

Supporting Information II  
Coordinates of [1.PF6] DB24C8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-2.189247	-3.365430	-1.030626
2	8	0	-4.333610	-1.458249	-0.764266
3	8	0	-4.242489	1.452130	-0.367558
4	8	0	-1.786070	3.158528	0.357173
5	6	0	-1.136468	-3.352924	-1.906770
6	6	0	0.142884	-3.435757	-1.323395
7	6	0	1.284229	-3.310781	-2.119065
8	6	0	1.158659	-3.155098	-3.499174
9	6	0	-0.103516	-3.118555	-4.084823
10	6	0	-1.250277	-3.213567	-3.292280
11	6	0	-3.502622	-3.634528	-1.511742
12	6	0	-4.263299	-2.359041	-1.882705
13	6	0	-5.442025	-0.554373	-0.903972
14	6	0	-5.299990	0.598109	0.086793
15	6	0	-4.154787	2.646778	0.423499
16	6	0	-3.066403	3.555925	-0.144876
17	8	0	0.559894	2.621123	1.489035
18	8	0	1.574366	0.087764	2.827243
19	8	0	1.663879	-2.807503	2.380496
20	8	0	0.187548	-3.564128	0.040893
21	6	0	0.560251	3.515367	0.437805
22	6	0	-0.688388	3.825502	-0.139557
23	6	0	-0.746660	4.754923	-1.189642
24	6	0	0.415399	5.350365	-1.684163
25	6	0	1.647909	5.021919	-1.136018
26	6	0	1.719728	4.111353	-0.081577
27	6	0	1.829228	2.394117	2.116269
28	6	0	1.692898	1.434948	3.300224
29	6	0	1.958368	-0.876320	3.821755
30	6	0	2.630434	-2.066119	3.134908
31	6	0	2.281348	-3.496106	1.285442
32	6	0	1.243361	-4.368593	0.583282
33	1	0	2.280398	-3.296931	-1.685505
34	1	0	2.051289	-3.050750	-4.111593
35	1	0	-0.194081	-2.995771	-5.161449
36	1	0	-2.211468	-3.152054	-3.787312
37	1	0	-4.027465	-4.114988	-0.678249
38	1	0	-3.497452	-4.358705	-2.334881
39	1	0	-3.767840	-1.825141	-2.697496
40	1	0	-5.272896	-2.638964	-2.205936
41	1	0	-6.363884	-1.109849	-0.700643
42	1	0	-5.464336	-0.161057	-1.927214

43	1	0	-6.235784	1.164590	0.120849
44	1	0	-5.053627	0.225422	1.085659
45	1	0	-3.944915	2.382402	1.463038
46	1	0	-5.116992	3.167098	0.364397
47	1	0	-3.089350	3.479134	-1.238283
48	1	0	-3.260816	4.585661	0.175648
49	1	0	-1.681050	5.035724	-1.660732
50	1	0	0.357992	6.060815	-2.504263
51	1	0	2.559495	5.467512	-1.527127
52	1	0	2.709662	3.876108	0.300353
53	1	0	2.523319	1.958985	1.391451
54	1	0	2.212492	3.347042	2.499795
55	1	0	0.813908	1.670040	3.906714
56	1	0	2.596310	1.536402	3.912103
57	1	0	2.663982	-0.447534	4.541022
58	1	0	1.052242	-1.186930	4.352419
59	1	0	3.058336	-2.739492	3.884492
60	1	0	3.431201	-1.702748	2.486372
61	1	0	2.680222	-2.756671	0.587068
62	1	0	3.095702	-4.123855	1.663047
63	1	0	0.770366	-5.023532	1.323662
64	1	0	1.708348	-5.018255	-0.167340
65	6	0	-4.203276	0.514390	4.449218
66	6	0	-3.106127	1.225723	3.968518
67	6	0	-2.191689	0.608956	3.112545
68	6	0	-2.363920	-0.727739	2.731086
69	6	0	-3.467426	-1.436888	3.229669
70	6	0	-4.384400	-0.816246	4.079515
71	6	0	-0.943408	-0.698053	0.624645
72	7	0	-1.768718	-0.325989	-0.364410
73	6	0	-1.078094	0.282892	-1.379515
74	6	0	0.256149	0.278214	-0.992682
75	7	0	0.282144	-0.305679	0.253997
76	6	0	-1.513044	0.815266	-2.584303
77	6	0	-0.516709	1.360549	-3.419067
78	6	0	0.856320	1.352150	-3.026326
79	6	0	1.259692	0.799593	-1.792998
80	6	0	-1.343530	-1.426010	1.870614
81	6	0	-0.935596	1.969521	-4.732853
82	6	0	1.922156	1.944244	-3.913458
83	1	0	-1.340788	1.182889	2.749049
84	1	0	-5.231752	-1.376386	4.464786
85	1	0	-2.772955	-0.506548	-0.353205
86	1	0	1.126698	-0.416745	0.828315
87	1	0	-2.564268	0.808070	-2.834369
88	1	0	2.290521	0.783623	-1.465096
89	1	0	-1.722591	-2.389360	1.517758
90	1	0	-0.439690	-1.597567	2.448232

91	1	0	2.913465	1.876072	-3.451585
92	1	0	1.963819	1.406378	-4.866110
93	1	0	1.718816	3.003890	-4.097255
94	1	0	-2.013165	1.863549	-4.897232
95	1	0	-0.701338	3.039387	-4.745368
96	1	0	-0.426196	1.471717	-5.563801
97	1	0	-2.954653	2.261925	4.260436
98	1	0	-4.910438	0.994977	5.120557
99	1	0	-3.612998	-2.483017	2.966728
100	15	0	4.602355	-0.096044	0.180866
101	9	0	3.011938	-0.382360	0.450084
102	9	0	4.775819	0.361992	1.745466
103	9	0	4.250955	1.452049	-0.228749
104	9	0	4.945444	-1.645746	0.588171
105	9	0	4.408520	-0.553948	-1.381093
106	9	0	6.190279	0.191043	-0.089445

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Coordinates of [1.C1O4]DB24C8

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-3.006597	2.410157	1.116062
2	8	0	-4.416183	0.287386	-0.214184
3	8	0	-3.624120	-2.384228	0.490143
4	8	0	-0.701344	-3.350061	0.629687
5	6	0	-2.222114	3.495531	1.405023
6	6	0	-1.321637	4.081351	0.499649
7	6	0	-0.542219	5.156488	0.940997
8	6	0	-0.652044	5.630824	2.253670
9	6	0	-1.531848	5.027118	3.145864
10	6	0	-2.309011	3.952624	2.724479
11	6	0	-3.941984	2.652348	0.057735
12	6	0	-5.004064	1.555498	0.126709
13	6	0	-5.357147	-0.779000	-0.013798
14	6	0	-4.716693	-2.112022	-0.396508
15	6	0	-3.075265	-3.687647	0.243161
16	6	0	-1.888027	-3.945222	1.169443
17	8	0	1.581134	-2.630449	-0.561032
18	8	0	2.149905	-0.100844	-2.153570
19	8	0	1.069110	2.599718	-2.464240
20	8	0	-1.228244	3.515178	-0.744286
21	6	0	1.675083	-3.213064	0.687873
22	6	0	0.469482	-3.591920	1.314961
23	6	0	0.513748	-4.163965	2.597390
24	6	0	1.730164	-4.369565	3.248593

25	6	0	2.916561	-4.005524	2.628560
26	6	0	2.890173	-3.432482	1.356202
27	6	0	2.821636	-2.204370	-1.148601
28	6	0	2.582103	-1.440393	-2.452635
29	6	0	2.622152	0.845996	-3.126715
30	6	0	2.463522	2.260804	-2.570633
31	6	0	0.916348	3.898296	-1.873313
32	6	0	-0.568456	4.251262	-1.783312
33	1	0	0.189679	5.639434	0.301639
34	1	0	-0.029950	6.460309	2.582150
35	1	0	-1.601384	5.383255	4.169759
36	1	0	-2.985226	3.466835	3.422260
37	1	0	-3.439401	2.596801	-0.911454
38	1	0	-4.419071	3.631297	0.181740
39	1	0	-5.413462	1.500015	1.142054
40	1	0	-5.809245	1.772176	-0.583723
41	1	0	-6.241915	-0.602461	-0.634498
42	1	0	-5.643895	-0.799115	1.043960
43	1	0	-5.463584	-2.909860	-0.315870
44	1	0	-4.338240	-2.068211	-1.420805
45	1	0	-2.772291	-3.769424	-0.803525
46	1	0	-3.856881	-4.426295	0.453351
47	1	0	-2.105786	-3.516208	2.153827
48	1	0	-1.739267	-5.030078	1.241630
49	1	0	-0.384921	-4.455643	3.127888
50	1	0	1.750294	-4.810689	4.241585
51	1	0	3.869205	-4.158616	3.130730
52	1	0	3.847689	-3.160272	0.919773
53	1	0	3.343176	-1.542406	-0.451401
54	1	0	3.424459	-3.092806	-1.373184
55	1	0	1.805877	-1.918038	-3.056882
56	1	0	3.517509	-1.424037	-3.022285
57	1	0	3.680229	0.670646	-3.344464
58	1	0	2.031221	0.717074	-4.040057
59	1	0	2.951868	2.976618	-3.241488
60	1	0	2.908363	2.323566	-1.573735
61	1	0	1.378833	3.891287	-0.881066
62	1	0	1.421619	4.632558	-2.510106
63	1	0	-1.062685	3.959607	-2.717457
64	1	0	-0.726807	5.330510	-1.673396
65	6	0	-3.001289	-3.000850	-4.331865
66	6	0	-1.901979	-3.190226	-3.497739
67	6	0	-1.357734	-2.111064	-2.798625
68	6	0	-1.905919	-0.828907	-2.927138
69	6	0	-3.004725	-0.647880	-3.781390
70	6	0	-3.552662	-1.729677	-4.473690
71	6	0	-0.877056	0.188719	-0.824546
72	7	0	-1.687679	-0.068991	0.209276

73	6	0	-0.981756	-0.114917	1.388380
74	6	0	0.343445	0.122837	1.049791
75	7	0	0.353524	0.287017	-0.309979
76	6	0	-1.393979	-0.344835	2.692400
77	6	0	-0.379777	-0.336926	3.674547
78	6	0	0.985572	-0.099574	3.322921
79	6	0	1.364757	0.142703	1.985966
80	6	0	-1.272663	0.361322	-2.259393
81	6	0	-0.768560	-0.601140	5.106568
82	6	0	2.069877	-0.114183	4.371915
83	1	0	-0.495172	-2.286151	-2.156227
84	1	0	-4.401156	-1.577925	-5.136861
85	1	0	-2.698331	-0.194453	0.123893
86	1	0	1.196080	0.399110	-0.884553
87	1	0	-2.437095	-0.525990	2.910138
88	1	0	2.388558	0.318697	1.679305
89	1	0	-1.950695	1.219137	-2.252654
90	1	0	-0.370208	0.632695	-2.808900
91	1	0	3.055247	0.078855	3.934493
92	1	0	1.883951	0.661677	5.120805
93	1	0	2.112337	-1.093786	4.858976
94	1	0	-1.850722	-0.737238	5.208741
95	1	0	-0.285029	-1.514330	5.467028
96	1	0	-0.482548	0.242456	5.740957
97	1	0	-1.459183	-4.177112	-3.391992
98	1	0	-3.418528	-3.841221	-4.880102
99	1	0	-3.434813	0.341224	-3.924010
100	17	0	5.561919	0.799127	-0.644576
101	8	0	5.582644	-0.482897	-1.320310
102	8	0	4.366933	0.884183	0.172638
103	8	0	6.733859	0.932884	0.194469
104	8	0	5.534363	1.859594	-1.632960

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