337
C	2.07993552483013	5.41338233711804	-6.39167762011311
H	3.18133016272335	5.41951362406020	-6.51006543302686
H	1.64365669065991	5.25246514934530	-7.39254214147256
H	1.78740978245207	6.41705050502168	-6.03616385375918
H	1.93082782114608	5.56904492425140	-3.64885510924499
H	1.28304663618972	3.77632309660081	-2.04078850614059
O	0.21080624655676	0.06466556266447	-3.08705571313733
Ru	-0.32554154523916	-1.45119933493209	-1.77918970678264
O	-0.85611059575536	-2.93278667886436	-0.43029540482756
C	-0.86211221565992	-2.66847839210312	0.82773845399860
O	-0.54628792257473	-1.52111028194324	1.30996728542542
C	-1.25528803375403	-3.75064548396451	1.77459192777803
C	-1.61671901070292	-5.02961040650060	1.29373480162777
C	-1.98928579343903	-6.04325024734065	2.18764013913420
C	-2.01233212147648	-5.81783483461607	3.58381782175481
C	-1.65186444829203	-4.53255804504319	4.05434556208947
C	-1.27819805209699	-3.51338166671497	3.16839904630123
H	-1.00401693334923	-2.52213392899746	3.54765465415679
H	-1.66764650296990	-4.32987779144090	5.13362566206598
C	-2.38619717448111	-6.91993412896455	4.54704216828159
H	-1.47854972519269	-7.41534487666214	4.94419513364810
H	-2.94466066529735	-6.52625410784967	5.41456958440136
H	-2.99771001097198	-7.69728847714740	4.05747617953782
H	-2.27111384431727	-7.03013892767590	1.79685551823982
H	-1.60624573368639	-5.21961594122297	0.21424496903295
O	-2.30389691395870	-0.84227791059132	-1.88390998355020
C	-2.73616028737975	0.04360924501987	-1.05873705971701
O	-2.00243847734036	0.58404098830095	-0.15409017478533
C	-4.16276884299067	0.46483449218723	-1.15719688288267
C	-5.00527577910162	-0.07823613789714	-2.15247972991895
C	-6.34688462821122	0.32180573055656	-2.24095572566786
C	-6.88998202597093	1.27025728968730	-1.34441008745915
C	-6.03668901087929	1.80813851317985	-0.35039078737889
C	-4.69581132207361	1.41568358874536	-0.25528571138490
H	-4.04793486803390	1.84060212793582	0.52011707232773
H	-6.43353591724471	2.54614683270650	0.35961125632889

C	-8.33447683257372	1.70312108380656	-1.43670739614988
H	-8.41176588917657	2.79174156059583	-1.61804767368132
H	-8.86392830395694	1.18169736673584	-2.25184413863561
H	-8.87147733993928	1.49937936727870	-0.49132290545553
H	-6.98759403304561	-0.10958287031509	-3.02155598686586
H	-4.59978904645899	-0.81440534180243	-2.85614280219506
O	1.66055482208940	-2.02545729945235	-1.63370192489830
C	2.40760417774951	-1.49174727440996	-0.73386475962024
O	1.98961763926790	-0.60733146107033	0.09784520193840
C	3.83204949412263	-1.92338418705576	-0.65146983493521
C	4.68868839208005	-1.39083105459298	0.34051898152413
C	6.02584181065908	-1.80012428773196	0.41571266196725
C	6.55472992620068	-2.74971146820326	-0.49215420533418
C	5.69059279138107	-3.27383555815536	-1.48049986722415
C	4.34945650907961	-2.87096531795473	-1.56237998351527
H	3.69290417201667	-3.28697964228981	-2.33531971656982
H	6.07681924075334	-4.00959179092271	-2.19844435571953
C	7.99788933100462	-3.18643841966345	-0.39709895262065
H	8.68127937765227	-2.31871622712685	-0.45371264928598
H	8.19725443510074	-3.68637191443556	0.56967446256254
H	8.26428875946235	-3.88803917132813	-1.20541300626059
H	6.67594828046646	-1.37662753519130	1.19313250764332
H	4.29339936115241	-0.65524964410237	1.05057797757412
N	0.32873648422999	1.40461474758049	1.74056574216177
H	1.32837437496633	1.52471311538813	1.94233827976245
H	-0.05729018113592	2.34150273984093	1.57516734280542
H	-0.10764934428536	1.04839855272289	2.59906164655512

BP-86 Geometry Optimized Coordinates for 5+ of **2e**

Ru	-0.00457442419703	0.01336883906510	0.00173938010113
O	0.51651425964916	1.47050867843636	-1.33952010821455
C	0.51982666145299	1.20841130512015	-2.60136070172321
C	0.90494959888400	2.26827791962079	-3.55579000857093
C	1.27408011471193	3.55205542699061	-3.08792401045352
C	1.63844244919454	4.55169502312249	-3.99690068481317
C	1.64826035770947	4.30699485318238	-5.39157205520960
C	1.27248424600003	3.02037149319971	-5.84613495004935
C	0.90658101910108	2.01137859773024	-4.94703415123136
H	0.61746841905405	1.02054502027456	-5.31550104554522
H	1.26584905056710	2.80986167589209	-6.92346667559355
C	2.07330697547601	5.38147116750449	-6.36190939828238
H	3.17533195517974	5.38428000853040	-6.47433746116711
H	1.64128802335074	5.21841734017855	-7.36392154735936

H	1.78173026234165	6.38535224144832	-6.00704720613640
H	1.91962467941667	5.54430624038594	-3.62171592811947
H	1.27057552218059	3.75792220418692	-2.01158632229134
O	0.19705698828377	0.04205450133488	-3.05647845255934
Ru	-0.32888147214334	-1.44938134105173	-1.77925036701901
O	-0.84677178339913	-2.89770139937653	-0.45041417105376
C	-0.85549060780372	-2.64861433446881	0.81816929849825
O	-0.53697352511272	-1.49057312742475	1.28576024061796
C	-1.24116595394978	-3.72332128727873	1.75545730435046
C	-1.60158605670404	-5.00122772400465	1.26718483299079
C	-1.96960665383811	-6.01501018301825	2.16011621176444
C	-1.98845678691338	-5.79052568815527	3.55720792570406
C	-1.62849477073979	-4.50580503620519	4.03225299634941
C	-1.25890556241490	-3.48418385683498	3.15037070190469
H	-0.98496671016453	-2.49462681173027	3.53345565636438
H	-1.64170627592697	-4.30690972496078	5.11177926325210
C	-2.35797546402450	-6.89366274976764	4.51810464527549
H	-1.44575223867287	-7.38080517108516	4.91494452725251
H	-2.91809476713280	-6.50245925498580	5.38538617493049
H	-2.96256390727809	-7.67510712929697	4.02722914072731
H	-2.25116673776915	-7.00128107410258	1.76895625352164
H	-1.59423297237347	-5.19068428087560	0.18782744419967
O	-2.26796744667177	-0.84729985532871	-1.87585121874331
C	-2.71778752855914	0.04295783604353	-1.05326648068497
O	-1.96747235177306	0.57564837489433	-0.15085239339764
C	-4.13160997541105	0.45984705103967	-1.15215091778931
C	-4.96998784412426	-0.08895977263209	-2.14970029515462
C	-6.30972787610549	0.31118353310686	-2.23834609228398
C	-6.85189613780582	1.26193865441447	-1.34256759758367
C	-6.00076708386915	1.80368551256278	-0.34756904068251
C	-4.66135934085461	1.41354833013858	-0.24925410638648
H	-4.01611372093716	1.84102124489446	0.52659187387514
H	-6.39932225235665	2.54254840205547	0.35984123102257
C	-8.29461751189270	1.69419994978926	-1.43624538185042
H	-8.36857705854252	2.78281889976570	-1.61839901499368
H	-8.82486461395913	1.17165750135650	-2.24963622260036
H	-8.82880551137644	1.49388033653997	-0.48867515962180
H	-6.95021544082390	-0.12114313822198	-3.01791821692664
H	-4.56570352108620	-0.82613893779202	-2.85262117935725
O	1.61982814103980	-2.00798852430138	-1.63169738417849
C	2.38396177465394	-1.48213707569141	-0.73104693194181
O	1.94875736772847	-0.59490539708572	0.09621801129784
C	3.79475750873064	-1.91260756384181	-0.64929328770745
C	4.64986524456607	-1.37739467693234	0.34445047062480

C	5.98409443954015	-1.79022048854284	0.41783159575069
C	6.50868825618440	-2.74277732569180	-0.49073257282936
C	5.64430795156758	-3.26765332402178	-1.47948129612208
C	4.30542849132175	-2.86356579406504	-1.56260834234206
H	3.64951713402085	-3.27988160637018	-2.33559570228796
H	6.02932517480458	-4.00462489634256	-2.19607808355695
C	7.94921678191838	-3.18188550495630	-0.39505157970406
H	8.63201311009838	-2.31361681434290	-0.44755972455402
H	8.14376264549813	-3.68148342735399	0.57278953906626
H	8.21617147974210	-3.88290046201089	-1.20317454480691
H	6.63613315993899	-1.36815324007813	1.19372204189481
H	4.25876523371980	-0.64047447299069	1.05505232792955
N	0.31298535651590	1.39145157993143	1.70409839749047
H	1.31362854643710	1.52484587124613	1.89626976516879
H	-0.08966240169221	2.32056480078671	1.53001327673007
H	-0.11566751218096	1.02995277844846	2.56519866482473

BP-86 Geometry Optimized Coordinates for 4+ of **2f**

Ru	0.10922589026389	-0.01297147633908	-0.03936562796083
O	-0.25522646001247	1.12157786215463	-1.75343654158683
C	0.49849403761674	0.96039388234599	-2.78581536990361
C	0.22511788101707	1.76849680004861	-3.99431024293864
C	-0.84089540134878	2.70188199258916	-4.02664761776468
C	-1.10726067945993	3.46715411624323	-5.16209020634058
C	-0.30831479503433	3.33691746949231	-6.34454294406797
C	0.76840703706735	2.39184930336367	-6.30493356537639
C	1.01959805044738	1.63526137283205	-5.16038464292996
H	1.85017827391613	0.91929851219604	-5.15875498561118
H	1.40980811930817	2.25393959768541	-7.18115973694917
N	-0.56305189266789	4.08487934333742	-7.46759944844848
C	0.26631622118463	3.93049930121716	-8.65828640970041
H	1.32805319635926	4.17561727867887	-8.45653561282969
H	0.22682853390340	2.89757362216999	-9.05801608059164
H	-0.09656741632949	4.61209749063580	-9.44158797492863
C	-1.66817226527793	5.03767951477322	-7.48336971039883
H	-2.64428267035721	4.54136312113427	-7.31285503835420
H	-1.54761289299861	5.82295845801990	-6.71077207217438
H	-1.70543133552193	5.53142348061076	-8.46576229943996
H	-1.94209904967858	4.17458402090340	-5.13725655031253
H	-1.46959777214036	2.82194368436779	-3.13621080252978
O	1.48061092471247	0.12444158529792	-2.81287059889696
Ru	1.88927204353107	-1.02431554844353	-1.13614217646167
O	2.26419479864191	-2.15400347228233	0.56070278591100

C	1.51877364123373	-2.00305841721696	1.60267472454139
O	0.53192340798049	-1.17589676615074	1.64354175901857
C	1.81212129148972	-2.81691200967421	2.80256384079555
C	2.89202861441632	-3.73461196493597	2.81779819119978
C	3.17923670984883	-4.50589050446332	3.94389088223574
C	2.38764331287647	-4.39893252501042	5.13367573898989
C	1.29714549904453	-3.46927880042017	5.11164202546339
C	1.02566274339400	-2.70557924511266	3.97628928622659
H	0.18500007550408	-2.00153397719800	3.98825418617328
H	0.661111104893359	-3.34882077521132	5.99434170038148
N	2.66230156137847	-5.15427862581869	6.24705756932256
C	3.78340709965557	-6.08820499758559	6.24482462881122
H	4.75042689805029	-5.57332630480422	6.07710985408193
H	3.83318003249839	-6.59496680318963	7.21985934729457
H	3.67244989248546	-6.86441026648327	5.46179833709864
C	1.84237583070668	-5.02272177745381	7.44695985364453
H	2.21978149574400	-5.70943049577766	8.21907784820634
H	1.87393193472787	-3.99409359443867	7.85858347983808
H	0.78166513104929	-5.27736240995610	7.25189671467004
H	4.02494239382078	-5.19975158778832	3.90558156040109
H	3.51525502427248	-3.83674455835701	1.92128694570388
O	0.60249472343108	-2.49195870338609	-1.83134867880802
C	-0.64718702001638	-2.44268059075603	-1.51481440776775
O	-1.14472122061594	-1.51675467690416	-0.77015282705489
C	-1.54597017846452	-3.49763386893951	-2.03196482418901
C	-1.05389054003933	-4.53243442837744	-2.86598591045302
C	-1.89194491146624	-5.53071353267870	-3.36216501573495
C	-3.28927346831332	-5.54773694723881	-3.04446244191464
C	-3.78004361835759	-4.50013810693094	-2.19857287069287
C	-2.92686078745486	-3.50875216170598	-1.71321980085730
H	-3.33010926460420	-2.71791487795556	-1.06932023241064
H	-4.83908587505847	-4.46682123446959	-1.92339546496836
N	-4.12142852135874	-6.52614691228395	-3.53007242939119
C	-3.59383021862112	-7.58213723689964	-4.38792662622061
H	-2.81400077810654	-8.18035712835795	-3.87584939132131
H	-4.41263537785142	-8.26058402495037	-4.66944716133539
H	-3.15188972178484	-7.17500445305562	-5.31898751676315
C	-5.53912064286814	-6.52592363703181	-3.18454035990606
H	-5.69855347087099	-6.62751018192874	-2.09237570197213
H	-6.04381146295502	-5.59682713894841	-3.51596117070313
H	-6.03164129422188	-7.37555489896559	-3.68044026772201
H	-1.46443361626810	-6.30849385813507	-4.00269826880509
H	0.01152754191091	-4.54483041439206	-3.12544392353377
O	3.14363556261478	0.46531594201643	-0.42213533896093

C	2.65946502135730	1.40184197777936	0.32098947791422
O	1.41567164945466	1.46028278696173	0.65212510056850
C	3.57257951485936	2.45509251456620	0.81603048600394
C	3.10081818304952	3.50345309410406	1.64487146532661
C	3.95407342365326	4.50031939228800	2.11781407071485
C	5.34676704228580	4.50228880693158	1.78009460548039
C	5.81692394994644	3.44076713335827	0.93977267822269
C	4.94891942387877	2.45130819617803	0.47785933053505
H	5.33666052138996	1.65014139691613	-0.16275925959089
H	6.87176615624310	3.39497568657301	0.65058477157658
N	6.19400129870210	5.47939750088378	2.24157256128152
C	7.60579003730158	5.46381790359100	1.87312748288217
H	8.11078630485203	6.32061244173547	2.34317328549246
H	8.11125004809294	4.53878779077343	2.21490729720028
H	7.74735217153097	5.54245628568428	0.77671103747787
C	5.68928141810489	6.54727165932894	3.09850018613415
H	6.51833830055522	7.22042227088963	3.36283414131855
H	4.90744659908936	7.14872051662925	2.59327722993687
H	5.25752875269175	6.15165274562445	4.03922810058210
H	3.54199014537057	5.28921197804438	2.75488077152908
H	2.03921973275600	3.52848295599065	1.91870599489522
N	-1.63335679203544	0.93651226374118	1.04368434379199
H	-1.64758467842322	1.95895316256075	0.95309634441362
H	-2.53340424974723	0.59242869258504	0.68940083409112
H	-1.60847528987185	0.72608834257108	2.04822747019479

BP-86 Geometry Optimized Coordinates for 5+ of **2f**

Ru	0.10017241218021	-0.00612789907006	-0.03678028531169
O	-0.25875483519014	1.10738095182628	-1.71908067663247
C	0.48998714697866	0.95838361086477	-2.76457572764797
C	0.22360216747861	1.75491516949725	-3.96175837108749
C	-0.84612975824361	2.68859751116844	-3.99636872106991
C	-1.10685183415281	3.44875833076884	-5.13215289965039
C	-0.30079650467463	3.31580274336161	-6.31226637204309
C	0.77817428726354	2.37023666021006	-6.26855940524541
C	1.02629219559489	1.61700771441170	-5.12540018558238
H	1.85754117423589	0.90226043195516	-5.12141078705248
H	1.42195249578874	2.23170275176295	-7.14244716610491
N	-0.55039379931460	4.05927205468995	-7.43308644636381
C	0.28297569684369	3.90404523826133	-8.62338870446757
H	1.34315100510295	4.14642676021926	-8.41505035450885
H	0.23921375661661	2.87195102072894	-9.02266213926949
H	-0.07602374449900	4.58842669505013	-9.40548602209112

C	-1.65859296194419	5.01148163904257	-7.45801379824370
H	-2.63320565333842	4.51088843556063	-7.29675586456689
H	-1.54306694129513	5.79451892732200	-6.68364770820214
H	-1.68698613268542	5.50525903362003	-8.44024905947824
H	-1.94203670513963	4.15535996832025	-5.11307023668535
H	-1.47929639541191	2.81114030399848	-3.10978032827301
O	1.47683810082825	0.11210677063652	-2.77324482902936
Ru	1.87882679611511	-1.01620172082752	-1.13337553300341
O	2.24417178434690	-2.12189886083467	0.52964912403536
C	1.50269684849495	-1.98427639305543	1.58870337480534
O	0.51458830395536	-1.14840036066960	1.61385878125427
C	1.79585919589229	-2.79205065735047	2.77195808599999
C	2.88127175770430	-3.70809233551081	2.77990019243230
C	3.16973872312991	-4.47891958210562	3.90165939145201
C	2.37662402186151	-4.37643272013571	5.09341434575667
C	1.28176351758009	-3.44826643645966	5.07681012298177
C	1.00662606647861	-2.68319544592945	3.94771848079020
H	0.16393574027548	-1.98210858352033	3.96473924498703
H	0.64733887964734	-3.33241326635832	5.96079283963891
N	2.65286820187261	-5.13162009877400	6.20004609543937
C	3.78014886689207	-6.06127666802710	6.19785889214262
H	4.74356763833302	-5.53805118403424	6.04045400107648
H	3.82514855240090	-6.57479736279999	7.16913296533976
H	3.67470899194899	-6.83012154548992	5.40813210542958
C	1.83546391073307	-5.00536651369142	7.40474313552114
H	2.21331799110366	-5.69873750014152	8.17011354370897
H	1.87329071869819	-3.97960589451710	7.82094480938270
H	0.77523491976966	-5.25648115857240	7.20765567546720
H	4.01713707821832	-5.17001574185369	3.86172765913519
H	3.50507785937825	-3.80736024008361	1.88382272852333
O	0.61565290165785	-2.45187385293455	-1.81300851180427
C	-0.64637655930554	-2.41976920051416	-1.50180508336843
O	-1.13059394676098	-1.48214271924473	-0.75237105360217
C	-1.53039005662396	-3.46663096482148	-2.01290217229685
C	-1.02946672326396	-4.49961692879316	-2.84912388877636
C	-1.86248958237549	-5.49832513973188	-3.34309049125847
C	-3.26138800705424	-5.52060756248368	-3.02305824055933
C	-3.75883323532763	-4.47478225886102	-2.17496791846581
C	-2.91353336929541	-3.48131447374985	-1.69044672068931
H	-3.32185863293010	-2.69391634037099	-1.04600622170975
H	-4.81755486291127	-4.44772914332238	-1.89940013922855
N	-4.08619367179136	-6.49891537859103	-3.50664172312061
C	-3.55550082768802	-7.55485033885228	-4.36612474622697
H	-2.77514881862965	-8.14917042312671	-3.85205489696768

H	-4.37311244407804	-8.23439273667686	-4.64688001061396
H	-3.11635867437484	-7.14359778878585	-5.29570350503165
C	-5.50592367284240	-6.50760429180742	-3.16088323682471
H	-5.66159301230569	-6.61505768040997	-2.06956645706644
H	-6.01225417297346	-5.57952900057005	-3.48978509155032
H	-5.99279421933212	-7.35765195338271	-3.66077993426783
H	-1.43291964939413	-6.27410720058284	-3.98400314277331
H	0.03523252336821	-4.50876870355345	-3.11042436532554
O	3.10553212781002	0.44335897109972	-0.43223830027252
C	2.63551959762820	1.39442003150078	0.31907482264678
O	1.38268218654805	1.43956166780978	0.64203997265622
C	3.54271129739123	2.43209378877642	0.80788466975802
C	3.07141260260775	3.48146240104870	1.64090941205710
C	3.92775502342596	4.47169948374888	2.11174275306904
C	5.32177292328595	4.46839099113486	1.76976246683565
C	5.78900002773553	3.40623893638556	0.92500134214640
C	4.92070855343796	2.42168105214024	0.46379128663882
H	5.30670831154892	1.62177759660911	-0.17896145759788
H	6.84274098348459	3.35910954367279	0.63365471449209
N	6.16995336039997	5.43804618380943	2.22974605518660
C	7.58299896755654	5.42111374430261	1.85801607576145
H	8.08975006862163	6.27423082476308	2.33191116895940
H	8.08373392435349	4.49295620844356	2.19547153027784
H	7.71940365916022	5.50552300458061	0.76218648046427
C	5.67182449423752	6.50912667397802	3.09003330154411
H	6.50612554334561	7.17437826992489	3.35628288412719
H	4.89609622616585	7.11571950678019	2.58326338068568
H	5.23772886374914	6.11155387300622	4.02782833806882
H	3.52050298489754	5.26111564506905	2.75060383140850
H	2.01101338345463	3.51084997694388	1.91789896501947
N	-1.61050084192319	0.93917396030716	1.02246493567350
H	-1.61409587444609	1.96115598293120	0.91970253053619
H	-2.50992979742282	0.59493831888924	0.66494005832240
H	-1.58593088067512	0.73500222004656	2.02892653937424

BP-86 Geometry Optimized Coordinates for 4+ of **3a**

Os	0.00432258673804	0.02642112215917	0.02367836016210
O	0.53008505429428	1.49308720805250	-1.34928852898859
C	0.52679280582592	1.20975088276173	-2.60501848990985
C	0.90850183143061	2.27471145591784	-3.56810047848641
C	1.27512652312369	3.55885976639587	-3.10267352010789
C	1.63759633070453	4.56937198118754	-4.00449394559502
C	1.63050158346160	4.28604251713275	-5.38208593309451

C	1.26985052140956	3.01740552067105	-5.87109963122126
C	0.91001832303687	2.01584653844461	-4.95829535713865
H	0.62697586190440	1.02250985963776	-5.32408617121073
H	1.26952846033101	2.81346707340766	-6.94769062881711
Br	2.12325884430632	5.65871070075438	-6.62038945480404
H	1.92165076836031	5.56296315613580	-3.64008042638181
H	1.27585843288932	3.76357728860680	-2.02631300571780
O	0.21101093386457	0.04987095342152	-3.07139947244986
Os	-0.32301271711748	-1.46067721826042	-1.77950773789586
O	-0.84768754987914	-2.92130341141360	-0.42861136419254
C	-0.85334718491915	-2.65593068173440	0.83308424135759
O	-0.53860845705575	-1.50552598391830	1.31786408341214
C	-1.24299479999027	-3.73658925429010	1.77522063633512
C	-1.60582963308499	-5.01351524374025	1.28750626539130
C	-1.97468241631396	-6.03765937356111	2.17105437392486
C	-1.97798636582792	-5.77540212186420	3.55298865087787
C	-1.62156253786866	-4.51443333372479	4.06396662843580
C	-1.25515433762334	-3.49899323932250	3.16920635444933
H	-0.97512259372109	-2.51110964624615	3.55160759289319
H	-1.62946018622672	-4.32699150903397	5.14352990804664
Br	-2.47952812288979	-7.16691196890442	4.76649445324477
H	-2.25567953833430	-7.02564147705671	1.78947527104489
H	-1.59865622213924	-5.20247696825784	0.20827397560477
O	-2.28507737656053	-0.84780691230958	-1.87722051260606
C	-2.72029484214368	0.04310028049526	-1.05310259136956
O	-1.98846101855577	0.58715254327580	-0.14430113072629
C	-4.14122174766492	0.46382154686363	-1.15913963499185
C	-4.97555517698140	-0.08072960539096	-2.16267346401047
C	-6.31630005735877	0.31509215780418	-2.26976597721702
C	-6.82052778366569	1.26289926873429	-1.36089014420197
C	-6.01247688733809	1.81873980228617	-0.35285179682240
C	-4.67301408812768	1.41524703465351	-0.25804969375352
H	-4.03077836788835	1.83893401305003	0.52204770593386
H	-6.42130612992062	2.55516200977278	0.34802239894048
Br	-8.64865191075263	1.80995552024539	-1.50055472420636
H	-6.95906015180028	-0.10734374114173	-3.05022159185587
H	-4.56814536352999	-0.81715849162814	-2.86425681710084
O	1.65010725438227	-2.02288709542888	-1.62377062207819
C	2.39970769398259	-1.48789921138508	-0.72134586025396
O	1.98341756777339	-0.59903002421107	0.11171128116580
C	3.81784966862283	-1.92294856274989	-0.63890511872062
C	4.67185070412680	-1.38900165481140	0.35373968187864
C	6.01048177926261	-1.79718095831751	0.43991398765015
C	6.49256894221968	-2.74667101043469	-0.47890045740353

C	5.66457684681447	-3.29222052843385	-1.47655830158224
C	4.32766282418217	-2.87637852221281	-1.55046580321283
H	3.67058375998868	-3.29243339251704	-2.32231133757707
H	6.05615392955395	-4.03025770300663	-2.18553714841407
Br	8.31748758562183	-3.31086024921617	-0.36789815403202
H	6.66855729607290	-1.38289854804021	1.21194820588210
H	4.28093504095215	-0.65112038186705	1.06311344181692
N	0.34191810338870	1.41634604135313	1.75227720302482
H	1.33802244277769	1.49797885319279	1.99189680519109
H	0.00891305894468	2.37100964515042	1.56850348538315
H	-0.13704085506828	1.10129501286717	2.60527726610133

BP-86 Geometry Optimized Coordinates for 5+ of **3a**

Os	0.00141839933153	0.02066034883094	0.01464486861616
O	0.51684164762729	1.46310249069206	-1.32747116682463
C	0.51957995827930	1.19600771208268	-2.59110958621787
C	0.90171412435505	2.25394553056017	-3.54563873280379
C	1.26716521412688	3.53714168699968	-3.07429128594293
C	1.63230378331715	4.54506442444943	-3.97533768855306
C	1.62906598430843	4.26063142617759	-5.35372089364912
C	1.26914892296741	2.99181891188111	-5.84503085801883
C	0.90598843257341	1.99035492067181	-4.93579081916509
H	0.62389074916060	0.99791100840575	-5.30429416905788
H	1.27227792076059	2.78845370913105	-6.92148496557742
Br	2.12527235455201	5.62933906563153	-6.58700167866540
H	1.91587149718713	5.53844640047924	-3.61072443717361
H	1.26551703620111	3.74385238189148	-1.99846929934294
O	0.19799729535586	0.02709809287250	-3.04733887447280
Os	-0.32446286765170	-1.45489682512319	-1.77691218403422
O	-0.83790572889579	-2.89286762021517	-0.45348783838329
C	-0.84477718009761	-2.64014008084164	0.81687004169361
O	-0.52710774365059	-1.47960878018483	1.28653126904380
C	-1.22830921490959	-3.71293232530118	1.75415833745878
C	-1.58959753495681	-4.98987224529486	1.26296959903777
C	-1.95530264925774	-6.01160602186854	2.14822260323955
C	-1.95684249130454	-5.74737411569623	3.53055580630879
C	-1.60117351616182	-4.48506296682362	4.04147179933238
C	-1.23746174188984	-3.46981077122270	3.14803282039635
H	-0.95853505033214	-2.48217704140772	3.53143792592155
H	-1.60802014670957	-4.29752844882042	5.12077801575101
Br	-2.45382136560657	-7.13474716864326	4.74248876251609
H	-2.23565448431679	-7.00016257570156	1.76834861055834
H	-1.58436241107534	-5.18121095416153	0.18429013060325

O	-2.25216799486716	-0.85669948479994	-1.87300010807894
C	-2.70141000834535	0.03666212380224	-1.04967201592822
O	-1.95240659007855	0.57254416767565	-0.14411703128423
C	-4.11235474177527	0.45530696991860	-1.15228907033244
C	-4.94508761195202	-0.09181499542541	-2.15693284470473
C	-6.28391740938074	0.30590434953483	-2.26106954879170
C	-6.78572163403916	1.25495600350638	-1.35098098907852
C	-5.97631031299652	1.81108927127398	-0.34281802124908
C	-4.63843733208493	1.40811113731542	-0.24807091115404
H	-3.99678459857480	1.83239865903528	0.53197604186713
H	-6.38422900167726	2.54775676302777	0.35794719960375
Br	-8.60838219435076	1.80260614280562	-1.48864605614162
H	-6.92815366578447	-0.11562234946763	-3.04047374105663
H	-4.54075940871213	-0.82847771414555	-2.85983061995925
O	1.61282950247654	-2.00886494416000	-1.62805303122459
C	2.37620515486812	-1.48037224198247	-0.72485412294916
O	1.94261363928514	-0.58871201172600	0.10289380146218
C	3.78394089418825	-1.91344253189001	-0.63972915495155
C	4.63346489885960	-1.37750083649301	0.35683717850802
C	5.96938472539134	-1.78846600641784	0.44462695075850
C	6.45152737410544	-2.73976370375241	-0.47379089037814
C	5.62524994766049	-3.28505045993537	-1.47407647410090
C	4.29032607123556	-2.86876309417914	-1.55251406158194
H	3.63594398573695	-3.28494888056328	-2.32637879978775
H	6.01772113300551	-4.02371361480486	-2.18153918236423
Br	8.27020979805220	-3.30552142356539	-0.35834236673536
H	6.62664805581571	-1.37551509092716	1.21772674075281
H	4.24420392748376	-0.63905999484161	1.06630656919580
N	0.32372927570006	1.40691894262680	1.71780093080505
H	1.31853361627100	1.48799391469867	1.96524721089881
H	-0.00717315824107	2.36002875047819	1.51983479997249
H	-0.16530659056282	1.09754374392714	2.56783273541398

BP-86 Geometry Optimized Coordinates for 4+ of **3b**

Os	0.01278210424047	0.05324698887787	0.05242000528129
O	0.53965981678142	1.51948637592722	-1.32066204899790
C	0.53653473992918	1.23639699851190	-2.57671445018336
C	0.91963547468607	2.30049708171290	-3.53935294135542
C	1.28726206460493	3.58486894082349	-3.07428685131546
C	1.65105184796031	4.59394654081907	-3.97573846379964
C	1.64576413283916	4.31331154391961	-5.35506086945018
C	1.28353611984235	3.04292143023050	-5.84161003908578
C	0.92218850099106	2.04208731701556	-4.92998733299310

H	0.63843737515040	1.04889260422599	-5.29553792647128
H	1.28588651980665	2.84512225621878	-6.91935665391888
Cl	2.09957066451651	5.57101155496855	-6.48951039301279
H	1.93660833429683	5.58935007750893	-3.61743891144134
H	1.28720175114122	3.78931003860291	-1.99790545901673
O	0.21950584227781	0.07643216021774	-3.04268779358540
Os	-0.31551410887841	-1.43363404404118	-1.75027678156848
O	-0.84117728946078	-2.89387681563101	-0.39915078214701
C	-0.84734359582893	-2.62859454934376	0.86280709065123
O	-0.53144886870579	-1.47803076342341	1.34713427886160
C	-1.23872718155557	-3.70822239505374	1.80454798201572
C	-1.60167704699900	-4.98565147384059	1.31722634574086
C	-1.97232960443190	-6.00820481703030	2.20036975390667
C	-1.97895399719827	-5.74824257883496	3.58389245677467
C	-1.62181073606294	-4.48521984925817	4.09240750016368
C	-1.25329814333535	-3.47068388160737	3.19887332095593
H	-0.97328587742971	-2.48272369076188	3.58102388296305
H	-1.63358519379657	-4.30359019347530	5.17293861053258
Cl	-2.44170511515193	-7.02304650086450	4.69538108877831
H	-2.25416356172245	-6.99829278081535	1.82488775733189
H	-1.59264520860567	-5.17465933773764	0.23804782054207
O	-2.27759287956265	-0.81998841701058	-1.84774013919860
C	-2.71283423705700	0.07091769806091	-1.02325358987119
O	-1.97982691270190	0.61496589197493	-0.11504660545847
C	-4.13357836189626	0.49077931610839	-1.12755130409560
C	-4.96979683251822	-0.05450970568209	-2.12960145989820
C	-6.31028687479064	0.33973057020417	-2.23376691858658
C	-6.81738775385838	1.28752090892089	-1.32470240792619
C	-6.00482636755701	1.84335115365781	-0.31866754295817
C	-4.66550085672810	1.44211802966328	-0.22589318806518
H	-4.02206706240188	1.86647652397014	0.55282230048085
H	-6.41914907197253	2.57889938884895	0.37990189431203
Cl	-8.49404346849093	1.78562974045626	-1.44831960954015
H	-6.95902454149939	-0.08007773898791	-3.01069719828337
H	-4.56250538808215	-0.79060048945885	-2.83156574471808
O	1.65756684884334	-1.99686100272202	-1.59494300832029
C	2.40815443087341	-1.46196797096931	-0.69293751754355
O	1.99174274661459	-0.57301956264662	0.14037084455899
C	3.82605735514043	-1.89618352165070	-0.61180753684258
C	4.68165256794295	-1.36158660524369	0.37960568304347
C	6.01995294636655	-1.76825455786383	0.46325123281312
C	6.50513347106246	-2.71778070426552	-0.45566084035689
C	5.67294668527474	-3.26315953833400	-1.45155143677112
C	4.33623800530495	-2.84949138974997	-1.52382881511095

H	3.67820497880930	-3.26610020619865	-2.29452116344042
H	6.07027946281082	-4.00030406508641	-2.15825275653416
Cl	8.17871048872159	-3.23167301870028	-0.35782935899437
H	6.68374079913961	-1.35667838367633	1.23184088743179
H	4.29067501590177	-0.62403511209222	1.08924430667388
N	0.35345264263378	1.44405058810690	1.78050849097085
H	1.34898958345427	1.51593736117639	2.02543859634835
H	0.03116528789102	2.40147554716736	1.59233406763478
H	-0.13359785756966	1.13594910416069	2.63142159208930

BP-86 Geometry Optimized Coordinates for 5+ of **3b**

Os	0.00946387087070	0.04789566909870	0.04365933845170
O	0.52604450930518	1.48987989158615	-1.29856646804747
C	0.52910280858215	1.22285092629391	-2.56247934133333
C	0.91317432650414	2.27954337872713	-3.51653342648934
C	1.27960805010496	3.56306232638115	-3.04562097177809
C	1.64693124220444	4.56924288431112	-3.94613911919969
C	1.64641838608792	4.28684150227508	-5.32614890439018
C	1.28491495422929	3.01631176600348	-5.81521205808997
C	0.91934369878352	2.01606768701225	-4.90711782877535
H	0.63657366446000	1.02368795932497	-5.27531160316406
H	1.29147665857189	2.81871586226226	-6.89275349309014
Cl	2.10474658645625	5.54013558415584	-6.45570747640617
H	1.93204467937153	5.56443639087307	-3.58761849534884
H	1.27648786219314	3.76972477033149	-1.96978496607809
O	0.20604748614411	0.05387216932033	-3.01837445870097
Os	-0.31756288225508	-1.42732685342338	-1.74743301812247
O	-0.83203829133933	-2.86488037412880	-0.42399030372433
C	-0.83907632613135	-2.61233546365903	0.84668940735657
O	-0.52020645263455	-1.45169388879875	1.31605368808524
C	-1.22390603886850	-3.68421817248000	1.78337689560659
C	-1.58538033373103	-4.96160976478582	1.29236572053512
C	-1.95241862771825	-5.98205325453855	2.17692155702235
C	-1.95665362711913	-5.72024597252137	3.56091048844515
C	-1.60027671590574	-4.45602930024339	4.06986004793913
C	-1.23498252628535	-3.44153786893964	3.17773242302387
H	-0.95601702851837	-2.45384182941711	3.56098900565037
H	-1.61054119151543	-4.27454207530887	5.15019659516747
Cl	-2.41440220294179	-6.99143494262690	4.67051585162714
H	-2.23360523564893	-6.97263509644433	1.80291233965646
H	-1.57866177319805	-5.15270602236221	0.21364683319349
O	-2.24489005574621	-0.82826336743694	-1.84350596597950
C	-2.69409755698783	0.06511969545999	-1.01973027895271

O	-1.94405888361902	0.60101063664277	-0.11466444868196
C	-4.10471074328532	0.48265586324577	-1.12074093463340
C	-4.93932108920205	-0.06598246092056	-2.12352754189569
C	-6.27797526086536	0.32953784272598	-2.22478206223271
C	-6.78258736372714	1.27887416281802	-1.31471049962609
C	-5.96885572270796	1.83605638314974	-0.30893343875321
C	-4.63108618411741	1.43575247916787	-0.21636975360065
H	-3.98816590729851	1.86129138799672	0.56196206433333
H	-6.38230957580013	2.57211327146501	0.38925275332512
Cl	-8.45418449234886	1.77649400383364	-1.43619229424940
H	-6.92816195507481	-0.09004591869421	-3.00030711247649
H	-4.53496967260071	-0.80258516329203	-2.82648967650563
O	1.61937939263575	-1.98267001002746	-1.59906002950982
C	2.38385850785581	-1.45432716167610	-0.69628285602045
O	1.95039702032086	-0.56255266431947	0.13184053098213
C	3.79116826848636	-1.88668239870313	-0.61274902725879
C	4.64285335595139	-1.34949991573169	0.38187649263758
C	5.97845997044547	-1.75869255254560	0.46669551323015
C	6.46300020547875	-2.71050844664394	-0.45174921353010
C	5.63215550879445	-3.25652839022615	-1.44952473081706
C	4.29747061687441	-2.84247388926963	-1.52570642995490
H	3.64167159533402	-3.25969268030686	-2.29782282231790
H	6.02994002395577	-3.99473580261472	-2.15451230747319
Cl	8.13075806199508	-3.22523694667066	-0.35078346207124
H	6.64180534981946	-1.34790508708750	1.23576362750012
H	4.25384012059232	-0.61095752656778	1.09139251539277
N	0.33392662844375	1.43445387908830	1.74645099638581
H	1.32810769618380	1.50941443977477	1.99878984911850
H	0.01101643578465	2.39006861605635	1.54671644389026
H	-0.16047921562912	1.13105790303070	2.59564779072299

BP-86 Geometry Optimized Coordinates for 4+ of **3c**

Os	0.00456570666965	0.02536739290121	0.02232070656547
O	0.53102051632439	1.49290696261900	-1.35028346791558
C	0.52837038366513	1.21152478366878	-2.60741234751647
C	0.91075767822245	2.27567873793565	-3.56850669670352
C	1.27951747552826	3.56034888812729	-3.10255035233654
C	1.64269135459459	4.56801804367409	-4.00449700619768
C	1.63658520032244	4.28949333569092	-5.38177604171470
C	1.27392239379119	3.02209271560022	-5.86869244384773
C	0.91247251806131	2.01936121645015	-4.96041219440540
H	0.62786571665573	1.02647401925794	-5.32607159789516
H	1.27989555128894	2.83916303247105	-6.94978347638311

F	1.98292334047473	5.24888153102283	-6.24504827441516
H	1.93152011046340	5.56774817760623	-3.65891602240785
H	1.27998964729269	3.76269548097342	-2.02580217751048
O	0.21146368526314	0.05071662641791	-3.07288352672479
Os	-0.32289603472034	-1.46051333203774	-1.77986586486982
O	-0.84798566173947	-2.92223195616699	-0.42861375944267
C	-0.85447122028834	-2.65830345869485	0.83420583807802
O	-0.53879381674521	-1.50657619530766	1.31766894267851
C	-1.24493375023781	-3.73753934589726	1.77497553778671
C	-1.60944213909340	-5.01527493015540	1.28711072010778
C	-1.97945058020212	-6.03616105916728	2.17106353300730
C	-1.98466532452459	-5.77806840055712	3.55245851415511
C	-1.62662832244249	-4.51802401079579	4.06099407271986
C	-1.25816749097196	-3.50185092617328	3.17049343074446
H	-0.97697254710999	-2.51416684491223	3.55244947694854
H	-1.64161439326754	-4.35115577719369	5.14460121697606
F	-2.33772418606110	-6.75038067122699	4.39840546774759
H	-2.26508269619408	-7.03069361975559	1.80828835906999
H	-1.60132074270203	-5.20241509334093	0.20763072500508
O	-2.28630869835243	-0.84782257852501	-1.87728249137285
C	-2.72295398308369	0.04374023539413	-1.05338031393843
O	-1.98866418257764	0.58728066896902	-0.14493645462146
C	-4.14236413877064	0.46389971022879	-1.15826665961672
C	-4.98099890890365	-0.08604907710956	-2.15698132022801
C	-6.32002383040234	0.31044288680416	-2.26026506200017
C	-6.82429897108402	1.26263914640088	-1.35807051942872
C	-6.01180909657167	1.82212296964743	-0.35741419856980
C	-4.67344065675976	1.42133017408113	-0.26122423461122
H	-4.02822906885701	1.84875692953951	0.51429124260946
H	-6.43795773748001	2.56199052157769	0.33052917827877
F	-8.10147267219666	1.64387902052305	-1.45416165411170
H	-6.98152032869626	-0.10523780058455	-3.02965029386792
H	-4.57427448345715	-0.82650557639088	-2.85461584571114
O	1.65140696887489	-2.02346587304145	-1.62457876580944
C	2.40296223948080	-1.48861018708974	-0.72257065529674
O	1.98456777355247	-0.59927160831011	0.11037972639457
C	3.81980563030633	-1.92222538406111	-0.64049269885808
C	4.67729955181006	-1.38257326442876	0.34776878889648
C	6.01423705033169	-1.79099004924495	0.43102630537732
C	6.49725748102808	-2.74484339608345	-0.48077105557169
C	5.66572538096574	-3.29421595458028	-1.47153406240077
C	4.32979420891611	-2.88149718817994	-1.54771535869054
H	3.67038676462838	-3.30153873562490	-2.31532273219797
H	6.07548278464360	-4.03576311704051	-2.16757425591323

F	7.77218998517015	-3.13782762593740	-0.40375096913037
H	6.69021451099456	-1.38341883404188	1.19212612560680
H	4.28635717450658	-0.64075723525613	1.05291725403978
N	0.34004684795382	1.41310042428012	1.75645799266131
H	1.33831827966519	1.52523401351347	1.97362256864454
H	-0.02801901243519	2.35818417885274	1.59100820568573
H	-0.10751211551791	1.07427931268472	2.61735640244846

BP-86 Geometry Optimized Coordinates for 5+ of **3c**

Os	0.00145493807926	0.02100335227526	0.01423706113210
O	0.51745668231685	1.46426536699049	-1.32735728348019
C	0.52102239834217	1.19891552704052	-2.59253201033301
C	0.90402178417652	2.25474626091096	-3.54487677020834
C	1.27179162325786	3.53892430644010	-3.07326792044831
C	1.63840589966662	4.54324622183089	-3.97425490137330
C	1.63651078367596	4.26161539470024	-5.35199841509128
C	1.27460311441561	2.99421803096733	-5.84197814594810
C	0.90914114990948	1.99277851506991	-4.93694810918641
H	0.62542991253231	1.00061968838513	-5.30476370899121
H	1.28492671282438	2.81184598369073	-6.92280518278271
F	1.98614514537653	5.21738399573396	-6.21184061559092
H	1.92703135825675	5.54295174549743	-3.62947841065697
H	1.26928148642729	3.74373783088407	-1.99716104208727
O	0.19805845308495	0.02856638584707	-3.04768225356533
Os	-0.32462131937083	-1.45313117663361	-1.77636799139581
O	-0.83834697287985	-2.89207561634007	-0.45377470391747
C	-0.84595759109361	-2.64126442707582	0.81824877248126
O	-0.52731350618403	-1.47932608846378	1.28692046854450
C	-1.22970795437243	-3.71247944783753	1.75295792356168
C	-1.59215495989265	-4.99047882669208	1.26087376424991
C	-1.95837771947641	-6.00939628230156	2.14556361231294
C	-1.96147231328296	-5.74867968707835	3.52734580376610
C	-1.60506378281347	-4.48765340376759	4.03756802378241
C	-1.24002038976097	-3.47168147607107	3.14881790279470
H	-0.96039522763189	-2.48423412534573	3.53199410574489
H	-1.61923073923432	-4.32175354044958	5.12100488143088
F	-2.31052681824221	-6.71841898124802	4.37165596207554
H	-2.24283385963963	-7.00461633843213	1.78473438661272
H	-1.58585809232959	-5.17938765009957	0.18186334992777
O	-2.25270649411712	-0.85551935116997	-1.87275119463486
C	-2.70400476079784	0.03844658435280	-1.04922027594150
O	-1.95260068260744	0.57393544968256	-0.14378760341825
C	-4.11263364438611	0.45542163393673	-1.15097139017992

C	-4.94917316347119	-0.09785931773377	-2.15127103035388
C	-6.28613081440612	0.29925099236562	-2.25211987057038
C	-6.78772388951681	1.25245419138911	-1.34815661982252
C	-5.97542492979658	1.81357082258201	-0.34675514087658
C	-4.63886725746431	1.41415436943843	-0.25064265897386
H	-3.99457658945223	1.84255280777865	0.52486216000128
H	-6.40184707467592	2.55329635571819	0.34065532065815
F	-8.06106270331750	1.63300687287357	-1.44298672707742
H	-6.94907149326757	-0.11555826146069	-3.02027819148600
H	-4.54474886253260	-0.83827780664894	-2.85001588365862
O	1.61270264070433	-2.00823514036976	-1.62860802359191
C	2.37861508746939	-1.48038815965867	-0.72537504300984
O	1.94323734139204	-0.58808267657141	0.10253361677255
C	3.78374752890418	-1.91270415744560	-0.64111499906096
C	4.63758626483546	-1.37126140031026	0.35099730777619
C	5.97118003147010	-1.78293389093356	0.43574129270100
C	6.45215818013385	-2.73916569325457	-0.47629063171540
C	5.62255823759880	-3.28869601758362	-1.46980337741814
C	4.28934401605630	-2.87460723908660	-1.54984212794459
H	3.63196371568029	-3.29440074069065	-2.31908214554617
H	6.03299252729346	-4.03120873879195	-2.16391057830068
F	7.72223593827943	-3.13385044823537	-0.39656516109238
H	6.64726289505990	-1.37744902436323	1.19739599431281
H	4.24887121510394	-0.62850811211309	1.05611350564124
N	0.32231804725021	1.40537595055610	1.72240684682281
H	1.32021683177287	1.52784830988919	1.93820557096158
H	-0.05662551446554	2.34508337678162	1.54802079772580
H	-0.12357570086736	1.06544895064969	2.58439318793981

BP-86 Geometry Optimized Coordinates for 4+ of **3d**

Os	0.01698798357203	0.03803615359191	0.06112896650097
O	0.61907601722329	1.67736424344874	-1.06352198038494
C	0.56958971508788	1.61218535065902	-2.34880385586812
C	1.00548762303609	2.79702528902228	-3.13467293784739
C	1.45693397558528	3.96365281940426	-2.47337453310904
C	1.86764727752124	5.08096603570327	-3.21643505006614
C	1.83253359355899	5.04581943154887	-4.62388318559723
C	1.38413693754314	3.88711171804163	-5.28731966049138
C	0.97210611468199	2.76729905442409	-4.54889511332942
H	0.62219108158907	1.86230268541786	-5.05838258618131
H	1.35594408798981	3.85728138163509	-6.38375861754341
H	2.15415546521189	5.92053367419537	-5.20323702414774
H	2.21620376931907	5.98255859203295	-2.69728182171638

H	1.48125655265649	3.98327007196519	-1.37794099814235
O	0.15939071818275	0.57078635413929	-2.98953648308462
Os	-0.45442445015380	-1.09772585101128	-1.95172496248136
O	-1.05086724609302	-2.72925381936905	-0.84793595734749
C	-1.00573846993908	-2.68425545499707	0.44028203961033
O	-0.60300463374319	-1.65286511076348	1.09788701886091
C	-1.44081650371943	-3.88457181369322	1.20274625509651
C	-1.88585718207627	-5.04108707531071	0.51971979646904
C	-2.29542594127631	-6.17237738400940	1.24179476974980
C	-2.26555121643403	-6.16152905000259	2.64989925284380
C	-1.82353382496789	-5.01310888368292	3.33488197633015
C	-1.41261427733796	-3.87926938957953	2.61737873009941
H	-1.06748808395010	-2.98185634779171	3.14321836357606
H	-1.79944231051597	-5.00217128468735	4.43178023780203
H	-2.58632680229967	-7.04725437103384	3.21275832908801
H	-2.63898528606278	-7.06597158734901	0.70578671181919
H	-1.90626117006983	-5.04221527549815	-0.57598135261107
O	-2.37019587115857	-0.34870398877597	-1.87993495821599
C	-2.72459623376022	0.41842683618720	-0.90570785334434
O	-1.93432023646672	0.75250143642848	0.05467005167607
C	-4.11681536333515	0.94105294944218	-0.89155834190537
C	-5.01813667563217	0.59892447629872	-1.92725416659777
C	-6.33110217270585	1.09372878683373	-1.91090791967585
C	-6.75750577464349	1.93309732864981	-0.86331725165290
C	-5.86469161321257	2.27656757873527	0.17025974463930
C	-4.55059099979783	1.78437466051787	0.15850985427765
H	-3.84953303660745	2.04637919985911	0.95902245209121
H	-6.19460093920532	2.93009413711974	0.98756354149963
H	-7.78467423111067	2.31915937300095	-0.85258241210264
H	-7.02490290291526	0.82451617744958	-2.71719131842303
H	-4.67930608445877	-0.05502018419858	-2.73876893133334
O	1.47761045620843	-1.80891480575308	-1.95680917591210
C	2.28473696725177	-1.48309205114358	-1.00512354271427
O	1.94826298538887	-0.72227579675138	-0.02215148491715
C	3.67361476170902	-2.01322463150290	-1.04582940511019
C	4.59163763076967	-1.68521283014192	-0.02028110104807
C	5.90186680200944	-2.18613401274447	-0.06046040424304
C	6.30875600397313	-3.01743338888377	-1.12198046844029
C	5.39917017804822	-3.34682137287038	-2.14565760911350
C	4.08783900324178	-2.84865049554551	-2.11001030802422
H	3.37438082992912	-3.10011952524273	-2.90293382802211
H	5.71388142584835	-3.99412131658092	-2.97382177138454
H	7.33375533712137	-3.40825707475971	-1.15148552437151
H	6.60869842305586	-1.92793232258007	0.73808729053709

H	4.26730511570456	-1.03751522674790	0.80206871844986
N	0.43240851439406	1.10039666119022	1.99509773704835
H	0.43105111610660	0.45662201826270	2.79620365911132
H	-0.27101337933759	1.82096158021747	2.20057407353570
H	1.34432593946762	1.57402470757939	2.00470714578923

BP-86 Geometry Optimized Coordinates for 5+ of **3d**

Os	0.01656040933108	0.03360725030672	0.05172218582834
O	0.60521634490528	1.64446018869015	-1.04661857799546
C	0.56181438712405	1.59638142683216	-2.33692073157365
C	0.99317697607947	2.77482259020745	-3.11518311661846
C	1.44400293471701	3.93876768546151	-2.44718529779133
C	1.85298900879224	5.05545740479198	-3.18957237366895
C	1.81582017510811	5.01975664022631	-4.59717941036389
C	1.36778653890416	3.86324661895751	-5.26474425214450
C	0.95674041057252	2.74216010689439	-4.52999670893986
H	0.60719340512093	1.83866612494501	-5.04201757444799
H	1.33936888896884	3.83654589228929	-6.36085034871366
H	2.13672798366949	5.89537458249182	-5.17526594300913
H	2.20174048876761	5.95668994547010	-2.67079606131245
H	1.46988768486675	3.95828139583813	-1.35196583614619
O	0.14987585184630	0.54329523658119	-2.96941143608941
Os	-0.45035072864327	-1.09371995660654	-1.94789888213195
O	-1.03529796651672	-2.69769294468904	-0.86752559280698
C	-0.99666237866442	-2.66486984092549	0.42716756616226
O	-0.58937301443285	-1.62202428652832	1.07179397337340
C	-1.43084578135050	-3.85530111318159	1.18540660428422
C	-1.87698840650355	-5.00953812169404	0.49770054220291
C	-2.28866755177914	-6.13764591170834	1.22121653895109
C	-2.25884412713011	-6.12307163111362	2.62930858013524
C	-1.81543806066522	-4.97622621804216	3.31648623470783
C	-1.40176803079126	-3.84395750236880	2.60073155908254
H	-1.05577590401073	-2.94783451411184	3.12782767144992
H	-1.79277919515784	-4.96595528683821	4.41300948556761
H	-2.58186718550737	-7.00757454709743	3.19250231896918
H	-2.63375853935058	-7.03129081800242	0.68710958843794
H	-1.89722372551115	-5.01292224708699	-0.59782183556738
O	-2.33247687705873	-0.36207216237669	-1.88024669018962
C	-2.70191801838103	0.40739895898272	-0.90565657828438
O	-1.89633232554017	0.73331554062446	0.05023962648165
C	-4.08462810344202	0.92550595008511	-0.88930575376349
C	-4.98298095973870	0.58099727834229	-1.92777077580612
C	-6.29464138260427	1.07576788141375	-1.90849639809943

C	-6.71801874494180	1.91363710491634	-0.85844327059161
C	-5.82668982046420	2.25787603730524	0.17647686299489
C	-4.51336423318272	1.76751410012100	0.16485475367650
H	-3.81336138108170	2.02990016919849	0.96590088006281
H	-6.15758129654182	2.91022699940180	0.99377130756758
H	-7.74514541202816	2.29934233681679	-0.84664842372993
H	-6.98966192035861	0.80818279276413	-2.71372274710148
H	-4.64590207944398	-0.07164541174952	-2.74083195108034
O	1.44590233850225	-1.79219857748429	-1.95619847385919
C	2.26550392799825	-1.47364107057915	-1.00470757357294
O	1.91153564302274	-0.70824670526478	-0.02615557949553
C	3.64409479203908	-2.00164558352663	-1.04167290636940
C	4.55745875336705	-1.67075505507556	-0.01189218072860
C	5.86519217500619	-2.17453106937069	-0.05050127391602
C	6.26981724995496	-3.00797586385824	-1.11150321862274
C	5.36358201531410	-3.33865428997682	-2.13777552095958
C	4.05388174242323	-2.83927494771613	-2.10680444027302
H	3.34261463118304	-3.09134369356272	-2.90126406039507
H	5.67985963815108	-3.98757646386803	-2.96353772442976
H	7.29396756537672	-3.40077381745606	-1.13853033577277
H	6.57185902238008	-1.91753348215422	0.74802064402760
H	4.23450034157857	-1.02160937119116	0.80962098947860
N	0.44008891688160	1.09129891997556	1.95768361632671
H	0.42579533255357	0.45356315700117	2.76436829424503
H	-0.25225014748990	1.82572062932594	2.15513463585347
H	1.36065721380610	1.54942059894706	1.96413821649492

BP-86 Geometry Optimized Coordinates for 4+ of **3e**

Os	-0.00097301668643	0.02129246837091	0.01977819769037
O	0.52550090002174	1.49082368283839	-1.35096928238483
C	0.52196249227029	1.21203938694800	-2.60903676660467
C	0.90668462669655	2.27679386518655	-3.56925199567652
C	1.28064126089266	3.56038539813585	-3.10619963736112
C	1.64374583807529	4.56307638377833	-4.01471228645600
C	1.64822871998773	4.32342876647856	-5.40950591374341
C	1.26800883569618	3.03797717710983	-5.86223028764503
C	0.90387099277098	2.02789716038489	-4.96146973516715
H	0.61102548184936	1.03788806216508	-5.32984007602087
H	1.25624079857790	2.82831620978209	-6.94025226492787
C	2.07209095691858	5.39965374322600	-6.38101123053434
H	3.17246491837301	5.39667990444112	-6.51002237945482
H	1.62527799077447	5.24561782288312	-7.37846605815350
H	1.79161174562497	6.40479621302934	-6.01975836328192

H	1.92824929259947	5.55463362694957	-3.63759847886533
H	1.28124681054349	3.76278869101598	-2.02897120284159
O	0.20301153354897	0.05159404711763	-3.07503737041092
Os	-0.32959380632501	-1.46151264279883	-1.78379482511851
O	-0.85314122971838	-2.92558248003871	-0.43422382341963
C	-0.86065143654601	-2.66370953599849	0.82935715012096
O	-0.54471416885037	-1.51181893278745	1.31326600414651
C	-1.25153951163235	-3.74377991533828	1.76975451421207
C	-1.61531348855534	-5.02211796779440	1.28643126866413
C	-1.98700928247276	-6.03727082543282	2.17847930422045
C	-2.00728999646056	-5.81584362839317	3.57548546492189
C	-1.64447991130716	-4.53200056821902	4.04857190990901
C	-1.27156689567046	-3.51069168028543	3.16525936368953
H	-0.99551075665539	-2.52130624867398	3.54794159268709
H	-1.65772197878555	-4.33219330803544	5.12849978041252
C	-2.38062569591927	-6.91991478310405	4.53644903194591
H	-1.47264766899036	-7.40969626851862	4.94011709462789
H	-2.94717753044856	-6.52942402909739	5.40036558163130
H	-2.98430707047406	-7.70113450192276	4.04315336032673
H	-2.27051651999921	-7.02287477344970	1.78547184313593
H	-1.60749615461322	-5.21066602847058	0.20670424665665
O	-2.29368887577060	-0.84999982598472	-1.87799561663789
C	-2.73060276856051	0.04062793193979	-1.05270586271754
O	-1.99406206977688	0.58367325402560	-0.14526548360560
C	-4.15100915116491	0.45998691971331	-1.15403971513235
C	-4.99417859061696	-0.08577506470534	-2.14857560712809
C	-6.33487656059625	0.31553374766856	-2.23907345624375
C	-6.87791104450819	1.26819441603256	-1.34658639513467
C	-6.02499403071350	1.80763405274635	-0.35298962137841
C	-4.68482044374008	1.41441827881977	-0.25500102054951
H	-4.03825160095122	1.84069486398224	0.52070558319756
H	-6.42202877802202	2.54760511950284	0.35498379460931
C	-8.31960589404513	1.70798059129420	-1.44729375487786
H	-8.38813882932966	2.77941933998652	-1.71637833784929
H	-8.86855640247793	1.13031638902224	-2.21011097004449
H	-8.84200759440340	1.58927823309974	-0.47978100979460
H	-6.97565445008047	-0.11847133467109	-3.01826901319643
H	-4.59031387647732	-0.82524074395380	-2.84965993129886
O	1.64550522810108	-2.02317764290395	-1.63212612789107
C	2.39845770380773	-1.49019524762741	-0.72968502962669
O	1.97880580560840	-0.60374111044786	0.10625139452972
C	3.81703930506398	-1.92049903145688	-0.65161351014945
C	4.67574278662986	-1.39131425428798	0.34151870948703
C	6.01273199359265	-1.80104655394627	0.41330332322732

C	6.54131821589078	-2.74632447391541	-0.49921582760877
C	5.67489576666022	-3.26925329271180	-1.48664268528789
C	4.33389507471503	-2.86685381405184	-1.56566787663933
H	3.67676593359069	-3.28339541016672	-2.33778905331763
H	6.05927458049455	-4.00510137239173	-2.20560470741519
C	7.98985355686631	-3.16783808852436	-0.42104903608986
H	8.65898990704892	-2.32994097546086	-0.69634067798906
H	8.26434549806119	-3.47013319045885	0.60641452284751
H	8.20562046181360	-4.00951250121113	-1.10068085761724
H	6.66308755979153	-1.38193413721063	1.19294305171249
H	4.28190702226753	-0.65969311064441	1.05641860166561
N	0.34069066880364	1.41194091754680	1.75116690238585
H	1.33583456126036	1.48271011987666	1.99847533765150
H	0.02105281831479	2.37052593685194	1.56371345173660
H	-0.14761398225894	1.10608729314178	2.60229396124019

BP-86 Geometry Optimized Coordinates for 5+ of **3e**

Os	-0.00587059823455	0.01787258056493	0.01046800969995
O	0.50949502591262	1.46261495522186	-1.32965817634847
C	0.51273306629076	1.19947178182482	-2.59561801783841
C	0.89822116514101	2.25581580617841	-3.54712336687495
C	1.27078031016321	3.53896073605276	-3.07838989870399
C	1.63757281510492	4.53830553689988	-3.98622524354756
C	1.64694750072272	4.29514933560804	-5.38130418703920
C	1.26788117336398	3.00978940206963	-5.83698681711202
C	0.89949103744598	2.00080145960117	-4.93926014614626
H	0.60817157973233	1.01130444505004	-5.30954384841113
H	1.26085820176467	2.80035909085491	-6.91460769697214
C	2.07491414137818	5.36952575206106	-6.35027184977643
H	3.17774248364879	5.37568193209634	-6.45578993931687
H	1.64960924490395	5.20420636102758	-7.35486989338486
H	1.77845337899461	6.37318046206505	-5.99836710454020
H	1.92145071411365	5.52983022515071	-3.60994640700845
H	1.26818602251309	3.74381695055477	-2.00185353918622
O	0.18810593592030	0.02932673926394	-3.05121793049547
Os	-0.33301699354463	-1.45384804236468	-1.78115670139735
O	-0.84517447937464	-2.89455468377642	-0.46002539114447
C	-0.85302089155006	-2.64572126522118	0.81274510126011
O	-0.53405873661952	-1.48358911731200	1.28169973935400
C	-1.23639984609633	-3.71792241188101	1.74719811103695
C	-1.59981770685009	-4.99576116724050	1.25921517442841
C	-1.96730790531382	-6.00940775850816	2.15208049196248
C	-1.98292751405807	-5.78624729714463	3.54953051998700

C	-1.61985659974826	-4.50231973974581	4.02461064682994
C	-1.25080532657984	-3.48054772257611	3.14308277591703
H	-0.97453977332093	-2.49201005482241	3.52713559123319
H	-1.63030965518178	-4.30427512449566	5.10440768220976
C	-2.35210511685481	-6.88949073525125	4.51023611472629
H	-1.43981917240544	-7.37951899828426	4.90376760830516
H	-2.90845281537870	-6.49797975478918	5.37994594007989
H	-2.96016367096435	-7.66907644685052	4.02044056489074
H	-2.25125189568656	-6.99497741708685	1.76063852446820
H	-1.59545323259477	-5.18523435366652	0.17986081757612
O	-2.26147299098478	-0.85732375562342	-1.87505490658741
C	-2.71330003432801	0.03561782239940	-1.05013568996296
O	-1.96004418750113	0.57055710963477	-0.14542433025831
C	-4.12297115237871	0.45156430979499	-1.14859544075522
C	-4.96362870293279	-0.09829749958133	-2.14449653992278
C	-6.30263527267735	0.30330083545048	-2.23287875779197
C	-6.84317866198003	1.25713199307737	-1.33916426155846
C	-5.99077666702558	1.79909401067784	-0.34528847856386
C	-4.65200614997388	1.40764665534761	-0.24687626491729
H	-4.00643374304872	1.83557216529436	0.52843541705411
H	-6.38821017239350	2.53931413560648	0.36147262751195
C	-8.28349504235209	1.69585559469556	-1.43755592199825
H	-8.34949461223373	2.77125436112788	-1.69039001561815
H	-8.83083320983198	1.12857363144476	-2.20872204640969
H	-8.80507404479549	1.56462932290877	-0.47129658149975
H	-6.94440667556574	-0.13039639894424	-3.01075208402714
H	-4.56164737512962	-0.83780173514493	-2.84627343267002
O	1.60478808663048	-2.00794233816781	-1.63635403290221
C	2.37226993189813	-1.48115364403783	-0.73331611267206
O	1.93584464460902	-0.59102256997488	0.09691410721413
C	3.77917559164653	-1.91009738892171	-0.65293532768054
C	4.63461334617800	-1.37755468469990	0.34268957522135
C	5.96862934305278	-1.79059800592086	0.41552098852227
C	6.49449112142721	-2.73955543266564	-0.49602767394028
C	5.62957841970067	-3.26405181983098	-1.48484619920233
C	4.29094270389438	-2.86033558217952	-1.56747935767027
H	3.63534096716670	-3.27751871161226	-2.34024199808275
H	6.01399971553746	-4.00176160718247	-2.20113897722564
C	7.94035136615360	-3.16324166943177	-0.41459603901151
H	8.60831549698372	-2.32483210534104	-0.69096609486713
H	8.21161800096113	-3.45962673378213	0.61525339859085
H	8.15675376711965	-4.00686371190311	-1.09099376217616
H	6.61955090710041	-1.37231236530841	1.19447088536606
H	4.24338326629643	-0.64394608164446	1.05663668332090

N	0.32141052523383	1.40430656065999	1.71620651770741
H	1.31363782316911	1.46234150749736	1.98003594202903
H	0.01807109145564	2.36482087072452	1.50986557560949
H	-0.18833270783935	1.11245221442787	2.56023253110387

BP-86 Geometry Optimized Coordinates for 4+ of **3f**

Os	0.00456570666965	0.02536739290121	0.02232070656547
O	0.53102051632439	1.49290696261900	-1.35028346791558
C	0.52837038366513	1.21152478366878	-2.60741234751647
C	0.91075767822245	2.27567873793565	-3.56850669670352
C	1.27951747552826	3.56034888812729	-3.10255035233654
C	1.64269135459459	4.56801804367409	-4.00449700619768
C	1.63658520032244	4.28949333569092	-5.38177604171470
C	1.27392239379119	3.02209271560022	-5.86869244384773
C	0.91247251806131	2.01936121645015	-4.96041219440540
H	0.62786571665573	1.02647401925794	-5.32607159789516
H	1.27989555128894	2.83916303247105	-6.94978347638311
F	1.98292334047473	5.24888153102283	-6.24504827441516
H	1.93152011046340	5.56774817760623	-3.65891602240785
H	1.27998964729269	3.76269548097342	-2.02580217751048
O	0.21146368526314	0.05071662641791	-3.07288352672479
Os	-0.32289603472034	-1.46051333203774	-1.77986586486982
O	-0.84798566173947	-2.92223195616699	-0.42861375944267
C	-0.85447122028834	-2.65830345869485	0.83420583807802
O	-0.53879381674521	-1.50657619530766	1.31766894267851
C	-1.24493375023781	-3.73753934589726	1.77497553778671
C	-1.60944213909340	-5.01527493015540	1.28711072010778
C	-1.97945058020212	-6.03616105916728	2.17106353300730
C	-1.98466532452459	-5.77806840055712	3.55245851415511
C	-1.62662832244249	-4.51802401079579	4.06099407271986
C	-1.25816749097196	-3.50185092617328	3.17049343074446
H	-0.97697254710999	-2.51416684491223	3.55244947694854
H	-1.64161439326754	-4.35115577719369	5.14460121697606
F	-2.33772418606110	-6.75038067122699	4.39840546774759
H	-2.26508269619408	-7.03069361975559	1.80828835906999
H	-1.60132074270203	-5.20241509334093	0.20763072500508
O	-2.28630869835243	-0.84782257852501	-1.87728249137285
C	-2.72295398308369	0.04374023539413	-1.05338031393843
O	-1.98866418257764	0.58728066896902	-0.14493645462146
C	-4.14236413877064	0.46389971022879	-1.15826665961672
C	-4.98099890890365	-0.08604907710956	-2.15698132022801
C	-6.32002383040234	0.31044288680416	-2.26026506200017
C	-6.82429897108402	1.26263914640088	-1.35807051942872

C	-6.01180909657167	1.82212296964743	-0.35741419856980
C	-4.67344065675976	1.42133017408113	-0.26122423461122
H	-4.02822906885701	1.84875692953951	0.51429124260946
H	-6.43795773748001	2.56199052157769	0.33052917827877
F	-8.10147267219666	1.64387902052305	-1.45416165411170
H	-6.98152032869626	-0.10523780058455	-3.02965029386792
H	-4.57427448345715	-0.82650557639088	-2.85461584571114
O	1.65140696887489	-2.02346587304145	-1.62457876580944
C	2.40296223948080	-1.48861018708974	-0.72257065529674
O	1.98456777355247	-0.59927160831011	0.11037972639457
C	3.81980563030633	-1.92222538406111	-0.64049269885808
C	4.67729955181006	-1.38257326442876	0.34776878889648
C	6.01423705033169	-1.79099004924495	0.43102630537732
C	6.49725748102808	-2.74484339608345	-0.48077105557169
C	5.66572538096574	-3.29421595458028	-1.47153406240077
C	4.32979420891611	-2.88149718817994	-1.54771535869054
H	3.67038676462838	-3.30153873562490	-2.31532273219797
H	6.07548278464360	-4.03576311704051	-2.16757425591323
F	7.77218998517015	-3.13782762593740	-0.40375096913037
H	6.69021451099456	-1.38341883404188	1.19212612560680
H	4.28635717450658	-0.64075723525613	1.05291725403978
N	0.34004684795382	1.41310042428012	1.75645799266131
H	1.33831827966519	1.52523401351347	1.97362256864454
H	-0.02801901243519	2.35818417885274	1.59100820568573
H	-0.10751211551791	1.07427931268472	2.61735640244846

BP-86 Geometry Optimized Coordinates for 5+ of **3f**

Os	0.00145493807926	0.02100335227526	0.01423706113210
O	0.51745668231685	1.46426536699049	-1.32735728348019
C	0.52102239834217	1.19891552704052	-2.59253201033301
C	0.90402178417652	2.25474626091096	-3.54487677020834
C	1.27179162325786	3.53892430644010	-3.07326792044831
C	1.63840589966662	4.54324622183089	-3.97425490137330
C	1.63651078367596	4.26161539470024	-5.35199841509128
C	1.27460311441561	2.99421803096733	-5.84197814594810
C	0.90914114990948	1.99277851506991	-4.93694810918641
H	0.62542991253231	1.00061968838513	-5.30476370899121
H	1.28492671282438	2.81184598369073	-6.92280518278271
F	1.98614514537653	5.21738399573396	-6.21184061559092
H	1.92703135825675	5.54295174549743	-3.62947841065697
H	1.26928148642729	3.74373783088407	-1.99716104208727
O	0.19805845308495	0.02856638584707	-3.04768225356533
Os	-0.32462131937083	-1.45313117663361	-1.77636799139581

O	-0.83834697287985	-2.89207561634007	-0.45377470391747
C	-0.84595759109361	-2.64126442707582	0.81824877248126
O	-0.52731350618403	-1.47932608846378	1.28692046854450
C	-1.22970795437243	-3.71247944783753	1.75295792356168
C	-1.59215495989265	-4.99047882669208	1.26087376424991
C	-1.95837771947641	-6.00939628230156	2.14556361231294
C	-1.96147231328296	-5.74867968707835	3.52734580376610
C	-1.60506378281347	-4.48765340376759	4.03756802378241
C	-1.24002038976097	-3.47168147607107	3.14881790279470
H	-0.96039522763189	-2.48423412534573	3.53199410574489
H	-1.61923073923432	-4.32175354044958	5.12100488143088
F	-2.31052681824221	-6.71841898124802	4.37165596207554
H	-2.24283385963963	-7.00461633843213	1.78473438661272
H	-1.58585809232959	-5.17938765009957	0.18186334992777
O	-2.25270649411712	-0.85551935116997	-1.87275119463486
C	-2.70400476079784	0.03844658435280	-1.04922027594150
O	-1.95260068260744	0.57393544968256	-0.14378760341825
C	-4.11263364438611	0.45542163393673	-1.15097139017992
C	-4.94917316347119	-0.09785931773377	-2.15127103035388
C	-6.28613081440612	0.29925099236562	-2.25211987057038
C	-6.78772388951681	1.25245419138911	-1.34815661982252
C	-5.97542492979658	1.81357082258201	-0.34675514087658
C	-4.63886725746431	1.41415436943843	-0.25064265897386
H	-3.99457658945223	1.84255280777865	0.52486216000128
H	-6.40184707467592	2.55329635571819	0.34065532065815
F	-8.06106270331750	1.63300687287357	-1.44298672707742
H	-6.94907149326757	-0.11555826146069	-3.02027819148600
H	-4.54474886253260	-0.83827780664894	-2.85001588365862
O	1.61270264070433	-2.00823514036976	-1.62860802359191
C	2.37861508746939	-1.48038815965867	-0.72537504300984
O	1.94323734139204	-0.58808267657141	0.10253361677255
C	3.78374752890418	-1.91270415744560	-0.64111499906096
C	4.63758626483546	-1.37126140031026	0.35099730777619
C	5.97118003147010	-1.78293389093356	0.43574129270100
C	6.45215818013385	-2.73916569325457	-0.47629063171540
C	5.62255823759880	-3.28869601758362	-1.46980337741814
C	4.28934401605630	-2.87460723908660	-1.54984212794459
H	3.63196371568029	-3.29440074069065	-2.31908214554617
H	6.03299252729346	-4.03120873879195	-2.16391057830068
F	7.72223593827943	-3.13385044823537	-0.39656516109238
H	6.64726289505990	-1.37744902436323	1.19739599431281
H	4.24887121510394	-0.62850811211309	1.05611350564124
N	0.32231804725021	1.40537595055610	1.72240684682281
H	1.32021683177287	1.52784830988919	1.93820557096158

H	-0.05662551446554	2.34508337678162	1.54802079772580
H	-0.12357570086736	1.06544895064969	2.58439318793981

BP-86 Geometry Optimized Coordinates for 4+ of **4a**

Rh	0.00941988765981	0.03678798850355	0.04097013678900
O	0.52938897615887	1.47977510770753	-1.34306714793260
C	0.52000365512382	1.18103709775904	-2.59200804250080
C	0.90576203899473	2.26018948745974	-3.55474708080641
C	1.27052513289661	3.54161013649914	-3.08430696696025
C	1.63334183516109	4.55608262203457	-3.98221580371247
C	1.62776630095709	4.27754543221229	-5.36055584673333
C	1.26848194964957	3.01068160832512	-5.85430405723621
C	0.90846141406595	2.00589285807554	-4.94459903405003
H	0.62607228174723	1.01316841340703	-5.31252067117286
H	1.26917988975006	2.81028347037859	-6.93156691725398
Br	2.12075426521522	5.65471134061823	-6.59352358364744
H	1.91622578784725	5.54858618265118	-3.61396717407972
H	1.26970048181415	3.74270302980507	-2.00730583454270
O	0.20866129936148	0.03800863210806	-3.08205690951513
Rh	-0.32973631674350	-1.49146257890397	-1.81932237267984
O	-0.84977627237716	-2.92833349862770	-0.44354687849284
C	-0.84615491391982	-2.64038491897096	0.80552701567204
O	-0.53410970877445	-1.49983112028713	1.30727422683185
C	-1.23777188242326	-3.72245039977063	1.76234761622060
C	-1.60046255824432	-5.00043765631974	1.28100995494385
C	-1.96907343564371	-6.02067338739744	2.16980830240591
C	-1.97175583153394	-5.75130185319422	3.55008372595020
C	-1.61527356839729	-4.48792722868096	4.05449414942414
C	-1.24922944295549	-3.47716300049980	3.15372347027032
H	-0.96925944797519	-2.48698085647697	3.53009337466937
H	-1.62276186902785	-4.29477367386123	5.13305347725931
Br	-2.47253228238411	-7.13649935263907	4.77084478971158
H	-2.25013831927573	-7.01059854881658	1.79334666179311
H	-1.59317309852800	-5.19330641922236	0.20246061032328
O	-2.28358667028750	-0.85763404450590	-1.89057021478237
C	-2.69048497113512	0.02857671011260	-1.05824682643370
O	-1.97457716452631	0.57996303705082	-0.14577154382809
C	-4.12039246155950	0.45965188001732	-1.15671377838869
C	-4.95740779052033	-0.07615800097927	-2.16100503495022
C	-6.29759817581489	0.32416542673712	-2.26321044004829
C	-6.79669539212534	1.26777883549030	-1.34763009176565
C	-5.98484756032683	1.81505368787637	-0.33825222565733
C	-4.64606161656844	1.40655253963594	-0.24933731289614

H	-4.00024002400937	1.82359641001947	0.53135902629473
H	-6.38971265650190	2.54852362318483	0.36799922784244
Br	-8.62332630941294	1.82120690744604	-1.47978474862169
H	-6.94327021656268	-0.09171279973925	-3.04479915825195
H	-4.55237056862227	-0.80959465328858	-2.86708933855071
O	1.64521315103452	-2.03200803717546	-1.63606983540968
C	2.36975492082216	-1.48651683538201	-0.73009643568502
O	1.97206444762414	-0.59938110312230	0.10934998433263
C	3.79963194428230	-1.91881086048233	-0.63969414891467
C	4.64597169297846	-1.38565991555389	0.35810650798886
C	5.98589805104544	-1.78972962426442	0.44955431401246
C	6.47508816685632	-2.73422550537027	-0.47034914049546
C	5.65378357015067	-3.27868578754915	-1.47370884906952
C	4.31558500616685	-2.86645933228798	-1.55189860478752
H	3.66211702782454	-3.28091786938270	-2.32766097139140
H	6.05097901186423	-4.01282023842671	-2.18361648725948
Br	8.30109233276920	-3.29297488915337	-0.35278210240669
H	6.63896865938982	-1.37604824575264	1.22614507215653
H	4.24870095644115	-0.65136487265099	1.06762030152198
N	0.32411560323356	1.39144320563311	1.71689529802589
H	1.32439582435764	1.51494124843603	1.91338677516865
H	-0.06923404432859	2.32353790538901	1.54247857143085
H	-0.11144205273808	1.03211401416232	2.57451624987136

BP-86 Geometry Optimized Coordinates for 5+ of **4a**

Rh	0.03121574470536	0.01759156634860	0.06027217010900
O	0.55187313666869	1.44367396026645	-1.29646727376904
C	0.53164176682630	1.16064244301583	-2.55177990558835
C	0.87681235423866	2.23389831397977	-3.51529956138308
C	1.19724349461519	3.53031348457198	-3.04953664723384
C	1.52447278238706	4.54695876016363	-3.95570759353319
C	1.52874941276855	4.25675840507688	-5.33291290798830
C	1.21252954917526	2.97426454023983	-5.81815839198953
C	0.88690831805006	1.96427045543445	-4.90370705335941
H	0.64009993871369	0.96061982391221	-5.26691445947095
H	1.22072490100658	2.76629268331577	-6.89367674044540
Br	1.97502999989868	5.63647554574405	-6.57242039352114
H	1.77307952655695	5.55131382122222	-3.59575879473786
H	1.18994716114480	3.74149211980364	-1.97466684970823
O	0.24670648807339	-0.00713515466137	-3.02495503630363
Rh	-0.30526831286461	-1.50434569932319	-1.78847918753076
O	-0.79312736712751	-2.92737009460535	-0.43505291764955
C	-0.82600896623374	-2.64330202467128	0.82374225129832

O	-0.49608994623809	-1.50029561547885	1.31510824951297
C	-1.25175689993366	-3.70938743674055	1.76370018788104
C	-1.60782046291442	-4.98674176503262	1.27189579192821
C	-2.01189279774747	-5.99727805607378	2.15392530452108
C	-2.05665994794076	-5.72022452756518	3.53279297087284
C	-1.70708726422237	-4.45624341366940	4.04371227987558
C	-1.30466694837480	-3.45255130291787	3.15335309391497
H	-1.02990307760588	-2.46370735925681	3.53641905307384
H	-1.74813788339897	-4.25829492113481	5.12037349919500
Br	-2.60479897469784	-7.09200766326827	4.74014351666213
H	-2.28792984774545	-6.98690955194652	1.77377751365883
H	-1.56752422002595	-5.18776486278681	0.19579296194828
O	-2.22933154772431	-0.89249261933455	-1.84465196331096
C	-2.64968673585100	0.01686011124796	-1.02914252766009
O	-1.92525708017545	0.55482750140221	-0.11123510161989
C	-4.06069591945327	0.45784848508942	-1.15192926663443
C	-4.88758473990027	-0.08585785288047	-2.16238896360831
C	-6.21965142682452	0.32958005983020	-2.28653723715915
C	-6.71944460425255	1.29229577374989	-1.39012013627331
C	-5.91476796641283	1.84539739424658	-0.37650528979256
C	-4.58360825568483	1.42477579096862	-0.26204660506918
H	-3.94566580973103	1.84650626920634	0.52232280503777
H	-6.32093538678152	2.59319157980390	0.31335234010058
Br	-8.53248729837969	1.86312232303125	-1.55365640885823
H	-6.85986934399882	-0.08946695014246	-3.07053743072030
H	-4.48451922330106	-0.83407747652748	-2.85353983946062
O	1.63584627772625	-2.05407048554796	-1.60335102399481
C	2.38295015363233	-1.49494779524019	-0.71174512423964
O	1.97135434067540	-0.61341942012397	0.13104322041307
C	3.80719810394853	-1.90818679488536	-0.64579234822101
C	4.66335078362781	-1.35596470501767	0.33489851289878
C	6.00729231716139	-1.74536260224980	0.40192520406617
C	6.48940969063757	-2.69143393719939	-0.52175897291747
C	5.65577623728153	-3.25240309626197	-1.50677915854245
C	4.31285148175454	-2.85748384926647	-1.56405522107617
H	3.65191141985103	-3.28605494507808	-2.32533900138990
H	6.04807278011128	-3.98668441655468	-2.21885722850444
Br	8.31862167298447	-3.22758899575511	-0.43472725289579
H	6.67035769171176	-1.31959916141664	1.16299208609275
H	4.27378994304192	-0.62161700086942	1.04829793297058
N	0.35629612827391	1.33457457919247	1.71495886976513
H	1.36106236756581	1.44539537661975	1.90004934183686
H	-0.03585305123328	2.26830870991025	1.54156746268850
H	-0.08049571803879	0.96436340609026	2.56832042583876

BP-86 Geometry Optimized Coordinates for 4+ of **4b**

Rh	0.01699836666231	0.06407494350343	0.06977944021499
O	0.53831111425700	1.50623633651186	-1.31479418599752
C	0.52994480761829	1.20716056655617	-2.56392823054771
C	0.91746320196815	2.28493674063205	-3.52652318574312
C	1.28192614706012	3.56717157847985	-3.05700002327270
C	1.64654775338420	4.57974268787506	-3.95487224065508
C	1.64465673812978	4.30271756843613	-5.33468970024753
C	1.28513083614898	3.03354278983325	-5.82552858810684
C	0.92302342798324	2.03002757083352	-4.91662666133295
H	0.64100409307539	1.03697484618838	-5.28386976624072
H	1.29002007711321	2.83841806145797	-6.90375528146251
Cl	2.09952796925913	5.56390352206087	-6.46463456230318
H	1.92994523037081	5.57451594865640	-3.59317850712703
H	1.27894749229212	3.76883474367419	-1.98013776949443
O	0.21797129092285	0.06369620366039	-3.05321402654022
Rh	-0.32160674246698	-1.46466950993678	-1.78957655222043
O	-0.84275310287675	-2.90067807386392	-0.41332068833976
C	-0.84007277418103	-2.61247356648516	0.83596114126929
O	-0.52766835056806	-1.47142309254492	1.33701361564882
C	-1.23296985439726	-3.69340006299217	1.79253464940118
C	-1.59614319770820	-4.97188605575160	1.31185635351872
C	-1.96605532774356	-5.99052767579281	2.20046427865883
C	-1.97104108730765	-5.72334442011721	3.58231778714880
C	-1.61349524429078	-4.45796087534400	4.08410485412747
C	-1.24596054130084	-3.44814994631124	3.18426047537987
H	-0.96571307753332	-2.45787060313946	3.56007734618412
H	-1.62412717216260	-4.27062245182695	5.16366584281683
Cl	-2.43233974923647	-6.99234258674533	4.70082517015045
H	-2.24832092741867	-6.98244500758670	1.83013991988371
H	-1.58774996382491	-5.16480984332907	0.23335886399077
O	-2.27548174763233	-0.83075767716168	-1.86194842930825
C	-2.68320547042931	0.05559261446414	-1.02979222545417
O	-1.96676768721587	0.60762656121318	-0.11775546868469
C	-4.11298540013022	0.48509349578105	-1.12731734305861
C	-4.95134531582549	-0.05238469674986	-2.13009460220383
C	-6.29144382784516	0.34564567358260	-2.23000114193484
C	-6.79402329465018	1.28951562449661	-1.31483454143407
C	-5.97829406446324	1.83777899620582	-0.30751757664500
C	-4.63950039943224	1.43217482633678	-0.22005879567386
H	-3.99287559829439	1.85057332009784	0.55920652439869
H	-6.38917754824555	2.57059959928180	0.39591933161657

Cl	-8.46953605298585	1.79253727460948	-1.43227412045923
H	-6.94267156569962	-0.06832747589457	-3.00797923910338
H	-4.54589330130848	-0.78569632573534	-2.83602725691800
O	1.65318297407388	-2.00557443017498	-1.60567256280654
C	2.37821845004388	-1.45942517831920	-0.70011290345188
O	1.97962506867878	-0.57229277614297	0.13928192551276
C	3.80805354889447	-1.88990707559218	-0.61072831564991
C	4.65585954883919	-1.35453571888583	0.38515413590063
C	5.99576531414973	-1.75609462756415	0.47414464078347
C	6.48839196033194	-2.70117458985605	-0.44507335245587
C	5.66308887303192	-3.24713063512465	-1.44595154504147
C	4.32481639867023	-2.83800585544617	-1.52256885198673
H	3.67048043933168	-3.25420280022976	-2.29662351980165
H	6.06630013230681	-3.98083888560504	-2.15289422207712
Cl	8.16341332023364	-3.20871252719181	-0.34119383909115
H	6.65449291180471	-1.34387783518863	1.24672580184089
H	4.25826752321312	-0.62008744168663	1.09430490926416
N	0.32977790336992	1.41911743161375	1.74642701650782
H	1.32994839787244	1.56273456850999	1.92921180464979
H	-0.08555074631127	2.34345214708636	1.58208786410452
H	-0.08572756760559	1.04697215267790	2.60852807989892

BP-86 Geometry Optimized Coordinates for 5+ of **4b**

Rh	0.04130871098153	0.03913218272476	0.09220419231524
O	0.56207282527044	1.46544499456918	-1.26435708834752
C	0.54126308454200	1.18283210243204	-2.52024294442708
C	0.88412117794540	2.25546187455295	-3.48358104434001
C	1.20314866790800	3.55302876838371	-3.01866886384688
C	1.52629060388177	4.56947451896818	-3.92496511344313
C	1.52892526579450	4.28187846124797	-5.30390851704555
C	1.21436347794982	2.99673879323375	-5.78655871345763
C	0.89278602479943	1.98640024469873	-4.87256464169395
H	0.64740341915739	0.98215719249274	-5.23500968183565
H	1.22276465833766	2.79538377447845	-6.86331712144524
Cl	1.93091552712619	5.54791949266998	-6.44028912341554
H	1.77430430941371	5.57635985553387	-3.57173583959654
H	1.19717540517037	3.76366191814645	-1.94371509675553
O	0.25563087134854	0.01432459391096	-2.99208071920017
Rh	-0.29461820900558	-1.48282880033346	-1.75472800551485
O	-0.78600205370255	-2.90561227723836	-0.40088616550895
C	-0.82005004500407	-2.62106435284953	0.85803276108708
O	-0.48901463227642	-1.47742081792374	1.34835948716267
C	-1.24935169842369	-3.68468939392645	1.79762520063123

C	-1.60538254744291	-4.96291755654681	1.30682438965267
C	-2.01399915392730	-5.97058947964912	2.18843787665144
C	-2.06500233761952	-5.69364071321786	3.56829488953403
C	-1.71465172085135	-4.42753335784089	4.07656163249234
C	-1.30739966887714	-3.42624240124058	3.18720798791483
H	-1.03283885564915	-2.43704531433130	3.56943569370018
H	-1.76208955015013	-4.23417663145006	5.15377814540780
Cl	-2.57507356757014	-6.94792435887091	4.67423378292814
H	-2.29129020056866	-6.96240461220648	1.81492644114022
H	-1.56114602871855	-5.16515366669319	0.23113791911845
O	-2.21853952688024	-0.87092764519939	-1.81137156027240
C	-2.63972260285031	0.04108039254744	-0.99873413704997
O	-1.91479509860431	0.57776994974722	-0.07986543575497
C	-4.04830650205818	0.48478443722138	-1.12497702824696
C	-4.87588581027571	-0.06036822140723	-2.13472115313577
C	-6.20578050792217	0.35776698687238	-2.26168548223571
C	-6.70722444936540	1.32568964754517	-1.36997220065978
C	-5.89971785561904	1.87948904978700	-0.35735256010104
C	-4.57067032840222	1.45654012254474	-0.23932859401082
H	-3.93237235813781	1.87931659957329	0.54415068271481
H	-6.31086595925454	2.63048814722479	0.32599930513620
Cl	-8.36719661649630	1.85194205282260	-1.52341701892801
H	-6.85109552724264	-0.05880649921470	-3.04278316660333
H	-4.47338132249621	-0.81214843174964	-2.82227669679462
O	1.64655808595373	-2.03292108337596	-1.56829589619057
C	2.39553259228226	-1.47115767875739	-0.67940664297986
O	1.98173828198642	-0.59095220607441	0.16432452716866
C	3.82037863912076	-1.87866053362252	-0.61770818350775
C	4.67878424400222	-1.32113866950098	0.35863658390111
C	6.02387089433359	-1.70388144207982	0.41996411220056
C	6.50948469373085	-2.64950412022220	-0.50413348142367
C	5.67129546709550	-3.21537774592138	-1.48416545943563
C	4.32715524733728	-2.82755409454108	-1.53646877078489
H	3.66459907754736	-3.26026142281754	-2.29396181926437
H	6.07014944268565	-3.94834472026875	-2.19391463468600
Cl	8.18878818147721	-3.13078991733126	-0.43280033450440
H	6.69334227405461	-1.27717546244113	1.17483629095213
H	4.28847148949855	-0.58744930385235	1.07226190816043
N	0.36614371563880	1.35448412234564	1.74859408903429
H	1.37080616030915	1.46182255118580	1.93623952617860
H	-0.02192395491614	2.29017356857503	1.57647967147439
H	-0.07357921637234	0.98485460666027	2.60068378978730

BP-86 Geometry Optimized Coordinates for 4+ of **4c**

Rh	0.00987236557724	0.03638379224226	0.04029841064590
O	0.52996357783893	1.47994378911115	-1.34352613951508
C	0.52145054036206	1.18321593578092	-2.59404925615831
C	0.90723179672106	2.26067806825625	-3.55476156756526
C	1.27371915879908	3.54309908161645	-3.08436680586289
C	1.63682619556286	4.55450981617933	-3.98278054090731
C	1.63218029148350	4.27996130702572	-5.36063726910205
C	1.27141611243460	3.01404966644072	-5.85202063626235
C	0.91021585318508	2.00840826718791	-4.94635495107655
H	0.62671236651972	1.01598125721896	-5.31392972939899
H	1.27842923019746	2.83416289457193	-6.93354243921628
F	1.97818753537461	5.24223682715939	-6.22043439583895
H	1.92410083068924	5.55338122224336	-3.63371780401519
H	1.27268584831030	3.74255897343462	-2.00717237855852
O	0.20935322974189	0.03854792329520	-3.08246799213857
Rh	-0.32880370141085	-1.49059607237661	-1.81845805327923
O	-0.84892863806051	-2.92811991497905	-0.44308065687238
C	-0.84671218458076	-2.64207793702223	0.80751642401337
O	-0.53376191492104	-1.49993357920577	1.30769942483372
C	-1.23935297824696	-3.72225177071559	1.76212202597027
C	-1.60342968744944	-5.00120014085883	1.28043689630814
C	-1.97378287466056	-6.01822334848213	2.16930292046886
C	-1.97925502753597	-5.75273000587012	3.54902290765665
C	-1.62153113623085	-4.49036885784448	4.05147663335069
C	-1.25284049410003	-3.47890877339079	3.15518268937807
H	-0.97209048597370	-2.48904500665551	3.53155740190451
H	-1.63689439338896	-4.31766877180176	5.13408406539687
F	-2.33246566663439	-6.72045889289332	4.39973650551581
H	-2.25919314049452	-7.01451023373672	1.81143798721374
H	-1.59462770837108	-5.19246292895220	0.20173198551102
O	-2.28336320618349	-0.85790486223257	-1.89014289280910
C	-2.69285750159968	0.02883755730088	-1.05804319562254
O	-1.97447877152949	0.57978382723471	-0.14578152345191
C	-4.12063975166508	0.45843151107682	-1.15583630872095
C	-4.96219631062528	-0.08490503413607	-2.15416845506871
C	-6.30074164133549	0.31558668937496	-2.25314827590151
C	-6.79960621856889	1.26544097911038	-1.34592098327593
C	-5.98343513618484	1.81863102086460	-0.34505042868601
C	-4.64570178097896	1.41312551731376	-0.25419255069352
H	-3.99702095327540	1.83563516361042	0.52103065982408
H	-6.40552642007750	2.55697011855442	0.34689974144419
F	-8.07567067122095	1.65072799673918	-1.43730973574110
H	-6.96508664186243	-0.09518109822302	-3.02261360604914

H	-4.55810430174854	-0.82365195439678	-2.85506229430699
O	1.64647335744140	-2.03163620851857	-1.63579945922430
C	2.37335423616419	-1.48671640774339	-0.72988672866259
O	1.97302469706419	-0.59897209499626	0.10925532973628
C	3.80098758742268	-1.91779424392263	-0.63966258225162
C	4.65162843372121	-1.37720485891806	0.35236247203929
C	5.98976159071700	-1.78175941942833	0.44108569184191
C	6.47883763440236	-2.73273293212233	-0.47019898320945
C	5.65346947202447	-3.28300477441698	-1.46523328730993
C	4.31643553437227	-2.87345583026607	-1.54586639186248
H	3.66030851851301	-3.29331424836463	-2.31630545938287
H	6.06803629298576	-4.02224819846896	-2.16075772823240
F	7.75433875432681	-3.12204531783367	-0.38854228279242
H	6.66123073588091	-1.37329050185214	1.20557311301281
H	4.25520115872396	-0.63740564074917	1.05644342638362
N	0.32510172927362	1.39175788532231	1.71847079464675
H	1.32538991968063	1.51702412746044	1.91353354125941
H	-0.07020584656293	2.32340436949371	1.54650302820464
H	-0.10800228003360	1.03068630615400	2.57653517246285

BP-86 Geometry Optimized Coordinates for 5+ of **4c**

Rh	0.03919887591356	0.01280855206758	0.06223628025814
O	0.55826613762930	1.44007953727353	-1.29374796166164
C	0.53580097979257	1.15968818963046	-2.55101649900528
C	0.87240790356676	2.23248938618687	-3.51274047654851
C	1.18899679519835	3.53193642445491	-3.04755575944364
C	1.50484277150638	4.54811627553170	-3.95469628255758
C	1.50347062781929	4.26226153401236	-5.33158734272804
C	1.19265490638331	2.97894710813871	-5.81459790889110
C	0.87773422444518	1.96566819210857	-4.90349135938627
H	0.63443770923321	0.96082818828804	-5.26563672122599
H	1.20200928109360	2.79329321199437	-6.89489051261328
F	1.80268518799515	5.22953870116762	-6.19711795100122
H	1.75238789739954	5.56056716857764	-3.61516496252142
H	1.18553995925868	3.74046272924326	-1.97220162322860
O	0.25191243055186	-0.01073494220242	-3.02234970360203
Rh	-0.29661914619362	-1.50733389013470	-1.78443775489595
O	-0.78785532298320	-2.93059020963823	-0.43279582520987
C	-0.82396912893044	-2.64772126997436	0.82772295235306
O	-0.49065735596063	-1.50368315337127	1.31791472057970
C	-1.25698284232240	-3.70929259407246	1.76406121985845
C	-1.61883872567155	-4.98654057864753	1.27123250325344
C	-2.03256854710025	-5.99105363236051	2.15195548970860

C	-2.08353317057277	-5.71587442183426	3.52974556145080
C	-1.72799115122462	-4.45469595849003	4.04010935096141
C	-1.31523921410824	-3.45328870938024	3.15539141087694
H	-1.03629294241466	-2.46573785069453	3.53868230853160
H	-1.78051591443686	-4.27683805885470	5.12048633454660
F	-2.47864916358344	-6.67100325615761	4.37019278858999
H	-2.31762363139890	-6.98587717179535	1.79044617861517
H	-1.57430635882781	-5.18659615009640	0.19517737981907
O	-2.22022602539769	-0.89589919619797	-1.84311257148039
C	-2.64354418274486	0.01498663975615	-1.02844492793391
O	-1.91708391256745	0.55160083409981	-0.10953500778205
C	-4.05057848963961	0.45639406290144	-1.15345371079601
C	-4.88155427561329	-0.09462849868557	-2.15902476537188
C	-6.21051580455243	0.32309191976212	-2.28300673966233
C	-6.70889279230526	1.29410338984492	-1.39673699704247
C	-5.90119284380289	1.85323430505311	-0.39050864246484
C	-4.57261572196191	1.43335598212000	-0.27130686799689
H	-3.93210504221890	1.86026655190720	0.50808799457021
H	-6.32471724441721	2.60763845409123	0.28261236268999
F	-7.97419258194105	1.69410518918383	-1.51305061266350
H	-6.86932631003400	-0.08980862752205	-3.05576003558052
H	-4.47951611688010	-0.84980141714051	-2.84307738876207
O	1.64465245701269	-2.05693280302765	-1.60112847484844
C	2.39453471411446	-1.49792396191572	-0.70962600955882
O	1.97981642834879	-0.61627942460967	0.13352685262439
C	3.81606392339298	-1.90835711510826	-0.64524220405997
C	4.67651505812823	-1.34856429464186	0.32984452624477
C	6.01861071353835	-1.73682384850413	0.39299505478405
C	6.50059995050175	-2.68788343932857	-0.52376059463338
C	5.66370831877515	-3.25521973048499	-1.50061731872190
C	4.32195707998761	-2.86452106535684	-1.55891341560630
H	3.65832679912877	-3.29848645082788	-2.31470950635581
H	6.07467834194592	-3.99316832909095	-2.19930841056671
F	7.77863894371542	-3.05977847379792	-0.46466714110111
H	6.70045795704405	-1.31647476927281	1.14137714828888
H	4.28709827340930	-0.60980928072691	1.03868292630756
N	0.36534569939554	1.32974028831583	1.71918841458648
H	1.37010643782380	1.43674646747805	1.90631238517115
H	-0.02225972885385	2.26569767916549	1.54764065418327
H	-0.07387597538971	0.96095764159007	2.57187266865609

BP-86 Geometry Optimized Coordinates for 4+ of **4d**

Rh	0.01767090410626	0.04766729588009	0.07996735596811
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O	0.61469447243718	1.66507606076691	-1.05756291098276
C	0.56117650410401	1.58286975962783	-2.33857347875176
C	1.00284814436698	2.78130276584497	-3.12096299476268
C	1.45861159448618	3.94116296327724	-2.45335054302118
C	1.87113920938876	5.06242785292873	-3.19022408748176
C	1.83263250421556	5.03587133736070	-4.59750540096990
C	1.37968794073492	3.88294618262605	-5.26719075448872
C	0.96623503334246	2.75965518358040	-4.53413018528899
H	0.61240518513658	1.85825380169147	-5.04723210426242
H	1.34887485150373	3.85987784547979	-6.36372489678589
H	2.15538347987158	5.91329075141517	-5.17217938153417
H	2.22353204345689	5.95973277174016	-2.66627558319584
H	1.48549290927532	3.95319491084221	-1.35790034776161
O	0.16024320613250	0.56005349083351	-3.00023651148729
Rh	-0.46364034512855	-1.12086652970731	-1.99493538367314
O	-1.05638396511672	-2.73280784570124	-0.86505809874872
C	-1.00270823419054	-2.66351220417309	0.41439828192726
O	-0.60507510969952	-1.64367102447626	1.08718462421534
C	-1.43763200033347	-3.86825748714120	1.19057473598801
C	-1.88824820013256	-5.02455621818187	0.51333432962429
C	-2.29495073290026	-6.15388416203975	1.24086541577999
C	-2.25549064252957	-6.13913634402476	2.64837580558041
C	-1.80724433557843	-4.99001834668404	3.32758347737231
C	-1.39956092017869	-3.85854393090901	2.60378888679717
H	-1.04898845754585	-2.96009400035586	3.12415744152502
H	-1.77549487121707	-4.97636248263287	4.42425302176950
H	-2.57372515176117	-7.02296285496751	3.21570609904334
H	-2.64340947616495	-7.04834479806779	0.70948796082016
H	-1.91522403491076	-5.02698404645064	-0.58221402496945
O	-2.36840116808932	-0.35404899756377	-1.89717727261735
C	-2.69829768444793	0.40361305483799	-0.91667010317349
O	-1.92480969719428	0.74642442537644	0.05036419839316
C	-4.09926145087860	0.93262278992071	-0.89375516039248
C	-5.00458003289935	0.58976491372009	-1.92409883936549
C	-6.31767477299613	1.08511538780083	-1.90199395512980
C	-6.73786206079492	1.92565027109606	-0.85325179376776
C	-5.83998822261194	2.26997153358696	0.17532653382041
C	-4.52598485891170	1.77661078557115	0.15703539576015
H	-3.81993469862924	2.03860304176791	0.95309473816065
H	-6.16534282820145	2.92469098197738	0.99349152420401
H	-7.76481223288247	2.31221441789675	-0.83766124337376
H	-7.01575240419555	0.81527484481117	-2.70436494245666
H	-4.66864172970716	-0.06535959607351	-2.73584155229162
O	1.47045803959310	-1.81693792240480	-1.96785672230218

C	2.25214213143557	-1.47815061102727	-1.00931924314837
O	1.93244600248184	-0.72063650910759	-0.02224492248968
C	3.65330690863715	-2.00680326617326	-1.04113554039445
C	4.56731335232345	-1.66928450704844	-0.01674056613661
C	5.87959444671742	-2.16640872232450	-0.05112863506270
C	6.29039115584387	-3.00322763642548	-1.10641503536965
C	5.38394341932009	-3.34201402984344	-2.12936046686291
C	4.07089032861704	-2.84699041847352	-2.09872637419272
H	3.35842426423374	-3.10457138673441	-2.89054329977110
H	5.70187271365236	-3.99372981510221	-2.95282145977308
H	7.31663684835064	-3.39115173741687	-1.13165991952005
H	6.58431103197511	-1.90078723363480	0.74683896212838
H	4.23964437548668	-1.01692413047305	0.80050071596498
N	0.42794589266472	1.09028924579596	1.94917087430466
H	0.49847324293013	0.43453174567826	2.73610990335699
H	-0.32085023042868	1.75561064389792	2.17504201191282
H	1.30616790343500	1.62073677770941	1.91494426134112

BP-86 Geometry Optimized Coordinates for 5+ of **4d**

Rh	-0.02053843070740	0.04402762253146	0.09552260146598
O	0.56080348959701	1.64627313498293	-1.01650816695737
C	0.52906856806420	1.57016055022015	-2.30155410232764
C	1.00689150004869	2.73611180245958	-3.08538248310507
C	1.50905596171019	3.87974221617259	-2.42041478448364
C	1.96172895658240	4.97746075512956	-3.16631196451022
C	1.91628591291221	4.94174093339275	-4.57361383343776
C	1.41689010533827	3.80477415618980	-5.23774366561588
C	0.96220069382383	2.70261298831443	-4.49942536425014
H	0.57126640713058	1.81450300446999	-5.00806472612378
H	1.38191345515652	3.77803471328874	-6.33354562453214
H	2.27129837745422	5.80229468270905	-5.15418647691483
H	2.35115830815292	5.86335533701830	-2.65032487558102
H	1.54149968413368	3.89920316263491	-1.32551312471946
O	0.08793908189551	0.54357264235458	-2.94998970017314
Rh	-0.50162574552901	-1.11812502667491	-1.96647046884127
O	-1.10584881718994	-2.69774577739956	-0.85561874133637
C	-1.02334807805082	-2.65669737216868	0.43225344469336
O	-0.63992263457902	-1.62159033456889	1.09512262727858
C	-1.41285895222034	-3.87009997099258	1.19396615783466
C	-1.86155823432221	-5.02229064107350	0.50590645395366
C	-2.22532611542905	-6.16831205841407	1.22777226046071
C	-2.14457428580006	-6.17217498912300	2.63368377831309
C	-1.69826086111719	-5.02655436727513	3.32081755767160

C	-1.33254368332065	-3.87655054048878	2.60659255593343
H	-0.98399708204989	-2.98138489826699	3.13329618936636
H	-1.63542094455027	-5.03070375989323	4.41571231313392
H	-2.42976221599995	-7.07036048987193	3.19546884718606
H	-2.57263862562241	-7.06094236858844	0.69362745894835
H	-1.92188412440698	-5.01048626473115	-0.58792138060889
O	-2.38669769161849	-0.38037013420605	-1.86677890456965
C	-2.72375252651706	0.40376973129888	-0.89863042094767
O	-1.94286494159888	0.73152549380397	0.07131709337000
C	-4.10515241423441	0.95035470991632	-0.89719871636972
C	-5.00240388320545	0.60489321683661	-1.93533832708894
C	-6.30562592832475	1.12310361987615	-1.93233446761996
C	-6.72015680943826	1.98489905643888	-0.89862779880025
C	-5.82899591266048	2.33015173301062	0.13593254783898
C	-4.52421491310058	1.81621954743432	0.14029749905987
H	-3.82433090147975	2.07911665472964	0.94104973800619
H	-6.15275833881477	3.00154328926150	0.94045234955074
H	-7.74021365971733	2.38887029243390	-0.89935838328696
H	-7.00024749513617	0.85467346273860	-2.73750436119123
H	-4.67166867311250	-0.06672020485684	-2.73520943049623
O	1.39556723793801	-1.81259521284615	-1.92989068340458
C	2.20312566787838	-1.46266579596593	-0.98431313641704
O	1.86762860994172	-0.71250395985604	0.00698414068816
C	3.59802508281453	-1.96784467357733	-1.03859602432484
C	4.52201435803705	-1.60970642867096	-0.02853492426598
C	5.83873513308521	-2.08856000943021	-0.08627691293910
C	6.24036128063295	-2.92380418703638	-1.14688165832897
C	5.32289237721473	-3.28130570805895	-2.15360496521913
C	4.00414184525005	-2.80684286946623	-2.10334441760777
H	3.28350890981251	-3.07989982909494	-2.88199270392708
H	5.63666674466299	-3.93151060248213	-2.97916797149387
H	7.27131408071813	-3.29670744599382	-1.18893662310638
H	6.55430254054794	-1.81037225099562	0.69691331507545
H	4.20186935155013	-0.95898245935781	0.79260239023596
N	0.35828431507467	1.06346740388733	1.93930634863408
H	0.41033600787125	0.39848869850122	2.72094513069516
H	-0.39517182069075	1.73103888946390	2.14566728657281
H	1.24221018551432	1.58650616992562	1.91347304895690

BP-86 Geometry Optimized Coordinates for 4+ of **4e**

Rh	0.00644740862380	0.03364019106136	0.03217275427827
O	0.52732358354154	1.47788352221698	-1.34939408446243
C	0.51918212001130	1.18272202139756	-2.60049187147973

C	0.90759757921765	2.26121449420371	-3.55997401624835
C	1.27732550048268	3.54297713035979	-3.09125218942840
C	1.64058289519321	4.54993678913338	-3.99511141577434
C	1.64856914232405	4.31488430205992	-5.39081205528982
C	1.27260063021935	3.03073406209195	-5.84874621048183
C	0.90838061214286	2.01666576057202	-4.95152952271858
H	0.61868233308030	1.02681269708434	-5.32258818654930
H	1.26405743212244	2.82453330838464	-6.92742008274196
C	2.06972845610953	5.39764050873629	-6.35624671321298
H	3.17412648405603	5.46551383492660	-6.40809678556199
H	1.70286354460063	5.19716161150145	-7.37742690605148
H	1.70130663641106	6.38902058720676	-6.03753551664688
H	1.92237587022369	5.54057332781255	-3.61361094962236
H	1.27452862437676	3.74107739663805	-2.01327596525151
O	0.20626516071048	0.03824772800159	-3.08982720528943
Rh	-0.33367549174603	-1.49206822913086	-1.82800577592913
O	-0.85654168098840	-2.93017192239677	-0.45438770499555
C	-0.85418718133340	-2.64561686813355	0.79686702691776
O	-0.53841726044097	-1.50419681135581	1.29767016422650
C	-1.24936141705767	-3.72589574243337	1.75142148663266
C	-1.62307851096212	-5.00254497953678	1.27390274805015
C	-1.99758410764247	-6.01252243443986	2.17083512934474
C	-2.00959832200557	-5.78588788514902	3.56710993723701
C	-1.63665392682326	-4.50322557564885	4.03397471630656
C	-1.26163755452915	-3.48712920193826	3.14465125746165
H	-0.97842149903768	-2.49778013395992	3.52194573587449
H	-1.64404505312293	-4.29954331449322	5.11318694615478
C	-2.38432426343444	-6.88541550791849	4.53268615441695
H	-1.48145850989839	-7.43117642153749	4.87082040952408
H	-2.87565944472933	-6.48132402780130	5.43514009433823
H	-3.05742742602894	-7.62482339181807	4.06514217024007
H	-2.28974056347092	-6.99735550081896	1.78228522841579
H	-1.62100954042086	-5.19331947911643	0.19456785028115
O	-2.28752776456241	-0.85754586094434	-1.89955310039312
C	-2.69765985749829	0.02695702353342	-1.06487863249883
O	-1.97819555823968	0.57634298494440	-0.15222078928846
C	-4.12703405872856	0.45455728672801	-1.15884073980929
C	-4.96849697973562	-0.07358805147232	-2.16317402858029
C	-6.30815865588298	0.33174866806910	-2.25086050585178
C	-6.85150033562131	1.26966149926231	-1.34283957781896
C	-5.99885841435205	1.79389758698215	-0.34176907733437
C	-4.65891186736469	1.39628093602151	-0.24773764922949
H	-4.01171018277099	1.81264079931728	0.53274982852397
H	-6.39453449098837	2.52714667774810	0.37385012635799

C	-8.30101930123491	1.68780706571829	-1.42020874452102
H	-8.41483852692243	2.77622545605342	-1.26789787257572
H	-8.75052839958933	1.42003854776907	-2.39148534449355
H	-8.89411952936847	1.18942152360928	-0.62874890898950
H	-6.94624522937398	-0.08586778361258	-3.04113242623839
H	-4.56250099801989	-0.80022273013157	-2.87630270284713
O	1.64127614246082	-2.03490505954375	-1.64471278643998
C	2.36925206508915	-1.49087620587849	-0.73878506417761
O	1.96856979723528	-0.60326093932905	0.10092622159814
C	3.79798260432871	-1.92067707694153	-0.64946410940679
C	4.64952916592909	-1.38645223349141	0.34478403254077
C	5.98708089459078	-1.79536718165068	0.42599679740705
C	6.52058412309864	-2.74427438156549	-0.47865945111359
C	5.65926591698212	-3.27389615705461	-1.46746636797129
C	4.31896533471058	-2.87148177141180	-1.55550388792147
H	3.66426782795914	-3.29254653910326	-2.32719813285349
H	6.04636907631591	-4.01534210010132	-2.17916182665527
C	7.97158555738281	-3.15675578935858	-0.40107218193427
H	8.61805338143754	-2.40283417048784	-0.89168467435829
H	8.31234282972449	-3.23953168002215	0.64638601112810
H	8.14860876966476	-4.12206874046344	-0.90551413630962
H	6.63267794278366	-1.37340075244472	1.20793492041556
H	4.25079212595630	-0.65246840413213	1.05439849365236
N	0.33023701881455	1.39441134877938	1.70484582857169
H	1.31803946903436	1.40613073039995	1.98480174691330
H	0.06856261098203	2.35951183157434	1.47261054188133
H	-0.21623818400155	1.12067251686923	2.52972269865661

BP-86 Geometry Optimized Coordinates for 5+ of **4e**

Rh	0.06223628140357	0.03654742472144	0.03599134772529
O	0.58016543115102	1.46504511648294	-1.32089211746972
C	0.55792476831964	1.18755711965956	-2.57909652873817
C	0.89171197181282	2.26382710339376	-3.53915500693199
C	1.20130201450799	3.56433925926950	-3.07568378285542
C	1.51376837852797	4.57809791572079	-3.98883249025572
C	1.52999469806649	4.33064727834513	-5.38264081411775
C	1.21409773859286	3.02623100887643	-5.83278062770428
C	0.90012102730952	2.00345370881351	-4.93013560267097
H	0.65802145923130	0.99896533206501	-5.29524779756889
H	1.21345300266123	2.81254292398199	-6.90958571352422
C	1.89951410841192	5.41972557954886	-6.35926758986566
H	2.98943634764428	5.40425981450756	-6.55725104584296
H	1.39051914731150	5.28445680282944	-7.32924027933967

H	1.65321702492616	6.42005001905240	-5.96348917791253
H	1.74807826986519	5.58415551603949	-3.61712754888355
H	1.19173598698211	3.77270073557010	-1.99993579043524
O	0.28096242946832	0.01593528670963	-3.05098896446984
Rh	-0.27234916039549	-1.48056925859246	-1.81224157553270
O	-0.75914307800430	-2.89916637809835	-0.46148530130693
C	-0.80260460238653	-2.61960445070952	0.80051818417752
O	-0.46390727530875	-1.47689375481177	1.29092556916147
C	-1.24504682756860	-3.68002916506816	1.73328987280018
C	-1.61741260294560	-4.95364262774392	1.24083536377770
C	-2.04344296595082	-5.95036034928200	2.12625698475799
C	-2.10875158750363	-5.71397092446765	3.52053678007227
C	-1.73536279287878	-4.43505346023769	3.99913123774337
C	-1.30866374905510	-3.42905839259181	3.12424620850210
H	-1.02634999717099	-2.44334195947897	3.51093618869995
H	-1.78444089633480	-4.22719069229658	5.07592351040183
C	-2.54142123179730	-6.80273694883325	4.47119862706538
H	-1.67310733111309	-7.42562465650079	4.76341850547251
H	-2.97173630939354	-6.38477009943948	5.39739957139288
H	-3.28208737837910	-7.47558997855452	4.00532413526842
H	-2.33483680711021	-6.93238309031349	1.73135006531700
H	-1.57364395633911	-5.15226635925883	0.16407134118484
O	-2.19223753249863	-0.85502084363748	-1.88597556561187
C	-2.62542247686491	0.02813634522813	-1.04612526121817
O	-1.89429840020433	0.57879497060935	-0.13906555647713
C	-4.04695085971527	0.43338250548849	-1.13880161867511
C	-4.87756830448811	-0.10356798930948	-2.15049863836264
C	-6.21972332990084	0.28586725726531	-2.23644324124373
C	-6.77487084589986	1.21247382237769	-1.32207809711599
C	-5.93185421597018	1.74335672149158	-0.31572483171726
C	-4.58808360197624	1.36409713659193	-0.22027421181916
H	-3.94954472407143	1.78541831439420	0.56431665840208
H	-6.33851055420120	2.46741300971407	0.40230759086460
C	-8.22969486813104	1.60499710403282	-1.39916841139710
H	-8.38468873232957	2.64933290621383	-1.07662470266771
H	-8.62953687303756	1.48481119991938	-2.42048431760201
H	-8.83684485913320	0.96424539092114	-0.72979744564904
H	-6.85137327499247	-0.13410605810039	-3.03001126150191
H	-4.46311210896944	-0.82005917087130	-2.86853567548651
O	1.67708934184388	-2.01655497201739	-1.64463778190422
C	2.41649819492093	-1.48334856665324	-0.72903417397396
O	2.00573086894160	-0.58963663616196	0.10378240749726
C	3.82869331040216	-1.92389724370530	-0.63610095245918
C	4.67491434955618	-1.40829592742071	0.37322782340047

C	6.00668595990673	-1.83245004974164	0.45710068527920
C	6.53592884585141	-2.77412789084231	-0.45747072504711
C	5.67736799510807	-3.28388600646482	-1.46119449226285
C	4.34367438111181	-2.86945107962296	-1.55452487606178
H	3.69247128120202	-3.27462890345485	-2.33720427755781
H	6.06316744837834	-4.01912811495888	-2.17943507779816
C	7.98029760140867	-3.20421520732531	-0.38292339194431
H	8.60018416828793	-2.59096023267002	-1.06619523697909
H	8.38979488128406	-3.07943923767210	0.63398720084685
H	8.10528574693322	-4.25729748981242	-0.68995181920298
H	6.65068329577864	-1.42813790566958	1.24892521947340
H	4.28082263299921	-0.68036194196811	1.09123747930438
N	0.40790845197149	1.38078482241713	1.66811275461218
H	1.35401885865259	1.24852913734224	2.04661861916570
H	0.32543248344784	2.36004606599468	1.36799189552161
H	-0.25919949216065	1.23193007877001	2.43517874927468

BP-86 Geometry Optimized Coordinates for 4+ of **4f**

Rh	0.08961102006797	0.00901101916790	-0.02266807831302
O	-0.25224434293000	1.11051014246677	-1.73741567919992
C	0.51327715078284	0.94060477899955	-2.76202523929554
C	0.23070966359346	1.75123273992802	-3.97056099974804
C	-0.84870908293155	2.66880810149464	-4.00508671775531
C	-1.12007781302431	3.43431210157578	-5.13908286135789
C	-0.31237159812769	3.32143169976845	-6.31747111161327
C	0.77727305386382	2.39146674980420	-6.27585506471631
C	1.03284559750820	1.63397591550011	-5.13310439009460
H	1.87378213867983	0.93032570524145	-5.12988862919460
H	1.42596349559885	2.26529065466513	-7.14847342592681
N	-0.57116991313059	4.07133215011131	-7.43775777914410
C	0.26625209034486	3.93463728828780	-8.62516216758700
H	1.32456727607108	4.18607576280681	-8.41418999877386
H	0.23706739939912	2.90549314971169	-9.03548345898532
H	-0.09731283862898	4.62138766490255	-9.40373791537974
C	-1.69139033830354	5.00656584499578	-7.45603740169029
H	-2.66050500946036	4.49327038644901	-7.29628840470430
H	-1.58906143864176	5.78838142262121	-6.67739390694150
H	-1.72845367258655	5.50569593919605	-8.43567962072898
H	-1.96583926248059	4.12886453150756	-5.11719496034295
H	-1.48459860838806	2.77686734836607	-3.11837395666407
O	1.50374969488698	0.11860317065088	-2.80917767962042
Rh	1.95088858536073	-1.03789579393816	-1.16929337944023
O	2.29190337829269	-2.13720869491262	0.53438490746035

C	1.53087431629643	-1.97990318883310	1.56143102953417
O	0.53848258928829	-1.15718522159668	1.62131449433144
C	1.81254987602310	-2.80199944841103	2.76210526071966
C	2.89067054774588	-3.72160336303432	2.78178983268615
C	3.16429601740708	-4.50155393822133	3.90511281187674
C	2.36013999924485	-4.40216483165436	5.08730691490280
C	1.27196795225876	-3.47000308216548	5.06075291842758
C	1.01396562744828	-2.69787165232199	3.92817502926983
H	0.17371484937309	-1.99344137098467	3.93618560515994
H	0.62597191147581	-3.35418145625146	5.93681880673056
N	2.62110126380263	-5.16708136729064	6.19687466535017
C	3.73693922549292	-6.10766982517539	6.19715633857736
H	4.70797871406315	-5.59669959359043	6.04178745770737
H	3.77478447604806	-6.62154418788581	7.16894107691296
H	3.62810345587546	-6.87715551504432	5.40722350163835
C	1.78824402756230	-5.04462089938451	7.38904965019693
H	2.15586113113063	-5.73929092773121	8.15885946874473
H	1.81802992608061	-4.01998019952134	7.81032119341502
H	0.72925546143562	-5.29494027629329	7.17976703551438
H	4.00897196795598	-5.19699303540859	3.87174059951652
H	3.52274031835950	-3.81917221093690	1.89109108414891
O	0.64455138589722	-2.47882157598895	-1.83426087593975
C	-0.59862267922484	-2.41742213152201	-1.50273675213685
O	-1.11641669595684	-1.49918170200595	-0.75899032120537
C	-1.50153365941761	-3.47747558005169	-2.01116070941614
C	-1.01094148698125	-4.52423343866709	-2.83101479936398
C	-1.85083830435532	-5.52653173480556	-3.31570894199907
C	-3.24897501896472	-5.53522569520780	-3.00099728434601
C	-3.73855108807771	-4.47380903405661	-2.17185850990743
C	-2.88326694017255	-3.47981449610071	-1.69645133734310
H	-3.28658118817329	-2.67996048916546	-1.06408289308887
H	-4.79844025866844	-4.43201805692983	-1.90125434533560
N	-4.08274550459372	-6.51797187557082	-3.47365004921321
C	-3.55687399814802	-7.58761505141654	-4.31575630796623
H	-2.77708735664496	-8.17759665212578	-3.79438097149194
H	-4.37611639159416	-8.27037077482143	-4.58528666571588
H	-3.11538241512440	-7.19567334915032	-5.25362006792586
C	-5.50334018068132	-6.50273289032363	-3.13988325678668
H	-5.67126176055560	-6.56891265418813	-2.04648424955299
H	-6.00330216493359	-5.58357469638627	-3.50497191698202
H	-5.99418306201076	-7.36675533944150	-3.61187360360565
H	-1.42451957811934	-6.31345150520467	-3.94592749455544
H	0.05475914731949	-4.54329857864194	-3.08844585154901
O	3.15242153993362	0.46395398081744	-0.44162070528099

C	2.64616094156511	1.38710974705041	0.30016510432445
O	1.40384125838054	1.45611091715513	0.64233336906548
C	3.55360346742934	2.44780239425544	0.79850064562533
C	3.07454101970325	3.50031058376228	1.61759820780277
C	3.92324707606279	4.50134463245461	2.08997554584545
C	5.31836088266116	4.50267153205241	1.76247013048452
C	5.79597716379991	3.43553919250293	0.93353737825413
C	4.93230110964061	2.44314717797982	0.47070119964148
H	5.32539481919770	1.63856203477943	-0.16209121987699
H	6.85309078189279	3.38801948320844	0.65331858218179
N	6.16101005297188	5.48379989097561	2.22269987163966
C	7.57749751267811	5.46197341748822	1.87235247506847
H	8.07648988372115	6.32700029311133	2.33357454983145
H	8.07888567704660	4.54328483888740	2.23667980599068
H	7.73272037671828	5.52155921503142	0.77671246999323
C	5.64881357910327	6.55915222785298	3.06592951527622
H	6.47478658519738	7.23680658016696	3.32825010505244
H	4.86929509752260	7.15352407101616	2.54901864548922
H	5.21147808101166	6.17230658088641	4.00781018902299
H	3.50607609263149	5.29324410227345	2.72011268519175
H	2.01124255189772	3.52523775394323	1.88419862090230
N	-1.57574087729923	0.95510837900336	1.03294926404142
H	-1.33849000016454	1.91099360549765	1.32275193928860
H	-2.42248390449768	1.01419263707984	0.45582311502023
H	-1.82266130980902	0.43413717490932	1.88239303994738

BP-86 Geometry Optimized Coordinates for 5+ of **4f**

Rh	0.04627180074954	0.04253604786467	0.03059928339820
O	-0.28311616181050	1.14033886604781	-1.68164947770215
C	0.47938270556100	0.96219028570852	-2.70293974520895
C	0.21312953883205	1.74852042083233	-3.92289149157475
C	-0.87089042303307	2.66219012964175	-3.97984750043100
C	-1.13212999190211	3.40484833380567	-5.12786531002597
C	-0.30934201720210	3.27024210714096	-6.29555318735572
C	0.78490142608416	2.34510304938750	-6.22981104076547
C	1.03154526053869	1.60983024015290	-5.07400975662400
H	1.87368279219757	0.90888915869584	-5.04940040615272
H	1.44068143612090	2.20731361695457	-7.09479806156039
N	-0.55980680166009	3.99596989311822	-7.42960022400838
C	0.28685147531930	3.83848873242270	-8.61017293415090
H	1.34093711321638	4.09598375368083	-8.39114621763381
H	0.25896998747200	2.80081429274933	-8.99564503357976
H	-0.07274090526127	4.50967710704546	-9.40301447816523

C	-1.68388847981175	4.92849320268545	-7.47988479804934
H	-2.65037190038593	4.41027838119770	-7.32724057809202
H	-1.59118622998103	5.71816687730556	-6.70977163280284
H	-1.70607402232131	5.41283713611068	-8.46669911739814
H	-1.98017719298704	4.09620327326779	-5.12832508408396
H	-1.51566097265692	2.78176576694470	-3.10152084482111
O	1.47659055474560	0.13358464823417	-2.73625662706240
Rh	1.90421645711668	-1.00883921714848	-1.11781861794560
O	2.24504169207642	-2.09554245335069	0.56165291915890
C	1.48258566203011	-1.94893194848775	1.59983234862834
O	0.49467528619616	-1.12596812194623	1.66575446436567
C	1.77933063204429	-2.78371557168499	2.77990170275436
C	2.87824167278989	-3.68163530538339	2.78010524429653
C	3.16732045232338	-4.47207193709580	3.88876315642766
C	2.35831582917251	-4.40678370311855	5.07133479570807
C	1.24873029325763	-3.49703017349435	5.06326010510621
C	0.97520882352752	-2.71200698155218	3.94667573041534
H	0.12140836499397	-2.02487611548756	3.96643210765267
H	0.60217907467894	-3.41101638643248	5.94183232310433
N	2.63379623953568	-5.18206130516776	6.16607668628101
C	3.77471583045471	-6.09483749947651	6.15775909362716
H	4.72969146114958	-5.55208923254412	6.01845216329286
H	3.81839235843482	-6.62546346943932	7.11960442409376
H	3.68671648877837	-6.84828185825723	5.35150977186435
C	1.79822264568528	-5.09947532713193	7.36209700853080
H	2.17712598677326	-5.80561415486813	8.11484567864627
H	1.81465107398253	-4.08336504327438	7.80191243274604
H	0.74580580957087	-5.36211224605844	7.14130240445442
H	4.02602366670727	-5.14869444418892	3.84451318374734
H	3.51210158948393	-3.75048747076361	1.88862525832250
O	0.61775042811054	-2.42982584520773	-1.77467518734978
C	-0.63752058151654	-2.37242182736817	-1.45318331929847
O	-1.15566061786920	-1.46007415582870	-0.70808144587297
C	-1.51805666405819	-3.43149723511877	-1.98273722955234
C	-1.00275869060055	-4.45788314550245	-2.81644909585575
C	-1.82560616230402	-5.45890490922464	-3.32433638529618
C	-3.22683880206130	-5.48668452779403	-3.01937055845236
C	-3.73987792815738	-4.44752095325280	-2.17339218842687
C	-2.90316074655603	-3.45237271982874	-1.67568711382261
H	-3.32026695260980	-2.66819662136613	-1.03328364340541
H	-4.80191948446612	-4.42617784482051	-1.91048740330288
N	-4.04336444770858	-6.46737620658210	-3.51646985943242
C	-3.50015636290054	-7.51662816185288	-4.37627490378170
H	-2.72267302718270	-8.10847239959666	-3.85562349769632

H	-4.31217287540492	-8.19745005992836	-4.66889505422028
H	-3.05282493388489	-7.09600235652593	-5.29739665839858
C	-5.46686510640908	-6.48475376908557	-3.18653210266266
H	-5.63103987450031	-6.59849679274580	-2.09742285296823
H	-5.97122899688785	-5.55603298291282	-3.51555550197466
H	-5.94405371805464	-7.33397177523344	-3.69655973707599
H	-1.38601516916089	-6.23062044056335	-3.96330716314744
H	0.06483672195946	-4.45964468548543	-3.06429310071949
O	3.10241611921581	0.46375589128896	-0.39918063747948
C	2.60468278531164	1.40377586083488	0.34199870464251
O	1.36721117942869	1.47789483613673	0.68898266018041
C	3.52750605791823	2.45248231530173	0.81761896525013
C	3.06333516288703	3.51447882414409	1.63600883283039
C	3.92551745872293	4.50835576639316	2.09032523447723
C	5.31749608056718	4.49192873966769	1.74291918403974
C	5.77869858023873	3.41607025629009	0.91380285606872
C	4.90310178130919	2.42921030955615	0.46961484765098
H	5.28092061832572	1.61689896691459	-0.16177125854658
H	6.83170915097617	3.35914980943344	0.62151066446880
N	6.17213190833026	5.46622344066957	2.18561482025805
C	7.58386921067818	5.43786543896861	1.80996719093734
H	8.09432813584806	6.29938016470208	2.26367058850282
H	8.08082503021630	4.51459697973638	2.16533083392179
H	7.71364108525030	5.49761224230219	0.71204789688149
C	5.68367595277012	6.55070401332444	3.03462808101253
H	6.52158958071296	7.21705201985173	3.28545733159155
H	4.90599150152280	7.15034251368065	2.52331219708926
H	5.25497036276102	6.16518995878910	3.97958136163069
H	3.52443742677941	5.30931017882547	2.71860597846111
H	2.00366229639042	3.55078115781958	1.91412314455074
N	-1.59133463171182	0.97821430650387	1.07252617645515
H	-1.36140894370988	1.94358892728989	1.33713220861780
H	-2.44421308443357	1.01121024471344	0.50164988141587
H	-1.81835265667032	0.47000022804418	1.93569031637627

BP-86 Geometry Optimized Coordinates for 4+ of **5a**

Ir	0.01043044846076	0.05050602753585	0.05397399750076
O	0.52759551466856	1.48223846852335	-1.33659771980501
C	0.51784704460441	1.18048152139247	-2.58851751122732
C	0.90340572400639	2.25388317957966	-3.54937483739031
C	1.27382341577706	3.53415684485765	-3.07825268788922
C	1.63825410938728	4.54805914393153	-3.97568566106093
C	1.62887612468547	4.27118388490950	-5.35441216358486

C	1.26426625877047	3.00599874316064	-5.84889359870428
C	0.90270076290637	2.00126292500405	-4.94013719910748
H	0.61652306407239	1.01044285738288	-5.30990833317306
H	1.26211883022659	2.80689190544416	-6.92637194303775
Br	2.12394219396653	5.64798418958518	-6.58667868060889
H	1.92543222154887	5.53907594681208	-3.60680003507692
H	1.27620408586432	3.73396852089285	-2.00110733265487
O	0.20447420887260	0.03314461507043	-3.08040972320994
Ir	-0.33306507897078	-1.49961890485702	-1.83190335963194
O	-0.84817915134793	-2.92338657286532	-0.45103104458722
C	-0.84461317198106	-2.63463910805256	0.80301254558761
O	-0.53351988593615	-1.49105963773893	1.30789829300655
C	-1.23351456972768	-3.71555374660848	1.75384755813842
C	-1.59871130629403	-4.99284746144820	1.27058741300686
C	-1.96586104427869	-6.01441996157741	2.15798537527437
C	-1.96473986935127	-5.74839495620779	3.53902197927896
C	-1.60568405616248	-4.48649693614902	4.04543714656847
C	-1.24113577001743	-3.47389185791078	3.14654340772112
H	-0.95919346363536	-2.48534339630151	3.52540809429298
H	-1.61005376169121	-4.29589817090693	5.12444910081250
Br	-2.46368109427390	-7.13587315921837	4.75762333403055
H	-2.24883564402156	-7.00312583397428	1.77981730139408
H	-1.59481160415928	-5.18449520483500	0.19193992876045
O	-2.27890975871361	-0.86134029356103	-1.89343823747670
C	-2.68821746397769	0.02812253893784	-1.05812881579437
O	-1.97189207461797	0.58340110207659	-0.14315145261527
C	-4.11389080363012	0.45430346884566	-1.15763137700738
C	-4.95113235404480	-0.08364392991066	-2.16147456281984
C	-6.29159458181040	0.31490315593874	-2.26328899601130
C	-6.79182823472066	1.25871719555102	-1.34836283371057
C	-5.98037440069572	1.80791001476603	-0.33963707029027
C	-4.64124485807788	1.40156823553455	-0.25055494322448
H	-3.99652539064701	1.82031337289076	0.52998201779829
H	-6.38597402179032	2.54133547938690	0.36621525979272
Br	-8.61902970793228	1.80955275340214	-1.48053175024021
H	-6.93686899442492	-0.10251117408402	-3.04435556962910
H	-4.54659827706716	-0.81706294195904	-2.86766991740584
O	1.63699924457030	-2.02869275024212	-1.63877795786099
C	2.36429447154424	-1.48158218201972	-0.72891314968019
O	1.96699233117061	-0.59172929094999	0.11361356085370
C	3.78833867795647	-1.91495494176322	-0.64059515166058
C	4.63677182434506	-1.38273313996391	0.35684750940547
C	5.97585751665271	-1.78890377979127	0.44731190415483
C	6.46317787504725	-2.73453435902448	-0.47249049099828

C	5.64028979569483	-3.27816686339210	-1.47515168745061
C	4.30291196863373	-2.86422853829924	-1.55293909097763
H	3.64951961917358	-3.27872950052804	-2.32855199293747
H	6.03582378039022	-4.01319726574004	-2.18503109381548
Br	8.28818772646260	-3.29599832782309	-0.35585076693225
H	6.62993995913968	-1.37593234081379	1.22340091530521
H	4.24197949906305	-0.64780490613612	1.06692654485761
N	0.32754794792542	1.39981812512721	1.72708214741291
H	1.32514420419817	1.51238721635526	1.94751833112154
H	-0.04091046982288	2.34332587657724	1.55411720490712
H	-0.12443064596374	1.06319585518121	2.58659509830575

BP-86 Geometry Optimized Coordinates for 5+ of **5a**

Ir	0.04486509937805	0.00965726013910	0.06199803834682
O	0.56380784622367	1.42746097233872	-1.29347788341653
C	0.52903975332363	1.15100081255854	-2.55445641490733
C	0.85444888216137	2.22606605646677	-3.51483616896452
C	1.18208045625612	3.52021554641455	-3.04653149306629
C	1.49261573298258	4.54258738651011	-3.95174863579095
C	1.47262029714877	4.26096451259175	-5.33055185433370
C	1.14854790446941	2.98121740059646	-5.81845629009082
C	0.84012167161452	1.96521220086296	-4.90518276648792
H	0.58758093337844	0.96394757782516	-5.27121338170252
H	1.13767555055442	2.78031207458885	-6.89533023978671
Br	1.89633513119399	5.64858711110441	-6.56902566168536
H	1.74718407120713	5.54479644530886	-3.58985823491487
H	1.19428481026962	3.72486893556591	-1.97043609669093
O	0.25289602340986	-0.02319044293464	-3.02015141750121
Ir	-0.28771999508390	-1.51845386227222	-1.78581902373159
O	-0.78001340428706	-2.93217784103660	-0.43575650056274
C	-0.82481160976843	-2.64968377323354	0.82477034588593
O	-0.48262965330763	-1.50466356654954	1.31252603016195
C	-1.26386835883660	-3.70629896134805	1.76114328282898
C	-1.63642655304585	-4.97937937676089	1.26943247426500
C	-2.05483508148326	-5.98368342787380	2.15132309839302
C	-2.09739256630423	-5.70523240634647	3.53018826050892
C	-1.73161870936476	-4.44586143996003	4.04108521038670
C	-1.31499005236648	-3.44806750953305	3.15097202243117
H	-1.02741546422356	-2.46306255932312	3.53458512847457
H	-1.77119062823979	-4.24696815172416	5.11766270792961
Br	-2.66499408533151	-7.06925780819432	4.73713288038474
H	-2.34385208445705	-6.96971983348432	1.77137872760447
H	-1.59807427142357	-5.18218888779653	0.19353527890119

O	-2.21674448280486	-0.90428639428653	-1.85139646649555
C	-2.63721194303306	0.00524077333869	-1.03560923688999
O	-1.91416399283381	0.54251605252454	-0.11067232010367
C	-4.04390170195898	0.45037655753381	-1.15998280486446
C	-4.87060409342109	-0.08447392039434	-2.17548580376521
C	-6.20084791948930	0.33608365179115	-2.30066105766455
C	-6.69973221249569	1.29545359967829	-1.40007675213874
C	-5.89589657138157	1.84002153521498	-0.38145428403554
C	-4.56647894937451	1.41417060774099	-0.26615516010582
H	-3.92951432604660	1.82934215890061	0.52248859805855
H	-6.30125042149437	2.58522538234733	0.31178920774053
Br	-8.51093912626244	1.87303406033130	-1.56504718941185
H	-6.84052608739672	-0.07630801647969	-3.08871667882804
H	-4.46882656143859	-0.82995688656206	-2.87037790414671
O	1.66164985653402	-2.05971204552499	-1.60805846783135
C	2.40586482766179	-1.49835444180212	-0.71441021109135
O	1.99057144209927	-0.61654442727717	0.13113262824774
C	3.82891905403753	-1.90576198341345	-0.64579751884429
C	4.68019703991433	-1.35429220424406	0.33981787995859
C	6.02526846352852	-1.73915215030861	0.41032756689153
C	6.51390968910374	-2.68010396365394	-0.51490050445870
C	5.68570891223598	-3.24055564599034	-1.50486397532765
C	4.34176364580210	-2.85008928172424	-1.56544092574195
H	3.68553306886723	-3.27844565737804	-2.33093424635088
H	6.08319849632420	-3.97090650130611	-2.21820180796833
Br	8.34503364526659	-3.21031169345986	-0.42352401235565
H	6.68411767015648	-1.31384776858141	1.17538886481574
H	4.28586080454847	-0.62406885352157	1.05482660816896
N	0.39220205286960	1.31504830471045	1.72825566650077
H	1.39158523832784	1.36454009729053	1.96568756700406
H	0.08107924574346	2.27703467946119	1.53989001568876
H	-0.10544746963743	1.00142166054377	2.57180853247603

BP-86 Geometry Optimized Coordinates for 4+ of **5b**

Ir	0.01878844675507	0.07790027164333	0.08255439282123
O	0.53624862443780	1.50868223628507	-1.30871385809070
C	0.52678015985166	1.20646969266830	-2.56083428970482
C	0.91295575411986	2.27866046569917	-3.52179408091900
C	1.28328607045936	3.55974331293924	-3.05173301265983
C	1.64842856926080	4.57194730519643	-3.94930288100732
C	1.64138436916354	4.29693457337831	-5.32960126730781
C	1.27626573352702	3.02939957760458	-5.82095397783226
C	0.91376025944124	2.02568024200943	-4.91286392334161

H	0.62774183018235	1.03455833626838	-5.28186347892854
H	1.27723847844003	2.83576113705316	-6.89944163445139
Cl	2.09665265602793	5.55802303734904	-6.45909720741327
H	1.93631510674369	5.56521405464563	-3.58702954356468
H	1.28450127885460	3.75989293740660	-1.97468353824130
O	0.21296324066211	0.05850048111873	-3.05158834267027
Ir	-0.32468387705495	-1.47349595821046	-1.80184016751074
O	-0.84000680401508	-2.89645154905244	-0.42021383774514
C	-0.83733749138440	-2.60703332294525	0.83396087430038
O	-0.52600205853627	-1.46278397322514	1.33776765150566
C	-1.22775253590842	-3.68657532110357	1.78478336532575
C	-1.59321249706503	-4.96449364593434	1.30231788877017
C	-1.96237263892063	-5.98416687669157	2.18954636253609
C	-1.96465724626283	-5.72000908738751	3.57211675764878
C	-1.60463906923344	-4.45597317519100	4.07570932710030
C	-1.23776991610292	-3.44459568510992	3.17778073212814
H	-0.95580009572439	-2.45589489593183	3.55615588357013
H	-1.61294963736276	-4.27083720345242	5.15565521682554
Cl	-2.42565108434265	-6.99053978728990	4.68858811915297
H	-2.24648515915819	-6.97492242961712	1.81756484715237
H	-1.58754340480983	-5.15647198727089	0.22377160145585
O	-2.27084233736579	-0.83578480876543	-1.86387236846728
C	-2.68081067477572	0.05413004351063	-1.02895318802019
O	-1.96374158708460	0.61057891662889	-0.11491929795353
C	-4.10646855979172	0.47846008337906	-1.12726636530044
C	-4.94515207453418	-0.06145392408807	-2.12935858783473
C	-6.28557194539956	0.33458539227406	-2.22870285887298
C	-6.78939480113309	1.27872608876723	-1.31429438968907
C	-5.97389041274416	1.82915088211525	-0.30787498496487
C	-4.63468883686880	1.42596475779530	-0.22038137977891
H	-3.98913985415199	1.84630605928669	0.55856736408675
H	-6.38551240326113	2.56196689038714	0.39511811455913
Cl	-8.46545056439518	1.77903638451167	-1.43153285761678
H	-6.93646396149568	-0.08115804669821	-3.00599237731925
H	-4.54020021590672	-0.79479577599224	-2.83534703886159
O	1.64568396742894	-2.00208123226962	-1.60842812055922
C	2.37348019714794	-1.45431541163982	-0.69899962945837
O	1.97528803006011	-0.56422688906116	0.14329235174229
C	3.79742624872159	-1.88603345580968	-0.61146425472257
C	4.64710444776987	-1.35207038117227	0.38452221994810
C	5.98607324016500	-1.75590357581351	0.47279314063170
C	6.47711456425746	-2.70183091522809	-0.44650816177257
C	5.65037839602571	-3.24645749198641	-1.44710508580768
C	4.31299628739395	-2.83550756164688	-1.52360213038816

H	3.65893632382192	-3.25142607374773	-2.29784882875430
H	6.05209246105971	-3.98083256057347	-2.15418644829152
Cl	8.15107551129169	-3.21200824833117	-0.34319724775033
H	6.64558818736192	-1.34475749438552	1.24524896146575
H	4.25182142452668	-0.61724215877810	1.09439734870369
N	0.33907459980863	1.43081592723648	1.75262769619817
H	1.33436411448752	1.51093577284686	1.99642218564903
H	0.00821818306870	2.38469047007478	1.56153738437998
H	-0.14523040753433	1.11915364432134	2.60387280591512

BP-86 Geometry Optimized Coordinates for 5+ of **5b**

Ir	0.05750060651942	0.03475148490951	0.09197940845713
O	0.57681770963130	1.45167800823075	-1.26396551767838
C	0.54099325797212	1.17547767739962	-2.52531864858677
C	0.86230560753169	2.25057740698036	-3.48569607693801
C	1.18619331554820	3.54651788765077	-3.01842028808168
C	1.49060022433936	4.56915116671117	-3.92382031863023
C	1.46950208010479	4.29010458406187	-5.30435160467951
C	1.14943509852228	3.00696149174996	-5.78938029475663
C	0.84689608209819	1.99019520046007	-4.87655779122863
H	0.59742576942325	0.98790593486716	-5.24180210604873
H	1.13892683625705	2.81253081049465	-6.86742843685226
Cl	1.84811918307063	5.56377815433331	-6.43981642649715
H	1.74231991190541	5.57449467269997	-3.56872866169852
H	1.19933404894840	3.75083228585482	-1.94230829292507
O	0.26631413635553	0.00013106764506	-2.99011126215520
Ir	-0.27477486143862	-1.49416998825761	-1.75533589558833
O	-0.76786058008251	-2.90677911939752	-0.40500524176315
C	-0.81520407543171	-2.62354224245286	0.85568573567538
O	-0.47116081533294	-1.47841676139069	1.34283973216196
C	-1.25932295963728	-3.67749191747441	1.79126819118861
C	-1.63278870929003	-4.95107505846837	1.30031244245659
C	-2.05773642164033	-5.95184458538833	2.18144261628417
C	-2.10770509110149	-5.67340511303791	3.56127552322915
C	-1.74000881061672	-4.41224539895807	4.06965846581091
C	-1.31649208146167	-3.41751606343423	3.18098020131130
H	-1.02838990290036	-2.43246896877169	3.56400095089348
H	-1.78691627975599	-4.21770855349187	5.14671771038848
Cl	-2.63857971630753	-6.91934022155431	4.66631097363104
H	-2.34878828664266	-6.93973002027556	1.80795343396171
H	-1.58974200911994	-5.15533656442688	0.22490270434499
O	-2.20368315826929	-0.87940986069390	-1.82215790448577
C	-2.62464918131055	0.03052939157665	-1.00651942955481

O	-1.90119267897238	0.56841275913520	-0.08180317122742
C	-4.03066037297857	0.47529741919180	-1.13094707532008
C	-4.85859696547976	-0.06070679924853	-2.14541364300842
C	-6.18789275726680	0.35961193991755	-2.27016371224965
C	-6.68943623952951	1.32100532267952	-1.37136624054089
C	-5.88214250486675	1.86582613744787	-0.35396694876594
C	-4.55361029165703	1.44065539660067	-0.23836060218062
H	-3.91599805850671	1.85675921254390	0.54921531014159
H	-6.29303397013461	2.61177960936339	0.33516347165285
Cl	-8.34907962225652	1.84998620960590	-1.52223699055837
H	-6.83293471429491	-0.05008789383542	-3.05521243576182
H	-4.45680862980430	-0.80713087639996	-2.83922819559810
O	1.67454568878849	-2.03573236364810	-1.57715599028855
C	2.41901657394668	-1.47389671344887	-0.68351653581753
O	2.00318059242695	-0.59174643017133	0.16188317424040
C	3.84176983798649	-1.87980521812200	-0.61571458032800
C	4.69415210417099	-1.32705272671272	0.36881933711373
C	6.03903366828839	-1.70930739267720	0.43703664398327
C	6.53136594978460	-2.64981752485687	-0.48849328374351
C	5.69966217837947	-3.21108348655934	-1.47676229608918
C	4.35579787312575	-2.82375961069685	-1.53571921771322
H	3.69904758480680	-3.25312427408969	-2.30014902546408
H	6.10356381616339	-3.94013039151018	-2.18780252819536
Cl	8.21066201290895	-3.13072878986954	-0.40886355021967
H	6.70325400284133	-1.28615355241230	1.19861172581461
H	4.29916737871635	-0.59740011037514	1.08399955678128
N	0.40471605429607	1.34132656418405	1.75786354438977
H	1.40439335779492	1.39422392791558	1.99340904011243
H	0.08945814746103	2.30226323250519	1.57119890825916
H	-0.08967633402677	1.02511770539201	2.60235336893533

BP-86 Geometry Optimized Coordinates for 4+ of 5c

Ir	0.01050214602280	0.04997397201008	0.05277055391815
O	0.52799119404645	1.48178976117881	-1.33822034594646
C	0.51975343039122	1.18129654432029	-2.59149697302268
C	0.90642249854529	2.25293130622479	-3.55054503606925
C	1.27927815135460	3.53394135152567	-3.07941497667421
C	1.64512907408933	4.54433962465288	-3.97727898398497
C	1.63718751432987	4.27150309028822	-5.35558188771434
C	1.27024296419561	3.00741930629818	-5.84755616950331
C	0.90635890804321	2.00220831250480	-4.94299144265059
H	0.61840002198176	1.01177489378559	-5.31223457057015
H	1.27481863600253	2.82881449667660	-6.92934571628153

F	1.98593681095170	5.23312276514518	-6.21484944855308
H	1.93738649480481	5.54161287005711	-3.62762643382257
H	1.28104974605076	3.73188175477063	-2.00199638444571
O	0.20567578344811	0.03243715318630	-3.08183865080831
Ir	-0.33300118017283	-1.49991680915283	-1.83176583845892
O	-0.84933406948430	-2.92335968491880	-0.44988415558021
C	-0.84626188938757	-2.63589651913503	0.80542349978112
O	-0.53345407224817	-1.49082613287197	1.30849960594700
C	-1.23627454906238	-3.71460909853925	1.75491952502368
C	-1.60376058233440	-4.99282703768776	1.27198311117385
C	-1.97246667309267	-6.01062957971191	2.16005124543759
C	-1.97307857448154	-5.74822237052770	3.54052726922179
C	-1.61183358093477	-4.48721650524544	4.04414203887789
C	-1.24483217239609	-3.47441407302694	3.14920041925679
H	-0.96129631312015	-2.48607857156927	3.52728057232080
H	-1.62320023761104	-4.31683358808114	5.12720825164836
F	-2.32471479382818	-6.71716223278567	4.39032252978237
H	-2.26048124403079	-7.00582786497537	1.80110895757174
H	-1.59903765357638	-5.18300919826531	0.19315832267989
O	-2.27954511138182	-0.86102232400753	-1.89386309054371
C	-2.69088200622690	0.02893744092333	-1.05862754362969
O	-1.97216136933067	0.58358325869772	-0.14369334425496
C	-4.11460534758465	0.45429437034133	-1.15732853538951
C	-4.95628849479826	-0.08994715791898	-2.15591706917701
C	-6.29491336446050	0.30919295285275	-2.25430190505648
C	-6.79510394557141	1.25837585936106	-1.34686092437909
C	-5.97920663955473	1.81216589307672	-0.34595445729537
C	-4.64128982635497	1.40850909688398	-0.25510326365304
H	-3.99355749989666	1.83162091856831	0.52047080149999
H	-6.40214167450301	2.54980715130386	0.34629758061293
F	-8.07148640028290	1.64221266769303	-1.43810628491644
H	-6.95894884927468	-0.10214314660213	-3.02378856179126
H	-4.55249972067758	-0.82807086954216	-2.85750424960968
O	1.63766321911101	-2.03019858235679	-1.63814728140528
C	2.36722013381403	-1.48271364979095	-0.72898384604545
O	1.96781104026495	-0.59144707198909	0.11261168294713
C	3.78940184988659	-1.91485205561869	-0.64063644183903
C	4.64155332620645	-1.37610503346575	0.35199772466907
C	5.97878820995351	-1.78263131670261	0.43995218652740
C	6.46679504276858	-2.73367583636038	-0.47198192158999
C	5.64023347047955	-3.28209657781564	-1.46726065352607
C	4.30402776786386	-2.87109112747186	-1.54771313693132
H	3.64821154769845	-3.29018966598861	-2.31869653463130
H	6.05376150246968	-4.02145947604989	-2.16334532793193

F	7.74163780144197	-3.12479540570233	-0.39071851805229
H	6.65092605474884	-1.37570685499389	1.20473826651993
H	4.24683849256033	-0.63648133378688	1.05711954658085
N	0.32695977188516	1.39981644671022	1.72768043040684
H	1.32518451780568	1.53254513070709	1.93364623592871
H	-0.06359321693963	2.33640053789208	1.56580416932717
H	-0.10427895061704	1.05032985502197	2.59272085807425

BP-86 Geometry Optimized Coordinates for 5+ of **5c**

Ir	0.03910875680241	0.00170532135415	0.07073311110638
O	0.55871911253883	1.42232786240142	-1.28652997951638
C	0.52788655822181	1.14263230953237	-2.54811617756250
C	0.85838537408927	2.21563736530163	-3.50642746291831
C	1.19005162127883	3.51051936982291	-3.03812146481630
C	1.50173246048807	4.52967769131450	-3.94314735272999
C	1.48081510987265	4.25196876337085	-5.32150344003869
C	1.15464597935532	2.97354867204226	-5.80790235947107
C	0.84429479888662	1.95728171999137	-4.89888208195795
H	0.58904633080793	0.95664694306521	-5.26434348380432
H	1.14871316088732	2.79434949517444	-6.88931771045851
F	1.77589521547452	5.22203327181068	-6.18531724077064
H	1.76104188356359	5.53827616994319	-3.60092644505390
H	1.20227564261851	3.71289588109220	-1.96172613769380
O	0.24536256742254	-0.03001800099233	-3.01761427802227
Ir	-0.29463147727392	-1.52748283617965	-1.77684037353000
O	-0.79468559807166	-2.94715203140113	-0.42554947787008
C	-0.83237839817456	-2.66206845754061	0.83571552494254
O	-0.49383043228517	-1.51514673817610	1.32452869369438
C	-1.26683624501188	-3.71772797414733	1.77296538382136
C	-1.64310014919702	-4.99222808170558	1.28325836647027
C	-2.05920971935377	-5.99290800391177	2.16686367261306
C	-2.09823227732942	-5.71713892228841	3.54511519423672
C	-1.72830424848652	-4.45901037395076	4.05266654685342
C	-1.31333647493853	-3.46136587948742	3.16490683896061
H	-1.02304358830104	-2.47647979076034	3.54646962298487
H	-1.77155913802119	-4.28063447621542	5.13336685710302
F	-2.49576044752241	-6.66881292035861	4.38831426117995
H	-2.35554234971496	-6.98525394105929	1.80759603006653
H	-1.60829506992334	-5.19327417659853	0.20705912158538
O	-2.21728124643499	-0.91611639026644	-1.83893541589827
C	-2.64044468888526	0.00409561867496	-1.03295417824198
O	-1.91522181759062	0.53253367341966	-0.10252890292017
C	-4.03814245260508	0.45898580498973	-1.16883783631405

C	-4.86685219713717	-0.08036981915068	-2.18283266208696
C	-6.18993583567925	0.35188741908060	-2.31674254337586
C	-6.68542867791471	1.32597539308694	-1.43189265350424
C	-5.88023284633689	1.87381931004017	-0.41751937035085
C	-4.55741813293607	1.43945718723944	-0.28848088423748
H	-3.91926186049535	1.85749530662437	0.49755350938044
H	-6.30127322453666	2.63091700469913	0.25413306379486
F	-7.94536218948629	1.73959711658002	-1.55769747514940
H	-6.84667305783374	-0.05170826329237	-3.09615023137607
H	-4.46780229356072	-0.83794459187004	-2.86596384853145
O	1.64561362500497	-2.07051631309361	-1.59284331359973
C	2.39981375341940	-1.50280741642468	-0.70828351356214
O	1.97802663097203	-0.62591897693346	0.14145982344786
C	3.82177961034025	-1.89877689120558	-0.65162434811126
C	4.68147195943755	-1.33230076631040	0.32069109126805
C	6.02747757662195	-1.70722589225443	0.37691460450167
C	6.51466472880308	-2.65166692401787	-0.54393634888777
C	5.67883041050110	-3.22560444156214	-1.51814877810920
C	4.33325034979971	-2.84829029190128	-1.56948422730339
H	3.67100665006475	-3.28769659465885	-2.32331938324997
H	6.09404863286452	-3.95796604499194	-2.22019449179817
F	7.79657423659249	-3.01068111762315	-0.49180536495992
H	6.70860542027907	-1.28153329087275	1.12291455860191
H	4.28839232022482	-0.59894084987834	1.03303592408253
N	0.37469999923533	1.29974228317568	1.74787343111892
H	1.37768965950244	1.41752691189285	1.94223816284197
H	-0.01231218777397	2.24087971198226	1.59936141326994
H	-0.05791469315953	0.93173593337835	2.60518190985640

BP-86 Geometry Optimized Coordinates for 4+ of **5d**

Ir	0.02538388254360	0.05790695210299	0.09429781735888
O	0.61629780929957	1.66666351068589	-1.04856476485856
C	0.56188450647484	1.58324917197357	-2.33337792319669
C	1.00228305435352	2.77614781725890	-3.11469001362793
C	1.45358108908457	3.93884265999110	-2.44765051753361
C	1.86726302410913	5.05883900311069	-3.18527067359729
C	1.83485358834998	5.02939266727129	-4.59271766975131
C	1.38635954993875	3.87422786891036	-5.26179345629842
C	0.97151672451308	2.75193744204709	-4.52854991897284
H	0.62143136958546	1.84951453356958	-5.04211406295791
H	1.36019308442720	3.84874567686225	-6.35835090947308
H	2.15877073244154	5.90603586547875	-5.16784363643263
H	2.21595912062612	5.95774155685748	-2.66166878631404

H	1.47594884594266	3.95399794100244	-1.35227017477297
O	0.15900515951926	0.55670559618184	-2.99746277526688
Ir	-0.46362251233320	-1.12789006239052	-2.00936365969133
O	-1.05102245950444	-2.72917837547661	-0.87413273877631
C	-0.99938937920865	-2.65946639241905	0.41041697588221
O	-0.59872600634438	-1.63918195244465	1.08731036270981
C	-1.43985535793019	-3.85984849028439	1.18042228828237
C	-1.88606409459050	-5.01723998645970	0.50080790923377
C	-2.30002829516684	-6.14497276829319	1.22617070321933
C	-2.27306183389718	-6.12878439118159	2.63406708227074
C	-1.82969857184183	-4.97911398180221	3.31563630523151
C	-1.41447133264507	-3.84896153625497	2.59452924816566
H	-1.06840547061259	-2.95074114136472	3.11805255375111
H	-1.80783554870539	-4.96393816092589	4.41248987369539
H	-2.59726140356834	-7.01154899747845	3.19959685385270
H	-2.64466693021564	-7.03961749948470	0.69270009576502
H	-1.90414718169541	-5.02228302460659	-0.59476370243627
O	-2.36019661257813	-0.35898159338510	-1.89789280728608
C	-2.69192614661217	0.39947784524848	-0.91216094927802
O	-1.91729728279971	0.74410575858696	0.05818760294389
C	-4.08926484696102	0.92348413479390	-0.88997708467599
C	-4.99294056733437	0.58526985502013	-1.92414266822035
C	-6.30632070742063	1.07905662555940	-1.90167263952688
C	-6.72986188061297	1.91331701832357	-0.84913840909024
C	-5.83431406082082	2.25278374392212	0.18312376757224
C	-4.51984007853060	1.76143825634652	0.16493718613819
H	-3.81673615528186	2.02046111076115	0.96439380354479
H	-6.16196476301371	2.90246428040310	1.00433497440737
H	-7.75723745377502	2.29863686953500	-0.83351650368497
H	-7.00231120827708	0.81289564424601	-2.70702320365997
H	-4.65601680332688	-0.06462775138029	-2.73948136533809
O	1.46693157540661	-1.81449669181749	-1.97247228703377
C	2.25103217288797	-1.47734825750869	-1.00868997273704
O	1.93316397198566	-0.71704620469762	-0.01845359789684
C	3.64487985246539	-2.01050991863397	-1.04005031170406
C	4.55766542126092	-1.68096129051654	-0.01114293770128
C	5.86748283539929	-2.18393049193939	-0.04321448308218
C	6.27819288745158	-3.01876800299500	-1.10019942819552
C	5.37342783090949	-3.34967429393088	-2.12736558480175
C	4.06267177295696	-2.84921068347801	-2.09953087042609
H	3.35272035767013	-3.10176718398542	-2.89502528813381
H	5.69106210180033	-3.99985243309358	-2.95210105937070
H	7.30268761619560	-3.41131179093209	-1.12343844500288
H	6.57061476053298	-1.92445823760432	0.75812143246136

H	4.23047133503109	-1.03055517733300	0.80770044625993
N	0.44604007735962	1.12640559423179	1.94014519931860
H	0.99444680023532	0.57022075583556	2.60776949099685
H	-0.41369958182011	1.40509525454406	2.42941823256671
H	0.97858110666645	1.98928479343670	1.77221789517613

BP-86 Geometry Optimized Coordinates for 5+ of **5d**

Ir	-0.00884718037804	0.09365280329927	0.06616555586105
O	0.57454956855841	1.69303181382752	-1.05196360786847
C	0.55003038004277	1.61810811412209	-2.34054069645758
C	1.03545215432973	2.78134465453563	-3.11780184184497
C	1.52379706482879	3.92801061357823	-2.44725712626508
C	1.98517598513050	5.02570224635397	-3.18755840782144
C	1.96273454881153	4.98743958929129	-4.59527183311509
C	1.47722747056732	3.84768530069456	-5.26521652310405
C	1.01380665074824	2.74574960416060	-4.53247435271289
H	0.63433112571705	1.85565042573902	-5.04642923428826
H	1.46032663047863	3.81881346541583	-6.36147684228999
H	2.32478010689726	5.84797314773638	-5.17169241757934
H	2.36345673261057	5.91375397034490	-2.66680918797526
H	1.53822646925201	3.94994391511979	-1.35200586465217
O	0.10519199203966	0.59348975588062	-2.99109599469217
Ir	-0.49305951979374	-1.06452177379138	-2.00302812723302
O	-1.08458231303896	-2.64160672643061	-0.89519245481699
C	-1.00307987521966	-2.60804035918816	0.39513605651907
O	-0.62810183340817	-1.56640076886515	1.06047190998578
C	-1.38669735829425	-3.82101242951962	1.15123960310546
C	-1.81990083255770	-4.97784463238033	0.46022902123962
C	-2.18031507310316	-6.12602340158126	1.17959235703031
C	-2.11197786103946	-6.12827765230159	2.58633851561213
C	-1.68121353508718	-4.97857161111071	3.27652931570564
C	-1.31864879370797	-3.82622538925233	2.56496401190831
H	-0.98253674623979	-2.92812583800136	3.09484161422113
H	-1.62818148791734	-4.98148362354578	4.37200279563255
H	-2.39484104510672	-7.02847060637314	3.14623542049448
H	-2.51552042860690	-7.02194611895663	0.64310646900760
H	-1.87102870689795	-4.96816362594935	-0.63413322249201
O	-2.36992319086932	-0.30620544288289	-1.91328345358258
C	-2.72444976524374	0.43110747857279	-0.91324999132435
O	-1.93072211150941	0.78247380548663	0.04203839553791
C	-4.12328891070535	0.91913690100827	-0.87105114765819
C	-5.02601900574489	0.56988843573175	-1.90345801463167
C	-6.34899269955331	1.03255382114927	-1.85992741256645

C	-6.77874883717010	1.84305550686112	-0.79133614979439
C	-5.88272532683258	2.19190760602916	0.23772043721069
C	-4.55811297283740	1.73341196733368	0.20156735075337
H	-3.85474911409224	1.99991977399335	0.99811009606999
H	-6.21835553348883	2.82286476860693	1.06973297945071
H	-7.81462282394681	2.20348075668591	-0.76032907698381
H	-7.04754198846160	0.76106381807835	-2.66076844105378
H	-4.68392164595103	-0.06086789211541	-2.73137943849516
O	1.41227446455573	-1.73918010316822	-1.98472978455194
C	2.20460548889574	-1.43727242284321	-1.00878587568462
O	1.88053557396704	-0.65473030534480	-0.03380037164374
C	3.57233807004052	-2.00545450501512	-1.02082554410699
C	4.47574280859048	-1.70108912507694	0.02527046993385
C	5.76878033459753	-2.24307968181531	0.01049815719661
C	6.16794341545532	-3.08846162493749	-1.04289952086844
C	5.27118871173458	-3.39300091579094	-2.08530313713332
C	3.97634908679636	-2.85512764756734	-2.07817157194586
H	3.27298349207592	-3.08654459430045	-2.88565057758375
H	5.58296135433710	-4.05145478536501	-2.90517878380156
H	7.18032839373555	-3.51142800221127	-1.05117609546737
H	6.46785320615110	-2.00654799156622	0.82188699009589
H	4.15753138737587	-1.04277908030226	0.84113541381331
N	0.37746239213996	1.18597424654484	1.87274047735880
H	0.89467142721873	0.62912008735947	2.56558121796430
H	-0.49394758225953	1.49163666865043	2.32529185524242
H	0.93663710138304	2.03007265535867	1.69239845713573

BP-86 Geometry Optimized Coordinates for 4+ of **5e**

Ir	0.00485847733726	0.04898535971556	0.04922663206671
O	0.52355048121568	1.48261875103632	-1.33933250953460
C	0.51598456215550	1.18445909069962	-2.59350227867301
C	0.90541195979017	2.25670835747226	-3.55151636697477
C	1.28272544124886	3.53690077910648	-3.08330066168656
C	1.64831614065275	4.54234634010660	-3.98784128347339
C	1.65159875875390	4.30819893182199	-5.38348610656997
C	1.26805952673910	3.02573439334285	-5.84119938756781
C	0.90161512190691	2.01309019913505	-4.94411974312984
H	0.60612753715822	1.02535410544277	-5.31592796910768
H	1.25529781479935	2.82026425500423	-6.91996733030216
C	2.07730470720964	5.38751014375472	-6.35059198278053
H	3.17887415973687	5.39214355955798	-6.46823600886850
H	1.64129416304349	5.23068942493922	-7.35227774864390
H	1.78645486734341	6.39052040429819	-5.99162280034717

H	1.93561443776430	5.53151079924921	-3.60672401255722
H	1.28417135505083	3.73514500323915	-2.00546146502974
O	0.20077280281988	0.03580089466498	-3.08443759167403
Ir	-0.33826048355079	-1.49811378173327	-1.83649482793725
O	-0.85527792973474	-2.92378132509977	-0.45695887517283
C	-0.85368160782504	-2.63826201073946	0.79912306385365
O	-0.54072805947132	-1.49316073529985	1.30274689862295
C	-1.24462897876849	-3.71784643871175	1.74809130221573
C	-1.61538773470495	-4.99536208154211	1.26916209014085
C	-1.98637210547547	-6.00735056510309	2.16508155403532
C	-1.99830718305747	-5.78291117900594	3.56164318920978
C	-1.62827802139565	-4.49970235002792	4.03014336679607
C	-1.25643411246070	-3.48152948168132	3.14255187026650
H	-0.97495349217524	-2.49254880501685	3.52181095239566
H	-1.63510170868277	-4.29756576711571	5.10963886938558
C	-2.37017046561427	-6.88387734926220	4.52654318119718
H	-1.46218251905250	-7.39316694045066	4.90526327023050
H	-2.90783371659992	-6.48656617793769	5.40550652886424
H	-3.00030201401046	-7.65114278757375	4.04452461448614
H	-2.27586392011964	-6.99248357761415	1.77539970756414
H	-1.61381593060440	-5.18583958573659	0.18990851852876
O	-2.28491422717593	-0.85985062142803	-1.89894292282196
C	-2.69760775761974	0.02899520442030	-1.06268420044921
O	-1.97805236119400	0.58272226870950	-0.14747699301607
C	-4.12252749670510	0.45259401914371	-1.15955249823469
C	-4.96381900734153	-0.07892301543117	-2.16380343010622
C	-6.30259805706682	0.32586061817349	-2.25381338335370
C	-6.84760628751543	1.26653199859473	-1.34845641430641
C	-5.99618795088576	1.79380363773457	-0.34864431928445
C	-4.65592872072730	1.39691994225603	-0.25184896300343
H	-4.01009897870255	1.81657478529358	0.52783739670801
H	-6.39228295623454	2.52947262973833	0.36414290443820
C	-8.29920925571789	1.67625239202756	-1.42843324536627
H	-8.44277146851838	2.72400730332019	-1.11087262174671
H	-8.69871367811617	1.55967307280215	-2.45065125769843
H	-8.91873084825671	1.04653158277670	-0.75987407340240
H	-6.93944589271352	-0.09373758370501	-3.04402923185298
H	-4.55768273207796	-0.80687722182141	-2.87531917248286
O	1.63256387045915	-2.02790852267146	-1.64323177268232
C	2.36288521442258	-1.48215740562098	-0.73317484119144
O	1.96186893424892	-0.59274628878117	0.11011953330076
C	3.78633989348507	-1.91229535030513	-0.64734438915789
C	4.63886699310724	-1.38549528447145	0.34942460983206
C	5.97694977607808	-1.79671743778935	0.42710094243540

C	6.50907609013162	-2.73914559984809	-0.48325982520106
C	5.64588202741017	-3.26206018254632	-1.47598705643938
C	4.30719459885764	-2.85889398576498	-1.56052285467340
H	3.65244953206880	-3.27482618935354	-2.33477270310568
H	6.03220349152687	-3.99899836731761	-2.19286951147080
C	7.95829694507823	-3.15976052299659	-0.41779426764411
H	8.55740539015695	-2.61236413143730	-1.17171917980072
H	8.39906385826530	-2.94880925543064	0.57147919366143
H	8.07641766258319	-4.23655078646480	-0.63405959284291
H	6.62307126357190	-1.38021106817312	1.21139100225413
H	4.24263580929418	-0.65571719270816	1.06462179577381
N	0.32672055423115	1.39917015952453	1.72302605454726
H	1.32212679658292	1.47745999421365	1.96739007458141
H	-0.00192310270275	2.35461965864251	1.53548819204643
H	-0.15728367371009	1.08741761375969	2.57453154192794

BP-86 Geometry Optimized Coordinates for 5+ of **5e**

Ir	0.05839656459053	-0.00384142070119	0.06832493989713
O	0.57798784053161	1.41525151976121	-1.28528698767297
C	0.54214902403975	1.14313526827015	-2.54884650713010
C	0.86427725767987	2.21845080502878	-3.50620469187950
C	1.19471106882141	3.51396069507773	-3.04077555808647
C	1.49854975954850	4.53018781287018	-3.95316618001185
C	1.48465918907844	4.29152109102856	-5.34887739575401
C	1.14770593895980	2.99311053508550	-5.80080315401648
C	0.84277184820154	1.96713786895189	-4.89874161937874
H	0.58434574793364	0.96765506779334	-5.26637912014466
H	1.12332123915397	2.78672058115729	-6.87871373524382
C	1.84488840552640	5.38503901856459	-6.32385523272293
H	2.94227648071672	5.42179026918376	-6.47141194869104
H	1.38604876460270	5.21508240568240	-7.31284592336176
H	1.53434756059670	6.37700847804062	-5.95193299746906
H	1.75004692817422	5.53143872689194	-3.57973029264112
H	1.20915562039558	3.71602129883690	-1.96391535525858
O	0.26708201797315	-0.03351002479371	-3.01455350035665
Ir	-0.27428182340413	-1.52936886252811	-1.78182923255986
O	-0.76686600271273	-2.94486520512759	-0.43430238202941
C	-0.81708217752682	-2.66451386823461	0.82852775451641
O	-0.47041050251125	-1.51901042643432	1.31638605968625
C	-1.26421272683860	-3.71759001891445	1.76105977438580
C	-1.64489963628611	-4.98976463379159	1.27205128167298
C	-2.07470223870965	-5.98245488542054	2.16052729573747
C	-2.13648388719437	-5.74307989677781	3.55404917264540

C	-1.75517958073997	-4.46480755280490	4.02968824322987
C	-1.32416099606869	-3.46368916076063	3.15242275603470
H	-1.03478153937569	-2.47925483159029	3.53704607387230
H	-1.80094551882823	-4.25425705882545	5.10615029373393
C	-2.57290500085959	-6.82520714175857	4.51049923640978
H	-1.69035174490917	-7.34904136487122	4.92754214371584
H	-3.13427398568940	-6.40712111324743	5.36437504390433
H	-3.19936804976982	-7.58236867763230	4.00882604928304
H	-2.37167977976471	-6.96391940217189	1.76855302035816
H	-1.60465275901388	-5.19180771975367	0.19578736504298
O	-2.20227302400027	-0.91493055117419	-1.84757703498381
C	-2.62585188773917	-0.00501980513310	-1.03071732805434
O	-1.89968054056862	0.53053876089576	-0.10495656674048
C	-4.03049619644860	0.43847011475009	-1.15400904381180
C	-4.86058388336792	-0.09046351196792	-2.17057170834138
C	-6.18825964046056	0.33799614175595	-2.28652842148406
C	-6.73037139042513	1.29706321623554	-1.39784127485895
C	-5.88860997574438	1.81957562614516	-0.38636506121577
C	-4.55893473184164	1.40128255148632	-0.26118802334450
H	-3.92133664121178	1.81719016343970	0.52697725599419
H	-6.28474117832425	2.56827818763065	0.31202313482864
C	-8.17120554745453	1.73143267850132	-1.50785222053264
H	-8.30371265820611	2.78014703164120	-1.18960085878313
H	-8.55083651670923	1.62158851695231	-2.53811391628773
H	-8.81188981846688	1.10864616042283	-0.85285103770345
H	-6.81909871643830	-0.07645486826816	-3.08368061837808
H	-4.45708317535105	-0.83210430177665	-2.86901660893562
O	1.67427051405380	-2.07152307749659	-1.60499530253332
C	2.42189596810232	-1.51152249585866	-0.71060686547118
O	2.00330855136946	-0.63098298838780	0.13709095237569
C	3.84369580906635	-1.91502126577019	-0.64628143139284
C	4.69998961422768	-1.36883528860545	0.33823755796418
C	6.04407563904564	-1.75790289984896	0.39442180607060
C	6.57593062734852	-2.69402676480611	-0.52379763260658
C	5.70743403629006	-3.23481370602535	-1.50294896939219
C	4.36208392480870	-2.85576722212012	-1.56830009413257
H	3.70395356385575	-3.28521442651812	-2.33196537716294
H	6.09556067829133	-3.96640162488523	-2.22372000658887
C	8.03160588511136	-3.08923307957979	-0.48066029003272
H	8.60849874289725	-2.51810837456942	-1.23435371935254
H	8.48049518305778	-2.88346697002063	0.50581294670386
H	8.16582109548031	-4.15982052649766	-0.71609232878127
H	6.69585722563484	-1.32963831665986	1.16705326293646
H	4.30466756465530	-0.64442301796015	1.05906987575943

N	0.40816806240502	1.30121593553017	1.73749527046022
H	1.40786518208588	1.35028992513491	1.97349047846129
H	0.09656610523819	2.26354859979318	1.55248055707611
H	-0.08717517658872	0.98570401753055	2.58157513255484

BP-86 Geometry Optimized Coordinates for 4+ of 5f

Ir	0.07248126972724	0.01717257732207	-0.01865524984263
O	-0.25201761978458	1.11000190558902	-1.73812495079317
C	0.51799909480778	0.93595260554254	-2.76336067066456
C	0.23963135318998	1.74242956609134	-3.96989582948169
C	-0.83789732495096	2.66327063271586	-4.00421957314122
C	-1.10907321942243	3.42789407626541	-5.13845342239928
C	-0.30309986198966	3.31190203866004	-6.31773539174377
C	0.78387427297063	2.37845686384691	-6.27688332207185
C	1.03976390315938	1.62154627334937	-5.13413946462889
H	1.87883176679960	0.91590741024491	-5.13301845191240
H	1.43014434685334	2.25040746614559	-7.15099345279854
N	-0.56051046877383	4.06171291130289	-7.43832818387362
C	0.26867504465106	3.91295373052993	-8.63008414382558
H	1.32936739417997	4.16126747373385	-8.42763175044815
H	0.23251489014656	2.88095008858761	-9.03253083291851
H	-0.09675015477504	4.59576927208485	-9.41113626182863
C	-1.67966594933705	4.99816461009439	-7.45729218390999
H	-2.65174242186926	4.48502804459505	-7.31463604722789
H	-1.58405045229848	5.76925107370136	-6.66758994998303
H	-1.70513889065018	5.51090093622966	-8.43029203387115
H	-1.95359461778222	4.12378891694094	-5.11517338169970
H	-1.47225719849989	2.77321477545331	-3.11681605830633
O	1.51118440986121	0.10937477008236	-2.80976441586098
Ir	1.96098045348613	-1.05065275688517	-1.17959227835924
O	2.28114801079092	-2.14063843970630	0.52838519696748
C	1.51827091166653	-1.97670916958956	1.55925313725757
O	0.52409679474649	-1.15021757923455	1.61944037492855
C	1.80230290469859	-2.79251855159115	2.75797757252145
C	2.88336756142757	-3.70962875435973	2.77941718844999
C	3.16175070259804	-4.48390461563313	3.90507804418345
C	2.36003893232189	-4.38195303980417	5.08872368021569
C	1.26863773899749	-3.45337975146295	5.06050917393316
C	1.00573697739821	-2.68617807144824	3.92603210311791
H	0.16377361746616	-1.98402791247682	3.93447256967168
H	0.62478287059597	-3.33681454634361	5.93802332882291
N	2.62594884754081	-5.14054243569679	6.20131546542802
C	3.74634816630622	-6.07561448019030	6.20455066853374

H	4.71468086121836	-5.56081217891871	6.04513068782251
H	3.78864013514956	-6.58485037296828	7.17863702221715
H	3.64013613537045	-6.84946257133645	5.41860370100832
C	1.79453220408185	-5.01539709369480	7.39421277877663
H	2.16729820615804	-5.70327666779087	8.16751545061988
H	1.81937887191205	-3.98795222827724	7.80894020907048
H	0.73654803397536	-5.27274570406612	7.18841709643613
H	4.00862076699797	-5.17657192766153	3.87146257581219
H	3.51459537339213	-3.80883035978657	1.88850513816678
O	0.64615836772716	-2.47806233702358	-1.83826985410219
C	-0.60176440715410	-2.41493486971072	-1.50578290845136
O	-1.12291113868188	-1.49470734454653	-0.76029430266655
C	-1.49862645059806	-3.47249290908041	-2.01635985982161
C	-1.00683737021221	-4.50628649695567	-2.85279652660779
C	-1.84314157705854	-5.50812447504281	-3.34328905510843
C	-3.23864211641610	-5.53154072747811	-3.01740837955095
C	-3.72913457829170	-4.48542023838490	-2.16937610697997
C	-2.87814539716490	-3.48999091086978	-1.68957929846319
H	-3.28264234936846	-2.70170733952269	-1.04374843177030
H	-4.78663310559848	-4.45668418546656	-1.88789646165181
N	-4.06864665150275	-6.51390782230125	-3.49709940303619
C	-3.54128368189655	-7.56796563293159	-4.35780223608352
H	-2.75371627417505	-8.16012645308805	-3.85080119824380
H	-4.35807675117219	-8.25196900619741	-4.63156158357764
H	-3.10945260367322	-7.15933899524257	-5.29288729047072
C	-5.48487529180985	-6.51899539424762	-3.14488707984789
H	-5.63829320787682	-6.61882232402803	-2.05178913419783
H	-5.99484560893606	-5.59274363223028	-3.47601755783065
H	-5.97590058307209	-7.37193644522692	-3.63654795099658
H	-1.41565096624378	-6.28418471414524	-3.98588731792835
H	0.05669139041772	-4.51505798952695	-3.11894887342854
O	3.14938196516838	0.45156440793767	-0.44153598267051
C	2.63996699944880	1.37972432844792	0.30025201809312
O	1.39289537279062	1.45496693606251	0.63829222712250
C	3.54530294542271	2.43417961998738	0.80176715765134
C	3.06562497724726	3.47646458301488	1.63461463998733
C	3.91212980340999	4.47508175933233	2.11461199855379
C	5.30592764452808	4.48594834668110	1.78125378094312
C	5.78398452919619	3.43123684640362	0.93646417006350
C	4.92313285514324	2.43952099181149	0.46740568022724
H	5.31777152886223	1.64440865781828	-0.17612721295161
H	6.83967767466662	3.39281410462383	0.64927586141854
N	6.14626900987456	5.46452913009488	2.25052451794639
C	7.55913258717804	5.45946515783253	1.88528236590667

H	8.05977904242428	6.31105152592571	2.36924125068649
H	8.06629852672175	4.53137445259687	2.21541287938949
H	7.70331764844431	5.55421479981370	0.79045563582656
C	5.63222642169784	6.52825347814711	3.10740929352906
H	6.45749141041626	7.20301407207873	3.37933321413595
H	4.85175672792742	7.12855289592423	2.59877600700471
H	5.19571274009532	6.12785626889317	4.04378567117526
H	3.49392215671312	5.25861529630321	2.75425202062616
H	2.00353136469972	3.49489771260947	1.90601330906076
N	-1.58595061338532	0.96916966808497	1.02617876203288
H	-1.35178717530322	1.92064096992710	1.33617769359060
H	-2.42719444066612	1.05167893947072	0.44208177497377
H	-1.86522545447415	0.44956581323798	1.86771039412194

BP-86 Geometry Optimized Coordinates for 5+ of **5f**

Ir	0.13041939894619	0.06992792935178	0.06408947038134
O	-0.19270811077602	1.15733961896384	-1.62191799562161
C	0.54946480968049	0.96413018296562	-2.66992044054318
C	0.24205213725839	1.70364433228206	-3.89151451470186
C	-0.86052149228198	2.59827769581046	-3.94734173200819
C	-1.16202141093748	3.30368312858421	-5.10742734787710
C	-0.36736020777334	3.15191207159790	-6.29338948800036
C	0.74528844447709	2.24721169011580	-6.22808299818192
C	1.03459579076938	1.54871038741054	-5.06077748436940
H	1.89165271829198	0.86570557381254	-5.04166646850612
H	1.38304858148395	2.09790072102429	-7.10459006366108
N	-0.65848822386109	3.84013298696174	-7.43844903591535
C	0.16160432222613	3.66456522267085	-8.63548562899750
H	1.21375650413544	3.96044069904348	-8.45774783382719
H	0.15456382525100	2.61382181396729	-8.98465956369087
H	-0.23923299656035	4.29548929204427	-9.44185761703608
C	-1.79455379244393	4.75870588852048	-7.48133752887340
H	-2.75061320688270	4.23669747756570	-7.28220238156879
H	-1.68767550801037	5.57494308962529	-6.74090261645252
H	-1.85423594597211	5.21092814406426	-8.48198416055783
H	-2.02169579293947	3.98067341657369	-5.10443439468714
H	-1.48669345838514	2.73339800781993	-3.05786165946704
O	1.57554611844014	0.15854249467679	-2.67855181470342
Ir	1.99715983790349	-0.98302772695711	-1.07916452582693
O	2.33640863117691	-2.04853640564801	0.59490623752164
C	1.54620215698756	-1.93550561739965	1.62572327988304
O	0.57089446585135	-1.08047292270573	1.68406980995508
C	1.79292784502727	-2.79679092736093	2.78029130328463

C	2.86798226737281	-3.72589791674299	2.78219225445049
C	3.10930531891972	-4.55152798621005	3.87515399296460
C	2.27655453326254	-4.49563131165583	5.04288706041743
C	1.19360521557519	-3.55319071141100	5.03349456523097
C	0.96572895799724	-2.73274836584540	3.93365317735808
H	0.13040055888268	-2.02335176714739	3.95632122954028
H	0.53048550347521	-3.47122025949132	5.90007864889489
N	2.50447465918308	-5.30662495978656	6.11991530750901
C	3.61564989910728	-6.25579820263403	6.10944158667674
H	4.59118233137137	-5.74319824050859	6.00092232531481
H	3.62473644283097	-6.80948846189821	7.05946376987590
H	3.51967138625278	-6.98923782016622	5.28539569072842
C	1.64236424599659	-5.23244343316314	7.29778940251767
H	1.98533959465201	-5.96710226312277	8.04067447665540
H	1.67356971894084	-4.22926216591023	7.76598795860277
H	0.58853842400815	-5.46243427120829	7.04771352626681
H	3.94980993443237	-5.25076102042569	3.83113246269052
H	3.52131016433858	-3.79178252570503	1.90454237499575
O	0.71880449093874	-2.39868475211256	-1.72605213366257
C	-0.54830519730677	-2.33558154133436	-1.42395842257604
O	-1.05874244170894	-1.41634696488884	-0.66256080170282
C	-1.43267427696170	-3.36743293259971	-1.96347715119552
C	-0.92736044453348	-4.39548794676412	-2.80406183652993
C	-1.76058264242298	-5.38058367095823	-3.32336825707281
C	-3.16472295216066	-5.39471834449813	-3.02644445315719
C	-3.66713381389485	-4.35377473344442	-2.17513417593569
C	-2.82163341196270	-3.37397696834359	-1.66475575205874
H	-3.23484648495816	-2.59119943667924	-1.01814256406298
H	-4.73017854043651	-4.32008470904477	-1.91748038593104
N	-3.98942441232424	-6.36037892828772	-3.53397396714168
C	-3.45379310709151	-7.41126032459557	-4.39692999418509
H	-2.68577805738429	-8.01643264139229	-3.87707487958666
H	-4.27230185203639	-8.08160873627366	-4.69658133465581
H	-2.99784647374092	-6.99321533037635	-5.31530060836853
C	-5.41522633614009	-6.36005084509970	-3.21305754425722
H	-5.59010419861547	-6.47497921827872	-2.12549883390826
H	-5.90788844901587	-5.42514192466027	-3.54333851417822
H	-5.89993840494252	-7.20218867725348	-3.72821316809430
H	-1.32721475342006	-6.15246828199092	-3.96649017068718
H	0.14104492351092	-4.41203915502072	-3.04820170108986
O	3.18704454193917	0.48471887916416	-0.35630223647641
C	2.68284455163889	1.43893108649894	0.37292680966009
O	1.43410746373877	1.49313894395824	0.72299040028589
C	3.57827092387196	2.50002996818856	0.83514380694846

C	3.09610376863310	3.55991096380241	1.64870271015239
C	3.93977236869575	4.57226752043272	2.09497730655636
C	5.33184756041149	4.58293670940042	1.74547380767494
C	5.81068471851886	3.50963043720938	0.92146380240252
C	4.95512157631606	2.50285137445457	0.48537624190449
H	5.35073528586317	1.69528563697448	-0.14139076978196
H	6.86391084483934	3.47146204534387	0.62658545672166
N	6.16711296955613	5.57535916568606	2.17928894124551
C	7.57836786303772	5.57194091586213	1.80019402947749
H	8.07307585498993	6.44622314437189	2.24757240421467
H	8.09637285220653	4.66169578087252	2.15988646266853
H	7.70681169078754	5.62866245792217	0.70166652425537
C	5.65802550052928	6.65500566176430	3.02240432514080
H	6.48250962989811	7.34090983225591	3.26591816185578
H	4.86626738660001	7.23644571733174	2.51103323441022
H	5.24075451102852	6.26917428210248	3.97269826919584
H	3.52374397791657	5.36874235899673	2.71931796521883
H	2.03704054355007	3.57984508807762	1.93071052385454
N	-1.48031824083668	1.02797059572862	1.12510224046932
H	-1.19925029960956	1.95079245411695	1.48047675393711
H	-2.30923323926404	1.17551334974923	0.53539634608645
H	-1.78738182593055	0.47587444128253	1.93604469531804

BP-86 Geometry Optimized Coordinates for 5+ of **6a**

Re	-0.00740485281518	-0.01866551644015	-0.03260725569263
O	0.52145981967095	1.46786233135243	-1.34497619861494
C	0.53074924861166	1.21959517747873	-2.61390767869586
C	0.91198783805046	2.27458589879625	-3.56666439730930
C	1.27667509292605	3.55864094338223	-3.09581241371115
C	1.64122688316475	4.56652235978208	-3.99704319834087
C	1.63849667132887	4.28199209101283	-5.37545673356297
C	1.27954898699409	3.01263993044160	-5.86641865771633
C	0.91688365252601	2.01108378417024	-4.95722690428089
H	0.63544355027129	1.01818771882359	-5.32552144416163
H	1.28305714961220	2.80911236795640	-6.94291273358908
Br	2.13386625481742	5.65099059702009	-6.60905939883457
H	1.92397461877326	5.56026232972195	-3.63254180559595
H	1.27465902569353	3.76557521174021	-2.01987067964276
O	0.20549556671928	0.04246931465207	-3.04866186800528
Re	-0.31393320629237	-1.40795570312009	-1.71700712051473
O	-0.84127052011677	-2.89782793605752	-0.43514043494791
C	-0.85515614634407	-2.66656464181211	0.84028560462659
O	-0.53423012043108	-1.49805028977778	1.29128261202498

C	-1.23722296762036	-3.73846339107566	1.77366441212478
C	-1.59664799458375	-5.01562061930372	1.28054424873447
C	-1.96125417597998	-6.03918424333516	2.16394788840273
C	-1.96391170082923	-5.77734918713561	3.54684972074474
C	-1.61029723481251	-4.51522519585749	4.05980872540531
C	-1.24751141477142	-3.49794596250803	3.16835884215498
H	-0.97007377191617	-2.51039681443142	3.55351665053877
H	-1.61797461101341	-4.32947139748483	5.13948904348381
Br	-2.45946991574193	-7.16760639166084	4.75638305385895
H	-2.23993980095604	-7.02761986202284	1.78232184621817
H	-1.59050752173487	-5.20511118151785	0.20138435977004
O	-2.26458204115455	-0.84554291569365	-1.86560936594087
C	-2.73497180324783	0.04699585995173	-1.05176910400061
O	-1.96926134786861	0.57191466577125	-0.15162345161910
C	-4.14277007078035	0.46347380907744	-1.15514698032052
C	-4.97562704117607	-0.08641669917720	-2.15872533292943
C	-6.31474066978746	0.30978218080862	-2.26341785205111
C	-6.81761423044790	1.26026948283372	-1.35523094916333
C	-6.00844980093878	1.81925312936501	-0.34836669971847
C	-4.67020332917418	1.41788341308016	-0.25280943101297
H	-4.02869319722630	1.84437653814751	0.52636956738213
H	-6.41707502257083	2.55703197080816	0.35092629670533
Br	-8.64108034347237	1.80568617476756	-1.49379216456873
H	-6.95874147964234	-0.11405052858113	-3.04186807036993
H	-4.57049089525152	-0.82428943679318	-2.86013983727634
O	1.62815060832632	-2.00917046585624	-1.61839113176343
C	2.40973626738459	-1.49294944977788	-0.72229388828756
O	1.95737333380765	-0.60166440004068	0.09775343623972
C	3.81422994223492	-1.92514332311374	-0.63909351262312
C	4.66595959915037	-1.38766450039847	0.35529153026906
C	6.00210233077438	-1.79810819838788	0.44115610977659
C	6.48306721005704	-2.75055967901950	-0.47676710734192
C	5.65489707661422	-3.29752025376437	-1.47473101959164
C	4.31976544663619	-2.88187278295539	-1.55142361728386
H	3.66388508041531	-3.29932975679196	-2.32356146800350
H	6.04641792488270	-4.03708950372906	-2.18188282060736
Br	8.30240816604319	-3.31547163058077	-0.36400415365713
H	6.66067887200553	-1.38379332732219	1.21251095708392
H	4.27762014590264	-0.64819858690695	1.06442971467555
N	0.31944494286349	1.43705353209578	1.73778040360293
H	1.31075376804171	1.51584430163260	1.99979843127306
H	-0.00108721637418	2.39112445125403	1.52671652172741
H	-0.18317168922761	1.14302593650694	2.58545413452372

BP-86 Geometry Optimized Coordinates for 6+ of **6a**

Re	-0.00788418727963	-0.01705036851281	-0.03171607065558
O	0.50896322746099	1.43596930129043	-1.31779443105122
C	0.52521885267456	1.20949547043956	-2.59729456872628
C	0.90401756155127	2.25330459128206	-3.54127154072625
C	1.26934425944282	3.53803391281268	-3.06639809742858
C	1.63464025657847	4.54170208579213	-3.96850642587352
C	1.63239818494130	4.25442308367884	-5.34795558317825
C	1.27233846806528	2.98402956358038	-5.83962680046976
C	0.90828749743069	1.98383107633297	-4.93286204570960
H	0.62632239534315	0.99130661980253	-5.30145419554396
H	1.27678390103214	2.78062320766917	-6.91590921434899
Br	2.12862398993693	5.61721603122717	-6.57820495835882
H	1.91819456759225	5.53566136211443	-3.60593865125644
H	1.26713789845402	3.74713767646459	-1.99099140875669
O	0.19254779566453	0.01847408990365	-3.01385279285193
Re	-0.31524660684220	-1.40441207404333	-1.71666254436813
O	-0.82774342550336	-2.85892432988340	-0.45917020435975
C	-0.84620789752192	-2.64916210199964	0.82862287024326
O	-0.52093563974451	-1.46722681011083	1.25990934559641
C	-1.22214581903489	-3.71233265582435	1.75182554722689
C	-1.58113316039236	-4.98936673491162	1.25201826143200
C	-1.94365849307625	-6.01147693935987	2.13451233189703
C	-1.94493445404019	-5.75034366163845	3.51904183147556
C	-1.59094297513572	-4.48791365198760	4.03532828333974
C	-1.22972018782569	-3.46937171196831	3.14827966783925
H	-0.95250625740976	-2.48280658066485	3.53582036684491
H	-1.59797979198315	-4.30503412078359	5.11527093770623
Br	-2.43791295191663	-7.13764586976360	4.72294067478633
H	-2.22251397527614	-6.99958156493422	1.75281047522886
H	-1.57641681553601	-5.17806407520005	0.17280509718448
O	-2.22226568948169	-0.85210846191602	-1.85533025357971
C	-2.71616770936564	0.04369626811837	-1.04528924810406
O	-1.92815029418356	0.55771966615132	-0.14893838025434
C	-4.11074282712423	0.45461677208059	-1.14774220993326
C	-4.94109791511341	-0.10188580993641	-2.15275484466084
C	-6.27805914692556	0.29406360394637	-2.25668107402269
C	-6.78088804827113	1.24782233245797	-1.34963674118372
C	-5.97211676945165	1.81103629493455	-0.34260848768529
C	-4.63551336325156	1.41271525412534	-0.24442792167465
H	-3.99526538351225	1.84219914766574	0.53399661529624
H	-6.38218785032503	2.55016443982644	0.35404128815219
Br	-8.59833913539059	1.79061071734236	-1.48956841186086

H	-6.92253791943865	-0.13140808252209	-3.03352590974288
H	-4.53651912033314	-0.84127769944684	-2.85274729599195
O	1.58487395318905	-1.98837272278221	-1.61670325380785
C	2.38874442810143	-1.48352817114339	-0.72143355202559
O	1.91321860860324	-0.58883702696390	0.09208811959574
C	3.77855822726204	-1.91455347310891	-0.63822991800691
C	4.62926426457150	-1.37502776510001	0.35896653345395
C	5.96166753554129	-1.78999234878472	0.44416218517709
C	6.43980762320927	-2.74598389595849	-0.47396844313597
C	5.61064988245322	-3.29266356563587	-1.47333218671220
C	4.27850878182159	-2.87528748034596	-1.55272462052176
H	3.62271276805808	-3.29225141063429	-2.32506610652694
H	6.00136954787381	-4.03386073697753	-2.17886573910704
Br	8.25115790053817	-3.31455154898923	-0.35955909724098
H	6.62174425711400	-1.37761739163223	1.21495431748167
H	4.24396985679786	-0.63386737367788	1.06783586442008
N	0.30655304804527	1.43087887085806	1.70452875038902
H	1.29561603742141	1.49915177252481	1.98117552531203
H	0.00166311266926	2.38794117607744	1.48004780473915
H	-0.21251593875239	1.15130555864246	2.54830776462513

BP-86 Geometry Optimized Coordinates for 5+ of **6b**

Re	-0.00012139139335	0.00836450218837	-0.00325263458597
O	0.53006584190267	1.49517931326906	-1.31492030602018
C	0.54019126027371	1.24754998933563	-2.58425342718874
C	0.92368421784562	2.30172282668334	-3.53597435708840
C	1.28900151644030	3.58595098402920	-3.06492094613030
C	1.65627056281262	4.59238849023256	-3.96513294982380
C	1.65714175002083	4.31010842983379	-5.34518907622725
C	1.29689077779228	3.03926383762477	-5.83459472892763
C	0.93123710320765	2.03868096578730	-4.92700995932387
H	0.64942696030846	1.04595752368495	-5.29541310788692
H	1.30458178553782	2.84188736431245	-6.91220429335100
Cl	2.11580975569815	5.56396708418416	-6.47454989348597
H	1.94042632559800	5.58781630733471	-3.60638497039738
H	1.28492676343598	3.79254000288297	-1.98894570367162
O	0.21383723657650	0.07048953501138	-3.01926639543101
Re	-0.30699793328852	-1.37983852796503	-1.68794776641713
O	-0.83568580655867	-2.87003718768271	-0.40699270381081
C	-0.85011073642615	-2.63956856104029	0.86889329810069
O	-0.52823878033083	-1.47113961681740	1.32021098487740
C	-1.23357702584305	-3.71113420432274	1.80103691922945
C	-1.59333378304107	-4.98835694567689	1.30721665151116

C	-1.95932270753769	-6.01121914667962	2.18926812870919
C	-1.96447221715062	-5.75262524607900	3.57394469081596
C	-1.61001846969923	-4.48904406157054	4.08586820366153
C	-1.24564574527808	-3.47193846023255	3.19634128935901
H	-0.96805647334298	-2.48465165077245	3.58201219945938
H	-1.62099011925947	-4.31018926389760	5.16667274182488
Cl	-2.42096163833342	-7.02732398022355	4.68062995278890
H	-2.23903296104764	-7.00139960608469	1.81298203366520
H	-1.58583109962497	-5.17684265162702	0.22791714795140
O	-2.25740147651024	-0.81635749914891	-1.83693887060509
C	-2.72803818786846	0.07602423201616	-1.02257869090448
O	-1.96157373703998	0.60025037460814	-0.12224747482108
C	-4.13534185410192	0.49202897806605	-1.12490499516739
C	-4.96969709027479	-0.05815454900186	-2.12762302308688
C	-6.30843756609323	0.33651127682717	-2.22988864584871
C	-6.81411731541164	1.28665685334324	-1.32111702829315
C	-6.00110920644956	1.84549545846380	-0.31563937581161
C	-4.66316100731507	1.44613465793076	-0.22185970599741
H	-4.02072611029499	1.87289897217043	0.55637548961036
H	-6.41544788482676	2.58214815155285	0.38144588368709
Cl	-8.48633751534521	1.78311963297477	-1.44394243203800
H	-6.95815622067738	-0.08433898728338	-3.00517275607900
H	-4.56444276038764	-0.79549080494299	-2.82949542114829
O	1.63474143199339	-1.98252678363441	-1.58945261872469
C	2.41706584553808	-1.46690190887466	-0.69320875889650
O	1.96457831387484	-0.57574474570828	0.12732853384549
C	3.82106100325622	-1.89869422826539	-0.61108206311129
C	4.67443472981134	-1.36075700385708	0.38219191348053
C	6.01014391159847	-1.76981466062288	0.46565793939668
C	6.49369377861118	-2.72233576568502	-0.45261075744800
C	5.66156052712325	-3.26924137494767	-1.44894728350311
C	4.32679036847388	-2.85542470916110	-1.52390559377685
H	3.66987375355347	-3.27327462498076	-2.29491541882762
H	6.05869985004787	-4.00799499936493	-2.15378291319639
Cl	8.16199522063866	-3.23691902112821	-0.35331650029286
H	6.67450551021875	-1.35834325568197	1.23353783757359
H	4.28613343086251	-0.62155390358542	1.09158974289566
N	0.33159881845839	1.46228077327640	1.76857791391379
H	1.32231595345266	1.52937799560749	2.03592784603078
H	0.02332283448385	2.41997367427803	1.55582156930406
H	-0.17901770869478	1.17414781903712	2.61341658565419

BP-86 Geometry Optimized Coordinates for 6+ of **6b**

Re	-0.00090472903916	0.00999122248502	-0.00221545020554
O	0.51793322327882	1.46302749092192	-1.28748275916289
C	0.53516585344544	1.23703587069538	-2.56739778798448
C	0.91689244080307	2.27963560931318	-3.51033266890434
C	1.28369823380350	3.56435998874638	-3.03531516451898
C	1.65256298738715	4.56622894906816	-3.93632806199325
C	1.65378693055466	4.28065654011575	-5.31732426464469
C	1.29169279146675	3.00905633836125	-5.80769670115021
C	0.92381310117993	2.01038077965792	-4.90240332800949
H	0.64077161166195	1.01819337820513	-5.27097328526064
H	1.30032400690575	2.81173267929271	-6.88504730614566
Cl	2.11391755634108	5.52822816204392	-6.44354536289736
H	1.93812812670015	5.56171462473632	-3.57966389609244
H	1.27936454061368	3.77326328760890	-1.95991130590094
O	0.20081193632526	0.04619647301035	-2.98417777105280
Re	-0.30891343260394	-1.37633767169983	-1.68737003253588
O	-0.82300298177000	-2.83102748478532	-0.43080338860587
C	-0.84190702158803	-2.62200543254154	0.85747774647977
O	-0.51572872363129	-1.44011534043154	1.28905807683874
C	-1.21907230533258	-3.68482048656263	1.77938937209272
C	-1.57736531241937	-4.96223605994675	1.27884444427940
C	-1.94099846326527	-5.98378166987893	2.15981640401146
C	-1.94558557268045	-5.72526153180857	3.54601572512645
C	-1.59197737370149	-4.46115885294950	4.06162771313656
C	-1.22929139023828	-3.44289810422079	3.17645004166970
H	-0.95274167015727	-2.45635324493419	3.56444131601233
H	-1.60311134098336	-4.28504281788681	5.14261864691462
Cl	-2.39932522210019	-6.99719958848983	4.64728658109313
H	-2.22001774835265	-6.97387413790859	1.78354992615832
H	-1.57063123684600	-5.15007140405959	0.19953262743670
O	-2.21543335160398	-0.82251015080934	-1.82658094885285
C	-2.70942957708791	0.07327307416058	-1.01601087318069
O	-1.92055078212741	0.58660431106430	-0.11952652827863
C	-4.10342252776569	0.48365942141116	-1.11730763812935
C	-4.93534078938609	-0.07340207644439	-2.12132501359380
C	-6.27199365820078	0.32054374950504	-2.22262181255512
C	-6.77733964602275	1.27382768258674	-1.31466844309692
C	-5.96490604065161	1.83747877764622	-0.30918214609250
C	-4.62856062289536	1.44145217478915	-0.21320517087892
H	-3.98729157725313	1.87137839118671	0.56408750543333
H	-6.38075528455398	2.57536512313385	0.38528399623196
Cl	-8.44407981633868	1.76703359858298	-1.43812301699750
H	-6.92230486682673	-0.10209929010582	-2.99606981248637
H	-4.53059703455724	-0.81219070329912	-2.82180129801582

O	1.59070623657842	-1.96208114017925	-1.58760606357991
C	2.39550918344858	-1.45763771542126	-0.69243648008830
O	1.91993086039136	-0.56327098084849	0.12185949134882
C	3.78495470150408	-1.88764415967494	-0.61099138881307
C	4.63760853786277	-1.34691429351660	0.38449316915522
C	5.96984697082226	-1.75951239479090	0.46658854635344
C	6.45020726126856	-2.71546711349700	-0.45221831356569
C	5.61703032294033	-3.26313321334748	-1.44935133828710
C	4.28503293808374	-2.84834458384958	-1.52611207758898
H	3.62794972725580	-3.26623138421848	-2.29680621786418
H	6.01339776548804	-4.00342694774902	-2.15260197139528
Cl	8.11145360736783	-3.23201379058086	-0.35261128027476
H	6.63596860542033	-1.34949113510607	1.23334953973225
H	4.25233263902885	-0.60610636626944	1.09368956058727
N	0.31631278026440	1.45484257910362	1.73685723877060
H	1.30482002873708	1.51604376047674	2.01713916300019
H	0.01886497041126	2.41424608543086	1.51248405001174
H	-0.20760576736022	1.17794921447217	2.57848743680654

BP-86 Geometry Optimized Coordinates for 5+ of **6c**

Re	-0.00778375760710	-0.01776264942319	-0.03403559571874
O	0.52027503100894	1.46953129753209	-1.34666836416626
C	0.53024197832132	1.22233688522014	-2.61695941549412
C	0.91154970100021	2.27532818913843	-3.56818522241234
C	1.27757249050537	3.56073846000372	-3.09761385347169
C	1.64261589391591	4.56505957629806	-3.99925751190716
C	1.64111119918981	4.28271725672325	-5.37684516179723
C	1.28118468515193	3.01436965945169	-5.86596562451107
C	0.91724849020595	2.01282392314999	-4.96045452747750
H	0.63499293911837	1.01987043928924	-5.32759338810371
H	1.29182590666833	2.83146186612351	-6.94671595280755
F	1.98918811313256	5.23875357641869	-6.23750447149462
H	1.92966760253799	5.56544183643910	-3.65506625475472
H	1.27476777122138	3.76615296553963	-2.02152277104521
O	0.20431307151959	0.04356166626137	-3.05015869475282
Re	-0.31415531575412	-1.40648106859621	-1.71654715873370
O	-0.84079984563201	-2.89732755702480	-0.43463614309950
C	-0.85518534736264	-2.66718236542071	0.84222580243608
O	-0.53372953203880	-1.49703649097414	1.29165526753430
C	-1.23693192627369	-3.73748940729078	1.77380537039685
C	-1.59713299249198	-5.01591423863719	1.28026548524090
C	-1.96170815556864	-6.03657583953409	2.16356313097988
C	-1.96563384611117	-5.77773478338553	3.54573983695220

C	-1.61167465483596	-4.51667827185993	4.05754634812785
C	-1.24813789618756	-3.49876538805984	3.17031337084307
H	-0.97031385937647	-2.51122663595943	3.55490238969639
H	-1.62644863989119	-4.35226684390215	5.14121838150574
F	-2.31312884165856	-6.74950039848439	4.38888124544334
H	-2.24421647424720	-7.03188710610959	1.80139362639669
H	-1.59012241803947	-5.20332269710156	0.20088619171681
O	-2.26594399793671	-0.84560265994617	-1.86505444634043
C	-2.73835933374175	0.04767127185117	-1.05130335037536
O	-1.97026828541512	0.57285849309131	-0.15172384846397
C	-4.14427141298391	0.46227566060896	-1.15356276781807
C	-4.98084459568002	-0.09350399417881	-2.15291465565967
C	-6.31823155049287	0.30195892294016	-2.25408163998429
C	-6.82086641282806	1.25607797579374	-1.35158393394565
C	-6.00893992318101	1.81973678401555	-0.35131720325579
C	-4.67186093150554	1.42208444861081	-0.25469483395392
H	-4.02778097231650	1.85240840728259	0.52007001642687
H	-6.43614891668903	2.56008983433118	0.33495526882411
F	-8.09499055155529	1.63499171239319	-1.44679848054263
H	-6.98091628170954	-0.11488986832356	-3.02138254745581
H	-4.57555628622594	-0.83472746751271	-2.85048070074689
O	1.62862933349608	-2.00831685032697	-1.61926957938124
C	2.41228674187162	-1.49226295077402	-0.72316353550936
O	1.95815675753518	-0.59968263986137	0.09619799539325
C	3.81438559628668	-1.92409053048365	-0.63973017104510
C	4.66952602038806	-1.38165013901114	0.35115051257410
C	6.00325100437603	-1.79318089969603	0.43508290688680
C	6.48362103034680	-2.75027331502516	-0.47634100834334
C	5.65306762651580	-3.30091022378475	-1.46850369212477
C	4.31973542376886	-2.88710546974372	-1.54786902584004
H	3.66153665939880	-3.30771091235852	-2.31613059846541
H	6.06304772766824	-4.04410149014526	-2.16218125086397
F	7.75414281931547	-3.14480349709004	-0.39740694492515
H	6.68000128084365	-1.38682481412789	1.19570793324473
H	4.28128222667968	-0.63809463024410	1.05584970122099
N	0.32513682039527	1.43820554394856	1.74009837734256
H	1.31384580103323	1.49235790297992	2.01695730758870
H	0.03150844270334	2.39895449500409	1.52137750958659
H	-0.19801611078257	1.15844707395726	2.57985583043001

BP-86 Geometry Optimized Coordinates for 6+ of **6c**

Re	-0.00975792347074	-0.01533172918249	-0.03273670247850
O	0.50645487022679	1.43764606332833	-1.31902692057292

C	0.52348232997918	1.21171855230555	-2.60006527154807
C	0.90259341887394	2.25265254055836	-3.54242048271873
C	1.26944132377508	3.53905532379842	-3.06788067185964
C	1.63609295842454	4.53849440905601	-3.97012274822333
C	1.63546572870473	4.25135901328803	-5.34833940605278
C	1.27450232685429	2.98230820712383	-5.83916951817511
C	0.90832276669676	1.98324678342072	-4.93586687633369
H	0.62538398314125	0.99051002523705	-5.30279568525650
H	1.28700229315452	2.79970855145629	-6.91968246149622
F	1.98505903357249	5.20242685879208	-6.20685586285714
H	1.92422449167352	5.53927751964952	-3.62887645665886
H	1.26578699116157	3.74696795334400	-1.99237245625970
O	0.19001681965986	0.01871482225631	-3.01456905355665
Re	-0.31677833700540	-1.40299504092254	-1.71526201237313
O	-0.82858412459159	-2.85792517356749	-0.45782862136834
C	-0.84728864216841	-2.64891994360612	0.83161377801106
O	-0.52178470634973	-1.46516791157068	1.26126316949026
C	-1.22202953971383	-3.71046722830513	1.75253175994144
C	-1.58017693618015	-4.98935072346080	1.25177111829957
C	-1.94122731172088	-6.00909570480156	2.13343232495535
C	-1.94367764734157	-5.74982841841712	3.51702525953334
C	-1.59155137420803	-4.48847453988473	4.03374423352270
C	-1.23103185335013	-3.46922929643156	3.15108624623572
H	-0.95476240439384	-2.48227963276637	3.53802189355214
H	-1.60625435987646	-4.32782157127878	5.11770572760468
F	-2.28752428967692	-6.72025622022851	4.35602070638268
H	-2.22249702471259	-7.00462330268896	1.77171456375547
H	-1.57415422925426	-5.17563573996966	0.17228318987539
O	-2.22429629317203	-0.85200027662499	-1.85449288586573
C	-2.72036150017847	0.04529914108872	-1.04512110630807
O	-1.92998886511890	0.55959180963983	-0.14894996093727
C	-4.11214150725352	0.45486010946651	-1.14740074127036
C	-4.94556199400967	-0.10678120674645	-2.14957397536291
C	-6.28017707678301	0.28866752475067	-2.25107333241994
C	-6.78190137321435	1.24564417055381	-1.34878820681532
C	-5.97213351289470	1.81338562187631	-0.34684319208578
C	-4.63737305097324	1.41817469234757	-0.24706618392603
H	-3.99488289457777	1.85057184928309	0.52773068488027
H	-6.40172797949062	2.55462656498462	0.33655143740765
F	-8.05158796405678	1.62307639041454	-1.44563142142892
H	-6.94335799664887	-0.12855311315819	-3.01736734671848
H	-4.54031662390557	-0.84918924041087	-2.84577020187280
O	1.58361536000750	-1.98749879252866	-1.61684540919630
C	2.38974608292714	-1.48221043291163	-0.72171999276495

O	1.91251190662518	-0.58633529922927	0.09139192901670
C	3.77686888283058	-1.91216925418556	-0.63913258612106
C	4.63130471034788	-1.36718849737756	0.35446198414835
C	5.96115847440302	-1.78233138157747	0.43719901514964
C	6.43731069150432	-2.74269520517201	-0.47543457492478
C	5.60657487795375	-3.29414459207976	-1.46908609859045
C	4.27645768480467	-2.87911335920754	-1.55007368568473
H	3.61796470487262	-3.29929970586635	-2.31818655006118
H	6.01633019774177	-4.03865150919821	-2.16106492180087
F	7.70247026849350	-3.13906814123019	-0.39613461901863
H	6.64013490733906	-1.37822637585109	1.19665714782281
H	4.24597785595218	-0.62215837221006	1.05906933215680
N	0.31530248554852	1.42500703363122	1.71236995161262
H	1.30325091047013	1.47345492916375	1.99637834349207
H	0.03008115297254	2.38792487999310	1.48791448888063
H	-0.21638403440082	1.15202762184014	2.55016539523663

BP-86 Geometry Optimized Coordinates for 5+ of **6d**

Re	0.00402711211191	0.00388598295521	-0.00166035529641
O	0.60619079690899	1.65371287610896	-1.06317157174647
C	0.57008316299529	1.62443374765122	-2.35584179163198
C	1.00137476370601	2.79908539800897	-3.13320931246708
C	1.45391436929436	3.96323708323688	-2.46594174975396
C	1.86456936805404	5.07886225036543	-3.20886863669378
C	1.82761183020706	5.04257901594037	-4.61654331316326
C	1.37792939946787	3.88619975392420	-5.28351513757137
C	0.96519639267527	2.76611796881966	-4.54838080638554
H	0.61447481615484	1.86259856204566	-5.05983060114234
H	1.34972233172188	3.85905736095681	-6.37964461785803
H	2.14994995706035	5.91739932169879	-5.19504385988058
H	2.21462412465442	5.97988783890317	-2.69054186749127
H	1.47975169283360	3.98304756410426	-1.37060418681141
O	0.15362745126476	0.56004034518757	-2.96814050028351
Re	-0.43588314406560	-1.05791992461832	-1.88181034848161
O	-1.03693962606685	-2.70657466953661	-0.85042047360146
C	-1.00687940560986	-2.69444776318361	0.44585804412935
O	-0.59578368136075	-1.64094121388995	1.07310823514596
C	-1.44197288099226	-3.88223222527403	1.20107544610822
C	-1.88911396151193	-5.03577158262978	0.51212663377899
C	-2.30330574765998	-6.16373063090599	1.23421909062700
C	-2.27525778375333	-6.15039828419803	2.64249306545679
C	-1.83093548100512	-5.00462539027220	3.33102654993948
C	-1.41471727407671	-3.87240146209220	2.61676371283242

H	-1.06812438497172	-2.97697974633328	3.14490065836123
H	-1.80970186140306	-4.99530745551962	4.42761700002944
H	-2.60037765474166	-7.03483431135641	3.20458712424911
H	-2.64914705987670	-7.05648548216055	0.69904054158791
H	-1.90804347480165	-5.03793653194908	-0.58355094152981
O	-2.34648356111652	-0.35589668541109	-1.86981595038908
C	-2.73698430226589	0.41652878966363	-0.90444958571033
O	-1.91563347054342	0.73308828048629	0.04295949782177
C	-4.11682180519812	0.93262245486786	-0.88952328610992
C	-5.01470481960904	0.58759860888200	-1.92871196910512
C	-6.32625969208902	1.08240888427326	-1.91098319223526
C	-6.75081232869917	1.92100021389339	-0.86179964856026
C	-5.86037441295796	2.26573757449597	0.17382458408227
C	-4.54706522451253	1.77544468327674	0.16383487536292
H	-3.84760840971013	2.03826428873774	0.96538957963879
H	-6.19213658386984	2.91859877073225	0.99040214487442
H	-7.77791523132670	2.30681199308549	-0.85130625973249
H	-7.02055262749385	0.81449375426013	-2.71677115604938
H	-4.67649188775864	-0.06551073704057	-2.74110139509151
O	1.46201528209302	-1.79204667029751	-1.94804101406104
C	2.29906806656942	-1.48442250493902	-1.00686635288905
O	1.92575021769090	-0.71633334996604	-0.03562310153400
C	3.67436435156350	-2.01116631360342	-1.04505405473588
C	4.58903453697002	-1.68100079383516	-0.01571765583349
C	5.89645078416996	-2.18535451202439	-0.05531214555533
C	6.30021453956393	-3.01877184037407	-1.11676572034487
C	5.39305367783542	-3.34874498741912	-2.14263029001055
C	4.08366442659582	-2.84893606603976	-2.11076443555923
H	3.37148619864463	-3.10047876228916	-2.90475260458527
H	5.70864735597968	-3.99762965126151	-2.96872335157858
H	7.32415659138287	-3.41206664162653	-1.14446843625264
H	6.60375116712031	-1.92895398538160	0.74288155448134
H	4.26674384887104	-1.03194971420842	0.80628395870070
N	0.45621476019172	1.10959517991371	1.98407915415624
H	0.47018669295163	0.46985199718617	2.78910186855215
H	-0.24513017413742	1.83062312369793	2.19803381525709
H	1.36792737588082	1.58511526227723	1.97586736253960

BP-86 Geometry Optimized Coordinates for 6+ of **6d**

Re	0.00483429474726	0.00559954764583	-0.00104337919357
O	0.58969777085796	1.61919866075946	-1.04240368998708
C	0.56107500888137	1.61264031829447	-2.34180100525187
C	0.98628584885855	2.77658226860156	-3.11196978013961

C	1.43813652978697	3.94036482953758	-2.43944634818260
C	1.84652872412913	5.05374590681476	-3.18353418441994
C	1.80754294960099	5.01416174425601	-4.59168393976801
C	1.35860645802364	3.85853296846645	-5.26153798241784
C	0.94723443007296	2.73851413054565	-4.52886469445121
H	0.59713409154599	1.83533764098029	-5.04090779216868
H	1.33054460903791	3.83330165997919	-6.35722713678640
H	2.12893106737818	5.88898289258480	-5.17028393703227
H	2.19645410966595	5.95558318563884	-2.66757053912461
H	1.46519539364960	3.96130188684155	-1.34437218116293
O	0.14007301440402	0.53098392942328	-2.93820139122198
Re	-0.43486227629288	-1.05536298839250	-1.88151089440415
O	-1.01839671029218	-2.66533556430624	-0.86761904952135
C	-0.99599597394109	-2.67498604672840	0.43718668001416
O	-0.57991596178708	-1.60557181700209	1.04690743699197
C	-1.42626252271464	-3.85266542287054	1.18343920155706
C	-1.87387150963345	-5.00383477294828	0.48684356693938
C	-2.28717142492318	-6.13062667373211	1.20787768515771
C	-2.25720950144563	-6.11692023349913	2.61662006475972
C	-1.81240780177854	-4.97376066703344	3.31042757705098
C	-1.39628443811930	-3.84072728032851	2.60098586496137
H	-1.04952495375898	-2.94719651657704	3.13175226599576
H	-1.79142139137199	-4.96855167166876	4.40655469492281
H	-2.58242569991227	-7.00211508759291	3.17702005896316
H	-2.63388093640927	-7.02272887354290	0.67317295546672
H	-1.89392287802356	-5.00482082015341	-0.60860786487551
O	-2.30254189542460	-0.36782316081377	-1.86277493696283
C	-2.71644526088625	0.40939450457742	-0.89979929428665
O	-1.87420227501934	0.71445042254000	0.04154712092679
C	-4.08328537141684	0.91988245451845	-0.88548750653489
C	-4.97732491627949	0.57243677297801	-1.92980227783357
C	-6.28671072775794	1.06806610785325	-1.91164221868527
C	-6.70949632264891	1.90613360102224	-0.86064957609363
C	-5.82240526044628	2.25176986928179	0.17839106642443
C	-4.51053176614063	1.76281414659585	0.17161825387254
H	-3.81313379647557	2.02558698649815	0.97468629660994
H	-6.15685146870120	2.90399341736125	0.99373034373255
H	-7.73623296777112	2.29231535372983	-0.85129644034207
H	-6.98116921302856	0.80227835227715	-2.71733363739565
H	-4.63922640898281	-0.07986996149388	-2.74260862229960
O	1.42268263540395	-1.76882353451896	-1.94185190680284
C	2.28036948558064	-1.47367154024449	-1.00385445952724
O	1.88425945532714	-0.69972467321268	-0.03802712944926
C	3.64089249406696	-1.99958805927932	-1.04061795049180

C	4.55355788612053	-1.66890886821802	-0.00700766794474
C	5.85682756497599	-2.17890569819430	-0.04697770380438
C	6.25517801568384	-3.01486055877447	-1.10929657993593
C	5.34961320736178	-3.34389327693567	-2.13757850484060
C	4.04339992125966	-2.84047561173102	-2.10903190044112
H	3.33169237745351	-3.09041195010489	-2.90367052608032
H	5.66502786360676	-3.99459498588001	-2.96166608472825
H	7.27729581255078	-3.41234711388548	-1.13577423274621
H	6.56566912598277	-1.92609044147598	0.75032794572447
H	4.23421760565122	-1.01826994621342	0.81462559062264
N	0.46071176192474	1.10142157920301	1.95134464622455
H	0.51275477046963	0.46012145220640	2.75459919598803
H	-0.26076252377699	1.79830368920195	2.18180466987818
H	1.35606936110028	1.60774257713817	1.92344458455155

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Re	-0.01328168457805	-0.01782041439379	-0.03405411846604
O	0.51696849925266	1.47102298032143	-1.34425753748224
C	0.52867813964789	1.22634412294782	-2.61539018444034
C	0.91422466173028	2.27993448766663	-3.56486370948660
C	1.28335972645070	3.56452360916636	-3.09622242919230
C	1.65013715512066	4.56407879212475	-4.00371760680064
C	1.66313295719111	4.32026293556174	-5.39872797874348
C	1.28797096017501	3.03378644249735	-5.85449345585198
C	0.91946209977631	2.02444750986486	-4.95715060598763
H	0.63101306338383	1.03404752165381	-5.32760538138773
H	1.28400250885632	2.82383648557269	-6.93203762298345
C	2.09051809522864	5.39574264142143	-6.36711020614230
H	3.19453161798224	5.41749934300901	-6.45632516079438
H	1.68175644328171	5.21958242338445	-7.37667188654243
H	1.77426117369197	6.39670883459910	-6.02465508727950
H	1.93113854630209	5.55639270972259	-3.62730721269667
H	1.27782149212899	3.76998425432777	-2.01971851483531
O	0.20152100693631	0.04786150030058	-3.04983914419275
Re	-0.31883464720674	-1.40346150512462	-1.71861967436143
O	-0.84755148142867	-2.89553129346489	-0.43924839849462
C	-0.86417628300329	-2.66774651902866	0.83847147473788
O	-0.54128682042987	-1.49781475583707	1.28881960165598
C	-1.24889887005074	-3.73840145823637	1.76893623923708
C	-1.61112567797877	-5.01619242392185	1.27887836108032
C	-1.98021614382623	-6.03093383883095	2.16968262055679
C	-1.99889030572487	-5.80951953208475	3.56746640209073
C	-1.63721015956509	-4.52606000937598	4.04481869505437

C	-1.26650130394158	-3.50299619946536	3.16539574436880
H	-0.99129350162596	-2.51477806075127	3.55134501597358
H	-1.65005442173520	-4.32941850293727	5.12485728394486
C	-2.36968408857491	-6.91455294050249	4.52587327491797
H	-1.45837516751729	-7.40875018781705	4.91638266480384
H	-2.92394044472594	-6.52387722399323	5.39726613948102
H	-2.98106259069661	-7.69057648538618	4.03448704940397
H	-2.26299971132944	-7.01615740971554	1.77648880301343
H	-1.60432042615024	-5.20426102876272	0.19918560772885
O	-2.27009505618312	-0.84166556798453	-1.86809604045019
C	-2.74412220914961	0.04999522875594	-1.05279994010416
O	-1.97553999812123	0.57320785827287	-0.15193530860495
C	-4.15088299681835	0.46342179617147	-1.15379170103514
C	-4.98703263920938	-0.08010485673461	-2.15859999894326
C	-6.32454481768216	0.32172178324226	-2.25205035399744
C	-6.87151338477212	1.26817148313537	-1.35252684799147
C	-6.02415766597857	1.80569199551890	-0.35336131815489
C	-4.68473742306117	1.41416060057172	-0.25019145143312
H	-4.04251092154859	1.84106597597579	0.52859408717106
H	-6.42430986723316	2.54489541323565	0.35281151371903
C	-8.32250270323242	1.67368411283551	-1.43800996803090
H	-8.47013660086900	2.71997909220012	-1.11840263972303
H	-8.71763006403756	1.55555395692078	-2.46150677742317
H	-8.93981053553644	1.03943677530140	-0.77165122445842
H	-6.95993840405686	-0.10374054319250	-3.03972717554571
H	-4.57954797716370	-0.81202718368803	-2.86532094526500
O	1.62343815993903	-2.00554840364451	-1.62120338793376
C	2.40822247232082	-1.49045251192522	-0.72484913413924
O	1.95222110396784	-0.60000603475409	0.09647603221387
C	3.81184335225809	-1.91915409685639	-0.64512025174163
C	4.66916093332809	-1.38312648900659	0.34485629524639
C	6.00490616916363	-1.79769543018213	0.41661539769949
C	6.52731662327269	-2.75027851772695	-0.48969644675516
C	5.65817708174387	-3.28069432098327	-1.47492725482736
C	4.32188152004708	-2.87628681888802	-1.55671166566266
H	3.66316074692456	-3.29697841137730	-2.32507975836544
H	6.03999647047355	-4.02371611620639	-2.18733765717147
C	7.97211271109000	-3.18132877416982	-0.42650806546609
H	8.54382482403693	-2.74800508651778	-1.27000818823787
H	8.45420587729017	-2.85432041770466	0.50995284742171
H	8.06614427952168	-4.27936658068286	-0.50761757643861
H	6.65784966784833	-1.37657830902560	1.19216819609814
H	4.28075562773141	-0.64580830952586	1.05665190441187
N	0.31498663094084	1.44500501188366	1.73685867053858

H	1.29358189734794	1.46010788413476	2.05158663997077
H	0.07242676370253	2.41377574874820	1.49244868195880
H	-0.25290748534275	1.20113197936024	2.55845292956290

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Re	-0.01789671937846	-0.01454226333689	-0.03234619500694
O	0.50163597134124	1.43990262186150	-1.31602567777551
C	0.52063438381809	1.21625405533067	-2.59776340652199
C	0.90470412902815	2.25737546187124	-3.53859087220631
C	1.27552175699885	3.54271311867504	-3.06643493020274
C	1.64475715191983	4.53689307286243	-3.97520908531758
C	1.65857158085892	4.28756140628819	-5.37062136303984
C	1.28141449767597	3.00069209017982	-5.82756799308715
C	0.90994161051193	1.99424797317109	-4.93183524469704
H	0.62047741950351	1.00404794167181	-5.30153428162915
H	1.27917469095253	2.79043239014010	-6.90458824213003
C	2.08941692838867	5.35862651819833	-6.33875633131239
H	3.19408099733379	5.37274993626314	-6.42281767900118
H	1.68335165137064	5.18145666232102	-7.34885418856497
H	1.77846092065920	6.36099101613122	-5.99633089376864
H	1.92751647791324	5.52944320698068	-3.60212967016265
H	1.26953793488008	3.75098029348796	-1.99064247519584
O	0.18554699516706	0.02369264282442	-3.01374979430940
Re	-0.32451164639264	-1.39882796109143	-1.71690172796073
O	-0.83914099048113	-2.85499787684454	-0.46231379189243
C	-0.85914607754053	-2.64858347147420	0.82807123050003
O	-0.53296774301389	-1.46489212250479	1.25865256427653
C	-1.23458223670067	-3.71115443720554	1.74807532246095
C	-1.59426311046033	-4.98941763212297	1.25074704754201
C	-1.95740869170370	-6.00422972261855	2.14031135914869
C	-1.97234466910943	-5.78302929888362	3.53945050889454
C	-1.61286193907731	-4.49926795913317	4.02172713341579
C	-1.24761084680378	-3.47384750131900	3.14658869668299
H	-0.97384854103793	-2.48629560136783	3.53477532608324
H	-1.62378543080188	-4.30690272216927	5.10208314974292
C	-2.33721929641551	-6.88909501763049	4.49531686878747
H	-1.42011842134067	-7.37445595123962	4.88364418910977
H	-2.89149230996081	-6.50108057048252	5.36759883624733
H	-2.94191471693189	-7.66931520986231	4.00311200344543
H	-2.23859986734886	-6.98953882110441	1.74751942266921
H	-1.58977418789448	-5.17581256473956	0.17091929136334
O	-2.23110857164434	-0.84578451376587	-1.85800880363159
C	-2.72832800527582	0.05032047051055	-1.04723791124592

O	-1.93760614572177	0.56246651160928	-0.14969229892081
C	-4.12087175939810	0.45908803753295	-1.14858690700554
C	-4.95398258742560	-0.09150683892321	-2.15532706270261
C	-6.28900816121485	0.31039101266525	-2.24927922241543
C	-6.83467876019443	1.26069399635594	-1.35105489490471
C	-5.98937179016871	1.80334006861743	-0.35097081307212
C	-4.65197038352979	1.41425342158265	-0.24444744291844
H	-4.01118558061429	1.84374460878555	0.53386695992102
H	-6.39163776781371	2.54409148127832	0.35163948441706
C	-8.28337838479947	1.66542013395309	-1.43874155767770
H	-8.43129191031904	2.71171994079651	-1.12023809388359
H	-8.67872709489310	1.54144438691278	-2.46110724221849
H	-8.89634617717378	1.03075753501082	-0.76858152871725
H	-6.92488779533155	-0.11644426521953	-3.03517062632501
H	-4.54672964466471	-0.82559805559956	-2.85967634261936
O	1.57519507285427	-1.98471213792674	-1.61781596681194
C	2.38249632963903	-1.48010884057828	-0.72265295461775
O	1.90349446876845	-0.58636723213658	0.09246776314607
C	3.77131951673924	-1.90646577581122	-0.64404949580061
C	4.62800187839422	-1.36619856349860	0.34753658574829
C	5.96052471534711	-1.78322956813215	0.41765626008679
C	6.47880001089127	-2.73955101670323	-0.48924357259227
C	5.60943865406214	-3.27239638322513	-1.47475841231335
C	4.27562115405490	-2.86788255037608	-1.55782781413406
H	3.61654147476181	-3.28921869736590	-2.32529876479770
H	5.99110561473140	-4.01690945895658	-2.18497725246917
C	7.92070915566428	-3.17230575391750	-0.42654677404456
H	8.48829734390942	-2.73877584577770	-1.27282003676578
H	8.40488919947000	-2.84531269702549	0.50837894537177
H	8.01141520073338	-4.27022136362989	-0.51075576220456
H	6.61565152751495	-1.36284566747097	1.19110192533148
H	4.24226075214450	-0.62693040585072	1.05850029627618
N	0.29984033189671	1.43034148382207	1.71249747998920
H	1.26927166797189	1.41392671964268	2.05684936689073
H	0.09738750564481	2.40534262979034	1.45360043709396
H	-0.30132213093844	1.20998020989674	2.51797412395019

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Re	0.14990755923954	-0.02811816669428	-0.06622624081858
O	-0.24795062545449	1.10976314803927	-1.72878939461774
C	0.49222286715236	0.97543475192185	-2.79027321086916
C	0.22188515569201	1.76592868611478	-3.98253088374303
C	-0.85028673447292	2.69801019357459	-4.01564537774626

C	-1.11703517934520	3.45464713755780	-5.15225004191644
C	-0.31789561039143	3.31843404475820	-6.33658920075998
C	0.76592765686689	2.37833786761415	-6.29337437587092
C	1.02099113285797	1.62868089508785	-5.14956268311122
H	1.85548511518884	0.91756092696941	-5.14744401219857
H	1.40828079603239	2.24139721742483	-7.16869100361331
N	-0.57780334147574	4.05416760458473	-7.46054750199078
C	0.26054041400483	3.90944058027896	-8.64863925923162
H	1.31371151021859	4.18557812127939	-8.44467217233819
H	0.24657491467023	2.87138920525258	-9.03372315057593
H	-0.11942879078590	4.57169849233105	-9.43997979150933
C	-1.67916852262022	5.01434853385801	-7.47848018721843
H	-2.65016380926324	4.52543752582507	-7.26906084371823
H	-1.53369238220530	5.82156432503844	-6.73377126110747
H	-1.73847956671813	5.47570250513040	-8.47512397084066
H	-1.95210470798028	4.16144681659984	-5.13083158040138
H	-1.47979553810722	2.82259291762336	-3.12664008989876
O	1.47979124278364	0.12328323826658	-2.77711086567293
Re	1.83533566162114	-0.98213892785190	-1.10396331450638
O	2.25049624984292	-2.12193784606423	0.53136999966551
C	1.51649865619536	-2.00250219170058	1.60333143844025
O	0.52807785732272	-1.15714953278849	1.60889884372498
C	1.80543536786697	-2.80894256062681	2.78064000799902
C	2.89027587459030	-3.72674271126646	2.79022426227642
C	3.17560831382522	-4.49917186271321	3.91153656501914
C	2.38077425044358	-4.39742578592506	5.10223442288236
C	1.28650231381782	-3.46873147256683	5.08425409857549
C	1.01386017629468	-2.70188491151809	3.95585203621850
H	0.17107959443408	-2.00078355834071	3.97286434313182
H	0.65005717007824	-3.35417110386355	5.96707051887769
N	2.65490410328142	-5.15382784943424	6.20892901298197
C	3.77887564288686	-6.08741516008868	6.20638410764221
H	4.74414706600630	-5.56742531794512	6.04896040275929
H	3.82238326416119	-6.60122716599955	7.17767937598472
H	3.67061266132202	-6.85596933038784	5.41656050147728
C	1.83553248326817	-5.02810039464089	7.41229186258613
H	2.21586557028058	-5.71733586715984	8.18030317399918
H	1.86854692477432	-4.00088235975362	7.82540992071195
H	0.77642344894705	-5.28454654756164	7.21496970956589
H	4.02240137646594	-5.19120972121942	3.87239590200506
H	3.51616049718713	-3.82605745343834	1.89548673192808
O	0.61777054455104	-2.44904370832375	-1.81739395471661
C	-0.65171888367134	-2.43727675854736	-1.51660751577458
O	-1.11965249388478	-1.48666894306510	-0.76212275607370

C	-1.53168898769179	-3.48050141052989	-2.02355603480848
C	-1.03181734660700	-4.51432047265234	-2.86061182742781
C	-1.86480125102507	-5.51416222437678	-3.35194847796932
C	-3.26292704523671	-5.53859673892752	-3.02854602947458
C	-3.75971895512311	-4.49226777817222	-2.18085317176087
C	-2.91498524037532	-3.49731107481549	-1.69862079403055
H	-3.32396533361356	-2.71035540644419	-1.05390429205469
H	-4.81812044715520	-4.46616029476794	-1.90360878944102
N	-4.08740830296323	-6.51928469719683	-3.50863603605614
C	-3.55817665854168	-7.57290776923028	-4.37178159623812
H	-2.77088625992193	-8.16286071965644	-3.86322256428274
H	-4.37444039252314	-8.25705770910349	-4.64555663600484
H	-3.12840835982983	-7.16014710999948	-5.30526713443409
C	-5.50682214068472	-6.52800121856478	-3.16175345567020
H	-5.66082952113947	-6.62543280626626	-2.06923299134109
H	-6.01611428971089	-5.60430916271120	-3.49905969735918
H	-5.99208028364928	-7.38431958211146	-3.65264625955659
H	-1.43576882129356	-6.28975160002526	-3.99361954082587
H	0.03228585737618	-4.52302793002846	-3.12472537888384
O	3.11414698762021	0.45291598261437	-0.42842524625896
C	2.66164545414329	1.41470683246838	0.32774769925127
O	1.39922189047800	1.44088504513913	0.64023969649353
C	3.56226144146897	2.44865063561030	0.81734157507967
C	3.08754577368897	3.49616229434513	1.65195428471957
C	3.94079184991086	4.48766704250450	2.12539289574781
C	5.33517068136216	4.48907911495456	1.78523202621459
C	5.80644167742782	3.42884153262189	0.94022742977466
C	4.94168236455922	2.44267040542849	0.47603787883127
H	5.33146556052856	1.64463967217521	-0.16694580563790
H	6.86105987342381	3.38459161979743	0.65108788078045
N	6.17996639878857	5.46115192761805	2.24720860678609
C	7.59375255734856	5.44820486490116	1.87843147302779
H	8.09681641783477	6.30402812646692	2.35159072826392
H	8.09711760058498	4.52230819247564	2.21867547671157
H	7.73188043233188	5.53110190559322	0.78261685613367
C	5.67790261558716	6.52871538846037	3.10948874670064
H	6.50910576653019	7.19854113754373	3.37431922475757
H	4.89776805835030	7.13140250598594	2.60467075604447
H	5.24800536420536	6.12809610216916	4.04810621650379
H	3.53073998650648	5.27489912208197	2.76530914161095
H	2.02679151637180	3.52257472276166	1.92811884414469
N	-1.63574918257187	0.98076617199020	1.04715271857350
H	-1.41937338125693	1.94444624478841	1.33155132777597
H	-2.48334117662035	1.03062285482203	0.46801667731724

H -1.89491945668973 0.47337806461687 1.90253518065956

BP-86 Geometry Optimized Coordinates for 6+ of **6f**

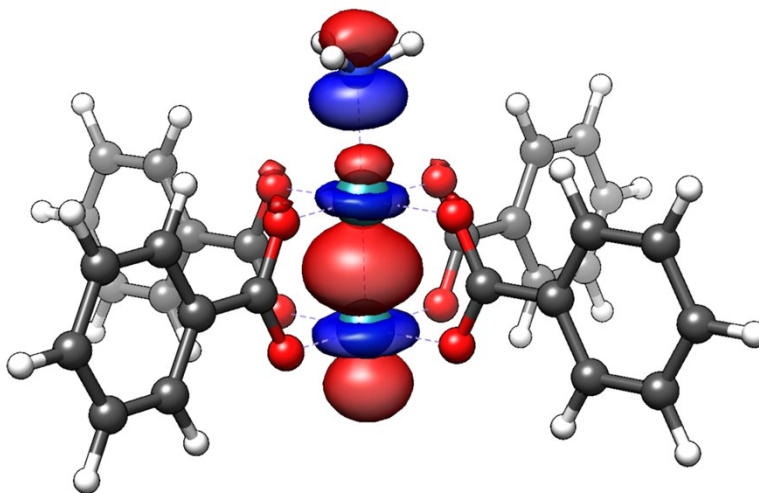
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C	0.48282788070272	0.96726599652937	-2.77465884085940
C	0.21979943398538	1.74947572336450	-3.95285326833594
C	-0.85593208437667	2.68340504045131	-3.98555822203041
C	-1.11612086553665	3.43899910245035	-5.11938454073746
C	-0.30812435367103	3.30451942268816	-6.30126587303850
C	0.77618204995506	2.36103255889676	-6.25829983100434
C	1.02698771489911	1.61051257948167	-5.11899255061944
H	1.86031291216879	0.89839430782538	-5.11571512082342
H	1.41941786793883	2.22507891895067	-7.13267060600330
N	-0.55989231898116	4.04233542807565	-7.41898499968828
C	0.27959040985912	3.89745072558422	-8.60890642753936
H	1.33576858813035	4.14720187083832	-8.39326729733137
H	0.24154624843694	2.86642579339224	-9.00910584650885
H	-0.08252950762945	4.58234978572971	-9.38852485647256
C	-1.67135562275917	4.99385828024506	-7.44711554585705
H	-2.63997479042655	4.49117879199817	-7.26452559788767
H	-1.54470379471062	5.78939789761113	-6.68827937419313
H	-1.71297449995641	5.46811864811577	-8.43808955318251
H	-1.95128033497041	4.14521823804659	-5.10208902581002
H	-1.48928435247809	2.80636344430341	-3.09930447602561
O	1.47297271439513	0.10105818416808	-2.73926432095452
Re	1.82333818975142	-0.97939858546645	-1.10525017736438
O	2.23017112549365	-2.08887998881876	0.49497198474889
C	1.50500582880354	-1.98400614285716	1.58834994234465
O	0.51292969524510	-1.12951306792385	1.57068211595479
C	1.79588046054998	-2.77862032643299	2.75166209041638
C	2.88602885144834	-3.69632873137222	2.75579735381583
C	3.17399965584549	-4.46388912408909	3.87476839802579
C	2.38017263673379	-4.36009920616876	5.06912546219355
C	1.28128990162412	-3.43258002552420	5.05517924156270
C	1.00354582643633	-2.66900074268503	3.93088224679325
H	0.15950024252875	-1.96983651868975	3.95014820368673
H	0.64823115270915	-3.31929122415079	5.94011719522115
N	2.65827291554386	-5.11102109252854	6.17168784556767
C	3.78495612408343	-6.04474294140268	6.16934203311960
H	4.74497562045965	-5.52216202248026	5.99620560484251
H	3.83817196652514	-6.54524344309880	7.14656082167728
H	3.66721152555201	-6.82132393584506	5.38980538545880

C	1.83759474710383	-4.99312055430309	7.37756542334817
H	2.22202953259694	-5.68345771316743	8.14192168390039
H	1.86867154184054	-3.96708131540672	7.79139530677507
H	0.78124931822483	-5.25419574123894	7.17639933445987
H	4.02078794492657	-5.15533453850293	3.83518802702044
H	3.50925744106713	-3.79635300888102	1.85956870365618
O	0.63264486571047	-2.41350872104301	-1.79862510782806
C	-0.65080084060278	-2.42324551741662	-1.50652284817025
O	-1.10058690038621	-1.45602628646966	-0.74700729823416
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C	-3.74241956409236	-4.46818047264430	-2.16454320850958
C	-2.90438634327858	-3.47336181933965	-1.68211794469398
H	-3.31666474958357	-2.68693126414663	-1.03926519721122
H	-4.80134414728333	-4.44520037060410	-1.89040568718992
N	-4.05748522009384	-6.49304817459090	-3.49238116597984
C	-3.52568975890388	-7.54973743468728	-4.35380341819431
H	-2.74375529524853	-8.13940072312879	-3.83847082590927
H	-4.34274431320790	-8.23071454321531	-4.63122418613450
H	-3.09132539738385	-7.13496920042829	-5.28319817548752
C	-5.48006810098875	-6.50657390586014	-3.14967148251522
H	-5.63378683768106	-6.61105672494926	-2.05862397056582
H	-5.98631357628277	-5.58141821029105	-3.48441734830462
H	-5.96086940282632	-7.36071189561172	-3.64768866375524
H	-1.40719801531271	-6.26726480712180	-3.97229049246135
H	0.05581198469359	-4.50059060766736	-3.10469696049957
O	3.07039879531025	0.42447078041647	-0.44569219321041
C	2.63729911111938	1.40330217521535	0.31970417765732
O	1.36287277213506	1.41050575703462	0.62176979088515
C	3.53080994584934	2.42143619256799	0.80382911372067
C	3.05621801638144	3.47154634292264	1.64196809400662
C	3.91268509569385	4.45466534434934	2.11519761104466
C	5.30958959587148	4.44808558049037	1.77398966861160
C	5.77879667735497	3.38647941464229	0.92517391127432
C	4.91355040812779	2.40714923082848	0.45974158458561
H	5.30027903326013	1.60894909186926	-0.18446526596522
H	6.83307910173064	3.33941640388099	0.63693982969600
N	6.15574447408592	5.41064866959344	2.23694712674135
C	7.57226817513804	5.39314970066177	1.87013909490241
H	8.07633595797491	6.24628553969257	2.34600217137778
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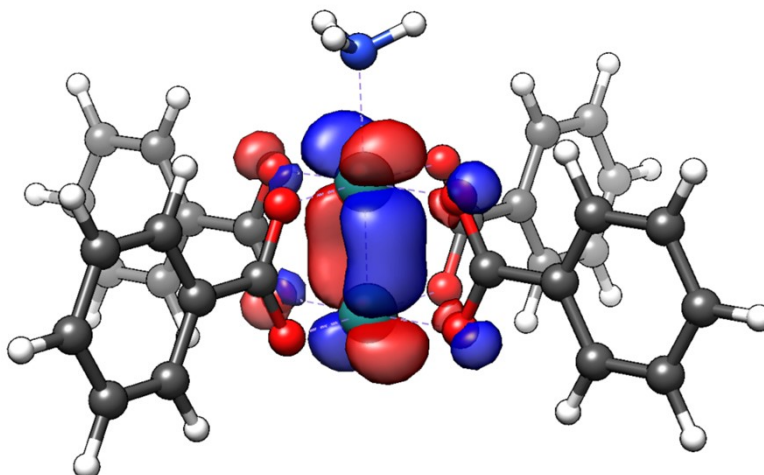
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H	4.88767864905084	7.08951364947991	2.59755647919194
H	5.22744727841648	6.07703779422197	4.03854934556154
H	3.50761859598727	5.24320515548725	2.75604976162518
H	1.99588612348010	3.50285914245142	1.91831949049927
N	-1.62906936087531	0.97038780956166	1.01997807580821
H	-1.40591934983839	1.92707765763029	1.32463287766497
H	-2.46535395486283	1.04073120577692	0.42565779736972
H	-1.91167850425663	0.45265758272670	1.86245107726960

Representative Molecular Orbital 3d Diagrams (2d)

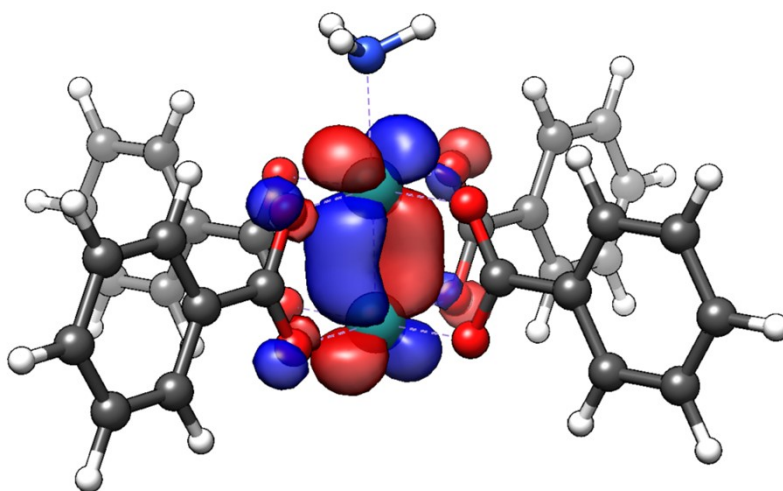
σ



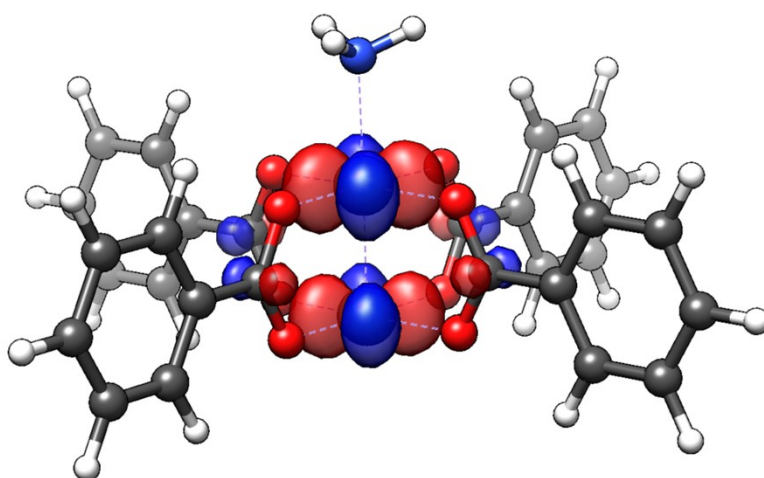
$\pi 1$



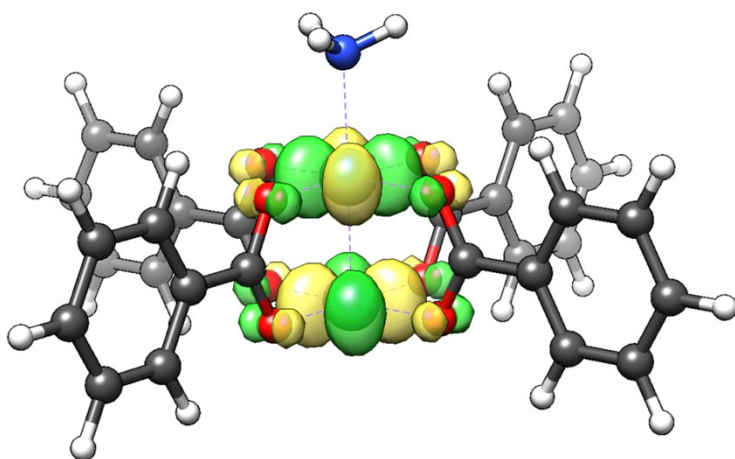
$\pi 2$



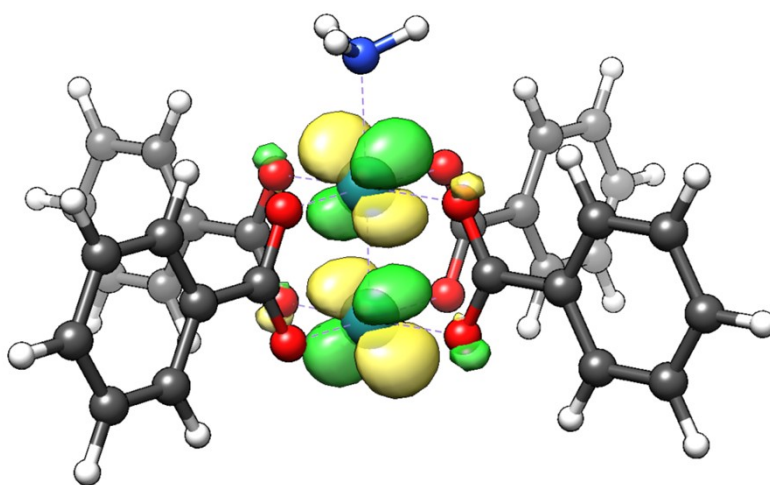
δ



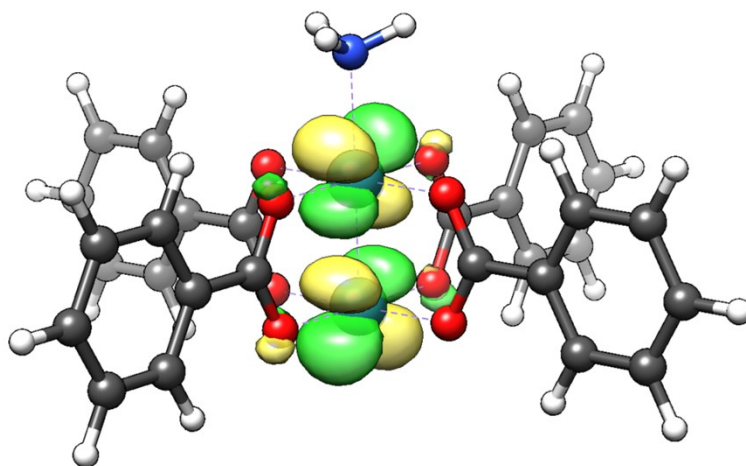
δ^*



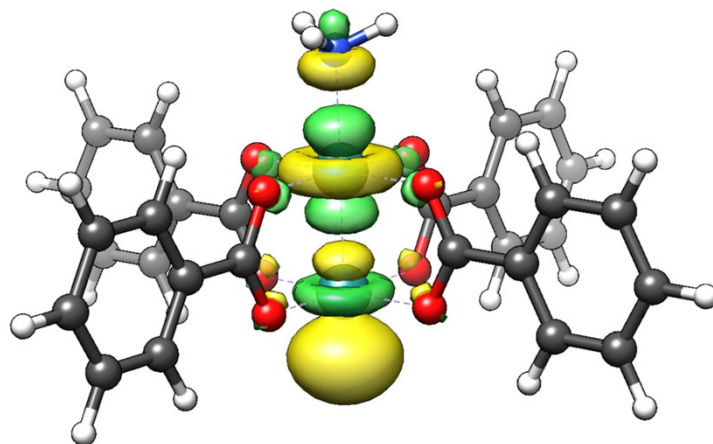
$\pi^* 1$



$\pi^* 2$

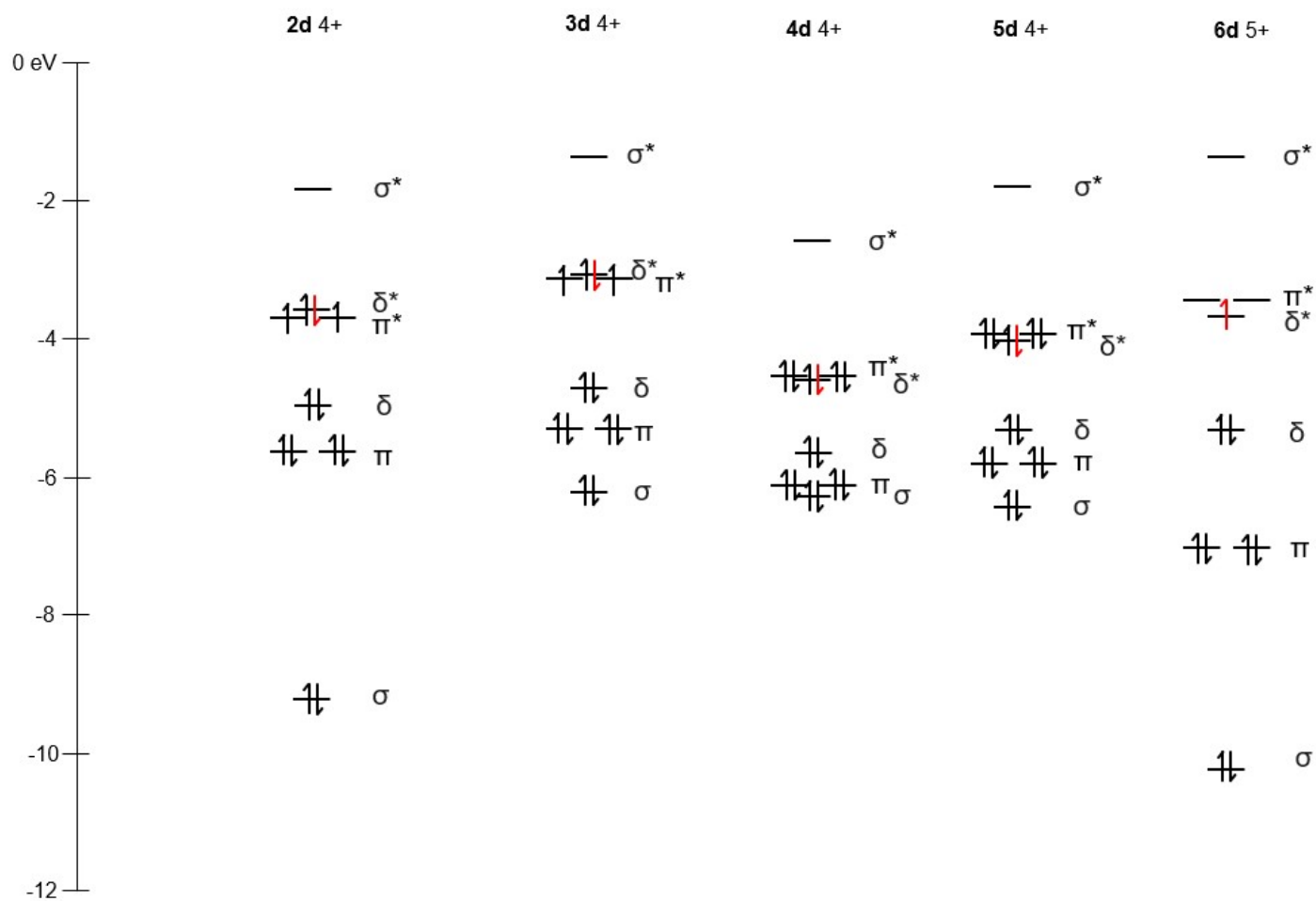


σ^*



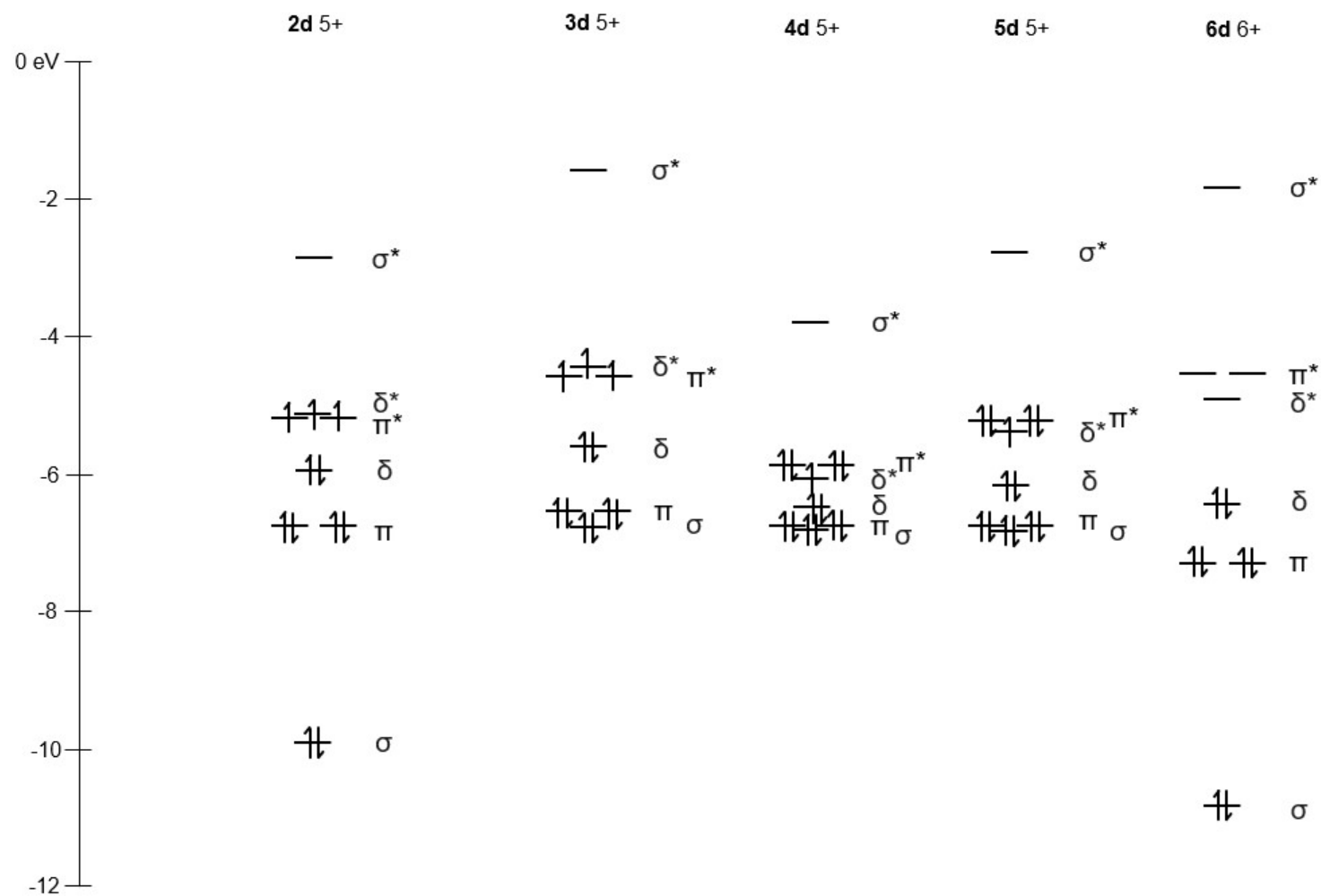
Quasi-Restricted Orbitals: Molecular Orbital Diagrams and Orbital Energy Level Tables of Benzoates

Reduced Species



	2a 4+	3a 4+	4a 4+	5a 4+	6a 5+
σ Energy	-9.204 eV	-6.220 eV	-6.276 eV	-6.421 eV	-10.209 eV
π 1 Energy	-5.617 eV	-5.297 eV	-6.100 eV	-5.780 eV	-7.032 eV
π 2 Energy	-5.617 eV	-5.296 eV	-6.100 eV	-5.779 eV	-7.030 eV
δ Energy	-4.968 eV	-4.720 eV	-5.655 eV	-5.330 eV	-5.319 eV
σ^* Energy	-3.569 eV	-3.043 eV	-4.582 eV	-4.003 eV	-3.659 eV
π^* 1 Energy	-3.688 eV	-3.112 eV	-4.524 eV	-3.920 eV	-3.424 eV
π^* 2 Energy	-3.688 eV	-3.112 eV	-4.523 eV	-3.920 eV	-3.423 eV
δ^* Energy	-1.850 eV	-1.368 eV	-2.584 eV	-1.792 eV	-1.353 eV

Oxidized Species



	2a 5+	3a 5+	4a 5+	5a 5+	6a 6+
σ Energy	-9.935 eV	-6.788 eV	-6.806 eV	-6.800 eV	-10.851 eV
π 1 Energy	-6.796 eV	-6.555 eV	-6.804 eV	-6.798 eV	-7.313 eV
π 2 Energy	-6.793 eV	-6.555 eV	-6.801 eV	-6.794 eV	-7.312 eV
δ Energy	-5.956 eV	-5.640 eV	-6.510 eV	-6.218 eV	-6.441 eV
σ^* Energy	-5.233 eV	-4.597 eV	-6.086 eV	-5.409 eV	-4.912 eV
π^* 1 Energy	-5.148 eV	-4.446 eV	-5.907 eV	-5.223 eV	-4.565 eV
π^* 2 Energy	-5.148 eV	-4.446 eV	-5.907 eV	-5.223 eV	-4.564 eV
δ^* Energy	-2.853 eV	-1.599 eV	-3.824 eV	-2.790 eV	-1.830 eV