

Supporting Information:

**A Density Functional Theory Study of Lewis Base Interactions with the
MgCl₂ Surface: Expanding the Role of the Donors**

Kumar Vanka,^{†*} Gurmeet Singh,[‡] Divya Iyer[†], Virendra K. Gupta^{‡*}

Table 1. The comparison between previous results using periodic DFT calculations¹, and analogous calculations done by us using the Partially Fixed and the Fully Fixed Models for the MgCl₂ surface (please refer to the manuscript): the calculations refer to the binding of the species TiCl₄ and the internal donor ethyl benzoate to the (110) MgCl₂ surface.

MgCl ₂ Surface	Species	ΔE (kcal/mol) (Partially Fixed Model)	ΔE (kcal/mol) (Fully Fixed Model)	ΔE (kcal/mol) (Previous Periodic DFT Calculations) ¹
110	TiCl ₄	-17.0	-19.3	-19.8
	Ethyl Benzoate	-28.0	-27.6	-29.8

¹ Taniike, T.; Terano, M. *Macromol. Symp.* **2007**, 260, 98.

The optimized geometries of the structures reported in the paper (the atomic symbol followed by the three Cartesian coordinates, in Å). The order in which the structures are presented follows the order in which they appear in the tables in the manuscript.

Zip_DIBP_Alpha_5.9

C	9.952	4.013	14.516
C	9.712	3.377	15.759
C	10.331	3.888	16.911
C	11.200	4.975	16.847
C	11.402	5.627	15.631
C	10.760	5.162	14.485
C	8.735	2.268	16.044
O	9.015	1.110	15.471
C	8.138	-0.024	15.812
C	8.843	-1.310	15.406
C	9.411	3.621	13.178
O	9.479	2.326	12.916
C	9.065	1.889	11.574
C	9.294	0.388	11.463
O	7.800	2.396	16.846
Mg	6.228	3.596	17.590
Cl	4.152	3.596	16.261
Mg	3.114	1.797	17.590
Cl	4.152	0.000	16.261
Mg	3.114	-1.798	17.590
Cl	1.038	-1.798	16.261
Mg	0.000	-3.595	17.590
Cl	1.038	-5.393	16.261
Mg	-0.000	-7.192	17.589
Cl	-1.038	-8.989	18.918
Cl	5.190	5.394	18.918
Mg	6.228	7.192	17.590
Cl	7.266	8.990	16.261
Mg	9.342	8.990	17.590
Cl	10.380	10.788	16.261
Mg	9.342	12.586	17.590
Cl	10.380	14.384	16.261
Cl	7.266	5.394	16.261
Cl	5.190	1.797	18.918
Cl	8.304	7.192	18.918
Cl	8.304	10.788	18.918
Cl	2.076	0.000	18.918
Cl	2.076	-3.596	18.918
Cl	-1.038	-5.394	18.918
O	9.039	4.464	12.344
Mg	7.266	5.394	11.726
Cl	5.190	5.394	10.398
Mg	4.152	3.596	11.726
Cl	5.190	1.797	10.398
Mg	4.152	0.000	11.726
Cl	2.076	0.000	10.398
Mg	1.038	-1.798	11.726
Cl	2.076	-3.596	10.397
Mg	1.038	-5.393	11.726
Cl	-0.000	-7.192	13.055
Cl	6.228	7.192	13.055
Mg	7.266	8.989	11.726
Cl	8.304	10.788	10.398
Mg	10.380	10.788	11.726
Cl	11.418	12.586	10.397

Mg	10.380	14.384	11.726
Cl	11.418	16.182	10.398
Cl	8.304	7.192	10.397
Cl	6.228	3.596	13.055
Cl	9.342	8.990	13.055
Cl	9.342	12.586	13.055
Cl	3.114	1.797	13.055
Cl	3.114	-1.798	13.055
Cl	0.000	-3.595	13.055
H	10.113	3.427	17.875
H	11.690	5.324	17.758
H	12.055	6.499	15.564
H	10.881	5.685	13.536
H	7.935	0.007	16.892
H	7.184	0.124	15.286
C	7.880	-2.486	15.623
C	10.154	-1.509	16.176
H	9.075	-1.244	14.329
H	8.004	2.149	11.447
H	9.666	2.446	10.838
C	8.809	-0.074	10.082
C	10.756	0.001	11.707
H	8.667	-0.095	12.233
H	10.888	-1.088	11.633
H	11.413	0.467	10.955
H	11.098	0.319	12.702
H	8.879	-1.168	9.997
H	7.768	0.224	9.889
H	9.431	0.357	9.283
H	10.659	-2.431	15.855
H	10.847	-0.672	16.016
H	9.962	-1.592	17.258
H	8.348	-3.429	15.304
H	7.622	-2.589	16.689
H	6.944	-2.362	15.057

Zip_DIBP_Alpha_6.3

Mg	3.596	8.305	11.727
Mg	1.798	11.418	11.727
Cl	3.596	10.380	10.398
Cl	1.798	9.343	13.055
Mg	3.596	14.532	11.727
Cl	3.596	12.456	13.055
Cl	1.797	13.494	10.398
Cl	3.595	16.608	10.398
Mg	1.797	17.646	11.727
Cl	1.797	15.570	13.055
Cl	1.797	19.723	10.398
Cl	3.596	6.229	13.055
Cl	1.798	7.267	10.398
Mg	1.798	5.190	11.726
Cl	3.596	4.152	10.397
Cl	1.797	3.114	13.055
Mg	3.595	2.076	11.727
Cl	3.595	0.000	13.055
Cl	1.797	1.038	10.398

Mg	1.797	-1.038	11.726
Cl	3.595	-2.076	10.397
Mg	3.595	-4.152	11.726
Cl	1.797	-3.114	13.054
Cl	3.595	-6.229	13.055
Mg	3.596	6.228	18.027
Cl	3.596	8.304	16.698
Cl	1.798	7.266	19.355
Cl	3.596	4.151	19.354
Cl	1.798	5.189	16.698
Mg	1.798	3.113	18.026
Cl	3.596	2.075	16.697
Mg	3.596	-0.000	18.026
Cl	1.798	1.037	19.354
Cl	3.596	-2.076	19.354
Cl	1.798	-1.038	16.697
Mg	1.798	-3.114	18.026
Cl	3.596	-4.152	16.697
Mg	3.596	-6.229	18.026
Cl	3.596	-8.305	19.354
Cl	1.798	-5.190	19.354
Mg	1.798	9.342	18.027
Cl	3.596	10.380	19.355
Cl	1.798	11.418	16.698
Mg	3.596	12.456	18.027
Cl	3.596	14.532	16.698
Cl	1.798	13.494	19.355
Mg	1.798	15.570	18.027
Cl	1.798	17.646	16.698
O	5.360	8.594	12.858
C	6.412	8.195	13.354
C	6.810	8.592	14.758
C	6.664	7.818	15.937
C	7.038	8.379	17.168
C	7.564	9.665	17.250
C	7.679	10.436	16.092
C	7.285	9.908	14.862
H	7.338	10.526	13.964
H	8.068	11.455	16.140
H	7.866	10.067	18.218
H	6.906	7.781	18.070
O	7.259	7.519	12.581
C	8.597	7.138	13.041
H	8.489	6.373	13.824
H	9.092	8.025	13.464
C	9.365	6.599	11.839
H	9.357	7.388	11.067
C	10.819	6.341	12.253
H	10.880	5.572	13.039
H	11.403	5.982	11.394
H	11.307	7.251	12.632
C	8.709	5.342	11.258
H	9.246	5.006	10.359
H	8.737	4.516	11.989
H	7.662	5.521	10.981
C	6.100	6.432	15.990
O	5.477	5.973	16.958

O	6.400	5.735	14.902
C	5.891	4.368	14.727
H	5.103	4.173	15.465
H	5.447	4.396	13.724
C	7.033	3.360	14.827
H	7.879	3.754	14.236
C	7.497	3.151	16.273
H	6.667	2.783	16.896
H	8.320	2.422	16.319
H	7.859	4.087	16.723
H	6.385	2.188	13.101
H	7.352	1.272	14.265
C	6.576	2.046	14.180
H	5.659	1.661	14.649

Zip_DIBP_Alpha_6.3

C	7.311	3.771	13.836
C	6.965	4.387	15.040
C	6.651	5.753	15.093
C	6.606	6.493	13.880
C	6.938	5.848	12.678
C	7.316	4.508	12.651
C	6.341	6.237	16.495
O	5.309	5.908	17.076
Mg	3.595	6.229	18.326
Cl	1.797	7.267	19.654
Mg	1.797	9.343	18.326
Cl	3.595	10.381	19.655
Mg	3.595	12.456	18.327
Cl	1.797	13.494	19.654
Mg	1.797	15.570	18.326
Cl	1.797	17.646	16.998
C	6.135	7.908	13.754
O	5.581	8.376	12.746
O	7.260	6.918	17.179
C	8.610	7.127	16.649
C	9.407	7.921	17.677
O	6.398	8.631	14.835
C	5.844	9.989	14.898
C	6.499	10.678	16.088
Cl	3.596	8.304	16.997
Cl	3.595	4.152	19.654
Mg	1.798	3.114	18.326
Cl	1.798	5.190	16.997
Cl	1.798	11.419	16.997
Cl	3.595	14.532	16.998
Cl	1.797	1.038	19.654
Mg	3.596	0.000	18.326
Cl	3.596	-2.076	19.654
Mg	1.798	-3.114	18.326
Cl	1.798	-5.190	19.654
Mg	3.596	-6.229	18.326
Cl	3.596	-8.305	19.654
Cl	3.596	2.076	16.997
Cl	1.798	-1.038	16.997
Cl	3.596	-4.151	16.997
Mg	3.596	8.305	11.726
Cl	1.797	9.343	13.055
Mg	1.798	11.418	11.727
Cl	3.596	12.456	13.055
Mg	3.596	14.532	11.727

Cl	1.797	15.570	13.055
Mg	1.797	17.646	11.727
Cl	1.797	19.723	10.398
Cl	3.596	10.380	10.398
Cl	3.596	6.229	13.054
Mg	1.798	5.190	11.726
Cl	1.798	7.267	10.397
Cl	1.797	13.494	10.398
Cl	3.595	16.608	10.398
Cl	3.596	4.152	10.397
Mg	3.595	2.076	11.726
Cl	1.797	3.114	13.054
Cl	1.798	1.038	10.397
Mg	1.797	-1.037	11.726
Cl	3.595	-2.075	10.397
Mg	3.595	-4.152	11.726
Cl	3.595	-6.229	13.054
Cl	3.595	0.000	13.054
Cl	1.797	-3.114	13.054
H	6.876	6.419	11.750
H	7.589	4.042	11.703
H	7.570	2.711	13.833
H	6.926	3.798	15.957
H	6.040	10.501	13.944
H	4.759	9.880	15.033
C	5.630	11.869	16.498
H	6.489	9.953	16.919
C	7.938	11.110	15.789
H	9.069	6.140	16.472
H	8.540	7.669	15.697
C	10.796	8.221	17.096
H	8.878	8.879	17.827
C	9.504	7.199	19.024
H	11.381	8.833	17.797
H	11.360	7.292	16.920
H	10.739	8.767	16.143
H	10.061	7.810	19.749
H	8.511	6.994	19.446
H	10.035	6.239	18.918
H	8.418	11.550	16.676
H	8.554	10.259	15.463
H	7.958	11.864	14.987
H	6.016	12.310	17.435
H	5.605	12.669	15.745
H	4.589	11.502	16.588

Zip_DIBP_Alpha_7.9

C	-0.021	-2.004	13.065
C	1.217	-2.121	12.428
C	1.879	-0.967	11.960
C	1.264	0.284	12.116
C	0.013	0.389	12.724
C	-0.623	-0.753	13.206
C	1.771	-3.507	12.278
O	1.721	-3.957	11.032
C	3.257	-1.091	11.404
O	3.696	0.062	10.845
O	3.922	-2.113	11.462
Mg	7.191	2.205	14.247
Cl	4.937	1.596	15.039
Mg	5.109	2.972	17.077

Cl	2.856	2.362	17.869
Mg	1.746	4.140	16.571
Cl	-0.506	3.531	17.363
Mg	-0.334	4.907	19.401
Cl	-2.588	4.298	20.193
Cl	9.445	2.813	13.455
Mg	10.554	1.036	14.753
Cl	12.807	1.644	13.961
Mg	12.636	0.269	11.923
Cl	10.383	-0.339	12.715
Cl	13.745	-1.508	13.221
Mg	15.999	-0.899	12.429
Cl	15.827	-2.275	10.391
Mg	18.081	-1.666	9.599
Cl	20.334	-1.058	8.807
Cl	14.889	0.877	11.131
Cl	18.252	-0.290	11.637
Cl	8.301	0.427	15.545
Cl	7.362	3.580	16.285
Cl	3.999	4.749	15.779
Cl	1.918	5.516	18.609
O	2.099	-4.204	13.244
Mg	2.769	-4.606	15.125
Cl	0.516	-5.215	15.917
Mg	0.687	-3.839	17.955
Cl	-1.565	-4.448	18.747
Mg	-2.674	-2.670	17.449
Cl	-4.928	-3.280	18.241
Mg	-4.756	-1.903	20.279
Cl	-7.010	-2.512	21.071
Cl	5.022	-3.997	14.333
Mg	6.133	-5.775	15.631
Cl	5.961	-7.151	13.593
Mg	8.214	-6.542	12.801
Cl	9.324	-8.320	14.099
Mg	11.577	-7.710	13.307
Cl	13.830	-7.102	12.515
Mg	13.659	-8.477	10.477
Cl	15.913	-7.869	9.685
Cl	10.467	-5.933	12.009
Cl	11.405	-9.086	11.269
Cl	8.386	-5.166	14.839
Cl	3.878	-6.384	16.423
Cl	2.940	-3.231	17.163
Cl	-0.421	-2.062	16.657
Cl	-2.503	-1.295	19.487
H	1.790	1.172	11.767
H	-0.456	1.368	12.837
H	-1.587	-0.672	13.709
H	-0.505	-2.897	13.462
C	2.270	-5.293	10.748
C	5.067	0.045	10.358
C	5.323	1.339	9.593
H	5.739	-0.062	11.225
H	5.210	-0.836	9.715
C	6.818	1.449	9.263
C	4.460	1.425	8.329
H	5.050	2.178	10.259
H	7.026	2.381	8.719
H	7.445	1.440	10.168
H	7.144	0.612	8.625
H	4.616	2.382	7.810

H	4.722	0.616	7.627
H	3.391	1.336	8.566
C	3.679	-5.192	10.167
H	2.252	-5.884	11.671
H	1.566	-5.718	10.019
C	4.248	-6.611	10.023
C	3.691	-4.438	8.834
H	4.293	-4.637	10.896
H	5.246	-6.573	9.560
H	4.344	-7.111	10.998
H	3.613	-7.234	9.372
H	4.719	-4.338	8.456
H	3.104	-4.976	8.071
H	3.271	-3.428	8.942

Zip_DIBP_Beta_5.9

C	6.571	5.710	15.591
C	6.568	6.985	15.008
C	6.882	7.123	13.637
C	7.223	5.987	12.894
C	7.285	4.733	13.503
C	6.945	4.592	14.848
C	6.674	8.390	12.845
O	7.682	9.212	12.585
C	9.033	9.009	13.116
C	10.047	9.327	12.021
C	6.310	8.130	15.924
O	7.072	9.183	15.632
C	7.045	10.358	16.521
C	7.944	10.178	17.743
O	5.546	8.073	16.895
Mg	3.596	8.305	17.654
Cl	3.596	10.381	16.324
Mg	1.798	11.419	17.654
Cl	1.798	13.495	16.325
Mg	3.596	14.533	17.653
Cl	3.596	16.609	16.325
Mg	1.798	17.647	17.654
Cl	1.798	19.724	16.324
Cl	3.596	6.229	18.982
Mg	1.798	5.190	17.654
Cl	1.798	3.114	18.982
Mg	3.596	2.076	17.654
Cl	3.596	4.152	16.325
Cl	1.798	1.038	16.325
Mg	1.798	-1.037	17.654
Cl	3.596	-2.075	16.325
Mg	3.596	-4.151	17.654
Cl	3.596	-6.228	18.982
Cl	3.596	0.000	18.982
Cl	1.798	-3.113	18.982
Cl	1.798	7.267	16.324
Cl	1.798	9.343	18.982
Cl	3.596	12.457	18.982
Cl	1.798	15.571	18.981
O	5.584	8.644	12.333
Mg	3.596	8.305	11.727
Cl	3.596	10.380	10.398
Mg	1.798	11.419	11.727
Cl	1.798	13.495	10.398
Mg	3.596	14.532	11.727

Cl	3.596	16.608	10.398
Mg	1.798	17.647	11.727
Cl	1.798	19.723	10.398
Cl	3.596	6.229	13.055
Mg	1.798	5.190	11.727
Cl	3.596	4.152	10.398
Mg	3.596	2.076	11.727
Cl	1.798	1.038	10.398
Mg	1.798	-1.037	11.727
Cl	1.797	-3.113	13.055
Mg	3.596	-4.151	11.727
Cl	3.596	-6.228	13.055
Cl	3.596	0.000	13.055
Cl	3.596	-2.075	10.398
Cl	1.798	3.114	13.055
Cl	1.798	7.267	10.398
Cl	1.798	9.343	13.055
Cl	3.596	12.456	13.055
Cl	1.798	15.571	13.055
H	7.425	6.083	11.825
H	7.581	3.864	12.913
H	6.960	3.609	15.320
H	6.284	5.614	16.638
H	9.131	9.697	13.967
H	9.135	7.976	13.476
H	11.028	9.181	12.510
C	9.948	8.346	10.846
C	9.953	10.786	11.558
H	6.003	10.561	16.793
H	7.413	11.167	15.873
C	7.800	11.424	18.628
H	7.566	9.312	18.313
C	9.405	9.920	17.362
H	8.408	11.321	19.538
H	8.151	12.326	18.098
H	6.756	11.587	18.935
H	10.021	9.773	18.260
H	9.512	9.023	16.734
H	9.823	10.777	16.808
H	10.741	11.011	10.826
H	8.983	10.986	11.082
H	10.069	11.484	12.402
H	10.744	8.539	10.114
H	10.047	7.302	11.180
H	8.986	8.454	10.323

Zip_DIBP_Beta_6.3

Mg	1.798	-1.038	11.727
Cl	3.596	0.000	13.055
Mg	3.596	2.076	11.727
Cl	1.798	3.114	13.055
Mg	1.798	5.190	11.727
Cl	3.596	6.229	13.055
Mg	3.596	8.305	11.727
Cl	1.798	9.343	13.055
Mg	1.798	11.418	11.727
Cl	3.596	12.456	13.055
Mg	3.596	14.532	11.727
Cl	1.797	15.570	13.055
Mg	1.797	17.646	11.727
Cl	3.595	16.608	10.398

Cl	1.798	1.038	10.398
Cl	3.596	-2.076	10.398
Mg	3.596	-4.152	11.727
Cl	3.596	-6.229	13.055
Cl	1.798	-3.114	13.055
Cl	1.798	7.267	10.398
Cl	3.596	4.152	10.398
Cl	1.797	13.494	10.398
Cl	3.596	10.380	10.398
Cl	1.797	19.723	10.398
Cl	1.798	1.038	16.698
Mg	3.596	2.076	18.027
Cl	3.596	0.000	19.355
Mg	1.798	-1.038	18.027
Cl	1.798	-3.114	19.355
Mg	3.596	-4.152	18.027
Cl	3.596	-6.229	19.355
Cl	3.596	-2.076	16.698
Cl	3.596	4.152	16.698
Mg	1.798	5.190	18.027
Cl	3.596	6.229	19.355
Mg	3.596	8.305	18.027
Cl	1.798	9.343	19.355
Mg	1.798	11.419	18.027
Cl	3.596	12.457	19.355
Mg	3.596	14.533	18.027
Cl	1.798	15.571	19.355
Mg	1.798	17.646	18.027
Cl	3.595	16.609	16.698
Cl	1.798	7.267	16.698
Cl	1.798	3.114	19.355
Cl	1.798	13.495	16.698
Cl	3.596	10.381	16.698
Cl	1.797	19.723	16.698
O	-0.068	5.566	12.554
O	0.084	4.668	16.924
C	-1.170	5.604	13.097
C	-0.856	5.105	16.257
C	-1.548	4.208	15.270
C	-1.742	4.457	13.893
C	-2.005	2.995	15.815
C	-2.701	2.074	15.037
C	-2.921	2.336	13.685
C	-2.428	3.510	13.118
H	-1.800	2.789	16.867
H	-3.060	1.147	15.488
H	-3.464	1.622	13.063
H	-2.564	3.692	12.051
O	-1.272	6.347	16.485
C	-2.592	6.867	16.132
C	-2.478	8.365	15.873
H	-2.996	6.338	15.259
H	-3.237	6.670	17.004
C	-3.879	8.914	15.573
C	-1.814	9.106	17.038
H	-1.847	8.495	14.978
H	-3.824	9.981	15.313
H	-4.360	8.387	14.736
H	-4.534	8.824	16.453
H	-1.768	10.183	16.815
H	-2.394	8.985	17.967
H	-0.794	8.736	17.217

O	-2.021	6.606	12.916
C	-1.571	7.683	12.002
C	-2.769	8.538	11.619
H	-0.787	8.246	12.529
H	-1.110	7.214	11.122
C	-3.831	7.734	10.861
H	-3.218	8.938	12.544
C	-2.261	9.723	10.781
H	-4.683	8.374	10.590
H	-3.415	7.319	9.929
H	-4.215	6.900	11.465
H	-3.093	10.382	10.499
H	-1.532	10.326	11.344
H	-1.775	9.376	9.857

Zip_DIBP_Beta_6.6

C	2.097	-0.777	2.581
C	0.718	-1.095	2.454
C	0.220	-1.502	1.205
C	1.058	-1.616	0.096
C	2.413	-1.312	0.222
C	2.919	-0.885	1.450
C	-0.289	-0.781	3.510
O	-1.290	-1.642	3.856
C	-1.321	-3.093	3.647
C	-2.780	-3.526	3.548
C	2.805	-0.323	3.837
O	2.724	-1.032	4.955
C	2.118	-2.357	5.029
C	2.868	-3.165	6.082
O	3.543	0.663	3.816
Mg	4.178	2.544	4.714
Cl	4.750	4.928	4.973
Mg	2.833	5.697	3.626
Cl	4.042	5.476	1.489
Mg	2.126	6.245	0.143
Cl	2.698	8.628	0.401
Mg	0.781	9.397	-0.944
Cl	1.991	9.176	-3.080
Mg	0.074	9.944	-4.427
Cl	-1.841	10.714	-5.774
O	-0.346	0.309	4.056
Mg	-2.017	0.209	5.605
Cl	-1.445	2.593	5.864
Mg	-3.362	3.362	4.517
Cl	-2.153	3.141	2.380
Mg	-4.069	3.909	1.034
Cl	-3.497	6.293	1.292
Mg	-5.414	7.062	-0.053
Cl	-4.204	6.840	-2.189
Mg	-6.121	7.609	-3.536
Cl	-8.037	8.379	-4.883
Cl	-3.932	0.978	4.259
Cl	-3.225	0.431	7.742
Mg	-1.310	-0.337	9.088
Cl	0.606	-1.106	10.434
Mg	0.034	-3.490	10.176
Cl	1.950	-4.259	11.522
Mg	0.741	-4.037	13.658
Cl	2.658	-4.807	15.005
Cl	-0.101	-0.559	6.951

Cl	2.262	3.313	3.368
Cl	2.970	2.766	6.851
Mg	4.885	1.997	8.197
Cl	6.801	1.228	9.543
Mg	6.230	-1.155	9.285
Cl	8.146	-1.924	10.631
Mg	6.937	-1.702	12.767
Cl	8.853	-2.471	14.114
Cl	6.094	1.775	6.060
Cl	-1.881	-2.721	8.829
Cl	-1.174	-3.268	12.312
Cl	4.314	-0.386	7.938
Cl	5.021	-0.933	11.421
Cl	-5.277	4.131	3.170
Cl	-5.985	4.678	-0.312
Cl	-7.329	7.831	-1.399
Cl	0.917	6.466	2.279
Cl	0.210	7.014	-1.203
Cl	-1.133	10.166	-2.290
H	3.079	-1.389	-0.638
C	-3.471	-2.937	2.315
H	3.974	-0.625	1.548
H	-0.754	-3.349	2.740
H	-3.291	-3.148	4.450
C	2.116	-4.480	6.321
H	1.075	-2.216	5.341
H	-0.850	-1.682	1.093
H	2.849	-2.564	7.005
H	2.170	-2.845	4.043
H	0.645	-1.923	-0.865
C	-2.850	-5.058	3.571
H	-0.832	-3.546	4.522
C	4.325	-3.407	5.683
H	-3.897	-5.389	3.528
H	-2.329	-5.498	2.706
H	-2.407	-5.475	4.488
H	2.612	-5.070	7.106
H	1.073	-4.301	6.630
H	2.095	-5.104	5.413
H	4.848	-3.988	6.457
H	4.390	-3.979	4.742
H	4.860	-2.456	5.551
H	-4.527	-3.238	2.285
H	-3.445	-1.838	2.323
H	-2.998	-3.298	1.387

Zip_DIBP_Beta_7.9

C	1.991	1.520	2.805
C	0.836	1.621	2.001
C	0.635	2.784	1.243
C	1.566	3.819	1.255
C	2.712	3.711	2.045
C	2.917	2.573	2.825
C	-0.222	0.566	1.904
O	0.181	-0.604	2.453
C	-0.824	-1.671	2.517
C	-0.143	-3.020	2.701
C	2.280	0.386	3.751
O	1.874	0.373	4.913
Mg	0.902	1.041	6.602
Cl	0.824	2.482	8.600

Mg	0.072	4.462	7.338
Cl	2.362	5.146	6.738
Mg	1.610	7.126	5.476
Cl	1.532	8.567	7.474
Mg	0.780	10.546	6.212
Cl	3.071	11.231	5.612
Mg	2.318	13.210	4.350
Cl	1.566	15.190	3.088
O	3.123	-0.576	3.390
C	3.649	-0.655	2.025
C	4.588	-1.852	1.959
O	-1.305	0.740	1.368
Cl	-1.388	0.356	7.203
Mg	-0.636	-1.622	8.465
Cl	0.116	-3.601	9.727
Mg	0.193	-5.043	7.729
Cl	0.945	-7.022	8.991
Mg	-1.344	-7.707	9.591
Cl	-0.592	-9.686	10.853
Cl	1.654	-0.937	7.864
Cl	0.149	3.020	5.340
Cl	-0.558	-3.064	6.467
Cl	-0.680	6.441	6.076
Cl	0.858	9.105	4.214
Cl	0.028	12.526	4.950
Cl	-2.096	-5.728	8.329
Cl	-4.274	-1.231	2.546
Mg	-6.565	-1.916	3.147
Cl	-5.812	-3.895	4.409
Mg	-5.735	-5.337	2.411
Cl	-4.983	-7.316	3.673
Mg	-7.273	-8.001	4.273
Cl	-6.521	-9.980	5.535
Mg	-5.026	0.747	1.284
Cl	-5.104	2.188	3.282
Mg	-5.856	4.168	2.020
Cl	-3.566	4.852	1.420
Mg	-4.318	6.832	0.158
Cl	-4.396	8.273	2.156
Mg	-5.148	10.252	0.894
Cl	-2.858	10.937	0.293
Mg	-3.610	12.916	-0.968
Cl	-4.362	14.895	-2.230
Cl	-7.317	0.062	1.885
Cl	-5.779	2.726	0.022
Cl	-6.487	-3.358	1.149
Cl	-6.609	6.147	0.758
Cl	-5.071	8.811	-1.103
Cl	-5.901	12.231	-0.367
Cl	-8.025	-6.022	3.011
H	0.477	-2.963	3.610
C	0.734	-3.399	1.504
H	4.008	-2.738	2.271
H	4.185	0.277	1.791
H	-0.279	2.854	0.654
H	3.794	2.509	3.472
C	5.036	-2.055	0.505
C	-1.236	-4.074	2.936
C	5.782	-1.689	2.904
H	2.801	-0.764	1.331
H	-1.490	-1.439	3.359
H	1.393	4.713	0.653

H	3.449	4.517	2.065
H	-1.416	-1.639	1.591
H	-0.787	-5.068	3.076
H	-1.838	-3.840	3.825
H	-1.907	-4.134	2.064
H	1.230	-4.367	1.672
H	0.130	-3.488	0.586
H	1.516	-2.649	1.320
H	5.699	-2.928	0.427
H	4.183	-2.220	-0.169
H	5.598	-1.181	0.136
H	6.423	-2.582	2.871
H	6.400	-0.825	2.609
H	5.459	-1.542	3.943

Zip_DEP_Alpha_5.9

Mg	7.266	5.394	11.726
Cl	6.228	7.192	13.055
Cl	8.304	7.192	10.397
Mg	7.266	8.989	11.726
Cl	9.342	8.990	13.055
Cl	8.304	10.788	10.398
Mg	10.380	10.788	11.726
Cl	9.342	12.586	13.055
Cl	11.418	12.586	10.397
Mg	10.380	14.384	11.726
Cl	11.418	16.182	10.398
Cl	6.228	3.596	13.055
Cl	5.190	5.394	10.398
Mg	4.152	3.596	11.726
Cl	3.114	1.797	13.055
Cl	5.190	1.797	10.398
Mg	4.152	0.000	11.726
Cl	3.114	-1.798	13.055
Cl	2.076	0.000	10.398
Mg	1.038	-1.798	11.726
Cl	0.000	-3.595	13.055
Cl	2.076	-3.596	10.398
Mg	1.038	-5.393	11.726
Cl	-0.000	-7.192	13.055
Mg	6.228	3.596	17.590
Cl	5.190	5.394	18.918
Cl	7.266	5.394	16.261
Mg	6.228	7.192	17.590
Cl	8.304	7.192	18.918
Cl	7.266	8.990	16.261
Mg	9.342	8.990	17.590
Cl	8.304	10.788	18.918
Cl	10.380	10.788	16.261
Mg	9.342	12.586	17.590
Cl	10.380	14.384	16.261
Mg	3.114	1.797	17.590
Cl	5.190	1.797	18.918
Cl	4.152	3.596	16.261
Mg	0.000	-3.595	17.590
Cl	2.076	-3.596	18.918
Cl	1.038	-1.798	16.261
Mg	-0.000	-7.192	17.590

Cl	-1.038	-5.394	18.918
Cl	1.038	-5.393	16.261
Cl	-1.038	-8.989	18.918
C	8.853	2.310	16.150
C	9.761	3.471	15.832
C	10.385	4.020	16.960
C	11.192	5.153	16.864
C	11.329	5.802	15.637
C	10.685	5.291	14.512
C	9.936	4.104	14.576
C	9.387	3.656	13.261
H	10.221	3.559	17.936
H	11.689	5.534	17.758
H	11.936	6.705	15.544
H	10.758	5.807	13.554
O	7.847	2.413	16.864
O	9.289	1.139	15.715
C	8.499	-0.044	16.099
H	8.295	0.016	17.177
H	7.534	0.014	15.573
C	9.310	-1.263	15.727
H	8.744	-2.168	15.992
H	10.264	-1.286	16.272
H	9.522	-1.294	14.650
O	9.039	4.459	12.378
O	9.408	2.343	13.080
C	8.971	1.837	11.770
C	9.059	0.329	11.814
H	7.944	2.182	11.596
H	9.635	2.272	11.008
H	8.759	-0.073	10.837
H	10.081	-0.013	12.028
H	8.384	-0.080	12.578

Zip_DEP_Alpha_6.6

C	7.279	4.797	15.183
C	6.766	6.102	15.244
C	6.638	6.847	14.042
C	7.079	6.268	12.840
C	7.646	4.997	12.805
C	7.734	4.252	13.982
C	6.354	6.508	16.640
O	7.123	7.329	17.352
C	5.986	8.187	13.898
O	6.081	8.954	14.977
C	5.397	10.260	14.915
C	5.795	11.053	16.140
O	5.384	5.988	17.192
Mg	3.595	6.229	18.326
Cl	3.596	8.304	16.997
Mg	1.797	9.343	18.326
Cl	1.798	11.419	16.997
Mg	3.595	12.456	18.327
Cl	3.595	14.532	16.998
Mg	1.797	15.570	18.326
Cl	1.797	17.646	16.998
Cl	3.595	4.152	19.654
Mg	1.798	3.114	18.326
Cl	1.797	1.038	19.654
Mg	3.596	0.000	18.326
Cl	3.596	2.076	16.997

Cl	1.798	-1.038	16.997
Mg	1.798	-3.114	18.326
Cl	3.596	-4.151	16.997
Mg	3.596	-6.229	18.326
Cl	3.596	-8.305	19.654
Cl	3.596	-2.076	19.654
Cl	1.798	-5.190	19.654
Cl	1.798	5.190	16.997
Cl	1.797	7.267	19.654
Cl	3.595	10.381	19.655
Cl	1.797	13.494	19.654
O	5.442	8.568	12.849
Mg	3.596	8.305	11.726
Cl	3.596	10.380	10.398
Mg	1.798	11.418	11.727
Cl	1.797	13.494	10.398
Mg	3.596	14.532	11.727
Cl	3.595	16.608	10.398
Mg	1.797	17.646	11.727
Cl	1.797	19.723	10.398
Cl	3.596	6.229	13.054
Mg	1.798	5.190	11.726
Cl	3.596	4.152	10.397
Mg	3.596	2.076	11.727
Cl	1.798	1.038	10.397
Mg	1.798	-1.038	11.726
Cl	1.797	-3.114	13.054
Mg	3.596	-4.152	11.727
Cl	3.596	-6.229	13.055
Cl	3.596	0.000	13.055
Cl	3.596	-2.076	10.398
Cl	1.797	3.114	13.054
Cl	1.798	7.267	10.397
Cl	1.797	9.343	13.055
Cl	3.596	12.456	13.055
Cl	1.797	15.570	13.055
H	6.956	6.838	11.919
H	7.996	4.585	11.857
H	8.144	3.241	13.971
H	7.314	4.202	16.097
H	5.693	10.753	13.980
H	4.318	10.064	14.886
H	5.310	12.040	16.058
H	5.472	10.528	17.053
H	6.881	11.224	16.188
C	8.404	7.826	16.832
C	9.100	8.531	17.975
H	8.987	6.970	16.463
H	8.194	8.507	15.998
H	10.066	8.922	17.625
H	8.498	9.374	18.343
H	9.287	7.845	18.811

Zip_DEP_Beta_5.9

Mg	1.798	-1.038	11.727
Cl	3.596	0.000	13.055
Mg	3.596	2.076	11.727
Cl	1.798	3.114	13.055
Mg	1.798	5.190	11.727
Cl	3.596	6.229	13.055
Mg	3.596	8.305	11.727

Cl	1.798	9.343	13.055
Mg	1.798	11.418	11.727
Cl	3.596	12.456	13.055
Mg	3.596	14.532	11.727
Cl	1.797	15.570	13.055
Mg	1.797	17.646	11.727
Cl	3.595	16.608	10.398
Cl	1.798	1.038	10.398
Cl	3.596	-2.076	10.398
Mg	3.596	-4.152	11.727
Cl	3.596	-6.229	13.055
Cl	1.798	-3.114	13.055
Cl	1.798	7.267	10.398
Cl	3.596	4.152	10.398
Cl	1.797	13.494	10.398
Cl	3.596	10.380	10.398
Cl	1.797	19.723	10.398
Cl	1.798	1.038	16.325
Mg	3.596	2.076	17.654
Cl	3.596	0.000	18.982
Mg	1.798	-1.037	17.654
Cl	1.798	-3.113	18.982
Mg	3.596	-4.151	17.654
Cl	3.596	-6.228	18.982
Cl	3.596	-2.076	16.325
Cl	3.596	4.152	16.325
Mg	1.798	5.190	17.654
Cl	3.596	6.229	18.982
Mg	3.596	8.305	17.654
Cl	1.798	9.343	18.982
Mg	1.798	11.419	17.653
Cl	3.596	12.457	18.981
Mg	3.596	14.533	17.653
Cl	1.798	15.571	18.981
Mg	1.798	17.647	17.653
Cl	3.596	16.609	16.324
Cl	1.798	7.267	16.324
Cl	1.798	3.114	18.982
Cl	1.798	13.495	16.324
Cl	3.596	10.381	16.324
Cl	1.798	19.724	16.324
O	5.549	8.072	16.912
O	5.582	8.663	12.344
C	6.311	8.137	15.941
C	6.670	8.415	12.861
C	6.883	7.145	13.647
C	6.570	6.999	15.017
C	7.227	6.014	12.898
C	7.291	4.757	13.501
C	6.950	4.608	14.843
C	6.574	5.721	15.593
H	7.427	6.115	11.829
H	7.589	3.891	12.905
H	6.966	3.623	15.311
H	6.286	5.618	16.639
O	7.675	9.248	12.614
C	9.018	9.047	13.163
C	10.020	9.358	12.072
H	9.106	9.739	14.011
H	9.115	8.019	13.538
H	11.038	9.270	12.478
H	9.924	8.659	11.230

H	9.886	10.380	11.694
O	7.073	9.194	15.661
C	7.053	10.352	16.575
H	6.013	10.554	16.856
C	7.958	10.113	17.768
H	7.415	11.170	15.939
H	7.980	11.024	18.385
H	7.587	9.294	18.398
H	8.988	9.887	17.458

Zip_DEP_Beta_6.6

C	2.678	0.304	-0.813
C	2.849	-0.024	0.538
C	3.648	1.032	-1.499
C	4.803	1.451	-0.834
C	4.990	1.129	0.510
C	4.030	0.374	1.199
C	4.332	0.058	2.635
O	4.400	0.945	3.481
O	4.640	-1.180	3.010
C	4.688	-2.287	2.052
C	5.516	-3.386	2.681
C	1.727	-0.755	1.204
O	0.874	-1.392	0.612
O	1.773	-0.607	2.555
C	0.758	-1.311	3.323
C	-0.577	-0.581	3.290
Mg	-2.017	0.209	5.605
Mg	4.178	2.544	4.714
H	5.561	2.036	-1.357
H	-0.469	0.442	3.689
H	5.890	1.460	1.033
H	0.653	-2.328	2.919
H	-1.305	-1.200	3.853
H	5.551	-4.250	2.003
H	3.657	-2.618	1.861
H	1.759	-0.016	-1.306
H	5.077	-3.712	3.634
H	5.125	-1.932	1.108
H	3.498	1.280	-2.551
H	-0.986	-0.499	2.276
H	1.167	-1.347	4.341
H	6.545	-3.050	2.866
Cl	-3.932	0.978	4.259
Cl	2.262	3.313	3.368
Cl	-3.225	0.431	7.742
Mg	-1.310	-0.337	9.088
Cl	-1.881	-2.721	8.829
Mg	0.034	-3.490	10.176
Cl	-1.174	-3.268	12.312
Mg	0.741	-4.037	13.658
Cl	2.970	2.766	6.851
Mg	4.885	1.997	8.197
Cl	4.314	-0.386	7.938
Mg	6.230	-1.155	9.285
Cl	5.021	-0.933	11.421
Mg	6.937	-1.702	12.767
Mg	-3.362	3.362	4.517
Cl	-5.277	4.131	3.170
Mg	-4.069	3.909	1.034
Cl	-5.985	4.678	-0.312

Mg	-5.414	7.062	-0.053
Cl	-7.329	7.831	-1.399
Mg	-6.121	7.609	-3.536
Mg	2.833	5.697	3.626
Cl	0.917	6.466	2.279
Mg	2.126	6.245	0.143
Cl	0.210	7.014	-1.203
Mg	0.781	9.397	-0.944
Cl	-1.133	10.166	-2.290
Mg	0.074	9.944	-4.427
Cl	-0.101	-0.559	6.951
Cl	-2.153	3.141	2.380
Cl	6.094	1.775	6.060
Cl	-3.497	6.293	1.292
Cl	2.698	8.628	0.401
Cl	0.606	-1.106	10.434
Cl	4.042	5.476	1.489
Cl	6.801	1.228	9.543
Cl	-4.204	6.840	-2.189
Cl	1.991	9.176	-3.080
Cl	1.950	-4.259	11.522
Cl	8.146	-1.924	10.631
Cl	-1.445	2.593	5.864
Cl	4.750	4.928	4.973
Cl	-1.841	10.714	-5.774
Cl	-8.037	8.379	-4.883
Cl	2.658	-4.807	15.005
Cl	8.853	-2.471	14.114

Zip_p-iso-propoxy_EB_Alpha_5.9

Mg	1.038	-1.798	11.726
Cl	3.114	-1.798	13.055
Mg	4.152	0.000	11.726
Cl	3.114	1.797	13.055
Mg	4.152	3.596	11.726
Cl	6.228	3.596	13.055
Mg	7.266	5.394	11.726
Cl	6.228	7.192	13.055
Mg	7.266	8.989	11.726
Cl	9.342	8.990	13.055
Mg	10.380	10.788	11.726
Cl	9.342	12.586	13.055
Mg	10.380	14.384	11.726
Cl	11.418	12.586	10.398
Cl	2.076	0.000	10.398
Cl	2.076	-3.596	10.398
Mg	1.038	-5.393	11.726
Cl	-0.000	-7.192	13.055
Cl	0.000	-3.595	13.055
Cl	5.190	5.394	10.398
Cl	5.190	1.797	10.398
Cl	8.304	10.788	10.398
Cl	8.304	7.192	10.397
Cl	11.418	16.182	10.398
Cl	1.038	-1.798	16.261
Mg	3.114	-1.798	17.590
Cl	2.076	-3.596	18.918
Mg	0.000	-3.595	17.590
Cl	-1.038	-5.394	18.918
Mg	-0.000	-7.192	17.590

Cl	-1.038	-8.989	18.918
Cl	1.038	-5.393	16.261
Cl	4.152	0.000	16.261
Mg	3.114	1.797	17.590
Cl	5.190	1.797	18.918
Mg	6.228	3.596	17.590
Cl	5.190	5.394	18.918
Mg	6.228	7.192	17.590
Cl	8.304	7.192	18.918
Mg	9.342	8.990	17.590
Cl	8.304	10.788	18.918
Mg	9.342	12.586	17.590
Cl	10.380	10.788	16.261
Cl	4.152	3.596	16.261
Cl	2.076	0.000	18.918
Cl	7.266	8.990	16.261
Cl	7.266	5.394	16.261
Cl	10.380	14.384	16.261
O	9.176	4.265	11.912
C	9.508	3.815	13.198
C	9.034	2.578	13.649
C	9.054	2.303	15.012
C	9.631	3.217	15.906
C	10.267	4.367	15.413
C	10.180	4.685	14.057
H	8.527	1.904	12.961
H	8.557	1.410	15.395
C	9.314	3.118	17.351
H	10.726	5.069	16.109
H	10.551	5.637	13.676
C	9.792	3.535	10.764
C	8.786	3.543	9.628
C	11.117	4.197	10.427
H	9.953	2.504	11.118
H	11.609	3.650	9.610
H	10.953	5.235	10.106
H	11.794	4.192	11.293
H	9.189	2.975	8.777
H	7.838	3.065	9.920
H	8.596	4.566	9.270
O	10.313	3.448	18.161
O	8.185	2.807	17.771
C	10.002	3.555	19.599
C	11.316	3.612	20.343
H	9.404	4.469	19.729
H	9.392	2.688	19.885
H	11.114	3.716	21.419
H	11.900	2.695	20.192
H	11.921	4.472	20.025

**Zip_p-
isopropoxy_EB_Alpha_6.3**

Mg	1.798	-1.038	11.727
Cl	3.596	0.000	13.055
Mg	3.596	2.076	11.727
Cl	1.798	3.114	13.055
Mg	1.798	5.190	11.727
Cl	3.596	6.229	13.055
Mg	3.596	8.305	11.727
Cl	1.798	9.343	13.055
Mg	1.798	11.418	11.727

Cl	3.596	12.456	13.055
Mg	3.596	14.532	11.727
Cl	1.797	15.570	13.055
Mg	1.797	17.646	11.727
Cl	3.595	16.608	10.398
Cl	1.798	1.038	10.398
Cl	3.596	-2.076	10.398
Mg	3.596	-4.152	11.727
Cl	3.596	-6.229	13.055
Cl	1.798	-3.114	13.055
Cl	1.798	7.267	10.398
Cl	3.596	4.152	10.398
Cl	1.797	13.494	10.398
Cl	3.596	10.380	10.398
Cl	1.797	19.723	10.398
Cl	1.798	-1.038	16.698
Mg	3.596	0.000	18.027
Cl	3.596	-2.076	19.355
Mg	1.798	-3.113	18.027
Cl	1.798	-5.189	19.355
Mg	3.596	-6.228	18.027
Cl	3.595	-8.304	19.355
Cl	3.596	-4.152	16.698
Cl	3.596	2.076	16.698
Mg	1.798	3.114	18.027
Cl	3.596	4.152	19.355
Mg	3.596	6.229	18.027
Cl	1.798	7.267	19.355
Mg	1.798	9.343	18.027
Cl	3.596	10.381	19.355
Mg	3.596	12.457	18.027
Cl	1.798	13.495	19.355
Mg	1.798	15.571	18.027
Cl	3.596	14.533	16.698
Cl	1.798	5.190	16.698
Cl	1.798	1.038	19.355
Cl	1.798	11.419	16.698
Cl	3.596	8.305	16.698
Cl	1.798	17.647	16.698
O	5.937	6.383	17.735
C	6.342	6.593	16.401
C	7.049	6.333	18.734
C	6.441	5.961	20.071
H	7.720	5.529	18.385
C	7.800	7.655	18.791
C	6.426	7.896	15.898
C	6.545	8.096	14.527
C	6.663	6.998	13.664
C	6.728	5.699	14.196
C	6.541	5.493	15.564
H	6.286	8.741	16.567
H	6.491	9.105	14.116
C	6.478	7.205	12.207
H	6.821	4.847	13.524
H	6.473	4.482	15.971
O	7.186	6.380	11.443
O	5.697	8.051	11.734
C	6.917	6.413	9.994
C	8.003	5.612	9.314
H	5.918	5.977	9.841
H	6.900	7.462	9.671
H	7.816	5.603	8.231

H	8.993	6.053	9.488
H	8.013	4.571	9.666
H	7.240	5.906	20.823
H	5.728	6.731	20.408
H	5.930	4.992	20.040
H	8.601	7.572	19.540
H	8.268	7.914	17.833
H	7.127	8.469	19.097

**Zip_p-
isopropoxy_EB_Alpha_6.6**

C	6.292	5.321	15.630
C	6.209	6.354	16.568
C	6.435	7.682	16.187
C	6.584	7.994	14.837
C	6.612	6.972	13.880
C	6.537	5.632	14.294
O	5.743	6.080	17.872
C	6.736	5.644	18.905
C	7.757	6.741	19.154
C	6.480	7.290	12.433
O	5.710	8.158	11.986
Mg	3.596	8.305	11.727
Cl	3.596	10.381	10.398
Mg	1.798	11.418	11.727
Cl	1.798	13.495	10.398
Mg	3.596	14.532	11.727
Cl	3.596	16.608	10.398
Mg	1.798	17.646	11.727
Cl	1.798	19.723	10.398
Cl	3.596	6.229	13.055
Mg	1.798	5.190	11.727
Cl	3.596	4.152	10.398
Mg	3.595	2.076	11.727
Cl	1.797	1.038	10.397
Mg	1.797	-1.037	11.726
Cl	1.797	-3.113	13.054
Mg	3.595	-4.151	11.726
Cl	3.595	-6.228	13.054
Cl	3.595	0.000	13.054
Cl	3.595	-2.076	10.397
Cl	1.797	3.114	13.055
Cl	1.798	7.267	10.398
Cl	1.798	9.343	13.055
Cl	3.596	12.456	13.055
Cl	1.798	15.570	13.055
Mg	3.596	6.229	18.326
Cl	3.596	8.305	16.997
Mg	1.798	9.343	18.326
Cl	1.798	11.419	16.997
Mg	3.596	12.457	18.327
Cl	3.595	14.533	16.997
Mg	1.797	15.571	18.326
Cl	1.797	17.647	16.998
Cl	3.596	4.152	19.654
Mg	1.798	3.114	18.326
Cl	1.798	1.038	19.654
Mg	3.596	0.000	18.326
Cl	3.596	2.076	16.997
Cl	1.798	-1.037	16.998
Mg	1.798	-3.113	18.326

Cl	3.596	-4.151	16.997
Mg	3.596	-6.228	18.326
Cl	3.596	-8.304	19.654
Cl	3.596	-2.075	19.654
Cl	1.798	-5.189	19.654
Cl	1.797	5.190	16.997
Cl	1.798	7.267	19.654
Cl	3.596	10.381	19.654
Cl	1.798	13.495	19.654
O	7.225	6.519	11.646
C	7.026	6.647	10.193
C	8.194	5.971	9.513
H	6.090	5.520	19.787
H	6.377	8.471	16.933
H	6.631	9.037	14.522
H	6.550	4.838	13.547
H	6.084	4.294	15.932
C	7.346	4.300	18.553
H	8.397	6.451	19.999
H	8.405	6.894	18.279
H	7.268	7.692	19.407
H	6.067	6.162	9.954
H	6.954	7.714	9.947
H	8.062	6.037	8.423
H	9.142	6.461	9.773
H	8.259	4.909	9.785
H	7.951	3.953	19.404
H	6.561	3.555	18.364
H	8.007	4.369	17.677

**Zip_p-
isopropoxy_EB_Alpha_7.9**

Mg	3.596	8.305	11.727
Cl	3.596	10.380	10.398
Cl	3.596	6.229	13.055
Mg	1.798	5.190	11.727
Cl	1.798	7.267	10.398
Cl	1.798	3.114	13.054
Mg	3.596	2.076	11.726
Cl	3.596	4.152	10.397
Cl	3.596	0.000	13.054
Mg	1.798	-1.037	11.726
Cl	1.798	1.038	10.397
Cl	1.798	-3.113	13.054
Mg	3.596	-4.151	11.726
Cl	3.596	-2.076	10.397
Cl	3.596	-6.228	13.054
Mg	1.798	11.418	11.727
Cl	1.798	9.343	13.055
Cl	1.797	13.494	10.398
Mg	3.596	14.532	11.727
Cl	3.596	12.456	13.055
Cl	3.595	16.608	10.398
Mg	1.797	17.646	11.727
Cl	1.797	15.570	13.055
Cl	1.797	19.723	10.398
Mg	3.596	6.229	19.627
Cl	3.596	8.305	18.298
Cl	3.596	4.151	20.955
Mg	1.798	9.343	19.627
Cl	1.798	7.267	20.955

Cl	1.798	11.419	18.298
Mg	3.596	12.457	19.627
Cl	3.596	10.380	20.955
Cl	3.596	14.533	18.298
Mg	1.798	15.571	19.627
Cl	1.798	13.495	20.955
Cl	1.798	17.647	18.298
Mg	1.797	3.114	19.626
Cl	1.798	5.190	18.298
Cl	1.797	1.038	20.954
Mg	3.595	0.000	19.626
Cl	3.595	2.076	18.297
Cl	3.595	-2.076	20.954
Mg	1.797	-3.114	19.626
Cl	1.797	-1.038	18.297
Cl	1.797	-5.189	20.954
Mg	3.595	-6.228	19.626
Cl	3.595	-4.152	18.297
Cl	3.595	-8.305	20.954
O	5.628	8.206	11.750
C	6.612	7.573	12.180
O	7.490	7.013	11.343
C	7.173	7.074	9.913
H	6.199	6.587	9.758
H	7.080	8.129	9.622
C	8.282	6.362	9.172
H	9.254	6.847	9.341
H	8.354	5.310	9.480
H	8.070	6.387	8.094
C	6.893	7.353	13.601
C	6.137	8.036	14.573
C	6.278	7.736	15.915
C	7.157	6.715	16.333
C	7.947	6.054	15.372
C	7.809	6.376	14.025
H	5.431	8.810	14.272
H	5.671	8.243	16.666
H	8.645	5.271	15.655
H	8.403	5.840	13.285
O	7.131	6.467	17.674
C	7.985	5.484	18.344
C	9.469	5.834	18.262
C	7.637	4.044	17.968
H	7.978	3.765	16.963
H	8.121	3.366	18.685
H	10.015	5.237	19.006
H	7.674	5.637	19.390
H	9.626	6.896	18.497
H	6.552	3.874	18.020
H	9.913	5.628	17.280

**Zip_p-
isopropoxy_EB_Beta_5.9**

Mg	1.798	-1.038	11.727
Cl	3.596	0.000	13.055
Mg	3.596	2.076	11.727
Cl	1.798	3.114	13.055
Mg	1.798	5.190	11.727
Cl	3.596	6.229	13.055
Mg	3.596	8.305	11.727
Cl	1.798	9.343	13.055

Mg	1.798	11.418	11.727
Cl	3.596	12.456	13.055
Mg	3.596	14.532	11.727
Cl	1.797	15.570	13.055
Mg	1.797	17.646	11.727
Cl	3.595	16.608	10.398
Cl	1.798	1.038	10.398
Cl	3.596	-2.076	10.398
Mg	3.596	-4.152	11.727
Cl	3.596	-6.229	13.055
Cl	1.798	-3.114	13.055
Cl	1.798	7.267	10.398
Cl	3.596	4.152	10.398
Cl	1.797	13.494	10.398
Cl	3.596	10.380	10.398
Cl	1.797	19.723	10.398
Cl	1.798	1.038	16.325
Mg	3.596	2.076	17.654
Cl	3.596	0.000	18.982
Mg	1.798	-1.037	17.654
Cl	1.798	-3.113	18.982
Mg	3.596	-4.151	17.654
Cl	3.596	-6.228	18.982
Cl	3.596	-2.076	16.325
Cl	3.596	4.152	16.325
Mg	1.798	5.190	17.654
Cl	3.596	6.229	18.982
Mg	3.596	8.305	17.654
Cl	1.798	9.343	18.982
Mg	1.798	11.419	17.653
Cl	3.596	12.457	18.981
Mg	3.596	14.533	17.653
Cl	1.798	15.571	18.981
Mg	1.798	17.647	17.653
Cl	3.596	16.609	16.324
Cl	1.798	7.267	16.324
Cl	1.798	3.114	18.982
Cl	1.798	13.495	16.324
Cl	3.596	10.381	16.324
Cl	1.798	19.724	16.324
O	-0.262	4.961	11.500
C	-1.228	4.555	12.153
C	-1.287	4.741	13.632
C	-1.110	3.642	14.486
C	-0.876	3.848	15.844
C	-0.843	5.151	16.344
C	-1.105	6.250	15.520
C	-1.296	6.042	14.157
H	-1.059	2.631	14.083
H	-0.649	3.011	16.505
O	-0.387	5.294	17.661
H	-1.058	7.265	15.910
H	-1.398	6.900	13.491
O	-2.201	3.932	11.492
C	-3.453	3.570	12.168
C	-4.470	3.270	11.089
H	-3.262	2.692	12.801
H	-3.764	4.406	12.811
H	-5.421	2.979	11.558
H	-4.649	4.149	10.457
H	-4.133	2.443	10.450
C	-1.085	6.258	18.556

C	-0.328	6.219	19.871
H	-0.982	7.255	18.098
C	-2.544	5.860	18.687
H	-3.064	6.593	19.321
H	-3.051	5.840	17.712
H	-2.635	4.870	19.155
H	-0.825	6.881	20.593
H	-0.308	5.201	20.284
H	0.701	6.593	19.769

**Zip_p-
isopropoxy_EB_Beta_6.3**

Mg	1.798	-1.038	11.727
Cl	1.798	-3.114	13.055
Mg	3.596	-4.152	11.727
Cl	3.596	-6.229	13.055
Cl	3.596	0.000	13.055
Mg	3.596	2.076	11.727
Cl	3.596	4.152	10.398
Mg	1.798	5.190	11.727
Cl	1.798	7.267	10.398
Mg	3.596	8.305	11.727
Cl	3.596	10.380	10.398
Mg	1.798	11.418	11.727
Cl	1.797	13.494	10.398
Mg	3.596	14.532	11.727
Cl	3.595	16.608	10.398
Mg	1.797	17.646	11.727
Cl	1.797	19.723	10.398
Cl	1.798	1.038	10.398
Cl	3.596	-2.076	10.398
Cl	1.798	3.114	13.055
Cl	3.596	6.229	13.055
Cl	1.798	9.343	13.055
Cl	3.596	12.456	13.055
Cl	1.797	15.570	13.055
Cl	1.798	7.267	16.698
Mg	3.595	8.305	18.027
Cl	3.595	10.381	16.698
Mg	1.797	11.419	18.027
Cl	1.797	13.495	16.698
Mg	3.595	14.533	18.027
Cl	3.595	16.609	16.698
Mg	1.797	17.646	18.027
Cl	1.797	19.723	16.698
Cl	3.596	6.229	19.355
Mg	1.798	5.190	18.027
Cl	1.798	3.114	19.355
Mg	3.596	2.076	18.027
Cl	3.596	4.152	16.698
Cl	1.798	1.038	16.698
Mg	1.798	-1.038	18.027
Cl	3.596	-2.076	16.698
Mg	3.596	-4.151	18.027
Cl	3.596	-6.228	19.355
Cl	3.596	0.000	19.355
Cl	1.798	-3.113	19.355
Cl	1.797	9.343	19.355
Cl	3.595	12.457	19.355
Cl	1.797	15.571	19.355
O	5.728	8.374	18.127

C	6.623	8.043	19.279
C	6.242	8.439	16.822
C	5.944	7.375	15.968
C	6.136	7.533	14.600
C	6.650	8.734	14.094
C	7.061	9.748	14.975
C	6.841	9.609	16.344
H	5.492	6.460	16.357
H	5.833	6.738	13.921
C	6.593	8.957	12.630
H	7.463	10.681	14.580
H	7.032	10.438	17.024
O	7.610	9.665	12.147
O	5.666	8.528	11.924
C	7.593	10.050	10.726
C	7.254	11.521	10.596
H	8.611	9.828	10.381
H	6.871	9.417	10.198
H	7.322	11.809	9.537
H	6.224	11.706	10.931
H	7.954	12.143	11.170
C	7.470	9.247	19.654
H	5.885	7.841	20.068
C	7.417	6.783	18.995
H	7.977	9.043	20.609
H	8.246	9.448	18.902
H	6.847	10.142	19.784
H	7.991	6.511	19.892
H	6.748	5.947	18.751
H	8.131	6.933	18.171

**Zip_p-
isopropoxy_EB_Beta_6.6**

Mg	1.798	5.190	11.727
Cl	3.596	4.1520	10.398
Cl	1.798	3.1140	13.055
Mg	3.596	8.3050	11.727
Cl	1.798	7.2670	10.398
Cl	3.596	6.2290	13.055
Mg	1.797	11.4189	11.727
Cl	3.596	10.3810	10.398
Cl	1.797	9.3430	13.055
Mg	3.595	14.5329	11.727
Cl	1.797	13.4949	10.398
Cl	3.595	12.4570	13.055
Mg	1.797	17.6469	11.727
Cl	3.595	16.6089	10.398
Cl	1.797	15.5709	13.055
Cl	1.797	19.7239	10.398
Mg	3.596	2.0760	11.727
Cl	1.798	1.0380	10.398
Cl	3.596	0.0000	13.055
Mg	1.798	-1.0379	11.727
Cl	1.798	-3.1139	13.055
Cl	3.596	-2.0759	10.398
Mg	3.596	-4.1519	11.727
Cl	3.596	-6.2289	13.055
Mg	1.797	5.1900	18.408
Cl	1.797	7.2670	17.079
Cl	3.595	6.2290	19.736
Cl	3.595	4.1520	17.079

Cl	1.797	3.1140	19.736
Mg	3.595	2.0760	18.408
Cl	1.797	1.0380	17.079
Cl	3.595	0.0000	19.736
Mg	1.797	-1.0379	18.408
Cl	3.595	-2.0759	17.079
Cl	1.797	-3.1139	19.736
Mg	3.595	-4.1519	18.408
Cl	3.595	-6.2289	19.736
Mg	3.595	8.3050	18.408
Cl	3.595	10.3810	17.078
Cl	1.797	9.3430	19.736
Mg	1.798	11.4190	18.408
Cl	1.797	13.4949	17.078
Cl	3.595	12.4570	19.735
Mg	3.595	14.5330	18.407
Cl	3.595	16.6089	17.079
Cl	1.797	15.5710	19.736
Mg	1.797	17.6470	18.408
Cl	1.797	19.7239	17.078
O	-0.204	5.5118	12.180
C	-1.054	6.0074	12.938
O	-1.981	6.8598	12.511
C	-1.921	7.2874	11.104
H	-0.868	7.3953	10.815
H	-2.373	6.4854	10.503
C	-2.689	8.5847	10.994
H	-3.734	8.4681	11.314
H	-2.685	8.9186	9.947
H	-2.220	9.3694	11.605
C	-1.115	5.7309	14.392
C	-0.590	4.5232	14.873
C	-0.445	4.3168	16.243
C	-0.801	5.3416	17.120
C	-1.406	6.5161	16.661
C	-1.575	6.7058	15.295
H	-0.242	3.7623	14.176
H	0.009	3.3939	16.613
H	-1.651	7.3028	17.374
H	-1.987	7.6425	14.919
O	-0.376	5.2736	18.457
C	-1.267	4.6354	19.487
C	-0.851	5.2364	20.816
C	-2.733	4.8546	19.168
H	-1.020	3.5626	19.458
H	-3.331	4.3379	19.933
H	-2.998	5.9210	19.194
H	-3.017	4.4424	18.190
H	-1.420	4.7556	21.625
H	0.212	5.0648	21.025
H	-1.056	6.3165	20.837

**Zip_p-
isopropoxy_EB_Beta_7.9**

Mg	1.798	-1.0381	11.726
Cl	3.596	0.0000	13.055
Mg	3.596	2.0762	11.726
Cl	1.798	3.1142	13.055
Mg	1.798	5.1904	11.726
Cl	3.596	6.2285	13.055
Mg	3.596	8.3047	11.726

Cl	1.798	9.3427	13.055
Mg	1.798	11.4188	11.726
Cl	3.596	12.4570	13.055
Mg	3.596	14.5332	11.726
Cl	1.798	15.5712	13.055
Mg	1.798	17.6473	11.726
Cl	3.596	16.6093	10.398
Cl	1.798	1.0381	10.398
Cl	3.596	-2.0762	10.398
Mg	3.596	-4.1523	11.726
Cl	3.595	-6.2285	13.055
Cl	1.798	-3.1142	13.055
Cl	1.798	7.2666	10.398
Cl	3.596	4.1523	10.398
Cl	1.798	13.4951	10.398
Cl	3.596	10.3808	10.398
Cl	1.798	19.7236	10.398
Cl	1.798	1.0381	18.368
Mg	3.596	2.0762	19.696
Cl	3.596	0.0000	21.025
Mg	1.798	-1.0380	19.696
Cl	1.798	-3.1142	21.025
Mg	3.596	-4.1523	19.696
Cl	3.596	-6.2284	21.025
Cl	3.596	-2.0762	18.368
Cl	3.596	4.1523	18.368
Mg	1.797	5.1904	19.696
Cl	3.595	6.2285	21.025
Mg	3.595	8.3047	19.696
Cl	1.797	9.3427	21.025
Mg	1.797	11.4188	19.696
Cl	3.595	12.4570	21.025
Mg	3.595	14.5332	19.696
Cl	1.797	15.5712	21.025
Mg	1.797	17.6473	19.696
Cl	3.595	16.6093	18.367
Cl	1.797	7.2666	18.368
Cl	1.798	3.1142	21.025
Cl	1.797	13.4951	18.367
Cl	3.595	10.3808	18.368
Cl	1.797	19.7236	18.367
O	5.563	8.4581	12.461
C	6.221	7.7191	13.216
O	7.034	6.7700	12.761
C	7.038	6.5267	11.312
C	8.201	5.6098	11.007
H	6.071	6.0676	11.055
H	7.123	7.4942	10.799
C	6.174	7.7880	14.698
C	6.090	6.6038	15.449
C	5.888	6.6579	16.827
C	5.846	7.8998	17.466
C	5.984	9.0851	16.736
C	6.101	9.0288	15.347
O	5.567	7.9525	18.851
H	8.212	5.3899	9.930
H	9.158	6.0786	11.272
H	8.114	4.6592	11.551
C	6.716	7.8345	19.801
H	6.203	7.8916	20.774
C	7.393	6.4796	19.692
C	7.660	9.0150	19.646

H	8.129	6.3849	20.504
H	6.658	5.6707	19.800
H	7.926	6.3678	18.738
H	8.418	8.9780	20.443
H	8.184	8.9855	18.681
H	7.121	9.9687	19.731
H	6.130	9.9510	14.764
H	5.928	10.0452	17.244
H	5.707	5.7471	17.397
H	6.101	5.6404	14.941

Zip_p-ethoxy_EB_Alpha_5.9

C	10.189	4.703	14.057
C	9.516	3.844	13.191
C	9.040	2.602	13.623
C	9.062	2.311	14.983
C	9.638	3.215	15.887
C	10.277	4.369	15.408
O	9.166	4.326	11.917
C	9.781	3.674	10.750
C	11.165	4.220	10.479
C	9.315	3.108	17.331
O	8.185	2.792	17.746
Mg	6.228	3.596	17.590
Cl	7.266	5.394	16.261
Mg	6.228	7.192	17.590
Cl	7.266	8.990	16.261
Mg	9.342	8.990	17.590
Cl	10.380	10.788	16.261
Mg	9.342	12.586	17.590
Cl	10.380	14.384	16.261
Cl	5.190	1.797	18.918
Mg	3.114	1.797	17.590
Cl	2.076	0.000	18.918
Mg	3.114	-1.798	17.589
Cl	4.152	0.000	16.261
Cl	1.038	-1.798	16.261
Mg	0.000	-3.595	17.589
Cl	1.038	-5.393	16.261
Mg	-0.000	-7.192	17.589
Cl	-1.038	-8.989	18.918
Cl	2.076	-3.596	18.918
Cl	-1.038	-5.394	18.918
Cl	4.152	3.596	16.261
Cl	5.190	5.394	18.918
Cl	8.304	7.192	18.918
Cl	8.304	10.788	18.918
O	10.310	3.440	18.144
C	9.992	3.549	19.580
C	11.301	3.667	20.324
H	9.096	3.887	9.917
Mg	7.266	5.394	11.726
Cl	8.304	7.192	10.397
Mg	7.266	8.989	11.726
Cl	8.304	10.788	10.398
Mg	10.380	10.788	11.726
Cl	11.418	12.586	10.398
Mg	10.380	14.384	11.726
Cl	11.418	16.182	10.398
Cl	6.228	3.596	13.055
Mg	4.152	3.596	11.726

Cl	5.190	1.797	10.398
Mg	4.152	0.000	11.726
Cl	2.076	0.000	10.398
Mg	1.038	-1.798	11.726
Cl	0.000	-3.595	13.055
Mg	1.038	-5.393	11.726
Cl	-0.000	-7.192	13.055
Cl	3.114	-1.798	13.055
Cl	2.076	-3.596	10.398
Cl	3.114	1.797	13.055
Cl	5.190	5.394	10.398
Cl	6.228	7.192	13.055
Cl	9.342	8.990	13.055
Cl	9.342	12.586	13.055
H	8.530	1.939	12.926
H	8.564	1.415	15.357
H	10.739	5.061	16.111
H	10.556	5.662	13.689
H	9.781	2.588	10.927
H	11.567	3.753	9.568
H	11.121	5.306	10.322
H	11.855	3.999	11.304
H	9.358	4.440	19.703
H	9.416	2.662	19.873
H	11.094	3.775	21.399
H	11.923	2.773	20.183
H	11.871	4.548	19.998

Zip_p-ethoxy_EB_Alpha_6.3

C	6.374	5.316	15.436
C	6.253	6.374	16.336
C	6.470	7.695	15.933
C	6.632	7.971	14.578
C	6.674	6.924	13.647
C	6.623	5.594	14.093
O	5.767	6.098	17.632
C	6.742	6.193	18.731
H	7.156	7.213	18.733
C	6.504	7.212	12.200
O	5.714	8.070	11.766
Mg	3.596	8.305	11.727
Cl	3.596	10.380	10.398
Mg	1.798	11.418	11.727
Cl	1.797	13.494	10.398
Mg	3.596	14.532	11.727
Cl	3.595	16.608	10.398
Mg	1.797	17.646	11.727
Cl	1.797	19.723	10.398
Cl	3.596	6.229	13.055
Mg	1.797	5.190	11.727
Cl	3.595	4.152	10.398
Mg	3.595	2.076	11.727
Cl	1.797	1.038	10.398
Mg	1.797	-1.038	11.727
Cl	1.797	-3.113	13.055
Mg	3.595	-4.152	11.727
Cl	3.595	-6.229	13.055
Cl	3.595	0.000	13.055
Cl	3.595	-2.076	10.398
Cl	1.797	3.114	13.055
Cl	1.798	7.267	10.398

Cl	1.798	9.343	13.055
Cl	3.596	12.456	13.055
Cl	1.797	15.570	13.055
H	6.137	6.055	19.637
O	7.222	6.430	11.403
C	6.954	6.520	9.957
C	7.971	5.651	9.253
Mg	3.596	6.229	18.027
Cl	3.596	8.305	16.698
Mg	1.798	9.343	18.027
Cl	1.798	11.419	16.698
Mg	3.596	12.457	18.027
Cl	3.596	14.533	16.698
Mg	1.798	15.571	18.027
Cl	1.798	17.647	16.698
Cl	3.596	4.152	19.355
Mg	1.798	3.114	18.027
Cl	1.798	1.038	19.355
Mg	3.596	0.000	18.027
Cl	3.596	2.076	16.698
Cl	1.798	-1.038	16.698
Mg	1.798	-3.113	18.027
Cl	3.596	-4.152	16.698
Mg	3.596	-6.228	18.027
Cl	3.595	-8.304	19.355
Cl	3.596	-2.076	19.355
Cl	1.798	-5.189	19.355
Cl	1.798	5.190	16.698
Cl	1.798	7.267	19.355
Cl	3.596	10.381	19.355
Cl	1.798	13.494	19.355
C	7.823	5.139	18.635
H	6.385	8.506	16.655
H	6.664	9.006	14.234
H	6.662	4.782	13.367
H	6.198	4.294	15.776
H	5.924	6.171	9.791
H	7.023	7.576	9.661
H	7.795	5.699	8.170
H	8.995	5.993	9.451
H	7.882	4.601	9.564
H	8.490	5.232	19.504
H	7.386	4.131	18.641
H	8.433	5.264	17.730

Zip_p-ethoxy_EB_Alpha_6.6

C	6.364	5.297	15.566
C	6.213	6.333	16.490
C	6.391	7.665	16.110
C	6.541	7.976	14.759
C	6.621	6.951	13.808
C	6.607	5.610	14.230
O	5.771	6.049	17.801
C	6.747	5.334	18.647
C	7.831	6.264	19.150
C	6.481	7.262	12.363
O	5.709	8.130	11.918
Mg	3.596	8.305	11.727
Cl	3.596	10.381	10.398
Mg	1.798	11.418	11.727
Cl	1.798	13.495	10.398

Mg	3.596	14.532	11.727
Cl	3.596	16.608	10.398
Mg	1.798	17.646	11.727
Cl	1.798	19.723	10.398
Cl	3.596	6.229	13.055
Mg	1.798	5.190	11.727
Cl	3.596	4.152	10.398
Mg	3.595	2.076	11.727
Cl	1.797	1.038	10.397
Mg	1.797	-1.037	11.726
Cl	1.797	-3.113	13.054
Mg	3.595	-4.151	11.726
Cl	3.595	-6.228	13.054
Cl	3.595	0.000	13.054
Cl	3.595	-2.076	10.397
Cl	1.797	3.114	13.055
Cl	1.798	7.267	10.398
Cl	1.798	9.343	13.055
Cl	3.596	12.456	13.055
Cl	1.798	15.570	13.055
Mg	3.596	6.229	18.326
Cl	3.596	8.305	16.997
Mg	1.798	9.343	18.326
Cl	1.798	11.419	16.997
Mg	3.596	12.457	18.327
Cl	3.595	14.533	16.997
Mg	1.797	15.571	18.326
Cl	1.797	17.647	16.998
Cl	3.596	4.152	19.654
Mg	1.798	3.114	18.326
Cl	1.798	1.038	19.654
Mg	3.596	0.000	18.326
Cl	3.596	2.076	16.997
Cl	1.798	-1.037	16.998
Mg	1.798	-3.113	18.326
Cl	3.596	-4.151	16.997
Mg	3.596	-6.228	18.326
Cl	3.596	-8.304	19.654
Cl	3.596	-2.075	19.654
Cl	1.798	-5.189	19.654
Cl	1.797	5.190	16.997
Cl	1.798	7.267	19.654
Cl	3.596	10.381	19.654
Cl	1.798	13.495	19.654
O	7.217	6.486	11.573
C	6.994	6.600	10.121
C	8.122	5.869	9.430
H	6.146	4.911	19.462
H	6.308	8.452	16.856
H	6.555	9.018	14.438
H	6.667	4.814	13.488
H	6.210	4.260	15.872
H	7.157	4.500	18.059
H	8.515	5.700	19.801
H	8.421	6.685	18.323
H	7.404	7.089	19.737
H	6.013	6.149	9.908
H	6.959	7.666	9.861
H	7.968	5.919	8.342
H	9.094	6.326	9.659
H	8.152	4.810	9.721

Zip_p-ethoxy_EB_Beta_5.9

C	-1.317	6.039	14.182
C	-1.297	4.741	13.652
C	-1.106	3.641	14.501
C	-0.866	3.845	15.859
C	-0.844	5.147	16.361
C	-1.123	6.246	15.545
C	-1.234	4.559	12.172
O	-2.201	3.932	11.506
C	-3.448	3.544	12.176
C	-4.483	3.319	11.096
O	-0.371	5.287	17.676
C	-1.020	6.272	18.553
C	-2.470	5.920	18.808
O	-0.267	4.971	11.523
Mg	1.798	5.190	11.727
Cl	3.596	4.152	10.398
Mg	3.596	2.076	11.727
Cl	1.798	1.038	10.398
Mg	1.798	-1.038	11.727
Cl	1.798	-3.113	13.055
Mg	3.596	-4.151	11.727
Cl	3.596	-6.228	13.055
Cl	3.596	0.000	13.055
Cl	3.596	-2.076	10.398
Cl	1.798	3.114	13.055
Cl	3.596	6.229	13.055
Mg	3.596	8.305	11.727
Cl	3.596	10.380	10.398
Mg	1.797	11.418	11.727
Cl	1.797	13.494	10.398
Mg	3.595	14.532	11.727
Cl	3.595	16.608	10.398
Mg	1.797	17.646	11.727
Cl	1.797	19.723	10.398
Cl	1.798	7.267	10.398
Cl	1.797	9.343	13.055
Cl	3.595	12.456	13.055
Cl	1.797	15.570	13.055
H	-0.428	6.221	19.476
Mg	1.798	5.190	17.654
Cl	1.798	3.114	18.982
Mg	3.596	2.076	17.654
Cl	3.596	4.152	16.325
Cl	1.798	1.038	16.325
Mg	1.798	-1.037	17.654
Cl	3.596	-2.075	16.325
Mg	3.596	-4.151	17.654
Cl	3.596	-6.228	18.982
Cl	3.596	0.000	18.982
Cl	1.798	-3.113	18.982
Cl	3.596	6.229	18.982
Mg	3.596	8.305	17.654
Cl	3.595	10.381	16.325
Mg	1.797	11.419	17.654
Cl	1.797	13.495	16.325
Mg	3.595	14.533	17.654
Cl	3.595	16.609	16.325
Mg	1.797	17.647	17.654
Cl	1.797	19.724	16.325
Cl	1.798	7.267	16.325

Cl	1.798	9.343	18.982
Cl	3.595	12.457	18.982
Cl	1.797	15.571	18.982
H	-1.047	2.632	14.096
H	-0.625	3.008	16.516
H	-1.082	7.260	15.938
H	-1.428	6.901	13.520
H	-3.256	2.627	12.751
H	-3.743	4.341	12.873
H	-5.431	3.006	11.560
H	-4.666	4.238	10.525
H	-4.162	2.532	10.401
H	-0.888	7.276	18.124
H	-2.892	6.636	19.529
H	-3.070	5.975	17.889
H	-2.560	4.912	19.234

Zip_p-ethoxy_EB_Beta_6.3

C	6.867	9.566	16.345
C	6.244	8.398	16.791
C	5.935	7.353	15.922
C	6.133	7.537	14.558
C	6.653	8.746	14.079
C	7.081	9.737	14.980
O	5.737	8.311	18.098
C	6.687	8.077	19.195
C	7.409	6.753	19.059
C	6.595	8.982	12.619
O	5.670	8.553	11.910
Mg	3.596	8.305	11.727
Cl	1.798	9.343	13.055
Mg	1.798	11.418	11.727
Cl	3.596	12.457	13.055
Mg	3.595	14.532	11.727
Cl	1.797	15.570	13.055
Mg	1.797	17.646	11.727
Cl	1.797	19.723	10.398
Cl	1.798	7.267	10.398
Mg	1.798	5.190	11.727
Cl	3.596	6.229	13.055
Cl	3.596	4.152	10.398
Mg	3.596	2.076	11.727
Cl	1.798	3.114	13.055
Cl	3.596	0.000	13.054
Mg	1.798	-1.038	11.726
Cl	3.596	-2.075	10.397
Mg	3.596	-4.152	11.726
Cl	3.596	-6.229	13.054
Cl	1.798	-3.114	13.054
Cl	1.798	1.038	10.397
Cl	3.596	10.380	10.398
Cl	1.797	13.494	10.398
Cl	3.595	16.608	10.398
Mg	3.595	8.305	18.027
Cl	1.797	9.343	19.355
Mg	1.797	11.419	18.027
Cl	3.595	12.457	19.355
Mg	3.595	14.533	18.027
Cl	1.797	15.571	19.355
Mg	1.797	17.646	18.027
Cl	1.797	19.723	16.698

Cl	1.798	7.267	16.698
Mg	1.798	5.190	18.027
Cl	3.596	4.152	16.698
Mg	3.596	2.076	18.026
Cl	3.596	0.000	19.355
Mg	1.798	-1.038	18.027
Cl	1.798	-3.113	19.355
Mg	3.596	-4.151	18.027
Cl	3.596	-6.228	19.355
Cl	3.595	10.381	16.698
Cl	3.596	6.229	19.355
Cl	1.797	13.495	16.698
Cl	3.595	16.609	16.698
Cl	1.798	3.114	19.355
Cl	1.798	1.038	16.698
Cl	3.596	-2.076	16.698
O	7.611	9.694	12.142
C	7.598	10.083	10.721
C	7.224	11.545	10.592
H	5.476	6.433	16.296
H	5.834	6.756	13.862
H	7.493	10.673	14.603
H	7.085	10.370	17.049
H	8.624	9.886	10.385
H	6.896	9.433	10.185
H	7.291	11.837	9.534
H	6.189	11.705	10.923
H	7.908	12.181	11.171
H	8.066	6.614	19.930
H	6.691	5.923	19.032
H	8.034	6.722	18.155
H	7.382	8.930	19.221
H	6.060	8.104	20.095

Zip_p-ethoxy_EB_Beta_6.6

C	-1.550	6.688	15.232
C	-1.141	5.710	14.309
C	-0.652	4.476	14.762
C	-0.489	4.244	16.123
C	-0.800	5.267	17.018
C	-1.369	6.468	16.595
C	-1.078	5.997	12.859
O	-1.999	6.852	12.428
C	-1.921	7.266	11.016
C	-2.891	8.409	10.828
O	-0.391	5.139	18.362
C	-1.253	4.287	19.207
C	-2.618	4.901	19.428
O	-0.226	5.500	12.102
Mg	1.798	5.189	11.727
Cl	3.596	6.229	13.055
Mg	3.596	8.305	11.727
Cl	1.798	9.342	13.055
Mg	1.798	11.418	11.727
Cl	3.595	12.456	13.055
Mg	3.596	14.532	11.727
Cl	1.797	15.570	13.054
Mg	1.797	17.646	11.726
Cl	1.797	19.723	10.397
Cl	3.596	4.151	10.398
Mg	3.596	2.076	11.727

Cl	3.595	0.000	13.055
Mg	1.798	-1.038	11.727
Cl	3.596	-2.076	10.398
Mg	3.596	-4.152	11.727
Cl	3.595	-6.229	13.055
Cl	1.797	3.114	13.055
Cl	1.798	7.266	10.398
Cl	3.596	10.380	10.398
Cl	1.798	13.494	10.398
Cl	3.595	16.608	10.398
Cl	1.798	1.037	10.398
Cl	1.798	-3.114	13.055
H	-0.690	4.182	20.141
Mg	1.797	5.190	18.408
Cl	1.797	3.114	19.736
Mg	3.595	2.076	18.408
Cl	3.595	0.000	19.736
Mg	1.797	-1.037	18.408
Cl	1.797	-3.113	19.736
Mg	3.595	-4.151	18.408
Cl	3.595	-6.228	19.736
Cl	1.797	7.267	17.079
Mg	3.595	8.305	18.407
Cl	1.797	9.343	19.735
Mg	1.797	11.419	18.407
Cl	3.595	12.457	19.735
Mg	3.595	14.533	18.407
Cl	1.797	15.571	19.735
Mg	1.797	17.647	18.407
Cl	1.797	19.723	17.078
Cl	3.595	6.229	19.736
Cl	3.595	4.152	17.079
Cl	1.797	1.038	17.079
Cl	3.595	-2.075	17.079
Cl	3.595	10.381	17.078
Cl	1.797	13.495	17.078
Cl	3.595	16.609	17.078
H	-0.881	7.544	10.796
H	-2.182	6.392	10.401
H	-3.921	8.110	11.067
H	-2.865	8.734	9.778
H	-2.620	9.267	11.458
H	-0.345	3.715	14.046
H	-0.049	3.305	16.472
H	-1.585	7.246	17.326
H	-1.935	7.644	14.877
H	-1.314	3.296	18.733
H	-3.191	4.247	20.102
H	-2.540	5.891	19.900
H	-3.185	4.995	18.492

Zip_t-butoxy_EB_Alpha_5.9

C	10.293	4.308	15.352
C	10.207	4.588	13.987
C	9.485	3.727	13.155
C	8.952	2.533	13.660
C	8.980	2.293	15.028
C	9.611	3.203	15.888
O	9.137	4.137	11.860
C	9.963	3.673	10.665
C	11.132	4.642	10.521

C	9.312	3.142	17.338
O	10.313	3.506	18.132
C	10.004	3.646	19.567
C	11.309	3.882	20.289
O	8.192	2.824	17.780
Mg	6.228	3.596	17.590
Cl	5.190	5.394	18.918
Mg	6.228	7.192	17.590
Cl	8.304	7.192	18.918
Mg	9.342	8.990	17.590
Cl	8.304	10.788	18.918
Mg	9.342	12.586	17.590
Cl	10.380	14.384	16.261
Cl	7.266	5.394	16.261
Cl	5.190	1.797	18.918
Mg	3.114	1.797	17.589
Cl	4.152	3.596	16.261
Cl	7.266	8.990	16.261
Cl	10.380	10.788	16.261
Cl	2.076	0.000	18.918
Mg	3.114	-1.798	17.589
Cl	2.076	-3.596	18.918
Mg	0.000	-3.595	17.589
Cl	-1.038	-5.394	18.918
Mg	-0.000	-7.192	17.589
Cl	-1.038	-8.989	18.918
Cl	4.152	0.000	16.261
Cl	1.038	-1.798	16.261
Cl	1.038	-5.393	16.261
Mg	7.266	5.394	11.726
Cl	6.228	7.192	13.055
Mg	7.266	8.989	11.726
Cl	9.342	8.990	13.055
Mg	10.380	10.788	11.726
Cl	9.342	12.586	13.055
Mg	10.380	14.384	11.726
Cl	11.418	16.182	10.398
Cl	8.304	7.192	10.397
Cl	6.228	3.596	13.055
Mg	4.152	3.596	11.726
Cl	5.190	5.394	10.398
Cl	8.304	10.788	10.398
Cl	11.418	12.586	10.398
Cl	5.190	1.797	10.398
Mg	4.152	0.000	11.726
Cl	3.114	1.797	13.055
Cl	2.076	0.000	10.398
Mg	1.038	-1.798	11.726
Cl	2.076	-3.596	10.398
Mg	1.038	-5.393	11.726
Cl	-0.000	-7.192	13.055
Cl	3.114	-1.798	13.055
Cl	0.000	-3.595	13.055
C	8.991	3.754	9.493
H	8.410	1.865	12.996
H	8.453	1.432	15.441
H	10.790	5.009	16.022
H	10.616	5.514	13.582
C	10.439	2.242	10.878
H	11.710	4.393	9.618
H	10.768	5.673	10.427
H	11.811	4.572	11.383

H	9.312	4.495	19.668
H	9.495	2.732	19.898
H	11.106	4.012	21.362
H	11.994	3.031	20.170
H	11.808	4.791	19.925
H	9.486	3.389	8.582
H	8.106	3.123	9.669
H	8.677	4.789	9.295
H	11.033	1.944	10.002
H	11.081	2.145	11.764
H	9.597	1.543	10.967

Zip-*t*-butoxy_EB_Alpha_6.3

C	6.629	5.627	14.062
C	6.370	5.337	15.400
C	6.242	6.387	16.308
C	6.456	7.711	15.915
C	6.624	7.998	14.563
C	6.680	6.960	13.625
O	5.764	6.094	17.603
C	6.751	6.192	18.691
C	7.905	5.228	18.509
C	6.515	7.249	12.180
O	7.247	6.474	11.389
C	6.963	6.532	9.946
C	7.982	5.647	9.268
O	5.714	8.091	11.737
Mg	3.596	8.305	11.727
Cl	1.798	9.343	13.055
Mg	1.798	11.418	11.727
Cl	3.596	12.456	13.055
Mg	3.596	14.532	11.727
Cl	1.797	15.570	13.055
Mg	1.797	17.646	11.727
Cl	1.797	19.723	10.398
Cl	3.596	10.380	10.398
Cl	3.596	6.229	13.055
Mg	1.797	5.190	11.727
Cl	1.798	7.267	10.398
Cl	1.797	13.494	10.398
Cl	3.595	16.608	10.398
Cl	3.595	4.152	10.398
Mg	3.595	2.076	11.727
Cl	1.797	3.114	13.055
Cl	1.797	1.038	10.398
Mg	1.797	-1.038	11.727
Cl	3.595	-2.076	10.398
Mg	3.595	-4.152	11.727
Cl	3.595	-6.229	13.055
Cl	3.596	0.000	13.055
Cl	1.797	-3.113	13.055
Mg	3.596	6.229	18.027
Cl	1.798	7.267	19.355
Mg	1.798	9.342	18.027
Cl	3.596	10.381	19.355
Mg	3.596	12.457	18.027
Cl	1.798	13.494	19.355
Mg	1.798	15.570	18.027
Cl	1.798	17.646	16.698
Cl	3.596	8.304	16.698
Cl	3.596	4.152	19.355

Mg	1.798	3.113	18.027
Cl	1.798	5.189	16.698
Cl	1.798	11.418	16.698
Cl	3.596	14.533	16.698
Cl	1.798	1.038	19.355
Mg	3.596	0.000	18.027
Cl	3.596	-2.076	19.355
Mg	1.798	-3.113	18.027
Cl	1.798	-5.189	19.355
Mg	3.596	-6.228	18.027
Cl	3.596	-8.304	19.355
Cl	3.596	2.075	16.698
Cl	1.798	-1.038	16.698
Cl	3.596	-4.152	16.698
C	7.203	7.567	18.766
C	5.991	5.882	19.886
H	6.366	8.518	16.641
H	6.652	9.035	14.227
H	6.677	4.820	13.332
H	6.197	4.312	15.731
H	5.934	6.170	9.800
H	7.020	7.580	9.625
H	7.769	5.598	8.191
H	9.000	6.034	9.404
H	7.938	4.624	9.668
H	8.604	5.348	19.350
H	7.552	4.188	18.497
H	8.455	5.430	17.577
H	6.646	5.929	20.755
H	5.184	6.604	20.000
H	5.573	4.880	19.801
H	7.936	7.666	19.565
H	7.659	7.852	17.819
H	6.354	8.218	18.970

Zip-*t*-butoxy_EB_Alpha_6.6

C	6.377	5.430	15.718
C	6.256	6.512	16.595
C	6.408	7.823	16.125
C	6.534	8.060	14.760
C	6.598	6.984	13.864
C	6.583	5.669	14.358
O	5.843	6.303	17.923
C	6.905	6.136	19.002
C	8.101	7.033	18.705
C	6.450	7.233	12.408
O	5.706	8.112	11.932
Mg	3.596	8.305	11.727
Cl	3.596	10.381	10.398
Mg	1.798	11.418	11.727
Cl	1.798	13.495	10.398
Mg	3.596	14.532	11.727
Cl	3.596	16.608	10.398
Mg	1.798	17.646	11.727
Cl	1.798	19.723	10.398
Cl	3.596	6.229	13.055
Mg	1.798	5.190	11.727
Cl	3.596	4.152	10.398
Mg	3.595	2.076	11.727
Cl	1.797	1.038	10.397
Mg	1.797	-1.037	11.726

Cl	1.797	-3.113	13.054
Mg	3.595	-4.151	11.726
Cl	3.595	-6.228	13.054
Cl	3.595	0.000	13.054
Cl	3.595	-2.076	10.397
Cl	1.797	3.114	13.055
Cl	1.798	7.267	10.398
Cl	1.798	9.343	13.055
Cl	3.596	12.456	13.055
Cl	1.798	15.570	13.055
Mg	3.596	6.229	18.326
Cl	3.596	8.305	16.997
Mg	1.798	9.343	18.326
Cl	1.798	11.419	16.997
Mg	3.596	12.457	18.327
Cl	3.595	14.533	16.997
Mg	1.797	15.571	18.326
Cl	1.797	17.647	16.998
Cl	3.596	4.152	19.654
Mg	1.798	3.114	18.326
Cl	1.798	1.038	19.654
Mg	3.596	0.000	18.326
Cl	3.596	2.076	16.997
Cl	1.798	-1.037	16.998
Mg	1.798	-3.113	18.326
Cl	3.596	-4.151	16.997
Mg	3.596	-6.228	18.326
Cl	3.596	-8.304	19.654
Cl	3.596	-2.075	19.654
Cl	1.798	-5.189	19.654
Cl	1.797	5.190	16.997
Cl	1.798	7.267	19.654
Cl	3.596	10.381	19.654
Cl	1.798	13.495	19.654
O	7.151	6.400	11.644
C	6.921	6.467	10.191
C	8.005	5.655	9.522
C	6.205	6.579	20.283
H	6.319	8.653	16.821
H	6.534	9.082	14.381
H	6.622	4.833	13.661
H	6.236	4.413	16.087
C	7.302	4.663	19.034
H	8.840	6.899	19.507
H	8.588	6.773	17.755
H	7.817	8.094	18.680
H	6.915	6.538	21.122
H	5.845	7.615	20.197
H	5.370	5.913	20.543
H	5.918	6.054	10.003
H	6.935	7.522	9.888
H	7.847	5.673	8.434
H	9.001	6.070	9.730
H	7.983	4.607	9.852
H	8.008	4.488	19.860
H	6.419	4.029	19.190
H	7.801	4.370	18.100

Zip_4-butoxy_EB_Beta_5.9

C	-1.229	6.005	14.115
C	-1.286	4.696	13.612

C	-1.169	3.605	14.485
C	-0.932	3.822	15.842
C	-0.843	5.129	16.327
C	-1.037	6.225	15.476
C	-1.216	4.500	12.136
O	-2.163	3.843	11.473
C	-3.415	3.453	12.130
C	-4.461	3.302	11.048
O	-0.360	5.312	17.630
C	-1.296	5.728	18.750
C	-2.373	4.660	18.877
O	-0.259	4.935	11.485
Mg	1.798	5.190	11.727
Cl	3.596	4.152	10.398
Mg	3.596	2.076	11.727
Cl	1.798	1.038	10.398
Mg	1.798	-1.038	11.727
Cl	1.798	-3.113	13.055
Mg	3.596	-4.151	11.727
Cl	3.596	-6.228	13.055
Cl	3.596	0.000	13.055
Cl	3.596	-2.076	10.398
Cl	1.798	3.114	13.055
Cl	3.596	6.229	13.055
Mg	3.596	8.305	11.727
Cl	3.596	10.380	10.398
Mg	1.797	11.418	11.727
Cl	1.797	13.494	10.398
Mg	3.595	14.532	11.727
Cl	3.595	16.608	10.398
Mg	1.797	17.646	11.727
Cl	1.797	19.723	10.398
Cl	1.798	7.267	10.398
Cl	1.797	9.343	13.055
Cl	3.595	12.456	13.055
Cl	1.797	15.570	13.055
C	-0.391	5.779	19.974
Mg	1.798	5.190	17.654
Cl	1.798	3.114	18.982
Mg	3.596	2.076	17.654
Cl	3.596	4.152	16.325
Cl	1.798	1.038	16.325
Mg	1.798	-1.037	17.654
Cl	3.596	-2.075	16.325
Mg	3.596	-4.151	17.654
Cl	3.596	-6.228	18.982
Cl	3.596	0.000	18.982
Cl	1.798	-3.113	18.982
Cl	3.596	6.229	18.982
Mg	3.596	8.305	17.654
Cl	3.595	10.381	16.325
Mg	1.797	11.419	17.654
Cl	1.797	13.495	16.325
Mg	3.595	14.533	17.654
Cl	3.595	16.609	16.325
Mg	1.797	17.647	17.654
Cl	1.797	19.724	16.325
Cl	1.798	7.267	16.325
Cl	1.798	9.343	18.982
Cl	3.595	12.457	18.982
Cl	1.797	15.571	18.982
H	-1.153	2.586	14.097

H	-0.729	2.984	16.509
H	-0.919	7.237	15.852
H	-1.274	6.855	13.432
H	-3.239	2.504	12.658
H	-3.690	4.221	12.867
H	-5.412	2.986	11.500
H	-4.626	4.252	10.522
H	-4.160	2.544	10.312
C	-1.879	7.105	18.447
H	-3.048	4.918	19.705
H	-2.979	4.591	17.961
H	-1.928	3.678	19.086
H	-0.985	6.067	20.853
H	0.067	4.802	20.178
H	0.396	6.541	19.857
H	-2.474	7.431	19.312
H	-1.076	7.838	18.288
H	-2.545	7.090	17.574

Zip_4-butoxy_EB_Beta_6.3

C	7.006	9.843	14.974
C	6.805	9.750	16.347
C	6.252	8.581	16.886
C	5.958	7.485	16.068
C	6.112	7.602	14.688
C	6.606	8.791	14.133
O	5.776	8.555	18.203
Mg	3.595	8.305	18.027
Cl	3.596	6.229	19.355
Mg	1.798	5.190	18.027
Cl	1.798	3.114	19.355
Mg	3.596	2.076	18.026
Cl	1.798	1.038	16.698
Mg	1.798	-1.038	18.027
Cl	3.596	-2.075	16.698
Mg	3.596	-4.151	18.027
Cl	3.596	-6.228	19.355
C	6.561	8.974	12.664
O	7.573	9.689	12.181
C	7.563	10.065	10.757
C	7.189	11.526	10.614
C	6.734	8.390	19.373
C	7.246	6.953	19.354
O	5.651	8.519	11.952
Mg	3.596	8.305	11.727
Cl	3.596	10.380	10.398
Mg	1.798	11.418	11.727
Cl	1.797	13.494	10.398
Mg	3.595	14.532	11.727
Cl	3.595	16.608	10.398
Mg	1.797	17.646	11.727
Cl	1.797	19.723	10.398
Cl	1.798	9.343	13.055
Cl	1.798	7.267	10.398
Mg	1.798	5.190	11.727
Cl	1.798	3.114	13.055
Mg	3.596	2.076	11.727
Cl	1.798	1.038	10.398
Mg	1.798	-1.038	11.727
Cl	1.798	-3.114	13.055
Mg	3.596	-4.152	11.727

Cl	3.596	-6.229	13.055
Cl	3.596	6.229	13.055
Cl	3.596	12.457	13.055
Cl	1.797	15.570	13.055
Cl	3.596	4.151	10.398
Cl	3.596	0.000	13.055
Cl	3.596	-2.075	10.398
Cl	1.797	9.343	19.355
Mg	1.797	11.419	18.027
Cl	1.797	13.495	16.698
Mg	3.595	14.533	18.027
Cl	3.595	16.609	16.698
Mg	1.797	17.646	18.027
Cl	1.797	19.723	16.697
Cl	1.798	7.267	16.698
Cl	3.595	10.381	16.698
Cl	3.595	12.457	19.355
Cl	1.797	15.571	19.355
Cl	3.596	4.152	16.698
Cl	3.596	0.000	19.355
Cl	1.798	-3.113	19.355
H	5.546	6.567	16.496
H	5.805	6.781	14.042
H	7.383	10.769	14.541
H	6.983	10.610	16.988
H	8.590	9.865	10.424
H	6.863	9.410	10.225
H	7.255	11.807	9.553
H	6.153	11.689	10.942
H	7.872	12.169	11.186
H	7.905	6.786	20.218
H	6.409	6.244	19.411
H	7.829	6.754	18.443
C	7.877	9.394	19.261
C	5.872	8.692	20.593
H	8.530	9.268	20.136
H	8.490	9.229	18.365
H	7.503	10.427	19.264
H	6.496	8.646	21.496
H	5.443	9.702	20.527
H	5.064	7.958	20.709

Zip_t-butoxy_EB_Beta_6.6

C	-1.527	6.770	15.236
C	-1.104	5.754	14.361
C	-0.607	4.550	14.879
C	-0.484	4.377	16.257
C	-0.818	5.431	17.112
C	-1.363	6.619	16.607
C	-1.056	5.985	12.900
O	-2.001	6.806	12.448
C	-1.952	7.158	11.019
C	-2.958	8.262	10.792
O	-0.403	5.353	18.448
C	-1.423	5.085	19.550
C	-2.625	6.010	19.389
O	-0.206	5.479	12.149
Mg	1.798	5.190	11.727
Cl	3.596	6.229	13.055
Mg	3.596	8.305	11.727
Cl	1.797	9.343	13.055

Mg	1.797	11.418	11.727
Cl	3.595	12.457	13.055
Mg	3.595	14.532	11.727
Cl	1.797	15.570	13.055
Mg	1.797	17.646	11.727
Cl	1.797	19.723	10.398
Cl	3.596	4.152	10.398
Mg	3.596	2.076	11.727
Cl	3.596	0.000	13.055
Mg	1.798	-1.037	11.727
Cl	3.596	-2.075	10.398
Mg	3.596	-4.151	11.726
Cl	3.596	-6.228	13.054
Cl	1.798	3.114	13.055
Cl	1.798	7.267	10.398
Cl	3.596	10.381	10.398
Cl	1.797	13.494	10.398
Cl	3.595	16.608	10.398
Cl	1.798	1.038	10.398
Cl	1.798	-3.113	13.054
Mg	1.797	5.190	18.408
Cl	1.797	3.114	19.736
Mg	3.595	2.076	18.408
Cl	3.595	0.000	19.736
Mg	1.797	-1.037	18.408
Cl	1.797	-3.113	19.736
Mg	3.595	-4.151	18.408
Cl	3.595	-6.228	19.736
Cl	1.797	7.267	17.079
Mg	3.595	8.305	18.408
Cl	1.797	9.343	19.736
Mg	1.798	11.419	18.408
Cl	3.595	12.457	19.735
Mg	3.595	14.533	18.407
Cl	1.797	15.571	19.736
Mg	1.797	17.647	18.408
Cl	1.797	19.723	17.079
Cl	3.595	6.229	19.736
Cl	3.595	4.152	17.079
Cl	1.797	1.038	17.079
Cl	3.595	-2.075	17.079
Cl	3.595	10.381	17.078
Cl	1.797	13.494	17.079
Cl	3.595	16.608	17.079
C	-0.668	5.409	20.833
H	-0.924	7.457	10.772
H	-2.196	6.251	10.447
H	-3.975	7.945	11.060
H	-2.954	8.538	9.728
H	-2.704	9.157	11.377
H	-0.276	3.759	14.208
H	-0.069	3.448	16.657
H	-1.568	7.448	17.282
H	-1.900	7.712	14.832
C	-1.832	3.619	19.455
H	-3.323	5.805	20.212
H	-2.331	7.067	19.452
H	-3.164	5.837	18.448
H	-1.346	5.292	21.690
H	0.179	4.729	20.989
H	-0.309	6.448	20.824
H	-2.530	3.380	20.271

H	-2.344	3.413	18.503
H	-0.954	2.966	19.544

Mono_DIBP_Alpha_5.9

Mg	1.038	-1.798	11.726
Cl	3.114	-1.798	13.055
Mg	4.152	0.000	11.726
Cl	3.114	1.797	13.055
Mg	4.152	3.596	11.726
Cl	6.228	3.596	13.055
Mg	7.266	5.394	11.726
Cl	6.228	7.192	13.055
Mg	7.266	8.989	11.726
Cl	9.342	8.990	13.055
Mg	10.380	10.788	11.726
Cl	9.342	12.586	13.055
Mg	10.380	14.384	11.726
Cl	11.418	12.586	10.398
Cl	2.076	0.000	10.398
Cl	2.076	-3.596	10.398
Mg	1.038	-5.393	11.726
Cl	-0.000	-7.192	13.055
Cl	0.000	-3.595	13.055
Cl	5.190	5.394	10.398
Cl	5.190	1.797	10.398
Cl	8.304	10.788	10.398
Cl	8.304	7.192	10.397
Cl	11.418	16.182	10.398
Cl	1.038	-1.798	16.261
Mg	3.114	-1.798	17.590
Cl	2.076	-3.596	18.918
Mg	0.000	-3.595	17.590
Cl	-1.038	-5.394	18.918
Mg	-0.000	-7.192	17.590
Cl	-1.038	-8.989	18.918
Cl	1.038	-5.393	16.261
Cl	4.152	0.000	16.261
Mg	3.114	1.797	17.590
Cl	5.190	1.797	18.918
Mg	6.228	3.596	17.590
Cl	5.190	5.394	18.918
Mg	6.228	7.192	17.590
Cl	8.304	7.192	18.918
Mg	9.342	8.990	17.590
Cl	8.304	10.788	18.918
Mg	9.342	12.586	17.590
Cl	10.380	10.788	16.261
Cl	4.152	3.596	16.261
Cl	2.076	0.000	18.918
Cl	7.266	8.990	16.261
Cl	7.266	5.394	16.261
Cl	10.380	14.384	16.261
O	1.462	2.963	17.943
C	0.687	3.797	17.466
O	0.895	4.248	16.241
C	-0.088	5.052	15.524
C	0.646	5.990	14.571
H	-0.727	4.339	14.981
H	-0.705	5.613	16.241
C	-0.386	6.825	13.804
H	1.261	6.671	15.186

C	1.583	5.226	13.624
H	0.116	7.543	13.140
H	-1.025	6.184	13.177
H	-1.039	7.396	14.481
H	2.103	5.940	12.964
H	2.327	4.653	14.195
H	1.006	4.525	12.999
C	-0.384	4.366	18.354
C	-1.536	3.612	18.649
C	-0.146	5.571	19.023
C	-1.066	6.036	19.967
C	-2.211	5.293	20.259
C	-2.442	4.080	19.609
C	-1.760	2.363	17.864
O	-2.512	1.455	18.513
O	-1.292	2.206	16.743
C	-2.737	0.192	17.807
C	-3.004	-0.915	18.821
H	-3.598	0.339	17.135
H	-1.848	-0.019	17.196
H	-3.201	-1.808	18.196
C	-1.776	-1.200	19.698
C	-4.260	-0.656	19.663
H	-1.919	-2.113	20.293
H	-0.849	-1.297	19.104
H	-1.587	-0.373	20.398
H	-4.462	-1.504	20.333
H	-4.134	0.240	20.286
H	-5.147	-0.510	19.027
H	0.769	6.132	18.825
H	-0.876	6.978	20.486
H	-2.924	5.656	21.002
H	-3.330	3.488	19.834

Mono_DIBP_Alpha_6.3

Mg	1.798	-1.038	11.727
Cl	3.596	0.000	13.055
Mg	3.596	2.076	11.727
Cl	1.798	3.114	13.055
Mg	1.798	5.190	11.727
Cl	3.596	6.229	13.055
Mg	3.596	8.305	11.727
Cl	1.798	9.343	13.055
Mg	1.798	11.418	11.727
Cl	3.596	12.456	13.055
Mg	3.596	14.532	11.727
Cl	1.797	15.570	13.055
Mg	1.797	17.646	11.727
Cl	3.595	16.608	10.398
Cl	1.798	1.038	10.398
Cl	3.596	-2.076	10.398
Mg	3.596	-4.152	11.727
Cl	3.596	-6.229	13.055
Cl	1.798	-3.114	13.055
Cl	1.798	7.267	10.398
Cl	3.596	4.152	10.398
Cl	1.797	13.494	10.398
Cl	1.797	19.723	10.398
Cl	1.798	-1.037	16.998
Cl	1.797	19.723	10.398
Cl	1.798	-1.037	16.998
Mg	3.596	0.000	18.327
Cl	3.596	-2.075	19.655
Mg	1.798	-3.113	18.327
Cl	1.798	-5.189	19.655
Mg	3.596	-6.228	18.327
Cl	3.596	-8.304	19.655
Cl	3.596	-4.151	16.998
Cl	3.596	2.076	16.997
Mg	1.798	3.114	18.326
Cl	3.596	4.152	19.654
Mg	3.596	6.229	18.326
Cl	1.798	7.267	19.654
Mg	1.798	9.343	18.326
Cl	3.596	10.381	19.654
Mg	3.596	12.457	18.326
Cl	1.798	13.495	19.654
Mg	1.798	15.571	18.326
Cl	3.596	14.533	16.997
Cl	1.798	5.190	16.997
Cl	1.798	1.038	19.654
Cl	1.798	11.419	16.997
Cl	3.596	8.305	16.997
Cl	1.798	17.647	16.997
O	-0.215	2.835	18.009
C	-1.320	3.383	17.946
O	-1.380	4.699	17.835
C	-2.627	5.459	17.874
C	-2.444	6.710	17.016
H	-3.455	4.837	17.505
H	-2.806	5.709	18.931
H	-3.421	7.224	17.058
C	-1.376	7.649	17.599

Cl	3.596	-2.076	19.355
Mg	1.798	-3.113	18.027
Cl	1.798	-5.189	19.355
Mg	3.596	-6.228	18.027
Cl	3.595	-8.304	19.355
Cl	3.596	-4.152	16.698
Cl	3.596	2.076	16.698
Mg	1.798	3.114	18.027
Cl	3.596	4.152	19.355
Mg	3.596	6.229	18.027
Cl	1.798	7.267	19.355
Mg	1.798	9.343	18.027
Cl	3.596	10.381	19.355
Mg	3.596	12.457	18.027
Cl	1.798	13.495	19.355
Mg	1.798	15.571	18.027
Cl	3.596	14.533	16.698
Cl	1.798	5.190	16.698
Cl	1.798	1.038	19.355
Cl	1.798	11.419	16.698
Cl	3.596	8.305	16.698
Cl	1.798	17.647	16.698
O	-0.228	2.824	17.758
C	-1.337	3.363	17.809
O	-1.441	4.657	17.546
C	-2.681	5.392	17.792
C	-2.373	6.876	17.629
H	-3.442	5.068	17.064
H	-3.026	5.159	18.810
C	-3.647	7.681	17.911
H	-1.616	7.129	18.392
C	-1.797	7.184	16.242
H	-3.445	8.759	17.841
H	-4.435	7.446	17.178
H	-4.047	7.481	18.917
H	-1.588	8.259	16.137
H	-0.863	6.632	16.065
H	-2.516	6.916	15.451
C	-2.559	2.525	18.053
C	-3.431	2.240	16.997
C	-2.748	1.911	19.307
C	-4.497	1.356	17.191
C	-4.690	0.751	18.435
C	-3.813	1.021	19.487
C	-1.825	2.301	20.416
O	-1.666	1.330	21.327
O	-1.281	3.397	20.454
C	-0.682	1.598	22.380
C	-0.402	0.299	23.122
H	0.224	1.992	21.901
H	-1.095	2.372	23.048
C	0.743	0.536	24.116
C	-1.649	-0.250	23.820
H	-0.057	-0.431	22.371
H	-1.429	-1.206	24.318
H	-2.007	0.453	24.590
H	-2.469	-0.421	23.109
H	1.002	-0.399	24.631
H	1.647	0.903	23.609
H	0.457	1.271	24.885
H	-3.263	2.688	16.015
H	-5.174	1.138	16.363

H	-5.524	0.064	18.585
H	-3.951	0.552	20.461

Mono_DIBP_Alpha_6.6

Mg	1.798	-1.038	11.727
Cl	3.596	0.000	13.055
Mg	3.596	2.076	11.727
Cl	1.798	3.114	13.055
Mg	1.798	5.190	11.727
Cl	3.596	6.229	13.055
Mg	3.596	8.305	11.727
Cl	1.798	9.343	13.055
Mg	1.798	11.418	11.727
Cl	3.596	12.456	13.055
Mg	3.596	14.532	11.727
Cl	1.797	15.570	13.055
Mg	1.797	17.646	11.727
Cl	3.595	16.608	10.398
Cl	1.798	1.038	10.398
Cl	3.596	-2.076	10.398
Mg	3.596	-4.152	11.727
Cl	3.596	-6.229	13.055
Cl	1.798	-3.114	13.055
Cl	1.798	7.267	10.398
Cl	3.596	4.152	10.398
Cl	1.797	13.494	10.398
Cl	3.596	10.380	10.398
Cl	1.797	19.723	10.398
Cl	1.798	-1.037	16.998
Mg	3.596	0.000	18.327
Cl	3.596	-2.075	19.655
Mg	1.798	-3.113	18.327
Cl	1.798	-5.189	19.655
Mg	3.596	-6.228	18.327
Cl	3.596	-8.304	19.655
Cl	3.596	-4.151	16.998
Cl	3.596	2.076	16.997
Mg	1.798	3.114	18.326
Cl	3.596	4.152	19.654
Mg	3.596	6.229	18.326
Cl	1.798	7.267	19.654
Mg	1.798	9.343	18.326
Cl	3.596	10.381	19.654
Mg	3.596	12.457	18.326
Cl	1.798	13.495	19.654
Mg	1.798	15.571	18.326
Cl	3.596	14.533	16.997
Cl	1.798	5.190	16.997
Cl	1.798	1.038	19.654
Cl	1.798	11.419	16.997
Cl	3.596	8.305	16.997
Cl	1.798	17.647	16.997
O	-0.215	2.835	18.009
C	-1.320	3.383	17.946
O	-1.380	4.699	17.835
C	-2.627	5.459	17.874
C	-2.444	6.710	17.016
H	-3.455	4.837	17.505
H	-2.806	5.709	18.931
H	-3.421	7.224	17.058
C	-1.376	7.649	17.599

C	-2.138	6.359	15.555
H	-2.093	7.270	14.941
H	-1.163	5.854	15.476
H	-2.911	5.704	15.124
H	-1.308	8.561	16.986
H	-1.623	7.940	18.632
H	-0.399	7.140	17.607
C	-2.555	2.528	17.890
C	-2.951	1.799	19.028
C	-3.220	2.335	16.673
C	-4.292	1.442	16.596
C	-4.696	0.730	17.729
C	-4.019	0.901	18.939
C	-2.214	2.052	20.306
O	-1.691	3.128	20.558
O	-2.177	0.972	21.102
C	-1.326	1.089	22.292
C	-1.194	-0.285	22.937
H	-0.351	1.476	21.967
H	-1.788	1.819	22.975
H	-0.502	-0.120	23.784
C	-2.525	-0.793	23.503
C	-0.543	-1.303	21.990
H	-2.387	-1.756	24.016
H	-2.952	-0.083	24.228
H	-3.263	-0.946	22.701
H	-0.343	-2.247	22.516
H	-1.211	-1.523	21.143
H	0.405	-0.923	21.587
H	-2.886	2.870	15.782
H	-4.807	1.299	15.645
H	-5.534	0.035	17.667
H	-4.317	0.341	19.826

Mono_DIBP_Beta_5.9

C	3.949	1.731	0.964
C	2.786	1.915	0.218
C	1.550	1.454	0.693
C	1.495	0.787	1.933
C	2.662	0.630	2.692
C	3.885	1.096	2.206
C	0.291	1.621	-0.086
O	0.399	2.549	-1.065
C	-0.797	2.750	-1.878
C	-0.480	3.777	-2.960
C	0.661	3.331	-3.880
C	0.205	0.323	2.560
O	-0.217	-0.923	2.414
C	0.351	-1.822	1.410
C	0.223	-3.255	1.916
C	-1.240	-3.660	2.132
C	-1.753	4.062	-3.773
O	-0.403	1.045	3.349
Mg	-0.998	2.621	4.469
Cl	-0.817	1.266	6.520
Mg	-2.873	2.202	7.508
Cl	-2.692	0.846	9.559
Mg	-3.858	-1.088	8.573
Cl	-3.678	-2.443	10.624
Mg	-5.733	-1.507	11.612
Cl	-5.553	-2.863	13.664

Cl	-1.177	3.976	2.418
Mg	-0.012	5.912	3.404
Cl	2.042	4.977	2.415
Mg	1.862	6.332	0.364
Cl	1.682	7.687	-1.685
Mg	2.847	9.622	-0.699
Cl	4.903	8.687	-1.688
Mg	4.722	10.042	-3.739
Cl	4.543	11.397	-5.790
Cl	0.167	4.556	5.455
Cl	-3.052	3.557	5.458
Cl	-0.192	7.267	1.353
Cl	3.028	8.267	1.351
Cl	2.668	10.977	-2.750
C	1.072	-3.492	3.171
Cl	-4.038	0.266	6.522
Cl	-5.913	-0.152	9.562
Cl	-5.874	1.795	3.474
Mg	-6.054	3.150	1.423
Cl	-8.109	4.085	2.411
Mg	-7.929	2.730	4.462
Cl	-7.749	1.375	6.513
Mg	-8.915	-0.559	5.527
Cl	-8.734	-1.914	7.578
Mg	-10.790	-0.979	8.566
Cl	-10.610	-2.334	10.618
Cl	-9.094	0.795	3.476
Cl	-10.969	0.375	6.516
Cl	-6.234	4.505	-0.627
Mg	-5.069	6.441	0.357
Cl	-3.013	5.505	-0.630
Mg	-3.194	6.860	-2.681
Cl	-3.373	8.215	-4.732
Mg	-2.208	10.151	-3.746
Cl	-2.388	11.506	-5.796
Mg	-0.333	10.570	-6.785
Cl	-0.513	11.926	-8.837
Cl	-4.889	5.085	2.409
Cl	-5.248	7.796	-1.692
Cl	-2.028	8.795	-1.695
Cl	-0.153	9.215	-4.734
H	-0.225	-1.657	0.489
H	1.403	-1.555	1.233
H	0.636	-3.873	1.097
H	1.031	-4.548	3.475
H	2.129	-3.235	2.999
H	0.705	-2.888	4.014
H	-1.836	-3.524	1.218
H	-1.699	-3.057	2.928
H	-1.306	-4.717	2.426
H	-1.092	1.781	-2.314
H	-1.604	3.101	-1.218
H	-0.182	4.711	-2.450
H	-1.594	4.910	-4.460
H	-2.037	3.201	-4.398
H	-2.612	4.260	-3.108
H	0.874	4.096	-4.640
H	1.585	3.148	-3.315
H	0.395	2.399	-4.404
H	4.906	2.089	0.581
H	4.788	0.967	2.805
H	2.610	0.149	3.671

H	2.823	2.413	-0.750
O	-0.719	0.971	0.131

Mono_DIBP_Beta_6.3

C	-4.207	3.677	18.648
C	-3.067	4.302	18.130
C	-2.560	5.455	18.763
C	-3.197	5.962	19.901
C	-4.337	5.331	20.407
C	-4.844	4.192	19.779
C	-1.250	6.058	18.341
O	-1.197	7.308	17.905
C	-2.389	8.024	17.459
C	-1.988	8.972	16.331
C	-0.917	9.980	16.777
C	-2.397	3.828	16.881
O	-0.204	5.426	18.511
Mg	1.798	5.189	18.027
Cl	3.596	4.151	16.698
Mg	3.596	2.075	18.027
Cl	1.798	1.037	16.698
Mg	1.797	-1.038	18.027
Cl	3.595	-2.076	16.698
Mg	3.596	-4.152	18.027
Cl	3.596	-6.229	19.355
Cl	3.596	6.228	19.355
Mg	3.596	8.304	18.027
Cl	3.596	10.380	16.698
Mg	1.798	11.418	18.027
Cl	1.798	13.494	16.698
Mg	3.595	14.532	18.027
Cl	3.595	16.608	16.698
Mg	1.797	17.646	18.027
Cl	1.797	19.723	16.698
Cl	1.798	7.266	16.698
Cl	1.798	3.114	19.355
Cl	3.595	-0.000	19.355
Cl	1.798	-3.114	19.355
Cl	1.798	9.342	19.355
Cl	3.596	12.456	19.355
Cl	1.797	15.570	19.355
C	-3.245	9.673	15.803
Cl	1.798	9.343	13.055
Mg	1.798	11.419	11.727
Cl	1.797	13.495	10.398
Mg	3.596	14.532	11.727
Cl	3.595	16.608	10.398
Mg	1.797	17.647	11.727
Cl	1.797	19.724	10.398
Mg	3.596	8.305	11.727
Cl	3.596	10.380	10.398
Cl	3.595	6.229	13.055
Mg	1.797	5.190	11.727
Cl	1.798	7.267	10.398
Cl	1.797	3.114	13.055
Mg	3.595	2.076	11.726
Cl	1.798	1.038	10.397
Mg	1.797	-1.037	11.726
Cl	3.595	-2.075	10.397
Mg	3.595	-4.152	11.726
Cl	3.595	-6.229	13.054

Cl	3.595	4.152	10.398
Cl	3.595	0.000	13.054
Cl	1.797	-3.113	13.054
Cl	3.596	12.456	13.055
Cl	1.797	15.570	13.055
H	-2.789	8.582	18.321
H	-3.143	7.301	17.116
H	-1.555	8.354	15.527
H	-3.716	10.292	16.583
H	-2.991	10.336	14.964
H	-3.995	8.952	15.444
H	-1.307	10.611	17.597
H	-0.645	10.632	15.933
H	-0.023	9.434	17.115
H	-2.784	6.834	20.412
H	-4.823	5.729	21.299
H	-5.735	3.700	20.172
H	-4.595	2.787	18.150
O	-2.580	2.512	16.666
O	-1.757	4.569	16.147
C	-1.882	1.951	15.509
C	-2.286	0.488	15.362
H	-2.151	2.538	14.618
H	-0.800	2.055	15.681
H	-1.683	0.124	14.509
C	-1.907	-0.342	16.596
C	-3.768	0.325	15.003
H	-2.091	-1.412	16.422
H	-0.840	-0.198	16.834
H	-2.489	-0.034	17.476
H	-4.018	-0.731	14.833
H	-4.412	0.694	15.816
H	-4.023	0.884	14.090

Mono_DIBP_Beta_6.6

Mg	1.798	-1.038	11.727
Cl	1.798	-3.114	13.055
Mg	3.596	-4.152	11.727
Cl	3.596	-6.229	13.055
Cl	3.596	0.000	13.055
Mg	3.596	2.076	11.727
Cl	3.596	4.152	10.398
Mg	1.798	5.190	11.727
Cl	1.798	7.267	10.398
Mg	3.596	8.305	11.727
Cl	3.596	10.380	10.398
Mg	1.798	11.418	11.727
Cl	1.797	13.494	10.398
Mg	3.596	14.532	11.727
Cl	3.595	16.608	10.398
Mg	1.797	17.646	11.727
Cl	1.797	19.723	10.398
Cl	1.798	1.038	10.398
Cl	3.596	-2.076	10.398
Cl	1.798	3.114	13.055
Cl	3.596	6.229	13.055
Cl	1.798	9.343	13.055
Cl	3.596	12.456	13.055
Cl	1.797	15.570	13.055
Cl	1.797	7.266	17.079
Mg	3.595	8.305	18.408

Cl	3.595	10.381	17.079
Mg	1.797	11.419	18.408
Cl	1.797	13.494	17.079
Mg	3.595	14.533	18.408
Cl	3.595	16.608	17.079
Mg	1.797	17.647	18.408
Cl	1.797	19.723	17.079
Cl	3.595	6.229	19.736
Mg	1.797	5.190	18.408
Cl	1.797	3.114	19.736
Mg	3.595	2.076	18.408
Cl	3.595	4.152	17.079
Cl	1.797	1.038	17.079
Mg	1.797	-1.037	18.408
Cl	3.595	-2.075	17.079
Mg	3.596	-4.151	18.408
Cl	3.596	-6.228	19.736
Cl	3.595	0.000	19.736
Cl	1.797	-3.113	19.736
Cl	1.797	9.343	19.736
Cl	3.595	12.457	19.736
Cl	1.797	15.571	19.736
O	-0.209	5.401	18.881
C	-1.277	5.959	18.618
O	-1.291	6.988	17.786
C	-2.539	7.550	17.278
C	-2.176	8.762	16.427
H	-3.035	6.770	16.681
H	-3.189	7.834	18.122
C	-3.445	9.300	15.754
C	-1.468	9.840	17.257
H	-1.478	8.414	15.648
H	-3.207	10.166	15.120
H	-3.921	8.540	15.116
H	-4.185	9.628	16.501
H	-1.176	10.681	16.609
H	-2.134	10.234	18.043
H	-0.569	9.421	17.734
C	-2.520	5.562	19.366
C	-3.234	4.399	19.022
C	-4.314	3.991	19.816
C	-4.685	4.736	20.935
C	-3.969	5.885	21.278
C	-2.884	6.296	20.499
C	-2.817	3.673	17.789
H	-4.860	3.087	19.544
H	-5.530	4.416	21.546
H	-4.246	6.462	22.162
H	-2.305	7.176	20.786
O	-3.209	2.385	17.771
O	-2.175	4.208	16.894
C	-2.756	1.604	16.620
C	-3.294	0.185	16.753
H	-3.120	2.093	15.703
H	-1.655	1.627	16.607
H	-2.897	-0.344	15.868
C	-2.760	-0.517	18.008
C	-4.826	0.140	16.684
H	-5.187	-0.898	16.700
H	-5.275	0.664	17.540
H	-5.200	0.612	15.763
H	-3.092	-1.564	18.044

H	-1.658	-0.506	18.029
H	-3.112	-0.018	18.922

Bridge_DIBP_Alpha_5.9

Mg	3.114	1.797	17.590
Cl	5.190	1.797	18.918
Cl	4.152	3.596	16.261
Mg	6.228	3.596	17.590
Cl	5.190	5.394	18.918
Cl	7.266	5.394	16.261
Mg	6.228	7.192	17.590
Cl	8.304	7.192	18.918
Cl	7.266	8.990	16.261
Mg	9.342	8.990	17.590
Cl	8.304	10.788	18.918
Cl	10.380	10.788	16.261
Mg	9.342	12.586	17.590
Cl	10.380	14.384	16.261
Cl	2.076	0.000	18.918
Cl	4.152	0.000	16.261
Mg	3.114	-1.797	17.590
Cl	1.038	-1.798	16.261
Cl	2.076	-3.596	18.918
Mg	0.000	-3.595	17.590
Cl	-1.038	-5.394	18.918
Cl	1.038	-5.393	16.261
Mg	-0.000	-7.192	17.590
Cl	-1.038	-8.989	18.918
Mg	4.152	3.596	11.726
Cl	6.228	3.596	13.055
Cl	5.190	5.394	10.398
Mg	7.266	5.394	11.726
Cl	6.228	7.192	13.055
Cl	8.304	7.192	10.398
Mg	7.266	8.989	11.726
Cl	9.342	8.990	13.055
Cl	8.304	10.788	10.398
Mg	10.380	10.788	11.726
Cl	9.342	12.586	13.055
Cl	11.418	12.586	10.398
Mg	10.380	14.384	11.726
Cl	11.418	16.182	10.398
Cl	3.114	1.797	13.055
Cl	5.190	1.797	10.398
Mg	4.152	0.000	11.726
Cl	3.114	-1.798	13.055
Cl	2.076	0.000	10.398
Mg	1.038	-1.798	11.726
Cl	0.000	-3.595	13.055
Cl	2.076	-3.596	10.397
Mg	1.038	-5.393	11.726
Cl	-0.000	-7.192	13.055
O	1.129	2.427	17.420
C	0.008	2.063	17.812
O	-0.511	2.442	18.965
C	0.344	3.236	19.858
C	-0.486	3.687	21.050
H	1.181	2.592	20.165
C	0.437	4.404	22.043
H	-0.125	4.715	22.934
H	0.876	5.310	21.594

H	1.264	3.758	22.374
C	-1.661	4.574	20.628
H	-2.259	4.867	21.503
H	-1.302	5.496	20.144
H	-2.328	4.057	19.924
O	-1.252	-2.060	18.324
C	-1.322	-0.822	18.415
O	-1.266	-0.175	19.562
C	-1.016	-0.941	20.795
H	-0.286	-0.327	21.341
H	-0.559	-1.902	20.531
C	-2.308	-1.119	21.587
H	-3.020	-1.660	20.940
C	-2.925	0.225	21.988
H	-2.251	0.773	22.667
H	-3.120	0.862	21.113
H	-3.877	0.075	22.517
C	-2.017	-1.998	22.811
H	-1.270	-1.526	23.470
H	-1.638	-2.988	22.519
H	-2.932	-2.147	23.399
H	0.737	4.092	19.287
C	-0.928	1.286	16.933
C	-1.553	0.045	17.214
H	-0.884	2.780	21.537
C	-2.397	-0.517	16.244
C	-2.653	0.123	15.035
C	-2.006	1.324	14.745
C	-1.133	1.881	15.677
H	-2.854	-1.485	16.455
H	-3.339	-0.327	14.317
H	-2.170	1.828	13.790
H	-0.596	2.802	15.441

Zip_DIBP_Alpha_6.6_011

Mg	-2.844	1.224	0.981
Cl	-5.299	1.725	0.981
Cl	-2.813	-2.225	-2.670
Mg	0.248	3.146	1.006
Cl	-2.206	3.647	1.006
Cl	0.278	-0.303	-2.646
Mg	-5.401	1.923	-1.513
Cl	-2.946	1.422	-1.513
Cl	-7.856	2.423	-1.513
Mg	-8.493	0.000	-1.538
Cl	-6.038	-0.499	-1.538
Cl	-10.948	0.501	-1.538
Mg	-5.936	-0.697	0.957
Cl	-3.481	-1.198	0.957
Cl	-8.391	-0.196	0.957
Mg	-2.309	3.845	-1.488
Cl	0.145	3.344	-1.488
Cl	-4.764	4.346	-1.489
Mg	3.340	5.069	1.031
Cl	3.370	1.618	-2.621
Cl	0.885	5.570	1.031
Cl	2.703	2.646	1.006
Mg	0.782	5.767	-1.464
Cl	3.237	5.266	-1.464
Cl	-1.672	6.267	-1.464
Cl	5.795	4.568	1.031

Mg	2.198	-3.424	-0.175
Mg	-0.358	-2.726	-2.670
Cl	4.653	-3.925	-0.175
Cl	2.836	-1.001	-0.150
H	6.248	-3.115	2.715
Mg	5.291	-1.502	-0.150
Mg	2.733	-0.804	-2.645
Cl	7.745	-2.003	-0.150
Mg	8.383	0.419	-0.125
Cl	5.188	-1.305	-2.645
Mg	5.825	1.118	-2.621
Cl	8.280	0.617	-2.621
Cl	10.837	-0.081	-0.125
Cl	5.928	0.920	-0.125
Mg	-0.893	-5.346	-0.199
Cl	1.561	-5.847	-0.199
Mg	-3.451	-4.648	-2.695
Cl	-0.256	-2.923	-0.175
Cl	-0.996	-5.149	-2.695
Cl	-3.348	-4.845	-0.199
Cl	2.096	-3.227	-2.670
Cl	-5.906	-4.147	-2.695
O	2.192	-3.426	1.927
C	1.765	-3.959	2.954
O	2.539	-4.387	3.935
C	4.005	-4.298	3.726
C	4.582	-2.952	4.150
C	4.362	-2.677	5.641
C	6.074	-2.930	3.786
H	4.901	-3.416	6.255
H	3.298	-2.722	5.910
H	4.210	-4.506	2.667
H	4.392	-5.112	4.353
H	4.067	-2.172	3.561
H	4.741	-1.681	5.913
H	6.629	-3.699	4.346
H	6.517	-1.958	4.043
C	0.318	-4.338	3.113
C	0.011	-5.671	2.786
C	-1.321	-6.095	2.711
C	-2.357	-5.198	3.002
C	-2.051	-3.888	3.355
C	-0.722	-3.440	3.415
H	0.821	-6.372	2.582
H	-1.545	-7.144	2.499
H	-3.396	-5.522	2.943
H	-2.837	-3.168	3.582
C	-0.526	-2.008	3.823
O	0.753	-1.750	4.171
C	1.059	-0.358	4.510
H	2.156	-0.313	4.456
H	0.632	0.273	3.718
C	0.558	0.069	5.892
H	-0.536	-0.043	5.896
C	0.884	1.557	6.081
H	1.971	1.737	6.050
H	0.414	2.176	5.302
H	0.517	1.911	7.054
C	1.148	-0.781	7.020
H	2.240	-0.652	7.084
H	0.941	-1.851	6.875
H	0.720	-0.486	7.990

O	-1.433	-1.195	3.862
Cl	-0.389	0.723	0.982

Zip_DIBP_Alpha_6.6_104

C	3.088	-4.702	9.606
C	2.324	-5.842	9.929
C	1.587	-5.773	11.244
C	1.814	-4.608	12.007
C	2.623	-3.534	11.636
C	3.254	-3.572	10.407
C	2.725	-6.881	8.757
O	3.215	-7.981	9.302
C	4.077	-8.876	8.507
C	0.558	-6.602	12.211
O	0.947	-7.771	12.679
C	2.177	-8.458	12.273
O	2.753	-6.642	7.502
Mg	2.076	-7.192	5.863
Cl	1.038	-5.393	7.191
Mg	2.076	-3.596	5.863
Cl	1.038	-1.798	7.191
Mg	-1.038	-1.798	5.863
Cl	-2.076	-0.000	7.191
Cl	3.114	-5.393	4.534
Cl	3.114	-8.990	4.534
Mg	2.076	-10.787	5.863
Cl	-0.000	-10.788	4.534
Mg	-1.038	-12.585	5.863
Cl	-2.076	-10.788	7.192
Mg	-1.038	-8.989	5.863
Cl	-2.076	-7.191	7.192
Mg	-1.038	-5.394	5.863
Cl	-2.076	-3.596	7.192
Cl	1.038	-8.989	7.192
Cl	-0.000	-7.192	4.534
Cl	1.038	-12.586	7.192
Mg	2.076	-14.383	5.863
Cl	3.114	-16.181	4.534
Cl	3.114	-12.586	4.534
Cl	0.000	-14.383	4.534
Cl	0.000	-3.595	4.534
O	-0.549	-6.161	12.685
Mg	-2.076	-7.191	11.726
Cl	-4.152	-7.191	10.397
Mg	-5.190	-8.989	11.726
Cl	-4.152	-10.788	10.397
Mg	-5.190	-12.585	11.726
Cl	-4.152	-14.384	10.397
Mg	-2.076	-14.383	11.726
Cl	-1.038	-16.182	10.397
Cl	-1.038	-5.394	10.398
Mg	-2.076	-3.595	11.726
Cl	-3.114	-5.394	13.055
Mg	-5.190	-5.393	11.726
Cl	-6.228	-3.596	13.055
Mg	-5.190	-1.797	11.726
Cl	-6.228	0.000	13.055
Cl	-3.114	-8.990	13.055
Mg	-2.076	-10.787	11.726
Cl	-1.038	-12.586	10.397
Cl	-1.038	-8.989	10.397

Cl	-3.114	-1.798	13.055
Cl	-4.152	-3.596	10.398
Cl	-6.228	-7.192	13.055
Cl	-3.114	-12.586	13.055
Cl	-6.228	-10.788	13.055
H	1.288	-4.530	12.961
H	2.731	-2.681	12.307
H	3.874	-2.745	10.059
H	3.617	-4.717	8.652
C	5.538	-8.436	8.535
H	3.937	-9.855	8.985
H	3.709	-8.906	7.475
C	2.568	-9.402	13.405
H	1.945	-9.001	11.345
H	2.954	-7.707	12.078
C	6.328	-9.383	7.620
H	5.584	-7.423	8.099
C	6.114	-8.397	9.953
H	7.382	-9.078	7.580
H	6.299	-10.417	7.999
H	5.937	-9.381	6.592
H	7.158	-8.054	9.932
H	5.551	-7.717	10.608
H	6.104	-9.400	10.409
C	3.927	-10.036	13.084
H	2.677	-8.790	14.317
C	1.496	-10.470	13.657
H	4.253	-10.679	13.914
H	3.871	-10.664	12.181
H	4.706	-9.276	12.925
H	1.793	-11.124	14.488
H	0.533	-10.010	13.924
H	1.358	-11.101	12.763

**Zip_DIBP_Alpha_5.9_Partial
y_Relaxed**

C	9.912	4.105	14.477
C	9.653	3.499	15.732
C	10.225	4.058	16.885
C	11.073	5.162	16.812
C	11.299	5.779	15.582
C	10.699	5.268	14.434
C	8.696	2.377	16.010
O	8.973	1.228	15.425
C	8.086	0.090	15.744
C	8.745	-1.187	15.249
C	9.387	3.679	13.144
O	9.505	2.394	12.874
C	9.091	1.952	11.529
C	9.435	0.479	11.369
O	7.759	2.496	16.817
Mg	6.195	3.638	17.510
Cl	4.152	3.596	16.261
Mg	3.114	1.797	17.590
Cl	4.267	-0.215	16.288
Mg	2.998	-1.732	17.588
Cl	1.038	-1.798	16.261
Mg	0.000	-3.595	17.590
Cl	0.172	-5.324	15.810
Mg	-0.281	-7.046	17.355
Cl	-0.137	-9.257	17.462

Cl	5.190	5.394	18.918
Mg	6.228	7.192	17.590
Cl	7.266	8.990	16.261
Mg	9.220	9.016	17.588
Cl	10.799	10.608	16.772
Mg	9.342	12.586	17.590
Cl	10.380	14.384	16.261
Cl	7.023	5.510	16.084
Cl	5.155	1.942	19.022
Cl	8.477	7.220	18.947
Cl	8.304	10.788	18.918
Cl	2.076	0.000	18.918
Cl	2.270	-3.732	18.717
Cl	-1.038	-5.394	18.918
O	8.971	4.508	12.315
Mg	7.242	5.452	11.765
Cl	5.190	5.394	10.398
Mg	4.152	3.596	11.726
Cl	5.322	1.559	10.433
Mg	4.013	0.063	11.716
Cl	2.076	0.000	10.398
Mg	1.038	-1.798	11.726
Cl	-0.748	-2.169	10.075
Mg	-1.581	-4.011	11.325
Cl	-3.195	-5.510	11.078
Cl	6.228	7.192	13.055
Mg	7.266	8.989	11.726
Cl	8.304	10.788	10.398
Mg	10.269	10.822	11.756
Cl	11.790	12.398	10.842
Mg	10.380	14.384	11.726
Cl	11.418	16.182	10.398
Cl	8.131	7.179	10.244
Cl	6.109	3.668	13.164
Cl	9.533	8.977	13.053
Cl	9.342	12.586	13.055
Cl	3.114	1.797	13.055
Cl	3.365	-2.079	12.649
Cl	0.000	-3.595	13.055
H	9.990	3.622	17.856
H	11.525	5.552	17.726
H	11.933	6.664	15.508
H	10.836	5.771	13.476
H	7.926	0.074	16.832
H	7.117	0.282	15.261
C	7.768	-2.352	15.463
C	10.088	-1.444	15.940
H	8.922	-1.077	14.164
H	8.010	2.131	11.436
H	9.626	2.574	10.794
C	8.980	0.030	9.972
C	10.923	0.196	11.597
H	8.848	-0.080	12.119
H	11.135	-0.875	11.477
H	11.540	0.740	10.863
H	11.246	0.496	12.603
H	9.133	-1.051	9.850
H	7.917	0.251	9.797
H	9.565	0.537	9.189
H	10.551	-2.365	15.558
H	10.794	-0.618	15.776
H	9.950	-1.566	17.027

H	8.196	-3.286	15.073
H	7.566	-2.502	16.535
H	6.805	-2.182	14.960

**Zip_DIBP_Alpha_6.3_Partial
y_Relaxed**

Mg	3.549	8.301	11.842
Mg	1.798	11.418	11.727
Cl	3.546	10.264	10.329
Cl	1.798	9.343	13.055
Mg	3.479	14.508	11.755
Cl	3.718	12.565	13.091
Cl	1.797	13.494	10.398
Cl	3.991	16.639	10.820
Mg	1.797	17.646	11.727
Cl	1.797	15.570	13.055
Cl	1.797	19.723	10.398
Cl	3.304	6.255	13.274
Cl	1.798	7.267	10.398
Mg	1.798	5.190	11.726
Cl	3.885	4.039	10.501
Cl	1.797	3.114	13.055
Mg	3.447	2.064	11.716
Cl	3.915	-0.106	12.695
Cl	1.797	1.038	10.398
Mg	1.797	-1.038	11.726
Cl	1.094	-2.425	9.818
Mg	1.310	-4.409	11.112
Cl	1.797	-3.114	13.054
Cl	1.116	-6.588	10.728
Mg	3.563	6.268	17.870
Cl	3.262	8.297	16.453
Cl	1.798	7.266	19.355
Cl	3.594	4.286	19.370
Cl	1.798	5.189	16.698
Mg	1.798	3.113	18.026
Cl	3.740	1.942	16.686
Mg	3.456	-0.000	18.011
Cl	1.798	1.037	19.354
Cl	3.867	-2.119	19.087
Cl	1.798	-1.038	16.697
Mg	1.798	-3.114	18.026
Cl	2.375	-4.549	16.108
Mg	2.931	-6.322	17.572
Cl	4.113	-8.196	17.524
Cl	1.798	-5.190	19.354
Mg	1.798	9.342	18.027
Cl	3.792	10.483	19.327
Cl	1.798	11.418	16.698
Mg	3.478	12.432	18.012
Cl	4.039	14.607	17.199
Cl	1.798	13.494	19.355
Mg	1.798	15.570	18.027
Cl	1.798	17.646	16.698
O	5.357	8.463	12.777
C	6.453	8.215	13.277
C	6.789	8.689	14.670
C	6.562	7.965	15.866
C	6.831	8.581	17.098
C	7.329	9.880	17.160
C	7.534	10.598	15.981

C	7.252	10.010	14.746
H	7.373	10.591	13.829
H	7.900	11.626	16.016
H	7.541	10.332	18.130
H	6.646	8.019	18.014
O	7.373	7.640	12.515
C	8.715	7.324	13.017
H	8.614	6.591	13.831
H	9.171	8.245	13.410
C	9.522	6.760	11.853
H	9.534	7.528	11.060
C	10.964	6.524	12.320
H	11.003	5.771	13.125
H	11.578	6.151	11.489
H	11.432	7.446	12.695
C	8.896	5.482	11.284
H	9.470	5.125	10.417
H	8.900	4.676	12.037
H	7.860	5.644	10.960
C	6.042	6.569	15.910
O	5.399	6.098	16.863
O	6.394	5.872	14.840
C	5.951	4.477	14.666
H	5.183	4.246	15.415
H	5.499	4.478	13.666
C	7.147	3.534	14.760
H	7.945	3.945	14.117
C	7.678	3.413	16.193
H	6.902	3.017	16.864
H	8.544	2.735	16.229
H	8.005	4.384	16.594
H	6.479	2.249	13.120
H	7.558	1.449	14.274
C	6.734	2.170	14.189
H	5.866	1.758	14.725

**Zip_DIBP_Alpha_6.6_Partial
y_Relaxed**

Mg	3.553	6.225	18.209
Cl	3.542	4.267	19.730
Cl	3.373	8.303	16.821
Mg	1.797	9.343	18.326
Cl	1.797	7.267	19.654
Cl	1.798	11.419	16.997
Mg	3.502	12.439	18.322
Cl	3.704	10.496	19.682
Cl	4.008	14.644	17.503
Mg	1.797	15.570	18.327
Cl	1.797	13.494	19.654
Cl	1.798	17.646	16.998
Mg	1.798	3.114	18.326
Cl	1.797	1.038	19.654
Cl	1.798	5.190	16.997
Mg	3.454	0.007	18.294
Cl	3.809	1.960	17.015
Cl	3.904	-2.163	19.297
Mg	1.798	-3.114	18.326
Cl	1.798	-1.038	16.997
Cl	1.798	-5.190	19.654
Mg	0.293	-6.237	18.122
Cl	0.178	-4.229	16.850

Cl	-0.627	-8.242	17.940
Mg	3.533	8.223	11.873
Cl	3.011	6.293	13.440
Cl	3.621	10.230	10.415
Mg	1.797	11.418	11.727
Cl	1.797	9.343	13.055
Cl	1.797	13.494	10.398
Mg	3.478	14.517	11.750
Cl	3.700	12.579	13.107
Cl	3.991	16.642	10.815
Mg	1.797	17.646	11.727
Cl	1.797	15.570	13.055
Cl	1.797	19.723	10.398
Mg	1.797	5.190	11.726
Cl	1.797	3.114	13.054
Cl	1.797	7.267	10.397
Mg	3.437	2.083	11.722
Cl	3.845	4.084	10.498
Cl	3.945	-0.095	12.669
Mg	1.797	-1.037	11.726
Cl	1.797	1.038	10.397
Cl	1.797	-3.113	13.054
Mg	1.257	-4.407	11.118
Cl	1.055	-2.420	9.832
Cl	1.150	-6.585	10.722
O	5.303	5.972	17.172
C	6.343	6.108	16.529
O	7.377	6.688	17.127
C	8.688	6.785	16.472
C	9.669	7.380	17.475
H	9.258	8.353	17.794
C	9.837	6.487	18.708
H	10.261	5.509	18.429
H	10.522	6.952	19.431
H	8.879	6.313	19.216
C	11.008	7.628	16.768
H	10.899	8.297	15.901
H	11.454	6.685	16.415
H	11.723	8.093	17.460
H	9.002	5.777	16.159
H	8.582	7.425	15.585
C	6.506	5.499	15.158
C	6.751	4.119	15.173
H	6.782	3.592	16.128
C	6.939	3.412	13.983
H	7.142	2.340	14.023
C	6.848	4.074	12.758
H	6.997	3.536	11.820
C	6.537	5.431	12.728
H	6.407	5.942	11.774
C	6.370	6.165	13.913
C	5.979	7.594	13.760
O	6.296	8.345	14.803
C	5.814	9.741	14.820
H	6.083	10.215	13.865
H	4.721	9.692	14.913
C	6.452	10.428	16.020
H	6.343	9.743	16.878
C	7.935	10.737	15.792
H	8.062	11.457	14.968
H	8.505	9.832	15.537
H	8.391	11.175	16.692

C	5.660	11.702	16.335
H	6.066	12.182	17.240
H	4.594	11.437	16.456
H	5.702	12.441	15.523
O	5.424	8.051	12.745

**Zip_DIBP_Alpha_7.9_Partial
y_Relaxed**

C	1.634	-0.553	13.639
C	2.888	-0.803	13.053
C	3.727	0.314	12.742
C	3.214	1.605	12.958
C	1.925	1.823	13.439
C	1.141	0.737	13.818
C	3.112	-2.270	12.818
O	3.783	-2.564	11.720
C	5.163	0.345	12.284
O	5.474	-0.486	11.311
O	5.983	1.169	12.737
Mg	7.025	2.003	14.348
Cl	5.101	1.062	15.697
Mg	5.109	2.972	17.077
Cl	2.856	2.362	17.869
Mg	1.812	4.101	16.678
Cl	-0.546	4.009	16.983
Mg	-0.334	4.907	19.401
Cl	-2.588	4.298	20.193
Cl	9.223	2.818	13.457
Mg	10.554	1.036	14.753
Cl	12.807	1.644	13.961
Mg	12.674	0.220	12.062
Cl	10.440	-0.397	12.556
Cl	13.745	-1.508	13.221
Mg	15.999	-0.899	12.429
Cl	17.023	-2.958	13.305
Mg	19.141	-2.376	12.385
Cl	21.141	-3.309	12.194
Cl	14.732	0.573	10.825
Cl	18.252	-0.290	11.637
Cl	8.301	0.427	15.545
Cl	7.362	3.580	16.285
Cl	3.813	4.654	15.524
Cl	1.918	5.516	18.609
O	2.583	-3.140	13.537
Mg	2.875	-4.434	15.143
Cl	0.635	-5.242	15.838
Mg	0.687	-3.839	17.955
Cl	-1.565	-4.448	18.747
Mg	-2.601	-2.667	17.546
Cl	-4.951	-2.826	17.871
Mg	-4.756	-1.903	20.279
Cl	-7.010	-2.512	21.071
Cl	5.282	-3.718	14.759
Mg	6.133	-5.775	15.631
Cl	5.962	-7.006	13.295
Mg	8.270	-6.569	12.946
Cl	9.324	-8.320	14.099
Mg	11.577	-7.710	13.307
Cl	13.830	-7.102	12.515
Mg	14.717	-9.184	13.270
Cl	16.701	-10.145	13.060

Cl	10.315	-6.269	11.670
Cl	12.595	-9.774	14.173
Cl	8.386	-5.166	14.839
Cl	3.878	-6.384	16.423
Cl	2.940	-3.231	17.163
Cl	-0.531	-1.939	16.639
Cl	-2.503	-1.295	19.487
H	3.852	2.461	12.743
H	1.554	2.846	13.532
H	0.151	0.877	14.254
H	1.027	-1.405	13.943
C	3.909	-3.984	11.359
C	6.844	-0.425	10.766
C	6.989	0.671	9.712
H	7.552	-0.291	11.593
H	6.979	-1.421	10.323
C	8.448	0.696	9.236
C	6.015	0.487	8.545
H	6.781	1.636	10.206
H	8.596	1.507	8.510
H	9.139	0.856	10.076
H	8.719	-0.249	8.740
H	6.124	1.306	7.820
H	6.214	-0.457	8.013
H	4.968	0.472	8.879
C	4.687	-4.085	10.054
H	4.427	-4.499	12.179
H	2.892	-4.395	11.255
C	4.841	-5.571	9.698
C	4.026	-3.301	8.916
H	5.692	-3.666	10.239
H	5.492	-5.689	8.820
H	5.269	-6.152	10.528
H	3.866	-6.017	9.448
H	4.615	-3.392	7.992
H	3.018	-3.694	8.708
H	3.934	-2.234	9.158

Zip_DIBP_Beta_5.9_Partially_Relaxed

C	6.571	5.710	15.591
C	6.568	6.985	15.008
C	6.882	7.123	13.637
C	7.223	5.987	12.894
C	7.285	4.733	13.503
C	6.945	4.592	14.848
C	6.674	8.390	12.845
O	7.682	9.212	12.585
C	9.033	9.009	13.116
C	10.047	9.327	12.021
C	6.310	8.130	15.924
O	7.072	9.183	15.632
C	7.045	10.358	16.521
C	7.944	10.178	17.743
O	5.546	8.073	16.895
Mg	3.575	8.268	17.586
Cl	3.442	10.335	16.199
Mg	1.798	11.419	17.654
Cl	1.798	13.495	16.325
Mg	3.478	14.509	17.649
Cl	4.005	16.668	16.773

Mg	1.798	17.647	17.654
Cl	1.798	19.724	16.324
Cl	3.501	6.322	19.105
Mg	1.798	5.190	17.654
Cl	1.798	3.114	18.982
Mg	3.449	2.049	17.681
Cl	3.808	3.986	16.393
Cl	1.798	1.038	16.325
Mg	1.798	-1.037	17.654
Cl	3.122	-2.269	15.979
Mg	3.661	-3.846	17.647
Cl	5.190	-5.422	17.943
Cl	3.789	-0.013	18.868
Cl	1.798	-3.113	18.982
Cl	1.798	7.267	16.324
Cl	1.798	9.343	18.982
Cl	3.775	12.574	18.978
Cl	1.798	15.571	18.981
O	5.584	8.644	12.333
Mg	3.583	8.348	11.786
Cl	3.427	10.281	10.233
Mg	1.798	11.419	11.727
Cl	1.798	13.495	10.398
Mg	3.485	14.509	11.728
Cl	3.989	16.649	10.818
Mg	1.798	17.647	11.727
Cl	1.798	19.723	10.398
Cl	3.455	6.283	13.171
Mg	1.798	5.190	11.727
Cl	3.813	4.037	10.423
Mg	3.448	2.087	11.698
Cl	1.798	1.038	10.398
Mg	1.798	-1.037	11.727
Cl	1.797	-3.113	13.055
Mg	1.167	-4.400	11.137
Cl	0.764	-6.556	10.813
Cl	3.931	-0.079	12.680
Cl	1.053	-2.424	9.831
Cl	1.798	3.114	13.055
Cl	1.798	7.267	10.398
Cl	1.798	9.343	13.055
Cl	3.781	12.564	13.032
Cl	1.798	15.571	13.055
H	7.425	6.083	11.825
H	7.581	3.864	12.913
H	6.960	3.609	15.320
H	6.284	5.614	16.638
H	9.131	9.697	13.967
H	9.135	7.976	13.476
H	11.028	9.181	12.510
C	9.948	8.346	10.846
C	9.953	10.786	11.558
H	6.003	10.561	16.793
H	7.413	11.167	15.873
C	7.800	11.424	18.628
H	7.566	9.312	18.313
C	9.405	9.920	17.362
H	8.408	11.321	19.538
H	8.151	12.326	18.098
H	6.756	11.587	18.935
H	10.021	9.773	18.260
H	9.512	9.023	16.734

H	9.823	10.777	16.808
H	10.741	11.011	10.826
H	8.983	10.986	11.082
H	10.069	11.484	12.402
H	10.744	8.539	10.114
H	10.047	7.302	11.180
H	8.986	8.454	10.323

Zip_DIBP_Beta_6.3_Partially_Relaxed

Mg	1.919	-1.009	11.731
Cl	3.596	0.000	13.055
Mg	3.596	2.076	11.727
Cl	2.099	3.141	13.274
Mg	1.843	5.175	11.840
Cl	3.596	6.229	13.055
Mg	3.596	8.305	11.727
Cl	1.664	9.500	13.045
Mg	1.946	11.434	11.721
Cl	3.596	12.456	13.055
Mg	3.596	14.532	11.727
Cl	2.561	15.855	13.525
Mg	1.943	17.472	11.915
Cl	3.595	16.608	10.398
Cl	1.588	0.938	10.431
Cl	3.596	-2.076	10.398
Mg	3.596	-4.152	11.727
Cl	3.596	-6.229	13.055
Cl	1.388	-3.166	12.611
Cl	1.851	7.149	10.328
Cl	3.596	4.152	10.398
Cl	1.555	13.525	10.593
Cl	3.596	10.380	10.398
Cl	0.455	19.103	11.709
Cl	1.576	0.920	16.744
Mg	3.596	2.076	18.027
Cl	3.596	0.000	19.355
Mg	1.914	-1.025	18.028
Cl	1.395	-3.163	18.927
Mg	3.596	-4.152	18.027
Cl	3.596	-6.229	19.355
Cl	3.596	-2.076	16.698
Cl	3.596	4.152	16.698
Mg	1.845	5.155	17.965
Cl	3.596	6.229	19.355
Mg	3.596	8.305	18.027
Cl	1.626	9.448	19.349
Mg	1.946	11.403	18.062
Cl	3.596	12.457	19.355
Mg	3.596	14.533	18.027
Cl	4.346	15.920	19.920
Mg	4.236	17.893	18.609
Cl	3.595	16.609	16.698
Cl	1.915	7.223	16.579
Cl	1.944	3.209	19.513
Cl	1.473	13.567	17.062
Cl	3.596	10.381	16.698
Cl	4.654	20.046	18.939
O	-0.009	5.449	12.735
O	0.060	4.685	17.110
C	-0.695	5.226	13.746

C	-1.083	4.516	16.694
C	-1.367	3.571	15.556
C	-1.102	3.871	14.201
C	-1.791	2.283	15.905
C	-1.981	1.310	14.922
C	-1.733	1.610	13.582
C	-1.282	2.879	13.227
H	-1.946	2.033	16.955
H	-2.315	0.312	15.211
H	-1.886	0.854	12.809
H	-1.074	3.117	12.184
O	-2.082	5.103	17.340
C	-3.461	5.033	16.842
C	-4.226	6.236	17.382
H	-3.444	5.029	15.744
H	-3.902	4.090	17.203
C	-5.629	6.249	16.760
C	-4.283	6.243	18.913
H	-3.686	7.138	17.044
H	-6.189	7.129	17.102
H	-5.591	6.281	15.661
H	-6.203	5.356	17.056
H	-4.803	7.142	19.274
H	-4.833	5.366	19.289
H	-3.278	6.233	19.356
O	-1.208	6.178	14.513
C	-0.965	7.598	14.197
C	-2.307	8.300	14.014
H	-0.394	7.981	15.052
H	-0.343	7.657	13.297
C	-3.075	7.758	12.804
H	-2.906	8.120	14.925
C	-2.069	9.811	13.893
H	-4.040	8.275	12.692
H	-2.501	7.912	11.877
H	-3.286	6.683	12.897
H	-3.027	10.343	13.813
H	-1.527	10.210	14.763
H	-1.478	10.041	12.994

**Zip_DIBP_Beta_6.6_Partially_
Relaxed**

Mg	4.045	2.542	4.753
Cl	2.970	2.766	6.851
Cl	6.109	1.911	6.006
Mg	4.885	1.997	8.197
Cl	4.344	-0.555	7.982
Cl	6.801	1.228	9.543
Mg	6.198	-1.059	9.352
Cl	5.021	-0.933	11.421
Cl	7.823	-2.407	10.443
Mg	6.937	-1.702	12.767
Cl	8.853	-2.471	14.114
Mg	2.833	5.697	3.626
Cl	2.009	3.430	3.606
Cl	4.750	4.928	4.973
Cl	0.917	6.466	2.279
Cl	4.009	5.362	1.294
Mg	2.130	6.351	0.255
Cl	0.599	6.955	-1.550
Cl	2.698	8.628	0.401

Mg	0.781	9.397	-0.944
Cl	-1.133	10.166	-2.290
Cl	1.759	11.618	-1.325
Mg	0.019	12.186	-2.839
Cl	-0.297	13.790	-4.332
Mg	-1.913	0.304	5.599
Cl	-3.225	0.431	7.742
Cl	-0.021	-0.438	7.021
Mg	-1.310	-0.337	9.088
Cl	-1.854	-2.903	8.836
Cl	0.606	-1.106	10.434
Mg	-0.012	-3.387	10.234
Cl	-1.174	-3.268	12.312
Cl	1.621	-4.740	11.329
Mg	0.741	-4.037	13.658
Cl	2.658	-4.807	15.005
Cl	-1.445	2.593	5.864
Cl	-3.991	0.906	4.404
Mg	-3.362	3.362	4.517
Cl	-2.205	3.019	2.166
Cl	-5.277	4.131	3.170
Mg	-4.063	4.021	1.129
Cl	-3.497	6.293	1.292
Cl	-5.634	4.624	-0.630
Mg	-5.414	7.062	-0.053
Cl	-4.515	9.338	-0.292
Cl	-7.329	7.831	-1.399
Mg	-6.309	9.965	-1.722
Cl	-6.855	11.774	-2.874
O	3.511	0.769	3.839
C	2.761	-0.211	3.756
O	2.624	-0.972	4.826
C	2.041	-2.310	4.832
H	2.074	-2.730	3.813
H	1.005	-2.200	5.182
H	2.846	-2.618	6.765
C	2.831	-3.171	5.812
C	2.087	-4.497	6.016
H	2.049	-5.086	5.085
H	1.053	-4.337	6.362
H	2.602	-5.113	6.766
C	4.274	-3.388	5.351
H	4.308	-3.927	4.389
H	4.827	-3.992	6.086
H	4.805	-2.433	5.239
C	2.108	-0.504	2.431
C	2.944	-0.278	1.323
C	2.483	-0.424	0.017
C	1.152	-0.771	-0.209
C	-0.297	-1.040	3.248
C	0.763	-0.888	2.198
C	0.305	-0.999	0.873
H	3.972	0.030	1.508
H	3.160	-0.244	-0.818
H	0.765	-0.854	-1.225
H	-0.745	-1.235	0.694
O	-1.025	-2.160	3.328
C	-0.665	-3.448	2.721
H	-0.024	-3.287	1.843
H	-0.098	-3.998	3.488
C	-1.941	-4.196	2.357
H	-2.548	-4.270	3.276

H	-0.942	-5.596	1.001
C	-1.563	-5.615	1.911
H	-2.467	-6.196	1.681
H	-1.008	-6.157	2.692
C	-2.758	-3.464	1.289
H	-2.195	-3.389	0.344
H	-3.687	-4.011	1.074
H	-3.039	-2.452	1.614
O	-0.604	-0.110	3.995

**Zip_DIBP_Beta_7.9_Partially_
Relaxed**

C	1.351	2.371	2.537
C	0.515	1.247	2.466
C	-0.684	1.333	1.705
C	-0.995	2.554	1.081
C	-0.137	3.648	1.139
C	1.052	3.550	1.854
C	1.003	0.117	3.343
O	1.607	-0.941	2.822
C	1.973	-1.024	1.403
C	3.257	-1.843	1.291
C	-1.667	0.242	1.434
O	-2.828	0.470	1.047
Mg	-4.873	0.701	1.482
Cl	-5.702	2.540	0.031
O	-1.162	-0.981	1.532
C	-1.990	-2.108	1.053
C	-1.287	-3.420	1.369
O	0.977	0.206	4.575
Mg	0.760	1.026	6.501
Cl	1.699	-0.805	7.895
Cl	-5.104	2.188	3.282
Mg	-5.856	4.168	2.020
Cl	-6.609	6.147	0.758
Mg	-4.399	6.877	0.278
Cl	-4.545	8.859	-1.108
Cl	-3.451	4.971	1.296
Cl	-4.396	8.273	2.156
Mg	-5.148	10.252	0.894
Cl	-5.901	12.231	-0.367
Mg	-6.070	13.531	1.626
Cl	-6.613	15.627	2.088
Cl	-5.407	11.641	2.912
Cl	-1.375	0.355	7.215
Mg	-0.616	-1.621	8.476
Cl	0.142	-3.599	9.737
Mg	0.123	-4.981	7.801
Cl	-2.073	-5.728	8.349
Mg	-1.314	-7.705	9.610
Cl	-0.555	-9.683	10.871
Cl	0.905	-7.147	8.410
Cl	-0.568	-3.190	6.406
Cl	-0.224	3.042	5.410
Mg	0.081	4.462	7.342
Cl	-0.676	6.440	6.081
Mg	1.531	7.147	5.608
Cl	1.384	9.141	4.207
Cl	0.840	2.485	8.603
Cl	2.483	5.173	6.482
Cl	1.539	8.569	7.468

Mg	0.780	10.547	6.207
Cl	0.021	12.524	4.947
Mg	-0.007	13.863	6.927
Cl	-0.427	15.997	7.346
Cl	0.665	11.974	8.203
Cl	-4.380	-1.003	3.305
Mg	-6.565	-1.916	3.147
Cl	-7.317	0.062	1.885
Cl	-5.812	-3.895	4.409
Mg	-5.805	-5.292	2.501
Cl	-8.025	-6.022	3.011
Mg	-7.273	-8.001	4.273
Cl	-6.521	-9.980	5.535
Cl	-5.048	-7.470	3.092
Cl	-6.155	-3.444	1.051
C	-1.139	-3.643	2.876
H	-0.285	-3.400	0.905
C	3.060	-3.288	1.768
H	2.110	-0.007	1.009
H	-1.935	2.632	0.536
H	2.251	2.325	3.153
H	3.470	-1.863	0.206
C	-2.086	-4.551	0.705
C	4.435	-1.163	2.000
H	1.138	-1.506	0.879
H	-2.963	-2.054	1.556
H	-0.416	4.575	0.638
H	1.736	4.397	1.918
H	-2.123	-1.962	-0.029
H	5.364	-1.723	1.826
H	4.589	-0.136	1.636
H	4.269	-1.123	3.087
H	3.978	-3.873	1.615
H	2.816	-3.318	2.840
H	2.248	-3.788	1.220
H	-1.630	-5.526	0.927
H	-3.120	-4.567	1.085
H	-2.140	-4.439	-0.387
H	-0.648	-4.606	3.077
H	-0.541	-2.859	3.357
H	-2.121	-3.653	3.373

**Zip_p-
isopropoxy_EB_Alpha_5.9_Pa
rtially_Relaxed**

Mg	1.038	-1.798	11.726
Cl	3.342	-2.000	12.777
Mg	4.031	0.054	11.754
Cl	3.114	1.797	13.055
Mg	4.152	3.596	11.726
Cl	6.026	3.780	13.208
Mg	7.219	5.411	11.750
Cl	6.228	7.192	13.055
Mg	7.266	8.989	11.726
Cl	9.547	8.968	13.045
Mg	10.272	10.824	11.757
Cl	9.342	12.586	13.055
Mg	10.380	14.384	11.726
Cl	11.790	12.399	10.838
Cl	2.076	0.000	10.398
Cl	1.286	-3.891	10.063

Mg	0.620	-5.442	11.773
Cl	-0.000	-7.192	13.055
Cl	0.000	-3.595	13.055
Cl	5.190	5.394	10.398
Cl	5.317	1.575	10.452
Cl	8.304	10.788	10.398
Cl	8.139	7.181	10.248
Cl	11.418	16.182	10.398
Cl	1.038	-1.798	16.261
Mg	3.004	-1.722	17.579
Cl	2.270	-3.678	18.768
Mg	0.000	-3.595	17.590
Cl	-1.038	-5.394	18.918
Mg	-0.254	-7.039	17.323
Cl	-0.216	-9.247	17.562
Cl	0.349	-5.284	15.878
Cl	4.269	-0.181	16.293
Mg	3.114	1.797	17.590
Cl	5.112	1.937	19.057
Mg	6.192	3.611	17.593
Cl	5.190	5.394	18.918
Mg	6.228	7.192	17.590
Cl	8.631	7.149	18.874
Mg	9.342	8.990	17.590
Cl	8.304	10.788	18.918
Mg	9.342	12.586	17.590
Cl	10.854	10.635	16.790
Cl	4.152	3.596	16.261
Cl	2.076	0.000	18.918
Cl	7.266	8.990	16.261
Cl	6.996	5.474	16.097
Cl	10.380	14.384	16.261
O	9.035	4.280	11.914
C	9.370	3.869	13.215
C	8.869	2.656	13.699
C	8.913	2.409	15.066
C	9.527	3.331	15.927
C	10.171	4.462	15.402
C	10.068	4.750	14.041
H	8.338	1.980	13.031
H	8.416	1.527	15.475
C	9.268	3.243	17.382
H	10.657	5.168	16.075
H	10.453	5.686	13.633
C	9.733	3.581	10.785
C	8.759	3.516	9.624
C	11.021	4.322	10.481
H	9.943	2.567	11.161
H	11.563	3.803	9.676
H	10.805	5.348	10.151
H	11.679	4.358	11.361
H	9.222	2.965	8.793
H	7.836	2.983	9.896
H	8.515	4.522	9.249
O	10.308	3.515	18.152
O	8.141	2.973	17.843
C	10.076	3.608	19.607
C	11.425	3.543	20.284
H	9.561	4.564	19.783
H	9.412	2.785	19.902
H	11.285	3.639	21.370
H	11.925	2.584	20.087

H	12.081	4.359	19.951
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**Zip_p-
isopropoxy_EB_Alpha_6.3_Pa
rtially_Relaxed**

Mg	1.798	-1.038	11.727
Cl	3.925	-0.109	12.689
Mg	3.446	2.060	11.731
Cl	1.798	3.114	13.055
Mg	1.798	5.190	11.727
Cl	3.236	6.298	13.304
Mg	3.542	8.284	11.757
Cl	1.798	9.343	13.055
Mg	1.798	11.418	11.727
Cl	3.692	12.560	13.110
Mg	3.480	14.503	11.758
Cl	1.797	15.570	13.055
Mg	1.797	17.646	11.727
Cl	3.989	16.634	10.820
Cl	1.798	1.038	10.398
Cl	1.023	-2.420	9.839
Mg	1.123	-4.391	11.159
Cl	0.669	-6.536	10.817
Cl	1.798	-3.114	13.055
Cl	1.798	7.267	10.398
Cl	3.881	4.041	10.498
Cl	1.797	13.494	10.398
Cl	3.516	10.294	10.314
Cl	1.797	19.723	10.398
Cl	1.798	-1.038	16.698
Mg	3.462	0.008	18.000
Cl	3.864	-2.113	19.086
Mg	1.798	-3.113	18.027
Cl	1.798	-5.189	19.355
Mg	2.937	-6.318	17.574
Cl	4.124	-8.188	17.520
Cl	2.373	-4.550	16.107
Cl	3.789	1.965	16.714
Mg	1.798	3.114	18.027
Cl	3.526	4.265	19.414
Mg	3.535	6.302	17.946
Cl	1.798	7.267	19.355
Mg	1.798	9.343	18.027
Cl	3.861	10.459	19.241
Mg	3.479	12.453	17.995
Cl	1.798	13.495	19.355
Mg	1.798	15.571	18.027
Cl	4.027	14.627	17.191
Cl	1.798	5.190	16.698
Cl	1.798	1.038	19.355
Cl	1.798	11.419	16.698
Cl	3.079	8.207	16.382
Cl	1.798	17.647	16.698
O	5.651	6.665	17.765
C	6.083	6.776	16.426
C	6.719	6.605	18.824
C	6.008	6.711	20.159
H	7.189	5.614	18.708
C	7.742	7.707	18.620
C	6.086	8.040	15.831
C	6.247	8.142	14.455

C	6.466	6.988	13.687
C	6.588	5.738	14.315
C	6.372	5.626	15.690
H	5.870	8.917	16.436
H	6.160	9.114	13.967
C	6.360	7.087	12.213
H	6.758	4.845	13.714
H	6.361	4.647	16.172
O	7.173	6.290	11.542
O	5.549	7.848	11.648
C	7.019	6.248	10.073
C	8.184	5.462	9.521
H	6.051	5.769	9.866
H	6.992	7.283	9.705
H	8.089	5.407	8.427
H	9.141	5.944	9.758
H	8.196	4.436	9.913
H	6.756	6.679	20.964
H	5.472	7.668	20.239
H	5.312	5.879	20.326
H	8.522	7.602	19.388
H	8.233	7.651	17.640
H	7.279	8.698	18.736

**Zip_p-
isopropoxy_EB_Alpha_6.6_Pa
rtially_Relaxed**

Mg	1.798	-1.038	11.727
Cl	3.919	-0.104	12.686
Mg	3.445	2.076	11.716
Cl	1.798	3.114	13.055
Mg	1.798	5.190	11.727
Cl	3.085	6.323	13.383
Mg	3.529	8.248	11.806
Cl	1.798	9.343	13.055
Mg	1.798	11.418	11.727
Cl	3.758	12.561	13.064
Mg	3.478	14.514	11.750
Cl	1.797	15.570	13.055
Mg	1.797	17.646	11.727
Cl	3.991	16.643	10.818
Cl	1.798	1.038	10.398
Cl	0.632	-2.317	9.986
Mg	0.788	-4.319	11.258
Cl	0.306	-6.453	10.897
Cl	1.798	-3.114	13.055
Cl	1.798	7.267	10.398
Cl	3.872	4.086	10.533
Cl	1.797	13.494	10.398
Cl	3.517	10.269	10.317
Cl	1.797	19.723	10.398
Cl	1.798	-1.037	16.998
Mg	3.453	0.008	18.290
Cl	3.902	-2.157	19.301
Mg	1.798	-3.113	18.327
Cl	1.798	-5.189	19.655
Mg	0.294	-6.241	18.121
Cl	-0.629	-8.246	17.955
Cl	0.181	-4.232	16.849
Cl	3.818	1.996	17.050
Mg	1.798	3.114	18.326

Cl	3.445	4.270	19.809
Mg	3.528	6.259	18.276
Cl	1.798	7.267	19.654
Mg	1.798	9.343	18.326
Cl	3.776	10.477	19.633
Mg	3.478	12.433	18.320
Cl	1.798	13.495	19.654
Mg	1.798	15.571	18.326
Cl	4.017	14.599	17.473
Cl	1.798	5.190	16.997
Cl	1.798	1.038	19.654
Cl	1.798	11.419	16.997
Cl	3.308	8.248	16.792
Cl	1.798	17.647	16.997
O	5.635	6.242	18.068
C	6.118	6.704	16.828
C	6.682	7.977	16.702
C	6.907	8.497	15.428
C	6.529	7.762	14.292
C	6.042	6.455	14.437
C	5.860	5.915	15.706
H	6.848	8.592	17.585
H	7.290	9.512	15.315
C	6.482	8.405	12.957
H	5.761	5.878	13.558
H	5.434	4.917	15.828
O	7.504	9.205	12.690
O	5.549	8.236	12.149
C	7.460	9.935	11.406
C	6.605	5.744	19.106
C	7.241	6.907	19.850
H	5.928	5.193	19.773
C	7.598	4.785	18.482
H	8.225	4.362	19.280
H	7.089	3.957	17.972
H	8.263	5.294	17.769
H	7.762	6.516	20.736
H	7.984	7.432	19.234
H	6.483	7.624	20.196
C	8.770	10.671	11.260
H	7.300	9.198	10.608
H	6.587	10.603	11.432
H	8.766	11.220	10.308
H	8.919	11.396	12.072
H	9.619	9.975	11.247

**Zip_p-
isopropoxy_EB_Alpha_7.9_Pa
rtially_Relaxed**

Mg	1.798	-1.038	11.727
Cl	3.908	-0.091	12.717
Mg	3.437	2.066	11.726
Cl	1.798	3.114	13.055
Mg	1.798	5.190	11.727
Cl	3.004	6.295	13.440
Mg	3.545	8.262	11.882
Cl	1.798	9.343	13.055
Mg	1.798	11.418	11.727
Cl	3.647	12.567	13.131
Mg	3.481	14.497	11.761
Cl	1.797	15.570	13.055

Mg	1.797	17.646	11.727
Cl	3.994	16.633	10.830
Cl	1.798	1.038	10.398
Cl	1.117	-2.427	9.819
Mg	1.303	-4.414	11.111
Cl	1.162	-6.589	10.707
Cl	1.798	-3.114	13.055
Cl	1.798	7.267	10.398
Cl	3.903	4.077	10.549
Cl	1.797	13.494	10.398
Cl	3.606	10.242	10.395
Cl	1.797	19.723	10.398
Cl	1.798	-1.038	18.298
Mg	3.453	0.001	19.593
Cl	3.897	-2.153	20.615
Mg	1.798	-3.114	19.627
Cl	1.798	-5.189	20.955
Mg	0.778	-6.399	19.159
Cl	0.231	-8.520	18.825
Cl	0.620	-4.390	17.893
Cl	3.798	1.972	18.322
Mg	1.798	3.114	19.627
Cl	3.583	4.313	20.990
Mg	3.532	6.293	19.457
Cl	1.798	7.267	20.955
Mg	1.798	9.343	19.627
Cl	3.828	10.444	20.863
Mg	3.478	12.438	19.616
Cl	1.798	13.495	20.955
Mg	1.798	15.571	19.627
Cl	4.010	14.598	18.762
Cl	1.798	5.190	18.298
Cl	1.798	1.038	20.955
Cl	1.798	11.419	18.298
Cl	3.122	8.247	17.970
Cl	1.798	17.647	18.298
O	5.495	7.910	12.481
C	6.131	7.018	13.076
O	6.920	6.163	12.437
C	6.978	6.251	10.967
C	8.133	5.391	10.510
H	6.016	5.885	10.580
H	7.102	7.308	10.693
H	8.194	5.430	9.413
H	9.087	5.751	10.919
H	7.992	4.343	10.805
C	6.094	6.791	14.545
C	6.064	7.878	15.430
C	5.951	7.657	16.803
C	5.787	6.354	17.284
C	5.799	5.263	16.411
C	5.993	5.483	15.048
O	5.502	6.152	18.656
H	5.987	4.639	14.359
H	5.614	4.258	16.788
H	6.119	8.897	15.046
H	5.920	8.496	17.495
C	6.642	5.761	19.559
C	7.692	6.856	19.582
H	6.132	5.703	20.533
C	7.178	4.386	19.208
H	7.883	4.074	19.992

H	6.366	3.647	19.167
H	7.721	4.390	18.252
H	8.452	6.606	20.337
H	8.202	6.947	18.612
H	7.255	7.827	19.850

Zip_p-
isopropoxy_EB_Beta_5.9_Part
ially_Relaxed

Mg	1.918	-1.003	11.716
Cl	3.596	0.000	13.055
Mg	3.596	2.076	11.727
Cl	1.980	3.182	13.182
Mg	1.850	5.214	11.673
Cl	3.596	6.229	13.055
Mg	3.596	8.305	11.727
Cl	1.510	9.488	12.973
Mg	1.928	11.427	11.704
Cl	3.596	12.456	13.055
Mg	3.596	14.532	11.727
Cl	2.288	15.772	13.407
Mg	1.724	17.327	11.726
Cl	3.595	16.608	10.398
Cl	1.669	0.922	10.374
Cl	3.596	-2.076	10.398
Mg	3.596	-4.152	11.727
Cl	3.596	-6.229	13.055
Cl	1.393	-3.160	12.612
Cl	1.996	7.212	10.218
Cl	3.596	4.152	10.398
Cl	1.604	13.509	10.525
Cl	3.596	10.380	10.398
Cl	0.194	18.904	11.435
Cl	1.546	0.920	16.390
Mg	3.596	2.076	17.654
Cl	3.596	0.000	18.982
Mg	1.907	-1.036	17.660
Cl	1.410	-3.164	18.579
Mg	3.596	-4.151	17.654
Cl	3.596	-6.228	18.982
Cl	3.596	-2.076	16.325
Cl	3.596	4.152	16.325
Mg	1.864	5.179	17.663
Cl	3.596	6.229	18.982
Mg	3.596	8.305	17.654
Cl	1.578	9.454	18.939
Mg	1.944	11.424	17.665
Cl	3.596	12.457	18.981
Mg	3.596	14.533	17.653
Cl	4.353	15.913	19.546
Mg	4.243	17.890	18.237
Cl	3.596	16.609	16.324
Cl	2.009	7.196	16.189
Cl	1.947	3.194	19.138
Cl	1.464	13.589	16.701
Cl	3.596	10.381	16.324
Cl	4.667	20.039	18.579
O	-0.172	4.965	11.474
C	-1.133	4.546	12.136
C	-1.185	4.749	13.612
C	-1.046	3.654	14.477

C	-0.808	3.868	15.834
C	-0.734	5.175	16.316
C	-0.954	6.274	15.481
C	-1.150	6.056	14.120
H	-1.029	2.636	14.088
H	-0.614	3.028	16.503
O	-0.278	5.327	17.635
H	-0.874	7.291	15.861
H	-1.224	6.911	13.445
O	-2.092	3.906	11.481
C	-3.336	3.508	12.153
C	-4.407	3.396	11.091
H	-3.153	2.543	12.647
H	-3.585	4.255	12.919
H	-5.347	3.069	11.558
H	-4.582	4.363	10.601
H	-4.128	2.660	10.325
C	-1.024	6.255	18.540
C	-0.270	6.243	19.856
H	-0.966	7.256	18.086
C	-2.462	5.788	18.661
H	-3.018	6.494	19.295
H	-2.964	5.749	17.684
H	-2.510	4.793	19.126
H	-0.790	6.892	20.573
H	-0.218	5.228	20.274
H	0.747	6.650	19.755

Zip_p-
isopropoxy_EB_Beta_6.3_Part
ially_Relaxed

Mg	1.798	-1.038	11.727
Cl	1.798	-3.114	13.055
Mg	1.156	-4.396	11.141
Cl	0.719	-6.543	10.800
Cl	3.915	-0.076	12.693
Mg	3.450	2.090	11.696
Cl	3.775	4.064	10.428
Mg	1.798	5.190	11.727
Cl	1.798	7.267	10.398
Mg	3.537	8.308	11.725
Cl	3.361	10.300	10.188
Mg	1.798	11.418	11.727
Cl	1.797	13.494	10.398
Mg	3.479	14.523	11.725
Cl	3.992	16.655	10.815
Mg	1.797	17.646	11.727
Cl	1.797	19.723	10.398
Cl	1.798	1.038	10.398
Cl	1.045	-2.420	9.832
Cl	1.798	3.114	13.055
Cl	3.347	6.301	13.226
Cl	1.798	9.343	13.055
Cl	3.841	12.558	12.989
Cl	1.797	15.570	13.055
Cl	1.798	7.267	16.698
Mg	3.519	8.310	18.032
Cl	3.389	10.314	16.549
Mg	1.797	11.419	18.027
Cl	1.797	13.495	16.698
Mg	3.477	14.501	18.032

Cl	3.996	16.655	17.136
Mg	1.797	17.646	18.027
Cl	1.797	19.723	16.698
Cl	3.382	6.322	19.560
Mg	1.798	5.190	18.027
Cl	1.798	3.114	19.355
Mg	3.459	2.065	18.026
Cl	3.871	4.049	16.803
Cl	1.798	1.038	16.698
Mg	1.798	-1.038	18.027
Cl	2.617	-2.394	16.167
Mg	3.141	-4.149	17.659
Cl	4.373	-5.989	17.645
Cl	3.843	-0.036	19.136
Cl	1.798	-3.113	19.355
Cl	1.797	9.343	19.355
Cl	3.734	12.561	19.371
Cl	1.797	15.571	19.355
O	5.619	8.299	18.046
C	6.534	7.905	19.171
C	6.124	8.399	16.736
C	5.887	7.332	15.867
C	6.084	7.519	14.502
C	6.545	8.753	14.021
C	6.892	9.776	14.918
C	6.664	9.606	16.282
H	5.479	6.391	16.239
H	5.830	6.719	13.809
C	6.487	9.000	12.563
H	7.245	10.735	14.539
H	6.807	10.432	16.977
O	7.477	9.740	12.089
O	5.567	8.555	11.850
C	7.443	10.157	10.673
C	7.025	11.608	10.575
H	8.473	9.996	10.332
H	6.759	9.494	10.130
H	7.070	11.918	9.521
H	5.991	11.739	10.924
H	7.696	12.257	11.155
C	7.496	9.037	19.485
H	5.814	7.778	19.991
C	7.204	6.578	18.873
H	8.045	8.790	20.405
H	8.235	9.176	18.684
H	6.959	9.981	19.653
H	7.783	6.268	19.755
H	6.458	5.800	18.663
H	7.900	6.657	18.025

Zip_p-
isopropoxy_EB_Beta_6.6_Part
ially_Relaxed

Mg	1.858	5.200	11.737
Cl	3.596	4.152	10.398
Cl	1.988	3.158	13.186
Mg	3.596	8.305	11.727
Cl	2.056	7.175	10.168
Cl	3.596	6.229	13.055
Mg	1.943	11.425	11.741
Cl	3.596	10.381	10.398

Cl	1.478	9.443	12.931
Mg	3.595	14.532	11.727
Cl	1.491	13.594	10.745
Cl	3.595	12.457	13.055
Mg	5.071	17.655	11.958
Cl	3.595	16.608	10.398
Cl	5.204	15.638	13.216
Cl	5.983	19.660	12.178
Mg	3.596	2.076	11.727
Cl	1.703	0.931	10.354
Cl	3.596	0.000	13.055
Mg	1.915	-0.998	11.711
Cl	1.403	-3.151	12.621
Cl	3.596	-2.075	10.398
Mg	3.596	-4.151	11.727
Cl	3.596	-6.228	13.055
Mg	1.872	5.230	18.388
Cl	2.111	7.188	16.850
Cl	3.595	6.229	19.736
Cl	3.595	4.152	17.079
Cl	1.947	3.205	19.876
Mg	3.595	2.076	18.408
Cl	1.609	0.949	17.107
Cl	3.595	0.000	19.736
Mg	1.910	-1.020	18.394
Cl	3.595	-2.075	17.079
Cl	1.404	-3.149	19.319
Mg	3.595	-4.151	18.408
Cl	3.595	-6.228	19.736
Mg	3.595	8.305	18.408
Cl	3.595	10.381	17.078
Cl	1.568	9.426	19.668
Mg	1.949	11.410	18.426
Cl	1.487	13.576	17.419
Cl	3.595	12.457	19.735
Mg	3.595	14.533	18.407
Cl	3.595	16.608	17.079
Cl	4.289	15.916	20.312
Mg	4.067	17.907	19.035
Cl	4.132	20.078	19.475
O	-0.100	5.586	12.116
C	-0.934	6.120	12.871
O	-1.817	7.004	12.433
C	-1.709	7.420	11.021
H	-0.663	7.693	10.826
H	-1.962	6.548	10.401
C	-2.666	8.570	10.817
H	-3.703	8.277	11.032
H	-2.613	8.897	9.769
H	-2.400	9.424	11.455
C	-1.002	5.848	14.323
C	-0.558	4.605	14.800
C	-0.409	4.394	16.169
C	-0.675	5.448	17.045
C	-1.193	6.664	16.591
C	-1.370	6.860	15.226
H	-0.283	3.816	14.102
H	-0.023	3.440	16.539
H	-1.364	7.471	17.303
H	-1.710	7.825	14.850
O	-0.245	5.353	18.380
C	-1.165	4.772	19.428

C	-0.753	5.415	20.738
C	-2.620	5.008	19.076
H	-0.937	3.695	19.439
H	-3.238	4.531	19.851
H	-2.864	6.080	19.060
H	-2.897	4.564	18.111
H	-1.339	4.973	21.556
H	0.304	5.232	20.967
H	-0.938	6.498	20.718

**Zip_p-
isopropoxy_EB_Beta_7.9_Part
ially_Relaxed**

Mg	1.798	-1.038	11.726
Cl	3.902	-0.086	12.721
Mg	3.441	2.072	11.717
Cl	1.798	3.114	13.055
Mg	1.798	5.190	11.726
Cl	3.225	6.277	13.326
Mg	3.539	8.324	11.801
Cl	1.798	9.342	13.055
Mg	1.798	11.418	11.726
Cl	3.685	12.557	13.103
Mg	3.481	14.498	11.750
Cl	1.798	15.571	13.055
Mg	1.798	17.647	11.726
Cl	3.998	16.639	10.836
Cl	1.798	1.038	10.398
Cl	1.003	-2.417	9.851
Mg	1.100	-4.397	11.161
Cl	0.711	-6.544	10.780
Cl	1.798	-3.114	13.055
Cl	1.798	7.266	10.398
Cl	3.872	4.058	10.497
Cl	1.798	13.495	10.398
Cl	3.505	10.282	10.298
Cl	1.798	19.723	10.398
Cl	1.798	1.038	18.368
Mg	3.449	2.066	19.676
Cl	3.896	-0.087	20.691
Mg	1.798	-1.038	19.696
Cl	1.798	-3.114	21.025
Mg	0.791	-4.324	19.223
Cl	0.244	-6.442	18.873
Cl	0.628	-2.314	17.957
Cl	3.808	4.034	18.415
Mg	1.797	5.190	19.696
Cl	3.534	6.365	21.110
Mg	3.534	8.331	19.567
Cl	1.797	9.342	21.025
Mg	1.797	11.418	19.696
Cl	3.769	12.537	20.997
Mg	3.478	14.505	19.701
Cl	1.797	15.571	21.025
Mg	1.797	17.647	19.696
Cl	3.999	16.657	18.813
Cl	1.797	7.266	18.368
Cl	1.798	3.114	21.025
Cl	1.797	13.495	18.367
Cl	3.277	10.351	18.130
Cl	1.797	19.723	18.367

O	5.497	8.233	12.388
C	6.137	7.521	13.188
O	6.941	6.547	12.784
C	6.977	6.249	11.342
C	8.083	5.245	11.116
H	5.992	5.844	11.063
H	7.145	7.192	10.803
C	6.080	7.672	14.660
C	6.075	6.534	15.484
C	5.883	6.662	16.857
C	5.761	7.938	17.414
C	5.812	9.082	16.611
C	5.932	8.946	15.229
O	5.488	8.067	18.795
H	8.124	4.995	10.046
H	9.059	5.650	11.412
H	7.900	4.317	11.675
C	6.645	8.040	19.753
H	6.131	8.190	20.716
C	7.319	6.681	19.767
C	7.582	9.202	19.481
H	8.051	6.659	20.588
H	6.586	5.883	19.942
H	7.861	6.487	18.830
H	8.352	9.234	20.266
H	8.093	9.087	18.515
H	7.045	10.160	19.490
H	5.908	9.830	14.590
H	5.696	10.067	17.060
H	5.771	5.779	17.485
H	6.146	5.543	15.037

Mono_DIBP_Alpha_Fully_Relaxed

Mg	1.548	-2.849	11.389
Cl	2.907	-2.221	13.278
Mg	3.283	-0.089	12.179
Cl	2.289	2.020	12.668
Mg	4.561	2.784	13.265
Cl	7.119	3.601	14.247
Mg	6.868	5.385	12.643
Cl	6.484	7.359	14.007
Mg	8.460	8.298	12.995
Cl	10.444	8.905	14.212
Mg	10.049	11.154	13.495
Cl	9.231	12.816	15.142
Mg	11.103	14.494	14.211
Cl	11.864	12.566	12.915
Cl	2.225	-0.963	10.135
Cl	1.646	-5.190	10.807
Mg	0.034	-5.431	12.562
Cl	-1.470	-7.003	13.442
Cl	-0.645	-3.144	12.385
Cl	4.933	4.536	11.606
Cl	5.514	0.728	12.376
Cl	8.223	10.512	12.085
Cl	8.724	6.399	11.534
Cl	10.353	16.401	13.340
Cl	0.330	-1.631	16.248
Mg	2.531	-1.072	17.132
Cl	3.007	-3.412	17.514

Mg	0.959	-3.931	16.396
Cl	-0.880	-5.309	17.032
Mg	-0.310	-7.204	15.605
Cl	0.419	-9.158	16.382
Cl	1.504	-5.535	14.573
Cl	3.717	0.433	15.672
Mg	3.554	2.208	17.418
Cl	5.791	2.787	18.110
Mg	6.233	4.538	16.509
Cl	5.133	6.521	17.591
Mg	7.263	7.535	17.773
Cl	8.265	8.441	19.814
Mg	8.926	10.331	18.540
Cl	8.746	12.710	18.944
Mg	10.488	12.855	17.300
Cl	11.173	10.597	17.684
Cl	4.025	3.938	15.371
Cl	2.735	0.414	18.958
Cl	7.562	9.672	16.667
Cl	8.408	5.626	16.915
Cl	12.055	14.398	16.475
O	1.988	3.355	17.889
C	0.986	3.955	17.460
O	0.940	4.285	16.187
C	-0.229	4.923	15.575
C	0.192	6.201	14.856
H	-0.620	4.173	14.871
H	-0.982	5.127	16.348
C	-1.055	6.867	14.261
H	0.617	6.881	15.617
C	1.250	5.943	13.779
H	-0.774	7.806	13.765
H	-1.524	6.221	13.502
H	-1.810	7.101	15.027
H	1.534	6.883	13.285
H	2.156	5.497	14.208
H	0.865	5.257	13.008
C	-0.039	4.440	18.447
C	-1.134	3.639	18.828
C	0.173	5.675	19.068
C	-0.713	6.123	20.051
C	-1.805	5.336	20.424
C	-2.014	4.098	19.817
C	-1.320	2.337	18.125
O	-2.317	1.600	18.637
O	-0.621	2.008	17.172
C	-2.593	0.312	17.989
C	-3.168	-0.656	19.015
H	-3.308	0.514	17.176
H	-1.661	-0.065	17.551
H	-3.360	-1.577	18.433
C	-2.151	-0.992	20.113
C	-4.503	-0.174	19.594
H	-2.548	-1.766	20.786
H	-1.209	-1.367	19.688
H	-1.920	-0.106	20.722
H	-4.931	-0.933	20.265
H	-4.370	0.750	20.176
H	-5.238	0.027	18.801
H	1.041	6.281	18.797
H	-0.541	7.087	20.531
H	-2.495	5.686	21.193

H	-2.861	3.475	20.102
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**Chelate_DIBP_Alpha_Fully_R
elaxed**

Mg	3.021	1.932	17.142
Cl	4.153	3.062	19.023
Cl	3.565	-0.359	16.618
Mg	5.341	4.467	17.541
Cl	4.533	6.735	17.324
Cl	5.098	2.780	15.760
Mg	6.842	7.443	17.174
Cl	7.629	5.163	17.510
Cl	7.855	8.396	19.251
Mg	8.527	10.307	18.057
Cl	7.189	9.651	16.146
Cl	8.416	12.651	18.638
Mg	10.067	12.905	16.921
Cl	10.729	10.614	17.084
Cl	11.557	14.488	16.034
Mg	2.352	-1.983	17.965
Cl	2.220	-1.429	20.165
Cl	0.211	-2.139	16.674
Mg	0.758	-4.437	16.240
Cl	2.848	-4.293	17.365
Cl	1.219	-6.109	14.375
Mg	-0.567	-7.758	15.482
Cl	-1.118	-5.819	16.832
Cl	0.123	-9.739	16.225
Mg	4.813	2.401	13.285
Cl	7.197	3.039	12.823
Cl	5.013	0.218	12.221
Mg	6.435	5.226	12.474
Cl	6.844	6.819	14.338
Cl	4.137	4.609	12.412
Mg	7.860	8.368	12.750
Cl	7.433	6.803	10.973
Cl	10.052	9.062	13.445
Mg	9.309	11.327	13.136
Cl	7.233	10.610	12.158
Cl	8.633	12.960	14.881
Mg	10.419	14.673	13.855
Cl	11.017	12.804	12.404
Cl	9.646	16.615	13.092
Mg	2.806	-0.410	12.822
Cl	2.386	1.707	13.839
Cl	1.154	-0.756	11.025
Mg	0.820	-2.951	11.846
Cl	2.519	-2.699	13.543
Cl	0.773	-5.082	10.708
Mg	-0.485	-5.803	12.619
Cl	-1.138	-3.536	13.145
Cl	-1.839	-7.560	13.359
O	2.126	3.679	16.523
C	0.994	4.118	16.279
C	-0.137	3.241	15.839
C	-0.723	3.521	14.595
C	-1.723	2.699	14.077
C	-2.179	1.606	14.815
C	-1.627	1.332	16.065
C	-0.587	2.121	16.577
C	0.009	1.714	17.887

O	0.838	5.431	16.358
C	-0.469	6.098	16.366
H	-0.664	6.446	15.340
H	-1.245	5.376	16.656
C	-0.400	7.276	17.333
H	-0.134	6.873	18.325
C	0.664	8.294	16.917
H	1.662	7.839	16.870
H	0.431	8.725	15.930
H	0.705	9.122	17.639
C	-1.796	7.907	17.427
H	-2.122	8.304	16.453
H	-2.551	7.185	17.774
H	-1.786	8.746	18.137
H	-0.365	4.370	14.011
H	-2.143	2.915	13.094
H	-2.962	0.960	14.417
H	-1.972	0.474	16.642
O	-0.894	1.464	18.809
C	-0.426	1.030	20.157
H	-0.197	1.959	20.700
H	0.490	0.437	20.035
C	-1.531	0.232	20.830
H	-1.099	-0.011	21.818
C	-1.804	-1.089	20.103
H	-2.231	-0.916	19.104
H	-2.524	-1.698	20.668
H	-0.880	-1.672	19.986
C	-2.808	1.051	21.053
H	-3.271	1.332	20.095
H	-2.607	1.974	21.618
H	-3.545	0.464	21.619
O	1.230	1.597	18.079

**Bridge_DIBP_Alpha_Fully_Re
laxed**

Mg	3.283	1.754	17.176
Cl	4.399	2.988	18.991
Cl	4.108	3.601	15.620
Mg	5.160	4.663	17.501
Cl	4.483	6.885	18.168
Cl	7.492	5.222	17.472
Mg	6.807	7.449	18.036
Cl	8.068	8.170	19.999
Cl	7.370	9.475	16.870
Mg	8.817	10.031	18.739
Cl	8.765	12.366	19.336
Cl	11.008	10.270	17.753
Mg	10.391	12.578	17.587
Cl	11.911	14.126	16.700
Cl	2.343	0.044	18.795
Cl	4.641	-0.142	16.300
Mg	3.124	-1.669	17.326
Cl	1.412	-2.275	15.627
Cl	2.545	-3.585	18.619
Mg	0.353	-3.668	17.493
Cl	-1.631	-4.917	18.076
Cl	1.088	-5.907	16.318
Mg	-0.915	-7.154	17.392
Cl	-0.640	-8.754	18.925
Mg	4.090	2.635	12.706

Cl	6.468	3.107	12.937
Cl	3.603	4.924	12.083
Mg	5.881	5.404	12.635
Cl	6.089	6.999	14.472
Cl	7.346	6.747	11.281
Mg	7.630	8.278	13.106
Cl	9.825	8.636	14.041
Cl	7.357	10.629	12.663
Mg	9.445	10.994	13.794
Cl	8.926	12.653	15.578
Cl	11.331	12.301	13.165
Mg	10.790	14.262	14.509
Cl	10.065	16.195	13.681
Cl	2.349	1.336	13.802
Cl	3.931	1.109	10.784
Mg	2.591	-0.368	12.077
Cl	3.492	-2.449	12.796
Cl	0.423	-1.318	11.725
Mg	1.155	-3.201	13.112
Cl	-1.109	-3.865	13.994
Cl	1.485	-5.593	12.578
Mg	-0.182	-6.060	14.200
Cl	-1.695	-7.625	15.093
O	1.352	2.398	17.096
C	0.192	2.107	17.437
O	-0.394	2.618	18.496
C	0.420	3.475	19.381
C	-0.421	3.846	20.592
H	1.318	2.907	19.662
C	0.478	4.561	21.611
H	-0.093	4.818	22.514
H	0.882	5.497	21.196
H	1.329	3.933	21.916
C	-1.639	4.692	20.207
H	-2.250	4.917	21.093
H	-1.325	5.651	19.764
H	-2.278	4.172	19.480
O	-0.453	-1.957	18.263
C	-0.811	-0.765	18.251
O	-0.964	-0.053	19.348
C	-0.624	-0.683	20.639
H	-0.274	0.160	21.249
H	0.201	-1.385	20.474
C	-1.836	-1.362	21.269
H	-2.190	-2.134	20.565
C	-2.974	-0.370	21.538
H	-2.658	0.399	22.260
H	-3.300	0.139	20.620
H	-3.847	-0.887	21.963
C	-1.381	-2.064	22.556
H	-0.989	-1.338	23.286
H	-0.600	-2.812	22.361
H	-2.229	-2.581	23.026
H	0.726	4.361	18.803
C	-0.678	1.220	16.602
C	-1.149	-0.059	16.980
H	-0.777	2.903	21.043
C	-1.911	-0.800	16.062
C	-2.233	-0.284	14.810
C	-1.745	0.965	14.431
C	-0.955	1.701	15.313
H	-2.251	-1.798	16.340

H	-2.832	-0.879	14.119
H	-1.955	1.358	13.435
H	-0.532	2.657	15.003

Zip_DIBP_Alpha_Fully_Relaxed

C	10.339	3.753	14.206
C	9.763	3.671	15.494
C	10.274	4.469	16.526
C	11.346	5.329	16.294
C	11.920	5.399	15.024
C	11.420	4.612	13.983
C	8.678	2.715	15.832
O	8.721	1.602	15.114
C	7.766	0.516	15.412
C	8.423	-0.810	15.056
C	9.726	3.079	13.020
O	10.457	2.117	12.492
C	9.905	1.434	11.302
C	10.673	0.141	11.079
O	7.854	2.904	16.739
Mg	6.337	3.828	17.734
Cl	3.963	3.829	17.071
Mg	3.793	1.567	17.732
Cl	3.778	-0.077	15.902
Mg	1.937	-1.150	17.001
Cl	0.036	-1.804	15.669
Mg	0.380	-4.047	16.439
Cl	1.257	-5.897	15.022
Mg	-0.742	-7.434	15.990
Cl	-0.167	-9.208	17.203
Cl	6.711	5.151	19.813
Mg	7.173	7.073	18.507
Cl	6.199	9.290	18.212
Mg	8.417	10.129	18.100
Cl	9.764	10.451	16.022
Mg	9.569	12.896	16.362
Cl	11.419	14.221	15.844
Cl	6.938	5.941	16.464
Cl	5.876	1.587	18.863
Cl	9.344	8.124	18.998
Cl	8.549	12.513	18.485
Cl	1.793	0.573	18.659
Cl	2.189	-3.397	17.861
Cl	-1.544	-5.342	16.947
O	8.642	3.441	12.545
Mg	7.097	4.655	12.043
Cl	5.844	3.541	10.248
Mg	4.894	2.066	11.844
Cl	5.854	-0.184	11.581
Mg	3.607	-1.011	11.607
Cl	2.661	-2.295	9.775
Mg	1.880	-3.845	11.401
Cl	2.064	-6.249	11.330
Mg	0.173	-6.196	12.805
Cl	-1.456	-7.657	13.648
Cl	6.419	6.787	12.985
Mg	8.256	7.872	11.929
Cl	7.853	10.249	11.707
Mg	9.587	10.675	13.325
Cl	11.542	11.930	12.782

Mg	10.847	14.157	13.429
Cl	10.838	15.990	12.168
Cl	8.711	5.982	10.567
Cl	5.712	3.249	13.705
Cl	10.197	8.322	13.299
Cl	8.555	13.055	14.157
Cl	2.657	1.172	11.806
Cl	3.123	-2.770	13.176
Cl	-0.415	-3.972	12.139
H	9.828	4.396	17.518
H	11.726	5.950	17.107
H	12.751	6.079	14.832
H	11.847	4.694	12.982
H	7.501	0.575	16.478
H	6.870	0.715	14.807
C	7.388	-1.930	15.235
C	9.680	-1.067	15.893
H	8.704	-0.769	13.989
H	8.838	1.250	11.482
H	10.005	2.127	10.452
C	9.967	-0.649	9.968
C	12.149	0.389	10.753
H	10.607	-0.442	12.014
H	12.680	-0.563	10.622
H	12.251	0.960	9.817
H	12.654	0.949	11.552
H	10.478	-1.607	9.799
H	8.918	-0.863	10.224
H	9.977	-0.094	9.017
H	10.144	-2.023	15.610
H	10.432	-0.277	15.755
H	9.432	-1.122	16.965
H	7.830	-2.899	14.965
H	7.053	-1.996	16.282
H	6.501	-1.773	14.605

Alpha_MgCl₂_one_DIBP

C	0.000	0.000	0.000
C	0.000	0.000	1.401
C	1.230	0.000	2.095
C	2.429	-0.037	1.367
C	2.418	-0.070	-0.024
C	1.201	-0.039	-0.709
C	-1.345	0.119	2.069
O	-2.103	-0.955	2.230
C	-1.599	-2.299	1.910
C	-2.578	-3.316	2.481
C	-3.973	-3.177	1.864
C	1.326	0.026	3.582
O	2.226	0.598	4.210
Mg	3.292	2.421	4.413
Cl	1.890	3.153	2.526
Mg	3.389	4.818	1.833
Cl	5.053	6.273	0.702
Mg	3.458	6.910	-0.934
Cl	3.538	8.176	-2.758
O	0.358	-0.686	4.147
C	0.260	-0.779	5.612
C	0.223	-2.249	6.016
C	1.567	-2.942	5.766
C	-0.191	-2.334	7.491

O	-1.814	1.211	2.391
Mg	-2.289	3.036	3.148
Cl	-1.077	5.004	2.592
Mg	-2.680	5.809	0.902
Cl	-3.929	3.727	1.397
Cl	-4.282	6.613	-0.789
Mg	-3.126	5.425	-2.499
Cl	-3.681	4.852	-4.574
Cl	-1.269	5.167	-1.084
Cl	5.134	1.393	5.643
Mg	4.270	2.568	7.573
Cl	5.872	1.763	9.264
Mg	4.579	-0.103	9.874
Cl	6.152	-1.068	11.389
Cl	4.991	4.013	3.524
Cl	1.786	5.623	0.143
Cl	2.749	3.906	6.413
Cl	2.972	0.322	8.171
Cl	3.549	1.122	11.622
Mg	5.152	0.318	13.313
Cl	6.754	-0.486	15.005
Mg	5.376	-2.364	15.574
Cl	6.581	-3.627	17.180
Cl	4.430	-1.127	17.363
Mg	6.033	-1.931	19.054
Cl	7.635	-2.736	20.745
Cl	3.773	-1.779	13.916
C	-2.000	-4.723	2.272
Cl	-3.401	4.363	4.950
Mg	-1.799	3.558	6.640
Cl	-0.542	2.523	4.878
Cl	-0.196	2.754	8.332
Mg	-1.475	0.884	8.953
Cl	0.044	-0.113	10.502
Cl	-3.049	1.288	7.211
Cl	-2.519	2.113	10.690
Mg	-0.917	1.308	12.381
Cl	0.685	0.504	14.072
Mg	-0.662	-1.378	14.633
Cl	0.442	-2.687	16.292
Cl	-2.313	-0.768	13.033
Cl	-1.638	-0.136	16.431
Mg	-0.035	-0.941	18.122
Cl	1.567	-1.745	19.813
H	2.363	-2.467	6.359
H	-4.386	-2.171	2.021
H	-1.889	-4.952	1.200
H	-3.942	-3.370	0.779
H	-2.672	-5.478	2.702
H	-1.528	-2.388	0.815
H	-0.599	-2.410	2.351
H	-0.947	0.048	-0.540
H	1.182	-0.036	-1.799
H	3.374	-0.046	1.913
H	3.359	-0.110	-0.574
H	1.111	-0.251	6.062
H	-0.674	-0.255	5.856
H	-0.556	-2.744	5.410
H	0.510	-1.786	8.138
H	-1.207	-1.930	7.641
H	-0.209	-3.379	7.832
H	-2.649	-3.126	3.566

H	-1.015	-4.839	2.749
H	-4.666	-3.902	2.312
H	1.517	-4.004	6.047
H	1.859	-2.893	4.707

Alpha_MgCl₂_two_DIBP

C	0.000	0.000	0.000
C	0.000	0.000	1.413
C	1.225	0.000	2.095
C	2.431	0.007	1.400
C	2.427	0.056	0.006
C	1.218	0.057	-0.690
C	-1.245	0.003	2.236
O	-2.193	-0.740	1.673
C	-3.515	-0.878	2.302
C	-3.967	-2.322	2.112
C	-3.175	-3.289	2.999
C	-1.236	0.039	-0.858
O	-1.781	1.103	-1.164
Mg	-2.999	2.682	-1.384
Cl	-5.226	3.724	-1.736
Mg	-5.959	3.065	0.521
Cl	-6.694	2.407	2.781
Mg	-7.592	0.334	2.098
Cl	-9.732	1.305	1.818
Mg	-10.466	0.646	4.076
Cl	-11.200	-0.011	6.335
Mg	-11.930	-2.234	5.685
Cl	-13.200	-3.417	7.442
Mg	-14.972	-1.772	7.631
Cl	-14.237	-1.114	5.373
O	-1.367	0.576	3.327
Mg	-1.186	2.471	4.350
Cl	-1.750	1.881	6.662
Cl	-3.338	3.570	4.187
Mg	-4.073	2.912	6.447
Cl	-4.807	2.253	8.705
Mg	-5.698	0.194	7.952
Cl	-4.892	0.552	5.739
Cl	-7.845	1.151	7.742
Mg	-8.578	0.492	10.001
Cl	-9.313	-0.165	12.260
Cl	-9.768	-1.407	9.117
Mg	-10.236	-2.348	11.348
Cl	-10.954	-3.313	13.484
O	-9.879	-4.152	10.440
C	-9.642	-5.280	10.002
O	-8.679	-6.057	10.480
C	-7.891	-5.529	11.607
C	-6.826	-6.551	11.972
C	-6.102	-6.070	13.237
C	-10.466	-5.963	8.951
C	-10.664	-5.461	7.644
C	-11.534	-6.137	6.778
C	-12.204	-7.288	7.187
C	-12.011	-7.779	8.478
C	-11.142	-7.123	9.351
C	-9.898	-4.315	7.075
O	-10.323	-3.531	6.214
C	-5.847	-6.791	10.817
O	-8.653	-4.306	7.537

C	-7.676	-3.320	7.067
C	-6.333	-4.037	6.956
C	-5.210	-3.000	6.860
C	-6.308	-5.019	5.780
Cl	-12.351	-1.267	11.297
Mg	-13.084	-1.926	13.556
Cl	-13.819	-2.585	15.815
Cl	-6.272	-0.785	10.065
C	-5.475	-2.412	2.373
O	-1.705	-1.073	-1.398
C	-1.120	-2.386	-1.083
C	-1.929	-3.446	-1.819
C	-1.427	-4.830	-1.387
C	-1.858	-3.265	-3.338
Cl	-3.696	2.316	0.951
Cl	-2.188	4.826	-0.773
Mg	-1.455	5.485	-3.032
Cl	-0.720	6.143	-5.291
Cl	-8.169	-0.555	4.225
Cl	-6.720	0.627	-0.110
Cl	-15.705	-2.431	9.890
Cl	-11.450	-1.604	3.363
Cl	0.754	4.335	-2.856
Mg	-0.029	3.748	-5.062
Cl	0.647	2.134	-6.458
Cl	-0.301	4.672	5.150
Mg	0.432	5.331	2.892
Cl	1.165	5.990	0.633
Mg	2.082	8.017	1.452
Cl	3.150	9.700	0.472
Cl	0.144	3.056	2.291
Cl	1.331	7.521	3.645
Cl	-2.401	3.305	-3.892
H	1.218	-0.004	3.185
H	3.374	0.000	1.949
H	3.366	0.104	-0.547
H	1.220	0.122	-1.780
H	-0.070	-2.388	-1.414
H	-1.162	-2.524	0.005
H	-0.373	-4.978	-1.672
H	-1.510	-4.979	-0.300
H	-2.979	-3.339	-1.497
H	-2.013	-5.618	-1.879
H	-0.823	-3.378	-3.699
H	-2.221	-2.276	-3.648
H	-2.472	-4.023	-3.846
H	-3.793	-2.584	1.054
H	-4.160	-0.162	1.773
H	-6.026	-1.844	1.603
H	-5.826	-3.451	2.311
H	-5.742	-2.027	3.369
H	-3.482	-4.329	2.820
H	-3.339	-3.065	4.064
H	-5.142	-2.426	7.801
H	-4.234	-3.485	6.720
H	-5.362	-2.307	6.018
H	-6.440	-4.488	4.824
H	-5.351	-5.559	5.740
H	-8.017	-2.896	6.112
H	-7.109	-5.768	5.867
H	-7.667	-2.529	7.830
H	-11.666	-5.756	5.765

H	-12.878	-7.797	6.497
H	-12.537	-8.675	8.811
H	-10.998	-7.502	10.364
H	-8.583	-5.333	12.440
H	-7.341	-7.499	12.205
H	-5.586	-5.113	13.060
H	-7.437	-4.577	11.288
H	-5.343	-6.803	13.545
H	-6.796	-5.930	14.079
H	-6.365	-7.140	9.912
H	-5.306	-5.864	10.569
H	-5.100	-7.549	11.093
H	-6.191	-4.607	7.891
H	-2.094	-3.222	2.805
H	-3.445	-0.587	3.359

Alpha_2DIBP_TiCl₄

C	1.411	0.057	1.919
C	0.305	0.349	1.081
C	0.518	0.520	-0.296
C	1.790	0.404	-0.852
C	2.875	0.094	-0.033
C	2.681	-0.070	1.335
C	-1.107	0.542	1.546
O	-1.957	-0.145	0.786
C	-3.399	-0.017	1.060
C	-4.159	-0.834	0.027
C	-3.798	-2.322	0.082
C	1.405	-0.183	3.405
O	0.617	-1.092	3.958
C	-0.277	-1.988	3.230
C	0.018	-3.438	3.606
C	-1.125	-4.321	3.089
O	-1.455	1.260	2.487
Mg	-2.393	2.725	3.684
Cl	-3.882	3.496	1.863
Cl	-0.808	1.954	5.357
Mg	-2.212	2.623	7.211
Cl	-3.810	3.598	5.606
Cl	-0.614	1.649	8.814
Mg	-1.788	-0.398	8.804
Cl	-3.518	0.453	7.367
Cl	0.205	-4.500	8.619
Mg	-1.366	-0.645	12.444
Cl	-2.963	0.328	10.840
Cl	-2.408	-2.955	12.516
Mg	-0.757	-3.795	14.147
Cl	0.232	-1.620	14.048
O	0.034	-5.590	13.283
C	0.872	-6.462	13.578
O	1.807	-6.908	12.757
C	1.973	-6.364	11.397
C	2.670	-7.453	10.585
C	1.764	-8.675	10.387
C	0.923	-7.187	14.879
C	-0.294	-7.487	15.505
C	-0.321	-8.172	16.717
C	0.877	-8.544	17.328
C	2.097	-8.262	16.711
C	2.135	-7.601	15.475
C	3.507	-7.279	14.933

O	4.244	-8.244	14.400
C	3.702	-9.589	14.149
C	4.792	-10.412	13.475
C	6.015	-10.587	14.381
O	4.017	-6.163	15.046
Mg	4.993	-4.373	15.240
Cl	3.577	-3.432	13.527
Mg	4.721	-1.222	13.564
Cl	6.319	-2.193	15.169
Cl	3.970	-3.514	17.195
Mg	5.569	-4.485	18.799
Cl	7.167	-5.458	20.405
Cl	4.426	-6.709	18.931
Mg	6.779	-7.264	18.731
Cl	7.631	-9.293	18.306
Ti	1.320	-2.596	8.317
Cl	2.646	-0.336	8.445
Mg	4.380	-1.114	10.149
Cl	3.122	-0.249	11.959
Cl	3.021	-3.240	9.865
Cl	-0.382	-1.570	7.039
Cl	6.157	-1.861	11.584
Cl	5.475	1.070	9.938
Mg	3.878	2.044	8.334
Cl	2.279	3.018	6.730
Mg	3.304	2.075	4.733
Cl	5.030	1.175	6.255
Cl	-1.460	4.919	3.581
Mg	-3.059	5.893	1.977
Cl	-4.656	6.867	0.373
C	-5.662	-0.606	0.241
O	2.219	0.381	4.149
Cl	2.503	3.021	2.592
Mg	3.031	5.313	3.101
Cl	4.629	4.339	4.705
C	1.375	-3.895	3.062
C	4.195	-11.763	13.058
Cl	1.432	6.288	1.497
C	3.157	-6.898	9.241
Cl	-2.117	-2.940	16.073
Mg	-0.519	-3.914	17.677
Cl	-2.204	-4.176	19.471
Mg	-0.572	-5.024	20.973
Cl	-0.595	-5.693	23.090
Cl	0.972	-4.280	15.918
Cl	1.078	-4.887	19.280
Cl	6.906	-5.393	16.854
H	6.444	-9.624	14.688
H	3.856	-12.336	13.936
H	5.752	-11.141	15.297
H	4.953	-12.371	12.544
H	3.409	-10.037	15.110
H	2.813	-9.483	13.510
H	3.029	-8.525	17.213
H	0.873	-9.055	18.292
H	-1.224	-7.184	15.020
H	-1.278	-8.413	17.185
H	5.096	-9.869	12.563
H	3.339	-11.644	12.376
H	6.801	-11.155	13.864
H	-3.580	-0.393	2.081
H	-3.664	1.048	1.019

H	-3.889	-0.438	-0.967
H	-6.242	-1.141	-0.523
H	-5.984	-0.983	1.225
H	-5.926	0.459	0.183
H	-4.348	-2.882	-0.687
H	-2.724	-2.487	-0.085
H	-4.063	-2.753	1.061
H	-0.331	0.763	-0.933
H	1.929	0.557	-1.923
H	3.877	-0.007	-0.454
H	3.530	-0.306	1.978
H	-1.290	-1.697	3.543
H	-0.166	-1.848	2.146
H	0.034	-3.492	4.706
H	-0.946	-5.371	3.356
H	-2.093	-4.026	3.520
H	-1.209	-4.268	1.992
H	1.591	-4.926	3.376
H	1.386	-3.870	1.960
H	2.195	-3.262	3.431
H	2.574	-5.451	11.496
H	0.981	-6.102	11.003
H	3.559	-7.760	11.165
H	2.302	-9.477	9.860
H	1.406	-9.083	11.343
H	0.883	-8.411	9.780
H	3.687	-7.683	8.682
H	2.315	-6.556	8.620
H	3.844	-6.051	9.373
Cl	-0.039	-1.515	10.285
Cl	2.490	-3.159	6.527

Donor_Pre_Pi_Complex

C	0.045	-0.017	-0.017
C	0.084	-0.037	1.382
C	1.304	-0.015	2.061
C	2.504	0.037	1.348
C	2.478	0.025	-0.044
C	1.261	-0.018	-0.738
C	1.306	-0.045	-2.228
O	0.320	0.682	-2.724
C	0.036	0.781	-4.166
C	-0.980	1.915	-4.295
C	-1.665	1.907	-5.666
C	-1.319	-0.120	-0.656
O	-2.160	0.901	-0.569
C	-1.759	2.205	-0.016
C	-2.817	3.229	-0.406
C	-4.194	2.877	0.165
O	2.169	-0.634	-2.903
Mg	3.139	-2.582	-2.865
Cl	4.926	-2.495	-4.566
Cl	2.299	-4.492	-4.038
Mg	4.012	-4.532	-5.811
Cl	5.724	-4.572	-7.584
Mg	4.651	-2.987	-9.145
Cl	3.535	-4.848	-10.133
Mg	5.247	-4.888	-11.905
Cl	6.959	-4.929	-13.678
Cl	3.875	-3.526	-13.349
Cl	3.393	-1.162	-10.179

Ti	1.380	-1.246	-8.744
C	1.209	0.836	-9.015
C	1.713	1.740	-7.885
C	3.193	1.495	-7.556
Cl	6.520	-3.121	-10.656
Cl	-0.007	-2.873	-9.923
Cl	-0.552	-1.133	-7.224
Cl	2.834	-2.604	-7.287
O	-1.724	-1.151	-1.197
Mg	-2.661	-2.804	-1.977
Cl	-1.147	-2.754	-3.853
Mg	-2.136	-4.761	-4.926
Cl	-0.422	-4.799	-6.699
Mg	-1.722	-3.192	-7.926
Cl	-3.589	-3.373	-6.426
Cl	-1.659	-4.448	-0.605
Mg	-3.372	-4.411	1.165
Cl	-5.085	-4.373	2.938
Mg	-4.760	-1.973	2.305
Cl	-2.382	-2.461	2.383
Cl	-5.710	0.008	2.750
Cl	-3.848	-4.724	-3.155
C	-2.345	4.614	0.058
C	-0.344	3.277	-3.990
C	1.473	3.225	-8.210
Cl	-2.616	-5.077	-9.245
Mg	-0.904	-5.117	-11.017
Cl	0.808	-5.157	-12.789
Mg	-0.277	-3.446	-14.132
O	0.467	-1.551	-13.631
C	1.016	-0.473	-13.888
O	1.057	0.433	-12.924
C	1.563	1.791	-13.135
C	0.537	2.799	-12.627
C	1.159	4.200	-12.690
Cl	-2.166	-3.569	-12.538
Cl	0.791	-3.212	-16.337
Mg	0.330	-5.473	-17.111
Cl	2.043	-5.513	-18.884
Cl	-1.381	-5.433	-15.339
C	1.501	-0.162	-15.285
C	0.491	0.171	-16.199
C	0.770	0.315	-17.558
C	2.057	0.068	-18.035
C	3.066	-0.286	-17.143
C	2.816	-0.372	-15.764
C	4.008	-0.652	-14.915
O	4.036	0.050	-13.792
C	5.229	-0.065	-12.927
C	6.418	0.740	-13.443
C	7.588	0.527	-12.472
O	4.924	-1.402	-15.282
Mg	5.679	-3.317	-15.083
Cl	4.770	-5.205	-16.227
Mg	6.482	-5.245	-18.000
Cl	8.194	-5.285	-19.772
Cl	7.249	-3.108	-16.934
C	-0.779	2.729	-13.406
C	6.080	2.227	-13.601
Cl	1.345	-3.045	-1.172
Mg	2.777	-4.176	0.282
Cl	1.065	-4.136	2.054

Mg	2.586	-5.050	3.632
Cl	2.491	-5.582	5.786
Cl	4.489	-4.216	-1.489
Cl	4.302	-5.107	1.993
Cl	-4.698	-2.753	-0.211
H	4.075	-0.493	-17.501
H	2.275	0.139	-19.101
H	-0.031	0.587	-18.246
H	-0.532	0.299	-15.841
H	1.785	1.942	-14.202
H	2.500	1.849	-12.566
H	1.387	4.489	-13.728
H	-0.621	2.962	-14.472
H	-1.244	1.735	-13.332
H	-1.500	3.458	-13.011
H	0.336	2.554	-11.570
H	0.463	4.946	-12.284
H	2.091	4.260	-12.108
H	4.872	0.319	-11.965
H	5.248	2.390	-14.301
H	6.710	0.336	-14.426
H	6.950	2.781	-13.984
H	5.802	2.670	-12.631
H	7.837	-0.537	-12.356
H	8.484	1.048	-12.837
H	7.351	0.927	-11.473
H	3.410	0.059	-0.613
H	3.458	0.086	1.876
H	1.309	-0.039	3.151
H	-0.845	-0.114	1.948
H	-1.372	4.889	-0.378
H	-2.876	3.234	-1.509
H	-1.696	2.106	1.077
H	-2.251	4.653	1.154
H	-3.074	5.382	-0.235
H	-4.941	3.620	-0.148
H	-4.538	1.890	-0.167
H	-4.176	2.865	1.266
H	-0.769	2.465	-0.417
H	0.415	3.530	-4.747
H	-1.102	4.074	-4.002
H	-1.758	1.713	-3.537
H	0.981	0.984	-4.691
H	-0.357	-0.191	-4.488
H	-0.948	2.095	-6.478
H	-2.159	0.948	-5.869
H	-2.426	2.701	-5.706
H	0.142	3.292	-3.004
H	1.741	1.051	-9.958
H	0.125	0.972	-9.188
H	1.125	1.502	-6.981
H	0.411	3.424	-8.418
H	2.052	3.524	-9.099
H	1.785	3.872	-7.374
H	3.379	0.471	-7.197
H	3.824	1.653	-8.444
H	3.541	2.183	-6.769
H	5.459	-1.131	-12.804

Pi_Complex_Re_Primary

C	-0.009	0.010	0.043
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C	-0.001	0.012	1.459
C	1.225	0.013	2.134
C	2.431	0.052	1.427
C	2.420	0.078	0.029
C	1.203	0.044	-0.655
C	-1.243	-0.109	2.309
O	-1.585	0.884	3.119
C	-0.899	2.186	3.107
C	-1.770	3.186	3.856
C	-1.991	2.771	5.314
C	-1.273	0.065	-0.748
O	-2.171	0.799	-0.113
C	-3.511	1.057	-0.663
C	-4.039	2.282	0.080
C	-5.520	2.509	-0.239
O	-1.445	-0.447	-1.868
Mg	-1.160	-2.384	-2.789
Cl	0.663	-3.978	-3.433
Mg	1.443	-4.023	-1.095
Cl	-0.555	-3.000	-0.435
Cl	-2.608	-4.290	-2.680
Mg	-3.388	-4.246	-5.019
Cl	-4.168	-4.201	-7.356
Mg	-6.055	-2.641	-6.995
Cl	-6.575	-2.589	-9.351
Cl	-7.440	-4.514	-6.605
Mg	-8.219	-4.468	-8.942
Cl	-10.137	-3.101	-8.345
Cl	-9.000	-4.424	-11.280
Cl	-1.881	-2.175	-5.141
Cl	2.222	-4.068	1.241
Mg	4.056	-2.699	0.651
Cl	5.682	-1.577	1.698
Cl	3.665	-3.050	-1.661
O	-1.921	-1.137	2.342
Mg	-3.078	-2.797	2.718
Cl	-1.394	-4.434	2.415
Mg	-0.616	-4.482	4.753
Cl	0.163	-4.528	7.091
Cl	-4.061	-2.621	0.535
C	-1.118	4.571	3.750
C	-3.208	3.533	-0.228
Cl	-7.550	-0.732	-6.271
Ti	-7.099	-0.725	-3.905
C	-5.540	0.695	-3.815
C	-4.859	1.216	-5.095
C	-5.644	2.349	-5.765
C	-3.420	1.678	-4.801
Cl	-6.970	-0.827	-1.431
Cl	-5.343	-2.501	-4.566
C	-9.313	0.188	-3.519
C	-8.730	1.354	-3.922
Mg	-10.838	-2.834	-10.728
O	-11.384	-0.932	-10.112
C	-11.672	-0.241	-9.126
O	-10.796	0.525	-8.487
C	-9.399	0.530	-8.969
C	-9.195	1.414	-10.197
C	-7.712	1.338	-10.586
Cl	-11.781	-2.537	-12.958
Cl	-12.272	-4.737	-10.528
Mg	-13.052	-4.692	-12.866

Cl	-13.832	-4.647	-15.204
C	-9.639	2.860	-9.950
C	-13.059	-0.118	-8.604
C	-14.088	-0.206	-9.555
C	-15.418	-0.019	-9.186
C	-15.736	0.245	-7.854
C	-14.728	0.285	-6.889
C	-13.385	0.105	-7.247
C	-12.412	-0.009	-6.098
O	-11.824	1.078	-5.613
C	-11.992	2.403	-6.215
C	-12.182	3.435	-5.109
C	-12.179	4.834	-5.740
C	-13.456	3.182	-4.297
O	-12.208	-1.075	-5.506
Mg	-12.715	-3.143	-5.094
Cl	-11.056	-4.876	-5.427
Mg	-10.276	-4.921	-3.089
Cl	-9.496	-4.966	-0.752
Mg	-7.923	-3.089	-0.945
Cl	-6.225	-4.651	-1.509
Mg	-5.446	-4.698	0.829
Cl	-4.667	-4.746	3.166
Cl	-14.066	-2.992	-7.123
Mg	-15.108	-5.144	-7.013
Cl	-14.328	-5.189	-4.676
Cl	-15.888	-5.099	-9.351
Cl	-12.131	-3.202	-2.717
Cl	-7.456	-3.327	1.427
Cl	0.960	-2.552	4.510
Mg	-0.204	-2.114	6.597
Cl	-0.181	-0.193	7.754
Cl	-8.606	-3.003	-3.401
Cl	-2.423	-2.815	5.341
H	-0.735	2.486	2.062
H	-16.204	-0.088	-9.939
H	-16.774	0.389	-7.554
H	-13.822	-0.414	-10.592
H	-14.990	0.431	-5.839
H	-14.350	3.253	-4.937
H	-13.561	3.930	-3.498
H	-12.268	5.605	-4.962
H	-13.029	4.961	-6.429
H	-11.255	5.029	-6.304
H	-11.312	3.355	-4.434
H	-12.850	2.393	-6.903
H	-11.077	2.593	-6.793
H	-10.705	2.926	-9.687
H	-9.481	3.471	-10.850
H	-9.054	3.315	-9.133
H	-8.843	0.916	-8.106
H	-9.096	-0.509	-9.143
H	-9.791	0.996	-11.025
H	-7.530	1.912	-11.505
H	-7.385	0.303	-10.760
H	-7.075	1.764	-9.793
H	3.379	0.075	1.969
H	3.356	0.147	-0.529
H	1.187	0.070	-1.746
H	-2.141	3.386	-0.004
H	0.071	2.065	3.609
H	-2.747	3.221	3.341

H	-0.990	4.890	2.704
H	-2.473	1.788	5.393
H	-1.739	5.323	4.256
H	-2.630	3.504	5.828
H	-1.037	2.716	5.862
H	-0.129	4.581	4.234
H	-3.956	2.056	1.158
H	-3.293	3.803	-1.293
H	-4.115	0.155	-0.482
H	-3.415	1.223	-1.745
H	-5.654	2.782	-1.296
H	-6.124	1.613	-0.039
H	-5.915	3.336	0.368
H	-4.829	0.052	-3.259
H	-3.417	2.521	-4.089
H	-2.819	0.859	-4.380
H	-2.921	2.019	-5.722
H	-4.782	0.384	-5.816
H	-5.129	2.700	-6.672
H	-6.653	2.027	-6.058
H	-5.739	3.213	-5.086
H	-9.757	-0.497	-4.245
H	-9.550	0.005	-2.471
C	-8.386	2.482	-3.002
H	-5.799	1.528	-3.139
H	-13.444	2.190	-3.823
H	1.244	-0.046	3.222
H	-3.561	4.391	0.361
H	-8.647	1.552	-4.994
H	-9.199	3.230	-3.038
H	-8.289	2.148	-1.961
H	-7.468	3.004	-3.303

Pi_Complex_Si_Primary

C	0.000	0.000	0.000
C	0.000	0.000	1.416
C	1.222	0.000	2.097
C	2.432	0.045	1.397
C	2.428	0.070	-0.001
C	1.216	0.028	-0.693
C	-1.246	-0.096	2.263
O	-1.590	0.931	3.029
C	-0.910	2.233	2.939
C	-1.740	3.250	3.710
C	-1.832	2.896	5.198
C	-1.257	0.051	-0.798
O	-2.164	0.787	-0.176
C	-3.494	1.028	-0.755
C	-4.021	2.302	-0.101
C	-5.503	2.495	-0.441
O	-1.421	-0.464	-1.918
Mg	-1.152	-2.399	-2.809
Cl	0.663	-3.978	-3.433
Mg	1.443	-4.023	-1.095
Cl	-0.560	-3.007	-0.442
Cl	-2.608	-4.290	-2.680
Mg	-3.388	-4.246	-5.019
Cl	-4.168	-4.201	-7.356
Mg	-6.064	-2.636	-6.995
Cl	-6.566	-2.605	-9.360
Cl	-7.440	-4.514	-6.605

Mg	-8.219	-4.468	-8.942
Cl	-10.136	-3.098	-8.348
Cl	-9.000	-4.424	-11.280
Cl	-1.866	-2.197	-5.166
Cl	2.222	-4.068	1.241
Mg	4.030	-2.657	0.660
Cl	5.640	-1.512	1.714
Cl	3.650	-3.018	-1.657
O	-1.920	-1.124	2.339
Mg	-3.070	-2.793	2.718
Cl	-1.394	-4.434	2.415
Mg	-0.616	-4.482	4.753
Cl	0.163	-4.528	7.091
Cl	-4.041	-2.641	0.526
C	-1.133	4.642	3.490
C	-3.193	3.529	-0.503
Cl	-7.481	-0.716	-6.273
Ti	-6.901	-0.615	-3.924
C	-5.344	0.758	-4.203
C	-4.468	0.999	-5.438
C	-5.128	1.987	-6.407
C	-3.071	1.506	-5.037
Cl	-6.853	-0.864	-1.495
Cl	-5.330	-2.514	-4.521
C	-9.031	0.557	-3.771
C	-8.371	1.589	-3.177
C	-8.112	2.907	-3.833
Mg	-10.841	-2.834	-10.731
O	-11.417	-0.943	-10.102
C	-11.688	-0.254	-9.109
O	-10.798	0.493	-8.467
C	-9.403	0.486	-8.955
C	-9.195	1.356	-10.192
C	-7.710	1.271	-10.576
Cl	-11.770	-2.540	-12.969
Cl	-12.272	-4.737	-10.528
Mg	-13.052	-4.692	-12.866
Cl	-13.832	-4.647	-15.204
C	-9.636	2.806	-9.964
C	-13.072	-0.113	-8.580
C	-14.107	-0.186	-9.526
C	-15.434	0.011	-9.152
C	-15.745	0.271	-7.817
C	-14.732	0.298	-6.858
C	-13.392	0.110	-7.222
C	-12.419	-0.012	-6.073
O	-11.815	1.072	-5.595
C	-11.964	2.395	-6.206
C	-12.179	3.434	-5.110
C	-12.137	4.831	-5.745
C	-13.484	3.202	-4.341
O	-12.233	-1.075	-5.473
Mg	-12.719	-3.148	-5.072
Cl	-11.056	-4.876	-5.427
Mg	-10.276	-4.921	-3.089
Cl	-9.496	-4.966	-0.752
Mg	-7.935	-3.094	-0.980
Cl	-6.225	-4.651	-1.509
Mg	-5.446	-4.698	0.829
Cl	-4.667	-4.746	3.166
Cl	-14.069	-2.987	-7.109
Mg	-15.108	-5.144	-7.013

Cl	-14.328	-5.189	-4.676
Cl	-15.888	-5.099	-9.351
Cl	-12.175	-3.258	-2.687
Cl	-7.448	-3.274	1.393
Cl	0.997	-2.599	4.478
Mg	-0.137	-2.106	6.564
Cl	-0.042	-0.132	7.625
Cl	-8.684	-2.922	-3.380
Cl	-2.393	-2.787	5.338
H	-0.813	2.501	1.877
H	-16.223	-0.045	-9.903
H	-16.782	0.421	-7.511
H	-13.847	-0.394	-10.565
H	-14.987	0.440	-5.805
H	-14.355	3.286	-5.012
H	-13.606	3.953	-3.547
H	-12.247	5.606	-4.973
H	-12.959	4.964	-6.466
H	-11.189	5.014	-6.273
H	-11.336	3.345	-4.403
H	-12.802	2.384	-6.917
H	-11.033	2.580	-6.760
H	-10.701	2.878	-9.701
H	-9.477	3.404	-10.873
H	-9.050	3.270	-9.153
H	-8.841	0.874	-8.097
H	-9.105	-0.557	-9.119
H	-9.788	0.930	-11.017
H	-7.523	1.829	-11.504
H	-7.385	0.232	-10.732
H	-7.074	1.707	-9.788
H	3.377	0.079	1.943
H	3.367	0.145	-0.554
H	1.205	0.049	-1.784
H	-2.127	3.401	-0.267
H	0.091	2.133	3.383
H	-2.756	3.240	3.274
H	-1.098	4.915	2.424
H	-2.264	1.899	5.358
H	-1.730	5.403	4.012
H	-2.459	3.626	5.728
H	-0.836	2.903	5.668
H	-0.109	4.697	3.891
H	-3.940	2.158	0.989
H	-3.278	3.719	-1.585
H	-4.108	0.144	-0.529
H	-3.383	1.131	-1.844
H	-5.642	2.629	-1.525
H	-6.108	1.633	-0.124
H	-5.892	3.393	0.059
H	-4.755	0.238	-3.412
H	-3.147	2.461	-4.491
H	-2.552	0.777	-4.399
H	-2.445	1.675	-5.926
H	-4.320	0.037	-5.959
H	-4.520	2.110	-7.316
H	-6.129	1.649	-6.710
H	-5.226	2.980	-5.938
H	-9.434	0.641	-4.780
H	-8.256	2.863	-4.921
H	-9.384	-0.300	-3.188
H	-8.811	3.656	-3.422

H	-7.101	3.289	-3.627
H	-8.109	1.506	-2.117
H	-5.672	1.724	-3.779
H	-13.505	2.212	-3.866
H	1.236	-0.057	3.187
H	-3.548	4.427	0.022

Pi_Complex_Si_Secondary

C	-13.344	0.124	-7.229
C	-13.019	-0.102	-8.586
C	-14.047	-0.168	-9.539
C	-15.375	0.039	-9.174
C	-15.691	0.307	-7.842
C	-14.685	0.327	-6.875
C	-11.634	-0.241	-9.107
O	-10.749	0.506	-8.459
C	-9.351	0.503	-8.941
C	-9.139	1.398	-10.158
C	-9.576	2.844	-9.898
C	-12.383	-0.015	-6.073
O	-12.202	-1.089	-5.487
Mg	-12.722	-3.148	-5.090
Cl	-12.151	-3.225	-2.705
O	-11.354	-0.927	-10.100
Mg	-10.838	-2.834	-10.725
Cl	-12.272	-4.737	-10.528
Mg	-13.052	-4.692	-12.866
Cl	-13.832	-4.647	-15.204
Cl	-11.786	-2.532	-12.952
C	-7.654	1.320	-10.542
O	-11.783	1.057	-5.569
C	-11.894	2.388	-6.173
C	-12.035	3.426	-5.066
C	-13.329	3.241	-4.266
C	-11.952	4.824	-5.695
Cl	-11.056	-4.876	-5.427
Mg	-10.276	-4.921	-3.089
Cl	-9.496	-4.966	-0.752
Mg	-7.920	-3.088	-0.951
Cl	-7.456	-3.307	1.418
Cl	-14.092	-2.974	-7.107
Mg	-15.108	-5.144	-7.013
Cl	-15.888	-5.099	-9.351
Cl	-6.225	-4.651	-1.509
Mg	-5.446	-4.698	0.829
Cl	-4.667	-4.746	3.166
Cl	-14.328	-5.189	-4.676
Cl	-9.000	-4.424	-11.280
Mg	-8.219	-4.468	-8.942
Cl	-10.146	-3.119	-8.340
Cl	-7.440	-4.514	-6.605
Mg	-6.056	-2.644	-6.979
Cl	-6.584	-2.571	-9.334
Cl	-4.168	-4.201	-7.356
Mg	-3.388	-4.246	-5.019
Cl	-2.608	-4.290	-2.680
Mg	-1.161	-2.383	-2.793
Cl	-1.874	-2.184	-5.148
O	-1.464	-0.442	-1.887
C	-1.303	0.081	-0.771
O	-2.209	0.820	-0.152

C	-3.538	1.073	-0.733
C	-4.074	2.321	-0.034
C	-3.236	3.561	-0.368
C	-0.044	0.036	0.029
C	-0.042	0.037	1.445
C	1.179	0.042	2.126
C	2.389	0.087	1.426
C	2.385	0.115	0.028
C	1.172	0.076	-0.662
C	-1.286	-0.085	2.292
O	-1.947	-1.123	2.347
Mg	-3.079	-2.797	2.723
Cl	-4.057	-2.630	0.534
O	-1.644	0.920	3.080
C	-0.983	2.234	3.029
C	-1.827	3.215	3.830
C	-1.225	4.618	3.669
C	-1.929	2.806	5.303
C	-5.552	2.542	-0.381
Cl	0.663	-3.978	-3.433
Mg	1.443	-4.023	-1.095
Cl	3.649	-3.009	-1.654
Mg	4.032	-2.661	0.660
Cl	5.646	-1.527	1.712
Cl	-0.549	-2.982	-0.438
Cl	2.222	-4.068	1.241
Cl	-1.394	-4.434	2.415
Mg	-0.616	-4.482	4.753
Cl	0.163	-4.528	7.091
Cl	-7.610	-0.792	-6.212
Ti	-7.044	-0.718	-3.875
C	-9.350	0.353	-3.497
C	-8.403	1.293	-3.806
C	-5.419	0.649	-3.919
C	-4.776	1.096	-5.249
C	-3.325	1.558	-5.024
Cl	-6.845	-0.853	-1.457
Cl	-5.346	-2.553	-4.552
C	-5.571	2.202	-5.953
Cl	0.953	-2.545	4.510
Mg	-0.207	-2.115	6.599
Cl	-0.197	-0.203	7.769
Cl	-8.656	-2.932	-3.370
Cl	-2.428	-2.819	5.342
H	-0.891	2.535	1.975
H	-16.158	-0.012	-9.931
H	-16.728	0.470	-7.543
H	-13.782	-0.377	-10.577
H	-14.947	0.476	-5.826
H	-14.213	3.364	-4.914
H	-13.401	3.990	-3.464
H	-12.011	5.598	-4.917
H	-12.784	4.996	-6.396
H	-11.010	4.970	-6.245
H	-11.176	3.298	-4.385
H	-12.753	2.414	-6.859
H	-10.972	2.536	-6.750
H	-10.643	2.913	-9.639
H	-9.410	3.463	-10.791
H	-8.993	3.287	-9.073
H	-8.793	0.874	-8.073
H	-9.057	-0.537	-9.126

H	-9.733	0.991	-10.993	Mg	-1.661	-1.865	4.708	Cl	-18.002	-5.964	-7.793
H	-7.466	1.901	-11.455	Cl	-0.014	-1.208	6.399	Mg	-17.557	-3.514	-7.860
H	-7.330	0.285	-10.723	Cl	-0.436	-3.916	4.551	Cl	-17.923	-3.533	-5.467
H	-7.018	1.736	-9.744	Mg	1.077	-3.487	6.448	C	-10.595	0.210	-5.647
H	3.335	0.114	1.974	Cl	2.592	-3.058	8.345	O	-15.482	-0.499	-5.875
H	3.324	0.189	-0.524	C	-5.063	2.844	2.860	C	-16.329	0.669	-6.158
H	1.162	0.102	-1.753	O	-1.795	-1.338	-1.021	C	-15.618	1.580	-7.153
H	-2.175	3.421	-0.118	Mg	-1.774	-3.490	-0.936	C	-16.539	2.775	-7.437
H	0.019	2.134	3.469	Cl	-3.107	-3.983	-2.948	C	-15.232	0.849	-8.443
H	-2.839	3.217	3.386	Cl	0.016	-3.153	0.666	Cl	-11.857	-3.318	-3.442
H	-1.185	4.932	2.615	Mg	1.055	-5.281	0.492	Cl	-18.079	-1.752	-9.150
H	-2.366	1.806	5.423	Cl	2.569	-4.852	2.389	Cl	-14.972	-3.319	1.977
H	-1.829	5.355	4.216	Cl	-3.285	-4.939	0.267	Mg	-16.486	-3.747	0.081
H	-2.558	3.518	5.857	Mg	-4.799	-5.368	-1.629	Cl	-18.401	-2.593	1.163
H	-0.938	2.793	5.782	Cl	-6.314	-5.796	-3.526	Mg	-19.576	-2.669	-0.894
H	-0.204	4.660	4.078	Mg	-7.727	-3.773	-3.278	Cl	-21.450	-1.627	-1.537
H	-4.008	2.128	1.051	Cl	-8.935	-4.428	-5.269	Cl	-18.000	-4.177	-1.815
H	-3.300	3.797	-1.442	Cl	-0.459	-5.709	-1.403	Cl	-14.742	-3.161	-1.365
H	-4.149	0.179	-0.540	C	-0.714	1.751	-4.486	Cl	-15.015	-4.111	-7.345
H	-3.421	1.208	-1.817	Cl	-9.136	-5.023	-1.851	H	-16.553	1.196	-5.221
H	-5.673	2.782	-1.448	Mg	-10.651	-5.454	-3.748	H	3.430	-0.027	1.889
H	-6.162	1.656	-0.160	Cl	-12.165	-5.886	-5.644	H	3.422	0.053	-0.611
H	-5.950	3.388	0.196	Cl	-3.154	-2.554	2.845	H	1.267	-0.039	3.122
H	-4.691	0.023	-3.366	Mg	-4.777	-3.573	4.325	H	1.272	0.006	-1.837
H	-3.294	2.423	-4.340	Cl	-3.262	-3.145	6.222	H	-3.035	0.597	-5.565
H	-2.714	0.749	-4.601	Cl	-6.291	-4.002	2.429	H	-3.140	2.366	-5.680
H	-2.859	1.866	-5.974	Mg	-7.404	-1.948	2.788	H	-0.636	2.603	-5.176
H	-4.728	0.225	-5.928	Cl	-6.134	-1.478	4.779	H	-0.475	0.838	-5.056
H	-5.055	2.533	-6.867	Cl	-6.334	-0.336	1.169	H	0.049	1.881	-3.706
H	-6.575	1.863	-6.246	Ti	-7.621	-0.867	-0.864	H	-2.324	2.594	-3.326
H	-5.680	3.081	-5.296	Cl	-6.169	-3.057	-1.426	H	-3.271	0.439	-2.493
H	-9.814	-0.207	-4.316	Cl	-8.900	-2.372	0.756	H	-2.026	-0.462	-3.392
C	-9.993	0.186	-2.159	C	-5.989	-0.019	-2.313	H	-2.456	3.855	2.816
H	-5.626	1.533	-3.290	C	-6.863	1.036	-2.450	H	-3.358	4.498	1.428
H	-13.379	2.248	-3.798	C	-7.622	1.314	-3.706	H	-2.041	3.333	1.164
H	1.193	-0.016	3.215	C	-8.563	1.033	-0.747	H	-3.961	0.339	2.529
H	-3.599	4.437	0.187	C	-8.241	2.323	0.019	H	-2.872	1.351	3.531
H	-8.182	1.567	-4.837	C	-9.005	2.369	1.354	H	-4.286	2.213	0.952
H	-7.986	1.938	-3.029	Cl	-8.874	-1.594	-2.830	H	-5.580	3.727	2.456
H	-10.959	0.722	-2.177	C	-8.556	3.577	-0.809	H	-4.711	3.100	3.872
H	-10.238	-0.863	-1.952	Cl	-9.117	-3.232	4.100	H	-5.797	2.031	2.953
H	-9.388	0.605	-1.345	Mg	-10.631	-3.660	2.203	H	-19.301	-0.178	-2.523
Re_Primary_Transition_State				Cl	-12.047	-4.101	0.437	H	-18.192	0.459	-0.371
C	0.047	-0.046	-0.063	Mg	-13.378	-2.088	0.428	H	-15.709	0.423	-0.206
C	0.054	-0.037	1.351	Cl	-11.948	-1.378	2.283	H	-12.976	2.589	-4.670
C	1.281	-0.037	2.031	O	-13.300	-0.489	-1.075	H	-17.257	0.267	-6.594
C	2.489	-0.018	1.338	C	-13.928	-0.144	-2.089	H	-14.703	1.956	-6.662
C	2.484	0.022	-0.054	O	-13.395	0.378	-3.181	H	-16.806	3.321	-6.518
C	1.271	0.010	-0.746	C	-11.960	0.301	-3.503	H	-14.534	0.023	-8.248
C	-1.147	0.093	2.218	C	-11.876	0.716	-4.975	H	-16.044	3.484	-8.115
O	-2.125	0.796	1.659	C	-12.049	2.230	-5.142	H	-14.745	1.545	-9.142
C	-3.260	1.184	2.515	C	-15.414	-0.209	-2.243	H	-16.118	0.425	-8.938
C	-3.888	2.452	1.954	C	-16.034	-0.552	-3.472	H	-17.470	2.446	-7.923
C	-2.875	3.595	1.830	C	-17.434	-0.564	-3.538	H	-12.722	0.212	-5.473
C	-1.138	-0.289	-0.954	C	-18.212	-0.206	-2.432	H	-11.206	2.772	-4.685
O	-1.318	0.713	-1.807	C	-17.593	0.157	-1.232	H	-11.628	-0.729	-3.325
C	-2.260	0.502	-2.916	C	-16.200	0.135	-1.138	H	-11.419	0.984	-2.830
C	-2.122	1.665	-3.888	C	-15.271	-1.034	-4.681	H	-9.706	0.715	-5.249
C	-3.189	1.518	-4.982	O	-14.466	-1.971	-4.616	H	-10.458	-0.870	-5.508
O	-1.174	-0.313	3.388	Mg	-13.490	-3.731	-5.140	H	-10.636	0.417	-6.726
				Cl	-14.992	-5.111	-3.984	H	-9.062	0.300	-0.035
				Mg	-16.496	-5.538	-5.888	H	-10.092	2.348	1.188

H	-8.743	1.514	1.992
H	-8.763	3.290	1.907
H	-7.164	2.327	0.265
H	-8.285	4.487	-0.252
H	-8.015	3.602	-1.766
H	-9.634	3.632	-1.031
H	-5.917	-0.785	-3.085
H	-5.200	-0.000	-1.558
H	-9.316	1.197	-1.533
H	-4.204	1.484	-4.559
H	-17.928	-0.889	-4.454
H	-12.082	2.506	-6.206
H	-6.678	1.905	-1.817
H	-7.039	2.050	-4.287
H	-7.748	0.412	-4.315
H	-8.606	1.764	-3.521

Donor_Si_Primary_Transition State

C	0.000	0.000	0.000
C	0.000	0.000	1.399
C	1.234	0.000	2.099
C	2.428	-0.032	1.368
C	2.417	-0.027	-0.029
C	1.199	-0.001	-0.715
C	-1.322	0.112	2.086
O	-1.211	0.892	3.150
C	-2.365	1.231	3.990
C	-1.921	2.413	4.850
C	-2.996	2.764	5.884
C	1.351	-0.117	3.598
O	2.022	0.787	4.295
C	2.573	2.026	3.727
C	2.598	3.090	4.818
C	3.427	2.652	6.030
O	-2.388	-0.383	1.683
C	-1.559	3.634	3.997
O	0.895	-1.085	4.211
Mg	0.608	-2.653	5.502
Cl	1.174	-4.368	3.976
Mg	3.578	-4.450	4.513
Cl	5.983	-4.530	5.048
Cl	-1.764	-2.441	5.206
C	3.133	4.392	4.204
Mg	-3.115	-2.344	1.031
Cl	-5.491	-2.062	0.455
Cl	-3.829	-4.169	2.407
Mg	-6.237	-4.083	1.883
Cl	-8.644	-3.996	1.359
Mg	-2.265	-4.409	6.655
Cl	0.139	-4.498	7.179
Cl	-4.673	-4.321	6.130
Mg	-4.981	-2.648	7.797
Cl	-2.729	-2.933	8.636
Cl	-5.696	-4.446	9.340
Mg	-8.102	-4.360	8.816
Cl	-10.509	-4.274	8.292
Mg	-11.031	-2.474	9.819
Cl	-8.689	-2.580	10.562
O	-11.215	-0.353	9.472
C	-11.905	0.670	9.590

O	-11.367	1.859	9.837
C	-9.913	1.916	10.050
C	-9.549	3.335	10.464
C	-10.211	3.736	11.787
C	-13.408	0.722	9.655
C	-13.915	0.970	10.938
C	-15.281	0.859	11.206
C	-16.163	0.499	10.188
C	-15.677	0.286	8.900
C	-14.309	0.405	8.612
C	-13.948	0.275	7.175
O	-14.615	-0.393	6.375
Mg	-14.872	-2.220	5.358
Cl	-15.513	-4.072	6.729
Mg	-17.920	-3.986	6.204
Cl	-20.327	-3.899	5.681
C	-8.020	3.447	10.543
O	-12.917	1.040	6.826
C	-12.600	1.170	5.394
C	-12.073	2.577	5.142
C	-11.672	2.688	3.665
C	-13.094	3.654	5.528
Cl	-13.448	-2.459	9.588
Mg	-13.944	-4.311	10.977
Cl	-11.537	-4.398	11.501
Cl	-16.351	-4.225	10.452
Cl	-12.467	-2.485	5.869
Mg	-12.078	-4.034	4.043
Cl	-9.672	-4.120	4.568
Mg	-9.262	-2.312	3.107
Cl	-11.534	-2.285	2.302
Cl	-17.267	-1.880	4.983
Cl	-14.485	-3.948	3.520
Cl	-0.805	-2.987	1.722
Mg	-0.396	-4.131	-0.277
Cl	-2.802	-4.045	-0.801
Cl	2.009	-4.218	0.247
Mg	2.475	-2.859	-1.635
Cl	4.254	-1.841	-2.541
Cl	0.271	-3.155	-2.466
Cl	-9.264	-0.259	4.535
Ti	-6.971	-0.377	5.497
C	-7.539	1.070	7.068
C	-6.991	2.080	6.255
C	-7.863	3.196	5.757
C	-6.346	1.257	4.202
C	-7.034	1.970	3.026
C	-6.239	3.209	2.578
Cl	-4.722	-0.542	6.449
Cl	-7.444	-2.266	7.289
Cl	-6.766	-2.377	3.795
C	-7.247	1.041	1.820
Cl	4.212	-2.600	2.950
Mg	5.416	-2.093	4.995
Cl	6.392	-0.111	5.414
Cl	3.209	-2.697	6.295
H	1.959	2.334	2.869
H	-17.229	0.390	10.391
H	-15.649	1.043	12.217
H	-16.356	0.027	8.086
H	-13.225	1.219	11.746
H	-7.612	2.776	11.315

H	-7.724	4.473	10.805
H	-9.949	4.770	12.054
H	-9.871	3.084	12.607
H	-11.306	3.673	11.727
H	-9.908	4.013	9.670
H	-9.420	1.621	9.114
H	-9.648	1.179	10.825
H	-14.014	3.551	4.932
H	-12.687	4.658	5.339
H	-13.367	3.596	6.591
H	-11.861	0.394	5.158
H	-13.519	0.983	4.821
H	-11.169	2.710	5.762
H	-11.243	3.680	3.459
H	-12.548	2.565	3.009
H	-10.931	1.926	3.385
H	3.360	-0.031	-0.581
H	1.181	0.037	-1.807
H	-0.953	0.026	-0.529
H	-0.772	3.408	3.264
H	3.595	1.798	3.387
H	1.554	3.260	5.138
H	2.527	4.726	3.348
H	3.013	1.750	6.500
H	3.127	5.196	4.954
H	3.448	3.450	6.787
H	4.465	2.427	5.742
H	4.172	4.268	3.862
H	-1.020	2.081	5.397
H	-2.440	3.999	3.445
H	-2.619	0.341	4.584
H	-3.208	1.481	3.328
H	-3.892	3.173	5.391
H	-3.294	1.890	6.479
H	-2.620	3.536	6.570
H	-6.059	0.210	3.865
H	-6.297	0.643	1.435
H	-7.879	0.185	2.086
H	-7.745	1.581	1.002
H	-8.036	2.297	3.352
H	-6.787	3.769	1.806
H	-6.030	3.902	3.408
H	-5.272	2.908	2.146
H	-6.946	0.647	7.881
H	-8.838	2.824	5.413
H	-8.625	0.990	7.161
H	-8.050	3.867	6.613
H	-7.406	3.797	4.964
H	-5.940	2.323	6.421
H	-5.375	1.719	4.425
H	-7.542	3.190	9.585
H	3.381	-0.094	1.894
H	-1.201	4.458	4.63

Si_Secondary_Transition_Stat e_

C	0.000	0.000	0.000
C	0.000	0.000	1.400
C	1.233	0.000	2.088
C	2.428	-0.051	1.354
C	2.415	-0.074	-0.037

C	1.197	-0.036	-0.716
C	-1.365	-0.119	2.025
O	-2.002	1.042	2.006
C	-3.423	1.096	2.375
C	-4.049	2.274	1.636
C	-5.479	2.493	2.146
C	1.384	0.103	3.563
O	0.405	0.782	4.152
C	0.562	1.100	5.583
C	-0.296	2.314	5.911
C	0.034	3.518	5.023
O	-1.901	-1.176	2.388
Mg	-1.838	-3.337	2.369
Cl	0.503	-3.087	1.799
Mg	0.740	-5.004	0.423
Cl	3.135	-4.580	0.022
Cl	-1.510	-4.930	4.156
Mg	-3.905	-5.354	4.556
Cl	-6.299	-5.778	4.957
Mg	-6.730	-3.858	6.483
Cl	-9.053	-4.524	6.530
Cl	-6.150	-5.278	8.288
Mg	-8.546	-5.704	8.689
Cl	-10.939	-6.131	9.089
Cl	-4.244	-3.795	2.565
C	-4.021	2.069	0.118
O	2.378	-0.324	4.166
Mg	3.237	-2.000	5.088
Cl	0.867	-2.627	5.478
Mg	1.377	-3.881	7.491
Cl	3.772	-3.458	7.090
Cl	5.523	-1.352	4.496
Cl	3.629	-3.956	3.758
Mg	6.024	-3.532	3.357
Cl	8.418	-3.108	2.956
C	-0.102	2.648	7.397
Cl	-1.653	-5.428	0.824
Cl	-1.016	-4.306	7.891
Mg	-1.193	-2.371	9.211
Cl	1.177	-1.940	9.097
Cl	-0.873	-3.808	11.223
Mg	-3.267	-4.232	11.624
Cl	-5.663	-4.655	12.025
Mg	-6.146	-2.724	13.360
Cl	-3.814	-2.057	12.945
O	-7.402	-0.965	12.879
C	-8.607	-0.668	12.875
O	-9.226	-0.051	11.879
C	-8.542	0.283	10.628
C	-9.495	1.201	9.865
C	-9.763	2.504	10.629
C	-9.561	-0.853	14.011
C	-10.945	-1.101	13.819
C	-11.784	-1.165	14.938
C	-11.282	-0.961	16.227
C	-9.921	-0.701	16.412
C	-9.067	-0.658	15.306
C	-11.550	-1.460	12.484
O	-11.127	-2.410	11.819
Mg	-11.084	-4.102	10.641
Cl	-8.828	-3.614	10.027
C	-8.952	1.488	8.463

O	-12.607	-0.812	12.017
C	-13.207	0.381	12.632
C	-13.713	1.299	11.524
C	-14.312	2.552	12.179
C	-14.726	0.600	10.612
Cl	-10.806	-5.629	12.417
Mg	-13.203	-6.050	12.805
Cl	-13.494	-4.160	14.395
Mg	-15.401	-3.997	12.912
Cl	-16.672	-2.144	12.832
Cl	-15.600	-6.470	13.195
Cl	-8.412	-3.718	13.644
Mg	-7.913	-4.582	15.758
Cl	-10.307	-5.007	16.157
Mg	-10.269	-3.490	17.973
Cl	-7.898	-3.434	17.968
Cl	-5.519	-4.158	15.356
Cl	-11.724	-2.559	19.396
Cl	-2.057	-0.583	7.696
Ti	-4.489	-1.128	7.663
C	-4.785	0.523	9.094
C	-3.926	1.700	9.550
C	-3.187	1.350	10.855
Cl	-6.821	-1.767	7.876
Cl	-4.364	-3.090	5.982
Cl	-3.699	-2.942	9.457
C	-5.414	1.088	7.005
C	-5.068	0.200	5.961
C	-6.094	-0.311	4.971
C	-4.760	2.975	9.747
Cl	-13.756	-4.490	10.901
H	-12.460	0.878	13.266
H	3.354	-0.122	-0.588
H	1.173	-0.044	-1.807
H	3.372	-0.067	1.902
H	-0.950	-0.002	-0.536
H	-6.116	1.621	1.933
H	-5.931	3.362	1.648
H	-4.458	2.935	-0.398
H	-4.606	1.180	-0.167
H	-2.995	1.943	-0.253
H	-3.451	3.169	1.882
H	-3.462	1.228	3.466
H	-3.895	0.137	2.116
H	1.085	3.821	5.152
H	-0.593	4.380	5.292
H	-0.128	3.298	3.959
H	0.264	0.208	6.151
H	1.627	1.307	5.765
H	-1.352	2.030	5.755
H	-0.749	3.488	7.688
H	0.938	2.946	7.600
H	-0.342	1.791	8.042
H	-11.956	-0.994	17.086
H	-9.527	-0.504	17.411
H	-8.006	-0.440	15.442
H	-10.174	2.315	11.631
H	-14.046	0.024	13.249
H	-12.838	1.605	10.924
H	-13.583	3.077	12.816
H	-14.283	-0.266	10.104
H	-14.650	3.258	11.407

H	-15.088	1.296	9.842
H	-15.593	0.240	11.187
H	-15.185	2.294	12.797
H	-10.445	0.649	9.756
H	-8.834	3.084	10.748
H	-8.333	-0.655	10.095
H	-7.592	0.780	10.881
H	-8.035	2.096	8.519
H	-8.728	0.561	7.916
H	-9.687	2.061	7.880
H	-4.341	-0.435	9.496
H	-3.890	1.089	11.660
H	-2.512	0.494	10.718
H	-2.580	2.203	11.194
H	-3.155	1.893	8.783
H	-4.115	3.820	10.030
H	-5.311	3.269	8.841
H	-5.495	2.834	10.555
H	-4.778	1.948	7.210
H	-7.060	-0.498	5.459
H	-6.467	1.205	7.262
H	-6.266	0.442	4.184
H	-5.761	-1.233	4.474
H	-4.051	0.321	5.557
H	-5.799	0.570	9.516
H	-5.503	2.679	3.231
H	-12.838	-1.408	14.810
H	-10.480	3.133	10.083

Just_3,3bis(methoxymethyl)2,4 dimethylpentane

C	0.000	0.000	0.000
O	0.000	0.000	1.415
C	1.324	0.000	1.928
C	1.433	-0.055	3.480
C	1.422	-1.534	3.919
O	0.379	-2.269	3.290
C	0.389	-3.627	3.692
C	2.899	0.490	3.741
C	3.048	2.013	3.581
C	0.307	0.785	4.183
C	-1.100	0.159	4.113
C	3.592	0.043	5.044
C	0.572	1.109	5.665
H	-1.048	0.019	-0.325
H	0.520	0.888	-0.411
H	1.883	-0.868	1.518
H	1.834	0.912	1.561
H	1.325	-1.611	5.022
H	2.396	-1.995	3.647
H	-0.429	-4.129	3.162
H	1.345	-4.125	3.433
H	0.229	-3.734	4.784
H	3.496	0.033	2.928
H	4.631	0.407	5.038
H	3.110	0.447	5.943
H	3.636	-1.048	5.147
H	4.116	2.274	3.522
H	2.568	2.398	2.670
H	2.628	2.564	4.433
H	0.265	1.744	3.637

H	-0.296	1.646	6.075
H	0.691	0.192	6.264
H	1.452	1.741	5.834
H	-1.835	0.894	4.477
H	-1.374	-0.145	3.100
H	-1.168	-0.725	4.764
H	0.487	-0.907	-0.408

DIBP_3,3bis(methoxymethyl)2,4dimethylpentane_Zip

C	0.000	0.000	0.000
C	0.000	0.000	1.396
C	1.206	0.000	2.107
C	2.430	0.046	1.401
C	2.410	0.047	-0.000
C	1.207	0.006	-0.699
C	1.093	0.053	3.608
O	1.125	1.120	4.222
Mg	1.476	2.647	5.512
Cl	-0.815	3.309	6.065
C	3.760	0.074	2.074
O	3.763	-0.690	3.161
C	4.974	-0.831	3.981
C	5.151	-2.311	4.305
C	6.150	-2.450	5.459
O	0.853	-1.055	4.294
C	0.854	-2.371	3.638
C	0.797	-3.438	4.724
C	0.968	-4.815	4.069
C	-0.496	-3.354	5.540
O	4.754	0.679	1.651
Mg	5.525	2.560	0.995
Cl	6.489	3.603	2.971
Mg	8.801	2.919	2.450
Cl	11.110	2.235	1.930
Mg	10.923	0.158	3.026
Cl	11.797	1.064	5.016
Mg	14.106	0.380	4.495
Cl	13.948	-1.479	5.995
Mg	16.029	-2.508	5.173
Cl	17.104	-1.475	7.061
Mg	19.414	-2.159	6.540
Cl	21.724	-2.843	6.020
Cl	7.809	1.953	0.320
C	5.590	-3.116	3.077
Cl	3.844	2.346	4.894
Mg	4.642	3.048	7.075
Cl	6.953	2.364	6.555
Mg	6.786	0.278	7.637
Cl	7.640	1.192	9.641
Mg	9.950	0.508	9.121
Cl	12.260	-0.175	8.599
Mg	12.001	-2.381	9.586
O	11.350	-3.936	8.235
C	10.075	-4.545	8.549
Cl	1.647	4.904	4.510
Mg	1.883	6.881	3.064
Cl	0.216	7.893	4.423
Cl	2.333	3.732	7.596
Mg	-0.662	5.588	5.031

Cl	-2.972	6.272	5.551
Mg	-3.720	5.214	3.569
Cl	-1.546	4.813	2.768
Cl	-5.756	4.749	2.790
Cl	13.048	-0.756	2.430
Cl	8.607	0.466	3.450
Cl	1.184	6.143	0.927
Mg	3.494	5.459	0.405
Cl	3.076	3.116	0.671
Cl	5.804	4.775	-0.114
Cl	4.124	7.040	2.289
Cl	16.417	-0.303	3.975
Cl	18.226	-3.495	4.726
Cl	8.900	-0.691	7.095
Cl	4.448	0.594	8.021
Cl	14.168	-3.549	9.598
Mg	15.256	-2.030	11.165
Cl	17.567	-2.714	10.644
Cl	9.793	-1.646	10.425
Cl	12.947	-1.346	11.686
C	11.670	-3.997	6.797
C	12.572	-5.148	6.217
C	12.110	-5.255	4.703
C	12.072	-3.917	3.942
C	14.102	-4.776	6.361
O	14.871	-4.375	5.165
C	15.518	-5.492	4.504
C	12.356	-6.541	6.925
C	12.819	-6.627	8.393
C	13.005	-7.716	6.171
C	10.751	-5.952	4.505
H	6.574	-2.775	2.720
H	-0.618	-2.367	6.007
H	0.149	-5.026	3.364
H	-1.374	-3.543	4.902
H	0.956	-5.604	4.834
H	-0.024	-2.430	2.978
H	1.769	-2.455	3.036
H	-0.947	0.020	1.938
H	-0.949	0.004	-0.537
H	3.359	0.078	-0.538
H	1.212	0.002	-1.790
H	5.833	-0.413	3.437
H	4.781	-0.225	4.876
H	4.174	-2.691	4.652
H	7.115	-1.978	5.220
H	5.741	-1.996	6.379
H	6.341	-3.509	5.687
H	1.653	-3.263	5.398
H	1.918	-4.895	3.519
H	-0.498	-4.107	6.341
H	5.666	-4.187	3.315
H	4.876	-3.012	2.247
H	10.695	-4.012	6.292
H	12.145	-3.036	6.570
H	14.653	-5.622	6.792
H	14.210	-3.941	7.060
H	12.859	-5.882	4.198
H	10.514	-5.968	3.431
H	10.730	-6.990	4.859
H	9.930	-5.411	5.001
H	11.965	-4.114	2.865

H	11.207	-3.305	4.243
H	12.972	-3.314	4.084
H	11.267	-6.719	6.917
H	12.509	-7.597	8.809
H	13.913	-6.578	8.485
H	12.412	-5.834	9.026
H	12.759	-8.657	6.685
H	12.673	-7.815	5.130
H	14.103	-7.639	6.171
H	14.780	-6.253	4.222
H	16.004	-5.100	3.602
H	16.286	-5.932	5.157
H	10.075	-5.602	8.252
H	9.929	-4.470	9.634
H	9.263	-3.999	8.046

Just_diphenylsilanediyl_diacetate

C	0.000	0.000	0.000
C	0.000	0.000	1.408
C	1.241	0.000	2.076
C	2.440	0.004	1.359
C	2.420	0.009	-0.038
C	1.198	0.006	-0.718
Si	-1.584	-0.060	2.424
C	-3.100	0.699	1.606
C	-3.012	1.716	0.636
C	-4.164	2.278	0.079
C	-5.425	1.835	0.486
C	-5.532	0.830	1.452
C	-4.381	0.266	2.007
O	-1.989	-1.630	2.927
C	-2.332	-2.799	2.291
C	-2.159	-2.818	0.790
O	-1.252	0.603	3.951
C	-0.928	1.853	4.421
C	-1.035	2.988	3.428
O	-2.734	-3.734	2.942
O	-0.590	1.986	5.573
H	-2.034	2.079	0.311
H	-4.076	3.064	-0.673
H	-6.326	2.274	0.051
H	-6.516	0.484	1.775
H	-4.480	-0.516	2.763
H	1.272	-0.007	3.168
H	3.392	0.003	1.893
H	3.357	0.013	-0.598
H	1.179	0.008	-1.809
H	-0.945	-0.006	-0.547
H	-1.105	-2.652	0.525
H	-2.487	-3.787	0.398
H	-2.749	-2.015	0.322
H	-0.393	2.799	2.554
H	-2.069	3.081	3.065
H	-0.730	3.922	3.910

DIBP_diphenylsilanediyl_diacetate_silane_Zip

C	0.000	0.000	0.000
C	0.000	0.000	1.407

C	1.236	0.000	2.083
C	2.437	0.010	1.371
C	2.421	0.012	-0.026
C	1.202	0.006	-0.710
Si	-1.584	-0.060	2.404
C	-2.066	-1.737	3.076
C	-1.493	-2.208	4.274
C	-1.706	-3.532	4.688
C	-2.514	-4.390	3.927
C	-3.108	-3.922	2.754
C	-2.866	-2.615	2.323
O	-2.764	0.490	1.255
C	-4.044	0.876	1.368
C	-4.738	1.081	0.057
O	-4.571	1.037	2.467
Mg	-6.045	1.762	3.766
Cl	-7.603	0.457	5.123
Mg	-5.751	-0.238	6.595
Cl	-3.900	-0.933	8.066
Mg	-3.396	-2.832	6.743
Cl	-4.777	-4.187	8.161
Mg	-2.926	-4.883	9.633
Cl	-1.074	-5.579	11.104
Mg	-0.428	-7.467	9.744
O	1.260	-6.838	8.553
C	2.495	-6.757	8.514
O	3.163	-5.635	8.261
C	2.458	-4.363	8.050
C	2.987	-3.736	6.763
C	2.568	-2.262	6.720
Cl	-6.726	3.712	5.028
Mg	-8.577	4.407	3.557
Cl	-10.428	5.102	2.085
Cl	-7.514	2.683	2.008
Cl	-4.338	1.404	5.501
Cl	-1.466	-3.450	8.131
Cl	-5.200	-2.253	5.215
Cl	-2.272	-6.923	8.223
C	3.427	-7.911	8.678
C	3.004	-9.158	8.196
C	3.815	-10.284	8.312
C	5.052	-10.184	8.949
C	5.491	-8.951	9.435
C	4.700	-7.804	9.283
C	5.258	-6.542	9.884
O	6.130	-5.812	9.208
C	6.471	-6.127	7.812
C	7.362	-5.011	7.286
C	7.607	-5.245	5.789
O	5.005	-6.211	11.046
Mg	4.331	-5.353	12.729
Cl	2.288	-4.767	11.487
Mg	2.029	-2.667	12.670
Cl	0.177	-1.971	11.198
Mg	1.520	-0.627	9.801
Cl	-0.019	0.013	8.119
Cl	3.002	-6.616	14.237
Mg	4.853	-7.311	15.708
Cl	6.704	-8.007	17.179
Cl	5.453	-9.281	14.311
Mg	7.586	-8.295	14.853
Cl	9.595	-8.663	13.935

Cl	3.879	-3.362	14.141
Cl	3.511	-1.409	10.875
Cl	1.053	1.282	11.103
Mg	-0.796	1.978	9.632
Cl	-2.648	2.673	8.160
Mg	-1.180	3.904	6.684
O	-0.774	2.547	5.151
C	-1.021	2.200	4.000
C	-0.987	3.127	2.821
Cl	0.658	3.522	8.261
C	8.676	-4.913	8.067
C	2.520	-4.498	5.519
O	-1.372	0.921	3.786
Cl	-2.452	5.206	4.960
Mg	-3.622	6.623	6.594
Cl	-5.473	7.318	5.122
Cl	-1.771	5.928	8.065
Cl	-1.952	-8.833	11.200
Mg	-0.101	-9.528	12.671
Cl	-1.571	-10.818	14.191
Mg	0.273	-11.450	15.535
Cl	0.491	-12.615	17.415
Cl	1.358	-8.763	10.966
Cl	1.749	-10.223	14.142
Cl	6.416	-5.938	14.274
H	2.822	-5.556	5.552
H	3.470	-11.244	7.927
H	5.680	-11.066	9.082
H	2.022	-9.233	7.727
H	6.448	-8.883	9.958
H	6.993	-7.096	7.793
H	5.536	-6.204	7.240
H	9.265	-5.838	7.961
H	8.501	-4.740	9.137
H	9.290	-4.083	7.688
H	8.147	-6.189	5.616
H	8.221	-4.434	5.373
H	6.806	-4.065	7.406
H	6.667	-5.282	5.218
H	1.376	-4.546	8.020
H	2.699	-3.760	8.936
H	1.423	-4.464	5.428
H	2.946	-4.060	4.605
H	1.476	-2.145	6.798
H	2.889	-1.790	5.780
H	3.044	-1.697	7.539
H	4.090	-3.773	6.809
H	-4.069	1.562	-0.666
H	-5.010	0.094	-0.350
H	-5.654	1.664	0.204
H	-0.622	2.626	1.914
H	-2.013	3.487	2.644
H	-0.374	4.005	3.046
H	-0.871	-1.549	4.887
H	-1.179	-3.917	5.565
H	-2.673	-5.420	4.254
H	-3.750	-4.579	2.165
H	-3.317	-2.279	1.387
H	1.269	0.002	3.177
H	3.387	0.021	1.908
H	3.360	0.021	-0.583
H	1.188	0.012	-1.802

H	-0.945	0.006	-0.545
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Just_diisobutyl pyridine-2,6-dicarboxylate

C	0.000	0.000	0.000
N	0.000	0.000	1.340
C	1.184	0.000	1.963
C	2.415	-0.004	1.289
C	2.402	-0.003	-0.103
C	1.175	0.000	-0.767
C	1.212	-0.001	3.473
O	-0.017	0.072	4.010
C	-0.077	0.058	5.462
C	-1.538	0.163	5.881
C	-2.370	-1.000	5.335
C	-1.370	-0.011	-0.638
O	-1.275	0.104	-1.994
C	-2.541	0.096	-2.708
C	-2.268	0.310	-4.192
C	-1.624	1.673	-4.462
O	2.250	-0.064	4.115
O	-2.418	-0.110	-0.037
C	-3.578	0.144	-4.972
C	-1.616	0.250	7.410
H	3.340	-0.010	1.866
H	3.337	-0.006	-0.667
H	1.117	0.001	-1.855
H	-3.041	-0.866	-2.522
H	-3.185	0.892	-2.298
H	-1.569	-0.481	-4.516
H	-3.404	0.264	-6.051
H	-4.027	-0.847	-4.813
H	-4.317	0.902	-4.669
H	-1.399	1.795	-5.532
H	-2.304	2.489	-4.168
H	-0.688	1.796	-3.901
H	0.379	-0.876	5.827
H	0.521	0.898	5.850
H	-1.933	1.103	5.457
H	-3.425	-0.895	5.629
H	-2.323	-1.044	4.239
H	-2.005	-1.961	5.735
H	-2.659	0.366	7.737
H	-1.221	-0.664	7.880
H	-1.044	1.105	7.803

DIBP_diisobutyl pyridine-2,6-dicarboxylate_Zip

N	0.000	0.000	0.000
C	0.000	0.000	1.340
C	1.156	0.000	2.128
C	2.391	0.038	1.483
C	2.418	0.156	0.095
C	1.196	0.127	-0.591
C	-1.349	0.160	1.984
O	-1.620	1.139	2.693
Mg	-1.407	3.060	3.371
Cl	-0.966	5.098	4.719
Mg	1.319	5.309	3.892
Cl	3.610	5.509	3.078

C	1.194	0.393	-2.067
O	0.550	-0.488	-2.797
C	0.469	-0.220	-4.249
C	-0.405	-1.290	-4.883
C	-0.600	-0.938	-6.364
O	-2.201	-0.805	1.712
C	-3.587	-0.686	2.211
C	-3.833	-1.625	3.390
C	-2.995	-1.261	4.620
C	-5.333	-1.595	3.715
O	1.776	1.384	-2.535
Mg	2.244	3.252	-1.741
Cl	2.888	4.989	-0.142
Mg	5.250	5.052	-0.845
Cl	7.612	5.114	-1.548
Cl	1.626	5.048	-3.268
Mg	-0.736	4.985	-2.565
Cl	-0.054	3.434	-0.785
Cl	4.651	2.887	-1.958
Cl	-3.096	4.922	-1.862
Mg	-3.712	3.306	-3.449
Cl	-1.451	3.013	-4.156
Cl	-4.359	4.981	-4.988
Mg	-6.721	4.918	-4.285
Cl	-8.808	5.549	-3.450
Cl	-7.534	3.259	-5.853
Mg	-9.690	3.547	-4.742
O	-9.653	1.614	-3.867
C	-10.358	0.762	-3.314
O	-10.032	0.143	-2.185
C	-8.794	0.498	-1.474
C	-7.990	-0.774	-1.232
C	-6.865	-0.460	-0.239
Cl	-10.345	4.914	-6.708
Mg	-12.706	4.851	-6.005
Cl	-12.094	3.441	-4.238
Cl	-13.530	5.902	-8.098
Mg	-15.777	5.755	-7.341
Cl	-15.067	4.789	-5.301
Cl	-17.777	6.259	-8.167
Cl	-5.949	2.870	-2.771
C	-11.648	0.258	-3.865
C	-11.765	0.169	-5.260
C	-12.940	-0.290	-5.849
C	-14.026	-0.643	-5.046
C	-13.924	-0.561	-3.656
C	-12.734	-0.132	-3.053
C	-12.754	-0.008	-1.551
O	-13.049	1.047	-0.991
Mg	-13.248	2.932	-0.247
Cl	-13.957	4.714	-1.648
Mg	-16.318	4.652	-0.944
Cl	-15.635	2.734	0.468
Cl	-18.680	4.589	-0.242
Mg	-19.184	3.059	-2.002
Cl	-17.140	3.564	-3.045
Cl	-20.889	1.705	-2.453
C	-7.443	-1.360	-2.538
O	-12.551	-1.078	-0.795
C	-12.151	-2.363	-1.386
C	-11.786	-3.309	-0.250
C	-12.977	-3.576	0.675

C	-11.231	-4.607	-0.852
C	0.176	-2.697	-4.707
Cl	-1.985	4.847	1.791
Mg	-4.347	4.785	2.494
Cl	-6.708	4.722	3.197
Mg	-7.297	3.111	1.588
Cl	-5.032	2.754	0.973
Cl	-7.971	4.781	0.071
Mg	-10.333	4.718	0.774
Cl	-10.897	3.260	-1.056
Cl	-12.694	4.656	1.477
Cl	-9.540	2.633	2.220
Cl	-3.691	3.164	4.285
Cl	1.051	2.901	3.431
H	-6.766	-0.645	-3.031
H	-14.785	-0.816	-3.034
H	-14.962	-0.976	-5.498
H	-13.012	-0.363	-6.935
H	-10.916	0.464	-5.879
H	-8.665	-1.512	-0.763
H	-9.136	0.961	-0.538
H	-8.235	1.231	-2.069
H	-8.250	-1.604	-3.246
H	-6.881	-2.285	-2.345
H	-7.269	-0.147	0.736
H	-6.206	0.337	-0.616
H	-6.248	-1.354	-0.069
H	-10.351	-4.424	-1.487
H	-10.929	-5.299	-0.053
H	-11.991	-5.120	-1.462
H	-11.296	-2.185	-2.054
H	-12.997	-2.756	-1.971
H	-10.985	-2.824	0.333
H	-13.793	-4.075	0.129
H	-13.370	-2.646	1.107
H	-12.681	-4.234	1.504
H	-5.947	-1.889	2.850
H	-5.646	-0.589	4.034
H	-5.560	-2.288	4.537
H	-3.783	0.362	2.469
H	-4.192	-0.972	1.342
H	-3.224	-0.240	4.964
H	-3.209	-1.954	5.446
H	-1.916	-1.322	4.417
H	1.091	-0.001	3.215
H	3.317	0.036	2.059
H	3.358	0.275	-0.446
H	-0.485	-3.449	-5.158
H	1.158	-2.777	-5.201
H	0.305	-2.952	-3.646
H	-1.388	-1.247	-4.383
H	0.050	0.786	-4.376
H	1.495	-0.236	-4.648
H	-1.039	0.061	-6.493
H	-1.268	-1.666	-6.846
H	0.358	-0.960	-6.906
H	-3.566	-2.646	3.065

Just_diethyl2,3diisopropylsuccinate

C	0.000	0.000	0.000
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C	0.000	0.000	1.536
C	1.442	0.000	2.064
C	-0.907	-1.141	2.104
C	-0.181	-2.482	2.160
O	-0.464	-3.200	3.276
C	0.131	-4.527	3.352
C	-0.087	-5.055	4.755
C	-1.747	-0.702	3.348
C	-1.006	-0.042	4.542
C	-0.145	-0.967	5.411
C	-2.776	-1.759	3.758
O	-3.457	-2.203	2.657
C	-4.520	-3.168	2.892
C	-3.999	-4.595	2.865
O	-3.035	-2.122	4.889
C	-1.985	0.759	5.417
O	0.539	-2.899	1.269
H	-2.380	0.105	2.932
H	-1.665	-1.333	1.325
H	-0.477	0.940	1.864
H	0.592	0.843	-0.386
H	0.435	-0.932	-0.385
H	-1.021	0.095	-0.401
H	1.963	0.908	1.726
H	1.491	-0.022	3.161
H	1.997	-0.866	1.679
H	-0.345	-5.163	2.590
H	1.198	-4.448	3.097
H	0.327	-6.071	4.833
H	0.413	-4.421	5.499
H	-1.156	-5.098	5.005
H	-0.331	0.697	4.079
H	-1.431	1.344	6.166
H	-2.578	1.466	4.815
H	-2.678	0.094	5.950
H	0.343	-0.375	6.201
H	-0.760	-1.739	5.890
H	0.642	-1.468	4.834
H	-5.233	-2.987	2.076
H	-4.998	-2.939	3.854
H	-4.841	-5.297	2.954
H	-3.476	-4.806	1.921
H	-3.312	-4.776	3.702

DIBP_diethyl2,3diisopropylsuccinate_Zip

C	0.000	0.000	0.000
C	0.000	0.000	1.414
C	1.221	0.000	2.101
C	2.431	-0.009	1.405
C	2.432	-0.006	0.010
C	1.223	-0.002	-0.682
C	-1.233	-0.105	2.261
O	-2.015	-1.057	2.224
Mg	-3.363	-2.596	2.381
Cl	-2.866	-4.801	1.651
Mg	-2.360	-5.760	3.865
Cl	-1.853	-6.720	6.077
C	-1.233	0.140	-0.827
O	-2.112	0.936	-0.233
C	-3.372	1.296	-0.893

C	-3.578	2.796	-0.709
C	-5.039	3.139	-1.018
O	-1.385	-0.335	-1.962
Mg	-1.269	-2.099	-3.135
Cl	-3.549	-2.946	-3.207
Mg	-4.055	-1.986	-5.421
Cl	-4.561	-1.027	-7.633
Mg	-5.201	1.069	-6.774
Cl	-5.542	2.250	-8.825
Cl	-1.605	-1.326	-5.449
Cl	0.064	-3.014	-1.263
Mg	-0.136	-5.339	-1.928
Cl	-0.643	-4.379	-4.141
O	-1.345	0.895	3.124
C	-2.455	0.825	4.092
C	-2.409	2.067	4.969
C	-3.473	1.928	6.066
C	-2.603	3.349	4.152
C	-2.610	3.613	-1.571
Cl	-2.642	-3.338	4.602
Cl	-3.925	-2.002	0.055
Mg	-6.279	-2.407	0.372
Cl	-6.785	-1.448	-1.840
Mg	-7.427	0.651	-0.991
Cl	-6.715	0.048	1.216
Cl	-5.772	-3.368	2.585
Cl	-7.762	1.750	-3.083
Cl	-9.691	-0.015	-0.906
Mg	-10.198	0.944	-3.119
Cl	-10.704	1.904	-5.333
Mg	-11.264	4.101	-4.416
O	-9.559	5.276	-4.694
C	-8.872	6.000	-5.430
C	-9.326	7.356	-5.945
C	-8.816	8.502	-4.979
C	-7.525	8.220	-4.193
Cl	-10.907	3.179	-2.174
Cl	-13.610	3.336	-4.399
Mg	-14.117	4.296	-6.611
Cl	-14.622	5.255	-8.824
Mg	-16.894	4.570	-8.670
Cl	-18.633	4.669	-10.049
Cl	-12.183	5.645	-6.269
Cl	-16.492	3.602	-6.542
O	-7.626	5.688	-5.755
C	-7.079	4.448	-5.168
C	-5.621	4.368	-5.555
C	-9.264	7.516	-7.521
C	-8.111	6.960	-8.367
O	-6.854	7.375	-8.353
C	-6.328	8.411	-7.475
C	-5.436	9.319	-8.296
C	-9.674	8.941	-8.040
C	-11.106	9.280	-7.600
C	-9.581	9.044	-9.570
C	-9.925	8.845	-3.969
Cl	0.369	-6.299	0.284
Cl	-7.467	0.405	-6.700
Mg	-7.974	1.366	-8.914
Cl	-8.938	3.352	-7.916
Mg	-9.095	4.480	-10.113
O	-8.369	6.110	-9.235

Cl	-4.522	0.479	-4.573
Cl	-8.480	2.325	-11.126
Cl	-11.386	3.758	-10.192
Mg	-11.892	4.716	-12.405
Cl	-12.399	5.677	-14.618
Cl	-12.501	6.951	-11.493
Mg	-11.119	7.461	-13.413
Cl	-10.126	9.402	-13.926
Cl	-9.510	5.493	-12.545
H	-5.216	4.221	-0.942
H	1.216	0.019	-1.772
H	3.374	-0.009	-0.540
H	3.371	-0.019	1.958
H	1.219	-0.012	3.191
H	-2.336	-0.099	4.675
H	-1.415	2.097	5.449
H	-3.397	0.773	3.523
H	-1.837	3.452	3.370
H	-3.593	3.354	3.667
H	-2.545	4.234	4.801
H	-3.318	1.025	6.675
H	-3.443	2.797	6.739
H	-4.485	1.877	5.634
H	-4.142	0.702	-0.381
H	-1.563	3.367	-1.343
H	-3.328	1.000	-1.950
H	-2.779	3.417	-2.642
H	-2.741	4.691	-1.397
H	-3.388	3.027	0.353
H	-5.710	2.659	-0.283
H	-5.324	2.824	-2.034
H	-5.186	3.477	-5.074
H	-5.052	5.235	-5.189
H	-5.498	4.298	-6.645
H	-7.668	3.610	-5.562
H	-7.229	4.497	-4.082
H	-4.636	8.744	-8.783
H	-4.970	10.065	-7.635
H	-6.006	9.849	-9.069
H	-5.756	7.882	-6.700
H	-7.150	8.958	-7.002
H	-8.650	9.394	-5.605
H	-8.990	9.692	-7.609
H	-11.388	10.269	-7.988
H	-11.818	8.545	-8.003
H	-11.228	9.310	-6.509
H	-9.894	10.046	-9.894
H	-8.565	8.881	-9.959
H	-10.254	8.321	-10.054
H	-7.236	9.122	-3.635
H	-7.685	7.421	-3.452
H	-6.679	7.926	-4.823
H	-9.609	9.673	-3.317
H	-10.860	9.145	-4.462
H	-10.147	7.980	-3.325
H	-10.084	6.858	-7.849
H	-10.411	7.328	-5.787

Just_ethyl4_tert_butoxybenzoate

C	0.000	0.000	0.000
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C	0.000	0.000	1.393
C	1.192	0.000	2.130
C	2.407	-0.044	1.422
C	2.421	-0.073	0.035
C	1.219	-0.038	-0.702
C	1.101	-0.091	3.618
O	0.235	-0.732	4.182
O	1.401	-0.056	-2.051
C	0.329	-0.050	-3.061
C	-0.489	1.243	-2.990
O	2.049	0.536	4.388
C	2.784	1.700	3.924
C	2.830	2.707	5.058
C	-0.531	-1.313	-2.957
C	1.128	-0.077	-4.367
H	3.355	-0.092	1.961
H	3.361	-0.129	-0.516
H	-0.953	0.016	-0.520
H	-0.948	-0.004	1.934
H	-1.215	-1.360	-3.817
H	0.107	-2.208	-2.979
H	-1.138	-1.349	-2.045
H	0.447	-0.082	-5.229
H	1.778	0.805	-4.438
H	1.758	-0.976	-4.412
H	3.802	1.382	3.646
H	2.300	2.122	3.032
H	3.419	3.585	4.753
H	1.818	3.043	5.326
H	3.296	2.269	5.951
H	-1.156	1.299	-3.862
H	-1.111	1.315	-2.090
H	0.179	2.115	-3.016

DIBP_diethyl2,3diisopropylsuccinate_Zip

C	0.000	0.000	0.000
C	0.000	0.000	1.402
C	1.214	0.000	2.102
C	2.419	0.139	1.408
C	2.397	0.209	0.013
C	1.199	0.063	-0.695
C	-1.285	0.235	2.101
O	-1.499	-0.520	3.163
C	-2.726	-0.254	3.938
C	-2.707	-1.174	5.136
O	3.566	0.542	-0.693
C	4.466	-0.586	-1.202
C	5.464	-0.898	-0.094
O	-2.097	1.097	1.714
Mg	-2.035	2.995	0.863
Cl	-1.581	4.828	-0.707
Mg	-3.901	5.005	-1.522
Cl	-6.220	5.183	-2.337
Cl	-2.402	4.728	2.561
Mg	-0.083	4.550	3.378
Cl	0.401	3.249	1.399
Cl	2.235	4.373	4.192
Mg	1.751	2.682	5.751
Cl	-0.468	2.433	4.923
Cl	1.415	4.274	7.462

Mg	3.734	4.096	8.277
Cl	6.054	3.918	9.093
Mg	5.589	2.077	10.608
Cl	3.228	2.270	9.958
O	6.198	0.276	9.599
C	7.142	-0.499	9.397
O	7.565	-0.860	8.189
C	6.947	-0.306	6.976
C	6.519	-1.464	6.078
C	6.231	-0.915	4.676
C	7.910	-1.200	10.467
C	9.289	-1.498	10.371
C	9.938	-2.115	11.449
C	9.223	-2.488	12.589
C	7.852	-2.237	12.667
C	7.209	-1.581	11.621
C	10.172	-1.113	9.214
O	10.467	-2.003	8.280
C	9.846	-3.338	8.270
C	10.325	-4.066	7.022
C	11.843	-4.270	7.025
C	5.312	-2.214	6.651
O	10.723	-0.011	9.155
Mg	11.305	1.862	8.728
Cl	11.124	3.552	10.385
Mg	13.443	3.375	11.200
Cl	15.763	3.197	12.016
Cl	8.970	2.306	8.071
Mg	9.626	3.829	6.301
Cl	7.306	4.007	5.485
Mg	7.586	2.414	3.768
Cl	9.750	1.829	4.576
Cl	11.945	3.652	7.116
Cl	5.377	2.210	2.898
Cl	8.127	4.106	2.216
Mg	5.808	4.284	1.400
Cl	3.488	4.462	0.585
Cl	3.929	2.136	6.499
Cl	-4.177	2.848	-0.280
C	3.621	-1.802	-1.563
C	5.136	-0.007	-2.444
C	9.573	-5.401	6.916
Cl	12.930	1.537	12.787
Mg	14.998	0.839	11.760
Cl	16.024	-1.147	11.756
Cl	6.262	2.811	-0.533
Mg	3.841	2.676	-1.113
Cl	1.825	2.505	-2.552
Mg	1.990	4.739	-3.498
Cl	-0.329	4.916	-4.313
Cl	4.309	4.561	-2.683
Cl	5.233	3.819	12.361
Mg	7.552	3.641	13.177
Cl	9.871	3.464	13.992
Mg	9.453	5.017	15.732
Cl	10.744	5.900	17.309
Cl	7.213	5.291	15.001
Cl	7.668	1.611	11.956
Cl	13.847	1.625	9.430
H	11.015	-2.289	11.405
H	9.746	-2.965	13.419
H	7.288	-2.532	13.553

H	6.145	-1.353	11.686
H	10.154	-3.871	9.183
H	8.756	-3.206	8.273
H	9.801	-6.054	7.773
H	10.051	-3.441	6.153
H	8.482	-5.259	6.877
H	9.875	-5.936	6.005
H	12.382	-3.316	7.098
H	12.151	-4.903	7.873
H	12.167	-4.770	6.102
H	7.738	0.303	6.519
H	6.104	0.336	7.258
H	5.519	-2.613	7.655
H	7.373	-2.161	6.004
H	7.149	-0.504	4.221
H	5.038	-3.064	6.008
H	4.439	-1.547	6.726
H	5.872	-1.711	4.009
H	5.464	-0.126	4.703
H	-1.845	-0.963	5.783
H	-3.621	-1.012	5.726
H	-2.678	-2.229	4.833
H	-2.717	0.805	4.223
H	-3.583	-0.437	3.275
H	-0.944	-0.016	-0.547
H	1.204	0.092	-1.782
H	3.359	0.277	1.945
H	1.206	-0.002	3.192
H	4.297	-2.590	-1.925
H	3.077	-2.202	-0.697
H	2.903	-1.580	-2.363
H	6.187	-1.648	-0.450
H	6.014	0.005	0.197
H	4.956	-1.313	0.787
H	5.770	-0.776	-2.908
H	4.385	0.301	-3.185
H	5.791	0.840	-2.197

**Just_1,2bis(diphenylphosphino)
ethane**

C	0.000	0.000	0.000
C	0.000	0.000	1.404
C	1.239	0.000	2.071
C	2.437	0.032	1.357
C	2.424	0.046	-0.040
C	1.201	0.024	-0.714
P	-1.553	-0.175	2.415
C	-2.868	0.425	1.237
C	-3.962	-0.420	1.000
C	-5.003	-0.026	0.151
C	-4.961	1.224	-0.468
C	-3.875	2.077	-0.241
C	-2.836	1.680	0.603
C	-1.384	1.335	3.544
C	-2.564	1.447	4.505
P	-2.568	2.859	5.764
C	-2.457	4.375	4.700
C	-3.053	4.433	3.428
C	-3.097	5.632	2.711
C	-2.550	6.798	3.250
C	-1.966	6.758	4.521

C	-1.927	5.562	5.240
C	-0.849	2.712	6.469
C	0.317	3.199	5.856
C	1.566	3.004	6.452
C	1.669	2.316	7.665
C	0.515	1.829	8.285
C	-0.733	2.033	7.694
H	-0.451	1.192	4.109
H	-1.263	2.247	2.942
H	-3.519	1.530	3.962
H	-2.651	0.534	5.116
H	0.249	3.742	4.912
H	2.464	3.390	5.964
H	2.646	2.165	8.128
H	0.586	1.299	9.237
H	-1.637	1.670	8.191
H	-3.493	3.538	2.982
H	-3.561	5.650	1.722
H	-2.583	7.734	2.689
H	-1.542	7.664	4.958
H	-1.474	5.551	6.234
H	-3.995	-1.397	1.489
H	-5.847	-0.696	-0.021
H	-5.772	1.535	-1.129
H	-3.835	3.053	-0.729
H	-1.988	2.350	0.761
H	1.274	-0.032	3.163
H	3.387	0.041	1.896
H	3.361	0.068	-0.600
H	1.177	0.027	-1.806
H	-0.946	-0.013	-0.544

**DIBP_1,2bis(diphenylphosphi
no)ethane_Zip**

C	0.000	0.000	0.000
C	0.000	0.000	1.402
C	1.221	0.000	2.094
C	2.425	0.001	1.387
C	2.420	0.005	-0.010
C	1.207	0.005	-0.704
P	-1.620	0.056	2.288
C	-1.320	-0.898	3.840
C	-1.150	-2.288	3.704
C	-0.956	-3.087	4.831
C	-0.945	-2.510	6.106
C	-1.128	-1.133	6.247
C	-1.316	-0.326	5.121
Mg	-3.641	-1.113	1.279
Cl	-2.452	-2.865	0.016
Cl	-4.061	-0.106	-0.840
Mg	-3.126	-1.916	-2.227
Cl	-2.190	-3.726	-3.614
C	-1.750	1.849	2.836
C	-1.684	2.805	1.644
P	-1.951	4.629	2.078
C	-0.641	5.533	1.129
C	-0.109	5.033	-0.069
C	0.806	5.792	-0.802
C	1.191	7.058	-0.356
C	0.648	7.570	0.825
C	-0.267	6.818	1.562

Mg	-3.964	5.779	1.143
Cl	-4.211	7.614	2.741
Mg	-6.642	7.160	2.916
Cl	-6.415	5.521	1.088
Cl	-6.869	8.799	4.743
Mg	-6.738	7.127	6.411
Cl	-6.216	5.443	4.813
Cl	-9.075	6.978	6.529
Mg	-9.301	8.617	8.357
Cl	-9.528	10.255	10.183
Cl	-10.364	6.908	9.618
Mg	-10.862	8.367	11.474
O	-9.859	7.184	12.772
C	-8.825	6.729	13.272
O	-7.721	7.451	13.201
C	-6.444	6.960	13.743
C	-5.354	7.941	13.333
C	-3.998	7.374	13.774
C	-8.853	5.440	14.049
C	-8.801	4.154	13.464
C	-8.930	3.025	14.286
C	-9.110	3.156	15.660
C	-9.192	4.427	16.230
C	-9.070	5.563	15.427
C	-8.593	3.923	12.007
O	-9.055	2.963	11.376
Mg	-10.847	1.975	10.777
Cl	-9.979	0.064	9.529
O	-7.802	4.849	11.476
C	-7.388	4.760	10.065
C	-5.900	4.419	10.002
C	-5.404	4.656	8.569
C	-5.613	2.987	10.467
C	-5.598	9.339	13.909
Cl	-13.139	1.032	10.756
Mg	-14.075	2.841	12.144
Cl	-16.295	1.762	12.356
Mg	-17.067	3.499	13.771
Cl	-18.947	3.946	14.864
Cl	-11.379	2.983	8.604
Mg	-10.467	1.259	7.320
Cl	-9.531	-0.549	5.933
Mg	-7.354	0.363	5.894
Cl	-6.151	-1.357	4.781
Cl	-15.010	4.652	13.530
Cl	-11.817	3.420	12.618
Cl	-7.966	2.108	7.397
Cl	-7.794	1.487	3.883
Mg	-6.859	-0.322	2.497
Cl	-4.794	0.916	2.247
Cl	-5.923	-2.131	1.108
Cl	-6.731	8.408	8.460
Cl	-4.209	7.342	-0.697
Mg	-3.982	5.704	-2.524
Cl	-3.349	4.456	-0.858
Cl	-3.755	4.065	-4.351
C	-1.408	4.803	3.834
C	-2.378	5.020	4.823
C	-1.993	5.128	6.164
C	-0.648	5.019	6.522
C	0.320	4.801	5.537
C	-0.055	4.694	4.198

Cl	-11.916	10.234	12.788
Mg	-14.098	9.030	12.776
Cl	-15.034	10.839	14.164
Mg	-12.953	10.236	15.346
Cl	-11.642	11.130	16.919
Cl	-13.486	7.937	14.928
Cl	-13.163	7.219	11.390
H	-6.139	2.258	9.832
H	-6.560	9.753	13.580
H	-3.942	7.280	14.870
H	-5.592	9.316	15.011
H	-3.186	8.044	13.459
H	-6.535	6.901	14.839
H	-6.263	5.956	13.335
H	-9.171	6.555	15.874
H	-9.364	4.543	17.301
H	-8.883	2.036	13.828
H	-9.202	2.266	16.285
H	-8.006	4.013	9.552
H	-7.598	5.758	9.662
H	-5.371	5.125	10.666
H	-5.996	4.087	7.836
H	-5.450	5.732	8.328
H	-4.354	4.347	8.468
H	-5.368	8.004	12.231
H	-3.803	6.382	13.337
H	-4.808	10.031	13.586
H	-4.535	2.773	10.419
H	-5.930	2.823	11.508
H	-0.932	2.054	3.542
H	-2.708	1.932	3.368
H	-0.702	2.730	1.157
H	-2.450	2.565	0.892
H	1.232	-0.022	3.186
H	3.372	-0.009	1.930
H	3.362	-0.003	-0.561
H	1.198	-0.007	-1.795
H	-0.948	-0.027	-0.540
H	0.706	4.543	3.431
H	1.374	4.722	5.813
H	-0.351	5.114	7.569
H	-2.751	5.310	6.927
H	-3.432	5.122	4.553
H	-0.689	7.234	2.481
H	0.934	8.564	1.174
H	1.905	7.649	-0.931
H	1.215	5.388	-1.730
H	-0.418	4.061	-0.454
H	-1.461	0.746	5.254
H	-1.125	-0.680	7.240
H	-0.801	-3.137	6.987
H	-0.823	-4.163	4.712
H	-1.163	-2.748	2.712

Just_ethyl 4-cyanobenzoate

C	0.000	0.000	0.000
C	0.000	0.000	1.403
C	1.218	0.000	2.100
C	2.423	0.000	1.404
C	2.420	0.000	-0.004
C	1.198	0.000	-0.704

C	-1.325	0.000	2.098
O	-2.399	-0.001	1.521
C	3.656	0.002	-0.721
N	4.664	0.003	-1.309
O	-1.191	0.005	3.449
C	-2.438	0.007	4.204
C	-2.083	0.017	5.675
H	1.215	-0.000	3.189
H	3.373	0.000	1.940
H	1.202	0.000	-1.794
H	-0.957	-0.000	-0.522
H	-3.023	0.891	3.910
H	-3.018	-0.884	3.922
H	-3.005	0.018	6.274
H	-1.498	-0.870	5.950
H	-1.504	0.913	5.939

DIBP_ethyl4cyanobenzoate_Zi p

C	0.000	0.000	0.000
C	0.000	0.000	1.414
C	1.226	0.000	2.095
C	2.432	0.006	1.400
C	2.428	0.053	0.005
C	1.218	0.053	-0.690
C	-1.244	-0.004	2.237
O	-2.193	-0.740	1.667
C	-3.508	-0.904	2.302
C	-3.824	-2.395	2.376
C	-2.958	-3.112	3.417
C	-1.235	0.043	-0.859
O	-1.700	-1.065	-1.411
C	-1.117	-2.379	-1.098
C	-1.952	-3.441	-1.800
C	-1.452	-4.825	-1.363
O	-1.780	1.109	-1.157
Mg	-2.992	2.695	-1.352
Cl	-2.217	4.843	-0.699
Mg	-1.478	5.552	-2.941
Cl	-0.735	6.260	-5.182
Cl	-3.691	2.304	0.979
Mg	-5.970	3.000	0.534
Cl	-5.229	3.709	-1.705
Cl	-6.711	2.292	2.777
Mg	-7.584	0.217	2.047
Cl	-6.653	0.544	-0.133
Cl	-9.723	1.157	1.771
Mg	-10.464	0.449	4.012
Cl	-11.633	-1.498	3.064
Mg	-12.007	-2.398	5.303
Cl	-14.217	-1.393	5.247
Mg	-14.958	-2.102	7.488
Cl	-15.699	-2.810	9.730
N	-10.543	-4.009	5.232
C	-9.889	-4.530	6.043
C	-9.226	-4.989	7.210
C	-7.841	-4.815	7.379
C	-7.305	-4.872	8.661
C	-8.159	-5.056	9.757
C	-9.514	-5.369	9.568
C	-10.055	-5.353	8.292

C	-7.727	-4.633	11.116
O	-6.570	-5.118	11.525
C	-6.028	-4.641	12.819
C	-4.896	-3.668	12.568
O	-8.424	-3.839	11.763
Mg	-10.133	-2.647	11.441
Cl	-11.168	-3.859	13.283
Mg	-13.115	-2.325	13.425
Cl	-13.857	-3.034	15.666
Cl	-12.375	-1.617	11.184
Cl	-9.634	-1.887	9.132
Mg	-8.624	0.225	9.948
Cl	-7.880	0.933	7.707
Mg	-5.726	0.011	7.937
Cl	-4.905	0.347	5.743
Cl	-9.363	-0.482	12.190
Cl	-11.205	-0.259	6.253
Cl	-8.207	-0.795	4.117
C	-1.919	-3.280	-3.323
Cl	-6.260	-0.978	10.042
Cl	-4.869	2.068	8.713
Mg	-4.127	2.776	6.472
Cl	-3.386	3.485	4.229
Mg	-1.207	2.420	4.396
Cl	-1.809	1.768	6.691
O	-1.364	0.556	3.335
C	-5.319	-2.569	2.665
Cl	0.742	4.456	-2.749
Mg	0.005	3.877	-4.974
Cl	0.751	2.297	-6.372
Cl	-13.025	-3.647	7.244
Cl	-0.375	4.619	5.236
Mg	0.365	5.328	2.995
Cl	1.105	6.036	0.754
Mg	1.498	8.247	1.522
Cl	2.078	10.157	0.548
Cl	0.204	3.039	2.393
Cl	0.828	7.652	3.714
Cl	-2.369	3.364	-3.844
H	3.375	0.001	1.949
H	1.218	-0.004	3.185
H	3.366	0.099	-0.548
H	1.220	0.118	-1.780
H	-1.885	-2.990	3.208
H	-4.202	-0.363	1.645
H	-3.495	-0.429	3.293
H	-3.152	-2.713	4.424
H	-3.172	-4.191	3.429
H	-3.617	-2.827	1.380
H	-5.614	-2.060	3.595
H	-5.578	-3.633	2.767
H	-5.926	-2.174	1.833
H	-0.076	-2.391	-1.457
H	-1.130	-2.506	-0.006
H	-0.407	-4.986	-1.673
H	-1.508	-4.958	-0.272
H	-2.994	-3.320	-1.452
H	-2.058	-5.613	-1.830
H	-0.895	-3.409	-3.708
H	-2.554	-4.037	-3.804
H	-4.484	-3.347	13.536
H	-5.247	-2.775	12.033

H	-4.087	-4.137	11.992
H	-5.690	-5.561	13.310
H	-6.849	-4.192	13.390
H	-2.279	-2.291	-3.636
O	-10.159	-5.563	10.429
H	-11.126	-5.491	8.136
H	-6.249	-4.662	8.827
H	-7.216	-4.553	6.525

Just_dicyclopentylidimethoxysilane

C	0.000	0.000	0.000
C	0.000	0.000	1.548
C	1.510	0.000	1.944
C	2.292	0.388	0.655
C	1.224	0.857	-0.348
Si	-1.057	-1.344	2.367
C	-1.538	-1.011	4.167
C	-0.360	-0.884	5.161
C	-0.988	-0.163	6.363
C	-1.871	0.913	5.711
C	-2.385	0.281	4.385
O	-0.287	-2.851	2.434
C	0.179	-3.550	1.284
O	-2.421	-1.441	1.367
C	-3.526	-2.291	1.665
H	-0.547	-3.520	0.453
H	1.138	-3.139	0.922
H	0.343	-4.601	1.565
H	-3.210	-3.328	1.876
H	-4.103	-1.921	2.531
H	-4.192	-2.303	0.790
H	0.081	-1.859	5.409
H	0.446	-0.257	4.742
H	-1.609	-0.873	6.934
H	-0.244	0.255	7.056
H	-2.692	1.244	6.364
H	-1.261	1.804	5.490
H	-2.282	0.996	3.554
H	-3.455	0.034	4.442
H	-2.139	-1.881	4.487
H	-0.436	0.964	1.866
H	1.697	0.714	2.759
H	1.839	-0.982	2.314
H	3.059	1.153	0.845
H	2.815	-0.493	0.253
H	0.986	1.921	-0.183
H	1.546	0.750	-1.394
H	-0.943	0.379	-0.415
H	0.137	-1.019	-0.398

DIBP_dicyclopentylidimethoxysilane_Zip

C	0.000	0.000	0.000
C	0.000	0.000	1.566
C	1.494	0.000	1.976
C	2.161	-0.805	0.851
C	1.467	-0.292	-0.420
Si	-1.164	1.276	2.329
C	-2.977	0.986	1.912

C	-3.962	2.113	2.333
C	-5.349	1.421	2.493
C	-5.132	-0.065	2.142
C	-3.641	-0.310	2.422
O	-0.821	2.863	1.895
C	0.387	3.410	1.376
O	-1.023	1.223	4.080
C	0.078	1.978	4.669
Mg	-1.915	-0.048	5.459
Cl	-3.394	-1.901	6.174
Mg	-1.745	-3.694	5.802
Cl	-0.095	-5.488	5.430
Cl	-1.286	0.123	7.855
Mg	-2.936	1.916	8.227
Cl	-3.829	1.447	5.997
Cl	-4.585	3.709	8.600
Mg	-3.065	5.411	8.021
Cl	-4.527	7.298	8.059
Cl	-2.478	5.734	10.281
Mg	-4.128	7.529	10.653
Cl	-2.457	9.253	10.328
Mg	-4.123	11.095	10.380
Cl	-3.669	11.346	12.706
Mg	-5.319	13.138	13.079
Cl	-6.968	14.933	13.451
Mg	-5.313	16.588	13.025
Cl	-3.619	14.978	13.243
O	-2.868	12.007	9.052
C	-2.125	12.307	8.117
O	-2.595	12.196	6.881
C	-1.747	12.484	5.714
C	-2.547	12.155	4.462
C	-1.626	12.282	3.241
C	-0.759	12.900	8.350
C	-0.691	14.299	8.377
C	0.518	14.946	8.632
C	1.673	14.201	8.872
C	1.607	12.810	8.886
C	0.400	12.143	8.629
C	0.418	10.652	8.647
O	-0.366	10.154	7.699
C	-0.504	8.702	7.512
C	-0.352	8.401	6.024
C	-0.882	6.989	5.751
C	-3.789	13.043	4.330
O	1.117	9.965	9.403
Mg	1.647	9.573	11.427
Cl	0.147	7.793	12.142
Mg	1.797	5.998	11.770
Cl	3.446	4.205	11.398
Mg	2.872	3.895	9.139
Cl	1.338	2.180	9.717
Mg	2.988	0.388	9.345
Cl	4.637	-1.406	8.972
Mg	4.000	-1.686	6.679
Cl	2.477	0.130	6.814
Cl	3.393	7.865	11.147
Cl	2.255	9.817	13.823
Mg	0.606	11.610	14.196
Cl	-1.043	13.402	14.568
Mg	-1.220	12.850	16.856
Cl	-2.617	13.586	18.425

C	1.096	8.564	5.553
Cl	-5.777	9.321	11.025
Cl	-5.769	12.946	10.649
Cl	-5.450	18.760	12.571
Cl	0.625	11.867	11.825
Cl	4.571	2.298	8.635
Cl	1.364	5.727	9.166
Cl	0.448	11.182	16.648
Cl	5.452	-3.304	5.737
Cl	2.529	-3.431	7.291
Mg	4.179	-5.224	6.919
Cl	5.828	-7.017	6.547
Cl	-1.404	3.795	7.429
Cl	-0.487	-1.929	4.648
H	1.756	7.852	6.073
H	-4.449	12.947	5.203
H	-1.254	13.313	3.129
H	-3.503	14.103	4.230
H	-2.172	12.027	2.323
H	-1.467	13.549	5.737
H	-0.840	11.867	5.791
H	-1.596	14.887	8.213
H	0.552	16.037	8.652
H	2.498	12.218	9.097
H	2.622	14.701	9.070
H	0.245	8.183	8.125
H	-1.509	8.467	7.888
H	-0.990	9.116	5.475
H	-0.358	6.235	6.358
H	-1.965	6.938	5.962
H	-0.754	6.715	4.694
H	-2.871	11.103	4.547
H	-0.754	11.613	3.311
H	-4.368	12.769	3.438
H	1.181	8.379	4.472
H	1.474	9.578	5.747
H	-2.978	0.926	0.806
H	-3.662	2.565	3.288
H	-3.974	2.918	1.586
H	-5.691	1.517	3.533
H	-6.116	1.881	1.855
H	-5.787	-0.738	2.715
H	-5.328	-0.245	1.073
H	-3.512	-0.434	3.514
H	-3.247	-1.220	1.947
H	-0.410	-0.967	1.908
H	-0.343	0.954	-0.429
H	-0.687	-0.770	-0.377
H	1.954	0.635	-0.757
H	1.526	-1.005	-1.255
H	3.253	-0.684	0.819
H	1.950	-1.877	0.997
H	1.916	1.018	1.997
H	1.640	-0.444	2.971
H	0.154	4.403	0.965
H	1.150	3.530	2.163
H	0.813	2.793	0.569
H	0.028	3.020	4.330
H	-0.029	1.961	5.760
H	1.041	1.521	4.402

Just_3,3'-dimethyl-4,4'-bipyridine

C	0.000	0.000	0.000
C	0.000	0.000	1.405
C	1.263	0.000	2.022
C	2.410	0.000	1.230
N	2.405	0.000	-0.108
C	1.202	0.000	-0.717
C	-1.261	-0.000	2.195
C	-2.526	-0.000	1.581
C	-3.697	-0.000	2.349
N	-3.675	-0.000	3.697
C	-2.472	-0.000	4.287
C	-1.259	0.000	3.601
C	-5.057	-0.000	1.705
C	1.218	-0.000	-2.222
H	-2.619	-0.000	0.495
H	-0.331	0.000	4.172
H	-2.479	-0.000	5.382
H	1.371	-0.000	3.106
H	3.398	0.000	1.703
H	-0.936	0.000	-0.558
H	-4.994	-0.000	0.609
H	-5.629	-0.883	2.025
H	-5.629	0.883	2.025
H	0.204	0.000	-2.644
H	1.756	0.883	-2.596
H	1.756	-0.883	-2.596

DIBP_3,3'-dimethyl-4,4'-bipyridine_Zip

C	0.000	0.000	0.000
C	0.000	0.000	1.406
C	1.256	0.000	2.031
C	2.410	0.279	1.298
N	2.326	0.663	-0.007
C	1.163	0.394	-0.645
C	-1.182	0.397	2.199
C	-2.148	1.207	1.582
C	-2.857	2.102	2.368
N	-2.654	2.235	3.694
C	-1.918	1.290	4.332
C	-1.198	0.341	3.604
Mg	-2.372	4.305	3.907
Cl	-2.161	5.891	2.015
Mg	-4.585	6.341	1.984
Cl	-7.008	6.790	1.952
C	-1.823	1.391	5.824
C	3.770	0.193	1.916
Mg	2.633	2.705	-0.210
Cl	2.659	4.383	-1.969
Mg	0.221	4.606	-2.253
Cl	0.168	2.764	-0.621
Cl	-1.830	6.176	5.359
Mg	0.593	5.726	5.391
Cl	0.102	3.909	3.799
Cl	3.015	5.277	5.422
Mg	2.857	3.813	7.266
Cl	5.071	2.977	7.318
Cl	3.347	5.562	8.766

Mg	5.770	5.112	8.798
Cl	8.072	4.724	8.813
Mg	8.031	3.075	10.617
Cl	5.634	3.521	10.790
O	8.019	1.142	9.720
C	8.738	0.209	9.339
O	8.690	-0.320	8.122
C	7.783	0.225	7.100
C	6.868	-0.892	6.609
C	5.850	-1.306	7.677
C	9.721	-0.504	10.204
C	9.397	-0.657	11.560
C	10.261	-1.311	12.434
C	11.483	-1.796	11.965
C	11.822	-1.652	10.618
C	10.942	-1.029	9.723
C	11.435	-0.885	8.306
O	11.303	-1.896	7.456
C	10.564	-3.110	7.830
C	10.419	-3.978	6.588
C	11.778	-4.413	6.030
C	6.179	-0.426	5.322
O	12.051	0.112	7.932
Mg	12.757	1.815	7.051
Cl	13.328	3.663	8.436
Mg	15.751	3.214	8.467
Cl	15.192	1.253	7.058
Cl	10.383	2.557	7.111
Mg	10.574	3.827	5.061
Cl	8.150	4.277	5.029
Mg	7.660	2.541	3.527
Cl	9.873	1.684	3.628
Cl	12.997	3.378	5.092
Cl	8.525	4.948	12.172
Mg	10.948	4.498	12.204
Cl	13.370	4.049	12.235
Mg	13.654	5.401	14.158
Cl	15.403	5.871	15.447
Cl	11.361	6.009	14.126
Cl	10.425	2.456	11.119
Cl	0.484	3.983	7.344
Cl	-4.779	4.649	3.747
C	9.536	-5.184	6.937
Cl	18.174	2.764	8.499
Mg	17.914	1.387	10.429
Cl	19.211	-0.137	11.398
Cl	15.780	2.298	10.797
Cl	5.279	2.724	3.534
Cl	7.819	3.992	1.686
Mg	5.396	4.441	1.654
Cl	5.076	2.808	-0.157
Cl	2.972	4.891	1.622
Cl	-2.216	4.828	-2.537
H	5.198	-0.459	7.940
H	12.407	-3.549	5.777
H	10.006	-5.809	7.713
H	12.321	-5.031	6.763
H	9.385	-5.817	6.052
H	11.133	-3.634	8.614
H	9.585	-2.810	8.230
H	12.789	-2.012	10.262
H	12.182	-2.282	12.646

H	8.450	-0.253	11.920
H	9.989	-1.427	13.483
H	7.218	1.064	7.526
H	8.454	0.593	6.312
H	7.505	-1.761	6.363
H	5.608	0.500	5.487
H	6.917	-0.252	4.521
H	5.481	-1.192	4.954
H	9.899	-3.373	5.825
H	8.544	-4.877	7.303
H	11.647	-5.014	5.120
H	5.216	-2.128	7.314
H	6.341	-1.651	8.599
H	-3.537	2.829	1.913
H	-2.224	1.287	0.499
H	-0.551	-0.349	4.146
H	-0.917	-0.116	-0.576
H	1.148	0.608	-1.716
H	1.340	-0.068	3.116
H	-1.152	2.217	6.115
H	-2.810	1.590	6.261
H	-1.420	0.468	6.261
H	4.502	0.793	1.363
H	3.769	0.502	2.969
H	4.101	-0.857	1.867