Supporting information

Optimized Coordinates of **A-H**

A

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.191096	-1.961088	-1.454745
2	6	0	-0.193868	-1.988660	1.406127
3	1	0	0.280843	-1.594536	-2.377740
4	1	0	0.384692	-2.824699	-1.099106
5	1	0	0.084466	-1.598845	2.396188
6	1	0	0.544148	-2.747009	1.122821
7	77	0	-0.442148	-0.438289	-0.008445
8	1	0	-1.155144	-2.509569	1.513141
9	1	0	-1.185581	-2.341521	-1.723996
10	15	0	1.816614	-0.089930	0.000124
11	6	0	-2.707955	-0.241876	-0.012160
12	6	0	-2.253918	0.456464	1.173058
13	6	0	-2.253116	0.516472	-1.160958
14	6	0	-1.480491	1.579397	0.763132
15	6	0	-1.482937	1.617854	-0.692419
16	6	0	-0.928684	2.736003	-1.530068
17	1	0	-1.648508	3.562776	-1.619305
18	1	0	-0.014561	3.157068	-1.097551
19	1	0	-0.691265	2.403134	-2.545355
20	6	0	-0.932158	2.653964	1.660828
21	1	0	-1.685227	3.430816	1.858825
22	1	0	-0.614916	2.253860	2.629036
23	1	0	-0.067988	3.154846	1.212880
24	6	0	-2.610816	0.092996	2.585482
25	1	0	-3.613510	0.461568	2.843295
26	1	0	-2.609581	-0.990821	2.736114
27	1	0	-1.906290	0.525273	3.302567
28	6	0	-3.678882	-1.387500	-0.041508
29	1	0	-4.721460	-1.037515	-0.031236
30	1	0	-3.548656	-1.999347	-0.940054
31	1	0	-3.547122	-2.045831	0.823409
32	6	0	-2.616992	0.227461	-2.588934
33	1	0	-3.620032	0.611370	-2.822303
34	1	0	-1.914994	0.693216	-3.287143
35	1	0	-2.621832	-0.847029	-2.795344
36	6	0	2.407501	0.781347	-1.551035
37	6	0	3.708871	1.596575	-1.545617
38	1	0	1.574081	1.435495	-1.826049
39	1	0	2.439721	0.006574	-2.327997
40	1	0	3.865635	2.053562	-2.530622
41	1	0	3.669022	2.410601	-0.813825

42	1	0	4.588621	0.987277	-1.322410
43	6	0	2.372017	0.990027	1.428479
44	6	0	3.831392	0.960877	1.905441
45	1	0	1.712689	0.699558	2.254343
46	1	0	2.080328	2.013713	1.162780
47	1	0	3.957864	1.641574	2.756473
48	1	0	4.123953	-0.038265	2.244374
49	1	0	4.534577	1.271971	1.128041
50	6	0	2.861628	-1.634932	0.133477
51	6	0	4.307635	-1.632789	-0.381135
52	1	0	2.292074	-2.400367	-0.400497
53	1	0	2.832976	-1.927403	1.190014
54	1	0	4.747208	-2.628927	-0.247197
55	1	0	4.354998	-1.401246	-1.450226
56	1	0	4.946205	-0.919667	0.147427

B

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	0.341318	-0.004615	-0.021598
2	15	0	-1.940101	0.228545	-0.049467
3	6	0	2.412629	-1.018765	0.347839
4	6	0	1.498058	-1.634963	1.294384
5	6	0	1.989126	-1.405142	-0.972759
6	6	0	0.515812	-2.345604	0.549437
7	6	0	0.807381	-2.197251	-0.861898
8	6	0	0.160848	-2.948718	-1.992172
9	1	0	0.701514	-3.881865	-2.211799
10	1	0	-0.872838	-3.225198	-1.763994
11	1	0	0.149805	-2.359749	-2.915629
12	6	0	-0.527331	-3.266821	1.117863
13	1	0	-0.169904	-4.306459	1.113033
14	1	0	-0.772560	-3.017491	2.154584
15	1	0	-1.457765	-3.248765	0.539966
16	6	0	1.673095	-1.680244	2.786645
17	1	0	2.314060	-2.523138	3.084601
18	1	0	2.140034	-0.769184	3.169724
19	1	0	0.716254	-1.799328	3.304943
20	6	0	3.740617	-0.402459	0.690465
21	1	0	4.529960	-1.167733	0.731552
22	1	0	4.045882	0.344352	-0.048843
23	1	0	3.717116	0.094979	1.662743
24	6	0	2.731126	-1.159294	-2.255263
25	1	0	3.211202	-2.085736	-2.600025
26	1	0	2.066180	-0.819107	-3.056540
27	1	0	3.517348	-0.410455	-2.134719
28	6	0	-2.687879	-0.300886	1.586766
29	6	0	-4.124562	-0.838165	1.652393
30	1	0	-2.568243	0.559658	2.256450
31	1	0	-1.999239	-1.062115	1.964477
32	1	0	-4.364421	-1.128215	2.682793

33	1	0	-4.867217	-0.100180	1.338272
34	1	0	-4.250311	-1.729207	1.027883
35	6	0	-2.750673	-0.838767	-1.359631
36	6	0	-4.180839	-0.539712	-1.831332
37	1	0	-2.068290	-0.779845	-2.214815
38	1	0	-4.465737	-1.248620	-2.618558
39	1	0	-4.917233	-0.627172	-1.028158
40	1	0	-4.262534	0.465539	-2.257121
41	6	0	-2.624701	1.944619	-0.360743
42	6	0	-4.013331	2.314154	0.179801
43	1	0	-2.589961	2.095775	-1.446098
44	1	0	-1.883237	2.628907	0.060614
45	1	0	-4.232217	3.361963	-0.059784
46	1	0	-4.812729	1.706161	-0.252372
47	1	0	-4.063776	2.215474	1.268903
48	6	0	0.497517	1.399931	-1.616775
49	6	0	1.776791	2.246026	-1.676172
50	1	0	-0.347854	2.098538	-1.631427
51	1	0	0.420394	0.814490	-2.548157
52	6	0	1.853310	3.123420	-2.936879
53	1	0	1.836050	2.893913	-0.793460
54	1	0	2.664780	1.603186	-1.639056
55	1	0	2.768679	3.729322	-2.954408
56	1	0	1.840670	2.511303	-3.848049
57	1	0	0.998629	3.810109	-2.991950
58	6	0	0.358542	1.711362	1.268861
59	6	0	1.669298	2.057664	1.985024
60	1	0	-0.413138	1.599534	2.048373
61	1	0	0.069025	2.595121	0.681621
62	6	0	1.574252	3.358401	2.799775
63	1	0	1.954886	1.244054	2.663135
64	1	0	2.484915	2.153413	1.258102
65	1	0	2.516481	3.583430	3.316517
66	1	0	1.337048	4.212412	2.152452
67	1	0	0.784502	3.293070	3.559537
68	1	0	-2.680688	-1.870659	-0.994007

C

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	0.427676	-0.346065	-0.056712
2	15	0	-1.909282	0.100455	0.011928
3	6	0	2.704760	-0.094268	-0.065919
4	6	0	2.180666	0.752463	-1.112549
5	6	0	2.221792	0.414553	1.202867
6	6	0	1.320302	1.724229	-0.512643
7	6	0	1.350629	1.514536	0.940133
8	6	0	0.832654	2.455411	1.991032
9	1	0	1.641841	3.121109	2.319732
10	1	0	0.028908	3.095921	1.623147
11	1	0	0.467015	1.922853	2.873188

12	6	0	0.771493	2.923465	-1.232029
13	1	0	1.578086	3.648430	-1.404297
14	1	0	0.355995	2.657154	-2.207895
15	1	0	-0.003662	3.435581	-0.661105
16	6	0	2.551011	0.689994	-2.564608
17	1	0	3.430372	1.321625	-2.749737
18	1	0	2.807763	-0.324036	-2.881311
19	1	0	1.743645	1.052427	-3.205619
20	6	0	3.765561	-1.142782	-0.240605
21	1	0	4.761128	-0.680686	-0.220664
22	1	0	3.743993	-1.889183	0.558524
23	1	0	3.674150	-1.667997	-1.195925
24	6	0	2.645696	-0.060543	2.560898
25	1	0	3.541169	0.487947	2.882973
26	1	0	1.867398	0.107307	3.309257
27	1	0	2.897014	-1.124027	2.565935
28	6	0	-0.196812	-2.453467	-0.334906
29	6	0	0.530016	-2.381396	0.878011
30	6	0	0.368019	-1.990717	-1.554563
31	1	0	1.414679	-2.184163	-1.770479
32	1	0	-0.271943	-1.922466	-2.428603
33	1	0	1.593823	-2.598375	0.882798
34	1	0	0.018833	-2.586604	1.812351
35	6	0	-2.310364	1.926531	0.019400
36	6	0	-3.662209	2.397091	0.581832
37	1	0	-2.193849	2.255723	-1.020305
38	1	0	-1.516188	2.413189	0.585385
39	1	0	-3.750518	3.478803	0.432411
40	1	0	-4.519558	1.929198	0.093167
41	1	0	-3.740326	2.211282	1.656907
42	6	0	-2.894780	-0.539300	1.463114
43	6	0	-3.077408	-2.056579	1.602808
44	1	0	-3.881346	-0.069112	1.400504
45	1	0	-2.412095	-0.132376	2.359890
46	1	0	-3.737723	-2.265561	2.450980
47	1	0	-3.544696	-2.499146	0.716176
48	1	0	-2.136011	-2.576954	1.793077
49	6	0	-2.791859	-0.533862	-1.506157
50	6	0	-4.302038	-0.286453	-1.635635
51	1	0	-2.595074	-1.609222	-1.571298
52	1	0	-2.258365	-0.081017	-2.351161
53	1	0	-4.679436	-0.799222	-2.526890
54	1	0	-4.861987	-0.670308	-0.776764
55	1	0	-4.535199	0.775350	-1.749731
56	1	0	-1.262444	-2.646713	-0.289613

D

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	0.265952	-0.346514	0.102862
2	15	0	1.832698	1.297526	-0.217977

3	6	0	-0.651993	-2.486476	0.197414
4	6	0	0.381285	-2.551604	-0.822155
5	6	0	0.005880	-2.256978	1.459313
6	6	0	1.634228	-2.320074	-0.190502
7	6	0	1.407067	-2.128693	1.228909
8	6	0	2.462349	-2.074664	2.298571
9	1	0	2.667871	-3.076454	2.704744
10	1	0	3.410968	-1.684602	1.918551
11	1	0	2.158506	-1.443736	3.140545
12	6	0	2.985119	-2.455332	-0.835758
13	1	0	3.394776	-3.462380	-0.671863
14	1	0	2.937364	-2.301599	-1.918160
15	1	0	3.714538	-1.746033	-0.428917
16	6	0	0.186958	-2.982180	-2.249219
17	1	0	0.312513	-4.070095	-2.351427
18	1	0	-0.813939	-2.738389	-2.613761
19	1	0	0.906749	-2.506160	-2.923373
20	6	0	-2.077057	-2.935332	0.029079
21	1	0	-2.169430	-4.018583	0.197534
22	1	0	-2.747314	-2.436771	0.735802
23	1	0	-2.453095	-2.727242	-0.975268
24	6	0	-0.639744	-2.289868	2.814448
25	1	0	-0.499789	-3.274619	3.282130
26	1	0	-0.208652	-1.543427	3.489786
27	1	0	-1.715058	-2.106028	2.757458
28	6	0	2.707631	1.082162	-1.864410
29	6	0	4.139611	1.598168	-2.066635
30	1	0	2.034514	1.519569	-2.612220
31	1	0	2.685472	0.004060	-2.047593
32	1	0	4.482138	1.347873	-3.078312
33	1	0	4.219870	2.682207	-1.952511
34	1	0	4.839147	1.132047	-1.364520
35	6	0	3.173505	1.270646	1.089924
36	6	0	4.066324	2.499546	1.311963
37	1	0	2.639511	1.037067	2.018005
38	1	0	4.761946	2.306383	2.137825
39	1	0	4.663229	2.750974	0.431466
40	1	0	3.478068	3.381602	1.584604
41	6	0	1.231826	3.073307	-0.221600
42	6	0	2.017770	4.132863	-1.007528
43	1	0	1.149793	3.370262	0.830640
44	1	0	0.207150	3.033444	-0.601433
45	1	0	1.510741	5.101825	-0.923736
46	1	0	3.038469	4.263924	-0.638003
47	1	0	2.072425	3.888731	-2.073417
48	6	0	-0.731346	0.899753	1.519357
49	6	0	-2.255962	0.764607	1.623377
50	1	0	-0.516937	1.961020	1.344438
51	1	0	-0.286021	0.660743	2.498883
52	6	0	-2.852362	1.615158	2.771588
53	1	0	-2.730333	1.078039	0.686597
54	1	0	-2.547666	-0.282797	1.775531
55	1	0	-2.395876	1.290809	3.720129
56	1	0	-2.568718	2.667535	2.632624
57	6	0	-0.895084	0.679030	-1.377807
58	6	0	-2.142286	-0.029748	-1.918050
59	1	0	-0.259831	0.925712	-2.244297

60	1	0	-1.224237	1.641472	-0.961247
61	6	0	-2.973559	0.865279	-2.869594
62	1	0	-1.857899	-0.938051	-2.464408
63	1	0	-2.791714	-0.351430	-1.096093
64	1	0	-3.315125	1.757197	-2.327304
65	1	0	-2.315015	1.220987	-3.677872
66	1	0	3.788835	0.389165	0.872785
67	6	0	-4.348971	1.505380	2.871719
68	6	0	-5.212342	2.509909	2.708542
69	6	0	-4.155463	0.151086	-3.465624
70	6	0	-5.436192	0.467427	-3.263504
71	1	0	-4.738626	0.505560	3.075961
72	1	0	-6.287222	2.362140	2.776690
73	1	0	-4.874075	3.523731	2.501024
74	1	0	-3.920213	-0.708318	-4.097840
75	1	0	-6.247019	-0.101369	-3.711913
76	1	0	-5.722704	1.312446	-2.639903

E

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	0.364734	-0.026818	-0.050941
2	15	0	-1.922576	0.119879	-0.048906
3	6	0	2.512818	-0.880990	0.089801
4	6	0	1.804901	-1.403446	1.240885
5	6	0	1.926930	-1.488080	-1.085184
6	6	0	0.774585	-2.265848	0.776374
7	6	0	0.853586	-2.321982	-0.675549
8	6	0	0.100502	-3.281485	-1.554511
9	1	0	0.638999	-4.236664	-1.643780
10	1	0	-0.892161	-3.512708	-1.157618
11	1	0	-0.031272	-2.890528	-2.568270
12	6	0	-0.116763	-3.129103	1.625934
13	1	0	0.304033	-4.137982	1.746654
14	1	0	-0.247474	-2.713490	2.630273
15	1	0	-1.113529	-3.252016	1.187269
16	6	0	2.170171	-1.140895	2.673895
17	1	0	2.963199	-1.823389	3.010712
18	1	0	2.535347	-0.119085	2.814425
19	1	0	1.314674	-1.277160	3.342987
20	6	0	3.845674	-0.185893	0.117640
21	1	0	4.668595	-0.914480	0.063961
22	1	0	3.966177	0.501923	-0.725253
23	1	0	3.986891	0.390420	1.036169
24	6	0	2.460616	-1.346710	-2.480696
25	1	0	3.292905	-2.044033	-2.651859
26	1	0	1.694906	-1.558532	-3.233559
27	1	0	2.837368	-0.336237	-2.668510
28	6	0	-2.607292	-0.264678	1.654415
29	6	0	-4.035902	-0.799116	1.826952
30	1	0	-2.463979	0.651049	2.241405

31	1	0	-1.899055	-0.988536	2.069357
32	1	0	-4.233795	-0.990701	2.888890
33	1	0	-4.795696	-0.097586	1.473229
34	1	0	-4.178407	-1.746272	1.295722
35	6	0	-2.736419	-1.100964	-1.213468
36	6	0	-4.187874	-0.888995	-1.667206
37	1	0	-2.078457	-1.115103	-2.089618
38	1	0	-4.478631	-1.685880	-2.362775
39	1	0	-4.895631	-0.904915	-0.834140
40	1	0	-4.310654	0.061831	-2.195969
41	6	0	-2.672730	1.770085	-0.523675
42	6	0	-4.041514	2.174155	0.040841
43	1	0	-2.696990	1.790623	-1.619749
44	1	0	-1.929069	2.515707	-0.230947
45	1	0	-4.297456	3.183253	-0.304808
46	1	0	-4.845639	1.505307	-0.278501
47	1	0	-4.036556	2.199268	1.135370
48	6	0	0.510570	1.386346	-1.647139
49	6	0	1.497847	2.565813	-1.560928
50	6	0	1.016247	3.741844	-0.684992
51	6	0	0.345090	1.544979	1.402133
52	6	0	1.610001	2.422638	1.492816
53	6	0	1.544224	3.773829	0.760810
54	1	0	-2.626661	-2.086532	-0.745146
55	1	0	0.797017	0.770583	-2.512459
56	1	0	-0.461904	1.816751	-1.915735
57	1	0	2.488729	2.229482	-1.225317
58	1	0	1.649525	2.943905	-2.585470
59	1	0	1.290864	4.694292	-1.159366
60	1	0	-0.082099	3.731472	-0.674051
61	1	0	0.919483	4.469953	1.339969
62	1	0	2.554532	4.209359	0.762749
63	1	0	2.476784	1.867247	1.123224
64	1	0	1.831445	2.641368	2.550456
65	1	0	-0.524346	2.211183	1.309258
66	1	0	0.210473	1.024622	2.362024

F

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	0.004518	0.374591	0.066457
2	15	0	-1.652328	-1.204511	-0.001992
3	6	0	1.077909	2.424800	-0.180175
4	6	0	0.088798	2.361876	-1.240460
5	6	0	0.363798	2.495507	1.069272
6	6	0	-1.199301	2.353482	-0.637301
7	6	0	-1.033988	2.434846	0.803135
8	6	0	-2.132889	2.662080	1.804494
9	1	0	-2.319982	3.736039	1.953678
10	1	0	-3.079116	2.216138	1.483765
11	1	0	-1.886668	2.240282	2.784544

12	6	0	-2.514688	2.445265	-1.359316
13	1	0	-2.848236	3.490259	-1.434553
14	1	0	-2.447784	2.055874	-2.379847
15	1	0	-3.309362	1.895209	-0.843622
16	6	0	0.375735	2.442540	-2.713167
17	1	0	0.435259	3.488057	-3.048880
18	1	0	1.325997	1.964340	-2.966349
19	1	0	-0.404303	1.953988	-3.305906
20	6	0	2.533366	2.759843	-0.353180
21	1	0	2.689053	3.848419	-0.312735
22	1	0	3.152667	2.315331	0.432977
23	1	0	2.921381	2.412021	-1.313526
24	6	0	0.998472	2.719915	2.410803
25	1	0	1.170653	3.791709	2.583066
26	1	0	0.367151	2.355067	3.226781
27	1	0	1.965749	2.214247	2.488208
28	6	0	-2.387504	-1.322295	-1.723134
29	6	0	-3.829587	-1.804894	-1.930564
30	1	0	-1.686966	-1.940643	-2.298008
31	1	0	-2.283869	-0.310906	-2.128917
32	1	0	-4.078665	-1.780108	-2.998704
33	1	0	-3.987612	-2.828262	-1.580728
34	1	0	-4.548200	-1.157962	-1.416046
35	6	0	-3.075004	-0.788494	1.141121
36	6	0	-4.078048	-1.873635	1.558958
37	1	0	-2.585754	-0.380697	2.032590
38	1	0	-4.806202	-1.453611	2.263745
39	1	0	-4.637376	-2.279873	0.711990
40	1	0	-3.581603	-2.707579	2.065909
41	6	0	-1.198596	-2.961619	0.466051
42	6	0	-1.975336	-4.134799	-0.147648
43	1	0	-1.250695	-3.008468	1.560086
44	1	0	-0.139089	-3.063152	0.218391
45	1	0	-1.541936	-5.081377	0.197767
46	1	0	-3.032169	-4.137409	0.134153
47	1	0	-1.916729	-4.132999	-1.240991
48	6	0	0.895133	-0.621352	1.757653
49	6	0	2.412829	-0.907064	1.763103
50	6	0	2.760525	-2.314010	1.239356
51	6	0	1.088131	-0.856634	-1.317768
52	6	0	2.570673	-0.478505	-1.565053
53	6	0	3.605872	-1.640448	-1.677359
54	1	0	-3.598682	0.056714	0.678176
55	6	0	4.616899	-1.714764	-0.506380
56	6	0	4.190648	-2.540459	0.726959
57	1	0	0.660685	0.056405	2.589672
58	1	0	0.386147	-1.561374	2.004301
59	1	0	2.799497	-0.822831	2.792720
60	1	0	2.949421	-0.141375	1.191818
61	1	0	2.557255	-3.040880	2.039666
62	1	0	2.071208	-2.572291	0.431488
63	1	0	4.913490	-2.356982	1.535789
64	1	0	4.287319	-3.607182	0.475581
65	1	0	3.089399	-2.604694	-1.789146
66	1	0	4.182297	-1.509227	-2.602585
67	1	0	2.922853	0.190577	-0.778601
68	1	0	2.623209	0.115873	-2.487347

69	1	0	1.039247	-1.910004	-1.024875
70	1	0	0.551319	-0.796976	-2.276636
71	1	0	4.863519	-0.688574	-0.200341
72	1	0	5.560152	-2.144043	-0.872204

G

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	-0.108679	0.312918	0.052638
2	15	0	-1.504516	-1.391223	-0.052127
3	6	0	0.585792	2.530370	-0.147581
4	6	0	-0.324427	2.275036	-1.248184
5	6	0	-0.180858	2.459172	1.074198
6	6	0	-1.608902	2.001851	-0.697959
7	6	0	-1.524119	2.120095	0.749517
8	6	0	-2.685112	2.050926	1.700427
9	1	0	-3.228032	3.006702	1.735183
10	1	0	-3.394128	1.273455	1.405573
11	1	0	-2.353974	1.827108	2.719380
12	6	0	-2.876470	1.782860	-1.477024
13	1	0	-3.376081	2.739392	-1.687179
14	1	0	-2.677800	1.295213	-2.435814
15	1	0	-3.582251	1.155977	-0.925416
16	6	0	-0.004523	2.404725	-2.710033
17	1	0	-0.181709	3.430934	-3.062973
18	1	0	1.040989	2.161927	-2.916130
19	1	0	-0.623496	1.736812	-3.316986
20	6	0	1.958010	3.133895	-0.260501
21	1	0	1.907030	4.229857	-0.180460
22	1	0	2.629166	2.782607	0.530224
23	1	0	2.427127	2.899750	-1.219088
24	6	0	0.346983	2.789546	2.439468
25	1	0	0.290559	3.871460	2.624318
26	1	0	-0.224527	2.292138	3.228783
27	1	0	1.393929	2.491614	2.549545
28	6	0	-2.933511	-2.711281	-1.909196
29	1	0	-2.901183	-2.875006	-2.988603
30	1	0	-2.813254	-3.670707	-1.393452
31	1	0	-3.896591	-2.268937	-1.634813
32	6	0	-3.670975	-1.928404	1.526017
33	1	0	-4.612860	-1.421086	1.749035
34	1	0	-3.877007	-2.923937	1.121837
35	1	0	-3.085166	-2.032128	2.443846
36	6	0	-0.247550	-3.762361	0.239963
37	1	0	0.721273	-3.465282	0.648183
38	1	0	-0.519429	-4.746679	0.630683
39	1	0	-0.185551	-3.809093	-0.852160
40	6	0	0.936734	-0.533476	1.736564
41	6	0	2.480190	-0.473101	1.761788
42	6	0	3.145369	-1.784489	1.299229
43	6	0	1.208859	-0.740485	-1.285529

44	6	0	2.574681	-0.071791	-1.578245
45	6	0	3.831917	-0.994130	-1.637800
46	6	0	4.823306	-0.817084	-0.460046
47	6	0	4.590902	-1.693110	0.790642
48	1	0	0.540745	0.041262	2.584318
49	1	0	0.626433	-1.568482	1.918550
50	1	0	2.825208	-0.260176	2.786998
51	1	0	2.841098	0.366501	1.157710
52	1	0	3.110636	-2.504211	2.130615
53	1	0	2.540579	-2.229366	0.504354
54	1	0	5.250407	-1.332651	1.593945
55	1	0	4.928160	-2.715136	0.562700
56	1	0	3.529939	-2.047961	-1.722394
57	1	0	4.380564	-0.773713	-2.562909
58	1	0	2.785213	0.706236	-0.841965
59	1	0	2.494540	0.458376	-2.536875
60	1	0	1.377234	-1.754207	-0.915529
61	1	0	0.656334	-0.857423	-2.226297
62	1	0	4.830196	0.244004	-0.174284
63	1	0	5.841603	-1.028676	-0.814765
64	8	0	-1.861065	-1.812431	-1.601139
65	8	0	-1.274687	-2.859687	0.664336
66	8	0	-2.996454	-1.101060	0.571404

H

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	0.727139	-0.654089	-0.099848
2	15	0	-1.270221	0.465615	0.043684
3	6	0	2.251597	-2.336347	-0.430930
4	6	0	1.746374	-2.562077	0.904851
5	6	0	1.166451	-2.624716	-1.354214
6	6	0	0.369233	-2.901087	0.814306
7	6	0	0.010135	-2.935346	-0.590723
8	6	0	-1.317442	-3.413890	-1.109367
9	1	0	-1.381152	-4.510111	-1.055053
10	1	0	-2.149916	-3.012525	-0.522579
11	1	0	-1.480232	-3.129263	-2.152182
12	6	0	-0.488902	-3.403250	1.938853
13	1	0	-0.396331	-4.495311	2.040660
14	1	0	-0.198394	-2.965021	2.898455
15	1	0	-1.547348	-3.180013	1.782826
16	6	0	2.562852	-2.620287	2.164024
17	1	0	2.807768	-3.664176	2.407389
18	1	0	3.504355	-2.077136	2.066117
19	1	0	2.023500	-2.204110	3.020813
20	6	0	3.698053	-2.229558	-0.825972
21	1	0	4.136341	-3.225411	-0.989471
22	1	0	3.822815	-1.661767	-1.752874
23	1	0	4.296258	-1.734439	-0.055956
24	6	0	1.317540	-2.731728	-2.843530

25	1	0	1.797730	-3.681938	-3.117031
26	1	0	0.352016	-2.697923	-3.358070
27	1	0	1.940000	-1.928790	-3.252246
28	6	0	1.342862	0.628147	-1.723411
29	6	0	2.731795	1.298627	-1.688077
30	6	0	2.706049	2.740343	-1.147900
31	6	0	1.527138	0.755199	1.311682
32	6	0	3.050432	0.720275	1.597734
33	6	0	3.774882	2.095098	1.736272
34	6	0	4.684413	2.497189	0.548796
35	6	0	4.034792	3.287357	-0.607421
36	1	0	1.298071	-0.037298	-2.595141
37	1	0	0.599058	1.406103	-1.929559
38	1	0	3.150838	1.324737	-2.708018
39	1	0	3.431054	0.691019	-1.107244
40	1	0	2.351493	3.409349	-1.946286
41	1	0	1.956225	2.817294	-0.356976
42	1	0	4.768742	3.362439	-1.423817
43	1	0	3.859194	4.318615	-0.266973
44	1	0	3.042161	2.890018	1.935057
45	1	0	4.412134	2.055039	2.629879
46	1	0	3.579295	0.143255	0.832658
47	1	0	3.207188	0.165277	2.530539
48	1	0	1.239381	1.762243	1.009758
49	1	0	1.002848	0.582470	2.264644
50	1	0	5.160882	1.588135	0.155931
51	1	0	5.509937	3.113842	0.931049
52	6	0	-2.265650	0.579416	-1.523227
53	6	0	-3.405335	1.397917	-1.619098
54	6	0	-1.878947	-0.163450	-2.645208
55	6	0	-4.143902	1.453821	-2.800990
56	1	0	-3.714071	1.998385	-0.768536
57	6	0	-2.615184	-0.105033	-3.831541
58	1	0	-0.984477	-0.773008	-2.583842
59	6	0	-3.750731	0.700751	-3.910949
60	1	0	-5.023066	2.090433	-2.857399
61	1	0	-2.294588	-0.683451	-4.694167
62	1	0	-4.323407	0.749797	-4.833418
63	6	0	-1.301190	2.260375	0.561927
64	6	0	-0.959502	3.246171	-0.381319
65	6	0	-1.609634	2.673703	1.866228
66	6	0	-0.920867	4.594915	-0.029030
67	1	0	-0.732011	2.965289	-1.403831
68	6	0	-1.571676	4.025171	2.218906
69	1	0	-1.897716	1.947406	2.617038
70	6	0	-1.224601	4.990809	1.274995
71	1	0	-0.654014	5.336084	-0.777769
72	1	0	-1.820106	4.318701	3.235558
73	1	0	-1.196244	6.041912	1.549577
74	6	0	-2.460596	-0.307438	1.246095
75	6	0	-2.023281	-0.522842	2.565655
76	6	0	-3.762359	-0.704033	0.904415
77	6	0	-2.876350	-1.071037	3.523459
78	1	0	-1.002049	-0.273000	2.838745
79	6	0	-4.607566	-1.278899	1.858452
80	1	0	-4.126283	-0.565398	-0.107358
81	6	0	-4.173759	-1.452181	3.172365

82	1	0	-2.521342	-1.215463	4.540579
83	1	0	-5.609933	-1.584685	1.569868
84	1	0	-4.835725	-1.889500	3.914998