

Electronic Supplementary Information - A Low Cost, High Accuracy Method for Halogen Bonding Complexes

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1 Iodine-Chloride Distances

Adduct	DFT	ONIOM (DFT:AM1)	ONIOM (DFT:PM6)	ONIOM (DFT:PM7)	AM1	PM6	PM7	GFN2-xTB
1-Cl	2.940	2.855	2.765	2.688	2.416	2.489	3.551	2.917
2-Cl	2.867	2.796	2.730	2.595	2.390	2.472	3.445	2.862
3-Cl	2.859	2.760	2.713	2.553	2.374	2.464	3.401	2.864
4-Cl	2.944	2.855	2.769	2.698	2.415	2.491	3.562	2.921
5-Cl	2.957	2.864	2.771	2.681	2.414	2.491	3.581	2.941
6-Cl	2.943	2.851	2.763	2.690	2.414	2.488	3.556	2.912
7-Cl	2.913	2.838	2.747	2.641	2.407	2.480	3.507	2.883
8-Cl	2.884	2.790	2.729	2.595	2.388	2.472	3.445	2.848
9-Cl	2.900	2.815	2.738	2.620	2.399	2.476	3.484	2.863
10-Cl	2.652	2.646	2.640	-	2.324	2.429	2.929	2.736
11-Cl	2.746	2.697	2.685	-	2.349	2.453	3.282	2.723
12-Cl	2.737	2.701	2.684	-	2.351	2.453	3.307	2.713
13-Cl	2.663	2.649	2.613	-	2.333	2.425	2.572	2.583
14-Cl	2.800	2.605	2.651	-	2.323	2.440	2.949	2.733
15-Cl	3.016	2.859	2.802	2.694	2.430	2.512	3.652	2.925
16-Cl	2.488	-	2.569	-	2.299	2.414	2.351	2.514
17-Cl	2.570	-	2.669	-	2.322	2.441	2.717	2.587
18-Cl	2.984	2.923	2.801	2.772	2.452	2.505	3.596	2.956
19-Cl	2.865	2.816	2.734	2.608	2.401	2.475	3.428	2.867
20-Cl	2.988	2.921	2.795	2.771	2.444	2.502	3.639	2.976
21-Cl	2.829	2.884	2.781	2.769	2.426	2.491	3.517	2.918
22-Cl	2.726	2.773	2.717	2.519	2.373	2.460	3.344	2.813
23-Cl	2.710	2.781	2.715	2.508	2.383	2.463	3.329	2.861
24-Cl	2.951	2.897	2.832	2.746	2.509	2.536	3.388	2.843
25-Cl	3.118	3.048	2.973	2.973	2.642	2.622	3.447	2.970
26-Cl	2.649	2.611	2.571	2.511	2.316	2.401	2.848	2.606
27-Cl	2.622	2.587	2.554	2.481	2.304	2.388	2.778	2.566
28-Cl	2.613	2.592	2.556	2.483	2.306	2.388	2.782	2.578
29-Cl	2.672	2.626	2.584	2.536	2.324	2.410	2.921	2.633
30-Cl	2.634	2.589	2.557	2.476	2.301	2.391	2.810	2.567
31-Cl	2.624	2.594	2.559	2.478	2.304	2.392	2.815	2.578
32-Cl	2.699	2.638	2.592	2.536	2.322	2.416	2.994	2.633
33-Cl	2.591	2.532	2.590	-	2.280	2.403	2.435	2.618
34-Cl	2.623	2.582	2.615	-	2.296	2.415	2.604	2.681
35-Cl	2.638	2.585	2.619	-	2.296	2.415	2.683	2.694
36-Cl	2.572	2.499	2.585	-	2.273	2.401	2.395	2.508
37-Cl	2.518	-	2.564	-	2.261	2.390	2.335	-
38-Cl	2.501	-	2.564	-	2.263	2.390	2.338	-
39-Cl	2.574	2.506	2.590	-	2.274	2.403	2.909	2.520
40-Cl	2.573	-	2.586	-	2.272	2.401	2.39	-

Table 1: Iodine-chloride distances in chloride adducts ($\text{\AA}$), where DFT is the method M052X-D3/[Def2TZVP + Def2TZVPD.ECP(I)]. Cases where the carbon-iodine (or carbon-nitrogen) bond was broken are omitted.

2 Iodine-Formaldehyde Distances

Adduct	DFT	ONIOM (DFT:AM1)	ONIOM (DFT:PM6)	ONIOM (DFT:PM7)	GFN2-xTB
1-OCH2	3.166	3.077	2.939	3.067	3.102
2-OCH2	3.084	3.048	2.889	3.034	3.040
3-OCH2	3.072	3.026	2.861	3.022	2.999
4-OCH2	3.178	3.079	2.948	3.073	3.115
5-OCH2	3.221	3.094	2.966	3.093	3.167
6-OCH2	3.180	3.075	2.941	3.068	3.109
7-OCH2	3.166	3.075	2.931	3.064	3.098
8-OCH2	3.101	3.046	2.887	3.036	3.018
9-OCH2	3.121	3.058	2.904	3.047	3.044
10-OCH2	2.880	2.943	2.692	2.942	2.844
11-OCH2	2.964	2.976	2.764	2.986	2.861
12-OCH2	2.976	2.990	2.769	3.004	2.876
13-OCH2	2.914	2.919	2.679	2.911	2.793
14-OCH2	2.986	2.842	2.705	2.916	2.859
15-OCH2	3.333	3.080	3.062	3.057	3.141
16-OCH2	2.735	2.864	2.627	2.754	2.779
17-OCH2	2.749	2.912	2.647	2.874	2.740
18-OCH2	3.173	3.092	2.951	3.064	3.106
19-OCH2	3.044	3.043	2.857	3.024	3.015
20-OCH2	3.220	3.117	2.977	3.108	3.184
21-OCH2	2.958	3.065	2.867	3.072	3.008
22-OCH2	2.886	3.014	2.776	3.030	2.920
23-OCH2	2.853	2.988	2.743	2.990	2.935
24-OCH2	3.131	3.131	2.919	3.128	2.949
25-OCH2	3.184	3.154	2.806	3.141	2.965
26-OCH2	2.916	2.794	2.702	2.721	2.729
27-OCH2	2.881	2.770	2.665	2.702	2.674
28-OCH2	2.867	2.776	2.668	2.706	2.694
29-OCH2	2.955	2.824	2.754	2.762	2.773
30-OCH2	2.878	2.770	2.683	2.687	2.669
31-OCH2	2.867	2.776	2.687	2.688	2.688
32-OCH2	2.961	2.780	2.708	2.692	2.770
33-OCH2	2.830	2.898	2.585	2.929	2.710
34-OCH2	2.856	2.908	2.629	2.990	2.753
35-OCH2	2.871	2.927	2.639	2.999	2.759
36-OCH2	2.787	2.788	2.574	2.962	2.697
37-OCH2	2.734	2.660	2.537	2.916	2.618
38-OCH2	2.717	2.681	2.538	2.922	2.647
39-OCH2	2.809	2.833	2.591	2.978	2.721
40-OCH2	2.809	2.790	2.584	2.972	2.707

Table 2: Iodine-oxygen distances in formaldehyde adducts (Å), where DFT is the method M052X-D3/[Def2TZVP + Def2TZVPD.ECP(I)].

3 Link Atom

Adduct	DFT	ONIOM(DFT:AM1)				
		H	F	Cl	Br	I
1-Cl	2.940	2.855	2.571	2.759	2.739	2.732
2-Cl	2.867	2.796	2.539	2.701	2.683	2.672
3-Cl	2.859	2.760	2.518	2.665	2.648	2.634
4-Cl	2.944	2.855	2.571	2.759	2.740	2.733
5-Cl	2.957	2.864	2.574	2.766	2.746	2.739
6-Cl	2.943	2.851	2.568	2.755	2.736	2.729
7-Cl	2.913	2.838	2.555	2.741	2.723	2.714
8-Cl	2.884	2.790	2.536	2.695	2.678	2.667
9-Cl	2.900	2.815	2.549	2.719	2.701	2.692
10-Cl	2.652	2.646	2.442	2.553	2.536	2.510
11-Cl	2.746	2.697	2.475	2.603	2.585	2.563
12-Cl	2.737	2.701	2.476	2.605	2.587	2.564
13-Cl	2.663	2.649	2.452	2.569	2.549	2.524
14-Cl	2.800	2.605	2.445	2.551	2.524	2.505
15-Cl	3.016	2.859	2.570	2.795	2.764	2.746
16-Cl	2.488	-	2.371	2.443	2.389	2.382
17-Cl	2.570	-	2.380	2.439	2.404	2.395
18-Cl	2.984	2.923	2.620	2.848	2.825	2.827
19-Cl	2.865	2.816	2.554	2.721	2.704	2.695
20-Cl	2.988	2.921	2.609	2.832	2.809	2.810
21-Cl	2.829	2.884	2.607	2.757	2.743	2.752
22-Cl	2.726	2.773	2.523	2.643	2.629	2.622
23-Cl	2.710	2.781	2.538	2.665	2.651	2.647
24-Cl	2.951	2.897	2.642	2.788	2.783	2.796
25-Cl	3.118	3.048	2.814	2.974	2.980	3.003
26-Cl	2.649	2.611	2.484	2.514	2.509	2.522
27-Cl	2.622	2.587	2.463	2.493	2.488	2.501
28-Cl	2.613	2.592	2.466	2.497	2.491	2.505
29-Cl	2.672	2.626	2.499	2.528	2.522	2.536
30-Cl	2.634	2.589	2.465	2.536	2.506	-
31-Cl	2.624	2.594	2.467	2.542	2.510	-
32-Cl	2.699	2.638	2.506	2.580	2.553	-
33-Cl	2.591	2.532	2.373	2.460	2.430	2.396
34-Cl	2.623	2.582	2.406	2.499	2.482	2.454
35-Cl	2.638	2.585	2.408	2.500	2.484	2.456
36-Cl	2.572	2.499	2.354	2.435	2.368	2.362
37-Cl	2.518	-	2.342	2.377	2.354	2.345
38-Cl	2.501	-	2.343	2.379	2.356	2.346
39-Cl	2.574	2.506	2.356	2.439	2.369	2.363
40-Cl	2.573	-	2.352	2.430	2.365	2.358

Table 3: Iodine-chloride distances in chloride adducts ($\text{\AA}$), where DFT is the method M052X-D3/[Def2TZVP + Def2TZVPD.ECP(I)]. The elements given for the ONIOM methods are the link atoms used in each case. The omitted values either did not converge or converged to a structure with a broken iodine-carbon (or iodine-nitrogen) bond.

4 Iodine-Lewis Base Distances

Adduct	DFT	ONIOM (DFT:AM1)	ONIOM (DFT:PM6)	ONIOM (DFT:PM7)	AM1	PM6	PM7	GFN2-xTB
11-NH3	2.962	2.953	2.736	2.927	2.829	2.023	3.325	2.789
11-DMF	2.879	2.902	2.730	2.903	3.878	2.014	2.992	2.711
11-I	3.183	3.123	3.138	-	2.626	2.718	3.983	3.063
11-Br	2.942	2.897	2.881	-	2.456	2.644	3.657	2.852
11-F	2.145	2.116	2.156	-	1.922	1.912	2.004	2.295
11-OMe	2.177	2.154	2.219	-	2.038	1.978	2.218	2.266

Table 4: Iodine-Lewis Base distances in pentafluoroiodobenzene adducts (Å), where DFT is the method M052X-D3/[Def2TZVP + Def2TZVPD.ECP(I)]. Cases where the carbon-iodine (or carbon-nitrogen) bond was broken are omitted.

5 Relaxed Scans

I-Cl Distance	DFT	ONIOM(DFT:AM1)	I-Cl Distance	GFN2-xTB
3.20	-1486.00738698	-758.8492838816	3.10	-45.096984518149
3.15	-1486.0085638	-758.8509318322	3.05	-45.09865245358
3.10	-1486.00968466	-758.8525422305	3.01	-45.100147379864
3.05	-1486.01074849	-758.8541132680	2.96	-45.101525110849
3.00	-1486.01174926	-758.8556356511	2.92	-45.102639581027
2.95	-1486.01266004	-758.8570711404	2.88	-45.103657868819
2.90	-1486.01344072	-758.8583632847	2.84	-45.104427728568
2.85	-1486.01405722	-758.8594679792	2.80	-45.104988565987
2.80	-1486.01447711	-758.8603507070	2.76	-45.105328771833
2.75	-1486.01465238	-758.8609558701	2.73	-45.105451345566
2.70	-1486.01451582	-758.8611967679	2.69	-45.105353328496
2.65	-1486.01399579	-758.8609807296	2.66	-45.105034604939
2.60	-1486.01301342	-758.8602135147	2.62	-45.104497306234
2.55	-1486.01147026	-758.8587761678	2.59	-45.103750389290
2.50	-1486.00925334	-758.8565246046	2.56	-45.102754029120
2.45	-1486.00623951	-758.8533053615	2.53	-45.101563742044
2.40	-1486.00227881	-758.8489405798	2.50	-45.100160726844
2.35	-1485.99719256	-758.8432230437	2.47	-45.098417999653
2.30	-1485.99077694	-758.8359277182	2.44	-45.096475084861
2.25	-1485.98277120	-758.8267809839	2.41	-45.094292420671
2.20	-1485.97286479	-758.8154825312		

Table 5: SCF energies with varying iodine-chloride distances (Å) for adduct **11-Cl**, where DFT is the method M052X-D3/[Def2TZVP + Def2TZVPD.ECP(I)].

I-O Distance	DFT	ONIOM(DFT:AM1)	I-O Distance	GFN2-xTB
3.50	-1140.23576944	-413.0721096353	3.17	-47.456381946423
3.45	-1140.23598989	-413.0723272311	3.12	-47.456829566648
3.40	-1140.23622336	-413.0725548939	3.07	-47.457262442058
3.35	-1140.23646139	-413.0727798604	3.02	-47.457629363802
3.30	-1140.23668949	-413.0729928004	2.97	-47.457946566407
3.25	-1140.23690212	-413.0731903100	2.93	-47.458165996581
3.20	-1140.23709961	-413.0733694433	2.88	-47.458281449612
3.15	-1140.23727611	-413.0735305389	2.84	-47.458277183728
3.10	-1140.23743124	-413.0736718938	2.79	-47.458140149508
3.05	-1140.23755648	-413.0737788133	2.75	-47.457859625919
3.00	-1140.23763327	-413.0738363766	2.71	-47.457421811009
2.95	-1140.23764901	-413.0738315798	2.67	-47.456824383201
2.90	-1140.23757579	-413.0737401716	2.63	-47.456060927972
2.85	-1140.23739023	-413.0735440861	2.59	-47.455112182026
2.80	-1140.23708142	-413.0732329209	2.56	-47.454017778798
2.75	-1140.23663426	-413.0727890375	2.52	-47.452641481458
2.70	-1140.23601196	-413.0721729464	2.48	-47.451184374572
2.65	-1140.23516004	-413.0713249527	2.43	-47.449446354003
2.60	-1140.23403562	-413.0702020699	2.39	-47.447779291606
2.55	-1140.23260813	-413.0687788320	2.36	-47.445914173602
2.50	-1140.23083324	-413.0670065931		

Table 6: SCF energies with varying iodine-oxygen distances (Å) for adduct **11-OCH2**, where DFT is the method M052X-D3/[Def2TZVP + Def2TZVPD.ECP(I)].

6 Computation Time

Adduct	DFT	ONIOM (DFT:AM1)	ONIOM (DFT:PM6)	ONIOM (DFT:PM7)	AM1	PM6	PM7	GFN2-xTB
1-Cl	14037.9	426.8	993.5	917.7	13.9	84.1	74.2	3.8
2-Cl	23498.7	431.6	903.9	1043.3	14.4	94.7	88.6	5.1
3-Cl	30101.0	435.9	1127.4	1175.3	16.6	112.6	85.7	5.1
4-Cl	23125.8	423.1	975.9	947.4	15.0	98.5	73.7	4.7
5-Cl	46059.3	419.9	1374.6	4863.1	17.7	123.9	94.2	7.4
6-Cl	29806.5	421.6	982.6	938.8	58.3	134.4	73.4	6.0
7-Cl	29872.3	405.7	1266.7	1425.3	63.3	195.1	80.9	6.8
8-Cl	36118.0	423.4	992.5	1048.3	60.2	236.9	67.5	5.6
9-Cl	21083.2	426.5	891.9	1059.0	63.0	94.0	87.0	5.0
10-Cl	102692.1	443.5	1072.7	-	18.6	71.6	115.3	11.4
11-Cl	34838.2	433.9	992.3	-	15.2	67.6	104.4	5.3
12-Cl	58326.0	426.2	840.7	-	16.6	59.7	94.8	6.9
13-Cl	6980.1	438.0	804.9	-	13.3	56.6	89.2	2.9
14-Cl	3289.3	434.2	813.9	-	12.9	81.1	114.1	1.8
15-Cl	11326.9	421.0	901.6	1019.2	13.5	67.6	86.8	2.7
16-Cl	11592.3	-	1205.0	-	13.5	67.0	100.3	3.9
17-Cl	16750.3	-	1006.6	-	15.5	95.5	82.7	4.0
18-Cl	2031.2	420.6	713.2	1049.7	14.7	59.2	80.6	3.7
19-Cl	4215.9	429.2	988.6	1059.6	16.9	57.9	82.3	2.2
20-Cl	12488.6	417.1	1491.5	1548.1	17.0	117.3	110.7	5.1
21-Cl	1371.0	429.2	1242.1	1205.3	12.5	81.4	99.8	1.8
22-Cl	2988.3	451.0	865.1	1143.9	13.5	53.8	79.1	1.8
23-Cl	1149.1	441.4	795.0	1166.7	13.9	53.8	102.5	1.3
24-Cl	853501.5	1662.0	2729.9	3111.9	51.2	86.3	58.7	52.6
25-Cl	3386171.8	4732.8	5750.9	6543.4	87.4	107.4	127.4	116.6
26-Cl	85778.1	576.3	1065.4	800.0	20.3	72.6	90.4	9.7
27-Cl	212557.2	572.8	1582.5	1574.8	22.7	216.2	363.1	19.7
28-Cl	135506.1	549.2	1064.0	1114.4	20.4	86.3	89.6	13.4
29-Cl	268712.0	582.8	2546.2	1965.9	27.2	194.2	236.0	27.7
30-Cl	213466.8	556.8	3873.8	4256.4	73.0	267.3	267.7	21.4
31-Cl	139007.8	573.3	1297.2	1349.3	22.9	145.1	137.9	15.2
32-Cl	261571.6	595.5	3107.1	2685.4	30.1	169.2	181.1	30.2
33-Cl	24658.1	442.4	982.3	-	70.4	131.1	131.2	4.6
34-Cl	23548.2	434.5	902.7	-	163.5	118.1	109.4	4.8
35-Cl	23328.4	444.9	2420.8	-	72.2	227.6	136.8	4.6
36-Cl	26074.3	440.6	3062.9	-	88.1	135.8	153.7	5.7
37-Cl	106649.9	-	2263.5	-	87.4	195.1	161.8	-
38-Cl	54988.2	-	1792.2	-	16.6	105.0	177.9	-
39-Cl	54677.5	440.8	981.2	-	73.5	377.5	3167.9	8.4
40-Cl	75814.4	-	4169.7	-	68.9	248.2	248.8	-

Table 7: Computation time in total CPU seconds (Intel Xeon E5462), where DFT is the method M052X-D3/[Def2TZVP + Def2TZVPD.ECP(I)]

7 Structures

7.1 DFT

OCH₂

O	2.8298	-5.5728	-2.1761
C	2.8331	-5.2031	-3.3129
H	2.8331	-5.9143	-4.1522
H	2.8360	-4.1342	-3.5736

SCF = -114.528846**ZPE = 0.027401****H₂₉₈ = -114.497637****G₂₉₈ = -114.523085****Cl**

Cl	2.8301	-5.5741	-2.1759
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SCF = -460.263546**ZPE = 0.000000****H₂₉₈ = -460.261186****G₂₉₈ = -460.278569****1**

H	2.6905	0.0586	-1.4459
C	2.1077	0.0787	-0.5388
C	0.6055	0.1142	1.7975
C	1.6685	-1.1008	0.0380
C	1.7867	1.2841	0.0677
C	1.0373	1.3048	1.2338
C	0.9190	-1.0989	1.2020
H	2.1260	2.2075	-0.3766
H	0.5845	-2.0269	1.6378
H	0.0214	0.1233	2.7052
I	2.1488	-2.9250	-0.8695
H	0.7905	2.2454	1.7015

SCF = -529.369785**ZPE = 0.091729****H₂₉₈ = -529.271326****G₂₉₈ = -529.309687****1-OCH₂**

H	3.1544	0.2488	-1.1300
C	2.3975	0.1945	-0.3634
C	0.4526	0.0417	1.6125
C	1.9354	-1.0354	0.0760
C	1.8765	1.3525	0.1952
C	0.9052	1.2793	1.1817
C	0.9659	-1.1235	1.0616
H	2.2343	2.3129	-0.1441
H	0.6165	-2.0876	1.3961
H	-0.3028	-0.0228	2.3812
I	2.7175	-2.7887	-0.7599
H	0.5032	2.1829	1.6136
O	3.4227	-5.3607	-2.4655
C	2.5982	-5.3397	-3.3337
H	2.5652	-6.1167	-4.1102
H	1.8422	-4.5434	-3.3882

SCF = -643.903023**ZPE = 0.120096****H₂₉₈ = -643.771378****G₂₉₈ = -643.821384****1-Cl**

H	2.6993	0.0354	-1.4417
C	2.1115	0.0548	-0.5353
C	0.6060	0.1044	1.7860
C	1.6778	-1.1437	0.0200
C	1.7961	1.2666	0.0633
C	1.0415	1.2974	1.2273
C	0.9220	-1.1069	1.1864
H	2.1414	2.1892	-0.3819
H	0.5804	-2.0335	1.6250
H	0.0171	0.1150	2.6925
I	2.1630	-3.0044	-0.9016
Cl	2.8305	-5.5701	-2.1722
H	0.7957	2.2403	1.6937

SCF = -989.660560**ZPE = 0.091623****H₂₉₈ = -989.559872****G₂₉₈ = -989.603712**

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H	0.3586	0.1743	0.0941
C	0.2190	0.1623	1.1629
C	-0.1383	0.1106	3.9232
C	0.3330	-1.0227	1.8729
C	-0.0759	1.3315	1.8406
C	-0.2544	1.3061	3.2204
C	0.1566	-1.0596	3.2473
H	-0.1682	2.2633	1.3054
H	0.2483	-1.9892	3.7853
H	-0.2789	0.1018	4.9925
I	0.7809	-2.7868	0.8516
C	-0.5599	2.5187	3.9220
N	-0.8037	3.4874	4.4827

SCF = -621.640108**ZPE = 0.090299****H₂₉₈ = -621.541272****G₂₉₈ = -621.583780****2-Cl**

H	0.3680	0.1583	0.0933
C	0.2258	0.1443	1.1639
C	-0.1375	0.0983	3.9141
C	0.3438	-1.0614	1.8516
C	-0.0691	1.3177	1.8329
C	-0.2520	1.2986	3.2146
C	0.1580	-1.0674	3.2321
H	-0.1593	2.2507	1.2971
H	0.2474	-1.9976	3.7736
H	-0.2805	0.0904	4.9843
I	0.8053	-2.8676	0.8086
Cl	1.4229	-5.2921	-0.5924
C	-0.5570	2.5098	3.9142
N	-0.8012	3.4809	4.4751

SCF = -1081.943847**ZPE = 0.090435****H₂₉₈ = -1081.842588****G₂₉₈ = -1081.890361****2-OCH2**

H	-0.5593	0.3817	0.0367
C	-0.3587	0.2987	1.0929
C	0.1581	0.0666	3.8170
C	-0.0592	-0.9341	1.6536
C	-0.3996	1.4224	1.8985
C	-0.1407	1.3069	3.2609
C	0.1987	-1.0567	3.0110
H	-0.6312	2.3883	1.4776
H	0.4282	-2.0207	3.4363
H	0.3560	-0.0122	4.8745
I	0.0009	-2.6308	0.4362
C	-0.1820	2.4716	4.0962
N	-0.2144	3.4024	4.7635
O	0.5785	-5.0604	-1.3734
C	1.7625	-5.1084	-1.5487
H	2.2175	-5.8928	-2.1684
H	2.4400	-4.3699	-1.0968

SCF = -736.174269**ZPE = 0.118802****H₂₉₈ = -736.042180****G₂₉₈ = -736.095630****3**

H	0.3713	0.1703	0.0898
C	0.2266	0.1580	1.1578
C	-0.1442	0.1008	3.9215
C	0.3310	-1.0287	1.8678
C	-0.0655	1.3294	1.8346
C	-0.2449	1.2769	3.2035
C	0.1483	-1.0690	3.2420
H	-0.1542	2.2704	1.3181
H	0.2332	-2.0006	3.7776
H	-0.2927	0.1096	4.9882
I	0.7746	-2.7922	0.8454
N	-0.5547	2.5200	3.9237
O	-0.6359	3.5339	3.2744
O	-0.7081	2.4475	5.1184

SCF = -733.931273**ZPE = 0.094706****H₂₉₈ = -733.827353****G₂₉₈ = -733.871648**

3-Cl

H	0.3644	0.1520	0.0877
C	0.2243	0.1390	1.1583
C	-0.1336	0.0909	3.9142
C	0.3443	-1.0670	1.8475
C	-0.0697	1.3139	1.8250
C	-0.2447	1.2724	3.1989
C	0.1612	-1.0735	3.2296
H	-0.1642	2.2523	1.3042
H	0.2524	-2.0036	3.7705
H	-0.2770	0.0995	4.9820
I	0.8053	-2.8723	0.8046
Cl	1.4216	-5.2893	-0.5928
N	-0.5537	2.5048	3.9110
O	-0.6455	3.5281	3.2679
O	-0.7039	2.4476	5.1124

SCF = -1194.236452**ZPE = 0.094881****H₂₉₈ = -1194.130071****G₂₉₈ = -1194.179592****4**

H	0.3800	0.1564	0.0884
C	0.2315	0.1404	1.1564
C	-0.1611	0.0995	3.8969
C	0.3367	-1.0458	1.8613
C	-0.0711	1.3072	1.8410
C	-0.2685	1.3071	3.2169
C	0.1409	-1.0782	3.2307
H	-0.1568	2.2338	1.2909
H	0.2193	-2.0074	3.7723
H	-0.3177	0.0747	4.9661
I	0.7929	-2.8152	0.8413
C	-0.5634	2.5829	3.9529
H	-1.1544	2.3907	4.8448
H	0.3618	3.0675	4.2638
H	-1.1077	3.2803	3.3210

SCF = -568.694961**ZPE = 0.119346****H₂₉₈ = -568.566985****G₂₉₈ = -568.609469****3-OCH2**

H	0.2375	0.0598	0.1249
C	0.1376	0.0884	1.1980
C	-0.1189	0.1411	3.9727
C	0.2543	-1.0762	1.9436
C	-0.1083	1.2895	1.8398
C	-0.2317	1.2919	3.2162
C	0.1276	-1.0570	3.3256
H	-0.2041	2.2119	1.2920
H	0.2204	-1.9690	3.8931
H	-0.2229	0.1920	5.0436
I	0.6270	-2.8880	0.9757
N	-0.4922	2.5649	3.9001
O	-0.5831	3.5561	3.2170
O	-0.5989	2.5400	5.1021
O	1.2486	-5.3297	-0.7821
C	1.5063	-4.9593	-1.8917
H	1.7615	-5.6716	-2.6877
H	1.4977	-3.8925	-2.1574

SCF = -848.465466**ZPE = 0.123264****H₂₉₈ = -848.328244****G₂₉₈ = -848.383536****4-OCH2**

H	1.2412	0.5610	0.2448
C	0.8065	0.4040	1.2195
C	-0.3170	0.0050	3.7171
C	0.7639	-0.8664	1.7696
C	0.2820	1.4705	1.9324
C	-0.2841	1.2900	3.1894
C	0.2030	-1.0739	3.0179
H	0.3129	2.4609	1.5001
H	0.1688	-2.0653	3.4417
H	-0.7573	-0.1596	4.6904
I	1.5486	-2.4867	0.7017
C	-0.8208	2.4591	3.9655
H	-1.5704	2.1384	4.6844
H	-0.0204	2.9539	4.5151
H	-1.2704	3.1937	3.3017
O	2.1402	-5.0054	-1.1440
C	1.0736	-5.2167	-1.6454
H	0.9282	-6.0443	-2.3538
H	0.1980	-4.5923	-1.4176

SCF = -683.228117**ZPE = 0.147734****H₂₉₈ = -683.066920****G₂₉₈ = -683.120984**

4-Cl

H	0.3779	0.1424	0.0858
C	0.2326	0.1226	1.1563
C	-0.1533	0.0881	3.8876
C	0.3499	-1.0826	1.8377
C	-0.0718	1.2940	1.8352
C	-0.2665	1.2973	3.2113
C	0.1510	-1.0855	3.2130
H	-0.1620	2.2218	1.2847
H	0.2324	-2.0149	3.7581
H	-0.3080	0.0631	4.9588
I	0.8197	-2.8839	0.7986
Cl	1.4685	-5.3716	-0.6363
C	-0.5607	2.5741	3.9504
H	-1.1789	2.3842	4.8257
H	0.3596	3.0496	4.2918
H	-1.0816	3.2834	3.3102

SCF = -1028.984586**ZPE = 0.119315****H₂₉₈ = -1028.854336****G₂₉₈ = -1028.902136****5**

H	1.3219	0.0891	0.2655
C	0.7571	0.0997	1.1846
C	-0.7065	0.1455	3.5326
C	0.3589	-1.0866	1.7733
C	0.4283	1.3100	1.7681
C	-0.3024	1.3645	2.9655
C	-0.3753	-1.0624	2.9450
H	0.7484	2.2144	1.2794
H	-0.6979	-1.9832	3.4055
H	-1.2849	0.1281	4.4405
I	0.8528	-2.9131	0.8831
N	-0.6061	2.5672	3.5637
C	-1.5829	2.5823	4.6296
C	-0.4132	3.7839	2.8067
H	-2.5526	2.1872	4.3110
H	-1.7176	3.6042	4.9667
H	-1.2354	1.9974	5.4792
H	-0.9897	3.7908	1.8763
H	-0.7234	4.6271	3.4140
H	0.6380	3.9228	2.5610

SCF = -663.369440**ZPE = 0.165963****H₂₉₈ = -663.192442****G₂₉₈ = -663.240046****5-Cl**

H	1.3296	0.0764	0.2756
C	0.7757	0.0828	1.2035
C	-0.6511	0.1416	3.5588
C	0.3782	-1.1208	1.7666
C	0.4737	1.2990	1.7982
C	-0.2391	1.3563	3.0005
C	-0.3410	-1.0663	2.9515
H	0.8041	2.2016	1.3110
H	-0.6738	-1.9854	3.4124
H	-1.2173	0.1215	4.4755
I	0.8403	-2.9812	0.8378
Cl	1.4776	-5.5640	-0.4544
N	-0.5156	2.5802	3.6288
C	-1.5920	2.5830	4.5936
C	-0.4389	3.7634	2.8019
H	-2.5399	2.2285	4.1700
H	-1.7289	3.5956	4.9623
H	-1.3442	1.9544	5.4454
H	-1.0946	3.7087	1.9240
H	-0.7217	4.6261	3.3983
H	0.5794	3.9232	2.4562

SCF = -1123.655599**ZPE = 0.166076****H₂₉₈ = -1123.476295****G₂₉₈ = -1123.528913****5-OCH2**

H	1.8455	0.2819	0.5123
C	1.1525	0.2311	1.3378
C	-0.6352	0.1221	3.4453
C	0.7445	-0.9961	1.8297
C	0.6735	1.4028	1.8962
C	-0.2244	1.3790	2.9746
C	-0.1520	-1.0458	2.8824
H	1.0094	2.3386	1.4830
H	-0.4831	-1.9971	3.2694
H	-1.3362	0.0438	4.2588
I	1.4711	-2.7642	0.9815
N	-0.6795	2.5444	3.5537
C	-1.8060	2.4706	4.4570
C	-0.4562	3.7922	2.8583
H	-2.6925	2.0371	3.9831
H	-2.0478	3.4715	4.7976
H	-1.5588	1.8745	5.3335
H	-0.8956	3.7948	1.8556
H	-0.8984	4.5979	3.4340
H	0.6087	3.9976	2.7673
O	2.0017	-5.3982	-0.7957
C	1.0947	-5.3241	-1.5737
H	0.9505	-6.0809	-2.3580
H	0.3715	-4.4972	-1.5344

SCF = -777.902299

ZPE = 0.194365
H₂₉₈ = -777.692074
G₂₉₈ = -777.750975

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H	0.2842	0.1544	0.0869
C	0.2065	0.1023	1.1613
C	0.0063	-0.0327	3.9317
C	0.3657	-1.1103	1.8187
C	-0.0524	1.2435	1.8918
C	-0.1541	1.1833	3.2800
C	0.2671	-1.1814	3.1928
H	-0.1804	2.1985	1.4063
H	0.3910	-2.1249	3.7006
H	-0.0672	-0.1076	5.0037
I	0.7571	-2.8411	0.7127
O	-0.4102	2.3563	3.9072
C	-0.5212	2.3367	5.3176
H	0.4083	1.9991	5.7756
H	-1.3420	1.6933	5.6338
H	-0.7239	3.3583	5.6159

SCF = -643.925933
ZPE = 0.125001
H₂₉₈ = -643.791673
G₂₉₈ = -643.835566

6-Cl

H	0.2971	0.1436	0.0852
C	0.2143	0.0870	1.1609
C	-0.0008	-0.0397	3.9194
C	0.3678	-1.1446	1.7934
C	-0.0416	1.2360	1.8863
C	-0.1503	1.1768	3.2709
C	0.2568	-1.1876	3.1724
H	-0.1612	2.1929	1.3998
H	0.3720	-2.1320	3.6845
H	-0.0796	-0.1175	4.9919
I	0.7629	-2.9122	0.6670
Cl	1.3094	-5.3556	-0.8800
O	-0.4052	2.3639	3.9080
C	-0.5164	2.3246	5.3102
H	0.4089	1.9731	5.7695
H	-1.3385	1.6787	5.6229
H	-0.7148	3.3426	5.6290

SCF = -1104.215304
ZPE = 0.124980
H₂₉₈ = -1104.078724
G₂₉₈ = -1104.128021

6-OCH2

H	0.9828	0.3825	0.1546
C	0.7117	0.2565	1.1911
C	0.0174	-0.0636	3.8630
C	0.8053	-0.9923	1.7920
C	0.2717	1.3391	1.9248
C	-0.0780	1.1857	3.2643
C	0.4610	-1.1516	3.1191
H	0.1914	2.3189	1.4799
H	0.5346	-2.1207	3.5873
H	-0.2456	-0.2107	4.8973
I	1.4735	-2.6351	0.6819
O	-0.4984	2.3069	3.9003
C	-0.8566	2.1927	5.2639
H	-0.0089	1.8585	5.8619
H	-1.6902	1.5020	5.3905
H	-1.1555	3.1852	5.5791
O	1.9115	-5.0776	-1.3062
C	0.8940	-5.0824	-1.9375
H	0.7175	-5.8206	-2.7324
H	0.0971	-4.3495	-1.7472

SCF = -758.459079
ZPE = 0.153404
H₂₉₈ = -758.291639
G₂₉₈ = -758.346561

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H	1.6297	0.2756	1.3775
C	0.8516	-0.0290	2.0597
C	-1.1449	-0.8057	3.8137
C	0.2893	-1.2866	1.9627
C	0.4119	0.8492	3.0415
C	-0.5901	0.4698	3.9265
C	-0.7107	-1.6823	2.8387
H	0.8637	1.8258	3.0990
H	-1.1477	-2.6653	2.7619
H	-1.9239	-1.1107	4.4976
I	0.9478	-2.6065	0.4817
S	-1.2304	1.4888	5.2036
C	-0.2802	3.0015	5.0220
H	-0.6438	3.6677	5.7982
H	-0.4521	3.4595	4.0523
H	0.7794	2.8210	5.1772

SCF = -966.891194
ZPE = 0.120992
H₂₉₈ = -966.760239
G₂₉₈ = -966.805911

7-Cl

H	0.9874	0.3989	0.6048
C	0.4375	0.1494	1.5007
C	-0.9817	-0.4858	3.7908
C	0.2904	-1.1862	1.8614
C	-0.1165	1.1580	2.2738
C	-0.8239	0.8472	3.4295
C	-0.4276	-1.4913	3.0129
H	-0.0055	2.1938	1.9854
H	-0.5543	-2.5250	3.3006
H	-1.5411	-0.7279	4.6833
I	1.1482	-2.7344	0.6702
Cl	2.3307	-4.8475	-0.9495
S	-1.5168	2.1355	4.4306
C	-0.0953	2.4697	5.5009
H	-0.3853	3.2648	6.1830
H	0.7543	2.7913	4.9062
H	0.1659	1.5804	6.0664

SCF = -1427.183870**ZPE = 0.120655****H₂₉₈ = -1427.050668****G₂₉₈ = -1427.102542****7-OCH2**

H	2.0920	0.2463	1.7624
C	1.2064	-0.0614	2.2961
C	-1.0645	-0.8436	3.6708
C	0.7032	-1.3380	2.1337
C	0.5720	0.8318	3.1497
C	-0.5689	0.4491	3.8445
C	-0.4350	-1.7334	2.8223
H	0.9833	1.8217	3.2600
H	-0.8279	-2.7303	2.6981
H	-1.9505	-1.1514	4.2076
I	1.6599	-2.6818	0.8477
S	-1.4580	1.4848	4.9486
C	-0.5181	3.0139	4.9056
H	-1.0313	3.6902	5.5823
H	-0.5139	3.4450	3.9088
H	0.4972	2.8607	5.2596
O	2.6295	-4.5546	-1.5138
C	1.8136	-4.3518	-2.3665
H	1.8643	-4.8606	-3.3393
H	0.9825	-3.6495	-2.2100

SCF = -1081.424489**ZPE = 0.149457****H₂₉₈ = -1081.260294****G₂₉₈ = -1081.316981****8**

H	0.5140	0.1754	0.1205
C	0.3077	0.1533	1.1782
C	-0.2234	0.0787	3.9092
C	0.3364	-1.0453	1.8756
C	0.0107	1.3196	1.8592
C	-0.2532	1.2780	3.2208
C	0.0737	-1.0956	3.2328
H	-0.0166	2.2622	1.3329
H	0.0995	-2.0353	3.7606
H	-0.4302	0.0549	4.9671
I	0.7881	-2.8101	0.8528
C	-0.5661	2.5651	3.9197
F	-0.8290	2.3891	5.2198
F	0.4559	3.4324	3.8323
F	-1.6319	3.1738	3.3742

SCF = -866.541836**ZPE = 0.096607****H₂₉₈ = -866.435816****G₂₉₈ = -866.480699****8-Cl**

H	0.5387	0.1621	0.1239
C	0.3233	0.1357	1.1819
C	-0.2295	0.0646	3.8983
C	0.3486	-1.0850	1.8535
C	0.0270	1.3068	1.8548
C	-0.2495	1.2702	3.2162
C	0.0687	-1.1050	3.2148
H	0.0093	2.2509	1.3288
H	0.0852	-2.0458	3.7450
H	-0.4447	0.0385	4.9553
I	0.8122	-2.8891	0.8076
Cl	1.4367	-5.3233	-0.6070
C	-0.5638	2.5496	3.9106
F	-0.8099	2.3876	5.2213
F	0.4422	3.4445	3.8150
F	-1.6467	3.1632	3.3880

SCF = -1326.841698**ZPE = 0.096590****H₂₉₈ = -1326.733371****G₂₉₈ = -1326.783547**

8-OCH2

H	1.3081	0.5517	0.3058
C	0.8384	0.4023	1.2648
C	-0.3660	0.0042	3.7400
C	0.7258	-0.8738	1.7987
C	0.3440	1.4804	1.9761
C	-0.2565	1.2776	3.2105
C	0.1289	-1.0802	3.0307
H	0.4269	2.4793	1.5744
H	0.0498	-2.0757	3.4374
H	-0.8314	-0.1449	4.7012
I	1.4693	-2.5071	0.7265
C	-0.7993	2.4668	3.9403
F	-1.2089	2.1630	5.1779
F	0.1189	3.4405	4.0495
F	-1.8497	3.0033	3.2955
O	2.0906	-4.9566	-1.0711
C	1.0818	-5.1989	-1.6699
H	1.0269	-6.0315	-2.3843
H	0.1721	-4.5981	-1.5283

SCF = -981.075744**ZPE = 0.125153****H₂₉₈ = -980.935522****G₂₉₈ = -980.993544****9**

H	0.3544	0.1678	0.0947
C	0.2169	0.1547	1.1640
C	-0.1378	0.1163	3.9222
C	0.3313	-1.0290	1.8732
C	-0.0767	1.3296	1.8390
C	-0.2505	1.2973	3.2109
C	0.1561	-1.0581	3.2463
H	-0.1684	2.2596	1.3011
H	0.2469	-1.9843	3.7907
H	-0.2770	0.1102	4.9914
I	0.7781	-2.7984	0.8555
Br	-0.6496	2.9018	4.1342

SCF = -3102.871245**ZPE = 0.081398****H₂₉₈ = -3102.781665****G₂₉₈ = -3102.824372****9-OCH2**

H	-0.5357	0.3131	0.0678
C	-0.3211	0.2444	1.1226
C	0.2288	0.0655	3.8419
C	-0.0335	-0.9814	1.7008
C	-0.3338	1.3886	1.9058
C	-0.0580	1.2857	3.2572
C	0.2404	-1.0767	3.0556
H	-0.5566	2.3486	1.4682
H	0.4617	-2.0335	3.5016
H	0.4401	0.0051	4.8976
I	-0.0151	-2.7044	0.5163
Br	-0.0738	2.8487	4.3284
O	0.5696	-5.1567	-1.3232
C	1.7372	-5.0806	-1.5787
H	2.2317	-5.8221	-2.2211
H	2.3596	-4.2664	-1.1808

SCF = -3217.404925**ZPE = 0.109940****H₂₉₈ = -3217.282070****G₂₉₈ = -3217.335552****9-Cl**

H	0.3513	0.1523	0.0921
C	0.2170	0.1354	1.1640
C	-0.1294	0.1028	3.9152
C	0.3438	-1.0672	1.8500
C	-0.0784	1.3159	1.8322
C	-0.2475	1.2815	3.2034
C	0.1667	-1.0671	3.2291
H	-0.1748	2.2471	1.2954
H	0.2619	-1.9933	3.7771
H	-0.2654	0.0978	4.9857
I	0.8054	-2.8748	0.8093
Cl	1.4315	-5.3292	-0.6031
Br	-0.6508	2.8975	4.1353

SCF = -3563.168269**ZPE = 0.081451****H₂₉₈ = -3563.076294****G₂₉₈ = -3563.124336**

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C	0.2286	-0.0235	1.1319
C	-0.1332	0.0056	3.9168
C	0.1327	-1.2200	1.8445
C	0.1446	1.1878	1.8209
C	-0.0358	1.2022	3.2076
C	-0.0477	-1.2056	3.2312
I	0.4893	-0.0454	-0.9187
C	0.2167	-2.4820	1.1754
N	0.2826	-3.4992	0.6551
C	-0.1458	-2.4379	3.9506
N	-0.2244	-3.4229	4.5273
C	-0.3192	0.0203	5.3340
N	-0.4687	0.0320	6.4682
C	-0.1218	2.4492	3.9029
N	-0.1908	3.4459	4.4604
C	0.2412	2.4355	1.1272
N	0.3170	3.4414	0.5869

SCF = -990.671861**ZPE = 0.083114****H₂₉₈ = -990.572644****G₂₉₈ = -990.631399****10-OCH2**

C	0.2044	-0.3497	0.9842
C	-0.1080	0.0574	3.7512
C	0.1122	-1.4359	1.8566
C	0.1386	0.9421	1.5118
C	-0.0167	1.1470	2.8858
C	-0.0428	-1.2352	3.2319
I	0.4349	-0.6287	-1.0594
C	0.1742	-2.7774	1.3610
N	0.2219	-3.8563	0.9821
C	-0.1352	-2.3588	4.1127
N	-0.2093	-3.2559	4.8190
C	-0.2672	0.2641	5.1567
N	-0.3949	0.4309	6.2814
C	-0.0822	2.4776	3.4070
N	-0.1345	3.5427	3.8218
C	0.2294	2.0830	0.6505
N	0.3020	2.9966	-0.0350
O	0.7628	-0.3877	-3.9104
C	0.8027	0.7692	-4.2291
H	0.9250	1.0634	-5.2783
H	0.7186	1.5732	-3.4847

SCF = -1105.211350**ZPE = 0.112029****H₂₉₈ = -1105.078756****G₂₉₈ = -1105.147264****10-Cl**

C	0.2261	-0.0233	1.0845
C	-0.1282	0.0050	3.9053
C	0.1345	-1.2071	1.8268
C	0.1355	1.1751	1.8031
C	-0.0389	1.1997	3.1902
C	-0.0398	-1.2038	3.2142
I	0.4940	-0.0454	-1.0903
Cl	0.8180	-0.0712	-3.7227
C	0.2186	-2.4843	1.1745
N	0.2777	-3.5342	0.7218
C	-0.1303	-2.4338	3.9428
N	-0.2040	-3.4093	4.5370
C	-0.3074	0.0192	5.3233
N	-0.4512	0.0306	6.4591
C	-0.1286	2.4439	3.8941
N	-0.2018	3.4311	4.4688
C	0.2208	2.4389	1.1254
N	0.2809	3.4794	0.6515

SCF = -1451.010493**ZPE = 0.083484****H₂₉₈ = -1450.908740****G₂₉₈ = -1450.972383****11**

C	0.2169	-0.0249	1.1634
C	-0.1298	0.0090	3.9213
C	0.1061	-1.2052	1.8761
C	0.1523	1.1726	1.8526
C	-0.0202	1.1970	3.2236
C	-0.0665	-1.1959	3.2473
I	0.4718	-0.0508	-0.8891
F	0.1626	-2.3797	1.2593
F	-0.1718	-2.3357	3.9188
F	-0.2955	0.0252	5.2353
F	-0.0815	2.3531	3.8725
F	0.2542	2.3317	1.2128

SCF = -1025.701600**ZPE = 0.050811****H₂₉₈ = -1025.639661****G₂₉₈ = -1025.688039**

11-I

C	0.0048	0.0136	1.1398
C	0.0212	0.0436	3.8829
C	0.0363	-1.1961	1.8047
C	-0.0183	1.2230	1.8096
C	-0.0100	1.2368	3.1899
C	0.0437	-1.1497	3.1848
I	0.0758	-3.0734	0.7365
F	0.0739	-2.2728	3.9086
F	0.0293	0.0593	5.2199
F	-0.0321	2.3972	3.8503
F	-0.0488	2.3803	1.1405
F	-0.0042	0.0621	-0.1957
I	0.1352	-5.8393	-0.8386

SCF = -1323.493172**ZPE = 0.050518****H₂₉₈ = -1323.428935****G₂₉₈ = -1323.484306****11-F**

C	0.0071	-0.0082	1.1401
C	0.0192	0.0319	3.8746
C	0.0358	-1.2228	1.7945
C	-0.0152	1.2059	1.8024
C	-0.0090	1.2251	3.1822
C	0.0408	-1.1599	3.1730
I	0.0753	-3.1528	0.6991
F	0.0681	-2.2810	3.9118
F	0.0252	0.0509	5.2156
F	-0.0303	2.3901	3.8425
F	-0.0428	2.3659	1.1298
F	-0.0001	0.0495	-0.2015
F	0.1147	-5.0163	-0.3624

SCF = -1125.652787**ZPE = 0.051276****H₂₉₈ = -1125.588500****G₂₉₈ = -1125.640798****11-OCH2**

C	0.0009	-0.2042	1.1130
C	-0.0006	-0.0767	3.8637
C	0.0003	-1.3821	1.8375
C	0.0008	1.0265	1.7412
C	0.0001	1.0890	3.1217
C	-0.0005	-1.2987	3.2181
F	-0.0012	-2.3984	3.9647
F	-0.0013	-0.0155	5.1904
F	-0.0000	2.2654	3.7328
F	0.0015	2.1472	1.0280
F	0.0017	-0.2246	-0.2174
I	0.0004	-3.2231	0.8782
O	0.0002	-5.6187	-0.8670
C	-0.0005	-5.2880	-2.0194
H	-0.0006	-6.0330	-2.8255
H	-0.0010	-4.2288	-2.3121

SCF = -1140.237662**ZPE = 0.079428****H₂₉₈ = -1140.142437****G₂₉₈ = -1140.201410****11-OMe**

C	0.0770	0.1155	1.2243
C	-0.0339	0.1060	3.9554
C	0.1030	-1.1076	1.8564
C	-0.0015	1.3180	1.9036
C	-0.0574	1.3109	3.2827
C	0.0453	-1.0703	3.2317
I	0.2357	-3.0763	0.6940
F	0.0644	-2.2073	3.9528
F	-0.0885	0.1029	5.2968
F	-0.1342	2.4635	3.9623
F	-0.0246	2.4920	1.2527
F	0.1284	0.1982	-0.1186
O	0.3614	-4.9501	-0.4067
C	0.2763	-4.7579	-1.7760
H	0.3406	-5.7215	-2.2978
H	1.0855	-4.1213	-2.1679
H	-0.6708	-4.2853	-2.0816

SCF = -1140.903394**ZPE = 0.090496****H₂₉₈ = -1140.797599****G₂₉₈ = -1140.854948**

11-Cl

C	0.2182	-0.0255	1.1308
C	-0.1267	0.0101	3.9151
C	0.1031	-1.1891	1.8645
C	0.1545	1.1566	1.8408
C	-0.0152	1.1929	3.2128
C	-0.0673	-1.1904	3.2368
I	0.4869	-0.0539	-1.0365
F	0.1526	-2.3857	1.2658
F	-0.1758	-2.3370	3.9194
F	-0.2913	0.0271	5.2418
F	-0.0735	2.3568	3.8720
F	0.2562	2.3376	1.2182
Cl	0.8245	-0.0895	-3.7611

SCF = -1486.014654**ZPE = 0.050748****H₂₉₈ = -1485.950473****G₂₉₈ = -1486.004077****11-Br**

C	0.0055	0.0121	1.1405
C	0.0210	0.0415	3.8818
C	0.0378	-1.1994	1.8020
C	-0.0189	1.2217	1.8100
C	-0.0110	1.2354	3.1902
C	0.0448	-1.1508	3.1819
I	0.0777	-3.0852	0.7273
F	0.0758	-2.2739	3.9078
F	0.0287	0.0566	5.2197
F	-0.0345	2.3961	3.8518
F	-0.0503	2.3802	1.1413
F	-0.0033	0.0639	-0.1961
Br	0.1309	-5.6408	-0.7300

SCF = -3599.923173**ZPE = 0.050599****H₂₉₈ = -3599.858961****G₂₉₈ = -3599.913610****11-DMF**

C	0.1070	0.5678	2.2658
C	0.6910	0.0262	4.9000
C	0.2583	-0.7501	2.6575
C	0.2424	1.6084	3.1647
C	0.5355	1.3354	4.4869
C	0.5517	-1.0009	3.9858
F	0.7089	-2.2470	4.4229
F	0.9730	-0.2361	6.1720
F	0.6673	2.3277	5.3575
F	0.0928	2.8680	2.7667
F	-0.1755	0.8730	1.0012
I	0.0496	-2.3024	1.2919
O	-0.2613	-4.3791	-0.6774
C	-0.4610	-4.8086	-1.7991
H	-0.5081	-5.8866	-1.9971
N	-0.6437	-4.0689	-2.9021
C	-0.6169	-2.6229	-2.8489
H	0.1795	-2.2415	-3.4871
H	-0.4422	-2.3118	-1.8264
H	-1.5681	-2.2203	-3.1950
C	-0.8730	-4.6748	-4.1926
H	-0.0916	-4.3829	-4.8937
H	-1.8356	-4.3598	-4.5943
H	-0.8704	-5.7562	-4.0941

SCF = -1274.282082**ZPE = 0.155741****H₂₉₈ = -1274.106823****G₂₉₈ = -1274.174523****11-NH3**

C	0.1903	-0.0260	1.3258
C	-0.1460	0.0112	4.0928
C	0.0902	-1.2009	2.0480
C	0.1185	1.1678	2.0195
C	-0.0483	1.1974	3.3911
C	-0.0767	-1.1935	3.4199
I	0.4425	-0.0538	-0.7458
F	0.1523	-2.3815	1.4364
F	-0.1710	-2.3344	4.0954
F	-0.3063	0.0290	5.4096
F	-0.1154	2.3561	4.0389
F	0.2087	2.3317	1.3798
N	0.8054	-0.0893	-3.6852
H	1.7738	0.0592	-3.9282
H	0.2574	0.6372	-4.1219
H	0.5172	-0.9760	-4.0721

SCF = -1082.280178**ZPE = 0.087563****H₂₉₈ = -1082.177478****G₂₉₈ = -1082.233974**

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C	0.5648	-0.2795	1.0914
C	-0.0071	0.5757	3.6599
C	0.2455	-1.1836	2.0891
C	0.5893	1.0651	1.4169
C	0.3072	1.5155	2.6943
C	-0.0439	-0.7788	3.3801
I	0.9941	-0.9194	-0.8304
I	-0.5171	-2.1579	4.8508
I	0.3557	3.5356	3.1473
F	-0.2817	0.9859	4.8916
F	0.2161	-2.4781	1.7988
F	0.8927	1.9497	0.4754

SCF = -1421.299881**ZPE = 0.045831****H₂₉₈ = -1421.241395****G₂₉₈ = -1421.295482****12-Cl**

C	0.5726	-0.2901	1.0568
C	-0.0068	0.5738	3.6585
C	0.2521	-1.1728	2.0689
C	0.5899	1.0451	1.4078
C	0.3080	1.5031	2.6866
C	-0.0395	-0.7754	3.3658
I	1.0233	-0.9630	-0.9753
Cl	1.5878	-1.8012	-3.5191
I	-0.5154	-2.1593	4.8415
I	0.3549	3.5296	3.1444
F	-0.2840	0.9859	4.8990
F	0.2157	-2.4812	1.8041
F	0.8918	1.9580	0.4811

SCF = -1881.612062**ZPE = 0.045868****H₂₉₈ = -1881.551212****G₂₉₈ = -1881.610498****12-OCH2**

C	0.5418	-0.5095	1.0118
C	0.0134	0.6250	3.4859
C	0.2552	-1.2949	2.1143
C	0.5550	0.8624	1.1891
C	0.2939	1.4524	2.4133
C	-0.0116	-0.7522	3.3592
I	0.9377	-1.3608	-0.8421
I	-0.4342	-1.9648	4.9843
I	0.3200	3.5115	2.6361
F	-0.2388	1.1687	4.6709
F	0.2354	-2.6155	1.9744
F	0.8275	1.6428	0.1479
O	1.5109	-2.1585	-3.6515
C	1.6058	-1.1767	-4.3328
H	1.8147	-1.2478	-5.4081
H	1.4874	-0.1702	-3.9080

SCF = -1535.835596**ZPE = 0.074399****H₂₉₈ = -1535.743874****G₂₉₈ = -1535.808304****13**

C	-0.0014	-0.0040	1.1587
I	-0.0038	-0.0158	-0.9894
Br	-0.9338	-1.5672	1.8176
Br	1.8230	-0.0260	1.8058
Br	-0.8899	1.5919	1.7998

SCF = -8058.046786**ZPE = 0.006993****H₂₉₈ = -8058.031991****G₂₉₈ = -8058.075399****13-OCH2**

C	-0.0366	0.0510	0.8922
I	-0.3651	-0.3539	-1.1912
Br	-0.5899	-1.4721	1.9560
Br	1.8478	0.3934	1.2054
Br	-1.0615	1.6078	1.4294
O	-0.5763	-0.5808	-4.0883
C	0.0576	0.2832	-4.6267
H	0.0984	0.3599	-5.7206
H	0.6195	1.0281	-4.0468

SCF = -8172.583386**ZPE = 0.035771****H₂₉₈ = -8172.535241****G₂₉₈ = -8172.588864**

13-Cl

C	0.0000	-0.0040	1.1251
I	-0.0019	-0.0170	-1.1276
Cl	-0.0055	-0.0332	-3.7903
Br	-0.9306	-1.5759	1.8419
Br	1.8307	-0.0186	1.8308
Br	-0.8985	1.5950	1.8230

SCF = -8518.367695**ZPE = 0.007268****H₂₉₈ = -8518.350285****G₂₉₈ = -8518.398995****14**

C	-0.0004	-0.0020	1.1408
I	0.0065	-0.0197	-0.9968
F	-0.6302	-1.0697	1.6095
F	1.2405	-0.0064	1.6062
F	-0.6156	1.0817	1.5919

SCF = -635.408369**ZPE = 0.014354****H₂₉₈ = -635.388389****G₂₉₈ = -635.424177****14-Cl**

C	-0.0003	-0.0028	1.0797
I	0.0013	-0.0186	-1.1032
Cl	0.0011	-0.0387	-3.9034
F	-0.6287	-1.0734	1.6149
F	1.2436	-0.0059	1.6089
F	-0.6172	1.0820	1.5994

SCF = -1095.717902**ZPE = 0.014351****H₂₉₈ = -1095.695612****G₂₉₈ = -1095.737033****14-OCH2**

C	-0.0045	0.0804	0.8531
I	0.0801	-0.4465	-1.2146
F	-0.7321	-0.7977	1.5360
F	1.2136	0.1099	1.3850
F	-0.5525	1.2822	1.0117
O	0.1360	-0.7765	-4.1821
C	0.0011	0.2794	-4.7331
H	-0.0083	0.3539	-5.8281
H	-0.1179	1.2126	-4.1649

SCF = -749.943974**ZPE = 0.042901****H₂₉₈ = -749.890756****G₂₉₈ = -749.938107****15**

C	0.0032	-0.0003	1.1681
I	0.0141	0.0013	-1.0335
C	-0.7229	-1.2544	1.6114
H	-0.2169	-2.1488	1.2577
H	-1.7484	-1.2643	1.2515
H	-0.7374	-1.2718	2.7040
C	1.4489	-0.0009	1.6222
H	1.9727	-0.8850	1.2685
H	1.4633	-0.0017	2.7149
H	1.9730	0.8835	1.2698
C	-0.7225	1.2533	1.6133
H	-0.2162	2.1481	1.2609
H	-0.7370	1.2691	2.7058
H	-1.7479	1.2641	1.2533

SCF = -455.552840**ZPE = 0.123263****H₂₉₈ = -455.421894****G₂₉₈ = -455.460948****15-Cl**

C	0.0001	-0.0042	1.1097
I	0.0006	-0.0177	-1.0945
Cl	-0.0024	-0.0359	-4.1108
C	-0.7209	-1.2478	1.5988
H	-0.2223	-2.1488	1.2463
H	-1.7483	-1.2667	1.2400
H	-0.7339	-1.2627	2.6951
C	1.4399	-0.0021	1.5919
H	1.9680	-0.8860	1.2390
H	1.4647	0.0046	2.6879
H	1.9692	0.8766	1.2281
C	-0.7192	1.2463	1.5835
H	-0.2196	2.1423	1.2198
H	-0.7322	1.2748	2.6794
H	-1.7467	1.2621	1.2245

SCF = -915.833964**ZPE = 0.122915****H₂₉₈ = -915.701009****G₂₉₈ = -915.745902**

15-OCH2

C	0.0793	-0.0919	0.9749
I	0.3687	-0.5784	-1.1459
C	-0.7631	-1.1970	1.5817
H	-0.2658	-2.1602	1.5011
H	-1.7343	-1.2624	1.0979
H	-0.9162	-0.9723	2.6402
C	1.4519	-0.0256	1.6154
H	1.9703	-0.9776	1.5348
H	1.3271	0.2136	2.6745
H	2.0640	0.7466	1.1562
C	-0.6296	1.2466	1.0431
H	-0.0364	2.0302	0.5784
H	-0.7813	1.5034	2.0944
H	-1.5999	1.2033	0.5548
O	0.4314	-0.6208	-4.4780
C	-0.1389	0.4159	-4.6575
H	-0.3328	0.7953	-5.6714
H	-0.4915	1.0298	-3.8163

SCF = -570.084718
ZPE = 0.151629
H₂₉₈ = -569.920595
G₂₉₈ = -569.971242

16

C	-0.0009	-0.0047	1.1473
I	0.0019	-0.0158	-1.0394
C	-0.6974	-1.2074	1.5953
N	-1.2430	-2.1498	1.9406
C	1.3899	-0.0027	1.5922
N	2.4794	-0.0011	1.9355
C	-0.6970	1.2027	1.5831
N	-1.2422	2.1486	1.9189

SCF = -614.328594
ZPE = 0.033188
H₂₉₈ = -614.286488
G₂₉₈ = -614.329851

16-OCH2

C	0.0239	-0.0419	1.0037
I	0.1689	-0.3920	-1.1699
C	-0.7348	-1.1468	1.5799
N	-1.3316	-2.0174	2.0175
C	1.3821	0.0064	1.5342
N	2.4515	0.0442	1.9349
C	-0.6648	1.2309	1.1907
N	-1.2047	2.2301	1.3161
O	0.2801	-0.6066	-3.8937
C	-0.0219	0.3686	-4.5279
H	-0.0001	0.3545	-5.6231
H	-0.3274	1.3004	-4.0357

SCF = -728.870068
ZPE = 0.062300
H₂₉₈ = -728.794469
G₂₉₈ = -728.847635

16-Cl

C	-0.0013	-0.0037	1.3221
I	0.0013	-0.0160	-1.2221
Cl	0.0051	-0.0278	-3.7100
C	-0.6992	-1.2113	1.6510
N	-1.2606	-2.1825	1.8939
C	1.3943	-0.0016	1.6475
N	2.5167	-0.0001	1.8875
C	-0.7001	1.2065	1.6395
N	-1.2622	2.1795	1.8732

SCF = -1074.690508
ZPE = 0.033818
H₂₉₈ = -1074.645604
G₂₉₈ = -1074.694088

17

I	0.0933	-1.3349	-1.5250
N	-0.6153	-0.3996	0.1114
C	0.0680	-0.3763	1.3230
C	-1.8289	0.2804	0.1240
O	1.1249	-0.8974	1.5271
O	-2.5696	0.3830	-0.8092
C	-2.0150	0.8472	1.5187
H	-2.1264	1.9243	1.4318
H	-2.9426	0.4505	1.9215
C	-0.7745	0.4199	2.3016
H	-0.1765	1.2534	2.6588
H	-0.9944	-0.2179	3.1530

SCF = -657.806120
ZPE = 0.082387
H₂₉₈ = -657.715369
G₂₉₈ = -657.757675

17-Cl

I	0.1797	-1.4395	-1.7167
Cl	1.0870	-2.6313	-3.8046
N	-0.6117	-0.3991	0.1064
C	0.0395	-0.3658	1.3087
C	-1.8009	0.2757	0.1428
O	1.1061	-0.8736	1.5666
O	-2.5828	0.4105	-0.7695
C	-2.0193	0.8590	1.5400
H	-2.1293	1.9363	1.4448
H	-2.9532	0.4634	1.9313
C	-0.7881	0.4285	2.3206
H	-0.1812	1.2547	2.6824
H	-1.0039	-0.2197	3.1662

SCF = -1118.136894**ZPE = 0.082628****H₂₉₈ = -1118.043717****G₂₉₈ = -1118.091127****17-OCH2**

I	0.5406	-1.3337	-1.4597
N	-0.3882	-0.4113	0.0962
C	0.0923	-0.4443	1.3979
C	-1.5631	0.3090	-0.0510
O	1.0885	-1.0075	1.7516
O	-2.1515	0.4689	-1.0836
C	-1.9541	0.8446	1.3146
H	-2.0194	1.9269	1.2473
H	-2.9449	0.4681	1.5534
C	-0.8654	0.3527	2.2655
H	-0.3046	1.1539	2.7386
H	-1.2337	-0.3013	3.0509
O	1.5161	-2.4449	-3.7774
C	0.8177	-2.1850	-4.7195
H	1.0663	-2.5523	-5.7220
H	-0.0875	-1.5743	-4.6085

SCF = -772.346598**ZPE = 0.111472****H₂₉₈ = -772.222419****G₂₉₈ = -772.274394****18**

I	-0.0014	-0.0029	-0.8049
C	0.0015	-0.0615	1.2799
H	0.0053	0.9174	1.7280
C	-0.0011	-1.1867	1.9630
H	0.0007	-1.1526	3.0435
H	-0.0049	-2.1539	1.4855

SCF = -375.665096**ZPE = 0.042503****H₂₉₈ = -375.617930****G₂₉₈ = -375.650037****18-OCH2**

I	-0.5871	-0.4220	-1.1363
C	-0.2919	-0.0573	0.8969
H	-0.5942	0.9298	1.2043
C	0.2123	-0.9540	1.7199
H	0.3400	-0.7093	2.7654
H	0.5069	-1.9382	1.3900
O	-0.6304	-0.5165	-4.3077
C	0.1076	0.3735	-4.6193
H	0.3108	0.6056	-5.6741
H	0.6112	0.9933	-3.8638

SCF = -490.198232**ZPE = 0.070999****H₂₉₈ = -490.117841****G₂₉₈ = -490.162024****18-Cl**

I	-0.0027	0.0108	-0.8991
Cl	-0.0066	0.1067	-3.8815
C	0.0002	-0.0631	1.2185
H	0.0021	0.9017	1.7072
C	-0.0001	-1.1766	1.9338
H	0.0015	-1.1454	3.0170
H	-0.0020	-2.1496	1.4624

SCF = -835.953275**ZPE = 0.042578****H₂₉₈ = -835.903770****G₂₉₈ = -835.942013****19**

I	-0.0021	-0.0454	-0.8129
C	0.0013	-0.0597	1.2543
H	0.0049	0.9157	1.7114
C	-0.0009	-1.1834	1.9570
H	-0.0045	-2.1582	1.4943
C	0.0016	-1.1377	3.3866
N	0.0036	-1.1139	4.5322

SCF = -467.934126**ZPE = 0.041662****H₂₉₈ = -467.886145****G₂₉₈ = -467.922922**

19-Cl

I	-0.0031	-0.0205	-0.9139
Cl	-0.0073	0.0088	-3.7787
C	0.0001	-0.0551	1.2040
H	0.0021	0.9022	1.7076
C	-0.0000	-1.1721	1.9321
H	-0.0019	-2.1504	1.4736
C	0.0022	-1.1341	3.3616
N	0.0040	-1.1154	4.5105

SCF = -928.241068**ZPE = 0.041848****H₂₉₈ = -928.190688****G₂₉₈ = -928.232845****19-OCH2**

I	-0.0679	-0.5416	-1.0930
C	-0.0217	-0.1840	0.9452
H	-0.0161	0.8554	1.2299
C	-0.0008	-1.1603	1.8428
H	-0.0064	-2.2033	1.5655
C	0.0303	-0.8574	3.2406
N	0.0551	-0.6252	4.3627
O	-0.0921	-0.7024	-4.1323
C	0.0046	0.3883	-4.6188
H	0.0190	0.5290	-5.7076
H	0.0826	1.2903	-3.9954

SCF = -582.468953**ZPE = 0.070233****H₂₉₈ = -582.387693****G₂₉₈ = -582.436122****20**

I	-0.0538	-0.0066	-0.8376
C	-0.3126	-0.1163	1.2254
H	-0.7076	0.7815	1.6620
C	0.0361	-1.2148	1.8974
H	0.4069	-2.0779	1.3613
N	0.0051	-1.3715	3.2613
C	-0.2569	-2.7090	3.7541
H	0.2882	-3.4290	3.1497
H	-1.3219	-2.9603	3.7210
H	0.0887	-2.7886	4.7819
C	-0.5773	-0.3047	4.0380
H	-0.0590	0.6281	3.8273
H	-0.4633	-0.5336	5.0937
H	-1.6426	-0.1708	3.8167

SCF = -509.670181**ZPE = 0.117833****H₂₉₈ = -509.543811****G₂₉₈ = -509.585699****20-Cl**

I	-0.0739	-0.0105	-0.9073
Cl	0.2196	0.1533	-3.8760
C	-0.2866	-0.1397	1.2015
H	-0.7380	0.7171	1.6766
C	0.1297	-1.1941	1.8957
H	0.5676	-2.0393	1.3787
N	0.1099	-1.3552	3.2909
C	-0.2861	-2.6815	3.7150
H	0.2733	-3.4230	3.1494
H	-1.3574	-2.8663	3.5588
H	-0.0614	-2.8093	4.7730
C	-0.5511	-0.3102	4.0298
H	-0.0735	0.6443	3.8217
H	-0.4668	-0.5202	5.0945
H	-1.6152	-0.2268	3.7678

SCF = -969.953951**ZPE = 0.117816****H₂₉₈ = -969.825434****G₂₉₈ = -969.872456****20-OCH2**

I	0.8069	-0.1341	-0.9331
C	0.1696	-0.1397	1.0500
H	-0.1986	0.8074	1.3982
C	0.2736	-1.2393	1.7980
H	0.6411	-2.1562	1.3568
N	-0.0156	-1.3404	3.1389
C	-0.5165	-2.6221	3.5933
H	0.0468	-3.4191	3.1152
H	-1.5782	-2.7572	3.3611
H	-0.3821	-2.7012	4.6694
C	-0.6126	-0.1915	3.7740
H	0.0305	0.6759	3.6432
H	-0.7155	-0.3893	4.8373
H	-1.6006	0.0400	3.3586
O	1.1266	0.0596	-4.1311
C	0.0175	0.3848	-4.4433
H	-0.2526	0.5607	-5.4944
H	-0.7734	0.5199	-3.6919

SCF = -624.202945**ZPE = 0.146230****H₂₉₈ = -624.043403****G₂₉₈ = -624.096595****21**

I	0.0000	0.0000	-0.5324
C	0.0000	0.0000	1.4519
H	0.0000	0.0000	3.7102
C	0.0000	0.0000	2.6488

SCF = -374.406016**21-Cl**

I	0.0255	-0.0550	-0.8657
Cl	0.3162	-0.1499	-3.6777
C	-0.1885	0.0153	1.2009
H	-0.4222	0.0927	3.4540
C	-0.3124	0.0567	2.3996

SCF = -834.711840**21-OCH2**

I	-0.0551	-0.5115	-1.0334
C	-0.1866	-0.0188	0.8961
H	-0.3373	0.5355	3.0814
C	-0.2667	0.2760	2.0545
O	0.1736	-0.8662	-3.9608
C	0.3093	0.1877	-4.5157
H	0.4115	0.2478	-5.6070
H	0.3369	1.1322	-3.9547

SCF = -488.942182**22**

I	0.0000	0.0000	-1.2562
C	0.0000	0.0000	0.7187
C	0.0000	0.0000	1.9198
C	0.0000	0.0000	3.2950
N	0.0000	0.0000	4.4429

SCF = -466.675056**22-OCH2**

I	-0.0287	-0.5029	-0.9366
C	-0.1981	-0.1513	1.0141
C	-0.3004	0.0638	2.1929
C	-0.4172	0.3110	3.5405
N	-0.5147	0.5192	4.6655
O	0.2209	-0.7654	-3.7999
C	0.2966	0.2408	-4.4489
H	0.3902	0.2060	-5.5412
H	0.2755	1.2320	-3.9761

SCF = -581.213395**22-Cl**

I	0.0258	-0.0546	-0.8610
Cl	0.3056	-0.1429	-3.5715
C	-0.1900	0.0152	1.2206
C	-0.3156	0.0565	2.4262
C	-0.4574	0.1017	3.7895
N	-0.5767	0.1398	4.9346

SCF = -927.001693**23**

I	0.0000	0.0000	-0.5123
C	0.0000	0.0000	1.4755
N	0.0000	0.0000	2.6216

SCF = -390.506157**23-OCH2**

I	-0.0025	-0.3307	-0.9348
C	-0.1695	0.1600	1.0020
N	-0.2656	0.4442	2.1085
O	0.2325	-0.7862	-3.7417
C	0.2890	0.1753	-4.4576
H	0.3798	0.0675	-5.5451
H	0.2524	1.1956	-4.0527

SCF = -505.045254**23-Cl**

I	0.0204	-0.0532	-0.8161
Cl	0.2997	-0.1414	-3.5100
C	-0.1989	0.0187	1.3024
N	-0.3182	0.0578	2.4467

SCF = -850.833230

24				24-OCH2			
C	4.9698	2.0504	0.3277	C	-0.9959	0.4392	1.5956
C	3.5879	-0.2936	-0.1692	C	1.0325	-0.4454	3.2620
C	3.5879	2.0592	0.3293	C	-1.1192	-0.7816	2.2315
C	5.6643	0.8828	0.0801	C	0.1282	1.2182	1.7858
C	4.9699	-0.2848	-0.1675	C	1.1365	0.7718	2.6179
C	2.8840	0.8828	0.0800	C	-0.1046	-1.2317	3.0707
C	1.4023	0.8828	0.0799	C	-0.2053	-2.5355	3.7676
C	-1.4023	0.8828	0.0798	C	-0.1461	-4.9549	5.1825
C	0.6898	1.0377	-1.0958	C	0.2469	-3.6984	3.1708
C	0.6898	0.7279	1.2557	C	-0.6592	-2.6089	5.0722
C	-0.6899	0.7279	1.2556	C	-0.6301	-3.7991	5.7682
C	-0.6898	1.0377	-1.0959	C	0.2760	-4.8890	3.8669
C	-2.8841	0.8828	0.0798	C	0.0106	-6.1986	5.9726
C	-5.6643	0.8827	0.0797	C	0.3441	-8.5144	7.4670
C	-3.5880	2.0589	0.3299	C	-0.9777	-7.1783	5.9768
C	-3.5880	-0.2934	-0.1703	C	1.1718	-6.3867	6.7234
C	-4.9699	-0.2846	-0.1687	C	1.3260	-7.5429	7.4631
C	-4.9699	2.0501	0.3282	C	-0.8042	-8.3284	6.7232
I	-2.6241	-2.0960	-0.5466	I	2.6934	-4.9638	6.7527
I	2.6241	-2.0964	-0.5444	I	2.5915	-1.0704	4.4955
F	-6.9893	0.8827	0.0797	F	0.5030	-9.6206	8.1809
F	-5.6698	-1.3870	-0.4022	F	2.4161	-7.7596	8.1898
F	-5.6699	3.1525	0.5617	F	-1.7263	-9.2829	6.7508
F	-1.3412	1.1869	-2.2469	F	0.7527	-5.9804	3.2718
F	1.3413	1.1869	-2.2469	F	0.6970	-3.6651	1.9181
F	1.3412	0.5787	2.4067	F	-1.0927	-1.5078	5.6824
F	-1.3414	0.5787	2.4066	F	-1.0373	-3.8226	7.0356
F	5.6698	3.1529	0.5604	F	-1.9446	0.8997	0.7895
F	6.9893	0.8828	0.0801	F	0.2387	2.3885	1.1720
F	5.6698	-1.3873	-0.4002	F	2.2024	1.5486	2.7736
I	2.6241	3.8620	0.7044	O	4.6125	-2.4819	6.4257
I	-2.6243	3.8615	0.7063	C	5.6822	-2.1541	6.8595
SCF = -2875.466931				H	6.2434	-2.8023	7.5442
ZPE = 0.141059				H	6.1387	-1.1941	6.5874
H₂₉₈ = -2875.295390				I	-2.7339	-6.9671	4.8855
G₂₉₈ = -2875.386260				I	-2.8413	-1.8962	1.8990
				SCF = -2990.010455			
				ZPE = 0.169561			
				H₂₉₈ = -2989.805664			
				G₂₉₈ = -2989.906623			

24-Cl

C	-0.8577	0.4239	1.5703
C	0.9694	-0.4752	3.4756
C	-1.0363	-0.8106	2.1615
C	0.2206	1.2095	1.9220
C	1.1199	0.7547	2.8667
C	-0.1275	-1.2629	3.1130
C	-0.2896	-2.5853	3.7647
C	-0.2806	-5.0155	5.1696
C	0.2782	-3.7224	3.2210
C	-0.8966	-2.6974	5.0018
C	-0.8926	-3.8909	5.6916
C	0.2826	-4.9161	3.9110
C	-0.1101	-6.2394	5.9901
C	0.2506	-8.5030	7.5391
C	-1.0135	-7.2944	5.9084
C	0.9880	-6.3125	6.8528
C	1.1448	-7.4528	7.6153
C	-0.8287	-8.4216	6.6834
I	2.3984	-4.7246	6.9905
I	2.3860	-1.1411	4.9182
F	0.4228	-9.5945	8.2849
F	2.1688	-7.5884	8.4575
F	-1.6728	-9.4538	6.6337
F	0.8807	-5.9784	3.3689
F	0.8726	-3.6586	2.0282
F	-1.4548	-1.6242	5.5632
F	-1.4475	-3.9430	6.9031
F	-1.7071	0.8929	0.6543
F	0.3867	2.4008	1.3470
F	2.1429	1.5556	3.1647
Cl	4.1621	-2.3583	6.9358
I	-2.6848	-1.9457	1.5878
I	-2.6628	-7.2345	4.6378

SCF = -3335.807336**ZPE = 0.141185****H₂₉₈ = -3335.633571****G₂₉₈ = -3335.727975****25**

C	0.3024	-1.3048	0.2410
C	-0.3193	1.3785	-0.0060
C	1.3426	-0.3941	0.1922
C	-1.0322	-0.9461	0.1745
C	-1.3011	0.4055	0.0527
C	0.9900	0.9378	0.0674
C	2.7572	-0.8234	0.2671
C	5.4167	-1.6352	0.4093
C	3.3903	-1.3713	-0.8483
C	3.4759	-0.6877	1.4546
C	4.7958	-1.0920	1.5163
C	4.7101	-1.7732	-0.7688
C	-2.1137	-1.9555	0.2212
C	-4.1470	-3.8554	0.3038
C	-2.4914	-2.5349	1.4321
C	-2.7690	-2.3418	-0.9480
C	-3.7782	-3.2844	-0.8980
C	-3.5008	-3.4782	1.4641
C	-0.6524	2.8137	-0.1484
C	-1.2835	5.5116	-0.4195
C	-0.5379	3.4461	-1.3863
C	-1.0870	3.5523	0.9517
C	-1.3996	4.8907	0.8082
C	-0.8519	4.7859	-1.5119
I	2.6244	0.1054	3.1780
I	2.4144	-1.6036	-2.6699
I	-2.2734	-1.5480	-2.8048
I	-1.5875	-2.0218	3.2332
I	0.0908	2.4339	-3.0905
I	-1.2785	2.7083	2.8419
F	0.6021	-2.5977	0.3571
F	-2.5744	0.7911	-0.0148
F	1.9641	1.8449	0.0130
F	-4.4193	-3.6727	-1.9929
F	-5.1151	-4.7597	0.3434
F	-3.8830	-4.0463	2.6007
F	5.5047	-0.9771	2.6321
F	6.6825	-2.0218	0.4771
F	5.3393	-2.2973	-1.8128
F	-1.5842	6.7959	-0.5486
F	-1.8150	5.6197	1.8361
F	-0.7543	5.4146	-2.6762

SCF = -3899.261918**ZPE = 0.185020****H₂₉₈ = -3899.036429****G₂₉₈ = -3899.147810**

25-OCH2

C	0.3001	-1.2978	0.3182
C	-0.3149	1.3900	0.1076
C	1.3420	-0.3891	0.2810
C	-1.0332	-0.9345	0.2564
C	-1.2988	0.4190	0.1533
C	0.9928	0.9453	0.1756
C	2.7582	-0.8223	0.3088
C	5.4224	-1.6223	0.3476
C	3.4442	-1.0501	-0.8844
C	3.4228	-1.0046	1.5199
C	4.7465	-1.4015	1.5309
C	4.7672	-1.4464	-0.8551
C	-2.1165	-1.9444	0.2534
C	-4.1466	-3.8464	0.2346
C	-2.7683	-2.2928	1.4348
C	-2.4969	-2.5589	-0.9400
C	-3.5052	-3.5030	-0.9392
C	-3.7759	-3.2383	1.4175
C	-0.6447	2.8234	-0.0686
C	-1.2755	5.5085	-0.4207
C	-0.8185	3.3440	-1.3517
C	-0.7864	3.6641	1.0329
C	-1.1005	4.9974	0.8500
C	-1.1323	4.6789	-1.5153
I	2.4802	-0.7009	3.3471
I	2.5164	-0.8214	-2.7312
I	-1.5899	-2.0763	-2.7482
I	-2.2748	-1.4245	3.2577
I	-0.5934	2.1484	-3.0397
I	-0.5311	2.9752	2.9774
F	0.5973	-2.5942	0.4049
F	-2.5714	0.8072	0.0750
F	1.9700	1.8499	0.1189
F	-3.8912	-4.1059	-2.0574
F	-5.1141	-4.7531	0.2259
F	-4.4152	-3.5917	2.5259
F	5.4073	-1.5816	2.6680
F	6.6926	-2.0025	0.3664
F	5.4481	-1.6712	-1.9724
F	-1.5771	6.7891	-0.5881
F	-1.2435	5.8241	1.8789
F	-1.3037	5.2068	-2.7219
O	0.0960	-0.1840	-5.0952
C	0.1098	-0.1301	-6.2944
H	0.4151	-0.9921	-6.9010
H	-0.1819	0.7828	-6.8292

SCF = -4013.790942**ZPE = 0.213332****H₂₉₈ = -4013.532165****G₂₉₈ = -4013.654366****25-Cl**

C	0.2954	-1.2944	0.3934
C	-0.3245	1.3883	0.1480
C	1.3362	-0.3854	0.3460
C	-1.0383	-0.9358	0.3239
C	-1.3055	0.4155	0.2043
C	0.9834	0.9461	0.2247
C	2.7535	-0.8211	0.3264
C	5.4046	-1.6326	0.2718
C	3.3698	-1.0978	-0.8981
C	3.4731	-0.9553	1.5111
C	4.7929	-1.3596	1.4780
C	4.6904	-1.5002	-0.9028
C	-2.1182	-1.9510	0.2800
C	-4.1351	-3.8513	0.1810
C	-2.7364	-2.3828	1.4507
C	-2.5170	-2.4764	-0.9532
C	-3.5226	-3.4219	-0.9799
C	-3.7403	-3.3291	1.3955
C	-0.6532	2.8156	-0.0848
C	-1.2670	5.4816	-0.5389
C	-0.7561	3.2908	-1.3961
C	-0.8587	3.6828	0.9853
C	-1.1640	5.0092	0.7533
C	-1.0627	4.6214	-1.5999
I	2.6136	-0.5602	3.3660
I	2.3049	-0.9080	-2.7033
I	-1.6075	-1.8350	-2.7387
I	-2.1923	-1.6359	3.3161
I	-0.4434	2.0059	-3.0330
I	-0.7193	3.0385	2.9601
Cl	0.1470	-0.4240	-4.9020
F	0.5952	-2.5917	0.4877
F	-2.5806	0.8000	0.1129
F	1.9605	1.8527	0.1518
F	-3.9420	-3.9563	-2.1255
F	-5.1043	-4.7644	0.1348
F	-4.3543	-3.7653	2.4960
F	5.5120	-1.4981	2.5924
F	6.6785	-2.0221	0.2470
F	5.3271	-1.7763	-2.0396
F	-1.5618	6.7627	-0.7556
F	-1.3670	5.8674	1.7536
F	-1.1729	5.1278	-2.8268

SCF = -4359.608344**ZPE = 0.185144****H₂₉₈ = -4359.380619****G₂₉₈ = -4359.495563**

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H	-1.4175	0.8796	-2.0659
C	-1.3267	1.6028	-1.2717
C	-1.0880	3.4699	0.8100
C	-1.1290	1.2408	0.0398
C	-1.4053	2.9636	-1.5297
C	-1.2863	3.8833	-0.4949
C	-1.0030	2.1126	1.1150
H	-1.5598	3.3004	-2.5425
H	-1.3495	4.9380	-0.7114
H	-0.9985	4.2019	1.5971
C	-0.7968	1.5450	2.4464
C	-0.4092	0.2246	4.8933
C	-0.7378	0.1618	2.5704
C	-0.6502	2.2678	3.6290
C	-0.4593	1.6119	4.8316
C	-0.5504	-0.5346	3.7409
H	-0.6857	3.3456	3.6054
H	-0.3477	2.1884	5.7363
H	-0.5132	-1.6114	3.7757
H	-0.2600	-0.2735	5.8381
I	-0.9747	-0.7493	0.6934

SCF = -759.585353**ZPE = 0.162540****H₂₉₈ = -759.412096****G₂₉₈ = -759.459048****26-Cl**

H	-1.4186	0.8685	-2.0509
C	-1.3291	1.6048	-1.2682
C	-1.0871	3.4556	0.8134
C	-1.1320	1.2145	0.0356
C	-1.4055	2.9665	-1.5219
C	-1.2850	3.8836	-0.4862
C	-1.0054	2.0952	1.1053
H	-1.5596	3.3061	-2.5342
H	-1.3461	4.9406	-0.6950
H	-0.9951	4.1791	1.6083
C	-0.7981	1.5327	2.4428
C	-0.4114	0.2293	4.8753
C	-0.7469	0.1475	2.5201
C	-0.6513	2.2703	3.6162
C	-0.4596	1.6180	4.8204
C	-0.5560	-0.5174	3.7165
H	-0.6858	3.3485	3.5928
H	-0.3463	2.1935	5.7261
H	-0.5190	-1.5964	3.7557
H	-0.2614	-0.2691	5.8207
I	-0.9888	-0.8029	0.6277
Cl	-1.3250	-1.5674	-1.8860

SCF = -1220.040641**ZPE = 0.163640****H₂₉₈ = -1219.864416****G₂₉₈ = -1219.915522****26-OCH2**

H	-1.3658	1.2843	-2.0915
C	-1.2889	1.9545	-1.2521
C	-1.0821	3.6553	0.9710
C	-1.1024	1.4913	0.0286
C	-1.3724	3.3313	-1.4025
C	-1.2695	4.1691	-0.2991
C	-0.9923	2.2787	1.1695
H	-1.5186	3.7457	-2.3876
H	-1.3365	5.2373	-0.4330
H	-1.0050	4.3232	1.8144
C	-0.7952	1.6130	2.4567
C	-0.4237	0.1165	4.7965
C	-0.7291	0.2241	2.4633
C	-0.6664	2.2480	3.6902
C	-0.4832	1.5043	4.8416
C	-0.5480	-0.5506	3.5874
H	-0.7095	3.3241	3.7486
H	-0.3852	2.0106	5.7889
H	-0.5032	-1.6271	3.5425
H	-0.2806	-0.4509	5.7025
I	-0.9429	-0.5438	0.5310
O	-1.2900	-1.0768	-2.3148
C	-1.3710	-1.8790	-3.2098
H	-1.2986	-2.9555	-3.0209
H	-1.5203	-1.5563	-4.2454

SCF = -874.135334**ZPE = 0.191598****H₂₉₈ = -873.928417****G₂₉₈ = -873.985474**

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H	-0.0620	0.1545	0.1864
C	-0.0597	0.1512	1.2643
C	-0.0526	0.1253	4.0761
C	-0.0652	-1.0094	2.0045
C	-0.0502	1.3363	1.9793
C	-0.0466	1.3104	3.3698
C	-0.0620	-1.0889	3.3909
H	-0.0444	2.2807	1.4562
H	-0.0487	0.1454	5.1540
C	-0.0685	-2.4136	4.0081
C	-0.0824	-5.0545	4.9569
C	-0.0773	-3.5262	3.1771
C	-0.0669	-2.6701	5.3786
C	-0.0738	-3.9732	5.8316
C	-0.0842	-4.8395	3.5897
H	-0.0604	-1.8575	6.0872
H	-0.0908	-5.6670	2.8988
H	-0.0876	-6.0625	5.3434
I	-0.0786	-2.9326	1.1650
C	-0.0428	2.6334	4.0954
C	-0.0720	-4.2696	7.3112
F	1.0032	3.3703	3.7158
F	0.0192	2.4700	5.4167
F	-1.1502	3.3228	3.8117
F	-0.0667	-3.1523	8.0376
F	-1.1520	-4.9797	7.6450
F	1.0041	-4.9874	7.6408

SCF = -1433.909462**ZPE = 0.172009****H₂₉₈ = -1433.719374****G₂₉₈ = -1433.783033****27-OCH2**

H	-0.0659	0.5645	0.3100
C	-0.0622	0.4833	1.3851
C	-0.0519	0.2620	4.1847
C	-0.0669	-0.7342	2.0329
C	-0.0519	1.6162	2.1786
C	-0.0467	1.4939	3.5642
C	-0.0623	-0.8983	3.4124
H	-0.0470	2.5952	1.7236
H	-0.0472	0.2061	5.2612
C	-0.0684	-2.2638	3.9338
C	-0.0820	-4.9604	4.7010
C	-0.0781	-3.3165	3.0270
C	-0.0656	-2.6121	5.2838
C	-0.0724	-3.9424	5.6479
C	-0.0851	-4.6543	3.3510
H	-0.0583	-1.8489	6.0451
H	-0.0927	-5.4215	2.5957
H	-0.0873	-5.9922	5.0184
I	-0.0812	-2.5822	1.0598
C	-0.0397	2.7620	4.3795
C	-0.0689	-4.3375	7.1028
F	1.0171	3.5158	4.0649
F	0.0054	2.5091	5.6878
F	-1.1372	3.4830	4.1335
F	-0.0658	-3.2727	7.9051
F	-1.1465	-5.0723	7.3915
F	1.0091	-5.0741	7.3857
O	-0.0950	-5.3452	0.2454
C	-0.0954	-6.1486	-0.6538
H	-0.1029	-7.2236	-0.4484
H	-0.0885	-5.8325	-1.7021

SCF = -1548.461971**ZPE = 0.201171****H₂₉₈ = -1548.238142****G₂₉₈ = -1548.311868**

27-Cl

H	-0.0640	0.1379	0.2043
C	-0.0613	0.1291	1.2843
C	-0.0534	0.1106	4.0811
C	-0.0661	-1.0599	1.9922
C	-0.0523	1.3194	1.9869
C	-0.0483	1.2980	3.3787
C	-0.0624	-1.0932	3.3785
H	-0.0476	2.2647	1.4653
H	-0.0497	0.1287	5.1588
C	-0.0683	-2.4251	3.9885
C	-0.0806	-5.0487	4.9543
C	-0.0767	-3.5313	3.1466
C	-0.0663	-2.6687	5.3608
C	-0.0724	-3.9668	5.8266
C	-0.0828	-4.8361	3.5873
H	-0.0601	-1.8490	6.0603
H	-0.0891	-5.6519	2.8824
H	-0.0853	-6.0560	5.3423
I	-0.0791	-3.0043	1.1078
Cl	-0.0948	-5.5438	0.4545
C	-0.0431	2.6140	4.0985
C	-0.0705	-4.2512	7.3003
F	1.0132	3.3598	3.7411
F	-0.0002	2.4674	5.4272
F	-1.1391	3.3314	3.8083
F	-0.0633	-3.1322	8.0336
F	-1.1501	-4.9606	7.6588
F	1.0037	-4.9712	7.6539

SCF = -1894.381738**ZPE = 0.173333****H₂₉₈ = -1894.188472****G₂₉₈ = -1894.256371****28**

H	-0.1640	0.1528	0.1759
C	-0.1284	0.1482	1.2533
C	-0.0362	0.1177	4.0633
C	-0.1236	-1.0125	1.9914
C	-0.0851	1.3360	1.9634
C	-0.0393	1.3134	3.3574
C	-0.0791	-1.0921	3.3793
H	-0.0864	2.2795	1.4411
H	-0.0002	0.1410	5.1409
C	-0.0811	-2.4185	3.9953
C	-0.0942	-5.0670	4.9368
C	-0.1277	-3.5302	3.1605
C	-0.0399	-2.6767	5.3609
C	-0.0466	-3.9876	5.8190
C	-0.1360	-4.8430	3.5711
H	-0.0024	-1.8686	6.0742
H	-0.1728	-5.6691	2.8794
H	-0.0983	-6.0749	5.3205
I	-0.1836	-2.9332	1.1511
C	0.0057	2.5507	4.0815
N	0.0418	3.5353	4.6629
C	-0.0038	-4.2329	7.2315
N	0.0302	-4.4243	8.3589

SCF = -944.096422**ZPE = 0.159018****H₂₉₈ = -943.922906****G₂₉₈ = -943.978052**

28-OCH2

H	-0.1407	0.5945	0.3366
C	-0.1104	0.5008	1.4104
C	-0.0322	0.2456	4.2060
C	-0.1096	-0.7230	2.0435
C	-0.0706	1.6285	2.2115
C	-0.0319	1.4944	3.5994
C	-0.0718	-0.9021	3.4227
H	-0.0694	2.6114	1.7677
H	-0.0016	0.1823	5.2821
C	-0.0775	-2.2749	3.9282
C	-0.0975	-4.9865	4.6589
C	-0.1201	-3.3168	3.0066
C	-0.0439	-2.6387	5.2697
C	-0.0539	-3.9810	5.6239
C	-0.1316	-4.6572	3.3142
H	-0.0098	-1.8884	6.0436
H	-0.1657	-5.4148	2.5498
H	-0.1044	-6.0211	4.9628
I	-0.1656	-2.5588	1.0494
C	0.0091	2.6698	4.4207
N	0.0419	3.6053	5.0787
C	-0.0187	-4.3372	7.0131
N	0.0095	-4.6191	8.1216
O	-0.2211	-5.3002	0.2123
C	-0.2498	-6.0814	-0.7064
H	-0.2591	-7.1608	-0.5268
H	-0.2673	-5.7396	-1.7463

SCF = -1058.649946**ZPE = 0.188224****H₂₉₈ = -1058.442666****G₂₉₈ = -1058.507676****28-Cl**

H	-0.1594	0.1358	0.1952
C	-0.1255	0.1273	1.2747
C	-0.0379	0.1053	4.0708
C	-0.1210	-1.0605	1.9825
C	-0.0859	1.3204	1.9725
C	-0.0422	1.3019	3.3674
C	-0.0778	-1.0943	3.3700
H	-0.0882	2.2653	1.4525
H	-0.0035	0.1294	5.1485
C	-0.0788	-2.4280	3.9783
C	-0.0893	-5.0598	4.9363
C	-0.1226	-3.5335	3.1330
C	-0.0391	-2.6736	5.3457
C	-0.0444	-3.9795	5.8151
C	-0.1293	-4.8380	3.5707
H	-0.0041	-1.8593	6.0515
H	-0.1645	-5.6521	2.8643
H	-0.0929	-6.0666	5.3224
I	-0.1777	-3.0050	1.0950
Cl	-0.2357	-5.5350	0.4448
C	-0.0007	2.5417	4.0886
N	0.0323	3.5313	4.6638
C	-0.0032	-4.2159	7.2300
N	0.0297	-4.4015	8.3594

SCF = -1404.576069**ZPE = 0.160548****H₂₉₈ = -1404.399228****G₂₉₈ = -1404.458315**

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H	0.0219	0.1663	0.1963
C	-0.0508	0.1379	1.2718
C	-0.2395	0.0639	4.0608
C	-0.0446	-1.0459	1.9766
C	-0.1541	1.3116	1.9850
C	-0.2510	1.3073	3.3972
C	-0.1362	-1.1269	3.3615
H	-0.1597	2.2393	1.4402
H	-0.3117	0.0277	5.1331
C	-0.1160	-2.4633	3.9673
C	-0.0585	-5.1050	4.8940
C	-0.0058	-3.5558	3.1146
C	-0.1986	-2.7243	5.3248
C	-0.1725	-4.0427	5.8225
C	0.0249	-4.8657	3.5402
H	-0.2845	-1.8958	6.0051
H	0.1110	-5.6915	2.8520
H	-0.0349	-6.1257	5.2332
I	0.1029	-2.9452	1.1187
N	-0.3518	2.4652	4.0884
N	-0.2540	-4.2884	7.1497
C	-0.3620	3.7349	3.3862
H	0.5596	3.8831	2.8232
H	-0.4479	4.5344	4.1113
H	-1.2087	3.8023	2.7028
C	-0.4510	2.4400	5.5335
H	0.4292	1.9776	5.9822
H	-1.3400	1.8983	5.8595
H	-0.5219	3.4568	5.8986
C	-0.3708	-3.1879	8.0847
H	0.4930	-2.5245	8.0244
H	-0.4218	-3.5854	9.0905
H	-1.2760	-2.6075	7.9015
C	-0.2273	-5.6534	7.6412
H	0.7045	-6.1520	7.3735
H	-1.0635	-6.2318	7.2481
H	-0.3046	-5.6374	8.7210

SCF = -1027.605461**ZPE = 0.310669****H₂₉₈ = -1027.275016****G₂₉₈ = -1027.340460****29-Cl**

H	-0.0066	0.1478	0.2089
C	-0.0364	0.1125	1.2886
C	-0.1315	0.0552	4.0653
C	-0.0163	-1.0933	1.9619
C	-0.1002	1.2953	1.9994
C	-0.1375	1.2921	3.4076
C	-0.0664	-1.1328	3.3475
H	-0.1206	2.2237	1.4549
H	-0.1771	0.0178	5.1392
C	-0.0503	-2.4737	3.9478
C	-0.0229	-5.0959	4.8956
C	0.0137	-3.5635	3.0881
C	-0.0984	-2.7238	5.3134
C	-0.0755	-4.0318	5.8165
C	0.0252	-4.8647	3.5351
H	-0.1531	-1.8881	5.9880
H	0.0679	-5.6802	2.8303
H	-0.0191	-6.1164	5.2369
I	0.0722	-3.0159	1.0642
Cl	0.1702	-5.5950	0.3733
N	-0.1735	2.4718	4.1151
N	-0.1002	-4.2696	7.1676
C	-0.4473	3.7031	3.4071
H	0.3360	3.9149	2.6816
H	-0.4646	4.5198	4.1200
H	-1.4073	3.6759	2.8829
C	-0.4539	2.4237	5.5319
H	0.3250	1.8769	6.0614
H	-1.4171	1.9511	5.7485
H	-0.4684	3.4354	5.9214
C	-0.3668	-3.1724	8.0686
H	0.4111	-2.4130	7.9958
H	-0.3696	-3.5459	9.0863
H	-1.3326	-2.6986	7.8681
C	-0.3025	-5.6215	7.6415
H	0.5109	-6.2704	7.3215
H	-1.2450	-6.0468	7.2860
H	-0.3127	-5.6140	8.7256

SCF = -1488.041905**ZPE = 0.311961****H₂₉₈ = -1487.708492****G₂₉₈ = -1487.777586**

29-OCH2

H	-0.0220	0.4946	0.2617
C	-0.0859	0.4113	1.3353
C	-0.2516	0.2036	4.1156
C	-0.0764	-0.8115	1.9734
C	-0.1800	1.5501	2.1044
C	-0.2654	1.4770	3.5146
C	-0.1571	-0.9501	3.3547
H	-0.1872	2.5039	1.6067
H	-0.3151	0.1152	5.1854
C	-0.1351	-2.3152	3.8933
C	-0.0746	-4.9952	4.6952
C	-0.0361	-3.3664	2.9882
C	-0.2049	-2.6395	5.2386
C	-0.1766	-3.9785	5.6732
C	-0.0041	-4.6944	3.3521
H	-0.2822	-1.8435	5.9575
H	0.0734	-5.4779	2.6166
H	-0.0499	-6.0307	4.9860
I	0.0573	-2.6588	1.0225
N	-0.3578	2.6018	4.2635
N	-0.2448	-4.2858	6.9907
C	-0.3711	3.9032	3.6243
H	0.5470	4.0787	3.0628
H	-0.4519	4.6668	4.3878
H	-1.2215	4.0048	2.9496
C	-0.4433	2.5055	5.7057
H	0.4395	2.0190	6.1232
H	-1.3303	1.9499	6.0138
H	-0.5079	3.5032	6.1216
C	-0.3478	-3.2296	7.9757
H	0.5160	-2.5644	7.9352
H	-0.3870	-3.6723	8.9632
H	-1.2538	-2.6393	7.8309
C	-0.2150	-5.6711	7.4175
H	0.7127	-6.1587	7.1169
H	-1.0559	-6.2305	7.0068
H	-0.2809	-5.7057	8.4978
O	0.2036	-5.4960	0.2087
C	0.2750	-6.3056	-0.6787
H	0.3006	-7.3796	-0.4643
H	0.3167	-5.9999	-1.7302

SCF = -1142.152274**ZPE = 0.339759****H₂₉₈ = -1141.788089****G₂₉₈ = -1141.863652****30**

H	1.5899	-0.2480	1.7798
C	0.6474	0.1223	2.1500
C	-1.8107	1.0675	3.0900
C	-0.4696	-0.6832	2.2431
C	0.5160	1.4455	2.5489
C	-0.7040	1.9024	3.0146
C	-1.7048	-0.2545	2.6961
H	1.3615	2.1122	2.4919
H	-2.7542	1.4500	3.4496
C	1.4407	-3.5971	3.9618
C	-0.6646	-4.6388	5.4872
C	0.1261	-3.5692	3.5308
C	1.6891	-4.1620	5.2001
C	0.6388	-4.6746	5.9497
C	-0.9388	-4.0756	4.2484
H	2.6988	-4.2087	5.5798
H	-1.9483	-4.0453	3.8711
H	-1.4652	-5.0483	6.0822
I	-0.2794	-2.6979	1.6561
C	-0.8685	3.3315	3.4697
C	0.9628	-5.2692	7.2980
F	-1.1155	3.3740	4.7825
F	-1.8990	3.9063	2.8452
F	0.2229	4.0553	3.2290
F	1.4401	-4.3273	8.1171
F	-0.1102	-5.8121	7.8696
F	1.8983	-6.2145	7.1798
H	-2.5574	-0.9130	2.7403
H	2.2466	-3.2023	3.3643

SCF = -1435.101530**ZPE = 0.193448****H₂₉₈ = -1434.888485****G₂₉₈ = -1434.957002**

30-OCH2

H	1.3186	0.0762	1.2342
C	0.5151	0.3896	1.8820
C	-1.5716	1.1833	3.5593
C	-0.5139	-0.4649	2.2270
C	0.4880	1.6800	2.3950
C	-0.5478	2.0617	3.2275
C	-1.5667	-0.1023	3.0510
H	1.2717	2.3773	2.1460
H	-2.3724	1.5070	4.2071
C	1.0887	-2.9761	3.9714
C	-0.6252	-4.9629	4.9371
C	-0.0375	-3.3823	3.2831
C	1.3482	-3.5895	5.1855
C	0.4929	-4.5750	5.6562
C	-0.9099	-4.3558	3.7223
H	2.2128	-3.2997	5.7624
H	-1.7729	-4.6467	3.1464
H	-1.2815	-5.7266	5.3235
I	-0.4722	-2.4188	1.4583
C	-0.5949	3.4493	3.8148
C	0.8218	-5.2608	6.9577
F	-0.4907	3.3955	5.1468
F	-1.7562	4.0431	3.5258
F	0.3912	4.2173	3.3537
F	1.3525	-4.4028	7.8320
F	-0.2634	-5.8025	7.5123
F	1.7116	-6.2394	6.7590
H	-2.3588	-0.7929	3.2940
H	1.7433	-2.2073	3.5919
O	-0.5263	-5.1994	0.7197
C	-0.1693	-6.1176	0.0264
H	-0.6671	-7.0913	0.0814
H	0.6615	-6.0122	-0.6797

SCF = -1549.651148**ZPE = 0.222598****H₂₉₈ = -1549.404411****G₂₉₈ = -1549.482033****30-Cl**

H	1.2241	-0.2516	0.9560
C	0.4977	0.0515	1.6963
C	-1.3605	0.8295	3.6107
C	-0.4043	-0.8600	2.2131
C	0.4736	1.3693	2.1391
C	-0.4522	1.7459	3.0935
C	-1.3404	-0.4785	3.1649
H	1.1721	2.0906	1.7463
H	-2.0791	1.1446	4.3527
C	0.8994	-2.9149	4.1622
C	-0.4917	-5.1269	5.1268
C	-0.0225	-3.5889	3.3866
C	1.1269	-3.3686	5.4515
C	0.4265	-4.4656	5.9264
C	-0.7229	-4.6901	3.8316
H	1.8444	-2.8665	6.0812
H	-1.4047	-5.2111	3.1798
H	-1.0307	-5.9790	5.5094
I	-0.3940	-2.8763	1.4300
Cl	-0.3673	-5.4117	0.7156
C	-0.5032	3.1537	3.6079
C	0.7073	-4.9732	7.3106
F	-0.2458	3.2000	4.9247
F	-1.7192	3.6929	3.4333
F	0.3812	3.9507	2.9993
F	1.0507	-3.9799	8.1418
F	-0.3555	-5.5923	7.8388
F	1.7191	-5.8539	7.3123
H	-2.0441	-1.1957	3.5623
H	1.4288	-2.0544	3.7857

SCF = -1895.560748**ZPE = 0.194547****H₂₉₈ = -1895.344763****G₂₉₈ = -1895.416592**

31

H	1.5845	-0.3121	2.0792
C	0.6027	0.0594	2.3253
C	-1.9596	1.0116	2.9363
C	-0.5278	-0.7296	2.2197
C	0.4338	1.3634	2.7580
C	-0.8416	1.8320	3.0629
C	-1.8089	-0.2954	2.5056
H	1.2857	2.0176	2.8566
H	-2.9394	1.3965	3.1712
C	1.3373	-3.7679	3.8939
C	-0.8530	-4.7109	5.3630
C	0.0353	-3.6522	3.4434
C	1.5370	-4.3721	5.1234
C	0.4449	-4.8374	5.8514
C	-1.0708	-4.1097	4.1353
H	2.5347	-4.4858	5.5171
H	-2.0706	-4.0124	3.7437
H	-1.6843	-5.0839	5.9403
I	-0.2828	-2.7219	1.5807
H	-2.6679	-0.9380	2.3976
H	2.1755	-3.4098	3.3180
C	-1.0067	3.1840	3.5121
N	-1.1378	4.2618	3.8730
C	0.6607	-5.4604	7.1251
N	0.8323	-5.9552	8.1424

SCF = -945.289732**ZPE = 0.180371****H₂₉₈ = -945.093310****G₂₉₈ = -945.152704****31-Cl**

H	1.3572	-0.7349	3.1638
C	0.4044	-0.2639	2.9690
C	-2.0524	0.9480	2.4628
C	-0.5641	-0.9139	2.2179
C	0.1428	0.9939	3.4799
C	-1.0875	1.5974	3.2245
C	-1.7865	-0.3161	1.9591
H	0.8811	1.5146	4.0694
H	-2.9996	1.4289	2.2746
C	1.2766	-4.4240	3.4789
C	-0.4769	-3.7519	5.5486
C	0.1801	-3.6125	3.2715
C	1.5023	-4.8983	4.7597
C	0.6280	-4.5624	5.7890
C	-0.7044	-3.2644	4.2733
H	2.3521	-5.5308	4.9614
H	-1.5529	-2.6284	4.0776
H	-1.1531	-3.5102	6.3532
I	-0.1566	-2.8473	1.3300
Cl	0.4072	-5.2737	0.5038
H	-2.5368	-0.8274	1.3732
H	1.9179	-4.7058	2.6599
C	-1.3605	2.9025	3.7540
N	-1.5789	3.9437	4.1781
C	0.8661	-5.0583	7.1141
N	1.0568	-5.4493	8.1734

SCF = -1405.755863**ZPE = 0.181832****H₂₉₈ = -1405.556220****G₂₉₈ = -1405.618891**

31-OCH2

H	1.5239	-0.1701	2.8897
C	0.5162	0.2143	2.8683
C	-2.1004	1.2025	2.7861
C	-0.5110	-0.4758	2.2481
C	0.2156	1.4234	3.4688
C	-1.0885	1.9122	3.4253
C	-1.8139	-0.0136	2.1882
H	0.9861	1.9918	3.9655
H	-3.1028	1.5998	2.7604
C	1.3932	-4.0258	3.3525
C	-0.6918	-4.1156	5.2209
C	0.1780	-3.4065	3.1399
C	1.5576	-4.7145	4.5430
C	0.5202	-4.7547	5.4701
C	-0.8752	-3.4298	4.0328
H	2.4889	-5.2151	4.7560
H	-1.8103	-2.9333	3.8262
H	-1.4848	-4.1614	5.9505
I	-0.0755	-2.3227	1.3491
H	-2.5913	-0.5729	1.6917
H	2.1835	-3.9914	2.6208
C	-1.3924	3.1675	4.0493
N	-1.6353	4.1675	4.5497
C	0.7018	-5.4669	6.7019
N	0.8470	-6.0357	7.6842
O	0.7290	-4.9102	0.4136
C	0.5669	-5.8702	-0.2965
H	1.3420	-6.6375	-0.3908
H	-0.3564	-6.0087	-0.8692

SCF = -1059.840168**ZPE = 0.209375****H₂₉₈ = -1059.610126****G₂₉₈ = -1059.679295****32**

H	1.5892	-0.2130	2.3745
C	0.5942	0.1420	2.5942
C	-1.9773	1.0604	3.1480
C	-0.5123	-0.6813	2.4446
C	0.4134	1.4346	3.0276
C	-0.8780	1.9347	3.3184
C	-1.7969	-0.2327	2.7156
H	1.2797	2.0635	3.1365
H	-2.9790	1.3973	3.3507
C	1.3537	-3.8729	4.0246
C	-0.8361	-4.9173	5.3940
C	0.0602	-3.6988	3.5541
C	1.5537	-4.5740	5.1907
C	0.4652	-5.1178	5.9128
C	-1.0364	-4.2172	4.2274
H	2.5621	-4.7050	5.5426
H	-2.0387	-4.0828	3.8509
H	-1.6946	-5.3173	5.9048
I	-0.2398	-2.6368	1.7915
H	-2.6528	-0.8777	2.5893
H	2.2016	-3.4718	3.4908
N	-1.0553	3.2030	3.7396
N	0.6614	-5.8075	7.0544
C	-2.3904	3.6978	4.0202
H	-2.3207	4.7284	4.3445
H	-2.8651	3.1210	4.8139
H	-3.0201	3.6603	3.1312
C	0.0860	4.0860	3.8944
H	0.6068	4.2275	2.9473
H	0.7893	3.6950	4.6295
H	-0.2628	5.0516	4.2382
C	2.0062	-6.0131	7.5597
H	2.4937	-5.0634	7.7795
H	2.6157	-6.5664	6.8453
H	1.9516	-6.5869	8.4762
C	-0.4697	-6.3652	7.7726
H	-0.1065	-6.8740	8.6565
H	-1.0097	-7.0869	7.1596
H	-1.1599	-5.5830	8.0880

SCF = -1028.802542**ZPE = 0.332689****H₂₉₈ = -1028.448773****G₂₉₈ = -1028.517973**

32-Cl

H	1.5546	-0.5302	3.1051
C	0.5485	-0.1453	3.0158
C	-2.0223	0.8637	2.7944
C	-0.4213	-0.8756	2.3457
C	0.2420	1.0753	3.5833
C	-1.0580	1.6089	3.4938
C	-1.7025	-0.3619	2.2364
H	1.0203	1.6164	4.0940
H	-3.0271	1.2343	2.6838
C	1.3101	-4.5815	3.4852
C	-0.3363	-3.8379	5.5970
C	0.3164	-3.6406	3.3128
C	1.4863	-5.1488	4.7327
C	0.6750	-4.7874	5.8223
C	-0.5100	-3.2641	4.3512
H	2.2607	-5.8875	4.8470
H	-1.2849	-2.5270	4.2085
H	-1.0006	-3.5418	6.3905
I	0.0490	-2.7419	1.4213
Cl	0.6694	-5.1469	0.3659
H	-2.4687	-0.9157	1.7117
H	1.9133	-4.8994	2.6500
N	-1.3706	2.8120	4.0715
N	0.8641	-5.3423	7.0628
C	-2.6477	3.4226	3.7769
H	-2.7127	4.3700	4.2999
H	-3.4671	2.7943	4.1230
H	-2.7803	3.6045	2.7067
C	-0.3073	3.6424	4.5918
H	0.4217	3.9101	3.8217
H	0.2174	3.1385	5.4021
H	-0.7380	4.5532	4.9921
C	1.7486	-6.4797	7.1932
H	2.7668	-6.2113	6.9171
H	1.4323	-7.3221	6.5716
H	1.7595	-6.7973	8.2298
C	-0.1357	-5.1281	8.0849
H	0.1661	-5.6508	8.9855
H	-1.1216	-5.4930	7.7821
H	-0.2200	-4.0699	8.3276

SCF = -1489.222634**ZPE = 0.333372****H₂₉₈ = -1488.866330****G₂₉₈ = -1488.939113****32-OCH2**

H	1.6371	0.0358	2.5261
C	0.6211	0.3583	2.6953
C	-1.9988	1.1950	3.1233
C	-0.4515	-0.4627	2.3771
C	0.3848	1.6020	3.2335
C	-0.9333	2.0590	3.4649
C	-1.7594	-0.0494	2.5867
H	1.2281	2.2266	3.4714
H	-3.0194	1.5008	3.2746
C	1.4420	-3.8129	3.6936
C	-0.7854	-4.6481	5.1410
C	0.1584	-3.4859	3.2885
C	1.6140	-4.5635	4.8351
C	0.5059	-5.0000	5.5961
C	-0.9569	-3.9019	3.9967
H	2.6163	-4.8118	5.1381
H	-1.9535	-3.6501	3.6679
H	-1.6600	-4.9629	5.6832
I	-0.0951	-2.3426	1.5686
H	-2.5918	-0.6873	2.3311
H	2.3029	-3.4969	3.1252
N	-1.1660	3.2807	3.9906
N	0.6746	-5.7321	6.7194
C	-2.5271	3.7334	4.2047
H	-2.5025	4.7280	4.6318
H	-3.0562	3.0778	4.8964
H	-3.0817	3.7772	3.2670
C	-0.0564	4.1549	4.3196
H	0.5343	4.3948	3.4352
H	0.5955	3.7006	5.0658
H	-0.4474	5.0784	4.7280
C	2.0092	-6.0818	7.1656
H	2.6014	-5.1911	7.3767
H	2.5311	-6.6820	6.4200
H	1.9332	-6.6627	8.0763
C	-0.4780	-6.1688	7.4828
H	-0.1364	-6.7339	8.3410
H	-1.1270	-6.8112	6.8871
H	-1.0589	-5.3191	7.8424
O	0.7197	-4.9853	0.5110
C	0.6660	-6.0756	0.0090
H	1.5713	-6.6739	-0.1467
H	-0.2874	-6.5122	-0.3116

SCF = -1143.345497**ZPE = 0.361209****H₂₉₈ = -1142.958334****G₂₉₈ = -1143.038254**

33

I	-1.3525	1.0879	-3.3275
C	-0.7400	0.4733	-1.4495
C	0.0808	-0.3347	1.0483
N	-0.9418	-0.7963	-1.0430
C	-0.1175	1.3784	-0.6090
C	0.2961	0.9758	0.6465
C	-0.5401	-1.1944	0.1812
H	0.0346	2.3885	-0.9511
H	0.7822	1.6791	1.3050
H	0.3871	-0.6907	2.0178
C	-1.6035	-1.7831	-1.9182
H	-1.0214	-1.8982	-2.8261
H	-2.6007	-1.4310	-2.1584
H	-1.6574	-2.7242	-1.3872
H	-0.7376	-2.2233	0.4304

SCF = -585.090389**ZPE = 0.121975****H₂₉₈ = -584.960231****G₂₉₈ = -585.001708****33-Cl**

I	-1.4004	1.1351	-3.4782
Cl	-2.1354	1.9842	-5.8136
C	-0.7495	0.4602	-1.4654
C	0.0842	-0.3468	1.0662
N	-0.9327	-0.7992	-1.0208
C	-0.1193	1.3566	-0.5995
C	0.2961	0.9689	0.6516
C	-0.5337	-1.2058	0.2051
H	0.0299	2.3663	-0.9488
H	0.7821	1.6728	1.3102
H	0.3928	-0.6954	2.0373
C	-1.5933	-1.7730	-1.9022
H	-1.0153	-1.8711	-2.8146
H	-2.5823	-1.4059	-2.1536
H	-1.6577	-2.7233	-1.3862
H	-0.7316	-2.2350	0.4544

SCF = -1045.514319**ZPE = 0.121972****H₂₉₈ = -1045.381869****G₂₉₈ = -1045.428648****33-OCH2**

I	-1.2086	1.0421	-3.3684
C	-0.6673	0.4433	-1.4578
C	0.0581	-0.3389	1.0856
N	-0.9521	-0.7975	-1.0112
C	-0.0031	1.3303	-0.6254
C	0.3620	0.9436	0.6480
C	-0.5989	-1.1834	0.2323
H	0.2178	2.3182	-0.9942
H	0.8790	1.6353	1.2952
H	0.3241	-0.6827	2.0712
C	-1.6578	-1.7662	-1.8697
H	-1.0695	-1.9421	-2.7637
H	-2.6262	-1.3599	-2.1407
H	-1.7799	-2.6868	-1.3144
H	-0.8650	-2.1900	0.5073
O	-1.9035	1.9558	-5.9553
C	-2.1704	2.3911	-7.0436
H	-1.4489	2.3443	-7.8673
H	-3.1444	2.8494	-7.2494

SCF = -699.635171**ZPE = 0.150511****H₂₉₈ = -699.472503****G₂₉₈ = -699.523034****34**

I	-1.3053	1.1301	-3.3462
C	-0.7064	0.5380	-1.4557
C	0.0610	-0.3400	1.0263
C	-0.8530	-0.7798	-1.0795
C	-0.1545	1.4359	-0.5500
C	0.2306	0.9863	0.7020
N	-0.4715	-1.1904	0.1389
H	-1.2726	-1.5290	-1.7315
H	-0.0266	2.4723	-0.8222
H	0.6637	1.6567	1.4263
H	0.3392	-0.7521	1.9823
H	-0.5490	-3.2217	-0.3601
C	-0.6867	-2.6013	0.5172
H	0.0381	-2.8720	1.2748
H	-1.6951	-2.7114	0.9034

SCF = -585.091458**ZPE = 0.121743****H₂₉₈ = -584.961179****G₂₉₈ = -585.003900**

34-Cl

I	-1.4124	1.1643	-3.4667
Cl	-2.2183	1.8667	-5.8615
C	-0.7391	0.5558	-1.4562
C	0.0733	-0.3489	1.0414
C	-0.8631	-0.7613	-1.0623
C	-0.1776	1.4281	-0.5273
C	0.2301	0.9781	0.7213
N	-0.4676	-1.1916	0.1487
H	-1.2855	-1.5140	-1.7121
H	-0.0573	2.4705	-0.7877
H	0.6699	1.6441	1.4464
H	0.3637	-0.7718	1.9887
H	-0.6649	-3.1999	-0.3789
C	-0.6743	-2.5965	0.5205
H	0.1282	-2.9097	1.1781
H	-1.6307	-2.6980	1.0241

SCF = -1045.499905**ZPE = 0.121695****H₂₉₈ = -1045.367412****G₂₉₈ = -1045.415089****35**

I	-1.4028	1.0025	-3.2824
C	-0.6956	0.4820	-1.4173
N	0.2387	-0.2068	1.0670
C	-0.7255	-0.8431	-0.9953
C	-0.1840	1.4530	-0.5620
C	0.2758	1.0761	0.6745
C	-0.2498	-1.1555	0.2538
H	-1.1151	-1.6266	-1.6243
H	-0.1439	2.4911	-0.8481
H	0.6832	1.7822	1.3802
H	-0.2468	-2.1638	0.6352
H	1.8492	-0.7570	2.2924
C	0.7824	-0.5795	2.3857
H	0.5958	0.2299	3.0811
H	0.2820	-1.4767	2.7283

SCF = -585.094207**ZPE = 0.121793****H₂₉₈ = -584.963920****G₂₉₈ = -585.006185****34-OCH2**

I	-1.3466	0.9726	-3.4152
C	-0.7188	0.4633	-1.5012
C	0.0713	-0.3119	1.0160
C	-0.8952	-0.8279	-1.0488
C	-0.1237	1.3848	-0.6468
C	0.2730	0.9897	0.6203
N	-0.5041	-1.1888	0.1824
H	-1.3484	-1.5972	-1.6533
H	0.0255	2.4033	-0.9713
H	0.7344	1.6839	1.3035
H	0.3561	-0.6844	1.9862
H	0.2122	-3.1537	0.3218
C	-0.6716	-2.5916	0.6067
H	-0.8029	-2.6167	1.6815
H	-1.5492	-3.0002	0.1210
O	-2.2521	1.5321	-6.0653
C	-2.3615	2.3471	-6.9415
H	-2.8246	2.0868	-7.9001
H	-2.0045	3.3766	-6.8167

SCF = -699.634308**ZPE = 0.150438****H₂₉₈ = -699.470641****G₂₉₈ = -699.523758****35-OCH2**

I	-1.3478	1.0938	-3.2689
C	-0.6577	0.5269	-1.4055
N	0.2483	-0.2219	1.0802
C	-0.7857	-0.7895	-0.9678
C	-0.0596	1.4553	-0.5560
C	0.3828	1.0518	0.6778
C	-0.3238	-1.1330	0.2771
H	-1.2440	-1.5430	-1.5872
H	0.0591	2.4858	-0.8483
H	0.8523	1.7272	1.3748
H	-0.3969	-2.1358	0.6662
H	1.8109	-0.9377	2.2821
C	0.7750	-0.6324	2.3929
H	0.7028	0.2054	3.0758
H	0.1799	-1.4572	2.7656
O	-2.4191	1.9479	-5.7923
C	-2.3828	2.0697	-6.9869
H	-1.5362	1.6978	-7.5766
H	-3.1990	2.5594	-7.5305

SCF = -699.636865**ZPE = 0.150306****H₂₉₈ = -699.473225****G₂₉₈ = -699.526416**

35-Cl

I	-1.4370	1.0333	-3.4007
Cl	-2.3193	1.7004	-5.7953
C	-0.7033	0.4856	-1.4336
N	0.2385	-0.2097	1.0829
C	-0.7213	-0.8398	-0.9816
C	-0.1849	1.4423	-0.5514
C	0.2742	1.0766	0.6834
C	-0.2509	-1.1593	0.2622
H	-1.1108	-1.6246	-1.6122
H	-0.1457	2.4821	-0.8389
H	0.6816	1.7789	1.3936
H	-0.2453	-2.1658	0.6499
H	1.8557	-0.7621	2.2993
C	0.7884	-0.5807	2.3879
H	0.6086	0.2262	3.0890
H	0.2907	-1.4775	2.7378

SCF = -1045.501186**ZPE = 0.121726****H₂₉₈ = -1045.368683****G₂₉₈ = -1045.416128****36**

N	-0.3816	0.6053	-0.1627
C	-0.5792	1.8465	-0.6068
N	-0.3281	2.6959	0.3895
C	0.0061	0.6667	1.1529
H	0.2219	-0.2163	1.7227
C	0.0399	1.9749	1.4983
H	0.2908	2.4503	2.4266
I	-1.1693	2.3603	-2.4940
H	0.2582	4.5248	-0.4382
C	-0.4269	4.1521	0.3160
H	-0.1578	4.5515	1.2860
H	-1.4451	4.4356	0.0709
H	0.1302	-0.6061	-1.7895
C	-0.5493	-0.6185	-0.9437
H	-0.3178	-1.4571	-0.2987
H	-1.5755	-0.6917	-1.2880

SCF = -602.354611**ZPE = 0.132439****H₂₉₈ = -602.212701****G₂₉₈ = -602.256950****36-OCH2**

N	-0.3776	0.5936	-0.1406
C	-0.5434	1.8233	-0.6313
N	-0.3260	2.6931	0.3570
C	-0.0474	0.6843	1.1892
H	0.1337	-0.1851	1.7909
C	-0.0150	2.0002	1.5012
H	0.1999	2.4977	2.4269
I	-1.0456	2.2874	-2.5703
H	0.3224	4.4922	-0.4872
C	-0.4050	4.1460	0.2397
H	-0.1846	4.5706	1.2115
H	-1.4050	4.4319	-0.0689
H	0.1929	-0.6634	-1.7112
C	-0.5232	-0.6475	-0.8963
H	-0.3306	-1.4721	-0.2209
H	-1.5327	-0.7190	-1.2870
O	-1.7178	2.7363	-5.2374
C	-1.9933	3.4703	-6.1497
H	-2.1975	3.0726	-7.1495
H	-2.0496	4.5567	-6.0152

SCF = -716.900777**ZPE = 0.161039****H₂₉₈ = -716.725454****G₂₉₈ = -716.780823****36-Cl**

N	-0.3757	0.6111	-0.1371
C	-0.5812	1.8471	-0.6087
N	-0.3204	2.6772	0.4087
C	0.0162	0.6593	1.1813
H	0.2333	-0.2240	1.7496
C	0.0502	1.9650	1.5266
H	0.3014	2.4406	2.4545
I	-1.2250	2.4099	-2.6672
H	0.1714	4.4869	-0.5006
C	-0.4337	4.1253	0.3238
H	-0.0824	4.5500	1.2574
H	-1.4691	4.4033	0.1547
H	0.2030	-0.6164	-1.7253
C	-0.5364	-0.5974	-0.9311
H	-0.4040	-1.4536	-0.2793
H	-1.5290	-0.6123	-1.3681
Cl	-1.9685	3.0599	-5.0422

SCF = -1062.784329**ZPE = 0.132219****H₂₉₈ = -1062.641057****G₂₉₈ = -1062.689171**

37			
N	-0.3371	0.5948	-0.1465
C	-0.5420	1.8402	-0.5782
N	-0.3325	2.6868	0.4312
C	0.0293	0.6493	1.1796
C	0.0021	1.9559	1.5491
I	-1.0929	2.3666	-2.4785
H	-0.1945	4.4406	-0.6757
C	-0.4114	4.1535	0.3450
H	0.3335	4.5789	1.0050
H	-1.4033	4.4821	0.6339
H	0.4392	-0.9065	-1.3928
C	-0.5097	-0.6259	-0.9496
H	-0.8721	-1.4156	-0.3044
H	-1.2450	-0.4206	-1.7168
C	0.4255	-0.6047	1.9230
C	0.2011	2.6342	2.8843
F	1.1542	-0.3261	2.9845
F	1.1520	-1.3795	1.1110
F	-0.6527	-1.2912	2.2932
F	1.4052	3.1967	2.9504
F	-0.7151	3.5980	3.0227
F	0.0576	1.7857	3.8818

SCF = -1276.656978
ZPE = 0.142776
H₂₉₈ = -1276.497869
G₂₉₈ = -1276.557251

37-OCH2			
N	-0.3049	0.5726	-0.1569
C	-0.5112	1.8080	-0.6209
N	-0.3299	2.6691	0.3839
C	0.0315	0.6502	1.1758
C	-0.0140	1.9619	1.5222
I	-1.0263	2.2948	-2.5607
H	-0.2042	4.3996	-0.7543
C	-0.4215	4.1312	0.2712
H	0.3154	4.5774	0.9267
H	-1.4177	4.4572	0.5481
H	0.5114	-0.9541	-1.3450
C	-0.4514	-0.6616	-0.9416
H	-0.8403	-1.4390	-0.2966
H	-1.1556	-0.4676	-1.7401
C	0.4187	-0.5861	1.9493
C	0.1542	2.6635	2.8473
F	1.1252	-0.2853	3.0213
F	1.1659	-1.3746	1.1692
F	-0.6622	-1.2735	2.3130
F	1.3549	3.2334	2.9310
F	-0.7675	3.6271	2.9528
F	-0.0060	1.8334	3.8590
O	-1.7565	2.7614	-5.1534
C	-1.8445	3.5027	-6.0978
H	-2.2630	3.1532	-7.0470
H	-1.5124	4.5453	-6.0416

SCF = -1391.205505
ZPE = 0.171617
H₂₉₈ = -1391.013803
G₂₉₈ = -1391.081337

37-Cl

N	-0.3177	0.6062	-0.1407
C	-0.5469	1.8461	-0.6005
N	-0.3471	2.6712	0.4391
C	0.0399	0.6481	1.1878
C	-0.0036	1.9512	1.5609
I	-1.1586	2.4369	-2.7366
H	-0.4185	4.3794	-0.7104
C	-0.4545	4.1274	0.3415
H	0.3793	4.5840	0.8625
H	-1.3912	4.4612	0.7727
H	0.4998	-0.9587	-1.2757
C	-0.4718	-0.5962	-0.9606
H	-0.9858	-1.3584	-0.3860
H	-1.0631	-0.3197	-1.8237
Cl	-1.8298	3.0844	-5.0758
C	0.4265	-0.5771	1.9600
C	0.2146	2.5926	2.8979
F	1.2506	-0.2832	2.9589
F	1.0577	-1.4485	1.1630
F	-0.6429	-1.1996	2.4647
F	1.4688	3.0334	3.0344
F	-0.5983	3.6464	3.0459
F	-0.0436	1.7493	3.8906

SCF = -1737.104387**ZPE = 0.142643****H₂₉₈ = -1736.943968****G₂₉₈ = -1737.006809****38-OCH2**

N	0.0317	-0.9304	-0.9157
C	-0.4706	0.1983	-1.4236
N	-0.4808	1.1265	-0.4629
C	0.3516	-0.7182	0.4047
C	0.0290	0.5766	0.6896
I	-1.1264	0.4633	-3.3574
H	-2.0058	2.4866	-0.8955
C	-0.9592	2.5037	-0.6110
H	-0.3680	3.0048	-1.3699
H	-0.8406	3.0030	0.3434
H	0.8772	-2.0223	-2.4823
C	0.2096	-2.1894	-1.6440
H	0.6418	-2.9120	-0.9618
H	-0.7572	-2.5370	-1.9921
C	0.9090	-1.7176	1.2372
N	1.3592	-2.5462	1.8853
C	0.1582	1.2969	1.9009
N	0.2506	1.9050	2.8659
O	-2.1345	0.8224	-5.8544
C	-1.9218	0.9600	-7.0318
H	-0.9031	0.9577	-7.4350
H	-2.7481	1.0925	-7.7373

SCF = -901.400859**ZPE = 0.157743****H₂₉₈ = -901.225195****G₂₉₈ = -901.288325****38**

N	0.0652	-0.9666	-0.8718
C	-0.4939	0.1254	-1.3960
N	-0.5380	1.0810	-0.4658
C	0.3903	-0.7021	0.4381
C	0.0114	0.5844	0.6932
I	-1.1755	0.3045	-3.3112
H	-2.1261	2.3633	-0.9155
C	-1.0783	2.4331	-0.6436
H	-0.5148	2.9408	-1.4192
H	-0.9727	2.9595	0.2976
H	0.9460	-2.0614	-2.4190
C	0.2954	-2.2366	-1.5689
H	0.7699	-2.9171	-0.8717
H	-0.6576	-2.6408	-1.8933
C	1.0026	-1.6523	1.2892
N	1.4973	-2.4417	1.9535
C	0.1211	1.3425	1.8830
N	0.1961	1.9799	2.8302

SCF = -786.851330**ZPE = 0.128989****H₂₉₈ = -786.709148****G₂₉₈ = -786.761709****38-Cl**

N	0.0470	-0.9530	-0.8606
C	-0.4877	0.1417	-1.4266
N	-0.5024	1.0800	-0.4653
C	0.3702	-0.7097	0.4534
C	0.0215	0.5825	0.7046
I	-1.2154	0.3701	-3.6137
H	-1.3892	2.5411	-1.6210
C	-0.9934	2.4452	-0.6180
H	-0.1740	3.1416	-0.4694
H	-1.7733	2.6290	0.1141
H	-0.0522	-2.1260	-2.5550
C	0.2608	-2.2344	-1.5244
H	1.3142	-2.4917	-1.4758
H	-0.3305	-2.9989	-1.0302
Cl	-1.9934	0.6198	-5.9777
C	0.9509	-1.6820	1.3024
N	1.4204	-2.4917	1.9620
C	0.1350	1.3467	1.8905
N	0.2122	1.9926	2.8328

SCF = -1247.305783**ZPE = 0.128826****H₂₉₈ = -1247.161204****G₂₉₈ = -1247.219814**

39

N	-0.3511	0.6089	-0.1789
C	-0.5504	1.8503	-0.6214
N	-0.3356	2.6912	0.3903
C	0.0020	0.6550	1.1591
C	0.0116	1.9661	1.5175
I	-1.0963	2.3759	-2.5273
H	-0.7141	4.4708	-0.6216
C	-0.4362	4.1452	0.3719
H	0.5248	4.5726	0.6394
H	-1.1929	4.4598	1.0833
H	0.4880	-1.1422	-0.9355
C	-0.4698	-0.6320	-0.9344
H	-1.2242	-1.2603	-0.4721
H	-0.7608	-0.4039	-1.9511
C	0.2895	-0.5754	1.9381
H	1.1257	-1.1255	1.5105
H	-0.5765	-1.2340	1.9672
H	0.5464	-0.3120	2.9580
C	0.3131	2.6254	2.8128
H	1.1621	3.3006	2.7226
H	0.5567	1.8762	3.5577
H	-0.5419	3.1944	3.1730

SCF = -681.017685**ZPE = 0.188237****H₂₉₈ = -680.818157****G₂₉₈ = -680.866167****39-Cl**

N	-0.3459	0.6156	-0.1560
C	-0.5512	1.8520	-0.6274
N	-0.3292	2.6738	0.4063
C	0.0084	0.6505	1.1842
C	0.0189	1.9571	1.5411
I	-1.1439	2.4268	-2.7144
H	-0.7179	4.4101	-0.6417
C	-0.4354	4.1207	0.3627
H	0.5214	4.5687	0.6157
H	-1.1931	4.4564	1.0653
H	0.4794	-1.1301	-0.9497
C	-0.4722	-0.6063	-0.9290
H	-1.2315	-1.2454	-0.4873
H	-0.7627	-0.3407	-1.9376
Cl	-1.8254	3.0868	-5.1073
C	0.2946	-0.5826	1.9609
H	1.1287	-1.1354	1.5315
H	-0.5705	-1.2433	1.9867
H	0.5520	-0.3246	2.9830
C	0.3205	2.6197	2.8356
H	1.1669	3.2987	2.7444
H	0.5662	1.8740	3.5845
H	-0.5334	3.1917	3.1954

SCF = -1141.442232**ZPE = 0.188456****H₂₉₈ = -1141.238470****G₂₉₈ = -1141.295446****39-OCH2**

N	-0.3072	0.6437	-0.1974
C	-0.4731	1.8952	-0.6240
N	-0.2654	2.7114	0.4093
C	0.0115	0.6580	1.1499
C	0.0398	1.9621	1.5336
I	-0.9773	2.5141	-2.5226
H	0.3694	4.5449	-0.3697
C	-0.3500	4.1665	0.3490
H	-0.1251	4.5621	1.3306
H	-1.3526	4.4627	0.0576
H	0.3796	-1.2272	-0.7879
C	-0.4619	-0.5719	-0.9838
H	-1.3885	-1.0688	-0.7120
H	-0.4805	-0.3116	-2.0343
C	0.2573	-0.5930	1.9114
H	1.1523	-1.1018	1.5572
H	-0.5843	-1.2773	1.8235
H	0.3950	-0.3638	2.9621
C	0.3303	2.5728	2.8562
H	1.2019	3.2229	2.8090
H	0.5369	1.7909	3.5786
H	-0.5165	3.1513	3.2203
O	-1.6583	3.5416	-5.0463
C	-1.9821	3.3926	-6.1946
H	-2.1079	2.3946	-6.6307
H	-2.1626	4.2550	-6.8456

SCF = -795.562972**ZPE = 0.217092****H₂₉₈ = -795.328990****G₂₉₈ = -795.389396**

40

N	-0.1255	-1.0924	-1.0275
C	-0.5276	0.0759	-1.5378
N	-0.5492	0.9763	-0.5626
C	0.1216	-0.9313	0.3185
C	-0.1331	0.3744	0.6221
I	-1.0245	0.4504	-3.4875
H	-1.9113	2.4213	-1.1991
C	-0.9674	2.3701	-0.6680
H	-0.2112	2.9459	-1.1928
H	-1.0968	2.7451	0.3401
H	1.0905	-2.6668	-1.6465
C	0.0486	-2.3718	-1.7078
H	-0.5715	-3.1144	-1.2179
H	-0.2493	-2.2566	-2.7417
O	0.5195	-1.9910	0.9991
O	-0.0916	1.0464	1.7716
C	1.1473	1.7500	2.0234
H	1.9732	1.0437	2.0402
H	1.0281	2.2216	2.9901
H	1.3134	2.5010	1.2546
C	0.4421	-1.9021	2.4372
H	1.1858	-1.2026	2.8053
H	0.6551	-2.8995	2.7960
H	-0.5554	-1.5898	2.7308

SCF = -831.460468**ZPE = 0.198218****H₂₉₈ = -831.247020****G₂₉₈ = -831.303711****40-OCH2**

N	-0.0342	-1.0604	-1.0393
C	-0.3729	0.1204	-1.5677
N	-0.4339	1.0130	-0.5867
C	0.1331	-0.9161	0.3223
C	-0.1090	0.3936	0.6163
I	-0.7167	0.4779	-3.5627
H	-1.6949	2.4982	-1.3232
C	-0.8020	2.4174	-0.7133
H	0.0106	2.9750	-1.1692
H	-1.0047	2.7917	0.2830
H	0.9838	-2.2212	-2.4487
C	0.1415	-2.3117	-1.7706
H	0.3317	-3.0907	-1.0438
H	-0.7636	-2.5321	-2.3261
O	0.4661	-1.9782	1.0377
O	-0.1190	1.0591	1.7727
C	1.1277	1.7092	2.1072
H	1.9220	0.9699	2.1707
H	0.9680	2.1812	3.0681
H	1.3733	2.4565	1.3561
C	0.2070	-1.9056	2.4541
H	0.8987	-1.2139	2.9241
H	0.3688	-2.9080	2.8261
H	-0.8187	-1.5913	2.6226
O	-1.0865	0.8438	-6.3234
C	-1.6544	1.3643	-7.2466
H	-1.4002	1.1082	-8.2810
H	-2.4428	2.1097	-7.0890

SCF = -946.005653**ZPE = 0.226986****H₂₉₈ = -945.758733****G₂₉₈ = -945.825943**

40-Cl

N	-0.1267	-1.0973	-1.0034
C	-0.5265	0.0696	-1.5359
N	-0.5415	0.9482	-0.5320
C	0.1188	-0.9543	0.3439
C	-0.1343	0.3426	0.6547
I	-1.0184	0.5233	-3.6722
H	-1.7770	2.4087	-1.3296
C	-0.9412	2.3410	-0.6433
H	-0.1190	2.9418	-1.0226
H	-1.2371	2.6865	0.3412
H	1.0606	-2.6886	-1.6416
C	0.0304	-2.3547	-1.7143
H	-0.6242	-3.1023	-1.2778
H	-0.2349	-2.1817	-2.7499
Cl	-1.5691	1.0770	-6.1244
O	0.5134	-2.0285	1.0315
O	-0.0831	1.0162	1.8184
C	1.1292	1.7624	2.0064
H	1.9831	1.0878	2.0058
H	1.0368	2.2561	2.9664
H	1.2467	2.5013	1.2163
C	0.4602	-1.9019	2.4547
H	1.2036	-1.1872	2.7989
H	0.6813	-2.8863	2.8463
H	-0.5312	-1.5797	2.7626

SCF = -1291.884366**ZPE = 0.198780****H₂₉₈ = -1291.668355****G₂₉₈ = -1291.729531**

7.2 ONIOM(DFT:AM1)

1

H	2.7070	0.0652	-1.4701
C	2.1111	0.0702	-0.5443
C	0.6022	0.1084	1.8022
C	1.6752	-1.1259	0.0256
C	1.7911	1.2859	0.0612
C	1.0368	1.3059	1.2343
C	0.9209	-1.1086	1.1985
H	2.1356	2.2282	-0.3896
H	0.5730	-2.0483	1.6547
H	0.0072	0.1202	2.7271
I	2.1415	-2.9011	-0.8577
H	0.7850	2.2649	1.7109

SCF = -298.209657**ZPE = 0.092185****H₂₉₈ = -298.110685****G₂₉₈ = -298.149206****SCF_{DFT} = -529.366810****1-OCH2**

H	3.1634	0.2445	-1.1641
C	2.3963	0.1776	-0.3771
C	0.4563	0.0339	1.6219
C	1.9342	-1.0643	0.0582
C	1.8869	1.3475	0.1875
C	0.9166	1.2765	1.1870
C	0.9648	-1.1369	1.0582
H	2.2532	2.3256	-0.1571
H	0.5960	-2.1130	1.4100
H	-0.3078	-0.0260	2.4108
I	2.6801	-2.7759	-0.7665
H	0.5158	2.1992	1.6321
O	3.3740	-5.2779	-2.4174
C	2.5985	-5.3242	-3.3298
H	2.6346	-6.1350	-4.0698
H	1.8217	-4.5575	-3.4612

SCF = -412.744075**ZPE = 0.120690****H₂₉₈ = -412.611858****G₂₉₈ = -412.661536****SCF_{DFT} = -643.900132****1-Cl**

H	2.7037	0.0319	-1.4793
C	2.1107	0.0414	-0.5523
C	0.6118	0.0899	1.7924
C	1.6827	-1.1587	0.0136
C	1.7935	1.2613	0.0469
C	1.0425	1.2872	1.2217
C	0.9324	-1.1267	1.1882
H	2.1348	2.2025	-0.4061
H	0.5875	-2.0660	1.6466
H	0.0198	0.1058	2.7181
I	2.1613	-2.9903	-0.8930
Cl	2.8101	-5.4796	-2.1303
H	0.7914	2.2459	1.6951

SCF = -758.510794**ZPE = 0.092694****H₂₉₈ = -758.409030****G₂₉₈ = -758.452868****SCF_{DFT} = -989.658309**

2

H	0.3612	0.1815	0.0655
C	0.2210	0.1546	1.1579
C	-0.1391	0.1087	3.9295
C	0.3386	-1.0448	1.8601
C	-0.0764	1.3361	1.8357
C	-0.2570	1.3153	3.2258
C	0.1585	-1.0677	3.2430
H	-0.1686	2.2820	1.2805
H	0.2492	-2.0108	3.8053
H	-0.2807	0.0894	5.0210
I	0.7763	-2.7659	0.8640
C	-0.5594	2.5178	3.9215
N	-0.8066	3.5015	4.4911

SCF = -298.158261**ZPE = 0.092015****H₂₉₈ = -298.057835****G₂₉₈ = -298.100145****SCF_{DFT} = -621.636546****2-Cl**

H	0.3809	0.1575	0.0628
C	0.2342	0.1340	1.1538
C	-0.1395	0.0900	3.9171
C	0.3480	-1.0715	1.8460
C	-0.0639	1.3173	1.8260
C	-0.2526	1.2996	3.2159
C	0.1593	-1.0833	3.2278
H	-0.1518	2.2637	1.2732
H	0.2463	-2.0281	3.7866
H	-0.2868	0.0726	5.0066
I	0.8014	-2.8562	0.8140
Cl	1.4014	-5.2194	-0.5554
C	-0.5565	2.5007	3.9097
N	-0.8057	3.4858	4.4788

SCF = -758.468777**ZPE = 0.092468****H₂₉₈ = -758.365624****G₂₉₈ = -758.413108****SCF_{DFT} = -1081.941106****2-OCH2**

H	0.2964	0.0426	0.1035
C	0.1777	0.0663	1.1983
C	-0.1280	0.1500	3.9746
C	0.2861	-1.1041	1.9493
C	-0.0830	1.2824	1.8278
C	-0.2366	1.3267	3.2206
C	0.1330	-1.0610	3.3350
H	-0.1680	2.2047	1.2332
H	0.2165	-1.9805	3.9364
H	-0.2483	0.1815	5.0682
I	0.6691	-2.8819	1.0231
C	-0.5022	2.5645	3.8675
N	-0.7195	3.5776	4.3967
O	1.2956	-5.2809	-0.7495
C	1.4776	-4.9252	-1.8794
H	1.7165	-5.6447	-2.6739
H	1.4124	-3.8652	-2.1637

SCF = -412.693021**ZPE = 0.120593****H₂₉₈ = -412.559321****G₂₉₈ = -412.612335****SCF_{DFT} = -736.170734****3**

H	0.3765	0.1688	0.0554
C	0.2310	0.1401	1.1477
C	-0.1423	0.0864	3.9241
C	0.3391	-1.0609	1.8491
C	-0.0631	1.3247	1.8209
C	-0.2486	1.2912	3.2118
C	0.1526	-1.0867	3.2313
H	-0.1487	2.2761	1.2679
H	0.2358	-2.0317	3.7927
H	-0.2900	0.0683	5.0178
I	0.7727	-2.7822	0.8517
N	-0.5620	2.5500	3.9411
O	-0.6495	3.5746	3.3196
O	-0.7189	2.5075	5.1316

SCF = -298.201890**ZPE = 0.096843****H₂₉₈ = -298.095783****G₂₉₈ = -298.140278****SCF_{DFT} = -733.925893**

3-Cl

H	0.3777	0.1400	0.0513
C	0.2344	0.1185	1.1432
C	-0.1309	0.0710	3.9150
C	0.3518	-1.0859	1.8374
C	-0.0629	1.3047	1.8079
C	-0.2460	1.2778	3.2020
C	0.1674	-1.0977	3.2202
H	-0.1544	2.2532	1.2552
H	0.2574	-2.0426	3.7789
H	-0.2755	0.0566	5.0069
I	0.8062	-2.8798	0.8007
Cl	1.3961	-5.2125	-0.5505
N	-0.5619	2.5280	3.9238
O	-0.6598	3.5613	3.3101
O	-0.7186	2.5022	5.1191

SCF = -758.519561**ZPE = 0.097397****H₂₉₈ = -758.410676****G₂₉₈ = -758.460165****SCF_{DFT} = -1194.231674****3-OCH2**

H	0.3020	0.0600	0.0979
C	0.1812	0.0723	1.1932
C	-0.1297	0.1236	3.9764
C	0.2933	-1.1044	1.9341
C	-0.0858	1.2837	1.8282
C	-0.2404	1.3030	3.2234
C	0.1379	-1.0767	3.3201
H	-0.1747	2.2153	1.2432
H	0.2245	-2.0019	3.9132
H	-0.2527	0.1467	5.0729
I	0.6866	-2.8715	0.9912
N	-0.5251	2.5905	3.9124
O	-0.6171	3.5929	3.2557
O	-0.6554	2.5942	5.1070
O	1.3127	-5.2637	-0.7527
C	1.4804	-4.9556	-1.8990
H	1.7194	-5.7064	-2.6638
H	1.4013	-3.9095	-2.2277

SCF = -412.737030**ZPE = 0.125403****H₂₉₈ = -412.597652****G₂₉₈ = -412.652834****SCF_{DFT} = -848.460234****4**

H	0.3829	0.1684	0.0619
C	0.2317	0.1405	1.1524
C	-0.1583	0.0980	3.9124
C	0.3367	-1.0610	1.8523
C	-0.0672	1.3199	1.8323
C	-0.2634	1.3092	3.2184
C	0.1406	-1.0816	3.2327
H	-0.1501	2.2653	1.2756
H	0.2194	-2.0249	3.7955
H	-0.3133	0.0764	5.0014
I	0.7768	-2.7830	0.8596
C	-0.5638	2.5652	3.9425
H	-1.1734	2.3647	4.8576
H	0.3902	3.0586	4.2586
H	-1.1266	3.2782	3.2913

SCF = -298.222046**ZPE = 0.119817****H₂₉₈ = -298.094484****G₂₉₈ = -298.135163****SCF_{DFT} = -568.690196****4-OCH2**

H	1.2008	0.5190	0.2009
C	0.7773	0.3650	1.2057
C	-0.2973	0.0044	3.7519
C	0.7519	-0.9073	1.7760
C	0.2658	1.4555	1.9070
C	-0.2752	1.2849	3.1868
C	0.2143	-1.0858	3.0502
H	0.2876	2.4570	1.4519
H	0.1902	-2.0854	3.5118
H	-0.7210	-0.1424	4.7566
I	1.5022	-2.5031	0.7495
C	-0.8035	2.4461	3.9385
H	-1.6206	2.1348	4.6349
H	0.0152	2.9104	4.5449
H	-1.2072	3.2232	3.2437
O	2.0833	-4.9360	-1.0457
C	1.0753	-5.1652	-1.6517
H	1.0160	-5.9949	-2.3690
H	0.1718	-4.5544	-1.5132

SCF = -412.756430**ZPE = 0.148444****H₂₉₈ = -412.594667****G₂₉₈ = -412.648138****SCF_{DFT} = -683.223408**

4-Cl

H	0.3987	0.1463	0.0577
C	0.2447	0.1200	1.1473
C	-0.1519	0.0804	3.8998
C	0.3525	-1.0865	1.8371
C	-0.0584	1.3015	1.8229
C	-0.2586	1.2919	3.2077
C	0.1515	-1.0964	3.2164
H	-0.1421	2.2468	1.2679
H	0.2313	-2.0403	3.7771
H	-0.3095	0.0603	4.9876
I	0.8091	-2.8607	0.8141
Cl	1.4282	-5.2741	-0.5800
C	-0.5647	2.5462	3.9322
H	-1.2059	2.3466	4.8258
H	0.3823	3.0281	4.2842
H	-1.0987	3.2720	3.2707

SCF = -758.522679**ZPE = 0.120404****H₂₉₈ = -758.391356****G₂₉₈ = -758.439307****SCF_{DFT} = -1028.980422****5**

H	1.3418	0.0839	0.2356
C	0.7604	0.0881	1.1718
C	-0.7142	0.1306	3.5351
C	0.3612	-1.1112	1.7585
C	0.4322	1.3075	1.7512
C	-0.3084	1.3610	2.9592
C	-0.3762	-1.0788	2.9404
H	0.7656	2.2297	1.2530
H	-0.7038	-2.0161	3.4186
H	-1.2995	0.1099	4.4662
I	0.8458	-2.8880	0.8970
N	-0.5707	2.5836	3.5972
C	-1.5774	2.5996	4.6263
C	-0.4197	3.7887	2.8240
H	-2.5594	2.1826	4.2716
H	-1.7424	3.6499	4.9838
H	-1.2197	1.9860	5.4967
H	-1.0179	3.7649	1.8724
H	-0.7450	4.6751	3.4294
H	0.6649	3.9220	2.5635

SCF = -298.196608**ZPE = 0.165330****H₂₉₈ = -298.020104****G₂₉₈ = -298.068257****SCF_{DFT} = -663.361130****5-Cl**

H	1.3507	0.0669	0.2438
C	0.7811	0.0723	1.1866
C	-0.6553	0.1238	3.5644
C	0.3777	-1.1297	1.7605
C	0.4766	1.2958	1.7781
C	-0.2484	1.3489	2.9897
C	-0.3383	-1.0867	2.9531
H	0.8178	2.2158	1.2828
H	-0.6682	-2.0233	3.4298
H	-1.2237	0.1021	4.5049
I	0.8271	-2.9590	0.8435
Cl	1.4284	-5.4569	-0.4214
N	-0.4947	2.5885	3.6474
C	-1.5863	2.5850	4.5923
C	-0.4415	3.7606	2.8060
H	-2.5404	2.1711	4.1655
H	-1.7813	3.6289	4.9538
H	-1.2905	1.9605	5.4772
H	-1.0816	3.6749	1.8859
H	-0.7715	4.6618	3.3867
H	0.6226	3.9231	2.4871

SCF = -758.494911**ZPE = 0.165938****H₂₉₈ = -758.316544****G₂₉₈ = -758.367624****SCF_{DFT} = -1123.648206****5-OCH2**

H	1.8257	0.2469	0.4635
C	1.1238	0.1974	1.3117
C	-0.6520	0.1048	3.4553
C	0.7104	-1.0357	1.8116
C	0.6611	1.3836	1.8681
C	-0.2351	1.3684	2.9663
C	-0.1776	-1.0700	2.8848
H	1.0122	2.3340	1.4401
H	-0.5172	-2.0348	3.2954
H	-1.3533	0.0304	4.2994
I	1.3949	-2.7666	0.9838
N	-0.6400	2.5598	3.5910
C	-1.7775	2.4986	4.4717
C	-0.4539	3.7900	2.8664
H	-2.6803	2.0474	3.9763
H	-2.0418	3.5291	4.8273
H	-1.5113	1.8767	5.3686
H	-0.9210	3.7610	1.8441
H	-0.9013	4.6436	3.4402
H	0.6469	3.9836	2.7531
O	1.9507	-5.2971	-0.7067
C	1.1272	-5.2928	-1.5769
H	1.0897	-6.0899	-2.3319
H	0.3778	-4.4920	-1.6536

SCF = -412.730775
 ZPE = 0.193863
 H_{298} = -412.521016
 G_{298} = -412.580146

SCF_{DFT} = -777.894035

6			
H	0.2857	0.1587	0.0551
C	0.2078	0.0974	1.1524
C	0.0079	-0.0473	3.9418
C	0.3693	-1.1273	1.8061
C	-0.0530	1.2533	1.8780
C	-0.1529	1.1767	3.2814
C	0.2692	-1.1956	3.1935
H	-0.1824	2.2236	1.3782
H	0.3949	-2.1564	3.7176
H	-0.0681	-0.1172	5.0354
I	0.7511	-2.8102	0.7277
O	-0.4133	2.3766	3.9100
C	-0.5215	2.3344	5.3285
H	0.4366	1.9892	5.7867
H	-1.3658	1.6730	5.6399
H	-0.7307	3.3990	5.6041

SCF = -298.270610
 ZPE = 0.125501
 H_{298} = -298.135708
 G_{298} = -298.180042

SCF_{DFT} = -643.920346

6-Cl			
H	0.3094	0.1409	0.0494
C	0.2215	0.0795	1.1454
C	-0.0040	-0.0618	3.9264
C	0.3670	-1.1504	1.7879
C	-0.0347	1.2415	1.8684
C	-0.1463	1.1623	3.2668
C	0.2526	-1.2102	3.1733
H	-0.1500	2.2124	1.3696
H	0.3647	-2.1735	3.6947
H	-0.0900	-0.1328	5.0181
I	0.7570	-2.8902	0.6805
Cl	1.2920	-5.2601	-0.8115
O	-0.4018	2.3723	3.9018
C	-0.5146	2.3147	5.3147
H	0.4370	1.9527	5.7755
H	-1.3651	1.6571	5.6195
H	-0.7142	3.3756	5.6105

SCF = -758.571690
 ZPE = 0.125959

H_{298} = -758.434000
 G_{298} = -758.483720

SCF_{DFT} = -1104.210462

6-OCH2			
H	0.5006	0.0096	0.1118
C	0.3598	-0.0145	1.2040
C	0.0018	-0.0625	3.9795
C	0.4903	-1.2149	1.9073
C	0.0521	1.1644	1.8716
C	-0.1270	1.1363	3.2684
C	0.3112	-1.2342	3.2881
H	-0.0533	2.1156	1.3313
H	0.4122	-2.1753	3.8521
H	-0.1359	-0.0949	5.0688
I	0.9466	-2.9357	0.9140
O	-0.4294	2.3561	3.8384
C	-0.6068	2.3643	5.2505
H	0.3289	2.0406	5.7676
H	-1.4634	1.7102	5.5439
H	-0.8329	3.4372	5.4772
O	1.4803	-5.2645	-1.0226
C	1.1922	-4.8904	-2.1238
H	1.2934	-5.5499	-2.9963
H	0.8159	-3.8733	-2.3041

SCF = -412.804967
 ZPE = 0.154049
 H_{298} = -412.636809
 G_{298} = -412.691965

SCF_{DFT} = -758.453408

7			
H	1.6591	0.2626	1.3352
C	0.8649	-0.0446	2.0339
C	-1.1411	-0.7883	3.8172
C	0.2924	-1.3111	1.9456
C	0.4364	0.8514	3.0126
C	-0.5694	0.4911	3.9140
C	-0.7134	-1.6809	2.8412
H	0.9002	1.8479	3.0676
H	-1.1752	-2.6792	2.7830
H	-1.9344	-1.0837	4.5218
I	0.9169	-2.6200	0.5191
S	-1.1832	1.4727	5.1451
C	-0.3069	2.9821	5.0421
H	-0.7216	3.6176	5.8605
H	-0.4618	3.5013	4.0699
H	0.7866	2.8541	5.2050

SCF = -298.211365

ZPE = 0.120117
H₂₉₈ = -298.081030
G₂₉₈ = -298.127331
SCF_{DFT} = -966.884040

7-Cl

H	1.5897	0.3082	1.2602
C	0.8334	-0.0251	1.9874
C	-1.0750	-0.8355	3.8396
C	0.3058	-1.3111	1.9061
C	0.4153	0.8567	2.9850
C	-0.5421	0.4581	3.9189
C	-0.6514	-1.7079	2.8404
H	0.8462	1.8675	3.0293
H	-1.0806	-2.7205	2.7928
H	-1.8301	-1.1572	4.5722
I	0.9429	-2.6313	0.4004
Cl	1.8110	-4.4062	-1.6370
S	-1.1442	1.4247	5.1862
C	-0.3144	2.9593	5.0487
H	-0.7079	3.5894	5.8795
H	-0.5203	3.4661	4.0794
H	0.7880	2.8557	5.1622

SCF = -758.513716
ZPE = 0.120573
H₂₉₈ = -758.380575
G₂₉₈ = -758.432353

SCF_{DFT} = -1427.176716

7-OCH2

H	2.1668	0.3032	1.7430
C	1.2541	-0.0224	2.2669
C	-1.0527	-0.8145	3.6110
C	0.7390	-1.3007	2.0652
C	0.6183	0.8614	3.1383
C	-0.5403	0.4764	3.8188
C	-0.4176	-1.6944	2.7419
H	1.0404	1.8672	3.2851
H	-0.8350	-2.7031	2.5949
H	-1.9643	-1.1293	4.1430
I	1.6694	-2.5927	0.7914
S	-1.4115	1.4424	4.9000
C	-0.5611	2.9680	4.9777
H	-1.1439	3.5927	5.6960
H	-0.5258	3.4887	3.9946
H	0.4794	2.8589	5.3579
O	2.6120	-4.4503	-1.4709
C	1.7707	-4.4285	-2.3239
H	1.8770	-5.0151	-3.2465
H	0.8607	-3.8210	-2.2164

SCF = -412.745798
ZPE = 0.148666
H₂₉₈ = -412.582208
G₂₉₈ = -412.639237

SCF_{DFT} = -1081.417402

8

H	0.3563	0.1234	0.0446
C	0.2209	0.1047	1.1378
C	-0.1298	0.0839	3.9103
C	0.3496	-1.0869	1.8516
C	-0.0821	1.2903	1.8079
C	-0.2552	1.2752	3.1932
C	0.1733	-1.0988	3.2354
H	-0.1892	2.2336	1.2488
H	0.2708	-2.0355	3.8071
H	-0.2743	0.0798	5.0026
I	0.7975	-2.8144	0.8703
C	-0.5666	2.5727	3.9305
F	-1.3128	2.4147	5.0730
F	0.5474	3.2599	4.3500
F	-1.2701	3.4935	3.1926

SCF = -298.457059
ZPE = 0.098471
H₂₉₈ = -298.348157
G₂₉₈ = -298.395478

SCF_{DFT} = -866.533486

8-Cl

H	0.5588	0.1416	0.0776
C	0.3375	0.1077	1.1554
C	-0.2264	0.0413	3.8865
C	0.3576	-1.1108	1.8347
C	0.0389	1.2911	1.8278
C	-0.2432	1.2551	3.1966
C	0.0742	-1.1348	3.1999
H	0.0224	2.2532	1.2952
H	0.0860	-2.0891	3.7486
H	-0.4493	0.0183	4.9636
I	0.8131	-2.8990	0.8050
Cl	1.4137	-5.2584	-0.5574
C	-0.5663	2.5509	3.9160
F	-0.8307	2.4351	5.2610
F	0.4283	3.5020	3.8667
F	-1.6667	3.2217	3.4308

SCF = -758.768629
ZPE = 0.098922
H₂₉₈ = -758.657907
G₂₉₈ = -758.708172

SCF_{DFT} = -1326.834632

8-OCH2

H	1.2059	0.6812	0.1616
C	0.7821	0.4758	1.1576
C	-0.2952	-0.0182	3.6877
C	0.7469	-0.8246	1.6612
C	0.2792	1.5333	1.9158
C	-0.2584	1.2816	3.1795
C	0.2094	-1.0713	2.9246
H	0.3008	2.5614	1.5206
H	0.1786	-2.0943	3.3322
H	-0.7248	-0.2084	4.6842
I	1.4841	-2.3677	0.5470
C	-0.7939	2.4366	4.0175
F	-1.8179	2.0976	4.8686
F	0.1439	3.0176	4.8374
F	-1.2967	3.4866	3.2880
O	2.0920	-4.7861	-1.2015
C	1.0700	-5.3022	-1.5561
H	1.0722	-6.1915	-2.2003
H	0.0916	-4.9049	-1.2499

SCF = -412.991987

ZPE = 0.127049

H₂₉₈ = -412.849811

G₂₉₈ = -412.907688

SCF_{DFT} = -981.067573

9

H	0.3571	0.1762	0.0665
C	0.2187	0.1497	1.1590
C	-0.1379	0.1155	3.9263
C	0.3364	-1.0487	1.8619
C	-0.0767	1.3327	1.8364
C	-0.2554	1.3177	3.2227
C	0.1577	-1.0649	3.2446
H	-0.1669	2.2731	1.2702
H	0.2475	-2.0050	3.8117
H	-0.2766	0.0900	5.0186
I	0.7708	-2.7728	0.8701
Br	-0.6511	2.9041	4.1351

SCF = -298.201250

ZPE = 0.082152

H₂₉₈ = -298.110892

G₂₉₈ = -298.153694

SCF_{DFT} = -3102.868053

9-OCH2

H	0.2808	0.0131	0.0890
C	0.1737	0.0467	1.1846
C	-0.1039	0.1657	3.9578
C	0.2899	-1.1158	1.9456
C	-0.0809	1.2695	1.8052
C	-0.2202	1.3311	3.1947
C	0.1507	-1.0544	3.3316
H	-0.1705	2.1804	1.1929
H	0.2399	-1.9652	3.9449
H	-0.2118	0.2008	5.0533
I	0.6629	-2.9042	1.0366
Br	-0.5618	2.9710	4.0315
O	1.2858	-5.3124	-0.7426
C	1.4753	-4.9361	-1.8645
H	1.7160	-5.6414	-2.6712
H	1.4152	-3.8708	-2.1295

SCF = -412.735844

ZPE = 0.110712

H₂₉₈ = -412.612220

G₂₉₈ = -412.665732

SCF_{DFT} = -3217.401665

9-Cl

H	0.3472	0.1462	0.0583
C	0.2162	0.1239	1.1513
C	-0.1205	0.0962	3.9159
C	0.3482	-1.0773	1.8460
C	-0.0819	1.3093	1.8237
C	-0.2505	1.2948	3.2103
C	0.1778	-1.0811	3.2293
H	-0.1823	2.2480	1.2592
H	0.2781	-2.0204	3.7949
H	-0.2516	0.0745	5.0077
I	0.7999	-2.8607	0.8191
Cl	1.4029	-5.2415	-0.5563
Br	-0.6521	2.8871	4.1261

SCF = -758.507980

ZPE = 0.082618

H₂₉₈ = -758.414869

G₂₉₈ = -758.462828

SCF_{DFT} = -3563.165498

10

C	0.2302	-0.0236	1.1290
C	-0.1343	0.0056	3.9259
C	0.1332	-1.2276	1.8397
C	0.1452	1.1950	1.8160
C	-0.0369	1.2148	3.2135
C	-0.0489	-1.2183	3.2373
I	0.4929	-0.0442	-0.8930
C	0.2167	-2.4784	1.1652
N	0.2828	-3.5093	0.6306
C	-0.1464	-2.4444	3.9507
N	-0.2261	-3.4474	4.5343
C	-0.3182	0.0203	5.3357
N	-0.4687	0.0324	6.4889
C	-0.1222	2.4556	3.9027
N	-0.1920	3.4707	4.4663
C	0.2410	2.4314	1.1172
N	0.3172	3.4509	0.5624

SCF = -297.921711**ZPE = 0.091260****H₂₉₈ = -297.815310****G₂₉₈ = -297.872398****SCF_{DFT} = -990.666874****10-OCH2**

C	0.1880	-0.2798	1.0150
C	-0.1104	0.0497	3.8015
C	0.1059	-1.3999	1.8528
C	0.1203	1.0048	1.5711
C	-0.0287	1.1756	2.9620
C	-0.0431	-1.2408	3.2455
I	0.4072	-0.5140	-1.0065
C	0.1716	-2.7164	1.3153
N	0.2234	-3.7991	0.8934
C	-0.1250	-2.3832	4.0883
N	-0.1918	-3.3178	4.7774
C	-0.2601	0.2156	5.2057
N	-0.3824	0.3511	6.3543
C	-0.0959	2.4834	3.5163
N	-0.1509	3.5532	3.9693
C	0.2014	2.1581	0.7402
N	0.2663	3.1087	0.0730
O	0.7416	-0.4353	-3.9295
C	0.8362	0.6666	-4.3955
H	0.9597	0.8199	-5.4753
H	0.8024	1.5612	-3.7574

SCF = -412.458489**ZPE = 0.119931****H₂₉₈ = -412.318809****G₂₉₈ = -412.385944****SCF_{DFT} = -1105.206170****10-Cl**

C	0.2223	-0.0230	1.1129
C	-0.1293	0.0052	3.9193
C	0.1360	-1.2211	1.8305
C	0.1323	1.1893	1.8058
C	-0.0430	1.2137	3.2040
C	-0.0393	-1.2174	3.2290
I	0.4916	-0.0449	-1.0556
Cl	0.8134	-0.0728	-3.6817
C	0.2234	-2.4764	1.1634
N	0.2927	-3.5109	0.6358
C	-0.1262	-2.4409	3.9504
N	-0.1970	-3.4427	4.5377
C	-0.3064	0.0194	5.3295
N	-0.4514	0.0310	6.4839
C	-0.1337	2.4515	3.9003
N	-0.2076	3.4649	4.4670
C	0.2159	2.4310	1.1132
N	0.2821	3.4544	0.5641

SCF = -758.258714**ZPE = 0.091450****H₂₉₈ = -758.149849****G₂₉₈ = -758.212015****SCF_{DFT} = -1451.005251****11**

C	0.2210	-0.0255	1.1280
C	-0.1340	0.0095	3.9567
C	0.1084	-1.2274	1.8504
C	0.1553	1.1939	1.8264
C	-0.0215	1.2209	3.2360
C	-0.0687	-1.2195	3.2602
I	0.4754	-0.0502	-0.9002
F	0.1636	-2.4293	1.2376
F	-0.1742	-2.3852	3.9316
F	-0.3018	0.0260	5.2932
F	-0.0815	2.4029	3.8841
F	0.2568	2.3804	1.1899

SCF = -298.537913**ZPE = 0.054924****H₂₉₈ = -298.472221****G₂₉₈ = -298.520070****SCF_{DFT} = -1025.692933**

11-I

C	0.0050	0.0028	1.1018
C	0.0214	0.0404	3.9112
C	0.0369	-1.2146	1.7942
C	-0.0187	1.2459	1.7929
C	-0.0104	1.2632	3.2051
C	0.0447	-1.1883	3.1947
I	0.0751	-3.0852	0.7286
F	0.0746	-2.3251	3.9279
F	0.0296	0.0429	5.2642
F	-0.0325	2.4386	3.8745
F	-0.0492	2.4103	1.1044
F	-0.0046	0.0527	-0.2503
I	0.1350	-5.7988	-0.8160

SCF = -596.341954**11-F**

C	0.0137	-0.0097	1.1026
C	0.0141	0.0356	3.9089
C	0.0379	-1.2244	1.7938
C	-0.0105	1.2372	1.7874
C	-0.0103	1.2571	3.1998
C	0.0379	-1.1927	3.1912
I	0.0752	-3.1867	0.6800
F	0.0605	-2.3309	3.9268
F	0.0145	0.0440	5.2633
F	-0.0332	2.4357	3.8676
F	-0.0338	2.4030	1.0981
F	0.0121	0.0360	-0.2520
F	0.1104	-5.0258	-0.3661

SCF = -398.514757**11-OCH2**

C	0.0009	-0.2122	1.0880
C	-0.0006	-0.0678	3.8991
C	0.0003	-1.4051	1.8331
C	0.0008	1.0542	1.7316
C	0.0001	1.1274	3.1438
C	-0.0005	-1.3255	3.2371
F	-0.0011	-2.4334	4.0089
F	-0.0013	-0.0164	5.2476
F	-0.0000	2.3240	3.7630
F	0.0014	2.1848	0.9947
F	0.0016	-0.2226	-0.2630
I	0.0005	-3.2266	0.8887
O	-0.0006	-5.6161	-0.8860
C	-0.0006	-5.3077	-2.0451
H	-0.0008	-6.0674	-2.8376
H	-0.0001	-4.2532	-2.3560

SCF = -413.073851**ZPE = 0.083486****H₂₉₈ = -412.974904****G₂₉₈ = -413.033287****SCF_{DFT} = -1140.229171****11-OMe**

C	0.0200	0.0863	1.1730
C	0.0125	0.1150	3.9812
C	0.0737	-1.1274	1.8606
C	-0.0389	1.3284	1.8648
C	-0.0427	1.3391	3.2777
C	0.0704	-1.1082	3.2566
I	0.1597	-3.1256	0.7055
F	0.1217	-2.2519	3.9814
F	0.0094	0.1170	5.3355
F	-0.0990	2.5129	3.9520
F	-0.0914	2.4974	1.1832
F	0.0212	0.1356	-0.1813
O	0.2397	-4.9791	-0.3887
C	0.2996	-4.7297	-1.7649
H	0.3393	-5.6822	-2.3037
H	1.1898	-4.1457	-2.0436
H	-0.5785	-4.1728	-2.1252

SCF = -413.755121**11-Cl**

C	0.2202	-0.0258	1.1146
C	-0.1305	0.0103	3.9441
C	0.1052	-1.2201	1.8365
C	0.1591	1.1867	1.8126
C	-0.0155	1.2198	3.2239
C	-0.0701	-1.2173	3.2482
I	0.4880	-0.0534	-1.0409
F	0.1552	-2.4273	1.2271
F	-0.1791	-2.3830	3.9267
F	-0.2968	0.0273	5.2868
F	-0.0718	2.4025	3.8790
F	0.2630	2.3780	1.1792
Cl	0.8192	-0.0878	-3.7174

SCF = -758.861198**ZPE = 0.055317****H₂₉₈ = -758.792845****G₂₉₈ = -758.845810****SCF_{DFT} = -1486.007125**

11-Br

C	0.0090	0.0025	1.1017
C	0.0183	0.0387	3.9109
C	0.0390	-1.2152	1.7932
C	-0.0167	1.2454	1.7932
C	-0.0120	1.2618	3.2054
C	0.0435	-1.1895	3.1936
I	0.0776	-3.0925	0.7223
F	0.0718	-2.3269	3.9262
F	0.0230	0.0407	5.2641
F	-0.0363	2.4370	3.8754
F	-0.0456	2.4103	1.1054
F	0.0029	0.0531	-0.2505
Br	0.1298	-5.6079	-0.7128

SCF = -2872.771349**11-DMF**

C	0.1021	0.5897	2.2624
C	0.7032	0.0260	4.9532
C	0.2564	-0.7503	2.6603
C	0.2445	1.6532	3.1936
C	0.5464	1.3706	4.5457
C	0.5568	-1.0239	4.0065
F	0.7176	-2.2881	4.4531
F	0.9916	-0.2622	6.2399
F	0.6832	2.3728	5.4365
F	0.0913	2.9310	2.7864
F	-0.1864	0.9191	0.9842
I	0.0460	-2.2762	1.3020
O	-0.2743	-4.3518	-0.7002
C	-0.4691	-4.8034	-1.8148
H	-0.5134	-5.8853	-1.9928
N	-0.6486	-4.0830	-2.9303
C	-0.6243	-2.6361	-2.8993
H	0.1753	-2.2631	-3.5386
H	-0.4559	-2.3105	-1.8802
H	-1.5744	-2.2406	-3.2568
C	-0.8712	-4.7101	-4.2122
H	-0.0873	-4.4278	-4.9146
H	-1.8329	-4.4035	-4.6230
H	-0.8669	-5.7899	-4.0961

SCF = -547.118039**11-NH3**

C	0.1941	-0.0258	1.2946
C	-0.1500	0.0115	4.1256
C	0.0926	-1.2257	2.0200
C	0.1225	1.1927	1.9918
C	-0.0488	1.2220	3.4023
C	-0.0790	-1.2177	3.4308
I	0.4437	-0.0526	-0.7509
F	0.1537	-2.4292	1.4095
F	-0.1737	-2.3835	4.1046
F	-0.3125	0.0291	5.4635
F	-0.1146	2.4052	4.0487
F	0.2130	2.3798	1.3533
N	0.8050	-0.0898	-3.6813
H	1.7736	0.0584	-3.9237
H	0.2567	0.6365	-4.1179
H	0.5164	-0.9769	-4.0669

SCF = -355.116908**12**

C	0.5693	-0.2860	1.0722
C	-0.0132	0.5855	3.6886
C	0.2448	-1.2126	2.0840
C	0.5963	1.0858	1.3967
C	0.3078	1.5406	2.7009
C	-0.0497	-0.7951	3.3992
I	0.9925	-0.9187	-0.8276
I	-0.5145	-2.1477	4.8396
I	0.3540	3.5208	3.1450
F	-0.2925	1.0031	4.9424
F	0.2154	-2.5299	1.7871
F	0.9053	1.9846	0.4372

SCF = -298.334535**ZPE = 0.049589****H₂₉₈ = -298.272699****G₂₉₈ = -298.326041****SCF_{DFT} = -1421.292715**

12-Cl

C	0.5716	-0.2895	1.0564
C	-0.0103	0.5799	3.6760
C	0.2530	-1.2105	2.0639
C	0.5943	1.0739	1.3816
C	0.3060	1.5336	2.6890
C	-0.0426	-0.7977	3.3853
I	1.0205	-0.9590	-0.9619
Cl	1.5799	-1.7892	-3.4703
I	-0.5021	-2.1521	4.8290
I	0.3457	3.5155	3.1363
F	-0.2903	0.9982	4.9361
F	0.2253	-2.5315	1.7731
F	0.8994	1.9810	0.4252

SCF = -758.655377**ZPE = 0.049953****H₂₉₈ = -758.590908****G₂₉₈ = -758.649262****SCF_{DFT} = -1881.604887****12-OCH2**

C	0.5368	-0.5229	1.0044
C	0.0105	0.6385	3.5188
C	0.2492	-1.3293	2.1240
C	0.5553	0.8764	1.1699
C	0.2946	1.4767	2.4199
C	-0.0168	-0.7661	3.3905
I	0.9204	-1.3675	-0.8274
I	-0.4286	-1.9481	4.9885
I	0.3274	3.4951	2.6319
F	-0.2418	1.1954	4.7237
F	0.2273	-2.6723	1.9816
F	0.8291	1.6624	0.1050
O	1.5027	-2.1390	-3.6568
C	1.6140	-1.1703	-4.3549
H	1.8322	-1.2616	-5.4270
H	1.5017	-0.1554	-3.9473

SCF = -412.870241**ZPE = 0.078203****H₂₉₈ = -412.775130****G₂₉₈ = -412.838694****SCF_{DFT} = -1535.828454****13**

C	-0.0011	-0.0039	1.1746
I	-0.0036	-0.0155	-0.9088
Br	-0.9271	-1.5552	1.7853
Br	1.8093	-0.0258	1.7735
Br	-0.8834	1.5793	1.7679

SCF = -298.229816**ZPE = 0.007377****H₂₉₈ = -298.214634****G₂₉₈ = -298.258103****SCF_{DFT} = -8058.043593****13-OCH2**

C	-0.0323	0.0505	0.8972
I	-0.3423	-0.3572	-1.1311
Br	-0.6157	-1.4562	1.9066
Br	1.8295	0.3599	1.1654
Br	-1.0426	1.6003	1.3558
O	-0.5366	-0.5836	-4.0344
C	0.0566	0.2906	-4.6034
H	0.0806	0.3420	-5.6995
H	0.5965	1.0702	-4.0474

SCF = -412.766459**ZPE = 0.036067****H₂₉₈ = -412.717982****G₂₉₈ = -412.771823****SCF_{DFT} = -8172.579952****13-Cl**

C	0.0001	-0.0038	1.2004
I	-0.0021	-0.0162	-1.0386
Cl	-0.0049	-0.0320	-3.6872
Br	-0.9230	-1.5585	1.7525
Br	1.8113	-0.0215	1.7418
Br	-0.8870	1.5782	1.7340

SCF = -758.560771**ZPE = 0.007756****H₂₉₈ = -758.542955****G₂₉₈ = -758.591471****SCF_{DFT} = -8518.359490****14**

C	-0.0002	-0.0021	1.1050
I	0.0067	-0.0209	-1.1104
F	-0.6351	-1.0775	1.6591
F	1.2498	-0.0061	1.6563
F	-0.6204	1.0905	1.6416

SCF = -298.484337**ZPE = 0.015056****H₂₉₈ = -298.463463****G₂₉₈ = -298.499694**

SCF_{DFT} = -635.398480

14-Cl

C	-0.0003	-0.0030	1.0876
I	0.0004	-0.0195	-1.2984
Cl	0.0011	-0.0379	-3.9037
F	-0.6289	-1.0715	1.6776
F	1.2427	-0.0069	1.6708
F	-0.6151	1.0815	1.6626

SCF = -758.829510

ZPE = 0.015511

H₂₉₈ = -758.805884

G₂₉₈ = -758.847707

SCF_{DFT} = -1095.708736

14-OCH2

C	-0.0100	0.0673	0.8482
I	0.0107	-0.4309	-1.3187
F	-0.6590	-0.8539	1.6217
F	1.2353	0.1748	1.4020
F	-0.6220	1.2566	1.1337
O	0.0302	-0.7437	-4.1438
C	0.0149	0.2845	-4.7642
H	0.0194	0.2850	-5.8613
H	-0.0042	1.2580	-4.2546

SCF = -413.022156

ZPE = 0.043875

H₂₉₈ = -412.967951

G₂₉₈ = -413.014456

SCF_{DFT} = -749.934921

15

C	0.0034	-0.0003	1.1367
I	0.0134	0.0013	-1.0002
C	-0.7162	-1.2428	1.6068
H	-0.1986	-2.1655	1.2489
H	-1.7720	-1.2566	1.2426
H	-0.7339	-1.2656	2.7255
C	1.4356	-0.0009	1.6176
H	1.9783	-0.9093	1.2599
H	1.4559	-0.0017	2.7365
H	1.9786	0.9078	1.2612
C	-0.7158	1.2417	1.6086
H	-0.1978	2.1648	1.2520
H	-0.7335	1.2630	2.7274
H	-1.7716	1.2565	1.2444

SCF = -298.284931

ZPE = 0.121410

H₂₉₈ = -298.155468

G₂₉₈ = -298.195549

SCF_{DFT} = -455.547289

15-Cl

C	-0.0002	-0.0043	1.1045
I	0.0013	-0.0170	-1.0922
Cl	0.0026	-0.0321	-3.9512
C	-0.7156	-1.2394	1.5834
H	-0.2001	-2.1621	1.2222
H	-1.7708	-1.2543	1.2173
H	-0.7388	-1.2735	2.7028
C	1.4291	-0.0019	1.5774
H	1.9682	-0.9113	1.2168
H	1.4750	0.0048	2.6965
H	1.9687	0.9028	1.2059
C	-0.7150	1.2367	1.5687
H	-0.1985	2.1548	1.1973
H	-0.7391	1.2836	2.6876
H	-1.7699	1.2482	1.2015

SCF = -758.582173

ZPE = 0.121955

H₂₉₈ = -758.449872

G₂₉₈ = -758.495598

SCF_{DFT} = -915.828865

15-OCH2

C	0.0829	-0.0768	0.9341
I	0.3560	-0.4705	-1.1513
C	-0.7548	-1.1882	1.5218
H	-0.2483	-2.1766	1.4036
H	-1.7575	-1.2359	1.0322
H	-0.9100	-1.0053	2.6149
C	1.4426	-0.0333	1.5912
H	1.9753	-1.0080	1.4736
H	1.3259	0.1696	2.6854
H	2.0734	0.7776	1.1531
C	-0.6201	1.2522	1.0813
H	-0.0134	2.0778	0.6367
H	-0.7731	1.4792	2.1663
H	-1.6214	1.2327	0.5869
O	0.4528	-0.5758	-4.2280
C	-0.1452	0.3866	-4.6169
H	-0.2590	0.5934	-5.6897
H	-0.6030	1.0997	-3.9167

SCF = -412.818976

ZPE = 0.150022

H₂₉₈ = -412.656220

G₂₉₈ = -412.707286

SCF_{DFT} = -570.079022

16

C	-0.0009	-0.0047	1.1487
I	0.0022	-0.0155	-0.9905
C	-0.6939	-1.2013	1.5864
N	-1.2494	-2.1605	1.9331
C	1.3829	-0.0028	1.5832
N	2.4922	-0.0014	1.9274
C	-0.6934	1.1965	1.5742
N	-1.2489	2.1593	1.9111

SCF = -298.081194

ZPE = 0.036847

H₂₉₈ = -298.036006

G₂₉₈ = -298.078294

SCF_{DFT} = -614.325092

16-OCH2

C	-0.0124	-0.0530	1.0135
I	0.0138	-0.4486	-1.1011
C	-0.7017	-1.1572	1.6509
N	-1.2550	-2.0451	2.1555
C	1.3662	0.0399	1.4514
N	2.4732	0.1131	1.7957
C	-0.7178	1.1987	1.2064
N	-1.2840	2.2024	1.3527
O	0.0455	-0.6563	-3.9571
C	0.0347	0.3835	-4.5576
H	0.0499	0.4061	-5.6545
H	0.0090	1.3469	-4.0293

SCF = -412.618891

ZPE = 0.065594

H₂₉₈ = -412.540404

G₂₉₈ = -412.592872

SCF_{DFT} = -728.866201

17

I	0.1000	-1.3425	-1.5377
N	-0.5936	-0.4282	0.0608
C	0.0669	-0.3798	1.3103
C	-1.8203	0.2731	0.1179
O	1.1553	-0.9079	1.5442
O	-2.5999	0.3918	-0.8289
C	-2.0137	0.8468	1.5186
H	-2.1095	1.9584	1.4515
H	-2.9550	0.4347	1.9587
C	-0.7753	0.4197	2.3003
H	-0.1828	1.2944	2.6655
H	-1.0293	-0.2279	3.1753

SCF = -298.329738

ZPE = 0.083516

H₂₉₈ = -298.238072

G₂₉₈ = -298.279903

SCF_{DFT} = -657.796458

17-OCH2

I	0.5716	-1.3705	-1.3921
N	-0.3514	-0.4507	0.0949
C	0.0917	-0.4373	1.4368
C	-1.5477	0.2866	-0.0393
O	1.1103	-0.9999	1.8431
O	-2.1570	0.4427	-1.1007
C	-1.9584	0.8501	1.3183
H	-2.0094	1.9649	1.2552
H	-2.9715	0.4625	1.5878
C	-0.8811	0.3749	2.2880
H	-0.3337	1.2259	2.7629
H	-1.2963	-0.2761	3.0962
O	1.5412	-2.5115	-3.8892
C	0.8263	-2.1969	-4.8010
H	1.0301	-2.5350	-5.8250
H	-0.0555	-1.5602	-4.6414

SCF = -412.866946

ZPE = 0.112317

H₂₉₈ = -412.741957

G₂₉₈ = -412.794006

SCF_{DFT} = -772.336582

18

I	-0.0013	0.0233	-0.7813
C	0.0014	-0.0615	1.2457
H	0.0053	0.9324	1.7086
C	-0.0011	-1.1803	1.9548
H	0.0006	-1.1680	3.0556
H	-0.0050	-2.1862	1.5116

SCF = -298.222735
 ZPE = 0.041935
 H_{298} = -298.176102
 G_{298} = -298.208243

SCF_{DFT} = -375.662870

18-OCH2

I	-0.5297	-0.4380	-1.1388
C	-0.2678	-0.0764	0.8435
H	-0.5481	0.9447	1.1278
C	0.1862	-0.9594	1.7201
H	0.3067	-0.7097	2.7854
H	0.4711	-1.9884	1.4592
O	-0.5741	-0.5222	-4.2295
C	0.0991	0.3931	-4.6097
H	0.2556	0.5816	-5.6804
H	0.5861	1.0795	-3.9024

SCF = -412.756915
 ZPE = 0.070518
 H_{298} = -412.677020
 G_{298} = -412.721223

SCF_{DFT} = -490.196061

18-Cl

I	-0.0028	-0.0070	-0.8890
Cl	-0.0065	0.1280	-3.8085
C	0.0001	-0.0680	1.1837
H	0.0019	0.9276	1.6412
C	-0.0001	-1.1678	1.9201
H	0.0016	-1.1497	3.0198
H	-0.0018	-2.1786	1.4911

SCF = -758.519104
 ZPE = 0.042505
 H_{298} = -758.469706
 G_{298} = -758.507775

SCF_{DFT} = -835.951521

19

I	-0.0020	-0.0380	-0.7952
C	0.0012	-0.0538	1.2284
H	0.0049	0.9497	1.6733
C	-0.0009	-1.1669	1.9629
H	-0.0046	-2.1823	1.5225
C	0.0016	-1.1448	3.3836
N	0.0036	-1.1464	4.5474

SCF = -298.174073

ZPE = 0.042404
 H_{298} = -298.125475
 G_{298} = -298.162012

SCF_{DFT} = -467.931598

19-Cl

I	-0.0026	-0.0409	-0.9034
Cl	-0.0077	0.0140	-3.7193
C	0.0004	-0.0487	1.1879
H	0.0023	0.9524	1.6331
C	-0.0000	-1.1526	1.9337
H	-0.0020	-2.1647	1.4908
C	0.0020	-1.1443	3.3542
N	0.0037	-1.1516	4.5197

SCF = -758.484335
 ZPE = 0.042775
 H_{298} = -758.433145
 G_{298} = -758.475021

SCF_{DFT} = -928.238968

19-OCH2

I	0.0642	-0.5938	-1.0907
C	0.0570	-0.2042	0.8998
H	0.1240	0.8648	1.1389
C	-0.0205	-1.1455	1.8411
H	-0.0878	-2.2258	1.6106
C	-0.0231	-0.8410	3.2292
N	-0.0266	-0.6101	4.3699
O	0.0462	-0.7046	-4.1320
C	-0.0260	0.3985	-4.5953
H	-0.0461	0.5624	-5.6809
H	-0.0747	1.2880	-3.9509

SCF = -412.709024
 ZPE = 0.070972
 H_{298} = -412.627162
 G_{298} = -412.675150

SCF_{DFT} = -582.466512

20

I	-0.0308	0.0495	-0.8142
C	-0.2858	-0.1050	1.1808
H	-0.6655	0.8101	1.6418
C	0.0008	-1.2275	1.8667
H	0.3655	-2.1353	1.3400
N	-0.0363	-1.3780	3.2503
C	-0.2466	-2.7093	3.7603
H	0.3304	-3.4500	3.1468
H	-1.3323	-3.0010	3.7513
H	0.1262	-2.7513	4.8182
C	-0.5951	-0.3120	4.0400
H	-0.0497	0.6409	3.8060
H	-0.4608	-0.5466	5.1286
H	-1.6900	-0.1580	3.8358

SCF = -298.220109**ZPE = 0.115689****H₂₉₈ = -298.095510****G₂₉₈ = -298.138501****SCF_{DFT} = -509.663285****20-Cl**

I	-0.0649	-0.0175	-0.8934
Cl	0.2504	0.2316	-3.7862
C	-0.3160	-0.1781	1.1551
H	-0.8491	0.6691	1.5951
C	0.1334	-1.2128	1.8719
H	0.6623	-2.0574	1.3862
N	0.0943	-1.3683	3.2815
C	-0.3105	-2.6835	3.7202
H	0.2551	-3.4601	3.1422
H	-1.4111	-2.8749	3.5895
H	-0.0619	-2.7917	4.8091
C	-0.5321	-0.2997	4.0201
H	-0.0354	0.6678	3.7456
H	-0.3904	-0.4820	5.1180
H	-1.6340	-0.2039	3.8155

SCF = -758.513967**ZPE = 0.116291****H₂₉₈ = -758.386651****G₂₉₈ = -758.434580****SCF_{DFT} = -969.948081****20-OCH2**

I	0.4602	-0.5664	-1.0755
C	-0.0313	-0.4058	0.8779
H	-0.4431	0.5700	1.1467
C	0.1519	-1.4083	1.7571
H	0.5576	-2.3869	1.4221
N	-0.0472	-1.3448	3.1346
C	-0.3543	-2.5809	3.8087
H	0.2690	-3.4122	3.3862
H	-1.4393	-2.8594	3.7133
H	-0.1093	-2.4663	4.8981
C	-0.6694	-0.1675	3.6813
H	-0.0807	0.7357	3.3683
H	-0.6645	-0.2310	4.8011
H	-1.7306	-0.0426	3.3312
O	0.8116	-0.3041	-4.1613
C	0.1421	0.6415	-4.4659
H	0.0713	0.9795	-5.5088
H	-0.4270	1.2075	-3.7147

SCF = -412.754100**ZPE = 0.144227****H₂₉₈ = -412.597182****G₂₉₈ = -412.648691****SCF_{DFT} = -624.196068****21**

I	0.0000	0.0000	-0.4893
C	0.0000	0.0000	1.4367
H	0.0000	0.0000	3.6966
C	0.0000	0.0000	2.6344

SCF = -298.165728**21-Cl**

I	0.0190	-0.0519	-0.8000
Cl	0.3138	-0.1478	-3.6673
C	-0.1863	0.0138	1.1802
H	-0.4182	0.0909	3.4248
C	-0.3096	0.0548	2.3734

SCF = -758.468762**21-OCH2**

I	-0.0686	-0.5766	-0.9739
C	-0.1887	-0.0389	0.8774
H	-0.3284	0.5845	3.0447
C	-0.2629	0.2917	2.0261
O	0.1654	-0.8892	-4.0138
C	0.3102	0.1926	-4.5093
H	0.4157	0.3144	-5.5956
H	0.3429	1.1041	-3.8951

SCF = -412.700609

22

I	0.0000	0.0000	-1.2158
C	0.0000	0.0000	0.7090
C	0.0000	0.0000	1.9077
C	0.0000	0.0000	3.2774
N	0.0000	0.0000	4.4420

SCF = -298.113787

22-OCH2

I	-0.0419	-0.6348	-0.8901
C	-0.1986	-0.2067	0.9866
C	-0.2968	0.0562	2.1523
C	-0.4092	0.3571	3.4836
N	-0.5050	0.6130	4.6159
O	0.2255	-0.8192	-3.8864
C	0.2947	0.2544	-4.4162
H	0.4005	0.3488	-5.5049
H	0.2547	1.1842	-3.8306

SCF = -412.649548

22-Cl

I	0.0181	-0.0522	-0.7995
Cl	0.3057	-0.1412	-3.5556
C	-0.1907	0.0129	1.2062
C	-0.3141	0.0536	2.4039
C	-0.4538	0.1008	3.7619
N	-0.5734	0.1416	4.9215

SCF = -758.432728

23

I	0.0000	0.0000	-0.4861
C	0.0000	0.0000	1.4545
N	0.0000	0.0000	2.6164

SCF = -298.201375

23-OCH2

I	-0.0079	-0.3881	-0.8722
C	-0.1683	0.1691	0.9871
N	-0.2638	0.5005	2.0968
O	0.2410	-0.8343	-3.8165
C	0.2897	0.1726	-4.4663
H	0.3849	0.1432	-5.5597
H	0.2406	1.1628	-3.9906

SCF = -412.737472

23-Cl

I	0.0311	-0.0427	-0.7502
Cl	0.2922	-0.1497	-3.5164
C	-0.1901	0.0211	1.2668
N	-0.3301	0.0532	2.4227

SCF = -758.520209

24

C	5.0016	2.0773	0.3070
C	3.5760	-0.3178	-0.1484
C	3.5944	2.0868	0.3098
C	5.7035	0.8665	0.0754
C	4.9822	-0.3334	-0.1527
C	2.9004	0.8889	0.0818
C	1.4273	0.8976	0.0836
C	-1.4274	0.8976	0.0835
C	0.7114	1.1269	-1.1085
C	0.7114	0.6726	1.2765
C	-0.7115	0.6726	1.2765
C	-0.7114	1.1269	-1.1086
C	-2.9004	0.8889	0.0816
C	-5.7036	0.8665	0.0750
C	-3.5944	2.0867	0.3096
C	-3.5760	-0.3178	-0.1486
C	-4.9822	-0.3335	-0.1530
C	-5.0017	2.0773	0.3067
I	-2.5190	-2.0389	-0.4744
I	2.5190	-2.0389	-0.4742
F	-7.0527	0.8564	0.0716
F	-5.6869	-1.4636	-0.3694
F	-5.7265	3.1955	0.5193
F	-1.3538	1.3495	-2.2751
F	1.3539	1.3496	-2.2750
F	1.3538	0.4511	2.4432
F	-1.3539	0.4511	2.4431
F	5.7264	3.1956	0.5196
F	7.0526	0.8565	0.0721
F	5.6869	-1.4635	-0.3690
I	2.5737	3.8089	0.6391
I	-2.5738	3.8088	0.6390

SCF = -596.949790

ZPE = 0.152745

 $H_{298} = -596.767572$ $G_{298} = -596.856199$ SCF_{DFT} = -2875.447998

24-OCH2

C	-1.0573	0.4505	1.5931
C	1.0624	-0.4204	3.2441
C	-1.1470	-0.7895	2.2531
C	0.0949	1.2612	1.7570
C	1.1565	0.8182	2.5877
C	-0.0864	-1.2072	3.0689
C	-0.1621	-2.5016	3.7679
C	-0.1031	-4.9635	5.2080
C	0.3421	-3.6712	3.1644
C	-0.6952	-2.5813	5.0701
C	-0.6658	-3.8089	5.7883
C	0.3716	-4.8989	3.8826
C	0.0331	-6.2035	5.9914
C	0.3291	-8.5488	7.4944
C	-0.9946	-7.1566	5.9767
C	1.2049	-6.3951	6.7395
C	1.3566	-7.5702	7.4944
C	-0.8474	-8.3356	6.7314
I	2.6662	-4.9562	6.7133
I	2.5751	-1.0972	4.4523
F	0.4705	-9.6789	8.2181
F	2.4603	-7.8105	8.2332
F	-1.7996	-9.2919	6.7596
F	0.8825	-5.9891	3.2714
F	0.8262	-3.6519	1.9040
F	-1.2255	-1.4959	5.6736
F	-1.1696	-3.8333	7.0408
F	-2.0434	0.9097	0.7939
F	0.1811	2.4502	1.1246
F	2.2356	1.6185	2.7175
O	4.5971	-2.5072	6.3828
C	5.6706	-2.2091	6.8319
H	6.2032	-2.8749	7.5233
H	6.1554	-1.2609	6.5663
I	-2.6679	-6.8296	4.8779
I	-2.7846	-1.9661	2.0341

SCF = -711.489539**ZPE = 0.181398****H₂₉₈ = -711.274027****G₂₉₈ = -711.372390****SCF_{DFT} = -2989.986608****24-Cl**

C	-0.9124	0.4310	1.5629
C	0.9986	-0.4454	3.4544
C	-1.0614	-0.8237	2.1791
C	0.1938	1.2541	1.8897
C	1.1481	0.8065	2.8401
C	-0.1035	-1.2421	3.1148
C	-0.2386	-2.5532	3.7723
C	-0.2311	-5.0249	5.2011
C	0.3715	-3.6976	3.2209
C	-0.9178	-2.6723	5.0012
C	-0.9141	-3.9036	5.7130
C	0.3752	-4.9289	3.9326
C	-0.0879	-6.2482	6.0089
C	0.2250	-8.5536	7.5604
C	-1.0413	-7.2724	5.9077
C	1.0172	-6.3460	6.8654
C	1.1747	-7.5020	7.6437
C	-0.8844	-8.4316	6.6874
I	2.3930	-4.7567	6.9504
I	2.3821	-1.1572	4.8700
F	0.3735	-9.6696	8.3091
F	2.2161	-7.6620	8.4897
F	-1.7669	-9.4569	6.6380
F	0.9923	-5.9925	3.3721
F	0.9851	-3.6496	2.0178
F	-1.5684	-1.6192	5.5435
F	-1.5611	-3.9622	6.8980
F	-1.7996	0.8952	0.6519
F	0.3348	2.4604	1.2954
F	2.1863	1.6247	3.1208
Cl	4.0935	-2.4139	6.8426
I	-2.6379	-2.0202	1.7281
I	-2.6224	-7.0741	4.6502

SCF = -1057.300085**ZPE = 0.153406****H₂₉₈ = -1057.115179****G₂₉₈ = -1057.207364****SCF_{DFT} = -3335.784617**

	25		
C	0.3111	-1.3475	0.3028
C	-0.3253	1.3943	0.0419
C	1.3533	-0.3944	0.2461
C	-1.0439	-0.9530	0.2233
C	-1.3492	0.4216	0.1008
C	1.0218	0.9740	0.1230
C	2.7611	-0.8226	0.2887
C	5.4433	-1.6422	0.3577
C	3.4192	-1.1200	-0.9154
C	3.4164	-0.9259	1.5235
C	4.7611	-1.3367	1.5629
C	4.7643	-1.5312	-0.8829
C	-2.1182	-1.9591	0.2418
C	-4.1659	-3.8768	0.2638
C	-2.6807	-2.3497	1.4648
C	-2.5579	-2.5080	-0.9735
C	-3.5847	-3.4697	-0.9646
C	-3.7077	-3.3108	1.4807
C	-0.6556	2.8188	-0.1269
C	-1.2829	5.5327	-0.4614
C	-0.7638	3.3435	-1.4248
C	-0.8550	3.6224	1.0041
C	-1.1695	4.9837	0.8412
C	-1.0783	4.7043	-1.5946
I	2.4228	-0.4806	3.2546
I	2.4345	-0.9561	-2.6819
I	-1.7164	-1.9158	-2.7223
I	-2.0115	-1.5273	3.2137
I	-0.4686	2.1456	-3.0357
I	-0.6901	2.8193	2.8779
F	0.6149	-2.6564	0.4265
F	-2.6392	0.8110	0.0306
F	2.0078	1.8938	0.0740
F	-4.0499	-4.0333	-2.0992
F	-5.1508	-4.7989	0.2740
F	-4.2862	-3.7246	2.6274
F	5.4423	-1.4545	2.7218
F	6.7331	-2.0367	0.3904
F	5.4503	-1.8309	-2.0058
F	-1.5844	6.8379	-0.6227
F	-1.3718	5.8048	1.8928
F	-1.1959	5.2665	-2.8158

SCF = -895.242974

ZPE = 0.200306

H₂₉₈ = -895.003398G₂₉₈ = -895.112389SCF_{DFT} = -3899.228083

	25-OCH2		
C	0.3116	-1.3518	0.2884
C	-0.3214	1.3925	0.0442
C	1.3550	-0.3996	0.2393
C	-1.0428	-0.9550	0.2128
C	-1.3462	0.4203	0.0940
C	1.0252	0.9697	0.1205
C	2.7624	-0.8281	0.2936
C	5.4448	-1.6410	0.3888
C	3.4328	-1.1272	-0.9019
C	3.4041	-0.9285	1.5374
C	4.7501	-1.3361	1.5871
C	4.7774	-1.5344	-0.8583
C	-2.1196	-1.9584	0.2411
C	-4.1755	-3.8654	0.2877
C	-2.6779	-2.3342	1.4725
C	-2.5657	-2.5177	-0.9657
C	-3.5965	-3.4733	-0.9463
C	-3.7097	-3.2907	1.4978
C	-0.6506	2.8193	-0.1092
C	-1.2775	5.5350	-0.4190
C	-0.7624	3.3567	-1.4004
C	-0.8458	3.6112	1.0323
C	-1.1603	4.9743	0.8785
C	-1.0765	4.7168	-1.5602
I	2.3938	-0.4897	3.2411
I	2.4433	-0.9693	-2.6871
I	-1.7091	-1.9384	-2.7325
I	-1.9975	-1.5026	3.1933
I	-0.4627	2.1406	-3.0214
I	-0.6742	2.7908	2.8797
F	0.6138	-2.6617	0.4068
F	-2.6358	0.8114	0.0233
F	2.0127	1.8884	0.0752
F	-4.0671	-4.0440	-2.0754
F	-5.1655	-4.7821	0.3108
F	-4.2870	-3.6926	2.6499
F	5.4220	-1.4514	2.7522
F	6.7357	-2.0314	0.4352
F	5.4729	-1.8339	-1.9757
F	-1.5792	6.8420	-0.5669
F	-1.3594	5.7879	1.9372
F	-1.1967	5.2867	-2.7780
O	0.1337	-0.1806	-5.0720
C	0.1331	-0.0568	-6.2678
H	0.3831	-0.8976	-6.9275
H	-0.1176	0.9018	-6.7409

SCF = -1009.783774

ZPE = 0.228868

H₂₉₈ = -1009.510931G₂₉₈ = -1009.629515SCF_{DFT} = -4013.768691

25-Cl

C	0.3080	-1.3434	0.3493
C	-0.3254	1.3990	0.0906
C	1.3520	-0.3923	0.2944
C	-1.0467	-0.9486	0.2711
C	-1.3493	0.4265	0.1480
C	1.0208	0.9761	0.1710
C	2.7601	-0.8243	0.3042
C	5.4379	-1.6466	0.3065
C	3.3884	-1.1123	-0.9170
C	3.4407	-0.9384	1.5264
C	4.7849	-1.3510	1.5286
C	4.7296	-1.5244	-0.9168
C	-2.1211	-1.9560	0.2570
C	-4.1633	-3.8728	0.2139
C	-2.7033	-2.3640	1.4672
C	-2.5372	-2.4847	-0.9744
C	-3.5601	-3.4449	-0.9969
C	-3.7285	-3.3262	1.4465
C	-0.6535	2.8206	-0.1112
C	-1.2787	5.5215	-0.5120
C	-0.7543	3.3123	-1.4216
C	-0.8577	3.6492	1.0031
C	-1.1716	5.0051	0.8029
C	-1.0676	4.6650	-1.6233
I	2.4878	-0.5106	3.2666
I	2.2994	-0.9134	-2.6753
I	-1.6150	-1.8192	-2.7128
I	-2.0668	-1.5691	3.2228
I	-0.4334	2.0091	-3.0077
I	-0.6996	2.8906	2.8790
Cl	0.1450	-0.4076	-4.7720
F	0.6106	-2.6536	0.4767
F	-2.6402	0.8180	0.0818
F	2.0086	1.8961	0.1268
F	-4.0053	-3.9920	-2.1494
F	-5.1490	-4.7978	0.1955
F	-4.3297	-3.7613	2.5780
F	5.4960	-1.4802	2.6725
F	6.7303	-2.0432	0.3101
F	5.3907	-1.8163	-2.0585
F	-1.5808	6.8253	-0.7031
F	-1.3802	5.8552	1.8347
F	-1.1794	5.1990	-2.8595

SCF = -1355.609226**ZPE = 0.201077****H₂₉₈ = -1355.366949****G₂₉₈ = -1355.478894****SCF_{DFT} = -4359.578252****26**

H	-1.4213	0.8653	-2.0911
C	-1.3263	1.5915	-1.2679
C	-1.0858	3.4721	0.8242
C	-1.1283	1.2088	0.0438
C	-1.4055	2.9668	-1.5327
C	-1.2861	3.8911	-0.4958
C	-1.0028	2.1081	1.1177
H	-1.5633	3.3078	-2.5700
H	-1.3501	4.9714	-0.7160
H	-0.9936	4.2167	1.6313
C	-0.7974	1.5436	2.4414
C	-0.4082	0.2248	4.8976
C	-0.7400	0.1422	2.5447
C	-0.6522	2.2795	3.6207
C	-0.4591	1.6167	4.8378
C	-0.5508	-0.5398	3.7302
H	-0.6899	3.3806	3.5921
H	-0.3456	2.2085	5.7633
H	-0.5098	-1.6396	3.7831
H	-0.2554	-0.2880	5.8624
I	-0.9768	-0.7590	0.6891

SCF = -298.415956**ZPE = 0.163593****H₂₉₈ = -298.241681****G₂₉₈ = -298.288620****SCF_{DFT} = -759.580057****26-Cl**

H	-1.4241	0.8356	-2.0838
C	-1.3294	1.5870	-1.2688
C	-1.0848	3.4549	0.8228
C	-1.1311	1.1897	0.0395
C	-1.4067	2.9599	-1.5322
C	-1.2850	3.8805	-0.4929
C	-1.0040	2.0890	1.1113
H	-1.5640	3.3023	-2.5662
H	-1.3469	4.9591	-0.7079
H	-0.9907	4.1938	1.6323
C	-0.7977	1.5268	2.4390
C	-0.4099	0.2277	4.8848
C	-0.7446	0.1276	2.5170
C	-0.6532	2.2765	3.6100
C	-0.4600	1.6197	4.8273
C	-0.5538	-0.5301	3.7161
H	-0.6908	3.3752	3.5790
H	-0.3465	2.2102	5.7494
H	-0.5136	-1.6284	3.7669
H	-0.2572	-0.2793	5.8493
I	-0.9896	-0.8030	0.6209
Cl	-1.3297	-1.4737	-1.8792

SCF = -758.885828

ZPE = 0.165123

H₂₉₈ = -758.708118

G₂₉₈ = -758.759292

SCF_{DFT} = -1220.035764

26-OCH2

H	-1.3706	1.2495	-2.1291
C	-1.2892	1.9252	-1.2593
C	-1.0808	3.6463	0.9684
C	-1.1019	1.4474	0.0218
C	-1.3741	3.3162	-1.4225
C	-1.2706	4.1612	-0.3194
C	-0.9925	2.2652	1.1609
H	-1.5234	3.7318	-2.4328
H	-1.3387	5.2543	-0.4583
H	-1.0012	4.3300	1.8289
C	-0.7969	1.6045	2.4412
C	-0.4246	0.1092	4.7929
C	-0.7326	0.1997	2.4334
C	-0.6685	2.2522	3.6727
C	-0.4835	1.5011	4.8386
C	-0.5507	-0.5644	3.5694
H	-0.7127	3.3519	3.7270
H	-0.3833	2.0220	5.8067
H	-0.5034	-1.6646	3.5401
H	-0.2784	-0.4740	5.7174
I	-0.9458	-0.5629	0.5140
O	-1.2789	-1.0610	-2.2147
C	-1.3654	-1.8208	-3.1470
H	-1.2973	-2.9046	-3.0117
H	-1.5156	-1.4438	-4.1626

SCF = -412.970080

ZPE = 0.192848

H₂₉₈ = -412.762046

G₂₉₈ = -412.818737

SCF_{DFT} = -874.129826

27

H	-0.0076	0.1485	0.1287
C	-0.0141	0.1263	1.2314
C	-0.0288	0.1051	4.0588
C	-0.0446	-1.0466	1.9573
C	0.0093	1.3323	1.9511
C	0.0005	1.3100	3.3450
C	-0.0519	-1.1065	3.3629
H	0.0395	2.2944	1.4063
H	-0.0283	0.1208	5.1636
C	-0.0826	-2.4238	3.9765
C	-0.1477	-5.0736	4.9353
C	-0.1057	-3.5381	3.1180
C	-0.0912	-2.6708	5.3520
C	-0.1225	-3.9924	5.8151
C	-0.1389	-4.8484	3.5490
H	-0.0787	-1.8353	6.0749
H	-0.1583	-5.7065	2.8563
H	-0.1795	-6.1096	5.3215
I	-0.0839	-2.9498	1.1260
C	0.0064	2.6351	4.1239
C	-0.1119	-4.2494	7.3305
F	0.6285	3.6601	3.4614
F	0.6375	2.5538	5.3381
F	-1.2530	3.0978	4.4047
F	-0.7258	-3.2629	8.0578
F	-0.7390	-5.4111	7.6961
F	1.1534	-4.3429	7.8498

SCF = -298.885603

ZPE = 0.175897

H₂₉₈ = -298.691503

G₂₉₈ = -298.755467

SCF_{DFT} = -1433.891570

27-OCH2

H	-0.0217	0.5538	0.2457
C	-0.0329	0.4560	1.3438
C	-0.0592	0.2413	4.1606
C	-0.0438	-0.7680	1.9822
C	-0.0361	1.6100	2.1428
C	-0.0503	1.4926	3.5320
C	-0.0561	-0.9181	3.3808
H	-0.0224	2.6075	1.6664
H	-0.0632	0.1803	5.2633
C	-0.0643	-2.2755	3.9012
C	-0.0763	-4.9869	4.6713
C	-0.0594	-3.3272	2.9663
C	-0.0766	-2.6186	5.2553
C	-0.0836	-3.9701	5.6245
C	-0.0640	-4.6645	3.3044
H	-0.0754	-1.8362	6.0348
H	-0.0584	-5.4643	2.5410
H	-0.0751	-6.0471	4.9838
I	-0.0424	-2.6079	1.0188
C	-0.0735	2.7605	4.3983
C	-0.1167	-4.3318	7.1168
F	0.5375	3.8392	3.8146
F	0.5469	2.6094	5.6116
F	-1.3425	3.1852	4.6974
F	0.5154	-3.4171	7.9189
F	-1.3888	-4.4276	7.6195
F	0.4749	-5.5332	7.4070
O	-0.0447	-5.2704	0.2551
C	-0.0433	-6.1078	-0.6143
H	-0.0465	-7.1719	-0.3623
H	-0.0387	-5.8340	-1.6737

SCF = -413.441921**ZPE = 0.205224****H₂₉₈ = -413.214041****G₂₉₈ = -413.287442****SCF_{DFT} = -1548.444242****27-Cl**

H	-0.0006	0.1301	0.1422
C	-0.0140	0.1141	1.2427
C	-0.0463	0.1007	4.0580
C	-0.0336	-1.0728	1.9478
C	-0.0110	1.3218	1.9516
C	-0.0277	1.3047	3.3470
C	-0.0491	-1.1036	3.3495
H	0.0091	2.2829	1.4121
H	-0.0537	0.1156	5.1596
C	-0.0672	-2.4250	3.9614
C	-0.1012	-5.0658	4.9336
C	-0.0685	-3.5368	3.1027
C	-0.0832	-2.6636	5.3395
C	-0.1000	-3.9796	5.8099
C	-0.0851	-4.8435	3.5516
H	-0.0823	-1.8221	6.0517
H	-0.0856	-5.6956	2.8348
H	-0.1147	-6.0962	5.3254
I	-0.0428	-3.0248	1.0848
Cl	-0.0612	-5.5524	0.5337
C	-0.0430	2.6236	4.1154
C	-0.1177	-4.2529	7.3141
F	0.5878	3.6613	3.4743
F	0.5586	2.5693	5.3489
F	-1.3042	3.1027	4.3754
F	-0.1173	-3.1304	8.1039
F	-1.2126	-4.9671	7.7345
F	0.9572	-4.9838	7.7570

SCF = -759.375172**ZPE = 0.177445****H₂₉₈ = -759.178549****G₂₉₈ = -759.244264****SCF_{DFT} = -1894.365498**

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H	-0.1661	0.1586	0.1478
C	-0.1295	0.1381	1.2500
C	-0.0354	0.1123	4.0763
C	-0.1252	-1.0366	1.9746
C	-0.0851	1.3433	1.9654
C	-0.0385	1.3270	3.3655
C	-0.0792	-1.0965	3.3792
H	-0.0872	2.3018	1.4163
H	0.0017	0.1208	5.1790
C	-0.0809	-2.4158	3.9919
C	-0.0937	-5.0703	4.9436
C	-0.1277	-3.5276	3.1313
C	-0.0398	-2.6634	5.3653
C	-0.0464	-3.9902	5.8346
C	-0.1353	-4.8391	3.5612
H	-0.0022	-1.8265	6.0833
H	-0.1725	-5.6942	2.8656
H	-0.0985	-6.1082	5.3215
I	-0.1846	-2.9371	1.1423
C	0.0065	2.5525	4.0854
N	0.0434	3.5555	4.6731
C	-0.0046	-4.2310	7.2354
N	0.0295	-4.4294	8.3810

SCF = -298.292728**ZPE = 0.163367****H₂₉₈ = -298.115340****G₂₉₈ = -298.169660****SCF_{DFT} = -944.089744****28-OCH2**

H	-0.1384	0.6025	0.3032
C	-0.1092	0.4919	1.3998
C	-0.0340	0.2363	4.2128
C	-0.1091	-0.7413	2.0210
C	-0.0703	1.6349	2.2101
C	-0.0330	1.5048	3.6044
C	-0.0724	-0.9098	3.4169
H	-0.0693	2.6348	1.7418
H	-0.0043	0.1540	5.3123
C	-0.0777	-2.2754	3.9183
C	-0.0960	-4.9998	4.6460
C	-0.1189	-3.3119	2.9680
C	-0.0452	-2.6363	5.2662
C	-0.0545	-3.9978	5.6234
C	-0.1291	-4.6542	3.2873
H	-0.0123	-1.8623	6.0513
H	-0.1620	-5.4406	2.5110
H	-0.1031	-6.0648	4.9362
I	-0.1619	-2.5656	1.0326
C	0.0065	2.6675	4.4223
N	0.0388	3.6192	5.0901
C	-0.0209	-4.3536	7.0000
N	0.0063	-4.6461	8.1253
O	-0.2185	-5.2211	0.2242
C	-0.2489	-6.0503	-0.6520
H	-0.2587	-7.1167	-0.4098
H	-0.2675	-5.7671	-1.7088

SCF = -412.848506**ZPE = 0.192636****H₂₉₈ = -412.637374****G₂₉₈ = -412.701254****SCF_{DFT} = -1058.643188**

28-Cl

H	-0.1616	0.1447	0.1625
C	-0.1268	0.1272	1.2625
C	-0.0375	0.1040	4.0770
C	-0.1222	-1.0619	1.9640
C	-0.0860	1.3331	1.9712
C	-0.0415	1.3182	3.3717
C	-0.0783	-1.0967	3.3649
H	-0.0889	2.2915	1.4287
H	-0.0023	0.1092	5.1770
C	-0.0791	-2.4206	3.9734
C	-0.0894	-5.0685	4.9349
C	-0.1230	-3.5290	3.1112
C	-0.0396	-2.6637	5.3487
C	-0.0448	-3.9860	5.8226
C	-0.1291	-4.8369	3.5557
H	-0.0043	-1.8245	6.0606
H	-0.1647	-5.6845	2.8341
H	-0.0934	-6.1031	5.3131
I	-0.1774	-3.0091	1.0971
Cl	-0.2322	-5.5386	0.5358
C	0.0004	2.5445	4.0910
N	0.0347	3.5478	4.6786
C	-0.0040	-4.2232	7.2250
N	0.0293	-4.4180	8.3713

SCF = -758.778606**ZPE = 0.164725****H₂₉₈ = -758.597942****G₂₉₈ = -758.656451****SCF_{DFT} = -1404.569743****29**

H	0.0289	0.1470	0.1602
C	-0.0468	0.1224	1.2598
C	-0.2408	0.0622	4.0724
C	-0.0411	-1.0675	1.9668
C	-0.1512	1.3121	1.9648
C	-0.2510	1.3207	3.3890
C	-0.1366	-1.1270	3.3688
H	-0.1553	2.2556	1.3958
H	-0.3161	0.0280	5.1702
C	-0.1175	-2.4577	3.9720
C	-0.0591	-5.1208	4.8806
C	-0.0061	-3.5488	3.0915
C	-0.2005	-2.7147	5.3311
C	-0.1732	-4.0579	5.8271
C	0.0240	-4.8645	3.5201
H	-0.2880	-1.8685	6.0299
H	0.1116	-5.7057	2.8129
H	-0.0346	-6.1704	5.2150
I	0.1052	-2.9443	1.1218
N	-0.3539	2.5012	4.0852
N	-0.2544	-4.3147	7.1747
C	-0.3634	3.7587	3.3853
H	0.5894	3.8875	2.8023
H	-0.4525	4.6065	4.1147
H	-1.2350	3.8039	2.6765
C	-0.4543	2.4983	5.5195
H	0.4544	2.0169	5.9739
H	-1.3699	1.9333	5.8461
H	-0.5294	3.5498	5.9041
C	-0.3686	-3.2367	8.1192
H	0.5233	-2.5561	8.0452
H	-0.4206	-3.6421	9.1644
H	-1.3013	-2.6408	7.9215
C	-0.2274	-5.6698	7.6588
H	0.7343	-6.1708	7.3615
H	-1.0901	-6.2527	7.2344
H	-0.3048	-5.6821	8.7781

SCF = -298.407431**ZPE = 0.309760****H₂₉₈ = -298.077771****G₂₉₈ = -298.143996****SCF_{DFT} = -1027.589518**

29-Cl

H	-0.0042	0.1389	0.1719
C	-0.0403	0.1083	1.2720
C	-0.1392	0.0580	4.0748
C	-0.0335	-1.0918	1.9529
C	-0.0976	1.3057	1.9833
C	-0.1383	1.3076	3.3997
C	-0.0825	-1.1309	3.3525
H	-0.1060	2.2483	1.4163
H	-0.1769	0.0174	5.1730
C	-0.0706	-2.4635	3.9535
C	-0.0395	-5.1164	4.8837
C	-0.0131	-3.5576	3.0759
C	-0.1130	-2.7146	5.3210
C	-0.0888	-4.0484	5.8181
C	0.0030	-4.8677	3.5161
H	-0.1580	-1.8621	6.0141
H	0.0464	-5.7065	2.7851
H	-0.0302	-6.1645	5.2184
I	0.0412	-3.0176	1.0770
Cl	0.1139	-5.5715	0.4685
N	-0.1081	2.5111	4.1245
N	-0.0599	-4.2941	7.1907
C	-0.3685	3.7323	3.4077
H	0.4501	3.8965	2.6560
H	-0.3666	4.5991	4.1197
H	-1.3550	3.7121	2.8688
C	-0.5252	2.4724	5.5022
H	0.2399	1.9060	6.0991
H	-1.5247	1.9745	5.6332
H	-0.5881	3.5134	5.9149
C	-0.3871	-3.2262	8.0954
H	0.4071	-2.4330	8.0360
H	-0.4221	-3.6095	9.1489
H	-1.3807	-2.7600	7.8506
C	-0.2304	-5.6435	7.6572
H	0.6183	-6.2763	7.2798
H	-1.1993	-6.0903	7.3023
H	-0.2135	-5.6664	8.7785

SCF = -758.859916**ZPE = 0.311149****H₂₉₈ = -758.527082****G₂₉₈ = -758.597374****SCF_{DFT} = -1488.026237****29-OCH2**

H	-0.0207	0.4691	0.2174
C	-0.0852	0.3912	1.3150
C	-0.2503	0.1982	4.1212
C	-0.0763	-0.8338	1.9596
C	-0.1782	1.5469	2.0767
C	-0.2636	1.4870	3.4998
C	-0.1573	-0.9554	3.3583
H	-0.1845	2.5166	1.5542
H	-0.3143	0.1105	5.2165
C	-0.1360	-2.3137	3.8958
C	-0.0755	-5.0184	4.6727
C	-0.0380	-3.3608	2.9622
C	-0.2045	-2.6374	5.2418
C	-0.1760	-4.0032	5.6698
C	-0.0069	-4.6956	3.3247
H	-0.2816	-1.8263	5.9819
H	0.0705	-5.4943	2.5654
H	-0.0502	-6.0827	4.9549
I	0.0521	-2.6681	1.0214
N	-0.3560	2.6342	4.2537
N	-0.2437	-4.3252	7.0059
C	-0.3697	3.9230	3.6150
H	0.5774	4.0781	3.0291
H	-0.4500	4.7355	4.3845
H	-1.2477	4.0036	2.9173
C	-0.4434	2.5617	5.6864
H	0.4678	2.0562	6.1087
H	-1.3573	1.9835	5.9939
H	-0.5119	3.5932	6.1228
C	-0.3463	-3.2942	8.0020
H	0.5467	-2.6128	7.9530
H	-0.3904	-3.7490	9.0268
H	-1.2786	-2.6866	7.8416
C	-0.2140	-5.7016	7.4226
H	0.7426	-6.1895	7.0894
H	-1.0827	-6.2620	6.9803
H	-0.2782	-5.7690	8.5406
O	0.1971	-5.3719	0.2204
C	0.2711	-6.2415	-0.6097
H	0.2934	-7.2952	-0.3170
H	0.3185	-6.0119	-1.6787

SCF = -412.959129**ZPE = 0.338778****H₂₉₈ = -412.595776****G₂₉₈ = -412.672113****SCF_{DFT} = -1142.136115**

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H	1.6526	-0.3731	1.8859
C	0.6687	-0.0044	2.2189
C	-1.8348	0.9796	3.0368
C	-0.4711	-0.8016	2.2064
C	0.5452	1.3147	2.6652
C	-0.7013	1.7956	3.0741
C	-1.7256	-0.3415	2.5928
H	1.4310	1.9756	2.6839
H	-2.8183	1.3774	3.3474
C	1.4307	-3.6115	3.8260
C	-0.6824	-4.4765	5.4665
C	0.1037	-3.5227	3.4185
C	1.6968	-4.1371	5.0937
C	0.6414	-4.5611	5.9052
C	-0.9628	-3.9528	4.2010
H	2.7409	-4.2248	5.4461
H	-2.0086	-3.9007	3.8565
H	-1.5070	-4.8308	6.1117
I	-0.3011	-2.7564	1.5341
C	-0.8251	3.2391	3.5836
C	0.9400	-5.1175	7.3051
F	-0.6307	3.3482	4.9369
F	-2.0526	3.8026	3.3519
F	0.0791	4.1021	3.0217
F	0.9523	-4.1484	8.2755
F	0.0274	-6.0443	7.7366
F	2.1578	-5.7382	7.4040
H	-2.6265	-0.9756	2.5542
H	2.2691	-3.2906	3.1863

SCF = -298.896116**ZPE = 0.195825****H₂₉₈ = -298.680476****G₂₉₈ = -298.748792****SCF_{DFT} = -1435.082487****30-OCH2**

H	1.5001	-0.2233	1.6315
C	0.5901	0.1693	2.1142
C	-1.7265	1.2131	3.3122
C	-0.5769	-0.5826	2.2193
C	0.5931	1.4676	2.6297
C	-0.5619	1.9789	3.2282
C	-1.7410	-0.0870	2.7973
H	1.5025	2.0907	2.5545
H	-2.6379	1.6335	3.7746
C	0.9782	-2.8204	3.9851
C	-0.4716	-5.0465	4.9040
C	-0.0766	-3.3594	3.2558
C	1.3018	-3.4103	5.2087
C	0.5752	-4.5165	5.6601
C	-0.8058	-4.4651	3.6759
H	2.1281	-3.0016	5.8177
H	-1.6156	-4.8990	3.0626
H	-1.0389	-5.9207	5.2713
I	-0.5908	-2.5017	1.4347
C	-0.5439	3.3982	3.8121
C	0.9499	-5.1695	6.9972
F	-0.1378	3.4350	5.1220
F	-1.7662	4.0178	3.8004
F	0.2992	4.2558	3.1543
F	1.4742	-4.2934	7.9122
F	-0.1062	-5.7646	7.6372
F	1.8923	-6.1578	6.8700
H	-2.6674	-0.6819	2.8579
H	1.5535	-1.9494	3.6312
O	-0.7592	-5.1732	0.7205
C	-0.3297	-6.0257	-0.0177
H	-0.7429	-7.0380	0.0025
H	0.4785	-5.8188	-0.7263

SCF = -413.449420**ZPE = 0.225079****H₂₉₈ = -413.200060****G₂₉₈ = -413.277579****SCF_{DFT} = -1549.631695**

30-Cl

H	1.5030	-0.5328	1.5227
C	0.6141	-0.1266	2.0302
C	-1.6404	0.9393	3.2969
C	-0.5230	-0.9032	2.2216
C	0.6303	1.1958	2.4784
C	-0.4978	1.7204	3.1133
C	-1.6507	-0.3821	2.8434
H	1.5212	1.8264	2.3272
H	-2.5285	1.3673	3.7892
C	0.8671	-2.8809	4.0883
C	-0.4305	-5.1372	5.1296
C	-0.0986	-3.5611	3.3530
C	1.1820	-3.3368	5.3690
C	0.5297	-4.4609	5.8828
C	-0.7500	-4.6860	3.8451
H	1.9401	-2.8111	5.9724
H	-1.4837	-5.2455	3.2344
H	-0.9371	-6.0263	5.5407
I	-0.5697	-2.8929	1.4385
Cl	-0.5839	-5.4055	0.8128
C	-0.4746	3.1579	3.6236
C	0.8901	-4.9645	7.2797
F	-0.0025	3.2854	4.9081
F	-1.7024	3.7724	3.6533
F	0.3138	4.0098	2.8893
F	1.2684	-3.9761	8.1548
F	-0.1287	-5.6206	7.9249
F	1.9360	-5.8540	7.2973
H	-2.5576	-0.9904	2.9845
H	1.3780	-1.9904	3.6853

SCF = -759.377080**ZPE = 0.197807****H₂₉₈ = -759.157660****G₂₉₈ = -759.229359****SCF_{DFT} = -1895.543167****31**

H	1.6258	-0.3810	2.0299
C	0.6208	-0.0278	2.3131
C	-1.9377	0.9097	3.0081
C	-0.5081	-0.8339	2.2066
C	0.4614	1.2748	2.7893
C	-0.8153	1.7428	3.1386
C	-1.7872	-0.3943	2.5327
H	1.3419	1.9340	2.8840
H	-2.9422	1.2820	3.2748
C	1.3190	-3.6888	3.8404
C	-0.8828	-4.6186	5.3220
C	0.0178	-3.5897	3.3582
C	1.5168	-4.2582	5.0996
C	0.4178	-4.7206	5.8409
C	-1.0893	-4.0505	4.0636
H	2.5397	-4.3472	5.5051
H	-2.1132	-3.9867	3.6603
H	-1.7451	-4.9908	5.9022
I	-0.2804	-2.7617	1.4824
H	-2.6767	-1.0359	2.4223
H	2.1900	-3.3403	3.2615
C	-0.9731	3.0699	3.6236
N	-1.1015	4.1556	4.0205
C	0.6235	-5.2991	7.1231
N	0.7914	-5.7723	8.1723

SCF = -298.303167**ZPE = 0.183236****H₂₉₈ = -298.104237****G₂₉₈ = -298.162872****SCF_{DFT} = -945.281734**

31-Cl

H	1.6537	-0.3370	2.5435
C	0.5959	-0.0433	2.6294
C	-2.0837	0.7350	2.8393
C	-0.4216	-0.8942	2.2164
C	0.2790	1.2084	3.1603
C	-1.0637	1.5977	3.2665
C	-1.7555	-0.5148	2.3125
H	1.0797	1.8878	3.4908
H	-3.1374	1.0444	2.9163
C	1.2863	-4.4194	3.5084
C	-0.6012	-3.7444	5.4735
C	0.2349	-3.5532	3.2326
C	1.3995	-4.9507	4.7957
C	0.4588	-4.6123	5.7775
C	-0.7154	-3.2121	4.1898
H	2.2262	-5.6406	5.0287
H	-1.5467	-2.5260	3.9558
H	-1.3453	-3.4847	6.2427
I	0.0663	-2.7680	1.3130
Cl	0.7165	-5.1528	0.5278
H	-2.5622	-1.1825	1.9715
H	2.0087	-4.7200	2.7260
C	-1.3927	2.8715	3.8062
N	-1.6621	3.9134	4.2481
C	0.5746	-5.1526	7.0882
N	0.6695	-5.5938	8.1603

SCF = -758.780321**ZPE = 0.184989****H₂₉₈ = -758.577818****G₂₉₈ = -758.639918****SCF_{DFT} = -1405.748055****31-OCH2**

H	1.6576	0.0363	2.5221
C	0.5940	0.2902	2.6644
C	-2.1091	0.9744	3.0128
C	-0.4297	-0.5546	2.2473
C	0.2550	1.4978	3.2780
C	-1.0946	1.8396	3.4535
C	-1.7760	-0.2343	2.4008
H	1.0518	2.1816	3.6181
H	-3.1699	1.2494	3.1429
C	1.3146	-4.1604	3.3233
C	-0.7198	-3.9268	5.2505
C	0.1967	-3.3613	3.1150
C	1.4186	-4.8495	4.5344
C	0.4054	-4.7311	5.4970
C	-0.8309	-3.2356	4.0441
H	2.2991	-5.4867	4.7259
H	-1.7165	-2.6067	3.8565
H	-1.5190	-3.8412	6.0065
I	0.0645	-2.3370	1.3145
H	-2.5797	-0.9004	2.0461
H	2.0997	-4.2750	2.5549
C	-1.4377	3.0702	4.0775
N	-1.7180	4.0769	4.5881
C	0.5138	-5.4324	6.7292
N	0.6028	-6.0059	7.7371
O	0.9703	-4.7809	0.3602
C	0.7054	-5.7215	-0.3474
H	1.4281	-6.5294	-0.4920
H	-0.2560	-5.7993	-0.8651

SCF = -412.855922**ZPE = 0.212425****H₂₉₈ = -412.623311****G₂₉₈ = -412.691328****SCF_{DFT} = -1059.831481**

32

H	1.6361	-0.3540	2.2373
C	0.6245	-0.0126	2.5124
C	-1.9479	0.8700	3.1955
C	-0.4888	-0.8378	2.3564
C	0.4585	1.2632	3.0185
C	-0.8366	1.7512	3.3792
C	-1.7718	-0.4041	2.6885
H	1.3486	1.9016	3.1347
H	-2.9682	1.1963	3.4521
C	1.3313	-3.7647	3.8921
C	-0.8822	-4.7873	5.2769
C	0.0384	-3.6361	3.3856
C	1.5260	-4.4034	5.1026
C	0.4237	-4.9387	5.8402
C	-1.0667	-4.1471	4.0656
H	2.5538	-4.4965	5.4876
H	-2.0863	-4.0549	3.6565
H	-1.7661	-5.1852	5.8002
I	-0.2388	-2.7174	1.5718
H	-2.6516	-1.0544	2.5524
H	2.2043	-3.3706	3.3462
N	-1.0060	3.0160	3.8844
N	0.6117	-5.5713	7.0436
C	-2.3198	3.4960	4.2214
H	-2.2598	4.5462	4.6116
H	-2.7787	2.8455	5.0153
H	-2.9844	3.4886	3.3145
C	0.1221	3.8954	4.0404
H	0.6181	4.0765	3.0478
H	0.8718	3.4433	4.7458
H	-0.2111	4.8818	4.4584
C	1.9360	-5.7335	7.5823
H	2.4116	-4.7290	7.7517
H	2.5773	-6.3261	6.8740
H	1.8910	-6.2767	8.5629
C	-0.5081	-6.1212	7.7604
H	-0.1600	-6.5998	8.7137
H	-1.0277	-6.9000	7.1379
H	-1.2421	-5.3089	8.0157

SCF = -298.419338**ZPE = 0.329834****H₂₉₈ = -298.068044****G₂₉₈ = -298.138469****SCF_{DFT} = -1028.784220****32-Cl**

H	1.7536	-0.3105	2.7536
C	0.6909	-0.0303	2.8316
C	-1.9897	0.7157	3.0242
C	-0.3039	-0.8791	2.3633
C	0.3609	1.1922	3.4061
C	-0.9944	1.5931	3.5274
C	-1.6384	-0.5029	2.4549
H	1.1747	1.8392	3.7651
H	-3.0553	0.9830	3.0766
C	1.3518	-4.5572	3.4798
C	-0.3850	-3.8144	5.5458
C	0.3768	-3.5857	3.2805
C	1.4724	-5.1564	4.7269
C	0.6134	-4.7947	5.7990
C	-0.4972	-3.2184	4.2975
H	2.2482	-5.9257	4.8579
H	-1.2753	-2.4533	4.1332
H	-1.0883	-3.5078	6.3339
I	0.2099	-2.6989	1.4119
Cl	0.9040	-5.0525	0.4441
H	-2.4361	-1.1602	2.0733
H	2.0077	-4.8854	2.6486
N	-1.3437	2.7836	4.1818
N	0.7781	-5.3425	7.0706
C	-2.6762	3.2922	3.9844
H	-2.7821	4.2928	4.4801
H	-3.4107	2.5869	4.4590
H	-2.9348	3.4018	2.8958
C	-0.3070	3.7569	4.4069
H	0.2212	4.0466	3.4577
H	0.4466	3.3299	5.1223
H	-0.7441	4.6804	4.8699
C	1.6199	-6.4997	7.2189
H	2.6786	-6.2213	6.9650
H	1.2977	-7.3420	6.5473
H	1.5961	-6.8582	8.2814
C	-0.2569	-5.1418	8.0487
H	-0.0061	-5.6944	8.9920
H	-1.2582	-5.4963	7.6800
H	-0.3296	-4.0470	8.2913

SCF = -758.863070**ZPE = 0.331402****H₂₉₈ = -758.508482****G₂₉₈ = -758.582258****SCF_{DFT} = -1489.205502**

32-OCH2

H	1.7239	-0.0864	2.3043
C	0.6942	0.2108	2.5624
C	-1.9216	0.9857	3.2012
C	-0.3909	-0.6181	2.2802
C	0.4802	1.4327	3.1738
C	-0.8388	1.8636	3.5162
C	-1.6950	-0.2339	2.5896
H	1.3505	2.0727	3.3878
H	-2.9589	1.2705	3.4370
C	1.4096	-3.5563	3.6819
C	-0.8458	-4.6840	4.9053
C	0.1433	-3.4342	3.1114
C	1.5562	-4.2375	4.8768
C	0.4304	-4.8244	5.5332
C	-0.9811	-4.0008	3.7102
H	2.5637	-4.3196	5.3140
H	-1.9795	-3.9160	3.2501
H	-1.7463	-5.1206	5.3651
I	-0.0666	-2.4179	1.3419
H	-2.5543	-0.8828	2.3531
H	2.3000	-3.1205	3.1995
N	-1.0571	3.0742	4.1286
N	0.5701	-5.5005	6.7210
C	-2.3948	3.5020	4.4385
H	-2.3750	4.5123	4.9258
H	-2.8806	2.7744	5.1446
H	-3.0131	3.5684	3.5018
C	0.0437	3.9555	4.4115
H	0.5758	4.2369	3.4618
H	0.7743	3.4535	5.1030
H	-0.3274	4.8926	4.9042
C	1.8635	-5.6318	7.3362
H	2.2917	-4.6176	7.5645
H	2.5679	-6.1785	6.6514
H	1.7794	-6.2077	8.2954
C	-0.5749	-6.0870	7.3641
H	-0.2670	-6.5928	8.3170
H	-1.0515	-6.8514	6.6913
H	-1.3335	-5.2942	7.6090
O	0.3709	-4.8321	0.0351
C	0.5912	-6.0155	0.0190
H	0.6838	-6.5523	-0.9294
H	0.7061	-6.5938	0.9410

SCF = -412.969593**ZPE = 0.358908****H₂₉₈ = -412.584592****G₂₉₈ = -412.664935****SCF_{DFT} = -1143.326999****33**

I	-1.3434	1.1136	-3.3157
C	-0.7464	0.4729	-1.4652
C	0.0897	-0.3218	1.0619
N	-0.9561	-0.8205	-1.0606
C	-0.1150	1.3926	-0.6152
C	0.3082	0.9980	0.6588
C	-0.5434	-1.2110	0.1859
H	0.0453	2.4314	-0.9599
H	0.8063	1.7195	1.3326
H	0.4056	-0.6800	2.0578
C	-1.6103	-1.7899	-1.9309
H	-1.0101	-1.9155	-2.8741
H	-2.6471	-1.4323	-2.1819
H	-1.6838	-2.7834	-1.4111
H	-0.7314	-2.2666	0.4770

SCF = -297.938670**ZPE = 0.119125****H₂₉₈ = -297.811104****G₂₉₈ = -297.853268****SCF_{DFT} = -585.082032****33-OCH2**

I	-1.2038	1.0675	-3.3408
C	-0.6637	0.4387	-1.4612
C	0.0935	-0.3447	1.0957
N	-0.9816	-0.8183	-1.0172
C	0.0397	1.3273	-0.6340
C	0.4234	0.9393	0.6532
C	-0.6082	-1.2041	0.2436
H	0.2872	2.3373	-1.0098
H	0.9773	1.6368	1.3075
H	0.3746	-0.6966	2.1036
C	-1.7125	-1.7552	-1.8621
H	-1.1316	-1.9411	-2.8075
H	-2.7215	-1.3258	-2.1133
H	-1.8527	-2.7297	-1.3214
H	-0.8851	-2.2303	0.5653
O	-2.0489	1.9225	-5.9779
C	-2.1744	2.4094	-7.0703
H	-1.3550	2.9684	-7.5421
H	-3.1114	2.3045	-7.6331

SCF = -412.481165**ZPE = 0.147365****H₂₉₈ = -412.321284****G₂₉₈ = -412.372956****SCF_{DFT} = -699.626984**

33-Cl

I	-1.4160	1.1868	-3.5389
Cl	-2.1449	1.9720	-5.8328
C	-0.7474	0.4586	-1.4457
C	0.0924	-0.3509	1.0805
N	-0.9466	-0.8165	-1.0412
C	-0.1100	1.3805	-0.5774
C	0.3097	0.9856	0.6780
C	-0.5332	-1.2299	0.2123
H	0.0356	2.4105	-0.9396
H	0.8066	1.6874	1.3658
H	0.4143	-0.6978	2.0727
C	-1.5988	-1.7714	-1.9204
H	-1.0021	-1.8726	-2.8673
H	-2.6281	-1.3993	-2.1752
H	-1.6762	-2.7711	-1.4186
H	-0.7215	-2.2832	0.4894

SCF = -758.384463**ZPE = 0.119781****H₂₉₈ = -758.254627****G₂₉₈ = -758.300791****SCF_{DFT} = -1045.505995****34-Cl**

I	-1.4716	1.1948	-3.4393
Cl	-2.3252	1.9003	-5.7716
C	-0.7472	0.5643	-1.4403
C	0.1110	-0.3542	1.0317
C	-0.9149	-0.7636	-1.0628
C	-0.1348	1.4529	-0.5581
C	0.2987	0.9889	0.6904
N	-0.4906	-1.2231	0.1625
H	-1.3958	-1.5064	-1.7296
H	0.0073	2.5102	-0.8392
H	0.7864	1.6579	1.4154
H	0.4407	-0.7541	2.0084
H	-0.1437	-3.2660	-0.2187
C	-0.6827	-2.6147	0.5213
H	-0.2832	-2.8153	1.5500
H	-1.7798	-2.8558	0.4967

SCF = -758.364736**ZPE = 0.119564****H₂₉₈ = -758.235159****G₂₉₈ = -758.281234****SCF_{DFT} = -1045.491843****34**

I	-1.3599	1.1498	-3.3010
C	-0.7346	0.5585	-1.4635
C	0.0879	-0.3421	1.0286
C	-0.8953	-0.7782	-1.0805
C	-0.1451	1.4615	-0.5688
C	0.2680	1.0028	0.6865
N	-0.4878	-1.2205	0.1506
H	-1.3572	-1.5333	-1.7541
H	-0.0045	2.5248	-0.8435
H	0.7366	1.6857	1.4176
H	0.4043	-0.7380	2.0169
H	-0.3201	-3.2762	-0.3189
C	-0.6855	-2.6171	0.5151
H	-0.1136	-2.8558	1.4517
H	-1.7814	-2.8002	0.6892

SCF = -297.941657**ZPE = 0.118850****H₂₉₈ = -297.815087****G₂₉₈ = -297.855928****SCF_{DFT} = -585.082149****34-OCH2**

I	-1.2851	0.9593	-3.3982
C	-0.7037	0.4690	-1.5087
C	0.0582	-0.3067	1.0449
C	-0.8696	-0.8476	-1.0647
C	-0.1407	1.4156	-0.6438
C	0.2420	1.0207	0.6424
N	-0.4930	-1.2287	0.1966
H	-1.3114	-1.6362	-1.7128
H	0.0032	2.4644	-0.9660
H	0.6894	1.7399	1.3509
H	0.3515	-0.6525	2.0583
H	-0.0425	-3.2802	-0.0260
C	-0.6802	-2.6111	0.6146
H	-0.3838	-2.7340	1.6907
H	-1.7621	-2.8922	0.4933
O	-2.1434	1.5591	-6.1112
C	-2.3534	2.3580	-6.9844
H	-2.7334	2.0400	-7.9641
H	-2.1727	3.4308	-6.8325

SCF = -412.482495**ZPE = 0.147259****H₂₉₈ = -412.322652****G₂₉₈ = -412.374586****SCF_{DFT} = -699.625065**

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I	-1.4115	1.0029	-3.2828
C	-0.7103	0.4915	-1.4473
N	0.2570	-0.2150	1.0900
C	-0.7350	-0.8406	-1.0181
C	-0.1921	1.4638	-0.5834
C	0.2859	1.0904	0.6782
C	-0.2470	-1.1724	0.2516
H	-1.1332	-1.6498	-1.6584
H	-0.1483	2.5311	-0.8699
H	0.7028	1.8389	1.3849
H	-0.2538	-2.2207	0.6184
H	1.8856	-0.7692	2.3126
C	0.7797	-0.5822	2.3986
H	0.5948	0.2519	3.1284
H	0.2689	-1.5129	2.7660

SCF = -297.941136**ZPE = 0.118849****H₂₉₈ = -297.814566****G₂₉₈ = -297.855250****SCF_{DFT} = -585.085206****35-OCH2**

I	-1.2432	1.1691	-3.2629
C	-0.6076	0.5742	-1.4222
N	0.2631	-0.2375	1.1198
C	-0.6781	-0.7695	-1.0361
C	-0.0913	1.5036	-0.5111
C	0.3381	1.0792	0.7511
C	-0.2385	-1.1545	0.2354
H	-1.0767	-1.5461	-1.7144
H	-0.0126	2.5775	-0.7627
H	0.7520	1.7932	1.4937
H	-0.2821	-2.2126	0.5684
H	1.8301	-0.9044	2.3665
C	0.7339	-0.6605	2.4307
H	0.5760	0.1655	3.1758
H	0.1658	-1.5706	2.7640
O	-2.1583	2.1041	-5.8814
C	-2.4463	2.0398	-7.0462
H	-2.3677	1.0957	-7.6024
H	-2.7981	2.9242	-7.5936

SCF = -412.481810**ZPE = 0.147215****H₂₉₈ = -412.321028****G₂₉₈ = -412.375473****SCF_{DFT} = -699.627939****35-Cl**

I	-1.4573	1.0431	-3.4360
Cl	-2.3461	1.6916	-5.7747
C	-0.6999	0.4888	-1.4402
N	0.2596	-0.2174	1.1026
C	-0.7369	-0.8401	-0.9990
C	-0.1690	1.4550	-0.5760
C	0.3043	1.0899	0.6817
C	-0.2563	-1.1758	0.2644
H	-1.1462	-1.6350	-1.6443
H	-0.1196	2.5138	-0.8797
H	0.7306	1.8250	1.3898
H	-0.2692	-2.2145	0.6447
H	1.8808	-0.7863	2.3241
C	0.7786	-0.5830	2.4043
H	0.6079	0.2550	3.1315
H	0.2581	-1.5042	2.7790

SCF = -758.362902**ZPE = 0.119655****H₂₉₈ = -758.232326****G₂₉₈ = -758.280313****SCF_{DFT} = -1045.493550****36**

N	-0.3877	0.5738	-0.1873
C	-0.5927	1.8582	-0.6495
N	-0.3321	2.7358	0.3835
C	0.0079	0.6409	1.1545
H	0.2322	-0.2514	1.7496
C	0.0428	1.9965	1.5124
H	0.3022	2.4670	2.4674
I	-1.1716	2.3661	-2.5184
H	0.2802	4.5701	-0.4532
C	-0.4250	4.1710	0.3270
H	-0.1447	4.5929	1.3306
H	-1.4783	4.4769	0.0770
H	0.1514	-0.6388	-1.8239
C	-0.5488	-0.6403	-0.9434
H	-0.3087	-1.5157	-0.2803
H	-1.6105	-0.7286	-1.3046

SCF = -297.922127**ZPE = 0.128273****H₂₉₈ = -297.784135****G₂₉₈ = -297.828948****SCF_{DFT} = -602.339342**

36-OCH2

N	-0.3795	0.5448	-0.1519
C	-0.5572	1.8029	-0.6894
N	-0.3267	2.7314	0.3047
C	-0.0321	0.6800	1.1993
H	0.1625	-0.1804	1.8481
C	0.0009	2.0510	1.4858
H	0.2288	2.5699	2.4227
I	-1.0717	2.2067	-2.6173
H	0.3342	4.5136	-0.6015
C	-0.4054	4.1612	0.1691
H	-0.1634	4.6346	1.1593
H	-1.4445	4.4595	-0.1410
H	0.2078	-0.7544	-1.7023
C	-0.5228	-0.7062	-0.8483
H	-0.3139	-1.5469	-0.1325
H	-1.5710	-0.8060	-1.2439
O	-1.7846	2.6546	-5.2750
C	-2.0009	3.5150	-6.0889
H	-2.2781	3.2587	-7.1193
H	-1.9278	4.5791	-5.8264

SCF = -412.465614**ZPE = 0.156933****H₂₉₈ = -412.294258****G₂₉₈ = -412.349671****SCF_{DFT} = -716.885806****36-Cl**

N	-0.3447	0.5823	-0.1751
C	-0.5867	1.8570	-0.6381
N	-0.3572	2.7193	0.4114
C	0.0420	0.6402	1.1831
H	0.2839	-0.2515	1.7598
C	0.0342	1.9803	1.5510
H	0.2681	2.4552	2.5027
I	-1.2885	2.4536	-2.8507
H	-0.7967	4.4728	-0.6449
C	-0.4869	4.1430	0.3835
H	0.4962	4.6182	0.6463
H	-1.2631	4.4676	1.1276
H	0.5298	-1.1614	-0.9395
C	-0.4590	-0.6288	-0.9264
H	-1.2301	-1.2960	-0.4553
H	-0.7674	-0.3905	-1.9802
Cl	-2.0239	3.0707	-5.1580

SCF = -758.378677**ZPE = 0.128789****H₂₉₈ = -758.237530****G₂₉₈ = -758.288575****SCF_{DFT} = -1062.769066****37**

N	-0.3577	0.5754	-0.2094
C	-0.5634	1.8627	-0.6595
N	-0.3423	2.7363	0.3844
C	0.0079	0.6336	1.1455
C	0.0052	1.9883	1.5212
I	-1.0989	2.3836	-2.5451
H	-0.2946	4.5493	-0.7024
C	-0.4640	4.1744	0.3431
H	0.3078	4.6224	1.0313
H	-1.4923	4.4684	0.6974
H	0.5436	-0.9143	-1.3883
C	-0.4716	-0.6357	-0.9872
H	-0.8457	-1.4615	-0.3178
H	-1.1938	-0.4867	-1.8350
C	0.3248	-0.6341	1.9555
C	0.3077	2.6581	2.8716
F	0.8934	-0.3814	3.1673
F	1.1909	-1.4680	1.2985
F	-0.7953	-1.3829	2.1969
F	1.4915	3.3450	2.8504
F	-0.6457	3.5779	3.2210
F	0.3838	1.7823	3.9122

SCF = -298.375533**ZPE = 0.140770****H₂₉₈ = -298.217753****G₂₉₈ = -298.278652****SCF_{DFT} = -1276.626408**

37-OCH2

N	-0.3902	0.5778	-0.2429
C	-0.6831	1.8483	-0.6888
N	-0.4642	2.7357	0.3421
C	0.0308	0.6611	1.0963
C	-0.0273	2.0137	1.4671
I	-1.3466	2.3320	-2.5713
H	-0.6198	4.5369	-0.7496
C	-0.6707	4.1632	0.3083
H	0.1323	4.6597	0.9228
H	-1.6782	4.4013	0.7523
H	0.5381	-0.8971	-1.4173
C	-0.4791	-0.6435	-1.0059
H	-0.8204	-1.4726	-0.3237
H	-1.2155	-0.5228	-1.8457
C	0.4464	-0.5832	1.8932
C	0.2984	2.7074	2.7970
F	1.0598	-0.2990	3.0766
F	1.3204	-1.3800	1.2004
F	-0.6215	-1.3862	2.1919
F	1.4415	3.4576	2.7215
F	-0.6850	3.5785	3.1873
F	0.4692	1.8465	3.8395
O	-2.1971	2.9495	-5.0146
C	-1.6012	3.3732	-5.9745
H	-2.1268	3.5672	-6.9173
H	-0.5221	3.5750	-5.9301

SCF = -412.921365**ZPE = 0.169790****H₂₉₈ = -412.730143****G₂₉₈ = -412.800616****SCF_{DFT} = -1391.175398****38**

N	0.0662	-0.9999	-0.9036
C	-0.5115	0.1300	-1.4446
N	-0.5575	1.1186	-0.4836
C	0.3977	-0.7254	0.4374
C	0.0056	0.6068	0.7014
I	-1.1829	0.3091	-3.3480
H	-2.1753	2.3923	-0.9315
C	-1.0870	2.4489	-0.6508
H	-0.5122	2.9884	-1.4539
H	-0.9831	3.0092	0.3194
H	0.9695	-2.0847	-2.4679
C	0.2955	-2.2508	-1.5822
H	0.7892	-2.9687	-0.8702
H	-0.6858	-2.6831	-1.9238
C	1.0079	-1.6398	1.3191
N	1.5109	-2.3722	2.0696
C	0.1352	1.3250	1.9069
N	0.2557	1.8922	2.9151

SCF = -297.784795**ZPE = 0.128124****H₂₉₈ = -297.643612****G₂₉₈ = -297.696024****SCF_{DFT} = -786.834775****38-OCH2**

N	-0.0129	-0.9871	-0.9630
C	-0.5618	0.1650	-1.4837
N	-0.5274	1.1527	-0.5229
C	0.3838	-0.7282	0.3648
C	0.0601	0.6179	0.6416
I	-1.3207	0.3706	-3.3762
H	-2.1047	2.4868	-0.9326
C	-1.0111	2.5022	-0.6684
H	-0.4309	3.0271	-1.4767
H	-0.8717	3.0493	0.3044
H	0.8081	-2.1218	-2.5349
C	0.1310	-2.2481	-1.6454
H	0.5811	-2.9987	-0.9389
H	-0.8780	-2.6139	-1.9831
C	0.9884	-1.6685	1.2226
N	1.4886	-2.4233	1.9525
C	0.2672	1.3306	1.8394
N	0.4505	1.8938	2.8404
O	-2.3151	0.6332	-5.8525
C	-1.8258	1.0107	-6.8883
H	-0.7766	1.3330	-6.9373
H	-2.4202	1.0411	-7.8095

SCF = -412.330062**ZPE = 0.157045****H₂₉₈ = -412.155470****G₂₉₈ = -412.217733****SCF_{DFT} = -901.384351**

39

N	-0.3570	0.5775	-0.2077
C	-0.5618	1.8618	-0.6626
N	-0.3413	2.7332	0.3815
C	0.0021	0.6292	1.1537
C	0.0119	1.9913	1.5261
I	-1.0932	2.3797	-2.5455
H	-0.7324	4.5264	-0.6696
C	-0.4433	4.1675	0.3544
H	0.5516	4.6095	0.6398
H	-1.2218	4.4922	1.0994
H	0.5144	-1.1739	-0.9548
C	-0.4773	-0.6419	-0.9606
H	-1.2529	-1.2961	-0.4737
H	-0.7807	-0.4269	-2.0202
C	0.2970	-0.5604	1.9686
H	1.1613	-1.1303	1.5383
H	-0.5921	-1.2421	2.0098
H	0.5583	-0.2530	3.0126
C	0.3201	2.5968	2.8316
H	1.1979	3.2894	2.7490
H	0.5668	1.7971	3.5748
H	-0.5573	3.1803	3.2143

SCF = -297.951919**ZPE = 0.183164****H₂₉₈ = -297.757036****G₂₉₈ = -297.806164****SCF_{DFT} = -680.998905****39-Cl**

N	-0.3496	0.5811	-0.1842
C	-0.5564	1.8583	-0.6490
N	-0.3336	2.7183	0.4001
C	0.0119	0.6266	1.1890
C	0.0220	1.9756	1.5578
I	-1.1872	2.4658	-2.8586
H	-0.7283	4.4739	-0.6709
C	-0.4370	4.1438	0.3626
H	0.5516	4.6015	0.6377
H	-1.2144	4.4856	1.0983
H	0.5116	-1.1685	-0.9482
C	-0.4720	-0.6254	-0.9414
H	-1.2508	-1.2871	-0.4743
H	-0.7719	-0.3803	-1.9959
Cl	-1.8534	3.1061	-5.1881
C	0.3039	-0.5660	1.9978
H	1.1652	-1.1352	1.5636
H	-0.5854	-1.2463	2.0314
H	0.5642	-0.2669	3.0430
C	0.3277	2.5866	2.8597
H	1.2021	3.2812	2.7731
H	0.5745	1.7934	3.6077
H	-0.5500	3.1722	3.2357

SCF = -758.404596**ZPE = 0.184397****H₂₉₈ = -758.204304****G₂₉₈ = -758.262822****SCF_{DFT} = -1141.423371****39-OCH2**

N	-0.3354	0.6456	-0.2344
C	-0.5188	1.9507	-0.6354
N	-0.2824	2.7756	0.4419
C	0.0263	0.6361	1.1278
C	0.0594	1.9817	1.5550
I	-1.0538	2.5630	-2.4997
H	0.3567	4.6352	-0.3114
C	-0.3725	4.2112	0.4326
H	-0.1250	4.6001	1.4575
H	-1.4166	4.5270	0.1580
H	-0.2885	-1.4362	-0.4566
C	-0.4837	-0.5151	-1.0703
H	-1.5295	-0.5591	-1.4816
H	0.2536	-0.4721	-1.9185
C	0.3033	-0.5836	1.9050
H	1.1621	-1.1514	1.4622
H	-0.5952	-1.2531	1.9286
H	0.5670	-0.3117	2.9583
C	0.3812	2.5164	2.8887
H	1.2710	3.1961	2.8408
H	0.6179	1.6756	3.5887
H	-0.4860	3.0898	3.3073
O	-1.8203	3.5073	-5.0583
C	-2.0101	3.2979	-6.2279
H	-1.8592	2.2994	-6.6601
H	-2.3405	4.1012	-6.8989

SCF = -412.495295**ZPE = 0.212270****H₂₉₈ = -412.265815****G₂₉₈ = -412.327732****SCF_{DFT} = -795.544249**

40			
N	-0.0934	-1.1230	-0.9804
C	-0.5149	0.0725	-1.5315
N	-0.4718	1.0584	-0.5694
C	0.2518	-0.8842	0.3655
C	0.0150	0.4830	0.6251
I	-1.0991	0.3277	-3.4510
H	-1.9500	2.4724	-1.0758
C	-0.8825	2.4277	-0.7246
H	-0.2164	2.9452	-1.4682
H	-0.8001	2.9374	0.2755
H	0.8125	-2.2704	-2.4998
C	0.0654	-2.3778	-1.6663
H	0.4399	-3.1409	-0.9285
H	-0.9250	-2.7098	-2.0823
O	0.7971	-1.8578	1.1392
O	0.0635	1.1401	1.8138
C	1.2944	1.8544	2.0518
H	2.1602	1.1518	2.0230
H	1.1377	2.2664	3.0822
H	1.4115	2.6720	1.3023
C	0.1066	-2.0812	2.3882
H	0.0068	-1.1218	2.9503
H	0.7911	-2.7968	2.9127
H	-0.8895	-2.5416	2.1883

SCF = -298.029178

ZPE = 0.193502

H₂₉₈ = -297.820263

G₂₉₈ = -297.877448

SCF_{DFT} = -831.437511

40-OCH2			
N	0.0395	-1.0031	-1.0574
C	-0.2447	0.2341	-1.6016
N	-0.2509	1.1796	-0.5998
C	0.2443	-0.8350	0.3288
C	0.0620	0.5325	0.6176
I	-0.5825	0.6008	-3.5772
H	-1.5727	2.7055	-1.2007
C	-0.5541	2.5774	-0.7420
H	0.2183	3.0721	-1.3925
H	-0.5457	3.0480	0.2800
H	1.0385	-2.1439	-2.5213
C	0.2040	-2.2393	-1.7737
H	0.4584	-3.0483	-1.0341
H	-0.7527	-2.4993	-2.3034
O	0.6399	-1.8681	1.1181
O	0.0166	1.1451	1.8309
C	1.2563	1.7642	2.2309
H	2.0725	1.0049	2.2689
H	1.0133	2.1529	3.2532
H	1.5104	2.5954	1.5317
C	-0.2141	-2.1015	2.2586
H	-0.3346	-1.1611	2.8483
H	0.3586	-2.8757	2.8310
H	-1.1998	-2.4947	1.9151
O	-0.9967	1.1232	-6.2866
C	-1.8636	1.1039	-7.1217
H	-1.6537	1.3951	-8.1587
H	-2.8881	0.7952	-6.8725

SCF = -412.572232

ZPE = 0.222147

H₂₉₈ = -412.329931

G₂₉₈ = -412.397828

SCF_{DFT} = -945.982901

7.3 ONIOM(DFT:PM6)

SCF = -758.465500

1-OCH2

H	3.1581	0.2417	-1.1759
C	2.3993	0.1753	-0.3952
C	0.4571	0.0185	1.6152
C	1.9246	-1.0641	0.0346
C	1.8950	1.3442	0.1867
C	0.9244	1.2664	1.1907
C	0.9581	-1.1536	1.0366
H	2.2616	2.3145	-0.1440
H	0.5919	-2.1243	1.3733
H	-0.2970	-0.0445	2.3979
I	2.6732	-2.8088	-0.8321
H	0.5338	2.1769	1.6424
O	3.3689	-5.2096	-2.3779
C	2.5917	-5.2879	-3.2877
H	2.6450	-6.1109	-4.0125
H	1.7986	-4.5400	-3.4292

SCF = -412.730588

1-Cl

H	2.7112	0.0263	-1.4654
C	2.1196	0.0422	-0.5509
C	0.6032	0.0916	1.7934
C	1.6825	-1.1535	0.0164
C	1.8009	1.2667	0.0501
C	1.0412	1.2921	1.2244
C	0.9258	-1.1291	1.1867
H	2.1433	2.1951	-0.3955
H	0.5828	-2.0620	1.6325
H	0.0135	0.1055	2.7043
I	2.1709	-3.0287	-0.9130
Cl	2.7949	-5.4404	-2.1131
H	0.7926	2.2388	1.6918

SCF = -758.504988

2-Cl

H	0.3830	0.1485	0.0685
C	0.2361	0.1351	1.1493
C	-0.1395	0.0904	3.9239
C	0.3490	-1.0665	1.8495
C	-0.0640	1.3229	1.8214
C	-0.2526	1.2993	3.2146
C	0.1614	-1.0857	3.2320
H	-0.1520	2.2586	1.2752
H	0.2499	-2.0259	3.7780
H	-0.2857	0.0748	5.0009
I	0.8098	-2.8890	0.7970
Cl	1.3907	-5.1981	-0.5382
C	-0.5608	2.5093	3.9127
N	-0.8105	3.4891	4.4780

2-OCH2

H	1.0362	0.5599	0.1785
C	0.6556	0.3959	1.1894
C	-0.3151	-0.0203	3.7896
C	0.6709	-0.8794	1.7573
C	0.1512	1.4752	1.9205
C	-0.3349	1.2643	3.2215
C	0.1912	-1.0934	3.0508
H	0.1363	2.4747	1.4842
H	0.2091	-2.0923	3.4931
H	-0.6912	-0.1791	4.8010
I	1.4238	-2.4840	0.6609
C	-0.8548	2.3683	3.9750
N	-1.2745	3.2582	4.5821
O	2.1034	-4.7444	-1.0045
C	1.1359	-5.1030	-1.6165
H	1.1842	-5.9545	-2.3079
H	0.1681	-4.5934	-1.5075

SCF = -412.679981

3-Cl

H	0.3778	0.1365	0.0578
C	0.2343	0.1263	1.1396
C	-0.1305	0.0753	3.9203
C	0.3516	-1.0769	1.8420
C	-0.0645	1.3116	1.8088
C	-0.2470	1.2819	3.2044
C	0.1690	-1.0965	3.2280
H	-0.1589	2.2572	1.2719
H	0.2617	-2.0381	3.7719
H	-0.2755	0.0732	5.0021
I	0.8118	-2.9032	0.7865
Cl	1.3874	-5.1990	-0.5400
N	-0.5613	2.5178	3.9182
O	-0.6582	3.5586	3.2754
O	-0.7168	2.4700	5.1345

SCF = -758.529320

3-OCH₂

H	0.2694	0.0657	0.0730
C	0.1613	0.0765	1.1599
C	-0.1189	0.1043	3.9560
C	0.2758	-1.1032	1.8998
C	-0.0944	1.2837	1.8142
C	-0.2321	1.2870	3.2103
C	0.1370	-1.0966	3.2899
H	-0.1876	2.2203	1.2538
H	0.2268	-2.0234	3.8633
H	-0.2309	0.1317	5.0455
I	0.6620	-2.9029	0.9203
N	-0.5020	2.5644	3.9098
O	-0.5928	3.5730	3.2288
O	-0.6171	2.5309	5.1240
O	1.2496	-5.1998	-0.6804
C	1.4782	-4.9006	-1.8197
H	1.7263	-5.6644	-2.5683
H	1.4477	-3.8542	-2.1545

SCF = -412.737866**4-OCH₂**

H	1.2101	0.5137	0.1993
C	0.7807	0.3613	1.1908
C	-0.3161	-0.0147	3.7380
C	0.7281	-0.9143	1.7546
C	0.2810	1.4544	1.9034
C	-0.2720	1.2739	3.1821
C	0.1840	-1.1078	3.0245
H	0.3240	2.4488	1.4641
H	0.1463	-2.1044	3.4676
H	-0.7385	-0.1673	4.7289
I	1.4752	-2.5432	0.6917
C	-0.7915	2.4469	3.9472
H	-1.5305	2.1607	4.7072
H	0.0281	2.9620	4.4710
H	-1.2740	3.1871	3.2945
O	2.0856	-4.8729	-1.0079
C	1.0860	-5.1357	-1.6157
H	1.0549	-5.9730	-2.3254
H	0.1653	-4.5494	-1.4853

SCF = -412.746860**4-Cl**

H	0.3903	0.1344	0.0614
C	0.2405	0.1149	1.1407
C	-0.1454	0.0774	3.9061
C	0.3517	-1.0862	1.8372
C	-0.0634	1.3032	1.8167
C	-0.2587	1.2873	3.2055
C	0.1590	-1.1029	3.2166
H	-0.1463	2.2324	1.2641
H	0.2449	-2.0395	3.7671
H	-0.2921	0.0527	4.9801
I	0.8172	-2.9006	0.7897
Cl	1.4169	-5.2404	-0.5648
C	-0.5694	2.5579	3.9395
H	-1.1959	2.3775	4.8207
H	0.3576	3.0357	4.2831
H	-1.0981	3.2785	3.3049

SCF = -758.519679**5-Cl**

H	1.3771	0.0489	0.2588
C	0.8127	0.0619	1.1920
C	-0.6205	0.1146	3.5863
C	0.4033	-1.1343	1.7731
C	0.5075	1.2916	1.7865
C	-0.2201	1.3291	2.9932
C	-0.3028	-1.1019	2.9717
H	0.8494	2.2058	1.3142
H	-0.6186	-2.0334	3.4431
H	-1.1629	0.1064	4.5253
I	0.8402	-3.0047	0.8230
Cl	1.3901	-5.4219	-0.4164
N	-0.4454	2.5864	3.6749
C	-1.6264	2.5954	4.5889
C	-0.4806	3.7818	2.7806
H	-2.5858	2.4078	4.0838
H	-1.6806	3.5642	5.1065
H	-1.4856	1.8196	5.3620
H	-1.2841	3.7566	2.0294
H	-0.5918	4.6907	3.3898
H	0.4852	3.8600	2.2509

SCF = -758.502856

5-OCH2

H	1.8304	0.2249	0.4545
C	1.1355	0.1828	1.2960
C	-0.6379	0.0859	3.4582
C	0.7066	-1.0472	1.7972
C	0.6795	1.3705	1.8641
C	-0.2138	1.3428	2.9625
C	-0.1734	-1.0934	2.8796
H	1.0327	2.3174	1.4634
H	-0.5062	-2.0532	3.2809
H	-1.3164	0.0267	4.3056
I	1.3828	-2.8130	0.9340
N	-0.5711	2.5446	3.6353
C	-1.8046	2.5067	4.4678
C	-0.4754	3.8065	2.8512
H	-2.7262	2.3460	3.8869
H	-1.9016	3.4531	5.0247
H	-1.7182	1.7018	5.2198
H	-1.1810	3.8580	2.0074
H	-0.6595	4.6668	3.5154
H	0.5510	3.9207	2.4585
O	1.9519	-5.2550	-0.6508
C	1.1466	-5.2679	-1.5387
H	1.1303	-6.0771	-2.2809
H	0.3957	-4.4718	-1.6431

SCF = -412.731896**6-Cl**

H	0.2720	0.1332	0.0597
C	0.1987	0.0713	1.1465
C	0.0108	-0.0952	3.9466
C	0.3638	-1.1579	1.7873
C	-0.0600	1.2311	1.8815
C	-0.1484	1.1213	3.2801
C	0.2698	-1.2386	3.1710
H	-0.1906	2.1942	1.4040
H	0.3977	-2.1985	3.6732
H	-0.0586	-0.1761	5.0213
I	0.7703	-2.9216	0.6378
Cl	1.3019	-5.1992	-0.8332
O	-0.4070	2.3446	3.8947
C	-0.5126	2.3542	5.3334
H	0.4301	2.0319	5.7851
H	-1.3468	1.7247	5.6568
H	-0.7105	3.4106	5.5451

SCF = -758.570535**6-OCH2**

H	0.4886	0.0131	0.1082
C	0.3532	-0.0178	1.1913
C	0.0089	-0.1089	3.9850
C	0.4849	-1.2264	1.8882
C	0.0491	1.1529	1.8771
C	-0.1203	1.0927	3.2775
C	0.3151	-1.2733	3.2706
H	-0.0592	2.1054	1.3644
H	0.4192	-2.2173	3.8112
H	-0.1212	-0.1544	5.0603
I	0.9440	-2.9679	0.8515
O	-0.4162	2.3181	3.8275
C	-0.6078	2.3906	5.2615
H	0.3092	2.1010	5.7824
H	-1.4613	1.7765	5.5622
H	-0.8212	3.4581	5.4046
O	1.4683	-5.2101	-0.9778
C	1.1895	-4.8502	-2.0870
H	1.3002	-5.5223	-2.9483
H	0.8136	-3.8359	-2.2830

SCF = -412.796451**7-Cl**

H	0.9883	0.3722	0.5416
C	0.4488	0.1268	1.4561
C	-0.9423	-0.5070	3.8027
C	0.2904	-1.2065	1.8342
C	-0.0811	1.1549	2.2461
C	-0.7698	0.8225	3.4139
C	-0.4060	-1.5225	3.0007
H	0.0425	2.1931	1.9487
H	-0.5340	-2.5647	3.2922
H	-1.4855	-0.7558	4.7109
I	1.1301	-2.7747	0.6228
Cl	2.2112	-4.7731	-0.9205
S	-1.4821	2.1074	4.3923
C	-0.1393	2.5109	5.5448
H	-0.4897	3.3115	6.2031
H	0.7514	2.8533	5.0088
H	0.1335	1.6425	6.1525

SCF = -758.510680

7-OCH2

H	2.1120	0.2845	1.6678
C	1.2203	-0.0355	2.2100
C	-1.0663	-0.8471	3.6132
C	0.7061	-1.3197	2.0392
C	0.5891	0.8569	3.0870
C	-0.5484	0.4448	3.7809
C	-0.4328	-1.7314	2.7368
H	0.9995	1.8568	3.2100
H	-0.8313	-2.7390	2.6053
H	-1.9540	-1.1701	4.1584
I	1.6465	-2.6417	0.7322
S	-1.4427	1.4602	4.9006
C	-0.5286	3.0099	5.0168
H	-1.0611	3.6455	5.7397
H	-0.4924	3.5445	4.0609
H	0.4928	2.8637	5.3864
O	2.6033	-4.4207	-1.3923
C	1.7970	-4.3984	-2.2797
H	1.9390	-4.9922	-3.1924
H	0.8878	-3.7841	-2.2128

SCF = -412.732658

8-Cl

H	0.5656	0.1440	0.0934
C	0.3420	0.1156	1.1604
C	-0.2315	0.0413	3.8977
C	0.3582	-1.1028	1.8409
C	0.0410	1.3006	1.8362
C	-0.2472	1.2635	3.2108
C	0.0720	-1.1354	3.2054
H	0.0310	2.2450	1.2957
H	0.0841	-2.0863	3.7394
H	-0.4520	-0.0066	4.9618
I	0.8207	-2.9245	0.7861
Cl	1.4033	-5.2320	-0.5501
C	-0.5674	2.5454	3.9119
F	-0.8374	2.4731	5.2297
F	0.4053	3.4792	3.8613
F	-1.6398	3.2056	3.4273

SCF = -758.775234

8-OCH2

H	1.2607	0.5245	0.2340
C	0.8056	0.3662	1.2144
C	-0.3569	-0.0256	3.7355
C	0.7031	-0.9172	1.7537
C	0.3234	1.4613	1.9372
C	-0.2593	1.2638	3.1984
C	0.1273	-1.1190	3.0080
H	0.4053	2.4643	1.5131
H	0.0515	-2.1231	3.4317
H	-0.8047	-0.1971	4.7162
I	1.4227	-2.5489	0.6731
C	-0.7702	2.4628	3.9501
F	-1.3209	2.2258	5.1519
F	0.1694	3.3884	4.2128
F	-1.7244	3.1522	3.2992
O	2.0600	-4.8270	-0.9810
C	1.0974	-5.1477	-1.6211
H	1.1341	-5.9971	-2.3158
H	0.1458	-4.6043	-1.5355

SCF = -412.989815

9-OCH2

H	0.9996	0.5358	0.1775
C	0.6180	0.3701	1.1872
C	-0.3582	-0.0424	3.7862
C	0.6522	-0.9010	1.7630
C	0.0914	1.4475	1.9099
C	-0.3908	1.2250	3.2012
C	0.1702	-1.1136	3.0555
H	0.0633	2.4423	1.4635
H	0.2017	-2.1079	3.5063
H	-0.7354	-0.2046	4.7966
I	1.4356	-2.4996	0.6808
Br	-1.1134	2.6921	4.1931
O	2.1373	-4.7702	-0.9889
C	1.1649	-5.1206	-1.5975
H	1.2049	-5.9685	-2.2939
H	0.2002	-4.6066	-1.4807

SCF = -412.727574

9-Cl

H	0.3605	0.1397	0.0637
C	0.2241	0.1252	1.1456
C	-0.1274	0.0918	3.9268
C	0.3489	-1.0717	1.8487
C	-0.0769	1.3194	1.8167
C	-0.2464	1.2735	3.1987
C	0.1742	-1.0882	3.2312
H	-0.1736	2.2504	1.2656
H	0.2715	-2.0239	3.7828
H	-0.2631	0.0754	5.0044
I	0.8094	-2.8931	0.7986
Cl	1.3926	-5.2103	-0.5384
Br	-0.6624	2.9107	4.1411

SCF = -758.509313**10-OCH2**

C	0.1998	-0.2857	0.9661
C	-0.1057	0.0557	3.7574
C	0.1118	-1.4043	1.8072
C	0.1359	1.0029	1.5179
C	-0.0170	1.1817	2.9119
C	-0.0411	-1.2405	3.2042
I	0.4231	-0.5168	-1.0887
C	0.1750	-2.7355	1.2695
N	0.2233	-3.8148	0.8610
C	-0.1305	-2.3882	4.0606
N	-0.2025	-3.3115	4.7504
C	-0.2610	0.2287	5.1732
N	-0.3860	0.3683	6.3126
C	-0.0819	2.5026	3.4678
N	-0.1342	3.5663	3.9146
C	0.2257	2.1620	0.6723
N	0.2968	3.1030	0.0059
O	0.7185	-0.4577	-3.7637
C	0.8022	0.6637	-4.1917
H	0.9237	0.8451	-5.2671
H	0.7598	1.5366	-3.5245

SCF = -412.442085**10-Cl**

C	0.2232	-0.0230	1.1081
C	-0.1293	0.0053	3.9184
C	0.1392	-1.2220	1.8226
C	0.1318	1.1902	1.7974
C	-0.0445	1.2170	3.2009
C	-0.0369	-1.2207	3.2264
I	0.4918	-0.0451	-1.0634
Cl	0.8119	-0.0732	-3.6837
C	0.2294	-2.4902	1.1512
N	0.2976	-3.5286	0.6482
C	-0.1230	-2.4533	3.9560
N	-0.1926	-3.4446	4.5461
C	-0.3082	0.0195	5.3405
N	-0.4526	0.0310	6.4873
C	-0.1382	2.4641	3.9047
N	-0.2141	3.4670	4.4740
C	0.2142	2.4446	1.0997
N	0.2760	3.4726	0.5750

SCF = -758.254949**11-I**

C	0.0084	0.0071	1.1206
C	0.0179	0.0439	3.9038
C	0.0369	-1.2053	1.7995
C	-0.0154	1.2414	1.7996
C	-0.0105	1.2554	3.2006
C	0.0411	-1.1700	3.1889
I	0.0752	-3.0662	0.7393
F	0.0677	-2.3024	3.8818
F	0.0227	0.0496	5.2352
F	-0.0324	2.4111	3.8587
F	-0.0423	2.3888	1.1248
F	0.0030	0.0246	-0.2071
I	0.1345	-5.7933	-0.8127

SCF = -596.354941**11-F**

C	0.0134	-0.0127	1.1174
C	0.0144	0.0344	3.8981
C	0.0381	-1.2218	1.7976
C	-0.0111	1.2254	1.7906
C	-0.0105	1.2438	3.1915
C	0.0383	-1.1811	3.1844
I	0.0745	-3.1259	0.7156
F	0.0615	-2.3107	3.8840
F	0.0151	0.0450	5.2301
F	-0.0335	2.4024	3.8464
F	-0.0347	2.3718	1.1126
F	0.0121	0.0040	-0.2115
F	0.1110	-4.9963	-0.3552

SCF = -398.516706

11-OCH2

C	0.0005	-0.2242	1.0707
C	-0.0004	-0.1072	3.8566
C	-0.0003	-1.4218	1.7911
C	0.0008	1.0259	1.7129
C	0.0004	1.0831	3.1147
C	-0.0007	-1.3435	3.1864
F	-0.0014	-2.4591	3.9014
F	-0.0008	-0.0643	5.1846
F	0.0006	2.2552	3.7338
F	0.0015	2.1471	0.9997
F	0.0009	-0.2630	-0.2549
I	-0.0007	-3.2471	0.8233
O	-0.0005	-5.5051	-0.7700
C	-0.0001	-5.2065	-1.9337
H	0.0000	-5.9781	-2.7140
H	0.0001	-4.1551	-2.2548

SCF = -413.081337

11-OMe

C	0.0653	0.0693	1.1849
C	-0.0209	0.1012	3.9643
C	0.1004	-1.1393	1.8602
C	-0.0122	1.3036	1.8625
C	-0.0553	1.3135	3.2628
C	0.0568	-1.1089	3.2444
I	0.2221	-3.0635	0.7504
F	0.0877	-2.2420	3.9390
F	-0.0617	0.1052	5.2960
F	-0.1286	2.4678	3.9227
F	-0.0446	2.4537	1.1903
F	0.1045	0.0945	-0.1441
O	0.3435	-4.9704	-0.3786
C	0.2765	-4.6966	-1.7456
H	0.3348	-5.6353	-2.3135
H	1.1000	-4.0497	-2.0946
H	-0.6618	-4.1937	-2.0370

SCF = -413.773079

11-Cl

C	0.2192	-0.0245	1.1227
C	-0.1291	0.0078	3.9335
C	0.1040	-1.2049	1.8457
C	0.1576	1.1722	1.8250
C	-0.0151	1.2100	3.2230
C	-0.0697	-1.2104	3.2441
I	0.4855	-0.0496	-1.0230
F	0.1566	-2.3753	1.2199
F	-0.1774	-2.3569	3.9130
F	-0.2927	0.0230	5.2537
F	-0.0707	2.3715	3.8718
F	0.2627	2.3280	1.1789
Cl	0.8153	-0.0811	-3.6880

SCF = -758.875604

11-Br

C	0.0080	0.0053	1.1199
C	0.0189	0.0393	3.9028
C	0.0383	-1.2076	1.7971
C	-0.0170	1.2391	1.7999
C	-0.0114	1.2516	3.2009
C	0.0433	-1.1736	3.1861
I	0.0769	-3.0755	0.7298
F	0.0717	-2.3066	3.8782
F	0.0244	0.0438	5.2342
F	-0.0347	2.4067	3.8603
F	-0.0457	2.3873	1.1264
F	0.0021	0.0246	-0.2080
Br	0.1294	-5.5770	-0.6993

SCF = -2872.784086

11-DMF

C	0.0893	0.5175	2.1713
C	0.6857	-0.0128	4.8423
C	0.2460	-0.8128	2.5698
C	0.2240	1.5835	3.0774
C	0.5241	1.3150	4.4211
C	0.5448	-1.0586	3.9127
F	0.7009	-2.3075	4.3276
F	0.9702	-0.2783	6.1130
F	0.6540	2.3106	5.2871
F	0.0687	2.8379	2.6667
F	-0.1944	0.7879	0.9042
I	0.0412	-2.3645	1.2179
O	-0.2410	-4.3816	-0.5995
C	-0.4448	-4.7818	-1.7339
H	-0.4911	-5.8572	-1.9464
N	-0.6300	-4.0244	-2.8198
C	-0.6046	-2.5789	-2.7500
H	0.1859	-2.1905	-3.3921
H	-0.4232	-2.2722	-1.7282
H	-1.5590	-2.1745	-3.0870
C	-0.8637	-4.6110	-4.1189
H	-0.0851	-4.3063	-4.8183
H	-1.8279	-4.2891	-4.5122
H	-0.8604	-5.6941	-4.0396

SCF = -547.125208**11-NH3**

C	0.2011	-0.0246	1.2545
C	-0.1436	0.0091	4.0663
C	0.0969	-1.2109	1.9826
C	0.1297	1.1787	1.9580
C	-0.0411	1.2126	3.3534
C	-0.0744	-1.2112	3.3784
I	0.4539	-0.0501	-0.8108
F	0.1603	-2.3735	1.3476
F	-0.1704	-2.3577	4.0440
F	-0.3050	0.0249	5.3824
F	-0.1054	2.3747	3.9951
F	0.2248	2.3258	1.2990
N	0.7847	-0.0870	-3.5266
H	1.7553	0.0610	-3.7623
H	0.2327	0.6408	-3.9570
H	0.4933	-0.9785	-3.9010

SCF = -355.126892**12-Cl**

C	0.5729	-0.2915	1.0495
C	-0.0046	0.5727	3.6530
C	0.2554	-1.1927	2.0546
C	0.5933	1.0542	1.3837
C	0.3086	1.5235	2.6807
C	-0.0400	-0.7940	3.3726
I	1.0181	-0.9569	-0.9550
Cl	1.5735	-1.7849	-3.4472
I	-0.5125	-2.1828	4.8538
I	0.3511	3.5565	3.1401
F	-0.2779	0.9817	4.8852
F	0.2222	-2.4888	1.7880
F	0.8904	1.9555	0.4610

SCF = -758.687588**12-OCH2**

C	0.5547	-0.5178	0.9479
C	0.0205	0.6185	3.4569
C	0.2646	-1.3125	2.0624
C	0.5666	0.8673	1.1405
C	0.3042	1.4652	2.3794
C	-0.0063	-0.7742	3.3273
I	0.9468	-1.3489	-0.8955
I	-0.4322	-1.9977	4.9514
I	0.3346	3.5296	2.6105
F	-0.2312	1.1541	4.6385
F	0.2440	-2.6258	1.9195
F	0.8368	1.6496	0.1089
O	1.4847	-2.1241	-3.4987
C	1.5790	-1.1605	-4.2098
H	1.7933	-1.2682	-5.2807
H	1.4542	-0.1425	-3.8138

SCF = -412.894564**13-OCH2**

C	-0.0548	0.0605	0.7910
I	-0.4274	-0.2705	-1.2958
Br	-0.5013	-1.5103	1.8383
Br	1.8195	0.4736	1.0976
Br	-1.1103	1.5483	1.4564
O	-0.6776	-0.4753	-3.9547
C	0.0786	0.2651	-4.5269
H	0.1019	0.3036	-5.6230
H	0.7652	0.9215	-3.9736

SCF = -412.732390

13-Cl

C	-0.0001	-0.0038	1.1306
I	-0.0025	-0.0173	-1.1693
Cl	-0.0051	-0.0337	-3.7825
Br	-0.9245	-1.5697	1.8515
Br	1.8229	-0.0159	1.8397
Br	-0.8965	1.5866	1.8330

SCF = -758.540617**14-Cl**

C	-0.0011	-0.0016	1.0454
I	0.0015	-0.0197	-1.1915
Cl	0.0047	-0.0438	-3.8426
F	-0.6164	-1.0441	1.6351
F	1.2120	-0.0063	1.6298
F	-0.6008	1.0581	1.6202

SCF = -758.828133**14-OCH2**

C	0.0006	0.0686	0.7232
I	0.1014	-0.4175	-1.3468
F	-0.7412	-0.7728	1.4490
F	1.1872	0.0882	1.3378
F	-0.5232	1.2747	0.9676
O	0.1804	-0.7494	-4.0301
C	-0.0051	0.2794	-4.6244
H	-0.0039	0.3018	-5.7214
H	-0.1808	1.2247	-4.0920

SCF = -413.024380**15-Cl**

C	-0.0002	-0.0041	1.1286
I	0.0015	-0.0177	-1.1282
Cl	0.0035	-0.0339	-3.9302
C	-0.7274	-1.2594	1.5950
H	-0.2320	-2.1644	1.2241
H	-1.7567	-1.2834	1.2182
H	-0.7678	-1.3218	2.6867
C	1.4524	-0.0017	1.5889
H	1.9863	-0.8847	1.2182
H	1.5313	0.0051	2.6802
H	1.9868	0.8763	1.2072
C	-0.7267	1.2572	1.5795
H	-0.2305	2.1573	1.1979
H	-0.7674	1.3329	2.6704
H	-1.7559	1.2773	1.2021

SCF = -758.578887**15-OCH2**

C	0.0634	-0.0709	0.9740
I	0.3065	-0.4937	-1.1877
C	-0.7642	-1.2059	1.5500
H	-0.2794	-2.1833	1.4196
H	-1.7557	-1.2796	1.0835
H	-0.9252	-1.0692	2.6282
C	1.4592	-0.0247	1.5695
H	1.9995	-0.9726	1.4394
H	1.4213	0.1772	2.6487
H	2.0815	0.7591	1.1172
C	-0.6479	1.2662	1.0857
H	-0.0776	2.0824	0.6229
H	-0.8036	1.5413	2.1383
H	-1.6369	1.2539	0.6088
O	0.4041	-0.6256	-4.2456
C	-0.1153	0.3909	-4.6087
H	-0.2231	0.6272	-5.6759
H	-0.5038	1.1257	-3.8895

SCF = -412.815169**16-OCH2**

C	0.0505	-0.0352	0.9244
I	0.2803	-0.3789	-1.2087
C	-0.7517	-1.1248	1.4720
N	-1.3865	-1.9845	1.9074
C	1.3821	-0.0106	1.5218
N	2.4337	0.0101	1.9965
C	-0.6238	1.2488	1.0914
N	-1.1569	2.2642	1.2214
O	0.4413	-0.5759	-3.8229
C	-0.0599	0.3506	-4.4072
H	-0.0565	0.3836	-5.5037
H	-0.5313	1.1829	-3.8659

SCF = -412.601401**16-Cl**

C	-0.0010	-0.0036	1.2884
I	0.0011	-0.0163	-1.1453
Cl	0.0035	-0.0294	-3.7144
C	-0.6997	-1.2099	1.6260
N	-1.2633	-2.1831	1.9035
C	1.3938	-0.0023	1.6232
N	2.5188	-0.0010	1.8989
C	-0.6984	1.2062	1.6164
N	-1.2608	2.1823	1.8858

SCF = -758.427139

17-Cl

I	0.1119	-1.3506	-1.5561
Cl	1.0608	-2.5825	-3.7249
N	-0.5826	-0.4423	0.0364
C	0.0747	-0.3922	1.2910
C	-1.8112	0.2614	0.0972
O	1.1397	-0.8954	1.5609
O	-2.6008	0.4007	-0.8068
C	-2.0097	0.8421	1.5077
H	-2.1194	1.9370	1.4472
H	-2.9462	0.4556	1.9412
C	-0.7723	0.4130	2.2911
H	-0.1884	1.2671	2.6704
H	-1.0147	-0.2147	3.1639

SCF = -758.723037**17-OCH2**

I	0.5596	-1.3248	-1.4290
N	-0.3191	-0.4682	0.0039
C	0.1341	-0.4773	1.3670
C	-1.5338	0.2797	-0.1334
O	1.1318	-1.0405	1.7283
O	-2.1043	0.4278	-1.1830
C	-1.9302	0.8148	1.2344
H	-2.0028	1.9193	1.2046
H	-2.9406	0.4529	1.5066
C	-0.8512	0.3247	2.2052
H	-0.3276	1.1582	2.7124
H	-1.2650	-0.3085	3.0138
O	1.4952	-2.3893	-3.6646
C	0.7521	-2.1171	-4.5725
H	0.9643	-2.4674	-5.5900
H	-0.1535	-1.5145	-4.4094

SCF = -412.926186**18-OCH2**

I	-0.7274	-0.2541	-1.1760
C	-0.4005	-0.0453	0.8670
H	-0.8473	0.8626	1.2586
C	0.2677	-0.9191	1.6007
H	0.4239	-0.7906	2.6681
H	0.7131	-1.8300	1.2179
O	-0.8101	-0.2723	-4.1254
C	0.1503	0.3275	-4.5197
H	0.3412	0.4541	-5.5936
H	0.8743	0.7723	-3.8223

SCF = -412.744246**18-Cl**

I	-0.0028	-0.0062	-0.9375
Cl	-0.0062	0.1139	-3.7363
C	0.0000	-0.0576	1.1970
H	0.0015	0.9314	1.6276
C	-0.0000	-1.1657	1.9195
H	0.0014	-1.1749	2.9997
H	-0.0015	-2.1566	1.4883

SCF = -758.514351**19-Cl**

I	-0.0033	-0.0388	-0.9419
Cl	-0.0072	0.0063	-3.6755
C	-0.0001	-0.0435	1.1994
H	0.0011	0.9488	1.6262
C	0.0002	-1.1557	1.9285
H	-0.0011	-2.1560	1.4823
C	0.0023	-1.1464	3.3592
N	0.0040	-1.1512	4.5186

SCF = -758.480777**19-OCH2**

I	0.0251	-0.5626	-1.1690
C	0.0328	-0.1842	0.8645
H	0.0810	0.8766	1.1055
C	-0.0156	-1.1426	1.7876
H	-0.0639	-2.2154	1.5513
C	-0.0080	-0.8414	3.1892
N	-0.0026	-0.6118	4.3226
O	0.0074	-0.7150	-4.0214
C	-0.0158	0.3814	-4.5087
H	-0.0290	0.5182	-5.5979
H	-0.0247	1.2856	-3.8838

SCF = -412.693981

20-Cl

I	-0.0795	-0.0170	-0.9415
Cl	0.1572	0.2024	-3.7183
C	-0.2899	-0.1737	1.1698
H	-0.8143	0.6669	1.5824
C	0.1793	-1.2080	1.8565
H	0.7049	-2.0409	1.3734
N	0.1778	-1.3565	3.3016
C	-0.3236	-2.7055	3.7093
H	0.2767	-3.4792	3.2047
H	-1.3820	-2.8826	3.4675
H	-0.1833	-2.8317	4.7924
C	-0.5382	-0.2794	4.0436
H	-0.0619	0.6854	3.7976
H	-0.4233	-0.4416	5.1243
H	-1.6096	-0.2000	3.8068

SCF = -758.518239**20-OCH2**

I	-0.1695	-0.6983	-1.2247
C	-0.3785	-0.4821	0.8140
H	-0.8108	0.4665	1.0911
C	0.0023	-1.4362	1.6757
H	0.4216	-2.3922	1.3230
N	0.0406	-1.2904	3.0867
C	-0.1549	-2.5590	3.8420
H	0.5022	-3.3457	3.4356
H	-1.1920	-2.9292	3.8261
H	0.1425	-2.4026	4.8927
C	-0.7134	-0.1523	3.6737
H	-0.3193	0.7922	3.2575
H	-0.5496	-0.1187	4.7626
H	-1.7975	-0.1907	3.4833
O	0.1964	-0.4795	-4.1707
C	0.3627	0.6878	-4.3871
H	0.5319	1.0597	-5.4064
H	0.3521	1.4285	-3.5748

SCF = -412.750878**21-Cl**

I	0.0234	-0.0538	-0.8497
Cl	0.3099	-0.1480	-3.6147
C	-0.1874	0.0149	1.1859
H	-0.4164	0.0908	3.4057
C	-0.3109	0.0559	2.3840

SCF = -758.457630**21-OCH2**

I	-0.0533	-0.5467	-1.0855
C	-0.1814	-0.0235	0.8194
H	-0.3255	0.5611	2.9779
C	-0.2590	0.2912	1.9801
O	0.1682	-0.8868	-3.9242
C	0.3027	0.1886	-4.4391
H	0.4061	0.2882	-5.5275
H	0.3278	1.1106	-3.8407

SCF = -412.679937**22-OCH2**

I	-0.0232	-0.5980	-1.0263
C	-0.1890	-0.1857	0.9039
C	-0.2903	0.0655	2.0830
C	-0.4058	0.3537	3.4283
N	-0.5027	0.5962	4.5570
O	0.2206	-0.8293	-3.7815
C	0.2844	0.2448	-4.3156
H	0.3864	0.3291	-5.4052
H	0.2436	1.1767	-3.7334

SCF = -412.626257**22-Cl**

I	0.0238	-0.0532	-0.8442
Cl	0.3029	-0.1419	-3.5451
C	-0.1886	0.0146	1.2068
C	-0.3141	0.0550	2.4117
C	-0.4560	0.1009	3.7768
N	-0.5763	0.1402	4.9323

SCF = -758.421730**23-OCH2**

I	0.0068	-0.3853	-1.0419
C	-0.1598	0.1819	0.8822
N	-0.2550	0.5092	1.9837
O	0.2372	-0.8506	-3.7352
C	0.2817	0.1693	-4.3693
H	0.3727	0.1496	-5.4629
H	0.2325	1.1515	-3.8779

SCF = -412.715477**23-Cl**

I	0.0201	-0.0518	-0.7969
Cl	0.2974	-0.1413	-3.4959
C	-0.1964	0.0173	1.2838
N	-0.3180	0.0578	2.4319

SCF = -758.510232**24-OCH2**

C	-1.0097	0.5093	1.5902
C	1.0635	-0.4185	3.2334
C	-1.1344	-0.7277	2.2297
C	0.1411	1.2927	1.7610
C	1.1717	0.8143	2.5876
C	-0.0986	-1.1908	3.0507
C	-0.2014	-2.4948	3.7412
C	-0.1332	-4.9598	5.1885
C	0.2907	-3.6712	3.1525
C	-0.7253	-2.5906	5.0408
C	-0.6924	-3.8006	5.7510
C	0.3237	-4.8812	3.8627
C	0.0502	-6.1890	5.9910
C	0.4529	-8.5011	7.5327
C	-0.9356	-7.1824	6.0282
C	1.2433	-6.3418	6.7219
C	1.4325	-7.4946	7.4844
C	-0.7295	-8.3317	6.7976
I	2.6797	-4.8529	6.6411
I	2.5828	-1.1222	4.4490
F	0.6441	-9.5948	8.2624
F	2.5523	-7.6478	8.1764
F	-1.6605	-9.2734	6.8347
F	0.8212	-5.9673	3.2828
F	0.7571	-3.6284	1.9099
F	-1.2366	-1.5080	5.6153
F	-1.1728	-3.8468	6.9882
F	-1.9882	0.9493	0.8132
F	0.2552	2.4676	1.1514
F	2.2618	1.5491	2.7535
O	4.4585	-2.5621	6.3133
C	5.5130	-2.3802	6.8605
H	5.9295	-3.1242	7.5521
H	6.0924	-1.4646	6.6856
I	-2.7097	-6.9595	4.9435
I	-2.8637	-1.8713	1.9538

24-Cl

C	-0.8667	0.4703	1.5720
C	0.9982	-0.4487	3.4573
C	-1.0421	-0.7806	2.1672
C	0.2320	1.2718	1.9065
C	1.1566	0.7931	2.8546
C	-0.1092	-1.2374	3.1082
C	-0.2656	-2.5584	3.7558
C	-0.2582	-5.0369	5.1882
C	0.3366	-3.7087	3.2206
C	-0.9370	-2.6947	4.9820
C	-0.9334	-3.9095	5.6840
C	0.3402	-4.9237	3.9228
C	-0.0936	-6.2566	6.0093
C	0.2635	-8.5478	7.5838
C	-1.0224	-7.3039	5.9397
C	1.0176	-6.3425	6.8626
C	1.1839	-7.4834	7.6378
C	-0.8391	-8.4428	6.7267
I	2.3848	-4.7213	6.9258
I	2.3739	-1.1946	4.8900
F	0.4337	-9.6353	8.3315
F	2.2266	-7.5883	8.4519
F	-1.7173	-9.4374	6.6638
F	0.9416	-5.9833	3.3918
F	0.9346	-3.6370	2.0358
F	-1.5681	-1.6442	5.4964
F	-1.5610	-3.9910	6.8528
F	-1.7488	0.9067	0.6798
F	0.3948	2.4630	1.3361
F	2.1956	1.5568	3.1677
Cl	4.0425	-2.4276	6.8202
I	-2.6981	-1.9597	1.6466
I	-2.6840	-7.1744	4.6645

SCF = -1057.358702**SCF = -711.535879**

25-OCH2

C	0.3533	-1.4728	0.1073
C	-0.3020	1.2335	-0.2523
C	1.3957	-0.5350	0.0372
C	-1.0034	-1.1135	0.0261
C	-1.2969	0.2466	-0.1590
C	1.0331	0.8069	-0.1748
C	2.7917	-0.9242	0.3037
C	5.4219	-1.7029	0.9152
C	3.5726	-1.5610	-0.6715
C	3.3291	-0.6590	1.5771
C	4.6318	-1.0515	1.8777
C	4.8811	-1.9462	-0.3558
C	-2.0725	-2.1066	0.2247
C	-4.1263	-3.9681	0.6703
C	-2.4139	-2.4762	1.5372
C	-2.7476	-2.6701	-0.8691
C	-3.7691	-3.5970	-0.6353
C	-3.4373	-3.3988	1.7540
C	-0.6371	2.6637	-0.3679
C	-1.1593	5.4151	-0.5570
C	-0.7084	3.2717	-1.6311
C	-0.8715	3.4146	0.7957
C	-1.1219	4.7841	0.6965
C	-0.9604	4.6423	-1.7128
I	2.1586	0.4002	2.9609
I	2.8086	-1.9184	-2.5523
I	-2.2326	-2.1336	-2.7938
I	-1.3353	-1.6531	3.1379
I	-0.5159	2.0974	-3.3261
I	-0.9478	2.4585	2.6648
F	0.6589	-2.7479	0.2913
F	-2.5657	0.6184	-0.2228
F	1.9931	1.7116	-0.2884
F	-4.4119	-4.1354	-1.6604
F	-5.1011	-4.8466	0.8784
F	-3.7647	-3.7430	2.9900
F	5.1334	-0.8095	3.0793
F	6.6629	-2.0789	1.2044
F	5.6234	-2.5510	-1.2708
F	-1.3898	6.7205	-0.6477
F	-1.3303	5.4976	1.7929
F	-1.0163	5.2283	-2.9001
O	-0.2551	0.5066	-5.6224
C	-0.1951	1.2003	-6.6023
H	-0.1215	0.7579	-7.6041
H	-0.2112	2.2969	-6.5298

SCF = -1009.851340**25-Cl**

C	0.3032	-1.3215	0.3456
C	-0.3268	1.4042	0.0951
C	1.3565	-0.3931	0.2994
C	-1.0504	-0.9515	0.2761
C	-1.3277	0.4197	0.1477
C	1.0042	0.9608	0.1701
C	2.7670	-0.8265	0.2990
C	5.4503	-1.6517	0.2973
C	3.4051	-1.1182	-0.9202
C	3.4660	-0.9464	1.5093
C	4.8004	-1.3571	1.5028
C	4.7341	-1.5260	-0.9082
C	-2.1259	-1.9614	0.2515
C	-4.1723	-3.8824	0.2039
C	-2.7216	-2.3832	1.4495
C	-2.5495	-2.4973	-0.9782
C	-3.5637	-3.4480	-0.9890
C	-3.7390	-3.3390	1.4201
C	-0.6552	2.8270	-0.1171
C	-1.2810	5.5333	-0.5228
C	-0.7589	3.3291	-1.4271
C	-0.8630	3.6725	0.9827
C	-1.1740	5.0178	0.7753
C	-1.0693	4.6710	-1.6152
I	2.5008	-0.5070	3.3208
I	2.2774	-0.9076	-2.6771
I	-1.5974	-1.8039	-2.7144
I	-2.0791	-1.5745	3.2768
I	-0.4296	1.9869	-3.0059
I	-0.7048	2.9090	2.9316
Cl	0.1423	-0.4016	-4.6831
F	0.6003	-2.6075	0.4690
F	-2.5948	0.8038	0.0812
F	1.9736	1.8637	0.1251
F	-3.9756	-3.9640	-2.1397
F	-5.1421	-4.7930	0.1796
F	-4.3032	-3.7387	2.5534
F	5.4626	-1.4708	2.6478
F	6.7219	-2.0430	0.2948
F	5.3515	-1.8054	-2.0489
F	-1.5776	6.8158	-0.7167
F	-1.3707	5.8187	1.8157
F	-1.1711	5.1613	-2.8438

SCF = -1355.687183

26-Cl

H	-1.4293	0.8940	-2.1285
C	-1.3319	1.6041	-1.2940
C	-1.0856	3.4505	0.8238
C	-1.1348	1.1977	0.0111
C	-1.4072	2.9846	-1.5395
C	-1.2850	3.8963	-0.4877
C	-1.0057	2.0771	1.1001
H	-1.5622	3.3366	-2.5603
H	-1.3453	4.9673	-0.6890
H	-0.9915	4.1715	1.6364
C	-0.7973	1.5093	2.4402
C	-0.4065	0.2314	4.8995
C	-0.7411	0.1127	2.5255
C	-0.6555	2.2739	3.6079
C	-0.4607	1.6274	4.8332
C	-0.5484	-0.5350	3.7320
H	-0.6961	3.3607	3.5664
H	-0.3505	2.2178	5.7426
H	-0.5055	-1.6216	3.7904
H	-0.2544	-0.2630	5.8577
I	-0.9906	-0.8418	0.6075
Cl	-1.3282	-1.5505	-1.8407

SCF = -758.875897**26-OCH2**

H	-1.3850	1.3021	-2.1835
C	-1.3002	1.9565	-1.3067
C	-1.0811	3.6402	0.9549
C	-1.1123	1.4631	-0.0322
C	-1.3805	3.3527	-1.4451
C	-1.2717	4.1807	-0.3242
C	-0.9967	2.2511	1.1267
H	-1.5291	3.7861	-2.4386
H	-1.3359	5.2680	-0.4444
H	-0.9982	4.3043	1.8194
C	-0.7990	1.5707	2.4138
C	-0.4263	0.0728	4.7679
C	-0.7380	0.1651	2.4037
C	-0.6671	2.2204	3.6487
C	-0.4818	1.4689	4.8164
C	-0.5561	-0.5994	3.5415
H	-0.7080	3.3109	3.7049
H	-0.3795	1.9833	5.7782
H	-0.5116	-1.6896	3.5127
H	-0.2813	-0.5038	5.6863
I	-0.9585	-0.5917	0.4501
O	-1.2895	-0.8625	-2.2174
C	-1.3462	-1.7768	-3.0041
H	-1.2541	-2.8197	-2.6839
H	-1.4927	-1.5823	-4.0693

SCF = -412.945058**27-OCH2**

H	-0.0668	0.5385	0.2369
C	-0.0633	0.4379	1.3256
C	-0.0542	0.2209	4.1435
C	-0.0671	-0.7912	1.9574
C	-0.0548	1.5922	2.1263
C	-0.0504	1.4787	3.5232
C	-0.0628	-0.9395	3.3565
H	-0.0518	2.5781	1.6428
H	-0.0507	0.1328	5.2362
C	-0.0676	-2.3076	3.8926
C	-0.0782	-5.0113	4.7094
C	-0.0763	-3.3784	2.9815
C	-0.0642	-2.6324	5.2576
C	-0.0695	-3.9775	5.6561
C	-0.0817	-4.7108	3.3368
H	-0.0573	-1.8250	6.0003
H	-0.0886	-5.5196	2.5915
H	-0.0824	-6.0634	5.0240
I	-0.0799	-2.6624	0.9920
C	-0.0410	2.7498	4.3480
C	-0.0659	-4.3500	7.1251
F	1.0253	3.5262	4.1092
F	-0.0388	2.5802	5.6766
F	-1.0994	3.5386	4.1144
F	-0.0578	-3.3233	7.9847
F	-1.1306	-5.0801	7.4862
F	0.9944	-5.0902	7.4784
O	-0.0959	-5.2736	0.4592
C	-0.1000	-5.9469	-0.5447
H	-0.1070	-7.0376	-0.4771
H	-0.0969	-5.4955	-1.5422

SCF = -413.440714

27-Cl

H	-0.0673	0.1616	0.1592
C	-0.0641	0.1349	1.2494
C	-0.0556	0.0961	4.0670
C	-0.0680	-1.0629	1.9401
C	-0.0558	1.3384	1.9696
C	-0.0516	1.3124	3.3725
C	-0.0639	-1.1037	3.3394
H	-0.0527	2.2891	1.4311
H	-0.0523	0.0709	5.1584
C	-0.0688	-2.4389	3.9547
C	-0.0792	-5.0747	4.9579
C	-0.0772	-3.5641	3.1118
C	-0.0655	-2.6675	5.3395
C	-0.0707	-3.9792	5.8319
C	-0.0825	-4.8669	3.5702
H	-0.0589	-1.8100	6.0188
H	-0.0892	-5.7369	2.8931
H	-0.0833	-6.1008	5.3399
I	-0.0808	-3.0327	1.0522
Cl	-0.0961	-5.5160	0.4562
C	-0.0427	2.6249	4.1128
C	-0.0673	-4.2473	7.3172
F	1.0194	3.4004	3.8349
F	-0.0395	2.5530	5.4534
F	-1.0981	3.4115	3.8407
F	-0.0593	-3.1677	8.1139
F	-1.1292	-4.9512	7.7421
F	0.9902	-4.9619	7.7353

SCF = -759.387878**28-OCH2**

H	-0.1317	0.5726	0.2739
C	-0.1050	0.4641	1.3616
C	-0.0356	0.2117	4.1786
C	-0.1061	-0.7725	1.9819
C	-0.0683	1.6108	2.1693
C	-0.0340	1.4800	3.5669
C	-0.0721	-0.9367	3.3801
H	-0.0665	2.6056	1.7076
H	-0.0084	0.1346	5.2707
C	-0.0777	-2.3123	3.8999
C	-0.0953	-5.0337	4.6759
C	-0.1172	-3.3715	2.9737
C	-0.0464	-2.6536	5.2572
C	-0.0553	-4.0103	5.6366
C	-0.1271	-4.7103	3.3107
H	-0.0150	-1.8735	6.0263
H	-0.1585	-5.5065	2.5524
H	-0.1019	-6.0854	4.9871
I	-0.1583	-2.6300	0.9967
C	0.0034	2.6559	4.3900
N	0.0334	3.6015	5.0518
C	-0.0228	-4.3479	7.0315
N	0.0034	-4.6200	8.1533
O	-0.2141	-5.2358	0.4249
C	-0.2509	-5.8936	-0.5885
H	-0.2670	-6.9850	-0.5374
H	-0.2691	-5.4270	-1.5789

SCF = -412.821623

28-Cl

H	-0.1593	0.1671	0.1645
C	-0.1255	0.1433	1.2544
C	-0.0380	0.1001	4.0735
C	-0.1219	-1.0542	1.9473
C	-0.0850	1.3479	1.9701
C	-0.0415	1.3186	3.3742
C	-0.0788	-1.0973	3.3463
H	-0.0871	2.3029	1.4419
H	-0.0040	0.0956	5.1636
C	-0.0796	-2.4341	3.9599
C	-0.0879	-5.0793	4.9542
C	-0.1229	-3.5581	3.1153
C	-0.0397	-2.6652	5.3418
C	-0.0442	-3.9831	5.8300
C	-0.1281	-4.8636	3.5695
H	-0.0053	-1.8237	6.0384
H	-0.1624	-5.7303	2.8883
H	-0.0910	-6.1012	5.3437
I	-0.1799	-3.0221	1.0593
Cl	-0.2394	-5.5049	0.4569
C	-0.0000	2.5516	4.1074
N	0.0334	3.5449	4.6973
C	-0.0033	-4.2086	7.2471
N	0.0296	-4.3903	8.3877

SCF = -758.768521**29-Cl**

H	0.0463	0.1557	0.1572
C	0.0032	0.1194	1.2461
C	-0.1061	0.0460	4.0533
C	0.0038	-1.0909	1.9179
C	-0.0561	1.3134	1.9678
C	-0.1064	1.2938	3.3832
C	-0.0459	-1.1382	3.3144
H	-0.0477	2.2580	1.4292
H	-0.1350	0.0021	5.1388
C	-0.0331	-2.4857	3.9216
C	0.0057	-5.1330	4.8865
C	0.0258	-3.5955	3.0611
C	-0.0780	-2.7247	5.2949
C	-0.0517	-4.0509	5.8020
C	0.0501	-4.9053	3.5125
H	-0.1157	-1.8764	5.9762
H	0.1001	-5.7601	2.8213
H	0.0302	-6.1613	5.2440
I	0.0723	-3.0396	1.0191
Cl	0.1323	-5.5372	0.3594
N	-0.0235	2.5073	4.1245
N	0.0454	-4.2813	7.1931
C	-0.4532	3.7493	3.4249
H	0.1356	3.8746	2.4985
H	-0.2339	4.6235	4.0601
H	-1.5233	3.7649	3.1654
C	-0.5186	2.4696	5.5281
H	0.0395	1.7040	6.0952
H	-1.5958	2.2570	5.6126
H	-0.3144	3.4371	6.0163
C	-0.4239	-3.2055	8.1060
H	0.1096	-2.2651	7.8794
H	-0.1736	-3.4689	9.1476
H	-1.5084	-3.0206	8.0447
C	-0.2993	-5.6387	7.6930
H	0.3104	-6.3964	7.1671
H	-1.3633	-5.8962	7.5673
H	-0.0444	-5.7151	8.7633

SCF = -758.879534

29-OCH2

H	-0.0326	0.4464	0.1827
C	-0.0931	0.3737	1.2708
C	-0.2489	0.1678	4.0845
C	-0.0819	-0.8603	1.9127
C	-0.1827	1.5277	2.0319
C	-0.2629	1.4577	3.4597
C	-0.1590	-0.9809	3.3143
H	-0.1912	2.4917	1.5272
H	-0.3087	0.0834	5.1667
C	-0.1372	-2.3558	3.8680
C	-0.0774	-5.0616	4.6789
C	-0.0404	-3.4207	2.9515
C	-0.2054	-2.6599	5.2187
C	-0.1776	-4.0241	5.6605
C	-0.0092	-4.7571	3.3289
H	-0.2806	-1.8518	5.9427
H	0.0676	-5.5568	2.5816
H	-0.0535	-6.1063	4.9823
I	0.0479	-2.7241	0.9767
N	-0.3516	2.6024	4.2141
N	-0.2460	-4.3287	6.9982
C	-0.3665	3.9433	3.5892
H	0.5622	4.1266	3.0170
H	-0.4427	4.7377	4.3523
H	-1.2326	4.0569	2.9106
C	-0.4348	2.5570	5.6900
H	0.4622	2.0790	6.1249
H	-1.3345	2.0067	6.0213
H	-0.5003	3.5746	6.1150
C	-0.3490	-3.2762	8.0319
H	0.5296	-2.6057	8.0067
H	-0.3933	-3.7172	9.0439
H	-1.2670	-2.6749	7.8980
C	-0.2185	-5.7286	7.4762
H	0.7221	-6.2313	7.1830
H	-1.0725	-6.3041	7.0727
H	-0.2844	-5.7747	8.5775
O	0.1951	-5.4158	0.4109
C	0.2794	-6.0940	-0.5825
H	0.3243	-7.1833	-0.5106
H	0.3138	-5.6504	-1.5829

SCF = -412.965358**30-OCH2**

H	1.3715	-0.1403	1.3641
C	0.5248	0.2274	1.9503
C	-1.6410	1.2100	3.4454
C	-0.5903	-0.5627	2.2143
C	0.5541	1.5372	2.4471
C	-0.5263	2.0238	3.1949
C	-1.6775	-0.0994	2.9490
H	1.4286	2.1649	2.2378
H	-2.4918	1.5880	4.0263
C	0.9121	-2.8318	4.0481
C	-0.4462	-5.1510	4.8853
C	-0.1001	-3.4066	3.2912
C	1.2460	-3.4415	5.2656
C	0.5677	-4.5957	5.6806
C	-0.7922	-4.5504	3.6675
H	2.0424	-2.9988	5.8768
H	-1.5776	-4.9952	3.0420
H	-0.9794	-6.0556	5.2053
I	-0.6446	-2.5217	1.4452
C	-0.5223	3.4330	3.7502
C	0.9089	-5.2746	6.9903
F	-0.6264	3.4727	5.0870
F	-1.5421	4.1814	3.3059
F	0.5682	4.1622	3.4809
F	1.8783	-4.6965	7.7107
F	-0.1312	-5.3528	7.8327
F	1.3194	-6.5420	6.8356
H	-2.5545	-0.7236	3.1453
H	1.4491	-1.9341	3.7309
O	-0.7305	-5.1438	0.8843
C	-0.2424	-5.8525	0.0360
H	-0.4514	-6.9250	0.0254
H	0.4166	-5.4515	-0.7411

SCF = -413.446364

30-Cl

H	1.3831	-0.4403	1.2226
C	0.5607	-0.0911	1.8493
C	-1.5441	0.8355	3.4454
C	-0.5173	-0.9163	2.1443
C	0.5977	1.2147	2.3575
C	-0.4556	1.6727	3.1585
C	-1.5717	-0.4661	2.9294
H	1.4473	1.8568	2.1193
H	-2.3706	1.1897	4.0649
C	0.9320	-2.9181	4.0109
C	-0.5200	-5.0446	5.1489
C	-0.0916	-3.5590	3.3220
C	1.2230	-3.3520	5.3088
C	0.4954	-4.4114	5.8752
C	-0.8233	-4.6144	3.8486
H	2.0233	-2.8606	5.8697
H	-1.6069	-5.1284	3.2743
H	-1.0868	-5.8805	5.5698
I	-0.5544	-2.9310	1.3477
Cl	-0.5217	-5.4400	0.8531
C	-0.4512	3.0669	3.7292
C	0.8400	-4.8480	7.2770
F	-0.4946	3.1061	5.0727
F	-1.5002	3.8175	3.3508
F	0.6097	3.8325	3.4268
F	0.7098	-3.8728	8.1928
F	0.1128	-5.8566	7.7802
F	2.1091	-5.2635	7.4207
H	-2.4248	-1.1096	3.1506
H	1.5050	-2.0985	3.5694

SCF = -759.387616**31-Cl**

H	1.6003	-0.5195	2.6545
C	0.5694	-0.1623	2.6823
C	-2.0732	0.7795	2.7423
C	-0.4659	-0.9196	2.1473
C	0.2914	1.0803	3.2646
C	-1.0331	1.5465	3.2930
C	-1.7787	-0.4617	2.1661
H	1.0949	1.6830	3.6893
H	-3.0984	1.1504	2.7616
C	1.3041	-4.3420	3.5007
C	-0.6257	-3.7436	5.4668
C	0.1887	-3.5598	3.2243
C	1.4582	-4.8328	4.8031
C	0.4968	-4.5300	5.7814
C	-0.7871	-3.2536	4.1669
H	2.3221	-5.4557	5.0497
H	-1.6630	-2.6488	3.9178
H	-1.3734	-3.5200	6.2312
I	-0.0335	-2.8382	1.2431
Cl	0.5545	-5.2461	0.6057
H	-2.5877	-1.0536	1.7342
H	2.0447	-4.5972	2.7298
C	-1.3269	2.8190	3.8882
N	-1.5640	3.8435	4.3681
C	0.6586	-5.0304	7.1166
N	0.7892	-5.4315	8.1923

SCF = -758.768219

31-OCH2

H	1.6086	-0.0374	2.7695
C	0.5541	0.2548	2.7855
C	-2.1515	1.0314	2.8234
C	-0.4404	-0.5468	2.2299
C	0.1872	1.4690	3.3760
C	-1.1640	1.8548	3.3940
C	-1.7862	-0.1830	2.2354
H	0.9517	2.1175	3.8191
H	-3.2020	1.3426	2.8367
C	1.3576	-4.2405	3.3043
C	-0.6007	-3.9372	5.3107
C	0.2585	-3.4040	3.1455
C	1.4763	-4.9452	4.5079
C	0.5005	-4.7908	5.5077
C	-0.7288	-3.2317	4.1098
H	2.3307	-5.6132	4.6679
H	-1.5876	-2.5722	3.9597
H	-1.3581	-3.8255	6.0951
I	0.1090	-2.3570	1.3147
H	-2.5583	-0.8160	1.7890
H	2.1128	-4.3705	2.5176
C	-1.5410	3.1009	3.9997
N	-1.8444	4.1026	4.4874
C	0.6266	-5.5125	6.7420
N	0.7281	-6.0934	7.7347
O	0.9518	-4.7862	0.5351
C	0.5871	-5.5992	-0.2808
H	1.1326	-6.5376	-0.4073
H	-0.2897	-5.4277	-0.9137

SCF = -412.827314**32-Cl**

H	1.6353	-0.5476	2.8639
C	0.6058	-0.1842	2.8730
C	-2.0253	0.7647	2.8992
C	-0.4104	-0.9215	2.2746
C	0.3224	1.0317	3.4945
C	-1.0052	1.5246	3.5231
C	-1.7186	-0.4494	2.2857
H	1.1288	1.5874	3.9650
H	-3.0542	1.1140	2.9030
C	1.3787	-4.4375	3.4770
C	-0.4771	-3.8623	5.5104
C	0.2870	-3.6005	3.2554
C	1.5476	-4.9903	4.7431
C	0.6260	-4.7128	5.7863
C	-0.6475	-3.3092	4.2444
H	2.4011	-5.6433	4.9179
H	-1.5020	-2.6563	4.0482
H	-1.2008	-3.6265	6.2876
I	0.0341	-2.7933	1.3218
Cl	0.6372	-5.1833	0.5199
H	-2.5205	-1.0203	1.8139
H	2.0927	-4.6770	2.6785
N	-1.3305	2.6877	4.2738
N	0.8724	-5.1687	7.1017
C	-2.5898	3.3937	3.9105
H	-2.7895	4.1910	4.6452
H	-3.4391	2.6895	3.9645
H	-2.5703	3.8417	2.9046
C	-0.2237	3.6436	4.5511
H	0.1799	4.1269	3.6475
H	0.6000	3.1171	5.0657
H	-0.5788	4.4285	5.2389
C	1.7613	-6.3504	7.2632
H	2.7323	-6.1577	6.7721
H	1.3371	-7.2782	6.8457
H	1.9719	-6.5124	8.3333
C	-0.2753	-5.1936	8.0474
H	0.0856	-5.4386	9.0603
H	-1.0562	-5.9201	7.7704
H	-0.7328	-4.1896	8.1063

SCF = -758.879749

32-OCH2

H	1.7043	-0.0086	2.3138
C	0.6813	0.2985	2.5461
C	-1.9545	1.0720	3.1429
C	-0.4012	-0.5398	2.2504
C	0.4603	1.5313	3.1310
C	-0.8708	1.9597	3.4444
C	-1.7130	-0.1570	2.5580
H	1.3093	2.1748	3.3485
H	-2.9784	1.3592	3.3695
C	1.4311	-3.5824	3.6322
C	-0.8238	-4.8037	4.7904
C	0.1610	-3.4616	3.0567
C	1.5889	-4.3333	4.7823
C	0.4626	-4.9686	5.4012
C	-0.9671	-4.0499	3.6403
H	2.5797	-4.4237	5.2228
H	-1.9588	-3.9246	3.1966
H	-1.7052	-5.2592	5.2371
I	-0.0610	-2.3579	1.3080
H	-2.5540	-0.8186	2.3350
H	2.3003	-3.0944	3.1822
N	-1.1004	3.1819	4.0244
N	0.6151	-5.7317	6.5303
C	-2.4698	3.6507	4.3312
H	-2.4526	4.6484	4.8039
H	-2.9753	2.9639	5.0350
H	-3.0798	3.7327	3.4123
C	0.0039	4.1212	4.3196
H	0.5331	4.4194	3.3954
H	0.7325	3.6692	5.0178
H	-0.3741	5.0439	4.7937
C	1.9263	-5.8690	7.2024
H	2.2913	-4.8951	7.5782
H	2.6811	-6.2916	6.5136
H	1.8597	-6.5521	8.0680
C	-0.5442	-6.3504	7.2106
H	-0.2209	-6.9547	8.0770
H	-1.0876	-7.0288	6.5271
H	-1.2475	-5.5845	7.5871
O	0.3961	-4.8244	0.2883
C	0.6117	-5.8611	0.8633
H	0.7755	-6.7831	0.3024
H	0.6514	-5.9192	1.9594

SCF = -412.973929**33-OCH2**

I	-1.4581	0.7857	-3.6263
C	-0.7784	0.3338	-1.6970
C	0.1715	-0.1783	0.8789
N	-1.0441	-0.8643	-1.0818
C	-0.0233	1.2999	-1.0167
C	0.4554	1.0527	0.2708
C	-0.5795	-1.1289	0.1919
H	0.1909	2.2611	-1.5080
H	1.0464	1.8100	0.8024
H	0.5352	-0.4006	1.8912
C	-1.8388	-1.9012	-1.7776
H	-1.3526	-2.2122	-2.7302
H	-2.8539	-1.5249	-2.0397
H	-1.9745	-2.8125	-1.1656
H	-0.8171	-2.1048	0.6465
O	-2.2596	1.4155	-6.0019
C	-1.9772	2.4909	-6.4700
H	-1.3807	3.2240	-5.9093
H	-2.3163	2.7600	-7.4794

SCF = -412.491826**33-Cl**

I	-1.3868	1.1733	-3.4730
Cl	-2.1380	1.9758	-5.8178
C	-0.7444	0.4610	-1.4535
C	0.0947	-0.3376	1.0852
N	-0.9399	-0.8095	-1.0289
C	-0.1091	1.3819	-0.5953
C	0.3109	0.9963	0.6654
C	-0.5293	-1.2311	0.2349
H	0.0410	2.4068	-0.9560
H	0.8039	1.7010	1.3382
H	0.4194	-0.6593	2.0763
C	-1.6060	-1.7886	-1.9193
H	-1.0420	-1.8977	-2.8726
H	-2.6201	-1.4303	-2.2060
H	-1.7057	-2.7825	-1.4586
H	-0.7145	-2.2709	0.5229

SCF = -758.393009

34-Cl

I	-1.4593	1.1952	-3.4116
Cl	-2.3216	1.9148	-5.7736
C	-0.7476	0.5653	-1.4412
C	0.1178	-0.3445	1.0403
C	-0.9223	-0.7601	-1.0799
C	-0.1352	1.4558	-0.5618
C	0.3004	0.9960	0.6881
N	-0.4893	-1.2059	0.1562
H	-1.4033	-1.4828	-1.7570
H	0.0027	2.5055	-0.8486
H	0.7836	1.6726	1.3971
H	0.4502	-0.7262	2.0118
H	-0.1606	-3.2950	-0.1850
C	-0.6833	-2.6261	0.5282
H	-0.2985	-2.8552	1.5381
H	-1.7593	-2.8933	0.5154

SCF = -758.378225**34-OCH2**

I	-1.5123	0.7390	-3.6052
C	-0.8370	0.3826	-1.6754
C	0.0384	-0.1965	0.9058
C	-0.9393	-0.9098	-1.1597
C	-0.2888	1.4007	-0.8881
C	0.1495	1.1034	0.4084
N	-0.5035	-1.1875	0.1188
H	-1.3688	-1.7358	-1.7581
H	-0.2010	2.4255	-1.2784
H	0.5834	1.8874	1.0447
H	0.3775	-0.4505	1.9237
H	-0.0541	-3.2868	0.0148
C	-0.6244	-2.5674	0.6407
H	-0.2393	-2.6662	1.6753
H	-1.6842	-2.9004	0.6583
O	-2.3408	1.2419	-6.0488
C	-2.1526	2.3249	-6.5418
H	-2.4974	2.5386	-7.5623
H	-1.6358	3.1245	-5.9931

SCF = -412.493150**35-OCH2**

I	-1.7654	1.1437	-3.2705
C	-0.8836	0.5676	-1.4819
N	0.2593	-0.2033	0.9514
C	-0.9861	-0.7535	-1.0299
C	-0.1922	1.4931	-0.6912
C	0.3761	1.0997	0.5224
C	-0.4121	-1.1304	0.1861
H	-1.5232	-1.5100	-1.6244
H	-0.0913	2.5418	-1.0130
H	0.9230	1.8183	1.1554
H	-0.4857	-2.1673	0.5544
H	1.9213	-0.9543	2.0807
C	0.8742	-0.6137	2.2330
H	0.8972	0.2155	2.9696
H	0.3203	-1.4456	2.7146
O	-2.8218	1.8667	-5.5783
C	-2.1309	1.9681	-6.5596
H	-1.0512	1.7666	-6.5257
H	-2.5695	2.2676	-7.5207

SCF = -412.491867**35-Cl**

I	-1.4534	1.0388	-3.4121
Cl	-2.3589	1.7013	-5.7787
C	-0.6995	0.4870	-1.4424
N	0.2641	-0.2199	1.0811
C	-0.7960	-0.8304	-0.9822
C	-0.1081	1.4430	-0.6081
C	0.3715	1.0884	0.6493
C	-0.3146	-1.1807	0.2770
H	-1.2555	-1.5976	-1.6184
H	-0.0213	2.4831	-0.9479
H	0.8379	1.8197	1.3194
H	-0.3810	-2.2071	0.6555
H	1.8633	-0.3735	2.4999
C	0.7783	-0.5819	2.4211
H	0.2585	-0.0091	3.2140
H	0.6342	-1.6552	2.6449

SCF = -758.374507

36-OCH2

N	-0.4430	0.6404	-0.2483
C	-0.4419	1.9169	-0.7856
N	-0.2554	2.7959	0.2684
C	-0.2617	0.7214	1.1360
H	-0.2254	-0.1403	1.7920
C	-0.1441	2.0722	1.4597
H	0.0070	2.5276	2.4314
I	-0.6480	2.4196	-2.7881
H	0.6234	4.5593	-0.5590
C	-0.1807	4.2556	0.1470
H	0.0340	4.7319	1.1235
H	-1.1362	4.6764	-0.2326
H	0.1615	-0.6750	-1.8201
C	-0.6034	-0.5987	-1.0162
H	-0.4984	-1.4915	-0.3691
H	-1.6031	-0.6455	-1.4982
O	-0.9680	3.0484	-5.2634
C	-2.0772	3.1516	-5.7269
H	-2.2101	3.4209	-6.7835
H	-2.9749	2.9820	-5.1159

SCF = -412.508791**36-Cl**

N	-0.3490	0.5845	-0.1692
C	-0.5894	1.8564	-0.6371
N	-0.3551	2.7129	0.4145
C	0.0396	0.6395	1.1879
H	0.2800	-0.2330	1.7689
C	0.0357	1.9753	1.5543
H	0.2717	2.4305	2.4996
I	-1.2342	2.4170	-2.7002
H	-0.8061	4.5082	-0.6415
C	-0.4867	4.1735	0.3735
H	0.4764	4.6656	0.5990
H	-1.2467	4.5242	1.0946
H	0.4915	-1.1863	-1.0038
C	-0.4737	-0.6516	-0.9495
H	-1.2325	-1.3239	-0.5102
H	-0.7914	-0.4234	-1.9942
Cl	-1.9802	3.0626	-5.0893

SCF = -758.414313**37-OCH2**

N	-0.4047	0.5933	-0.2611
C	-0.7303	1.8608	-0.7121
N	-0.5080	2.7420	0.3318
C	0.0360	0.6783	1.0657
C	-0.0430	2.0274	1.4433
I	-1.4477	2.3452	-2.6109
H	-0.8633	4.5476	-0.7706
C	-0.7413	4.1899	0.2763
H	0.1038	4.7603	0.7154
H	-1.6689	4.4678	0.8245
H	0.4879	-0.9753	-1.4074
C	-0.5107	-0.6360	-1.0558
H	-0.9723	-1.4627	-0.4753
H	-1.1474	-0.4891	-1.9579
C	0.4927	-0.5039	1.8790
C	0.2949	2.6580	2.7685
F	1.1446	-0.1724	2.9947
F	1.3296	-1.3155	1.2193
F	-0.5202	-1.2849	2.2714
F	1.4337	3.3598	2.7308
F	-0.6348	3.5172	3.2054
F	0.4464	1.7808	3.7618
O	-2.2623	2.9347	-4.9401
C	-1.4803	3.2835	-5.7924
H	-1.8439	3.5344	-6.7985
H	-0.4023	3.3588	-5.5912

SCF = -412.987317**37-Cl**

N	-0.3133	0.5830	-0.1908
C	-0.5596	1.8586	-0.6432
N	-0.3725	2.7154	0.4166
C	0.0467	0.6296	1.1717
C	-0.0136	1.9745	1.5614
I	-1.1632	2.4410	-2.7547
H	-0.6249	4.4863	-0.7389
C	-0.5197	4.1742	0.3292
H	0.3618	4.7000	0.7392
H	-1.4305	4.5210	0.8548
H	0.5639	-1.0476	-1.2601
C	-0.4302	-0.6210	-1.0240
H	-1.0549	-1.3943	-0.5408
H	-0.9125	-0.3673	-2.0000
Cl	-1.8455	3.0978	-5.1375
C	0.4118	-0.5598	2.0023
C	0.2473	2.5591	2.9135
F	1.3563	-0.3139	2.9196
F	0.8979	-1.6109	1.3239
F	-0.6223	-1.0611	2.6922
F	1.5451	2.8033	3.1429
F	-0.3591	3.7299	3.1636
F	-0.1453	1.7786	3.9286

SCF = -758.909033**38-OCH2**

N	-0.0333	-0.9779	-0.9960
C	-0.6178	0.1647	-1.5146
N	-0.5541	1.1466	-0.5409
C	0.4101	-0.7152	0.3120
C	0.0818	0.6241	0.5989
I	-1.4609	0.3637	-3.4087
H	-2.1194	2.5109	-1.0534
C	-1.0701	2.5133	-0.6816
H	-0.4565	3.1002	-1.3992
H	-1.0648	3.0556	0.2867
H	0.8407	-2.1823	-2.5283
C	0.0993	-2.2570	-1.7033
H	0.4332	-3.0688	-1.0241
H	-0.8716	-2.5747	-2.1458
C	1.0619	-1.6623	1.1424
N	1.5940	-2.4244	1.8275
C	0.3218	1.3569	1.7892
N	0.5233	1.9435	2.7632
O	-2.4354	0.6217	-5.7380
C	-1.7384	0.9834	-6.6561
H	-0.6721	1.2107	-6.5169
H	-2.1698	1.0917	-7.6607

SCF = -412.369715**38-Cl**

N	0.0545	-0.9877	-0.8740
C	-0.4882	0.1441	-1.4389
N	-0.5104	1.1176	-0.4660
C	0.3840	-0.7317	0.4795
C	0.0270	0.5987	0.7373
I	-1.2070	0.3649	-3.5803
H	-1.3836	2.6413	-1.6729
C	-1.0098	2.4880	-0.6323
H	-0.2088	3.2298	-0.4513
H	-1.8485	2.6944	0.0593
H	-0.0871	-2.2131	-2.6114
C	0.2674	-2.2708	-1.5545
H	1.3409	-2.5387	-1.5754
H	-0.2926	-3.0850	-1.0568
Cl	-2.0164	0.6157	-6.0000
C	0.9631	-1.6884	1.3484
N	1.4358	-2.4666	2.0600
C	0.1495	1.3431	1.9359
N	0.2511	1.9474	2.9155

SCF = -758.292212**39-Cl**

N	-0.3452	0.5830	-0.1757
C	-0.5579	1.8581	-0.6462
N	-0.3364	2.7122	0.4090
C	0.0167	0.6270	1.1980
C	0.0222	1.9699	1.5669
I	-1.1463	2.4279	-2.7185
H	-0.7438	4.5006	-0.6758
C	-0.4531	4.1743	0.3500
H	0.5087	4.6580	0.5961
H	-1.2268	4.5376	1.0494
H	0.4874	-1.1871	-1.0174
C	-0.4725	-0.6429	-0.9731
H	-1.2444	-1.3106	-0.5512
H	-0.7714	-0.3979	-2.0190
Cl	-1.8300	3.0892	-5.1274
C	0.3107	-0.5789	1.9923
H	1.1597	-1.1461	1.5774
H	-0.5534	-1.2615	2.0362
H	0.5722	-0.3264	3.0319
C	0.3239	2.5985	2.8651
H	1.1816	3.2873	2.7974
H	0.5759	1.8480	3.6306
H	-0.5331	3.1741	3.2509

SCF = -758.445320**39-OCH2**

N	-0.1573	0.6214	-0.3399
C	-0.3024	1.9184	-0.8018
N	-0.2274	2.7505	0.3020
C	-0.0024	0.6333	1.0592
C	-0.0467	1.9775	1.4645
I	-0.5677	2.5036	-2.7752
H	-0.0578	4.6186	-0.7353
C	-0.3292	4.2143	0.2642
H	0.3538	4.6785	1.0029
H	-1.3629	4.5443	0.4932
H	0.5444	-1.3376	-0.8049
C	-0.1715	-0.5808	-1.1818
H	-1.1817	-1.0383	-1.1999
H	0.1148	-0.3499	-2.2311
C	0.1731	-0.5816	1.8699
H	1.1477	-1.0689	1.6868
H	-0.6123	-1.3345	1.6840
H	0.1381	-0.3626	2.9525
C	0.0700	2.5509	2.8141
H	1.0105	3.1151	2.9484
H	0.0670	1.7691	3.5951
H	-0.7620	3.2332	3.0602
O	-0.9817	3.2328	-5.2267
C	-2.1086	3.3645	-5.6356
H	-2.9797	3.1822	-4.9907
H	-2.2873	3.6733	-6.6743

SCF = -412.545070

40-OCH2

N	0.0656	-0.9615	-1.1385
C	-0.1924	0.2752	-1.7206
N	-0.2466	1.2096	-0.7065
C	0.2012	-0.7929	0.2537
C	-0.0050	0.5699	0.5304
I	-0.4252	0.6383	-3.7498
H	-1.5308	2.7815	-1.3766
C	-0.5550	2.6345	-0.8688
H	0.2247	3.1454	-1.4709
H	-0.6136	3.1306	0.1233
H	1.1608	-2.1664	-2.5252
C	0.2744	-2.2230	-1.8596
H	0.4413	-3.0534	-1.1404
H	-0.6092	-2.4751	-2.4805
O	0.5270	-1.8629	1.0043
O	-0.0939	1.2422	1.6962
C	1.2025	1.6304	2.2679
H	1.8138	0.7446	2.4603
H	0.8821	2.1092	3.2051
H	1.7070	2.3404	1.6087
C	-0.2107	-1.9698	2.2706
H	-0.1279	-1.0433	2.8477
H	0.3264	-2.7993	2.7544
H	-1.2520	-2.2315	2.0606
O	-0.7887	1.0774	-6.2702
C	-1.8906	0.9692	-6.7488
H	-2.0478	1.1545	-7.8199
H	-2.7588	0.6861	-6.1373

SCF = -412.620217

40-Cl

N	-0.0570	-1.0546	-0.9811
C	-0.5038	0.1267	-1.5435
N	-0.4872	1.0830	-0.5566
C	0.2733	-0.8306	0.3788
C	-0.0107	0.5075	0.6541
I	-1.1306	0.4193	-3.6619
H	-1.9587	2.5021	-1.1536
C	-0.9430	2.4704	-0.7066
H	-0.2686	3.0299	-1.3847
H	-0.9742	2.9772	0.2750
H	0.9487	-2.2261	-2.4501
C	0.1379	-2.3201	-1.7002
H	0.3996	-3.1305	-0.9956
H	-0.7875	-2.5986	-2.2457
Cl	-1.8559	0.7654	-6.1202
O	0.8009	-1.8415	1.1128
O	0.0270	1.2150	1.8100
C	1.3594	1.7315	2.1326
H	2.0645	0.9036	2.2450
H	1.1730	2.2363	3.0880
H	1.6841	2.4357	1.3630
C	0.1227	-2.0489	2.3941
H	0.1128	-1.1191	2.9726
H	0.7616	-2.8096	2.8585
H	-0.8885	-2.4240	2.2153

SCF = -758.521858

7.4 ONIOM(DFT:PM7)

1-OCH2

H	3.1962	0.2681	-1.1340
C	2.4235	0.1838	-0.3699
C	0.4462	0.0174	1.5961
C	1.9629	-1.0540	0.0717
C	1.8830	1.3446	0.1824
C	0.8960	1.2632	1.1628
C	0.9785	-1.1510	1.0519
H	2.2364	2.3182	-0.1552
H	0.6153	-2.1160	1.4054
H	-0.3239	-0.0466	2.3639
I	2.7716	-2.8152	-0.7605
H	0.4775	2.1726	1.5911
O	3.4070	-5.2970	-2.4472
C	2.5710	-5.2977	-3.3056
H	2.5396	-6.0845	-4.0711
H	1.8038	-4.5118	-3.3593

SCF = -412.729000

1-Cl

H	2.7035	0.0415	-1.4679
C	2.1153	0.0483	-0.5533
C	0.6075	0.0927	1.7932
C	1.6762	-1.1333	0.0257
C	1.7953	1.2656	0.0501
C	1.0416	1.2889	1.2231
C	0.9258	-1.1263	1.1923
H	2.1330	2.1965	-0.3934
H	0.5821	-2.0533	1.6452
H	0.0210	0.1110	2.7059
I	2.1878	-3.0889	-0.9428
Cl	2.7997	-5.4330	-2.1071
H	0.7937	2.2348	1.6906

SCF = -758.500155**2-Cl**

H	0.3740	0.1620	0.0726
C	0.2310	0.1442	1.1513
C	-0.1365	0.0977	3.9238
C	0.3426	-1.0402	1.8648
C	-0.0685	1.3249	1.8260
C	-0.2528	1.3008	3.2149
C	0.1633	-1.0776	3.2399
H	-0.1604	2.2624	1.2840
H	0.2536	-2.0123	3.7898
H	-0.2808	0.0881	5.0010
I	0.8319	-2.9860	0.7420
Cl	1.3860	-5.1819	-0.5249
C	-0.5591	2.4998	3.9062
N	-0.8098	3.4807	4.4716

SCF = -758.461389**2-OCH2**

H	0.3157	0.0086	0.1172
C	0.1918	0.0385	1.2006
C	-0.1332	0.1549	3.9786
C	0.2929	-1.1126	1.9799
C	-0.0739	1.2585	1.8172
C	-0.2360	1.3160	3.2054
C	0.1325	-1.0660	3.3636
H	-0.1555	2.1678	1.2189
H	0.2102	-1.9647	3.9789
H	-0.2610	0.2057	5.0618
I	0.6969	-2.9616	1.0479
C	-0.5067	2.5621	3.8332
N	-0.7270	3.5771	4.3438
O	1.3276	-5.3062	-0.7716
C	1.4637	-4.8781	-1.8825
H	1.6969	-5.5421	-2.7257
H	1.3604	-3.8052	-2.0999

SCF = -412.678490**3-Cl**

H	0.3870	0.1545	0.0690
C	0.2397	0.1403	1.1466
C	-0.1367	0.0864	3.9229
C	0.3475	-1.0441	1.8613
C	-0.0610	1.3210	1.8169
C	-0.2487	1.2862	3.2061
C	0.1646	-1.0847	3.2362
H	-0.1521	2.2648	1.2789
H	0.2536	-2.0217	3.7813
H	-0.2859	0.0817	5.0028
I	0.8404	-3.0215	0.7203
Cl	1.3790	-5.1837	-0.5262
N	-0.5627	2.5036	3.9085
O	-0.6585	3.5478	3.2743
O	-0.7252	2.4642	5.1225

SCF = -758.522418**3-OCH2**

H	0.2903	0.0252	0.1133
C	0.1747	0.0474	1.1980
C	-0.1289	0.1387	3.9840
C	0.2831	-1.1102	1.9684
C	-0.0875	1.2634	1.8229
C	-0.2368	1.2980	3.2117
C	0.1333	-1.0750	3.3545
H	-0.1761	2.1838	1.2346
H	0.2169	-1.9792	3.9616
H	-0.2498	0.1865	5.0725
I	0.6822	-2.9515	1.0187
N	-0.5104	2.5693	3.8673
O	-0.5990	3.5675	3.1713
O	-0.6376	2.5750	5.0806
O	1.3107	-5.2998	-0.7763
C	1.4779	-4.9072	-1.8962
H	1.7182	-5.5997	-2.7140
H	1.3971	-3.8398	-2.1473

SCF = -412.734336

4-OCH2

H	1.2674	0.5569	0.2279
C	0.8265	0.3831	1.2099
C	-0.3064	-0.0127	3.7311
C	0.7866	-0.8878	1.7779
C	0.2924	1.4599	1.9135
C	-0.2772	1.2685	3.1752
C	0.2254	-1.0961	3.0349
H	0.3215	2.4565	1.4763
H	0.1929	-2.0865	3.4898
H	-0.7453	-0.1690	4.7151
I	1.5896	-2.5225	0.7172
C	-0.8331	2.4286	3.9273
H	-1.5915	2.1290	4.6637
H	-0.0363	2.9529	4.4787
H	-1.3061	3.1660	3.2634
O	2.0991	-4.9516	-1.0943
C	1.0431	-5.1524	-1.6237
H	0.9113	-5.9735	-2.3410
H	0.1667	-4.5231	-1.4120

SCF = -412.744595**4-Cl**

H	0.3918	0.1511	0.0638
C	0.2426	0.1233	1.1414
C	-0.1444	0.0812	3.9031
C	0.3495	-1.0645	1.8490
C	-0.0618	1.3032	1.8211
C	-0.2573	1.2846	3.2036
C	0.1600	-1.0981	3.2224
H	-0.1463	2.2361	1.2744
H	0.2443	-2.0294	3.7789
H	-0.2933	0.0631	4.9772
I	0.8303	-2.9559	0.7577
Cl	1.4080	-5.2388	-0.5583
C	-0.5702	2.5503	3.9350
H	-1.1982	2.3710	4.8163
H	0.3542	3.0332	4.2815
H	-1.1006	3.2718	3.3015

SCF = -758.514529**5-Cl**

H	-0.2056	-0.1009	0.0105
C	-0.1118	-0.0275	1.0924
C	0.1239	0.1770	3.8709
C	0.3499	-1.0971	1.8451
C	-0.4624	1.1618	1.7300
C	-0.3436	1.2605	3.1208
C	0.4719	-1.0083	3.2233
H	-0.8248	2.0040	1.1523
H	0.8352	-1.8494	3.8111
H	0.2106	0.2708	4.9497
I	0.9061	-3.0106	0.8099
Cl	1.5645	-5.2964	-0.4259
N	-0.6850	2.4537	3.8685
C	-2.1225	2.7742	3.7235
C	0.1628	3.5953	3.4593
H	-2.4269	3.0545	2.7048
H	-2.3734	3.5974	4.4093
H	-2.7109	1.8912	4.0276
H	0.0073	3.9313	2.4239
H	-0.0265	4.4393	4.1396
H	1.2215	3.3036	3.5710

SCF = -758.498259**5-OCH2**

H	1.8773	0.2495	0.5035
C	1.1731	0.1930	1.3360
C	-0.6234	0.0953	3.4695
C	0.7541	-1.0314	1.8493
C	0.6923	1.3742	1.8858
C	-0.2111	1.3491	2.9697
C	-0.1394	-1.0827	2.9157
H	1.0341	2.3187	1.4724
H	-0.4734	-2.0352	3.3323
H	-1.3175	0.0330	4.3027
I	1.4762	-2.8185	1.0057
N	-0.5911	2.5362	3.6124
C	-1.8102	2.4878	4.4369
C	-0.4818	3.7811	2.8334
H	-2.6988	2.1437	3.8833
H	-2.0257	3.4844	4.8571
H	-1.6406	1.8147	5.2978
H	-1.0435	3.7542	1.8858
H	-0.8433	4.6360	3.4288
H	0.5836	3.9803	2.6137
O	1.9475	-5.3248	-0.7452
C	1.0819	-5.2458	-1.5699
H	0.9727	-6.0040	-2.3569
H	0.3647	-4.4123	-1.5706

SCF = -412.728879

6-Cl

H	0.2966	0.1573	0.0731
C	0.2139	0.0870	1.1574
C	-0.0003	-0.0852	3.9491
C	0.3612	-1.1311	1.8087
C	-0.0427	1.2388	1.8960
C	-0.1455	1.1314	3.2896
C	0.2572	-1.2290	3.1847
H	-0.1623	2.2038	1.4189
H	0.3726	-2.1859	3.6921
H	-0.0811	-0.1630	5.0238
I	0.7805	-2.9749	0.6068
Cl	1.2869	-5.1920	-0.8303
O	-0.3980	2.3367	3.8916
C	-0.5142	2.3325	5.3042
H	0.4200	2.0054	5.7709
H	-1.3561	1.7107	5.6238
H	-0.7080	3.3877	5.5306

SCF = -758.562840**6-OCH2**

H	0.4875	-0.0461	0.1436
C	0.3537	-0.0653	1.2266
C	0.0074	-0.0898	4.0125
C	0.4860	-1.2501	1.9554
C	0.0471	1.1146	1.8873
C	-0.1237	1.0908	3.2823
C	0.3158	-1.2697	3.3355
H	-0.0622	2.0533	1.3484
H	0.4183	-2.1927	3.9102
H	-0.1246	-0.1077	5.0893
I	0.9545	-3.0372	0.9437
O	-0.4192	2.3123	3.7956
C	-0.6049	2.3992	5.2024
H	0.3102	2.1238	5.7358
H	-1.4565	1.7913	5.5231
H	-0.8224	3.4677	5.3395
O	1.4645	-5.2911	-1.0746
C	1.1893	-4.8122	-2.1379
H	1.2711	-5.3952	-3.0650
H	0.8446	-3.7718	-2.2261

SCF = -412.792095**7-Cl**

H	0.9727	0.3805	0.5251
C	0.4415	0.1329	1.4416
C	-0.9305	-0.4862	3.7950
C	0.2877	-1.1852	1.8449
C	-0.0930	1.1572	2.2240
C	-0.7745	0.8411	3.3983
C	-0.3935	-1.5067	3.0096
H	0.0268	2.1914	1.9081
H	-0.5154	-2.5423	3.3200
H	-1.4668	-0.7378	4.7075
I	1.1691	-2.8471	0.5778
Cl	2.1928	-4.7836	-0.8976
S	-1.4874	2.1421	4.3769
C	-0.1449	2.4975	5.5664
H	-0.4820	3.2924	6.2367
H	0.7624	2.8300	5.0538
H	0.1015	1.6145	6.1631

SCF = -758.505563**7-OCH2**

H	2.0912	0.1814	1.7159
C	1.2038	-0.1306	2.2685
C	-1.0666	-0.8824	3.7111
C	0.6879	-1.4176	2.1546
C	0.5758	0.7872	3.1107
C	-0.5572	0.4141	3.8301
C	-0.4437	-1.8020	2.8718
H	0.9933	1.7908	3.1878
H	-0.8541	-2.8099	2.7933
H	-1.9522	-1.1944	4.2693
I	1.6293	-2.8055	0.8790
S	-1.4332	1.4923	4.9213
C	-0.5259	3.0667	4.8869
H	-1.0406	3.7600	5.5666
H	-0.5163	3.5218	3.8907
H	0.5065	2.9613	5.2376
O	2.5345	-4.5740	-1.4536
C	1.8264	-4.2580	-2.3671
H	1.9200	-4.7334	-3.3526
H	1.0568	-3.4809	-2.2536

SCF = -412.731441

8-Cl

H	0.5626	0.1654	0.1016
C	0.3401	0.1301	1.1659
C	-0.2327	0.0482	3.9016
C	0.3516	-1.0722	1.8574
C	0.0386	1.3075	1.8463
C	-0.2478	1.2629	3.2144
C	0.0700	-1.1264	3.2138
H	0.0271	2.2546	1.3109
H	0.0816	-2.0733	3.7494
H	-0.4532	0.0004	4.9653
I	0.8430	-3.0143	0.7304
Cl	1.3983	-5.2073	-0.5415
C	-0.5680	2.5432	3.9094
F	-0.8347	2.4610	5.2151
F	0.4040	3.4601	3.8507
F	-1.6328	3.1858	3.4173

SCF = -758.765884**9-OCH2**

H	0.3057	-0.0339	0.0975
C	0.1908	0.0118	1.1809
C	-0.1122	0.1725	3.9613
C	0.2983	-1.1269	1.9766
C	-0.0707	1.2441	1.7802
C	-0.2177	1.3034	3.1607
C	0.1494	-1.0589	3.3604
H	-0.1556	2.1379	1.1604
H	0.2322	-1.9474	3.9892
H	-0.2295	0.2296	5.0448
I	0.6946	-2.9894	1.0705
Br	-0.5730	2.9784	3.9764
O	1.3242	-5.3397	-0.7635
C	1.4589	-4.8807	-1.8622
H	1.6920	-5.5207	-2.7237
H	1.3542	-3.8023	-2.0496

SCF = -412.722471**8-OCH2**

H	1.2930	0.5393	0.2707
C	0.8340	0.3717	1.2463
C	-0.3448	-0.0105	3.7557
C	0.7484	-0.9021	1.8052
C	0.3230	1.4596	1.9506
C	-0.2656	1.2650	3.2013
C	0.1655	-1.1028	3.0540
H	0.3893	2.4599	1.5145
H	0.0984	-2.0961	3.5010
H	-0.7995	-0.1791	4.7347
I	1.5155	-2.5541	0.7407
C	-0.8055	2.4652	3.9238
F	-1.3619	2.2253	5.1101
F	0.1180	3.3941	4.1766
F	-1.7530	3.1127	3.2431
O	2.0672	-4.9451	-1.0469
C	1.0674	-5.1639	-1.6703
H	1.0144	-5.9892	-2.3930
H	0.1660	-4.5473	-1.5424

SCF = -412.983088**9-Cl**

H	0.3246	0.1470	0.0642
C	0.2040	0.1316	1.1456
C	-0.1083	0.1026	3.9295
C	0.3400	-1.0460	1.8639
C	-0.0931	1.3200	1.8184
C	-0.2422	1.2745	3.1978
C	0.1888	-1.0769	3.2413
H	-0.2017	2.2472	1.2642
H	0.2976	-2.0058	3.7975
H	-0.2287	0.0881	5.0084
I	0.8222	-2.9800	0.7512
Cl	1.3779	-5.1995	-0.5262
Br	-0.6498	2.8961	4.1298

SCF = -758.500824

10-OCH2

C	0.2011	-0.3774	0.9972
C	-0.1085	0.0606	3.7601
C	0.1086	-1.4662	1.8736
C	0.1385	0.9294	1.4997
C	-0.0161	1.1494	2.8790
C	-0.0460	-1.2473	3.2539
I	0.4373	-0.6911	-1.0865
C	0.1677	-2.8079	1.3990
N	0.2159	-3.8965	1.0120
C	-0.1394	-2.3559	4.1438
N	-0.2151	-3.2558	4.8659
C	-0.2644	0.2818	5.1568
N	-0.3911	0.4619	6.2920
C	-0.0788	2.4799	3.3840
N	-0.1295	3.5605	3.7922
C	0.2296	2.0552	0.6312
N	0.3052	2.9590	-0.0865
O	0.7728	-0.3525	-3.9895
C	0.8055	0.8200	-4.2409
H	0.9257	1.1771	-5.2722
H	0.7165	1.5774	-3.4481

SCF = -412.441795**11-OCH2**

C	0.0004	-0.2590	1.1100
C	-0.0003	-0.0474	3.8808
C	-0.0003	-1.4289	1.8714
C	0.0008	1.0049	1.7119
C	0.0004	1.1133	3.1044
C	-0.0007	-1.3036	3.2616
F	-0.0014	-2.3688	4.0388
F	-0.0007	0.0377	5.1951
F	0.0007	2.2971	3.6783
F	0.0015	2.0896	0.9646
F	0.0008	-0.3090	-0.2083
I	-0.0008	-3.3234	0.9472
O	-0.0011	-5.6560	-0.9172
C	-0.0001	-5.2367	-2.0404
H	-0.0002	-5.9166	-2.9026
H	0.0010	-4.1566	-2.2476

SCF = -413.071041**11-DMF**

C	0.1265	0.5451	2.2512
C	0.6779	0.0623	4.9311
C	0.2683	-0.7761	2.6778
C	0.2557	1.6189	3.1401
C	0.5327	1.3783	4.4875
C	0.5451	-0.9992	4.0272
F	0.6914	-2.2229	4.4969
F	0.9394	-0.1813	6.1989
F	0.6557	2.3816	5.3301
F	0.1158	2.8545	2.7052
F	-0.1354	0.8255	0.9888
I	0.0683	-2.3844	1.3209
O	-0.2455	-4.4443	-0.6999
C	-0.4490	-4.8446	-1.8324
H	-0.4871	-5.9179	-2.0584
N	-0.6456	-4.0760	-2.9112
C	-0.6316	-2.6316	-2.8160
H	0.1579	-2.2247	-3.4477
H	-0.4561	-2.3466	-1.7864
H	-1.5878	-2.2284	-3.1492
C	-0.8766	-4.6462	-4.2173
H	-0.1022	-4.3265	-4.9147
H	-1.8446	-4.3287	-4.6052
H	-0.8637	-5.7303	-4.1519

SCF = -547.115951**11-NH3**

C	0.1912	-0.0257	1.3195
C	-0.1499	0.0116	4.1229
C	0.0887	-1.2110	2.0467
C	0.1200	1.1786	2.0188
C	-0.0490	1.2074	3.4088
C	-0.0806	-1.2028	3.4369
I	0.4490	-0.0535	-0.7894
F	0.1483	-2.3837	1.4454
F	-0.1740	-2.3396	4.0957
F	-0.3087	0.0289	5.4292
F	-0.1125	2.3613	4.0408
F	0.2101	2.3350	1.3903
N	0.8069	-0.0900	-3.6946
H	1.7745	0.0584	-3.9445
H	0.2594	0.6352	-4.1363
H	0.5194	-0.9759	-4.0862

SCF = -355.114678

12-OCH2

C	0.5222	-0.5877	1.0037
C	0.0286	0.6452	3.4626
C	0.2414	-1.3408	2.1455
C	0.5477	0.8023	1.1334
C	0.3047	1.4427	2.3501
C	-0.0086	-0.7482	3.3853
I	0.8951	-1.5129	-0.8526
I	-0.4292	-1.9212	5.0879
I	0.3528	3.5459	2.5038
F	-0.2045	1.2278	4.6241
F	0.2110	-2.6570	2.0505
F	0.8107	1.5373	0.0680
O	1.4841	-2.1471	-3.7297
C	1.6122	-1.0930	-4.2861
H	1.8371	-1.0389	-5.3595
H	1.5091	-0.1427	-3.7423

SCF = -412.876943**13-OCH2**

C	-0.0791	0.0897	0.8928
I	-0.6353	-0.1437	-1.2369
Br	-0.3092	-1.5905	1.8603
Br	1.7917	0.6359	1.0596
Br	-1.1860	1.4478	1.7555
O	-0.8772	-0.2264	-4.1367
C	0.1152	0.2249	-4.6367
H	0.2266	0.2824	-5.7273
H	0.9472	0.5965	-4.0212

SCF = -412.736183**14-OCH2**

C	-0.0108	0.0766	0.8407
I	0.0204	-0.5012	-1.2797
F	-0.6539	-0.7970	1.6017
F	1.2045	0.1916	1.3570
F	-0.6053	1.2452	1.0389
O	0.0456	-0.7826	-4.1822
C	0.0147	0.2837	-4.7307
H	0.0185	0.3602	-5.8258
H	-0.0185	1.2213	-4.1570

SCF = -413.015809**15-Cl**

C	-0.0001	-0.0037	1.1510
I	-0.0023	-0.0205	-1.2368
Cl	-0.0053	-0.0404	-3.9310
C	-0.7234	-1.2591	1.5999
H	-0.2260	-2.1662	1.2371
H	-1.7566	-1.2853	1.2342
H	-0.7622	-1.3230	2.6926
C	1.4521	0.0018	1.5892
H	1.9888	-0.8830	1.2272
H	1.5348	0.0098	2.6812
H	1.9859	0.8830	1.2146
C	-0.7277	1.2553	1.5823
H	-0.2326	2.1590	1.2079
H	-0.7679	1.3337	2.6740
H	-1.7606	1.2735	1.2152

SCF = -758.579575**15-OCH2**

C	0.0639	-0.0922	0.9472
I	0.3012	-0.5644	-1.2370
C	-0.7593	-1.2069	1.5790
H	-0.2774	-2.1898	1.4909
H	-1.7609	-1.2952	1.1386
H	-0.9008	-1.0192	2.6524
C	1.4548	-0.0225	1.5637
H	2.0039	-0.9694	1.4750
H	1.3885	0.2051	2.6367
H	2.0793	0.7592	1.1125
C	-0.6521	1.2477	1.0605
H	-0.0908	2.0678	0.5953
H	-0.7909	1.5197	2.1164
H	-1.6506	1.2334	0.6053
O	0.3617	-0.6355	-4.2930
C	-0.1068	0.4183	-4.6180
H	-0.2199	0.6902	-5.6759
H	-0.4409	1.1522	-3.8711

SCF = -412.813343**16-OCH2**

C	0.0567	-0.0286	1.0410
I	0.3503	-0.4036	-1.2179
C	-0.7584	-1.1130	1.5372
N	-1.4117	-1.9835	1.9246
C	1.3743	-0.0173	1.6328
N	2.4322	-0.0088	2.0970
C	-0.6058	1.2502	1.1575
N	-1.1357	2.2738	1.2369
O	0.4958	-0.5398	-3.9648
C	-0.0782	0.3527	-4.5281
H	-0.0948	0.4100	-5.6237
H	-0.6034	1.1381	-3.9659

SCF = -412.598417**17-OCH2**

I	0.6929	-1.4002	-1.4063
N	-0.3142	-0.4507	0.1119
C	0.1026	-0.4401	1.4630
C	-1.5091	0.2781	-0.0694
O	1.0901	-0.9937	1.8514
O	-2.0486	0.4049	-1.1322
C	-1.9528	0.8385	1.2707
H	-2.0296	1.9410	1.2181
H	-2.9688	0.4777	1.5193
C	-0.8951	0.3668	2.2764
H	-0.3841	1.2073	2.7834
H	-1.3230	-0.2567	3.0843
O	1.5791	-2.4813	-3.9179
C	0.7766	-2.1718	-4.7552
H	0.9044	-2.4759	-5.8020
H	-0.1116	-1.5743	-4.5012

SCF = -412.898319**18-OCH2**

I	-0.9532	-0.0534	-1.1150
C	-0.5398	-0.0525	0.9423
H	-1.1387	0.6757	1.4756
C	0.3539	-0.8622	1.4969
H	0.5593	-0.8548	2.5611
H	0.9535	-1.5935	0.9739
O	-0.9361	0.0539	-4.1771
C	0.2003	0.2637	-4.4934
H	0.4926	0.3507	-5.5486
H	0.9934	0.3772	-3.7405

SCF = -412.744594**18-Cl**

I	-0.0020	0.0084	-0.9626
Cl	-0.0055	0.0888	-3.7331
C	0.0007	-0.0357	1.2300
H	0.0034	0.9536	1.6422
C	-0.0009	-1.1692	1.9155
H	0.0004	-1.2081	2.9927
H	-0.0037	-2.1532	1.4737

SCF = -758.511365**19-Cl**

I	-0.0056	-0.0312	-1.0339
Cl	-0.0100	-0.0218	-3.6415
C	-0.0009	-0.0190	1.2450
H	-0.0009	0.9767	1.6311
C	0.0014	-1.1518	1.9413
H	0.0012	-2.1408	1.4738
C	0.0043	-1.1655	3.3601
N	0.0067	-1.1831	4.5206

SCF = -758.477444**19-OCH2**

I	0.2468	-0.6094	-1.1291
C	0.1726	-0.2057	0.9206
H	0.3345	0.8442	1.1499
C	-0.0511	-1.1526	1.8369
H	-0.2127	-2.2139	1.6032
C	-0.0954	-0.8322	3.2200
N	-0.1342	-0.5809	4.3494
O	0.2196	-0.6826	-4.1519
C	-0.0718	0.3971	-4.5827
H	-0.1367	0.5820	-5.6634
H	-0.2850	1.2428	-3.9131

SCF = -412.693789**20-Cl**

I	-0.0753	-0.0018	-0.9751
Cl	0.2082	0.1986	-3.7239
C	-0.3126	-0.1539	1.1997
H	-0.7993	0.7089	1.5917
C	0.1310	-1.2199	1.8616
H	0.6166	-2.0703	1.3680
N	0.1538	-1.3607	3.2843
C	-0.3057	-2.6988	3.7165
H	0.2937	-3.4704	3.2052
H	-1.3691	-2.8907	3.5090
H	-0.1321	-2.8106	4.7975
C	-0.5374	-0.2928	4.0307
H	-0.0512	0.6707	3.7939
H	-0.4201	-0.4631	5.1110
H	-1.6102	-0.2067	3.8001

SCF = -758.512800

20-OCH2

I	0.8051	-0.2597	-1.0071
C	0.1764	-0.2394	0.9786
H	-0.1800	0.7276	1.2836
C	0.2522	-1.3366	1.7547
H	0.6097	-2.3054	1.3713
N	0.0156	-1.3407	3.1316
C	-0.4768	-2.6176	3.6767
H	0.1335	-3.4545	3.2958
H	-1.5335	-2.8158	3.4357
H	-0.3629	-2.6097	4.7754
C	-0.6558	-0.1688	3.7110
H	-0.0351	0.7292	3.5325
H	-0.7417	-0.2875	4.8043
H	-1.6612	0.0110	3.2973
O	1.0609	-0.0102	-4.0945
C	0.0187	0.4870	-4.4137
H	-0.2093	0.7100	-5.4648
H	-0.7491	0.7390	-3.6681

SCF = -412.749825**21-Cl**

I	0.0244	-0.0541	-0.8645
Cl	0.3107	-0.1486	-3.6173
C	-0.1884	0.0160	1.1906
H	-0.4161	0.0901	3.4089
C	-0.3120	0.0563	2.3933

SCF = -758.439453**21-OCH2**

I	-0.0650	-0.6441	-1.0033
C	-0.1871	-0.0471	0.8721
H	-0.3248	0.6270	3.0037
C	-0.2612	0.3174	2.0233
O	0.1763	-0.9139	-4.0536
C	0.3074	0.1947	-4.4889
H	0.4129	0.3765	-5.5669
H	0.3271	1.0721	-3.8261

SCF = -412.667998**22-OCH2**

I	-0.0389	-0.7106	-0.9204
C	-0.1982	-0.2386	0.9847
C	-0.2974	0.0535	2.1598
C	-0.4095	0.3836	3.4845
N	-0.5046	0.6640	4.6059
O	0.2288	-0.8374	-3.9356
C	0.2939	0.2627	-4.4067
H	0.3964	0.4153	-5.4895
H	0.2534	1.1606	-3.7725

SCF = -412.615853**22-Cl**

I	0.0395	-0.0577	-0.9975
Cl	0.3011	-0.1432	-3.5015
C	-0.1938	0.0174	1.2345
C	-0.3191	0.0572	2.4453
C	-0.4586	0.1020	3.8002
N	-0.5774	0.1399	4.9575

SCF = -758.406216**23-OCH2**

I	-0.0047	-0.4423	-0.9069
C	-0.1690	0.1859	0.9927
N	-0.2632	0.5485	2.0834
O	0.2443	-0.8673	-3.8560
C	0.2888	0.1703	-4.4547
H	0.3809	0.1944	-5.5487
H	0.2390	1.1363	-3.9311

SCF = -412.709947**23-Cl**

I	0.0327	-0.0546	-0.9456
Cl	0.2905	-0.1352	-3.4394
C	-0.2016	0.0184	1.3297
N	-0.3185	0.0533	2.4781

SCF = -758.501510

24-OCH2

C	-1.0409	0.4418	1.6158
C	1.0687	-0.4430	3.2254
C	-1.1404	-0.7869	2.2670
C	0.1026	1.2309	1.7622
C	1.1528	0.7824	2.5682
C	-0.0842	-1.2271	3.0713
C	-0.1654	-2.5164	3.7668
C	-0.1098	-4.9683	5.1989
C	0.3165	-3.6867	3.1739
C	-0.6719	-2.6037	5.0663
C	-0.6444	-3.8110	5.7715
C	0.3441	-4.8939	3.8792
C	0.0248	-6.2049	5.9769
C	0.3097	-8.5480	7.4666
C	-1.0029	-7.1538	5.9820
C	1.1980	-6.4212	6.7146
C	1.3309	-7.5938	7.4552
C	-0.8545	-8.3220	6.7281
I	2.7468	-4.9855	6.7048
I	2.6599	-1.1141	4.4414
F	0.4438	-9.6535	8.1694
F	2.4155	-7.8403	8.1641
F	-1.7983	-9.2426	6.7611
F	0.8293	-5.9703	3.2946
F	0.7765	-3.6511	1.9398
F	-1.1609	-1.5283	5.6495
F	-1.1082	-3.8474	7.0042
F	-2.0129	0.8949	0.8482
F	0.1904	2.3905	1.1445
F	2.2168	1.5532	2.6838
O	4.6794	-2.5012	6.3865
C	5.6984	-2.1153	6.8891
H	6.2450	-2.7312	7.6154
H	6.1203	-1.1324	6.6403
I	-2.7717	-6.8271	4.8699
I	-2.8782	-1.9694	2.0353

SCF = -711.527224**24-Cl**

C	-0.8751	0.4418	1.5813
C	0.9814	-0.4658	3.4569
C	-1.0496	-0.8063	2.1741
C	0.2216	1.2389	1.9201
C	1.1458	0.7742	2.8613
C	-0.1154	-1.2575	3.1145
C	-0.2634	-2.5664	3.7607
C	-0.2556	-5.0284	5.1839
C	0.3390	-3.7085	3.2257
C	-0.9357	-2.6990	4.9789
C	-0.9319	-3.9098	5.6788
C	0.3428	-4.9193	3.9256
C	-0.0996	-6.2408	5.9953
C	0.2526	-8.5197	7.5623
C	-1.0294	-7.2851	5.9204
C	1.0004	-6.3342	6.8486
C	1.1725	-7.4680	7.6258
C	-0.8473	-8.4206	6.7061
I	2.4590	-4.6495	6.9422
I	2.4472	-1.2183	4.9594
F	0.4143	-9.5997	8.3010
F	2.1993	-7.5959	8.4455
F	-1.6984	-9.4306	6.6689
F	0.9473	-5.9648	3.3969
F	0.9401	-3.6420	2.0542
F	-1.5621	-1.6604	5.4955
F	-1.5547	-3.9833	6.8383
F	-1.7304	0.9089	0.6890
F	0.3761	2.4186	1.3520
F	2.1693	1.5537	3.1571
Cl	4.0598	-2.4208	6.8300
I	-2.7116	-2.0017	1.6534
I	-2.6963	-7.1476	4.6301

SCF = -1057.347716

25-OCH2

C	0.2843	-1.3489	0.2669
C	-0.3406	1.3644	0.0121
C	1.3305	-0.4232	0.2026
C	-1.0616	-0.9734	0.2122
C	-1.3416	0.3905	0.0824
C	0.9857	0.9261	0.0760
C	2.7301	-0.8506	0.2606
C	5.3984	-1.6693	0.3774
C	3.4138	-1.1665	-0.9220
C	3.3776	-0.9422	1.4988
C	4.7087	-1.3515	1.5502
C	4.7451	-1.5742	-0.8539
C	-2.1345	-1.9672	0.2885
C	-4.1845	-3.8590	0.4442
C	-2.6659	-2.3190	1.5357
C	-2.6248	-2.5601	-0.8833
C	-3.6482	-3.5030	-0.7957
C	-3.6884	-3.2631	1.6064
C	-0.6693	2.7835	-0.1411
C	-1.3043	5.4870	-0.4415
C	-0.7944	3.3317	-1.4257
C	-0.8583	3.5842	0.9915
C	-1.1753	4.9324	0.8344
C	-1.1119	4.6809	-1.5667
I	2.3531	-0.4648	3.2867
I	2.4429	-1.0251	-2.7856
I	-1.8288	-2.0384	-2.7609
I	-1.9302	-1.4312	3.3090
I	-0.4965	2.1188	-3.1237
I	-0.6648	2.7639	2.9311
F	0.5786	-2.6263	0.3864
F	-2.5996	0.7735	0.0243
F	1.9495	1.8204	0.0131
F	-4.1403	-4.0855	-1.8720
F	-5.1511	-4.7501	0.5173
F	-4.2164	-3.6220	2.7605
F	5.3552	-1.4514	2.6955
F	6.6560	-2.0555	0.4325
F	5.4266	-1.8811	-1.9408
F	-1.6043	6.7613	-0.5827
F	-1.3620	5.7216	1.8745
F	-1.2397	5.2364	-2.7563
O	0.2719	-0.0856	-5.2244
C	0.3836	0.1777	-6.3905
H	0.8642	-0.5195	-7.0894
H	0.0091	1.1258	-6.8000

SCF = -1009.845499**25-Cl**

C	0.3013	-1.3160	0.3669
C	-0.3255	1.3971	0.1085
C	1.3477	-0.3895	0.3118
C	-1.0448	-0.9445	0.2886
C	-1.3250	0.4206	0.1693
C	1.0006	0.9601	0.1918
C	2.7488	-0.8201	0.3113
C	5.4153	-1.6410	0.2910
C	3.3785	-1.1082	-0.9064
C	3.4491	-0.9415	1.5176
C	4.7801	-1.3517	1.5010
C	4.7064	-1.5163	-0.9073
C	-2.1131	-1.9477	0.2641
C	-4.1451	-3.8586	0.1983
C	-2.7098	-2.3709	1.4579
C	-2.5300	-2.4777	-0.9638
C	-3.5423	-3.4287	-0.9874
C	-3.7236	-3.3252	1.4186
C	-0.6514	2.8104	-0.1025
C	-1.2716	5.4978	-0.5242
C	-0.7532	3.3039	-1.4096
C	-0.8587	3.6572	0.9930
C	-1.1681	4.9979	0.7761
C	-1.0625	4.6432	-1.6104
I	2.4991	-0.5070	3.3550
I	2.2609	-0.9067	-2.7456
I	-1.5816	-1.7966	-2.7830
I	-2.0812	-1.5713	3.3107
I	-0.4250	1.9616	-3.0722
I	-0.7049	2.9129	2.9652
Cl	0.1438	-0.4089	-4.7747
F	0.5966	-2.5941	0.4852
F	-2.5838	0.8019	0.0987
F	1.9640	1.8567	0.1427
F	-3.9671	-3.9554	-2.1207
F	-5.1053	-4.7614	0.1711
F	-4.3137	-3.7529	2.5202
F	5.4782	-1.4795	2.6150
F	6.6753	-2.0286	0.2853
F	5.3402	-1.7984	-2.0303
F	-1.5650	6.7681	-0.7195
F	-1.3717	5.8318	1.7800
F	-1.1688	5.1517	-2.8239

SCF = -1355.681271

26-Cl

H	-1.4269	0.9043	-2.1077
C	-1.3278	1.6027	-1.2657
C	-1.0840	3.4449	0.8305
C	-1.1307	1.1674	0.0357
C	-1.4036	2.9738	-1.5183
C	-1.2825	3.8895	-0.4755
C	-1.0060	2.0781	1.0977
H	-1.5584	3.3245	-2.5384
H	-1.3429	4.9585	-0.6794
H	-0.9902	4.1667	1.6397
C	-0.7986	1.5241	2.4352
C	-0.4107	0.2381	4.8794
C	-0.7445	0.1352	2.5193
C	-0.6555	2.2803	3.6004
C	-0.4621	1.6311	4.8188
C	-0.5536	-0.5232	3.7158
H	-0.6940	3.3671	3.5645
H	-0.3502	2.2166	5.7305
H	-0.5119	-1.6082	3.7771
H	-0.2591	-0.2564	5.8367
I	-0.9972	-0.8641	0.5659
Cl	-1.3229	-1.5501	-1.8277

SCF = -758.892027**26-OCH2**

H	-1.3756	1.2710	-2.1284
C	-1.2909	1.9216	-1.2533
C	-1.0792	3.6347	0.9666
C	-1.1030	1.4205	0.0229
C	-1.3737	3.3072	-1.4159
C	-1.2686	4.1548	-0.3150
C	-0.9942	2.2562	1.1487
H	-1.5219	3.7247	-2.4151
H	-1.3350	5.2389	-0.4540
H	-0.9987	4.3109	1.8204
C	-0.7975	1.5933	2.4366
C	-0.4273	0.1138	4.7803
C	-0.7376	0.1907	2.4142
C	-0.6682	2.2490	3.6603
C	-0.4837	1.5065	4.8268
C	-0.5550	-0.5598	3.5631
H	-0.7105	3.3393	3.7106
H	-0.3824	2.0233	5.7868
H	-0.5079	-1.6490	3.5498
H	-0.2822	-0.4566	5.7016
I	-0.9526	-0.6202	0.4826
O	-1.2785	-1.0213	-2.1887
C	-1.3598	-1.7890	-3.1169
H	-1.2882	-2.8712	-2.9743
H	-1.5085	-1.4179	-4.1337

SCF = -412.955830**27-OCH2**

H	-0.0659	0.5793	0.2837
C	-0.0627	0.4655	1.3694
C	-0.0543	0.2414	4.1777
C	-0.0666	-0.7715	1.9898
C	-0.0544	1.6102	2.1708
C	-0.0501	1.4911	3.5613
C	-0.0626	-0.9089	3.3865
H	-0.0514	2.5985	1.6929
H	-0.0514	0.1456	5.2696
C	-0.0675	-2.2753	3.9046
C	-0.0782	-4.9670	4.6693
C	-0.0757	-3.3077	2.9504
C	-0.0648	-2.6107	5.2586
C	-0.0702	-3.9548	5.6286
C	-0.0810	-4.6436	3.3094
H	-0.0585	-1.8143	6.0117
H	-0.0872	-5.4491	2.5673
H	-0.0825	-6.0233	4.9667
I	-0.0789	-2.6158	0.9696
C	-0.0411	2.7620	4.3795
C	-0.0676	-4.3608	7.0847
F	1.0194	3.5264	4.1267
F	-0.0334	2.5854	5.6970
F	-1.0999	3.5329	4.1398
F	-0.0594	-3.3534	7.9521
F	-1.1299	-5.0925	7.4146
F	0.9890	-5.1038	7.4077
O	-0.0949	-5.2327	0.2976
C	-0.0986	-6.0948	-0.5489
H	-0.1060	-7.1503	-0.2656
H	-0.0948	-5.8503	-1.6152

SCF = -413.444900

27-Cl

H	-0.0674	0.1526	0.1812
C	-0.0642	0.1243	1.2690
C	-0.0556	0.0928	4.0827
C	-0.0680	-1.0611	1.9721
C	-0.0559	1.3233	1.9862
C	-0.0516	1.2979	3.3831
C	-0.0639	-1.1048	3.3626
H	-0.0527	2.2731	1.4474
H	-0.0524	0.0714	5.1741
C	-0.0688	-2.4381	3.9620
C	-0.0792	-5.0518	4.9538
C	-0.0772	-3.5392	3.0903
C	-0.0655	-2.6591	5.3406
C	-0.0707	-3.9641	5.8258
C	-0.0825	-4.8380	3.5743
H	-0.0589	-1.8035	6.0198
H	-0.0891	-5.7141	2.9098
H	-0.0833	-6.0774	5.3342
I	-0.0811	-3.0784	1.0334
Cl	-0.0955	-5.4927	0.4637
C	-0.0427	2.6138	4.1082
C	-0.0673	-4.2424	7.3048
F	1.0156	3.3712	3.8149
F	-0.0384	2.5429	5.4378
F	-1.0954	3.3816	3.8221
F	-0.0591	-3.1698	8.0937
F	-1.1259	-4.9441	7.7111
F	0.9866	-4.9551	7.7041

SCF = -759.397769**28-OCH2**

H	-0.1339	0.6195	0.3226
C	-0.1060	0.4944	1.4070
C	-0.0332	0.2303	4.2122
C	-0.1073	-0.7501	2.0135
C	-0.0676	1.6299	2.2181
C	-0.0315	1.4944	3.6103
C	-0.0716	-0.9073	3.4088
H	-0.0657	2.6276	1.7644
H	-0.0046	0.1467	5.3035
C	-0.0779	-2.2814	3.9079
C	-0.0977	-4.9911	4.6277
C	-0.1189	-3.3004	2.9389
C	-0.0465	-2.6373	5.2534
C	-0.0567	-3.9929	5.6060
C	-0.1292	-4.6428	3.2758
H	-0.0141	-1.8721	6.0359
H	-0.1611	-5.4345	2.5191
H	-0.1051	-6.0470	4.9199
I	-0.1619	-2.5793	0.9701
C	0.0077	2.6578	4.4288
N	0.0394	3.6036	5.0929
C	-0.0247	-4.3569	6.9815
N	0.0013	-4.6533	8.0987
O	-0.2173	-5.1852	0.2420
C	-0.2498	-6.0443	-0.6066
H	-0.2557	-7.1009	-0.3269
H	-0.2741	-5.7962	-1.6717

SCF = -412.837277

28-Cl

H	-0.1594	0.1554	0.1813
C	-0.1255	0.1295	1.2690
C	-0.0377	0.0943	4.0828
C	-0.1210	-1.0551	1.9741
C	-0.0853	1.3295	1.9818
C	-0.0416	1.3050	3.3811
C	-0.0782	-1.1012	3.3647
H	-0.0877	2.2836	1.4539
H	-0.0034	0.0979	5.1728
C	-0.0796	-2.4356	3.9627
C	-0.0889	-5.0579	4.9461
C	-0.1239	-3.5361	3.0899
C	-0.0396	-2.6601	5.3379
C	-0.0443	-3.9713	5.8236
C	-0.1289	-4.8371	3.5693
H	-0.0046	-1.8229	6.0368
H	-0.1635	-5.7099	2.9006
H	-0.0924	-6.0791	5.3338
I	-0.1802	-3.0702	1.0357
Cl	-0.2362	-5.4837	0.4548
C	-0.0005	2.5306	4.1001
N	0.0329	3.5298	4.6829
C	-0.0030	-4.1979	7.2277
N	0.0306	-4.3817	8.3695

SCF = -758.789169**29-Cl**

H	0.0124	0.1468	0.1791
C	-0.0199	0.1054	1.2672
C	-0.1026	0.0424	4.0698
C	-0.0106	-1.0927	1.9494
C	-0.0747	1.2967	1.9858
C	-0.1102	1.2834	3.3969
C	-0.0497	-1.1397	3.3404
H	-0.0797	2.2360	1.4431
H	-0.1270	0.0022	5.1537
C	-0.0355	-2.4833	3.9340
C	-0.0079	-5.1074	4.8867
C	0.0148	-3.5675	3.0436
C	-0.0733	-2.7141	5.3018
C	-0.0515	-4.0346	5.8046
C	0.0307	-4.8716	3.5193
H	-0.1092	-1.8688	5.9810
H	0.0710	-5.7346	2.8381
H	0.0054	-6.1357	5.2366
I	0.0621	-3.0725	1.0101
Cl	0.1303	-5.5232	0.3600
N	-0.0330	2.4833	4.1239
N	0.0412	-4.2670	7.1783
C	-0.4626	3.7099	3.4307
H	0.2285	3.9158	2.5927
H	-0.3935	4.5749	4.1119
H	-1.4914	3.6545	3.0400
C	-0.4861	2.4393	5.5254
H	0.2035	1.8007	6.1084
H	-1.5136	2.0582	5.6410
H	-0.4352	3.4456	5.9737
C	-0.3812	-3.1863	8.0824
H	0.3030	-2.3248	7.9660
H	-0.3005	-3.5111	9.1332
H	-1.4157	-2.8499	7.9022
C	-0.3160	-5.6079	7.6669
H	0.4005	-6.3475	7.2615
H	-1.3388	-5.9123	7.3893
H	-0.2252	-5.6534	8.7648

SCF = -758.895726

29-OCH2

H	0.0102	0.4647	0.2237
C	-0.0733	0.3759	1.3091
C	-0.2788	0.1772	4.1077
C	-0.0723	-0.8603	1.9417
C	-0.1793	1.5265	2.0684
C	-0.2977	1.4585	3.4854
C	-0.1721	-0.9653	3.3404
H	-0.1740	2.4912	1.5673
H	-0.3522	0.0951	5.1883
C	-0.1505	-2.3333	3.8844
C	-0.0718	-5.0168	4.6744
C	-0.0324	-3.3694	2.9398
C	-0.2338	-2.6395	5.2278
C	-0.2105	-3.9976	5.6566
C	0.0103	-4.7014	3.3302
H	-0.3217	-1.8392	5.9571
H	0.1112	-5.5082	2.5965
H	-0.0315	-6.0615	4.9720
I	0.0752	-2.7050	0.9671
N	-0.4837	2.5887	4.2272
N	-0.3857	-4.3131	6.9751
C	-0.3546	3.9146	3.6190
H	0.6577	4.0820	3.2069
H	-0.5554	4.7114	4.3579
H	-1.0969	4.0380	2.8064
C	-0.4476	2.5375	5.6902
H	0.5216	2.1599	6.0651
H	-1.2593	1.8873	6.0704
H	-0.6101	3.5397	6.1264
C	-0.3395	-3.2689	8.0015
H	0.6256	-2.7298	8.0013
H	-0.4863	-3.6979	9.0091
H	-1.1591	-2.5419	7.8418
C	-0.1895	-5.6869	7.4441
H	0.8419	-6.0426	7.2663
H	-0.8968	-6.3693	6.9339
H	-0.3955	-5.7681	8.5267
O	0.2245	-5.3709	0.2615
C	0.2315	-6.1969	-0.6171
H	0.2844	-7.2622	-0.3811
H	0.1859	-5.9143	-1.6729

SCF = -412.974549**30-OCH2**

H	1.1134	0.0509	0.9324
C	0.3831	0.2761	1.7125
C	-1.4678	0.9331	3.7028
C	-0.6117	-0.6205	2.0851
C	0.4576	1.5149	2.3530
C	-0.4626	1.8334	3.3488
C	-1.5483	-0.3043	3.0635
H	1.2453	2.2172	2.0553
H	-2.2008	1.1855	4.4800
C	0.8720	-2.7668	3.7857
C	-0.5801	-4.9186	4.8230
C	-0.1716	-3.3376	3.0632
C	1.1826	-3.2727	5.0483
C	0.4536	-4.3435	5.5614
C	-0.8962	-4.4156	3.5606
H	2.0014	-2.8124	5.6149
H	-1.7035	-4.8891	2.9916
H	-1.1533	-5.7648	5.2220
I	-0.6807	-2.5393	1.1780
C	-0.4061	3.1568	4.0756
C	0.7579	-4.9180	6.9251
F	-0.2491	3.0113	5.3901
F	-1.5183	3.8733	3.9278
F	0.5794	3.9656	3.6988
F	1.7500	-4.3239	7.5805
F	-0.2852	-4.8610	7.7507
F	1.0991	-6.2044	6.8737
H	-2.3462	-0.9912	3.3566
H	1.4578	-1.9268	3.4050
O	-0.7165	-5.1830	0.6974
C	-0.0244	-6.0255	0.1769
H	-0.3194	-7.0773	0.2051
H	0.9085	-5.7681	-0.3345

SCF = -413.449012

30-Cl

H	1.2900	-0.3404	0.9952
C	0.5275	-0.0807	1.7280
C	-1.4121	0.6374	3.6043
C	-0.4633	-0.9704	2.1009
C	0.5582	1.1913	2.3059
C	-0.4102	1.5408	3.2443
C	-1.4385	-0.6304	3.0220
H	1.3434	1.8891	2.0120
H	-2.1730	0.9113	4.3382
C	0.9106	-2.8924	3.9071
C	-0.5464	-4.9502	5.1165
C	-0.0761	-3.5732	3.1985
C	1.1534	-3.2298	5.2364
C	0.4190	-4.2537	5.8369
C	-0.7957	-4.6076	3.7855
H	1.9202	-2.6879	5.7963
H	-1.5443	-5.1837	3.2294
H	-1.1159	-5.7686	5.5642
I	-0.4787	-3.0340	1.1952
Cl	-0.4213	-5.4611	0.7097
C	-0.4105	2.8928	3.8971
C	0.7072	-4.5791	7.2772
F	-0.2925	2.8407	5.2248
F	-1.5322	3.5836	3.6858
F	0.5606	3.7201	3.5137
F	0.5263	-3.5420	8.0962
F	-0.0328	-5.5505	7.8077
F	1.9655	-4.9645	7.4912
H	-2.2232	-1.3272	3.3145
H	1.4987	-2.0901	3.4556

SCF = -759.398021**31-Cl**

H	1.5023	-0.7853	2.8983
C	0.5046	-0.3526	2.8249
C	-2.0452	0.7862	2.6656
C	-0.5158	-0.9811	2.1325
C	0.2507	0.8640	3.4579
C	-1.0265	1.4293	3.3765
C	-1.7821	-0.4312	2.0372
H	1.0392	1.3721	4.0141
H	-3.0365	1.2354	2.6054
C	1.2735	-4.3480	3.4579
C	-0.5791	-3.5942	5.4151
C	0.1651	-3.5743	3.1277
C	1.4653	-4.7395	4.7822
C	0.5433	-4.3549	5.7592
C	-0.7722	-3.2097	4.0911
H	2.3302	-5.3494	5.0514
H	-1.6570	-2.6181	3.8424
H	-1.3015	-3.3046	6.1806
I	-0.1063	-2.9546	1.1265
Cl	0.4460	-5.2862	0.4953
H	-2.5838	-0.9208	1.4857
H	1.9963	-4.6802	2.7031
C	-1.2914	2.6687	4.0193
N	-1.5079	3.6786	4.5412
C	0.7437	-4.7414	7.1136
N	0.9073	-5.0525	8.2159

SCF = -758.789897

31-OCH2

H	1.4980	-0.4033	3.1126
C	0.4887	-0.0024	2.9860
C	-2.0776	1.0811	2.6976
C	-0.4395	-0.5775	2.1235
C	0.1237	1.1225	3.7236
C	-1.1596	1.6604	3.5805
C	-1.7151	-0.0455	1.9622
H	0.8405	1.5851	4.4116
H	-3.0778	1.5134	2.5845
C	1.4187	-4.0625	3.1746
C	-0.5885	-3.7707	5.1059
C	0.2822	-3.3016	2.9175
C	1.5570	-4.6774	4.4178
C	0.5558	-4.5280	5.3821
C	-0.7296	-3.1574	3.8640
H	2.4489	-5.2741	4.6384
H	-1.6318	-2.5709	3.6719
H	-1.3710	-3.6606	5.8653
I	0.0987	-2.3305	1.0555
H	-2.4477	-0.4772	1.2765
H	2.2093	-4.1997	2.4285
C	-1.5338	2.8064	4.3359
N	-1.8387	3.7374	4.9501
C	0.6989	-5.1521	6.6526
N	0.8152	-5.6598	7.6848
O	0.9268	-4.7734	0.3010
C	0.4381	-5.8185	-0.0576
H	1.0725	-6.6863	-0.2537
H	-0.6419	-5.9309	-0.1971

SCF = -412.841986**32-Cl**

H	1.4437	-0.8889	3.1827
C	0.4676	-0.4206	3.0402
C	-2.0175	0.8020	2.7204
C	-0.4978	-0.9933	2.2283
C	0.1986	0.7689	3.7069
C	-1.0569	1.3978	3.5646
C	-1.7322	-0.3900	2.0624
H	0.9637	1.1976	4.3455
H	-2.9913	1.2587	2.5830
C	1.3097	-4.4800	3.3914
C	-0.4488	-3.7602	5.4354
C	0.2349	-3.6327	3.1279
C	1.5200	-4.9586	4.6760
C	0.6517	-4.5968	5.7302
C	-0.6520	-3.2914	4.1467
H	2.3629	-5.6192	4.8548
H	-1.5140	-2.6435	3.9606
H	-1.1476	-3.4695	6.2131
I	-0.0648	-2.8987	1.1870
Cl	0.5255	-5.2224	0.3604
H	-2.5012	-0.8256	1.4236
H	1.9962	-4.7996	2.5968
N	-1.3865	2.5222	4.3375
N	0.9391	-4.9658	7.0446
C	-2.4875	3.3691	3.8471
H	-2.6233	4.2389	4.5120
H	-3.4319	2.7956	3.8832
H	-2.3321	3.7357	2.8198
C	-0.2673	3.3106	4.8810
H	0.4260	3.6772	4.1070
H	0.2966	2.6915	5.6034
H	-0.6523	4.1773	5.4446
C	1.8016	-6.1407	7.2477
H	2.8149	-5.9220	6.8622
H	1.4190	-7.0480	6.7499
H	1.9134	-6.3554	8.3233
C	-0.1404	-4.8598	8.0379
H	0.2208	-5.1796	9.0298
H	-1.0275	-5.4619	7.7794
H	-0.4435	-3.8010	8.1399

SCF = -758.896465

32-OCH2

H	1.5075	-0.7099	3.0559
C	0.5427	-0.2107	2.9282
C	-1.9124	1.0918	2.6269
C	-0.4178	-0.7007	2.0412
C	0.2852	0.9216	3.6742
C	-0.9594	1.6020	3.5537
C	-1.6398	-0.0434	1.8905
H	1.0452	1.2883	4.3590
H	-2.8663	1.5946	2.4923
C	1.5013	-3.7888	3.2314
C	-0.7211	-4.2484	4.8639
C	0.2201	-3.4322	2.8035
C	1.6836	-4.3774	4.4657
C	0.5730	-4.6290	5.3217
C	-0.8860	-3.6627	3.6259
H	2.6885	-4.6418	4.7844
H	-1.8959	-3.3779	3.3154
H	-1.5925	-4.4103	5.4935
I	-0.0360	-2.4668	0.9689
H	-2.3999	-0.4039	1.1922
H	2.3813	-3.6094	2.6063
N	-1.2515	2.6759	4.3409
N	0.7366	-5.2573	6.5175
C	-2.4602	3.4699	4.1084
H	-2.5437	4.2902	4.8444
H	-3.3627	2.8398	4.2265
H	-2.4687	3.9194	3.0980
C	-0.2220	3.2916	5.1813
H	0.6200	3.6821	4.5800
H	0.1703	2.5556	5.9094
H	-0.6383	4.1311	5.7672
C	2.0726	-5.5417	7.0448
H	2.6542	-4.6144	7.2047
H	2.6316	-6.1980	6.3502
H	2.0139	-6.0739	8.0120
C	-0.3807	-5.4006	7.4533
H	-0.0685	-5.9373	8.3677
H	-1.1959	-5.9926	6.9942
H	-0.7839	-4.4172	7.7607
O	0.4256	-4.9488	0.0334
C	0.3971	-5.9668	0.6792
H	0.5726	-6.9324	0.2021
H	0.1971	-5.9620	1.7593

SCF = -412.982867**33-OCH2**

I	-1.2214	1.0218	-3.4349
C	-0.6494	0.4189	-1.4725
C	0.1142	-0.3280	1.0866
N	-0.9873	-0.8102	-0.9930
C	0.0835	1.3051	-0.6729
C	0.4697	0.9386	0.6099
C	-0.6113	-1.1847	0.2740
H	0.3585	2.2985	-1.0559
H	1.0450	1.6295	1.2423
H	0.4053	-0.6463	2.0970
C	-1.7549	-1.7846	-1.7825
H	-1.2186	-2.0693	-2.7134
H	-2.7572	-1.3898	-2.0562
H	-1.9318	-2.7261	-1.2233
H	-0.9057	-2.1889	0.6228
O	-2.0726	1.7509	-6.1408
C	-2.1741	2.4651	-7.0992
H	-1.7288	3.4704	-7.1130
H	-2.7176	2.1350	-7.9965

SCF = -412.481790**34-OCH2**

I	-1.2822	1.0496	-3.3833
C	-0.6889	0.4781	-1.4385
C	0.0682	-0.3369	1.0966
C	-0.8552	-0.8440	-1.0283
C	-0.1310	1.4117	-0.5584
C	0.2470	0.9941	0.7141
N	-0.4761	-1.2280	0.2258
H	-1.2904	-1.6175	-1.6852
H	0.0133	2.4624	-0.8518
H	0.6882	1.7046	1.4278
H	0.3609	-0.6886	2.0999
H	-0.0912	-3.3126	-0.0358
C	-0.6646	-2.6276	0.6259
H	-0.3260	-2.8185	1.6646
H	-1.7365	-2.9172	0.5735
O	-2.1563	1.7982	-6.1431
C	-2.3942	2.3973	-7.1539
H	-2.8604	1.8968	-8.0151
H	-2.1552	3.4658	-7.2552

SCF = -412.481787

35-OCH2

I	-0.7216	0.6141	-2.1738
C	-0.0858	0.0653	-0.2524
N	0.7587	-0.6625	2.2972
C	-0.3141	-1.2266	0.2356
C	0.5774	0.9845	0.5713
C	0.9921	0.6045	1.8408
C	0.1146	-1.5735	1.5118
H	-0.8301	-1.9864	-0.3698
H	0.7815	2.0121	0.2361
H	1.5166	1.3068	2.5112
H	-0.0538	-2.5854	1.9181
H	2.3142	-0.9341	3.7335
C	1.2109	-1.0321	3.6435
H	0.7419	-0.3826	4.4136
H	0.9540	-2.0796	3.8999
O	-1.6361	1.4127	-4.9161
C	-1.9934	1.7227	-6.0175
H	-1.3531	1.5495	-6.8947
H	-2.9739	2.1907	-6.1883

SCF = -412.483215**36-OCH2**

N	0.2811	-1.4497	1.0795
C	0.1593	-0.1701	0.6016
N	0.4386	0.6900	1.6325
C	0.6411	-1.3968	2.4259
H	0.7986	-2.2790	3.0308
C	0.7398	-0.0542	2.7729
H	0.9954	0.3959	3.7221
I	-0.3620	0.3739	-1.3546
H	1.1667	2.5226	0.8352
C	0.4294	2.1421	1.5743
H	0.6943	2.5818	2.5591
H	-0.5751	2.5302	1.3004
H	0.7786	-2.7509	-0.5278
C	0.0749	-2.6769	0.3289
H	0.2420	-3.5685	0.9695
H	-0.9630	-2.7429	-0.0623
O	-1.1123	1.1516	-4.1128
C	-1.3883	1.4671	-5.2363
H	-0.6096	1.5719	-6.0059
H	-2.4294	1.6618	-5.5332

SCF = -412.498908**37-OCH2**

N	-0.2822	0.5800	-0.1780
C	-0.4948	1.8595	-0.6269
N	-0.3295	2.7190	0.4304
C	0.0395	0.6324	1.1776
C	-0.0257	1.9715	1.5674
I	-0.9930	2.4111	-2.6058
H	-0.2312	4.5868	-0.6130
C	-0.4402	4.1695	0.3921
H	0.2959	4.6551	1.0708
H	-1.4613	4.4979	0.6925
H	0.6199	-0.9467	-1.3483
C	-0.3798	-0.6406	-0.9644
H	-0.7962	-1.4816	-0.3664
H	-1.0595	-0.5349	-1.8333
C	0.4205	-0.5633	2.0114
C	0.1488	2.5499	2.9476
F	1.1510	-0.2359	3.0693
F	1.1514	-1.4530	1.3454
F	-0.6386	-1.2223	2.4682
F	1.3721	3.0276	3.1474
F	-0.6867	3.5530	3.2029
F	-0.0740	1.6599	3.9059
O	-1.6967	3.1681	-5.3327
C	-1.9326	3.5058	-6.4595
H	-2.8988	3.2733	-6.9312
H	-1.1903	4.0579	-7.0546

SCF = -412.964228**38-OCH2**

N	0.5227	-1.1923	0.7203
C	0.0488	-0.0262	0.1768
N	0.0055	0.9245	1.1638
C	0.7865	-0.9815	2.0788
C	0.4601	0.3542	2.3587
I	-0.5170	0.2562	-1.8336
H	-1.4961	2.3548	0.6904
C	-0.4353	2.3030	1.0195
H	0.1931	2.8526	0.2851
H	-0.3665	2.8541	1.9834
H	1.4615	-2.3415	-0.8038
C	0.7266	-2.4524	0.0231
H	1.1224	-3.2352	0.7073
H	-0.2272	-2.8397	-0.3969
C	1.2862	-1.9648	2.9544
N	1.6960	-2.7578	3.6894
C	0.5515	1.0417	3.5843
N	0.6341	1.5880	4.6000
O	-1.3035	0.6500	-4.6198
C	-1.6174	0.8178	-5.7654
H	-0.8747	1.1158	-6.5202
H	-2.6574	0.6787	-6.0957

SCF = -412.361927

39-OCH2

N	0.1349	-1.1876	0.1214
C	-0.0860	0.0887	-0.3251
N	0.1042	0.9450	0.7273
C	0.4715	-1.1439	1.4812
C	0.4522	0.2020	1.8636
I	-0.6214	0.6347	-2.2736
H	0.6825	2.8373	-0.0492
C	-0.0320	2.3917	0.6749
H	0.1747	2.8502	1.6637
H	-1.0621	2.6888	0.3847
H	0.2645	-3.2977	-0.0833
C	0.0363	-2.3938	-0.6845
H	-0.9882	-2.5220	-1.0936
H	0.7555	-2.3726	-1.5306
C	0.7740	-2.3360	2.2825
H	1.6488	-2.8945	1.9001
H	-0.0757	-3.0423	2.3313
H	1.0146	-2.0810	3.3321
C	0.7288	0.8025	3.1741
H	1.5874	1.4994	3.1496
H	0.9811	0.0401	3.9355
H	-0.1380	1.3573	3.5792
O	-1.3941	1.4212	-5.0404
C	-1.7058	1.7374	-6.1541
H	-2.7295	1.5822	-6.5250
H	-0.9784	2.1931	-6.8417

SCF = -412.536359**40-OCH2**

N	0.1922	-1.0931	-0.1422
C	-0.1834	0.0974	-0.7109
N	-0.1657	1.0654	0.2603
C	0.4575	-0.8754	1.2190
C	0.2286	0.4771	1.4726
I	-0.6944	0.3867	-2.7195
H	-1.6253	2.5430	-0.1991
C	-0.5653	2.4550	0.1184
H	0.0747	2.9828	-0.6186
H	-0.4689	2.9885	1.0903
H	1.1634	-2.2937	-1.6052
C	0.3832	-2.3645	-0.8189
H	0.7150	-3.1435	-0.0966
H	-0.5615	-2.7179	-1.2818
O	0.9496	-1.8710	1.9620
O	0.2130	1.2012	2.5955
C	1.5151	1.3611	3.1899
H	1.9602	0.3898	3.4294
H	1.2666	1.9177	4.1078
H	2.1685	1.9480	2.5383
C	0.0928	-2.2435	3.0581
H	-0.0927	-1.3916	3.7204
H	0.7065	-3.0078	3.5615
H	-0.8435	-2.6711	2.6882
O	-1.4001	0.8016	-5.5770
C	-1.7257	0.9669	-6.7190
H	-0.9747	1.0827	-7.5141
H	-2.7858	1.0081	-7.0089

SCF = -412.614278

7.5 AM1

Cl

Cl	0.0000	0.0000	0.0000
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SCF = -0.060011**ZPE = 0.000000****H₂₉₈ = -0.057651****G₂₉₈ = -0.075034**

		1	
H	2.7072	0.0644	-1.4704
C	2.1114	0.0694	-0.5444
C	0.6028	0.1078	1.8015
C	1.6765	-1.1288	0.0244
C	1.7914	1.2847	0.0609
C	1.0372	1.3051	1.2341
C	0.9218	-1.1090	1.1976
H	2.1352	2.2276	-0.3897
H	0.5733	-2.0484	1.6546
H	0.0072	0.1186	2.7262
I	2.1375	-2.8906	-0.8521
H	0.7850	2.2643	1.7100

SCF = 0.060601
ZPE = 0.092254
H₂₉₈ = 0.159622
G₂₉₈ = 0.121147

		1-Cl	
H	2.7002	-0.0010	-1.4995
C	2.1116	0.0068	-0.5695
C	0.6268	0.0592	1.7788
C	1.6913	-1.2001	-0.0069
C	1.7979	1.2279	0.0278
C	1.0529	1.2571	1.2064
C	0.9462	-1.1564	1.1729
H	2.1363	2.1689	-0.4278
H	0.6030	-2.0938	1.6363
H	0.0395	0.0758	2.7073
I	2.1616	-3.0041	-0.8999
Cl	2.7113	-5.1119	-1.9440
H	0.8039	2.2160	1.6797

SCF = -0.041707
ZPE = 0.092927
H₂₉₈ = 0.060111
G₂₉₈ = 0.016834

		2	
H	0.3842	0.1250	0.0370
C	0.2404	0.1004	1.1292
C	-0.1279	0.0615	3.8989
C	0.3548	-1.0996	1.8327
C	-0.0579	1.2835	1.8029
C	-0.2433	1.2665	3.1923
C	0.1706	-1.1164	3.2159
H	-0.1475	2.2284	1.2451
H	0.2590	-2.0580	3.7815
H	-0.2726	0.0444	4.9901
I	0.7869	-2.8105	0.8490
C	-0.5478	2.4708	3.8840
N	-0.7972	3.4562	4.4499

SCF = 0.111993
ZPE = 0.092079
H₂₉₈ = 0.212465
G₂₉₈ = 0.170198

		2-Cl	
H	0.3663	0.1215	0.0463
C	0.2296	0.1001	1.1385
C	-0.1201	0.0679	3.9010
C	0.3576	-1.1088	1.8274
C	-0.0686	1.2851	1.8054
C	-0.2459	1.2751	3.1973
C	0.1787	-1.1050	3.2131
H	-0.1661	2.2285	1.2497
H	0.2747	-2.0455	3.7772
H	-0.2580	0.0551	4.9916
I	0.8020	-2.8642	0.8183
Cl	1.3143	-4.8880	-0.3454
C	-0.5501	2.4770	3.8878
N	-0.7997	3.4638	4.4544

SCF = -0.002247
ZPE = 0.092700
H₂₉₈ = 0.100974
G₂₉₈ = 0.053970

		3	
H	0.3774	0.1680	0.0554
C	0.2319	0.1392	1.1478
C	-0.1407	0.0860	3.9237
C	0.3400	-1.0638	1.8477
C	-0.0618	1.3239	1.8206
C	-0.2477	1.2907	3.2117
C	0.1538	-1.0870	3.2306
H	-0.1475	2.2754	1.2676
H	0.2370	-2.0316	3.7928
H	-0.2881	0.0675	5.0175
I	0.7658	-2.7718	0.8567
N	-0.5632	2.5494	3.9407
O	-0.6525	3.5735	3.3186
O	-0.7196	2.5067	5.1312

SCF = 0.068362
ZPE = 0.096903
H₂₉₈ = 0.174506
G₂₉₈ = 0.130071

3-Cl

H	0.3683	0.1091	0.0371
C	0.2322	0.0885	1.1298
C	-0.1152	0.0493	3.9002
C	0.3607	-1.1205	1.8197
C	-0.0652	1.2755	1.7900
C	-0.2402	1.2552	3.1860
C	0.1830	-1.1182	3.2064
H	-0.1639	2.2216	1.2350
H	0.2799	-2.0597	3.7694
H	-0.2530	0.0380	4.9928
I	0.8055	-2.8795	0.8081
Cl	1.3138	-4.8899	-0.3482
N	-0.5561	2.5039	3.9041
O	-0.6628	3.5370	3.2896
O	-0.7057	2.4843	5.1014

SCF = -0.054708**ZPE = 0.097640****H₂₉₈ = 0.054266****G₂₉₈ = 0.005212****4-Cl**

H	0.3633	0.1111	0.0412
C	0.2279	0.0866	1.1332
C	-0.1227	0.0602	3.8877
C	0.3601	-1.1220	1.8193
C	-0.0743	1.2696	1.8053
C	-0.2520	1.2678	3.1932
C	0.1798	-1.1159	3.2035
H	-0.1756	2.2114	1.2473
H	0.2766	-2.0546	3.7701
H	-0.2622	0.0442	4.9780
I	0.8094	-2.8706	0.8132
Cl	1.3349	-4.9140	-0.3627
C	-0.5570	2.5240	3.9147
H	-1.1462	2.3212	4.8428
H	0.3913	3.0393	4.2114
H	-1.1446	3.2237	3.2707

SCF = -0.053604**ZPE = 0.120634****H₂₉₈ = 0.077775****G₂₉₈ = 0.030367****4**

H	0.3846	0.1680	0.0622
C	0.2330	0.1400	1.1526
C	-0.1568	0.0978	3.9120
C	0.3374	-1.0638	1.8510
C	-0.0653	1.3191	1.8324
C	-0.2622	1.3087	3.2184
C	0.1416	-1.0818	3.2320
H	-0.1479	2.2648	1.2761
H	0.2203	-2.0247	3.7957
H	-0.3116	0.0755	5.0011
I	0.7681	-2.7733	0.8642
C	-0.5647	2.5646	3.9419
H	-1.1734	2.3632	4.8577
H	0.3886	3.0600	4.2570
H	-1.1297	3.2758	3.2904

SCF = 0.048208**ZPE = 0.119930****H₂₉₈ = 0.176759****G₂₉₈ = 0.134065****5**

H	1.3410	0.0840	0.2351
C	0.7596	0.0873	1.1716
C	-0.7146	0.1299	3.5340
C	0.3621	-1.1139	1.7570
C	0.4311	1.3067	1.7504
C	-0.3090	1.3606	2.9585
C	-0.3760	-1.0790	2.9394
H	0.7639	2.2288	1.2515
H	-0.7038	-2.0161	3.4181
H	-1.3003	0.1089	4.4648
I	0.8448	-2.8771	0.9040
N	-0.5710	2.5829	3.5967
C	-1.5769	2.5992	4.6265
C	-0.4189	3.7883	2.8243
H	-2.5596	2.1834	4.2720
H	-1.7407	3.6494	4.9848
H	-1.2193	1.9846	5.4962
H	-1.0184	3.7662	1.8734
H	-0.7420	4.6748	3.4309
H	0.6656	3.9200	2.5625

SCF = 0.073602**ZPE = 0.165400****H₂₉₈ = 0.250156****G₂₉₈ = 0.202051**

5-Cl

H	2.0057	-0.0610	0.7362
C	1.1631	0.0074	1.4419
C	-0.9560	0.2177	3.2247
C	0.4130	-1.1324	1.7328
C	0.8779	1.2393	2.0241
C	-0.1944	1.3659	2.9324
C	-0.6433	-1.0046	2.6334
H	1.4956	2.1150	1.7766
H	-1.2536	-1.8854	2.8867
H	-1.8026	0.2730	3.9244
I	0.8497	-2.9507	0.8532
Cl	1.3538	-5.0742	-0.1775
N	-0.4318	2.6385	3.5493
C	-1.1729	2.5928	4.7862
C	-0.9265	3.6422	2.6333
H	-2.2705	2.3852	4.6495
H	-1.0681	3.5889	5.2932
H	-0.7387	1.7993	5.4482
H	-2.0041	3.4917	2.3476
H	-0.8297	4.6476	3.1219
H	-0.3063	3.6281	1.6996

SCF = -0.027122**ZPE = 0.166013****H₂₉₈ = 0.151980****G₂₉₈ = 0.099725****6**

H	0.2852	0.1585	0.0555
C	0.2077	0.0963	1.1529
C	0.0084	-0.0480	3.9410
C	0.3703	-1.1301	1.8046
C	-0.0534	1.2521	1.8779
C	-0.1531	1.1761	3.2808
C	0.2698	-1.1957	3.1929
H	-0.1831	2.2220	1.3773
H	0.3958	-2.1564	3.7177
H	-0.0672	-0.1180	5.0347
I	0.7494	-2.7996	0.7351
O	-0.4141	2.3759	3.9092
C	-0.5215	2.3340	5.3280
H	0.4375	1.9895	5.7857
H	-1.3657	1.6724	5.6401
H	-0.7311	3.3989	5.6031

SCF = -0.000382**ZPE = 0.125583****H₂₉₈ = 0.134569****G₂₉₈ = 0.090317****6-Cl**

H	0.2865	0.1160	0.0359
C	0.2114	0.0527	1.1325
C	0.0164	-0.0830	3.9119
C	0.3775	-1.1803	1.7673
C	-0.0490	1.2150	1.8542
C	-0.1456	1.1384	3.2528
C	0.2766	-1.2288	3.1562
H	-0.1793	2.1833	1.3545
H	0.4033	-2.1885	3.6805
H	-0.0574	-0.1527	5.0044
I	0.7636	-2.8921	0.6745
Cl	1.2147	-4.8934	-0.5972
O	-0.4076	2.3492	3.8896
C	-0.5097	2.2892	5.3018
H	0.4484	1.9367	5.7567
H	-1.3503	1.6217	5.6133
H	-0.7188	3.3469	5.6023

SCF = -0.102817**ZPE = 0.126169****H₂₉₈ = 0.034927****G₂₉₈ = -0.014408****7**

H	1.6572	0.2634	1.3338
C	0.8638	-0.0449	2.0331
C	-1.1396	-0.7897	3.8179
C	0.2925	-1.3129	1.9428
C	0.4364	0.8506	3.0125
C	-0.5685	0.4897	3.9148
C	-0.7126	-1.6816	2.8410
H	0.9003	1.8472	3.0672
H	-1.1745	-2.6801	2.7830
H	-1.9322	-1.0856	4.5233
I	0.9115	-2.6100	0.5247
S	-1.1811	1.4716	5.1471
C	-0.3068	2.9818	5.0414
H	-0.7215	3.6187	5.8590
H	-0.4626	3.4995	4.0684
H	0.7871	2.8553	5.2038

SCF = 0.058870**ZPE = 0.120185****H₂₉₈ = 0.189244****G₂₉₈ = 0.143017**

7-Cl

H	1.6195	0.2832	1.2620
C	0.8524	-0.0487	1.9784
C	-1.0802	-0.8463	3.8049
C	0.3203	-1.3340	1.8788
C	0.4322	0.8347	2.9731
C	-0.5386	0.4422	3.8952
C	-0.6512	-1.7172	2.8070
H	0.8706	1.8417	3.0260
H	-1.0897	-2.7255	2.7537
H	-1.8461	-1.1639	4.5279
I	0.9519	-2.6345	0.3994
Cl	1.6899	-4.1448	-1.3239
S	-1.1476	1.4112	5.1607
C	-0.3070	2.9410	5.0326
H	-0.7049	3.5750	5.8580
H	-0.4984	3.4475	4.0602
H	0.7933	2.8296	5.1574

SCF = -0.045422**ZPE = 0.120788****H₂₉₈ = 0.087785****G₂₉₈ = 0.036304****8-Cl**

H	0.3526	0.0816	0.0250
C	0.2242	0.0628	1.1181
C	-0.1077	0.0416	3.8825
C	0.3661	-1.1416	1.8121
C	-0.0785	1.2484	1.7838
C	-0.2448	1.2367	3.1712
C	0.1954	-1.1337	3.1990
H	-0.1924	2.1917	1.2297
H	0.3007	-2.0704	3.7675
H	-0.2444	0.0387	4.9739
I	0.8184	-2.8992	0.8083
Cl	1.3390	-4.9230	-0.3475
C	-0.5572	2.5237	3.9071
F	-1.2971	2.3787	5.0592
F	0.5445	3.2343	4.3310
F	-1.2711	3.4553	3.1872

SCF = -0.302425**ZPE = 0.099232****H₂₉₈ = -0.190662****G₂₉₈ = -0.242623****8**

H	0.3545	0.1251	0.0438
C	0.2202	0.1052	1.1373
C	-0.1272	0.0829	3.9093
C	0.3495	-1.0889	1.8483
C	-0.0819	1.2902	1.8080
C	-0.2541	1.2746	3.1934
C	0.1751	-1.0991	3.2330
H	-0.1893	2.2339	1.2495
H	0.2736	-2.0357	3.8049
H	-0.2700	0.0778	5.0018
I	0.7882	-2.8030	0.8725
C	-0.5665	2.5711	3.9319
F	-1.3170	2.4119	5.0715
F	0.5468	3.2562	4.3568
F	-1.2662	3.4942	3.1934

SCF = -0.186800**ZPE = 0.098531****H₂₉₈ = -0.077853****G₂₉₈ = -0.125146****9**

H	0.3586	0.1757	0.0665
C	0.2196	0.1489	1.1591
C	-0.1372	0.1148	3.9257
C	0.3373	-1.0515	1.8604
C	-0.0761	1.3316	1.8360
C	-0.2555	1.3169	3.2224
C	0.1587	-1.0653	3.2437
H	-0.1666	2.2723	1.2700
H	0.2490	-2.0051	3.8117
H	-0.2761	0.0890	5.0180
I	0.7649	-2.7628	0.8758
Br	-0.6528	2.9030	4.1341

SCF = 0.069002**ZPE = 0.082213****H₂₉₈ = 0.159403****G₂₉₈ = 0.116642**

9-Cl

H	0.3646	0.1200	0.0453
C	0.2296	0.0940	1.1376
C	-0.1192	0.0636	3.8973
C	0.3586	-1.1154	1.8234
C	-0.0689	1.2797	1.8083
C	-0.2437	1.2636	3.1940
C	0.1797	-1.1114	3.2078
H	-0.1654	2.2198	1.2460
H	0.2748	-2.0507	3.7740
H	-0.2555	0.0407	4.9881
I	0.8039	-2.8668	0.8118
Cl	1.3197	-4.8952	-0.3598
Br	-0.6469	2.8569	4.1118

SCF = -0.040595**ZPE = 0.082854****H₂₉₈ = 0.052583****G₂₉₈ = 0.005120****10**

C	0.2306	-0.0236	1.1259
C	-0.1340	0.0056	3.9253
C	0.1332	-1.2272	1.8389
C	0.1452	1.1945	1.8152
C	-0.0369	1.2145	3.2126
C	-0.0490	-1.2180	3.2364
I	0.4919	-0.0444	-0.8803
C	0.2165	-2.4785	1.1653
N	0.2823	-3.5095	0.6308
C	-0.1466	-2.4443	3.9495
N	-0.2266	-3.4474	4.5329
C	-0.3174	0.0203	5.3351
N	-0.4672	0.0323	6.4885
C	-0.1223	2.4556	3.9015
N	-0.1921	3.4706	4.4650
C	0.2409	2.4316	1.1173
N	0.3169	3.4512	0.5627

SCF = 0.348583**ZPE = 0.091315****H₂₉₈ = 0.455024****G₂₉₈ = 0.397970****10-Cl**

C	0.2253	-0.0239	1.0776
C	-0.1254	0.0054	3.8954
C	0.1288	-1.2195	1.8048
C	0.1438	1.1866	1.7816
C	-0.0300	1.2125	3.1791
C	-0.0452	-1.2164	3.2024
I	0.4855	-0.0455	-1.0180
Cl	0.7718	-0.0691	-3.3241
C	0.2052	-2.4773	1.1398
N	0.2653	-3.5132	0.6137
C	-0.1412	-2.4402	3.9229
N	-0.2194	-3.4418	4.5098
C	-0.3011	0.0200	5.3054
N	-0.4449	0.0320	6.4600
C	-0.1107	2.4510	3.8759
N	-0.1764	3.4645	4.4436
C	0.2357	2.4303	1.0927
N	0.3087	3.4552	0.5469

SCF = 0.201168**ZPE = 0.091685****H₂₉₈ = 0.310118****G₂₉₈ = 0.248347****11**

C	0.2216	-0.0255	1.1243
C	-0.1345	0.0095	3.9559
C	0.1087	-1.2269	1.8494
C	0.1557	1.1935	1.8254
C	-0.0216	1.2206	3.2348
C	-0.0690	-1.2192	3.2590
I	0.4735	-0.0501	-0.8879
F	0.1637	-2.4296	1.2378
F	-0.1734	-2.3851	3.9302
F	-0.3029	0.0259	5.2922
F	-0.0802	2.4028	3.8828
F	0.2572	2.3808	1.1902

SCF = -0.267559**ZPE = 0.054984****H₂₉₈ = -0.201825****G₂₉₈ = -0.249631**

11-I

C	0.0061	-0.0379	1.0821
C	0.0229	0.0055	3.8878
C	0.0397	-1.2600	1.7697
C	-0.0194	1.2067	1.7701
C	-0.0109	1.2278	3.1818
C	0.0478	-1.2232	3.1718
I	0.0770	-3.0976	0.7268
F	0.0797	-2.3566	3.9128
F	0.0314	0.0096	5.2416
F	-0.0349	2.4048	3.8499
F	-0.0517	2.3706	1.0793
F	-0.0039	0.0167	-0.2712
I	0.1231	-5.3814	-0.5694

SCF = -0.356270**11-F**

C	0.0095	-0.0336	1.0908
C	0.0187	0.0137	3.8939
C	0.0382	-1.2552	1.7760
C	-0.0147	1.2133	1.7749
C	-0.0101	1.2356	3.1868
C	0.0424	-1.2142	3.1763
I	0.0748	-3.1460	0.7046
F	0.0693	-2.3490	3.9185
F	0.0234	0.0205	5.2487
F	-0.0329	2.4143	3.8544
F	-0.0422	2.3782	1.0838
F	0.0035	0.0190	-0.2645
F	0.1088	-4.8181	-0.2426

SCF = -0.382633**11-OCH2**

C	1.2098	1.1843	-0.0000
C	-1.2198	2.6050	-0.0000
C	-0.0000	0.4643	-0.0000
C	1.2198	2.6050	-0.0000
C	-0.0000	3.3198	-0.0000
C	-1.2099	1.1842	0.0000
F	-2.4058	0.5568	0.0000
F	-2.3944	3.2698	0.0000
F	-0.0000	4.6670	-0.0000
F	2.3944	3.2698	-0.0000
F	2.4058	0.5568	-0.0000
I	-0.0000	-1.5634	0.0000
O	0.0004	-5.3246	0.0000
C	-0.0001	-6.5525	0.0000
H	-0.9404	-7.1432	0.0000
H	0.9397	-7.1440	0.0000

SCF = -0.318530**11-OMe**

C	0.0571	0.0919	1.1465
C	-0.0172	0.0404	3.9491
C	0.0798	-1.1533	1.7902
C	-0.0019	1.3130	1.8733
C	-0.0393	1.2860	3.2844
C	0.0421	-1.1621	3.1918
I	0.1689	-2.9782	0.6701
F	0.0603	-2.3203	3.8951
F	-0.0525	-0.0005	5.3025
F	-0.0956	2.4400	3.9914
F	-0.0225	2.5004	1.2219
F	0.0905	0.1927	-0.2049
O	0.2531	-4.7508	-0.3318
C	0.2878	-4.6748	-1.7004
H	0.3327	-5.7218	-2.1128
H	1.1905	-4.1174	-2.0766
H	-0.6272	-4.1758	-2.1259

SCF = -0.405331**11-Cl**

C	0.2254	-0.0256	1.0705
C	-0.1266	0.0083	3.9111
C	0.1208	-1.2176	1.8028
C	0.1513	1.1836	1.7778
C	-0.0232	1.2170	3.1888
C	-0.0542	-1.2173	3.2141
I	0.4863	-0.0508	-1.0273
F	0.1818	-2.4291	1.2000
F	-0.1516	-2.3848	3.8929
F	-0.2928	0.0244	5.2546
F	-0.0906	2.4004	3.8432
F	0.2430	2.3804	1.1500
Cl	0.7766	-0.0791	-3.3583

SCF = -0.397908**ZPE = 0.055572****H₂₉₈ = -0.329453****G₂₉₈ = -0.382000**

11-Br

C	0.0072	-0.0361	1.0834
C	0.0216	0.0079	3.8887
C	0.0396	-1.2587	1.7706
C	-0.0182	1.2087	1.7709
C	-0.0109	1.2301	3.1826
C	0.0465	-1.2208	3.1729
I	0.0771	-3.0975	0.7270
F	0.0772	-2.3539	3.9144
F	0.0290	0.0123	5.2427
F	-0.0348	2.4073	3.8506
F	-0.0492	2.3726	1.0798
F	-0.0014	0.0187	-0.2700
Br	0.1207	-5.2332	-0.4854

SCF = -0.380162**11-DMF**

C	-2.4206	1.1824	-0.0001
C	-3.5834	-1.3805	0.0075
C	-1.5796	0.0534	-0.0030
C	-3.8348	1.0459	0.0065
C	-4.4201	-0.2410	0.0103
C	-2.1713	-1.2241	0.0008
F	-1.4242	-2.3492	-0.0017
F	-4.1236	-2.6174	0.0110
F	-5.7603	-0.3799	0.0167
F	-4.6172	2.1457	0.0092
F	-1.9201	2.4368	-0.0035
I	0.4373	0.2622	-0.0125
O	4.3009	0.5907	-0.0155
C	5.5225	0.8201	0.0106
H	5.9390	1.8543	0.0358
N	6.4720	-0.1796	0.0108
C	6.1105	-1.5681	-0.0196
H	6.5439	-2.0589	-0.9324
H	4.9929	-1.6721	-0.0417
H	6.5106	-2.0902	0.8911
C	7.8720	0.1244	0.0412
H	8.3781	-0.2990	-0.8689
H	8.3455	-0.3310	0.9534
H	8.0406	1.2331	0.0637

SCF = -0.327841**11-NH3**

C	0.0005	0.1308	1.1713
C	0.0217	0.1696	3.9838
C	0.0350	-1.0923	1.8664
C	-0.0237	1.3721	1.8625
C	-0.0130	1.3927	3.2759
C	0.0455	-1.0605	3.2731
I	0.0695	-2.8596	0.8643
F	0.0790	-2.1959	4.0049
F	0.0330	0.1685	5.3337
F	-0.0353	2.5648	3.9409
F	-0.0562	2.5296	1.1686
F	-0.0106	0.1758	-0.1792
N	0.1170	-5.3220	-0.5270
H	1.0620	-5.6177	-0.6576
H	-0.3213	-5.2185	-1.4185
H	-0.3733	-6.0125	0.0025

SCF = -0.282298**ZPE = 0.091325****H₂₉₈ = -0.176929****G₂₉₈ = -0.231539****12**

C	0.5713	-0.2872	1.0688
C	-0.0136	0.5852	3.6875
C	0.2446	-1.2124	2.0826
C	0.5985	1.0848	1.3963
C	0.3089	1.5400	2.7000
C	-0.0515	-0.7951	3.3975
I	0.9922	-0.9153	-0.8151
I	-0.5213	-2.1473	4.8366
I	0.3556	3.5200	3.1445
F	-0.2933	1.0028	4.9412
F	0.2145	-2.5302	1.7874
F	0.9095	1.9849	0.4382

SCF = -0.064161**ZPE = 0.049649****H₂₉₈ = -0.002282****G₂₉₈ = -0.055587**

12-Cl

C	0.5822	-0.3035	1.0154
C	-0.0052	0.5710	3.6445
C	0.2601	-1.2182	2.0311
C	0.6023	1.0602	1.3497
C	0.3125	1.5218	2.6562
C	-0.0373	-0.8056	3.3523
I	1.0221	-0.9571	-0.9494
Cl	1.5108	-1.6834	-3.1315
I	-0.5000	-2.1592	4.7974
I	0.3511	3.5050	3.1033
F	-0.2863	0.9901	4.9049
F	0.2301	-2.5422	1.7483
F	0.9080	1.9735	0.3977

SCF = -0.191776**ZPE = 0.050180****H₂₉₈ = -0.127228****G₂₉₈ = -0.185202****13**

C	-0.0003	-0.0036	1.1644
I	-0.0042	-0.0159	-0.8980
Br	-0.9268	-1.5545	1.7845
Br	1.8082	-0.0256	1.7737
Br	-0.8828	1.5786	1.7678

SCF = 0.041017**ZPE = 0.007480****H₂₉₈ = 0.056275****G₂₉₈ = 0.012865****13-Cl**

C	0.0000	-0.0046	1.1029
I	-0.0026	-0.0157	-1.0505
Cl	-0.0052	-0.0282	-3.3832
Br	-0.9042	-1.5675	1.6868
Br	1.8091	-0.0026	1.6757
Br	-0.9028	1.5648	1.6711

SCF = -0.097730**ZPE = 0.008093****H₂₉₈ = -0.079751****G₂₉₈ = -0.127811****14**

C	-0.0002	-0.0024	1.0902
I	0.0066	-0.0204	-1.0852
F	-0.6338	-1.0755	1.6558
F	1.2474	-0.0063	1.6528
F	-0.6193	1.0884	1.6379

SCF = -0.211374**ZPE = 0.015222****H₂₉₈ = -0.190394****G₂₉₈ = -0.226487****14-Cl**

C	-0.0001	-0.0029	0.9836
I	0.0001	-0.0211	-1.2700
Cl	0.0008	-0.0393	-3.5934
F	-0.6171	-1.0708	1.6005
F	1.2372	0.0042	1.5923
F	-0.6210	1.0725	1.5833

SCF = -0.362092**ZPE = 0.015939****H₂₉₈ = -0.338274****G₂₉₈ = -0.379417****15**

C	0.0035	-0.0003	1.1245
I	0.0132	0.0013	-0.9839
C	-0.7154	-1.2414	1.6048
H	-0.1987	-2.1659	1.2501
H	-1.7723	-1.2569	1.2439
H	-0.7295	-1.2581	2.7234
C	1.4341	-0.0009	1.6156
H	1.9787	-0.9094	1.2614
H	1.4471	-0.0016	2.7344
H	1.9790	0.9079	1.2626
C	-0.7150	1.2404	1.6066
H	-0.1980	2.1652	1.2533
H	-0.7290	1.2555	2.7253
H	-1.7719	1.2567	1.2458

SCF = -0.013355**ZPE = 0.121594****H₂₉₈ = 0.116240****G₂₉₈ = 0.076272**

15-Cl

C	-0.0001	-0.0045	1.0534
I	0.0049	-0.0128	-1.0942
Cl	0.0087	-0.0217	-3.5241
C	-0.7142	-1.2365	1.5458
H	-0.2004	-2.1621	1.1893
H	-1.7706	-1.2544	1.1833
H	-0.7366	-1.2679	2.6661
C	1.4240	-0.0031	1.5454
H	1.9679	-0.9114	1.1891
H	1.4627	0.0011	2.6657
H	1.9684	0.9023	1.1824
C	-0.7133	1.2318	1.5358
H	-0.1984	2.1542	1.1725
H	-0.7363	1.2719	2.6559
H	-1.7695	1.2479	1.1726

SCF = -0.108268**ZPE = 0.122243****H₂₉₈ = 0.024096****G₂₉₈ = -0.020956****16**

C	-0.0008	-0.0048	1.1357
I	0.0019	-0.0156	-0.9764
C	-0.6931	-1.2001	1.5825
N	-1.2476	-2.1574	1.9363
C	1.3814	-0.0028	1.5794
N	2.4884	-0.0011	1.9308
C	-0.6927	1.1952	1.5705
N	-1.2468	2.1561	1.9147

SCF = 0.190438**ZPE = 0.036985****H₂₉₈ = 0.235718****G₂₉₈ = 0.193530****16-Cl**

C	-0.0007	-0.0046	1.2050
I	-0.0001	-0.0139	-1.0674
Cl	-0.0003	-0.0234	-3.3660
C	-0.6933	-1.2028	1.5739
N	-1.2602	-2.1834	1.8444
C	1.3845	-0.0031	1.5688
N	2.5181	-0.0020	1.8356
C	-0.6935	1.1966	1.5631
N	-1.2605	2.1794	1.8253

SCF = 0.030949**ZPE = 0.037286****H₂₉₈ = 0.078724****G₂₉₈ = 0.031569****17**

I	0.0935	-1.3396	-1.5269
N	-0.5922	-0.4288	0.0588
C	0.0680	-0.3785	1.3093
C	-1.8198	0.2726	0.1174
O	1.1570	-0.9056	1.5434
O	-2.5998	0.3915	-0.8290
C	-2.0132	0.8463	1.5175
H	-2.1091	1.9581	1.4499
H	-2.9549	0.4344	1.9571
C	-0.7749	0.4190	2.2995
H	-0.1828	1.2934	2.6663
H	-1.0289	-0.2302	3.1734

SCF = -0.058808**ZPE = 0.083635****H₂₉₈ = 0.032943****G₂₉₈ = -0.008805****17-Cl**

I	0.1673	-1.4107	-1.6763
Cl	0.9907	-2.4845	-3.5636
N	-0.5762	-0.4412	0.0279
C	0.0671	-0.3731	1.2634
C	-1.7920	0.2374	0.1052
O	1.1688	-0.8632	1.5662
O	-2.6305	0.3844	-0.8008
C	-2.0136	0.8277	1.5134
H	-2.1251	1.9347	1.4389
H	-2.9474	0.4040	1.9513
C	-0.7721	0.4198	2.2870
H	-0.1865	1.2976	2.6474
H	-1.0086	-0.2335	3.1592

SCF = -0.197015**ZPE = 0.084276****H₂₉₈ = -0.102480****G₂₉₈ = -0.149197****18**

I	-0.0012	0.0257	-0.7708
C	0.0013	-0.0637	1.2392
H	0.0053	0.9286	1.7077
C	-0.0012	-1.1801	1.9529
H	0.0008	-1.1634	3.0535
H	-0.0049	-2.1874	1.5126

SCF = 0.047422**ZPE = 0.042013****H₂₉₈ = 0.094116****G₂₉₈ = 0.062016**

18-Cl

I	-0.0029	-0.0212	-0.9509
Cl	-0.0056	0.1103	-3.3997
C	-0.0003	-0.0755	1.0911
H	0.0009	0.9215	1.5515
C	-0.0000	-1.1562	1.8574
H	0.0014	-1.1179	2.9568
H	-0.0012	-2.1766	1.4522

SCF = -0.047493**ZPE = 0.042657****H₂₉₈ = 0.001899****G₂₉₈ = -0.035539****19**

I	-0.0018	-0.0333	-0.7844
C	0.0011	-0.0568	1.2231
H	0.0048	0.9449	1.6742
C	-0.0009	-1.1685	1.9608
H	-0.0046	-2.1849	1.5225
C	0.0016	-1.1429	3.3815
N	0.0037	-1.1411	4.5453

SCF = 0.096033**ZPE = 0.042466****H₂₉₈ = 0.144679****G₂₉₈ = 0.108169****19-Cl**

I	-0.0020	-0.0569	-0.9419
Cl	-0.0065	0.0209	-3.3421
C	-0.0005	-0.0680	1.1100
H	-0.0004	0.9336	1.5600
C	0.0006	-1.1562	1.8820
H	0.0006	-2.1764	1.4593
C	0.0017	-1.1238	3.3016
N	0.0026	-1.1097	4.4677

SCF = -0.017576**ZPE = 0.042947****H₂₉₈ = 0.033627****G₂₉₈ = -0.007682****20**

I	0.7803	0.2451	-0.5744
C	0.0044	-0.0452	1.2477
H	-0.4482	0.8527	1.6776
C	0.0281	-1.2371	1.8749
H	0.5195	-2.1148	1.4029
N	-0.5881	-1.5432	3.0847
C	-0.0287	-2.6275	3.8513
H	-0.8135	-3.0114	4.5560
H	0.8654	-2.3054	4.4521
H	0.2786	-3.4616	3.1674
C	-1.1660	-0.4702	3.8508
H	-0.3925	0.2625	4.2100
H	-1.7011	-0.8950	4.7404
H	-1.9082	0.0775	3.2109

SCF = 0.049916**ZPE = 0.115756****H₂₉₈ = 0.174570****G₂₉₈ = 0.131606****20-Cl**

I	-0.0589	-0.0395	-0.9110
Cl	0.1920	0.2296	-3.3268
C	-0.3108	-0.2272	1.1079
H	-0.9031	0.5820	1.5500
C	0.1852	-1.2212	1.8490
H	0.7764	-2.0385	1.3917
N	0.1247	-1.3770	3.2651
C	-0.3727	-2.6683	3.6819
H	0.1659	-3.4723	3.1161
H	-1.4776	-2.7979	3.5141
H	-0.1686	-2.7986	4.7777
C	-0.4791	-0.2836	3.9866
H	0.0309	0.6697	3.6893
H	-0.3326	-0.4478	5.0870
H	-1.5815	-0.1708	3.7916

SCF = -0.042887**ZPE = 0.116476****H₂₉₈ = 0.084404****G₂₉₈ = 0.037176****21**

I	0.0000	0.0000	-0.5186
C	0.0000	0.0000	1.3937
H	0.0000	0.0000	3.6532
C	0.0000	0.0000	2.5915

SCF = 0.103223

21-Cl

I	0.0271	-0.0520	-0.8811
Cl	0.2747	-0.1321	-3.2930
C	-0.1749	0.0115	1.0809
H	-0.4090	0.0827	3.3274
C	-0.2994	0.0496	2.2768

SCF = -0.002719**22**

I	1.2371	0.0002	-0.0000
C	-0.6729	-0.0013	0.0000
C	-1.8720	-0.0022	0.0001
C	-3.2417	-0.0002	-0.0001
N	-4.4064	0.0015	0.0001

SCF = 0.155144**22-Cl**

I	0.0243	-0.0540	-0.8476
Cl	0.2685	-0.1351	-3.2064
C	-0.1805	0.0135	1.1290
C	-0.3055	0.0539	2.3301
C	-0.4470	0.0993	3.6864
N	-0.5681	0.1380	4.8469

SCF = 0.027957**23**

I	-0.0000	0.0000	-0.5028
C	0.0000	-0.0000	1.4242
N	0.0000	-0.0000	2.5865

SCF = 0.067769**23-Cl**

I	0.0000	0.0000	0.0765
Cl	-0.0000	-0.0000	-2.3069
C	0.0000	0.0000	2.0765
N	0.0000	0.0000	3.2435

SCF = -0.058092**24**

C	4.9922	2.0887	0.3064
C	3.5850	-0.3211	-0.1457
C	3.5849	2.0867	0.3057
C	5.7036	0.8828	0.0801
C	4.9922	-0.3231	-0.1463
C	2.9010	0.8828	0.0800
C	1.4276	0.8828	0.0800
C	-1.4276	0.8828	0.0799
C	0.7114	1.1065	-1.1131
C	0.7114	0.6591	1.2730
C	-0.7115	0.6591	1.2730
C	-0.7114	1.1065	-1.1132
C	-2.9010	0.8828	0.0798
C	-5.7037	0.8827	0.0797
C	-3.5850	2.0867	0.3055
C	-3.5850	-0.3212	-0.1459
C	-4.9922	-0.3232	-0.1466
C	-4.9923	2.0887	0.3061
I	-2.5506	-2.0368	-0.4665
I	2.5506	-2.0368	-0.4663
F	-7.0529	0.8827	0.0797
F	-5.7077	-1.4476	-0.3579
F	-5.7077	3.2131	0.5174
F	-1.3536	1.3255	-2.2805
F	1.3537	1.3255	-2.2804
F	1.3536	0.4400	2.4403
F	-1.3538	0.4400	2.4402
F	5.7076	3.2132	0.5177
F	7.0528	0.8828	0.0801
F	5.7077	-1.4476	-0.3575
I	2.5505	3.8024	0.6262
I	-2.5506	3.8023	0.6262

SCF = -0.408792**ZPE = 0.152867****H₂₉₈ = -0.226487****G₂₉₈ = -0.315065**

24-Cl

C	-0.8142	0.4954	1.5976
C	1.0140	-0.5238	3.5115
C	-1.0309	-0.7701	2.1695
C	0.3170	1.2580	1.9790
C	1.2261	0.7394	2.9376
C	-0.1159	-1.2566	3.1136
C	-0.3174	-2.5795	3.7293
C	-0.3097	-5.0493	5.1573
C	0.2745	-3.7287	3.1678
C	-1.0163	-2.7042	4.9468
C	-1.0125	-3.9352	5.6585
C	0.2783	-4.9597	3.8796
C	-0.1002	-6.2419	5.9961
C	0.3478	-8.4775	7.6082
C	-1.0103	-7.3071	5.9492
C	1.0321	-6.2572	6.8266
C	1.2518	-7.3837	7.6344
C	-0.7860	-8.4331	6.7601
I	2.3126	-4.6313	6.8197
I	2.3023	-1.3347	4.9137
F	0.5628	-9.5616	8.3883
F	2.3183	-7.4757	8.4611
F	-1.6241	-9.4968	6.7646
F	0.8904	-6.0253	3.3165
F	0.8830	-3.6823	1.9617
F	-1.6738	-1.6530	5.4853
F	-1.6664	-3.9960	6.8401
F	-1.6574	1.0260	0.6802
F	0.5247	2.4759	1.4281
F	2.2899	1.5068	3.2673
Cl	3.6911	-2.5443	6.6180
I	-2.6433	-1.8854	1.6422
I	-2.6265	-7.2154	4.7240

SCF = -0.561905**ZPE = 0.153764****H₂₉₈ = -0.376881****G₂₉₈ = -0.468383****25**

C	1.2019	0.7288	0.0003
C	-1.2149	-0.7369	-0.0007
C	1.2456	-0.6838	-0.0012
C	-0.0306	1.4205	0.0014
C	-1.2322	0.6763	0.0009
C	0.0303	-1.4054	-0.0017
C	2.5359	-1.3921	-0.0021
C	4.9938	-2.7410	-0.0037
C	3.1365	-1.7232	1.2221
C	3.1365	-1.7203	-1.2270
C	4.3701	-2.3971	-1.2302
C	4.3701	-2.4002	1.2236
C	-0.0624	2.8921	0.0030
C	-0.1229	5.6951	0.0062
C	-0.0776	3.5784	-1.2208
C	-0.0768	3.5757	1.2283
C	-0.1072	4.9824	1.2323
C	-0.1080	4.9852	-1.2216
C	-2.4735	-1.5002	-0.0011
C	-4.8709	-2.9539	-0.0018
C	-3.0587	-1.8570	1.2233
C	-3.0599	-1.8539	-1.2258
C	-4.2631	-2.5833	-1.2286
C	-4.2619	-2.5866	1.2253
I	2.2293	-1.2201	-2.9714
I	2.2293	-1.2275	2.9677
I	-0.0540	2.5391	2.9722
I	-0.0557	2.5457	-2.9670
I	-2.1731	-1.3226	2.9686
I	-2.1758	-1.3149	-2.9706
F	2.3556	1.4285	0.0008
F	-2.4150	1.3256	0.0018
F	0.0594	-2.7544	-0.0028
F	-0.1222	5.6965	2.3773
F	-0.1521	7.0442	0.0077
F	-0.1239	5.7018	-2.3650
F	4.9975	-2.7397	-2.3749
F	6.1769	-3.3899	-0.0045
F	4.9974	-2.7457	2.3675
F	-6.0249	-3.6532	-0.0022
F	-4.8757	-2.9525	-2.3730
F	-4.8732	-2.9590	2.3693

SCF = -0.431033**ZPE = 0.200471****H₂₉₈ = -0.191304****G₂₉₈ = -0.300674**

25-Cl

C	0.3021	-1.3266	0.5441
C	-0.3311	1.4135	0.2694
C	1.3454	-0.3763	0.4735
C	-1.0516	-0.9325	0.4503
C	-1.3556	0.4432	0.3422
C	1.0146	0.9931	0.3652
C	2.7475	-0.8147	0.3728
C	5.4051	-1.6494	0.1317
C	3.2637	-1.0721	-0.9093
C	3.5230	-0.9635	1.5309
C	4.8598	-1.3833	1.4114
C	4.5982	-1.4909	-1.0252
C	-2.1153	-1.9430	0.3257
C	-4.1287	-3.8617	0.0390
C	-2.7675	-2.4229	1.4698
C	-2.4414	-2.3962	-0.9646
C	-3.4527	-3.3593	-1.1034
C	-3.7804	-3.3880	1.3274
C	-0.6535	2.8161	-0.0415
C	-1.2628	5.4690	-0.6809
C	-0.7264	3.1877	-1.3954
C	-0.8765	3.7332	0.9948
C	-1.1831	5.0679	0.6749
C	-1.0325	4.5204	-1.7114
I	2.7148	-0.5749	3.3515
I	2.0418	-0.8226	-2.5392
I	-1.4238	-1.6273	-2.5725
I	-2.2472	-1.7256	3.3034
I	-0.3821	1.7652	-2.8341
I	-0.7556	3.1298	2.9288
Cl	0.1274	-0.3708	-4.3027
F	0.6048	-2.6367	0.6745
F	-2.6469	0.8348	0.2783
F	2.0024	1.9137	0.3235
F	-3.8212	-3.8429	-2.3112
F	-5.1028	-4.7898	-0.0982
F	-4.4491	-3.8925	2.3905
F	5.6625	-1.5467	2.4889
F	6.6907	-2.0531	0.0166
F	5.1645	-1.7572	-2.2239
F	-1.5576	6.7524	-0.9889
F	-1.4096	6.0029	1.6270
F	-1.1201	4.9521	-2.9898

SCF = -0.593393**ZPE = 0.201559****H₂₉₈ = -0.350917****G₂₉₈ = -0.462172****26**

H	-1.4241	0.8740	-2.1041
C	-1.3282	1.5965	-1.2778
C	-1.0851	3.4661	0.8257
C	-1.1299	1.2118	0.0317
C	-1.4067	2.9741	-1.5347
C	-1.2858	3.8917	-0.4925
C	-1.0028	2.1002	1.1139
H	-1.5650	3.3207	-2.5701
H	-1.3488	4.9735	-0.7063
H	-0.9922	4.2083	1.6353
C	-0.7974	1.5355	2.4384
C	-0.4073	0.2283	4.9043
C	-0.7381	0.1356	2.5552
C	-0.6528	2.2765	3.6154
C	-0.4594	1.6195	4.8360
C	-0.5493	-0.5435	3.7406
H	-0.6907	3.3777	3.5832
H	-0.3465	2.2169	5.7581
H	-0.5078	-1.6430	3.7984
H	-0.2543	-0.2793	5.8718
I	-0.9763	-0.7719	0.6836

SCF = 0.436446**ZPE = 0.163515****H₂₉₈ = 0.610661****G₂₉₈ = 0.563681****26-Cl**

H	-1.4296	0.8697	-2.1005
C	-1.3322	1.6052	-1.2796
C	-1.0833	3.4696	0.8165
C	-1.1340	1.2067	0.0280
C	-1.4071	2.9789	-1.5389
C	-1.2831	3.8978	-0.4974
C	-1.0051	2.1018	1.1005
H	-1.5645	3.3250	-2.5714
H	-1.3433	4.9766	-0.7113
H	-0.9871	4.2051	1.6288
C	-0.8001	1.5260	2.4218
C	-0.4162	0.2085	4.8497
C	-0.7541	0.1227	2.4702
C	-0.6530	2.2671	3.5969
C	-0.4612	1.6010	4.8085
C	-0.5635	-0.5347	3.6736
H	-0.6870	3.3660	3.5743
H	-0.3450	2.1821	5.7358
H	-0.5262	-1.6336	3.7186
H	-0.2645	-0.3091	5.8087
I	-0.9903	-0.8057	0.6420
Cl	-1.2828	-1.5255	-1.5402

SCF = 0.173120**ZPE = 0.165531****H₂₉₈ = 0.351192**

G₂₉₈ = 0.300145

27			
H	0.0009	0.1625	0.1234
C	-0.0070	0.1360	1.2259
C	-0.0251	0.0986	4.0542
C	-0.0412	-1.0375	1.9483
C	0.0183	1.3381	1.9528
C	0.0078	1.3071	3.3464
C	-0.0502	-1.1107	3.3529
H	0.0514	2.3033	1.4135
H	-0.0259	0.1100	5.1589
C	-0.0846	-2.4288	3.9668
C	-0.1563	-5.0762	4.9404
C	-0.1098	-3.5507	3.1189
C	-0.0949	-2.6704	5.3439
C	-0.1295	-3.9898	5.8136
C	-0.1460	-4.8587	3.5524
H	-0.0810	-1.8324	6.0637
H	-0.1668	-5.7195	2.8631
H	-0.1904	-6.1099	5.3323
I	-0.0857	-2.9563	1.1113
C	0.0158	2.6276	4.1332
C	-0.1210	-4.2379	7.3305
F	0.6353	3.6569	3.4749
F	0.6508	2.5393	5.3448
F	-1.2429	3.0881	4.4210
F	-0.7397	-3.2491	8.0507
F	-0.7451	-5.3994	7.7018
F	1.1435	-4.3240	7.8528

SCF = -0.033225**ZPE = 0.175829****H₂₉₈ = 0.160823****G₂₉₈ = 0.096824****27-Cl**

H	-0.1614	0.0876	0.1463
C	-0.1290	0.0753	1.2468
C	-0.0475	0.0850	4.0554
C	-0.1234	-1.1174	1.9495
C	-0.0931	1.2882	1.9429
C	-0.0521	1.2843	3.3379
C	-0.0836	-1.1219	3.3536
H	-0.1017	2.2449	1.3957
H	-0.0208	0.1056	5.1564
C	-0.0835	-2.4377	3.9758
C	-0.0926	-5.0786	4.9456
C	-0.1226	-3.5476	3.1184
C	-0.0475	-2.6770	5.3537
C	-0.0516	-3.9937	5.8225
C	-0.1290	-4.8550	3.5639
H	-0.0212	-1.8372	6.0671
H	-0.1617	-5.7097	2.8603
H	-0.1013	-6.1101	5.3350
I	-0.1720	-2.9953	1.0819
Cl	-0.2188	-5.2141	0.4620
C	0.0055	2.6080	4.0940
C	0.0073	-4.2474	7.3288
F	1.2807	3.0672	4.3210
F	-0.5673	2.5762	5.3422
F	-0.6209	3.6529	3.4600
F	-0.5797	-3.2677	8.0908
F	-0.6056	-5.4079	7.7312
F	1.2844	-4.3457	7.8243

SCF = -0.317678**ZPE = 0.177886****H₂₉₈ = -0.119741****G₂₉₈ = -0.187711**

28

H	-0.1655	0.1730	0.1433
C	-0.1292	0.1482	1.2453
C	-0.0357	0.1063	4.0726
C	-0.1249	-1.0269	1.9667
C	-0.0850	1.3497	1.9678
C	-0.0387	1.3247	3.3677
C	-0.0794	-1.1002	3.3704
H	-0.0869	2.3112	1.4242
H	0.0010	0.1107	5.1753
C	-0.0813	-2.4203	3.9833
C	-0.0937	-5.0726	4.9500
C	-0.1282	-3.5398	3.1336
C	-0.0398	-2.6625	5.3583
C	-0.0462	-3.9871	5.8342
C	-0.1359	-4.8492	3.5658
H	-0.0020	-1.8229	6.0732
H	-0.1731	-5.7070	2.8736
H	-0.0983	-6.1084	5.3338
I	-0.1848	-2.9434	1.1286
C	0.0061	2.5460	4.0947
N	0.0428	3.5458	4.6879
C	-0.0036	-4.2199	7.2364
N	0.0313	-4.4113	8.3831

SCF = 0.559691**ZPE = 0.163294****H₂₉₈ = 0.737025****G₂₉₈ = 0.682661****28-Cl**

H	-0.1694	0.0981	0.1623
C	-0.1321	0.0863	1.2627
C	-0.0365	0.0914	4.0712
C	-0.1267	-1.1074	1.9637
C	-0.0897	1.2988	1.9571
C	-0.0420	1.2997	3.3575
C	-0.0791	-1.1130	3.3674
H	-0.0937	2.2516	1.4052
H	0.0012	0.1046	5.1709
C	-0.0784	-2.4305	3.9882
C	-0.0866	-5.0753	4.9516
C	-0.1247	-3.5384	3.1289
C	-0.0354	-2.6704	5.3646
C	-0.0397	-3.9915	5.8390
C	-0.1299	-4.8465	3.5722
H	0.0017	-1.8292	6.0740
H	-0.1671	-5.6986	2.8655
H	-0.0897	-6.1088	5.3324
I	-0.1851	-2.9828	1.0946
Cl	-0.2407	-5.2016	0.4681
C	0.0012	2.5326	4.0649
N	0.0365	3.5418	4.6426
C	0.0042	-4.2297	7.2411
N	0.0400	-4.4255	8.3871

SCF = 0.279226**ZPE = 0.165107****H₂₉₈ = 0.460239****G₂₉₈ = 0.401813****29**

H	0.0282	0.1593	0.1530
C	-0.0471	0.1307	1.2524
C	-0.2399	0.0555	4.0659
C	-0.0414	-1.0593	1.9567
C	-0.1514	1.3170	1.9641
C	-0.2507	1.3173	3.3884
C	-0.1358	-1.1318	3.3576
H	-0.1558	2.2635	1.4001
H	-0.3148	0.0174	5.1635
C	-0.1166	-2.4631	3.9612
C	-0.0585	-5.1245	4.8846
C	-0.0054	-3.5622	3.0915
C	-0.1999	-2.7151	5.3221
C	-0.1731	-4.0560	5.8246
C	0.0250	-4.8758	3.5223
H	-0.2876	-1.8663	6.0176
H	0.1129	-5.7196	2.8185
H	-0.0342	-6.1722	5.2248
I	0.1052	-2.9524	1.1048
N	-0.3537	2.4944	4.0906
N	-0.2556	-4.3057	7.1737
C	-0.3631	3.7553	3.3969
H	0.5897	3.8870	2.8148
H	-0.4526	4.5996	4.1304
H	-1.2346	3.8038	2.6881
C	-0.4538	2.4845	5.5248
H	0.4554	2.0017	5.9768
H	-1.3689	1.9173	5.8490
H	-0.5297	3.5341	5.9145
C	-0.3712	-3.2230	8.1126
H	0.5214	-2.5435	8.0376
H	-0.4264	-3.6232	9.1595
H	-1.3029	-2.6273	7.9096
C	-0.2271	-5.6582	7.6648
H	0.7350	-6.1598	7.3699
H	-1.0893	-6.2441	7.2435
H	-0.3044	-5.6648	8.7841

SCF = 0.445337**ZPE = 0.309655****H₂₉₈ = 0.774922****G₂₉₈ = 0.708630**

29-Cl

H	-0.0666	0.1058	0.1677
C	-0.0713	0.0864	1.2690
C	-0.0887	0.0802	4.0679
C	-0.0770	-1.1150	1.9547
C	-0.0744	1.2949	1.9619
C	-0.0725	1.3197	3.3778
C	-0.0864	-1.1171	3.3576
H	-0.0731	2.2292	1.3812
H	-0.0946	0.0527	5.1670
C	-0.0956	-2.4394	3.9782
C	-0.1028	-5.0806	4.9315
C	-0.0878	-3.5414	3.1097
C	-0.1054	-2.6791	5.3494
C	-0.1106	-4.0068	5.8537
C	-0.0863	-4.8467	3.5573
H	-0.0852	-1.8230	6.0406
H	-0.0800	-5.6973	2.8485
H	-0.1125	-6.1254	5.2775
I	-0.0750	-2.9793	1.0848
Cl	-0.0841	-5.2093	0.4316
N	0.0161	2.5340	4.0843
N	-0.0374	-4.2213	7.2453
C	-0.2619	3.7465	3.3583
H	0.5286	3.8902	2.5732
H	-0.2241	4.6246	4.0553
H	-1.2684	3.7284	2.8577
C	-0.3628	2.5220	5.4738
H	0.3985	1.9330	6.0533
H	-1.3756	2.0629	5.6399
H	-0.3744	3.5683	5.8779
C	-0.9605	-3.4906	8.0808
H	-1.1373	-2.4610	7.6775
H	-0.5100	-3.4027	9.1057
H	-1.9524	-4.0137	8.1693
C	0.2160	-5.5684	7.6946
H	1.1124	-5.9772	7.1580
H	-0.6573	-6.2566	7.5270
H	0.4393	-5.5377	8.7942

SCF = 0.200560**ZPE = 0.311590****H₂₉₈ = 0.533633****G₂₉₈ = 0.463936****30**

H	1.5491	-0.3132	1.8555
C	0.5807	0.0878	2.1963
C	-1.8846	1.1463	3.0427
C	-0.5621	-0.6967	2.2957
C	0.4770	1.4401	2.5371
C	-0.7507	1.9583	2.9577
C	-1.7967	-0.2081	2.7054
H	1.3660	2.0940	2.4742
H	-2.8496	1.5694	3.3768
C	1.4167	-3.7040	3.8973
C	-0.6179	-4.5994	5.6216
C	0.0705	-3.5646	3.5821
C	1.7439	-4.3052	5.1168
C	0.7277	-4.7440	5.9696
C	-0.9608	-4.0003	4.4054
H	2.8044	-4.4388	5.3983
H	-2.0235	-3.8979	4.1317
H	-1.4113	-4.9640	6.2994
I	-0.4311	-2.7117	1.7348
C	-0.8597	3.4482	3.3137
C	1.0952	-5.3827	7.3170
F	-1.8125	3.7193	4.2610
F	-1.1863	4.2362	2.2405
F	0.3012	3.9816	3.8102
F	1.1982	-4.4679	8.3336
F	0.1826	-6.3054	7.7573
F	2.2966	-6.0418	7.3057
H	-2.6967	-0.8415	2.7647
H	2.2225	-3.3687	3.2243

SCF = -0.046846**ZPE = 0.195701****H₂₉₈ = 0.168729****G₂₉₈ = 0.100126**

30-Cl

H	1.5146	-0.5815	1.5959
C	0.6194	-0.1410	2.0630
C	-1.6394	1.0185	3.2236
C	-0.5394	-0.8954	2.2349
C	0.6587	1.1930	2.4707
C	-0.4730	1.7662	3.0541
C	-1.6672	-0.3144	2.8089
H	1.5700	1.7955	2.3286
H	-2.5311	1.4825	3.6746
C	0.7497	-2.8401	4.2341
C	-0.3396	-5.2719	5.1072
C	-0.1224	-3.5700	3.4348
C	1.0796	-3.3390	5.4957
C	0.5326	-4.5510	5.9245
C	-0.6738	-4.7780	3.8427
H	1.7653	-2.7765	6.1505
H	-1.3465	-5.3619	3.1870
H	-0.7670	-6.2272	5.4547
I	-0.6178	-2.8330	1.5305
Cl	-0.7462	-4.9764	0.7024
C	-0.4281	3.2167	3.5225
C	0.9096	-5.1016	7.2990
F	0.0069	3.3718	4.8175
F	-1.6392	3.8640	3.4960
F	0.4048	4.0273	2.7904
F	1.1827	-4.1375	8.2377
F	-0.0586	-5.8816	7.8810
F	2.0297	-5.8961	7.2904
H	-2.5953	-0.8927	2.9406
H	1.1750	-1.8792	3.8967

SCF = -0.319576**ZPE = 0.197915****H₂₉₈ = -0.100012****G₂₉₈ = -0.171971****31**

H	1.6017	-0.2879	2.0545
C	0.5947	0.0819	2.3074
C	-1.9711	1.0554	2.9297
C	-0.5328	-0.7292	2.2554
C	0.4276	1.4155	2.6867
C	-0.8523	1.9011	2.9991
C	-1.8143	-0.2797	2.5514
H	1.3047	2.0841	2.7354
H	-2.9773	1.4412	3.1691
C	1.3370	-3.7626	3.9355
C	-0.8462	-4.7699	5.3974
C	0.0281	-3.6342	3.4858
C	1.5524	-4.4101	5.1540
C	0.4630	-4.9111	5.8846
C	-1.0720	-4.1239	4.1799
H	2.5815	-4.5284	5.5357
H	-2.1022	-4.0264	3.8006
H	-1.7006	-5.1707	5.9701
I	-0.2977	-2.7144	1.6337
H	-2.6994	-0.9336	2.4901
H	2.1989	-3.3812	3.3642
C	-1.0170	3.2591	3.3862
N	-1.1518	4.3701	3.7030
C	0.6875	-5.5682	7.1252
N	0.8711	-6.1056	8.1403

SCF = 0.546127**ZPE = 0.183104****H₂₉₈ = 0.744985****G₂₉₈ = 0.686116**

31-Cl

H	1.5775	-0.6319	1.7073
C	0.6696	-0.1823	2.1400
C	-1.6214	0.9956	3.2172
C	-0.5140	-0.9126	2.2243
C	0.7206	1.1359	2.5921
C	-0.4287	1.7273	3.1355
C	-1.6561	-0.3213	2.7581
H	1.6560	1.7115	2.5201
H	-2.5261	1.4599	3.6386
C	0.6316	-2.9587	4.2160
C	-0.5500	-5.3962	4.9432
C	-0.2155	-3.6386	3.3489
C	0.8901	-3.5078	5.4722
C	0.2978	-4.7265	5.8363
C	-0.8097	-4.8485	3.6847
H	1.5591	-2.9833	6.1723
H	-1.4603	-5.3923	2.9745
H	-1.0116	-6.3558	5.2255
I	-0.6016	-2.8222	1.4528
Cl	-0.7400	-4.9313	0.5364
H	-2.6024	-0.8816	2.8221
H	1.0923	-1.9963	3.9337
C	-0.3843	3.0700	3.6017
N	-0.3478	4.1684	3.9835
C	0.5611	-5.2847	7.1178
N	0.7762	-5.7410	8.1659

SCF = 0.277393**ZPE = 0.185082****H₂₉₈ = 0.480036****G₂₉₈ = 0.417636****32**

H	1.5958	-0.2676	2.3062
C	0.5857	0.0950	2.5577
C	-1.9857	1.0265	3.1854
C	-0.5317	-0.7311	2.4590
C	0.4216	1.4036	2.9743
C	-0.8724	1.9167	3.3030
C	-1.8132	-0.2807	2.7680
H	1.3127	2.0473	3.0443
H	-3.0046	1.3711	3.4229
C	1.3291	-3.8289	4.0254
C	-0.8608	-4.9103	5.4070
C	0.0256	-3.6725	3.5595
C	1.5465	-4.5338	5.1953
C	0.4573	-5.1009	5.9286
C	-1.0699	-4.2041	4.2363
H	2.5822	-4.6534	5.5507
H	-2.0978	-4.0803	3.8581
H	-1.7351	-5.3287	5.9303
I	-0.2882	-2.6722	1.7696
H	-2.6929	-0.9393	2.6823
H	2.1909	-3.4095	3.4811
N	-1.0391	3.2143	3.7185
N	0.6687	-5.7995	7.0911
C	-2.3511	3.7172	4.0281
H	-2.2890	4.7923	4.3429
H	-2.8061	3.1246	4.8681
H	-3.0202	3.6463	3.1273
C	0.0908	4.0998	3.8138
H	0.5867	4.2111	2.8108
H	0.8400	3.6958	4.5483
H	-0.2402	5.1133	4.1629
C	2.0036	-5.9958	7.5906
H	2.4887	-5.0040	7.8028
H	2.6256	-6.5525	6.8374
H	1.9774	-6.5907	8.5415
C	-0.4384	-6.3775	7.8054
H	-0.0715	-6.9106	8.7219
H	-0.9812	-7.1165	7.1548
H	-1.1576	-5.5740	8.1232

SCF = 0.430317**ZPE = 0.329665****H₂₉₈ = 0.781507****G₂₉₈ = 0.710876**

32-Cl

H	1.3984	-0.6042	1.8919
C	0.4777	-0.1616	2.3059
C	-1.8279	0.9958	3.3490
C	-0.7028	-0.8993	2.3409
C	0.5263	1.1424	2.7839
C	-0.6355	1.7620	3.3103
C	-1.8490	-0.3063	2.8633
H	1.4813	1.6856	2.7350
H	-2.7576	1.4209	3.7546
C	0.3488	-3.0072	4.3397
C	-0.5833	-5.5993	4.8201
C	-0.3819	-3.6931	3.3774
C	0.6176	-3.6156	5.5583
C	0.1486	-4.9284	5.8365
C	-0.8465	-4.9832	3.6035
H	1.2001	-3.0542	6.3034
H	-1.4041	-5.5354	2.8229
H	-0.9569	-6.6228	4.9742
I	-0.7770	-2.7812	1.5397
Cl	-0.9253	-4.8221	0.4428
H	-2.7980	-0.8656	2.9007
H	0.7143	-1.9821	4.1525
N	-0.6226	3.1060	3.7150
N	0.3522	-5.5160	7.0847
C	-1.7196	3.5758	4.5195
H	-1.5340	4.6344	4.8404
H	-1.8783	2.9453	5.4368
H	-2.6592	3.5564	3.9037
C	0.6554	3.7296	3.9361
H	1.2039	3.7968	2.9579
H	1.2909	3.1568	4.6656
H	0.5108	4.7706	4.3279
C	1.3008	-4.9167	7.9840
H	0.9336	-3.8978	8.2841
H	2.3162	-4.8093	7.5131
H	1.3996	-5.5412	8.9105
C	0.0812	-6.9201	7.2393
H	0.3540	-7.2522	8.2753
H	0.6550	-7.5423	6.4991
H	-1.0173	-7.1034	7.0888

SCF = 0.196321
 ZPE = 0.331543
 H₂₉₈ = 0.551098
 G₂₉₈ = 0.477031

33

I	-1.3372	1.1106	-3.3038
C	-0.7474	0.4740	-1.4684
C	0.0896	-0.3210	1.0610
N	-0.9565	-0.8201	-1.0615
C	-0.1159	1.3923	-0.6163
C	0.3076	0.9981	0.6578
C	-0.5437	-1.2101	0.1845
H	0.0452	2.4316	-0.9593
H	0.8055	1.7202	1.3308
H	0.4056	-0.6797	2.0566
C	-1.6108	-1.7902	-1.9312
H	-1.0113	-1.9156	-2.8750
H	-2.6483	-1.4335	-2.1812
H	-1.6830	-2.7839	-1.4111
H	-0.7313	-2.2657	0.4762

SCF = 0.331708
 ZPE = 0.119216
 H₂₉₈ = 0.459324
 G₂₉₈ = 0.417251

33-Cl

I	-1.3746	1.1653	-3.4353
Cl	-2.0235	1.9077	-5.4905
C	-0.7585	0.4685	-1.4893
C	0.0757	-0.3417	1.0503
N	-0.9562	-0.8086	-1.0758
C	-0.1210	1.3866	-0.6102
C	0.2941	0.9938	0.6461
C	-0.5468	-1.2189	0.1792
H	0.0279	2.4178	-0.9689
H	0.7886	1.6974	1.3338
H	0.3934	-0.6885	2.0437
C	-1.6052	-1.7707	-1.9503
H	-1.0077	-1.8765	-2.8963
H	-2.6355	-1.4035	-2.2085
H	-1.6803	-2.7676	-1.4425
H	-0.7366	-2.2721	0.4565

SCF = 0.071519
 ZPE = 0.120376
 H₂₉₈ = 0.202550
 G₂₉₈ = 0.155335

34

I	-1.4082	1.1556	-3.2672
C	-0.7567	0.5643	-1.4563
C	0.1089	-0.3460	1.0201
C	-0.9213	-0.7713	-1.0685
C	-0.1404	1.4602	-0.5717
C	0.2940	0.9973	0.6744
N	-0.4934	-1.2181	0.1539
H	-1.4038	-1.5226	-1.7321
H	0.0045	2.5225	-0.8481
H	0.7835	1.6758	1.3959
H	0.4424	-0.7450	2.0015
H	-0.1441	-3.2672	-0.2266
C	-0.6861	-2.6169	0.5135
H	-0.2827	-2.8108	1.5435
H	-1.7847	-2.8560	0.4936

SCF = 0.328508**ZPE = 0.118909****H₂₉₈ = 0.455118****G₂₉₈ = 0.414324****35**

I	-1.4070	0.9998	-3.2708
C	-0.7114	0.4922	-1.4499
N	0.2568	-0.2148	1.0893
C	-0.7349	-0.8400	-1.0188
C	-0.1930	1.4635	-0.5840
C	0.2853	1.0906	0.6773
C	-0.2469	-1.1721	0.2505
H	-1.1327	-1.6495	-1.6589
H	-0.1494	2.5311	-0.8700
H	0.7021	1.8393	1.3839
H	-0.2531	-2.2205	0.6170
H	1.8849	-0.7717	2.3117
C	0.7794	-0.5820	2.3979
H	0.5969	0.2532	3.1272
H	0.2666	-1.5114	2.7664

SCF = 0.329038**ZPE = 0.118923****H₂₉₈ = 0.456593****G₂₉₈ = 0.413270****34-Cl**

I	-1.4542	1.1726	-3.3864
Cl	-2.2141	1.8012	-5.4604
C	-0.7612	0.5703	-1.4778
C	0.1064	-0.3440	1.0044
C	-0.9280	-0.7571	-1.0850
C	-0.1404	1.4555	-0.5929
C	0.2961	0.9966	0.6552
N	-0.5012	-1.2130	0.1397
H	-1.4132	-1.5026	-1.7456
H	0.0052	2.5117	-0.8766
H	0.7884	1.6676	1.3750
H	0.4381	-0.7411	1.9809
H	-0.1634	-3.2584	-0.2357
C	-0.6965	-2.6025	0.5043
H	-0.2930	-2.8009	1.5318
H	-1.7944	-2.8399	0.4857

SCF = 0.091392**ZPE = 0.119906****H₂₉₈ = 0.221157****G₂₉₈ = 0.175513****35-Cl**

I	-1.4266	1.0399	-3.3788
Cl	-2.2076	1.6258	-5.4571
C	-0.7107	0.5034	-1.4750
N	0.2464	-0.2144	1.0771
C	-0.7293	-0.8309	-1.0351
C	-0.1939	1.4651	-0.5902
C	0.2762	1.0968	0.6654
C	-0.2527	-1.1713	0.2261
H	-1.1241	-1.6267	-1.6882
H	-0.1554	2.5273	-0.8833
H	0.6891	1.8312	1.3819
H	-0.2543	-2.2130	0.5976
H	1.8678	-0.7754	2.3017
C	0.7631	-0.5842	2.3774
H	0.5804	0.2461	3.1103
H	0.2509	-1.5137	2.7426

SCF = 0.092672**ZPE = 0.119983****H₂₉₈ = 0.223444****G₂₉₈ = 0.175766**

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N	-0.3880	0.5739	-0.1881
C	-0.5936	1.8587	-0.6516
N	-0.3322	2.7361	0.3827
C	0.0074	0.6411	1.1532
H	0.2315	-0.2510	1.7487
C	0.0421	1.9969	1.5112
H	0.3013	2.4671	2.4665
I	-1.1714	2.3631	-2.5053
H	0.2821	4.5704	-0.4528
C	-0.4246	4.1716	0.3264
H	-0.1458	4.5928	1.3306
H	-1.4773	4.4778	0.0745
H	0.1516	-0.6387	-1.8247
C	-0.5485	-0.6406	-0.9442
H	-0.3079	-1.5155	-0.2807
H	-1.6102	-0.7294	-1.3053

SCF = 0.347948**ZPE = 0.128343****H₂₉₈ = 0.485972****G₂₉₈ = 0.441256****36-Cl**

N	-0.3897	0.5857	-0.1981
C	-0.6001	1.8654	-0.6704
N	-0.3350	2.7266	0.3752
C	0.0104	0.6413	1.1535
H	0.2327	-0.2520	1.7363
C	0.0447	1.9844	1.5131
H	0.3019	2.4554	2.4613
I	-1.2260	2.4169	-2.6662
H	0.2730	4.5556	-0.4555
C	-0.4270	4.1546	0.3271
H	-0.1517	4.5804	1.3276
H	-1.4765	4.4605	0.0663
H	0.1417	-0.6107	-1.8386
C	-0.5488	-0.6211	-0.9520
H	-0.3076	-1.5024	-0.3013
H	-1.6081	-0.7052	-1.3179
Cl	-1.8838	2.9968	-4.7632

SCF = 0.077483**ZPE = 0.129346****H₂₉₈ = 0.217140****G₂₉₈ = 0.170538****37**

N	-0.3587	0.5756	-0.2096
C	-0.5646	1.8631	-0.6611
N	-0.3416	2.7364	0.3838
C	0.0079	0.6338	1.1446
C	0.0060	1.9887	1.5202
I	-1.1005	2.3807	-2.5308
H	-0.2740	4.5500	-0.7010
C	-0.4615	4.1747	0.3414
H	0.2991	4.6220	1.0423
H	-1.4954	4.4695	0.6784
H	0.5391	-0.9118	-1.3942
C	-0.4744	-0.6359	-0.9867
H	-0.8423	-1.4627	-0.3152
H	-1.2022	-0.4888	-1.8300
C	0.3249	-0.6337	1.9551
C	0.3085	2.6580	2.8709
F	0.8952	-0.3806	3.1661
F	1.1897	-1.4686	1.2977
F	-0.7955	-1.3814	2.1982
F	1.4918	3.3457	2.8497
F	-0.6455	3.5768	3.2210
F	0.3854	1.7816	3.9110

SCF = -0.105370**ZPE = 0.140818****H₂₉₈ = 0.052448****G₂₉₈ = -0.008444****37-Cl**

N	-0.3497	0.5875	-0.2178
C	-0.5699	1.8693	-0.6815
N	-0.3543	2.7287	0.3776
C	0.0139	0.6375	1.1453
C	0.0003	1.9830	1.5224
I	-1.1544	2.4357	-2.7228
H	-0.5134	4.5053	-0.7232
C	-0.4825	4.1583	0.3452
H	0.3953	4.6208	0.8734
H	-1.4299	4.4624	0.8690
H	0.5788	-1.0031	-1.2237
C	-0.4516	-0.6191	-0.9890
H	-1.0066	-1.3938	-0.3928
H	-1.0017	-0.4046	-1.9451
Cl	-1.7556	3.0185	-4.8226
C	0.3252	-0.6198	1.9413
C	0.2988	2.6495	2.8560
F	0.8991	-0.3952	3.1617
F	1.1900	-1.4715	1.2988
F	-0.7860	-1.3837	2.1969
F	1.4835	3.3424	2.8579
F	-0.6447	3.5767	3.2253
F	0.3790	1.7917	3.9175

SCF = -0.399424

ZPE = 0.142158
H₂₉₈ = -0.238130
G₂₉₈ = -0.304057

38

N	0.0669	-0.9994	-0.9049
C	-0.5125	0.1303	-1.4468
N	-0.5586	1.1184	-0.4839
C	0.3981	-0.7253	0.4355
C	0.0046	0.6067	0.7003
I	-1.1813	0.3081	-3.3347
H	-2.1794	2.3908	-0.9246
C	-1.0895	2.4486	-0.6502
H	-0.5194	2.9867	-1.4575
H	-0.9801	3.0101	0.3188
H	0.9780	-2.0834	-2.4653
C	0.2982	-2.2501	-1.5841
H	0.7861	-2.9697	-0.8698
H	-0.6819	-2.6797	-1.9324
C	1.0088	-1.6388	1.3177
N	1.5123	-2.3706	2.0687
C	0.1339	1.3235	1.9066
N	0.2539	1.8897	2.9155

SCF = 0.485335
ZPE = 0.128213
H₂₉₈ = 0.626555
G₂₉₈ = 0.574279

38-Cl

N	0.0746	-0.9805	-0.9148
C	-0.4967	0.1469	-1.4717
N	-0.5496	1.1178	-0.4909
C	0.3895	-0.7225	0.4399
C	-0.0039	0.6000	0.7071
I	-1.1920	0.3566	-3.5372
H	-2.1548	2.3857	-0.9555
C	-1.0735	2.4436	-0.6535
H	-0.4966	2.9797	-1.4557
H	-0.9834	3.0061	0.3134
H	0.9981	-2.0431	-2.4699
C	0.3139	-2.2205	-1.5957
H	0.7885	-2.9529	-0.8902
H	-0.6604	-2.6372	-1.9711
Cl	-1.9093	0.5731	-5.6724
C	0.9853	-1.6442	1.3233
N	1.4765	-2.3907	2.0677
C	0.1071	1.3085	1.9198
N	0.2073	1.8764	2.9298

SCF = 0.195125
ZPE = 0.128925
H₂₉₈ = 0.337704

G₂₉₈ = 0.283545

39

N	-0.3570	0.5779	-0.2086
C	-0.5626	1.8624	-0.6651
N	-0.3413	2.7332	0.3806
C	0.0019	0.6295	1.1524
C	0.0117	1.9917	1.5248
I	-1.0934	2.3769	-2.5330
H	-0.7327	4.5277	-0.6692
C	-0.4428	4.1677	0.3543
H	0.5526	4.6087	0.6392
H	-1.2205	4.4920	1.1004
H	0.5147	-1.1744	-0.9528
C	-0.4769	-0.6422	-0.9607
H	-1.2534	-1.2955	-0.4742
H	-0.7785	-0.4282	-2.0211
C	0.2967	-0.5599	1.9678
H	1.1614	-1.1296	1.5381
H	-0.5923	-1.2417	2.0085
H	0.5571	-0.2520	3.0119
C	0.3197	2.5968	2.8306
H	1.1973	3.2897	2.7483
H	0.5665	1.7968	3.5735
H	-0.5580	3.1799	3.2134

SCF = 0.318196
ZPE = 0.183224
H₂₉₈ = 0.513111
G₂₉₈ = 0.464049

39-Cl

N	-0.3462	0.5899	-0.2155
C	-0.4905	1.8716	-0.6991
N	-0.2977	2.7280	0.3624
C	-0.0573	0.6312	1.1732
C	-0.0267	1.9808	1.5380
I	-0.9366	2.4345	-2.7439
H	-0.5850	4.4989	-0.7226
C	-0.3543	4.1568	0.3226
H	0.6343	4.5815	0.6464
H	-1.1551	4.5210	1.0216
H	-0.6949	-0.3798	-2.0415
C	-0.4628	-0.6207	-0.9687
H	0.5029	-1.1925	-0.9134
H	-1.2868	-1.2526	-0.5397
Cl	-1.4045	3.0252	-4.8890
C	0.1559	-0.5660	1.9999
H	1.0234	-1.1609	1.6151
H	-0.7528	-1.2208	1.9864
H	0.3669	-0.2698	3.0570
C	0.2275	2.5886	2.8526
H	1.1235	3.2593	2.8097
H	0.4141	1.7918	3.6141
H	-0.6526	3.1985	3.1813

SCF = 0.051193**ZPE = 0.184904****H₂₉₈ = 0.251719****G₂₉₈ = 0.193781****40**

N	-0.0949	-1.1278	-0.9781
C	-0.5151	0.0668	-1.5341
N	-0.4708	1.0549	-0.5730
C	0.2501	-0.8859	0.3667
C	0.0150	0.4825	0.6226
I	-1.0950	0.3172	-3.4398
H	-1.9452	2.4702	-1.0876
C	-0.8793	2.4246	-0.7317
H	-0.2092	2.9403	-1.4730
H	-0.8007	2.9354	0.2681
H	0.8117	-2.2807	-2.4931
C	0.0632	-2.3848	-1.6604
H	0.4356	-3.1464	-0.9199
H	-0.9271	-2.7166	-2.0768
O	0.7936	-1.8583	1.1432
O	0.0640	1.1422	1.8099
C	1.2934	1.8604	2.0441
H	2.1608	1.1597	2.0172
H	1.1365	2.2759	3.0730
H	1.4079	2.6755	1.2914
C	0.1064	-2.0727	2.3956
H	0.0134	-1.1103	2.9537
H	0.7891	-2.7894	2.9208
H	-0.8928	-2.5290	2.2011

SCF = 0.240916**ZPE = 0.193565****H₂₉₈ = 0.449867****G₂₉₈ = 0.392748****40-Cl**

N	-0.0235	-1.0121	-0.8776
C	-0.4958	0.1461	-1.4634
N	-0.4490	1.1501	-0.5161
C	0.3378	-0.7343	0.4664
C	0.0568	0.6154	0.6973
I	-1.1882	0.3515	-3.5070
H	-1.9779	2.5105	-0.9847
C	-0.8919	2.4995	-0.6964
H	-0.2927	2.9899	-1.5105
H	-0.7543	3.0605	0.2666
H	0.8432	-2.1738	-2.3966
C	0.1404	-2.2779	-1.5261
H	0.5628	-3.0131	-0.7900
H	-0.8537	-2.6437	-1.9007
Cl	-1.9139	0.5671	-5.6488
O	0.9390	-1.6408	1.2932
O	0.1310	1.3211	1.8649
C	1.3832	2.0031	2.0419
H	2.2274	1.2737	2.0226
H	1.2757	2.4700	3.0528
H	1.5120	2.7801	1.2514
C	0.0075	-2.4132	2.0680
H	-0.6282	-1.7410	2.6917
H	0.6736	-3.0461	2.7061
H	-0.6218	-3.0428	1.3951

SCF = -0.027966**ZPE = 0.194789****H₂₉₈ = 0.182856****G₂₉₈ = 0.123914**

7.6 PM6

1-Cl

H	2.6964	0.0051	-1.4866
C	2.1130	0.0196	-0.5670
C	0.6192	0.0726	1.7883
C	1.6864	-1.1801	0.0025
C	1.7979	1.2456	0.0329
C	1.0490	1.2732	1.2138
C	0.9397	-1.1480	1.1802
H	2.1344	2.1731	-0.4179
H	0.6018	-2.0792	1.6327
H	0.0380	0.0869	2.7041
I	2.1693	-3.0354	-0.9145
Cl	2.7342	-5.2087	-1.9884
H	0.8031	2.2199	1.6813

SCF = -0.080566

2-Cl			
H	0.3802	0.1264	0.0585
C	0.2363	0.1136	1.1394
C	-0.1321	0.0755	3.9129
C	0.3529	-1.0907	1.8374
C	-0.0625	1.3030	1.8084
C	-0.2476	1.2834	3.2022
C	0.1675	-1.1010	3.2217
H	-0.1521	2.2372	1.2607
H	0.2575	-2.0389	3.7709
H	-0.2754	0.0620	4.9900
I	0.8084	-2.8922	0.8019
Cl	1.3375	-4.9858	-0.4020
C	-0.5538	2.4944	3.8984
N	-0.8020	3.4757	4.4625

SCF = -0.042546

3-Cl			
H	0.3820	0.1160	0.0500
C	0.2380	0.1064	1.1315
C	-0.1279	0.0607	3.9098
C	0.3554	-1.1005	1.8312
C	-0.0596	1.2930	1.7971
C	-0.2431	1.2677	3.1932
C	0.1705	-1.1112	3.2189
H	-0.1527	2.2376	1.2589
H	0.2618	-2.0511	3.7654
H	-0.2734	0.0606	4.9912
I	0.8105	-2.9026	0.7947
Cl	1.3374	-4.9890	-0.4056
N	-0.5553	2.5029	3.9036
O	-0.6513	3.5446	3.2605
O	-0.7114	2.4595	5.1209

SCF = -0.107124**4-Cl**

H	0.3800	0.1136	0.0525
C	0.2366	0.0941	1.1324
C	-0.1337	0.0639	3.8976
C	0.3565	-1.1087	1.8261
C	-0.0669	1.2843	1.8058
C	-0.2544	1.2717	3.1954
C	0.1703	-1.1164	3.2073
H	-0.1554	2.2114	1.2515
H	0.2615	-2.0502	3.7613
H	-0.2743	0.0406	4.9720
I	0.8168	-2.9048	0.7927
Cl	1.3576	-5.0123	-0.4202
C	-0.5646	2.5443	3.9274
H	-1.1532	2.3610	4.8334
H	0.3643	3.0452	4.2295
H	-1.1323	3.2445	3.3041

SCF = -0.095133**5-Cl**

H	1.4105	0.0367	0.2753
C	0.8311	0.0473	1.1991
C	-0.6385	0.1016	3.5682
C	0.4030	-1.1521	1.7615
C	0.5299	1.2775	1.7955
C	-0.2160	1.3149	2.9903
C	-0.3223	-1.1137	2.9491
H	0.8890	2.1906	1.3349
H	-0.6561	-2.0436	3.4109
H	-1.1958	0.0920	4.4978
I	0.8372	-3.0021	0.8204
Cl	1.3364	-5.1748	-0.2918
N	-0.4394	2.5726	3.6766
C	-1.6331	2.5840	4.5745
C	-0.4636	3.7691	2.7825
H	-2.5866	2.4047	4.0559
H	-1.6880	3.5499	5.0969
H	-1.5069	1.8023	5.3441
H	-1.2610	3.7471	2.0249
H	-0.5756	4.6779	3.3911
H	0.5063	3.8425	2.2599

SCF = -0.078316

6-Cl

H	0.2957	0.1241	0.0544
C	0.2170	0.0584	1.1404
C	0.0142	-0.1104	3.9369
C	0.3763	-1.1755	1.7748
C	-0.0431	1.2191	1.8747
C	-0.1396	1.1067	3.2717
C	0.2748	-1.2525	3.1586
H	-0.1690	2.1825	1.3979
H	0.3979	-2.2122	3.6619
H	-0.0604	-0.1937	5.0106
I	0.7701	-2.9196	0.6339
Cl	1.2323	-4.9691	-0.6989
O	-0.4007	2.3310	3.8879
C	-0.5213	2.3355	5.3248
H	0.4160	2.0095	5.7851
H	-1.3592	1.7052	5.6370
H	-0.7201	3.3910	5.5396

SCF = -0.146321**7-Cl**

H	0.9845	0.3531	0.5260
C	0.4495	0.1087	1.4432
C	-0.9305	-0.5166	3.7957
C	0.2995	-1.2265	1.8229
C	-0.0794	1.1400	2.2293
C	-0.7633	0.8116	3.4010
C	-0.3936	-1.5329	2.9955
H	0.0408	2.1767	1.9269
H	-0.5185	-2.5735	3.2935
H	-1.4694	-0.7631	4.7066
I	1.1300	-2.7794	0.6314
Cl	2.1080	-4.5903	-0.7529
S	-1.4739	2.0993	4.3768
C	-0.1322	2.5029	5.5317
H	-0.4827	3.3039	6.1889
H	0.7590	2.8432	4.9956
H	0.1385	1.6338	6.1390

SCF = -0.087030**8-Cl**

H	0.5406	0.1264	0.0798
C	0.3292	0.0974	1.1491
C	-0.2133	0.0268	3.8904
C	0.3613	-1.1238	1.8269
C	0.0296	1.2827	1.8243
C	-0.2432	1.2482	3.2022
C	0.0888	-1.1485	3.1961
H	0.0086	2.2255	1.2821
H	0.1115	-2.0973	3.7332
H	-0.4216	-0.0201	4.9565
I	0.8192	-2.9219	0.7866
Cl	1.3515	-5.0121	-0.4220
C	-0.5613	2.5289	3.9040
F	-0.8173	2.4592	5.2252
F	0.4058	3.4686	3.8426
F	-1.6417	3.1855	3.4310

SCF = -0.352291**9-Cl**

H	0.3782	0.1243	0.0555
C	0.2362	0.1064	1.1365
C	-0.1303	0.0704	3.9145
C	0.3543	-1.0958	1.8338
C	-0.0644	1.3017	1.8068
C	-0.2411	1.2529	3.1873
C	0.1711	-1.1088	3.2164
H	-0.1549	2.2335	1.2572
H	0.2621	-2.0447	3.7683
H	-0.2717	0.0523	4.9907
I	0.8097	-2.8951	0.7967
Cl	1.3394	-4.9910	-0.4104
Br	-0.6571	2.8927	4.1323

SCF = -0.086027

10-Cl

C	0.2246	-0.0242	1.0852
C	-0.1269	0.0055	3.9025
C	0.1310	-1.2214	1.8055
C	0.1415	1.1880	1.7814
C	-0.0335	1.2162	3.1845
C	-0.0441	-1.2201	3.2089
I	0.4899	-0.0459	-1.0415
Cl	0.7900	-0.0702	-3.4515
C	0.2107	-2.4916	1.1359
N	0.2700	-3.5317	0.6350
C	-0.1389	-2.4526	3.9379
N	-0.2156	-3.4435	4.5280
C	-0.3043	0.0205	5.3245
N	-0.4474	0.0326	6.4716
C	-0.1176	2.4637	3.8889
N	-0.1856	3.4668	4.4590
C	0.2320	2.4441	1.0869
N	0.3000	3.4743	0.5670

SCF = 0.164168**11-I**

C	0.0111	-0.0226	1.1056
C	0.0171	0.0188	3.8876
C	0.0392	-1.2341	1.7846
C	-0.0142	1.2134	1.7821
C	-0.0111	1.2294	3.1829
C	0.0418	-1.1956	3.1731
I	0.0774	-3.1023	0.7236
F	0.0682	-2.3264	3.8697
F	0.0201	0.0270	5.2194
F	-0.0348	2.3865	3.8398
F	-0.0409	2.3606	1.1061
F	0.0074	-0.0046	-0.2227
I	0.1254	-5.4652	-0.6186

SCF = -0.428116**11-F**

C	0.0136	-0.0356	1.1047
C	0.0147	0.0107	3.8827
C	0.0383	-1.2515	1.7783
C	-0.0105	1.2021	1.7782
C	-0.0098	1.2212	3.1786
C	0.0383	-1.2034	3.1677
I	0.0743	-3.1028	0.7289
F	0.0612	-2.3310	3.8712
F	0.0155	0.0193	5.2151
F	-0.0324	2.3794	3.8345
F	-0.0338	2.3488	1.1000
F	0.0121	-0.0125	-0.2243
F	0.1071	-4.7663	-0.2141

SCF = -0.513806**11-OCH2**

C	0.0001	-0.1125	1.0205
C	-0.0000	-0.2447	3.8027
C	0.0001	-1.3671	1.6273
C	-0.0000	1.0770	1.7708
C	-0.0001	1.0074	3.1716
C	0.0001	-1.4142	3.0202
F	0.0001	-2.5898	3.6347
F	-0.0001	-0.3217	5.1297
F	-0.0001	2.1195	3.8946
F	-0.0001	2.2587	1.1618
F	0.0001	-0.0284	-0.3043
I	0.0002	-3.1212	0.4817
O	-0.0000	-4.8713	-0.5856
C	-0.0001	-5.1823	-1.7710
H	-0.0002	-6.2459	-2.0384
H	0.0001	-4.4272	-2.5680

SCF = -0.357806**11-OMe**

C	0.0560	0.1160	1.1663
C	-0.0173	0.0398	3.9416
C	0.0788	-1.1273	1.7851
C	-0.0022	1.3233	1.8914
C	-0.0390	1.2800	3.2908
C	0.0413	-1.1411	3.1740
I	0.1676	-2.9378	0.6484
F	0.0602	-2.2976	3.8296
F	-0.0520	-0.0100	5.2727
F	-0.0942	2.4081	3.9964
F	-0.0225	2.4988	1.2638
F	0.0895	0.2000	-0.1610
O	0.2488	-4.6493	-0.3405
C	0.2896	-4.7001	-1.7289
H	0.3304	-5.7646	-1.9983
H	1.1836	-4.1864	-2.1084
H	-0.6120	-4.2424	-2.1590

SCF = -0.484290

11-Cl

C	0.2225	-0.0264	1.0959
C	-0.1264	0.0106	3.9118
C	0.1154	-1.2038	1.8264
C	0.1518	1.1698	1.7997
C	-0.0211	1.2110	3.1977
C	-0.0582	-1.2082	3.2249
I	0.4847	-0.0544	-1.0178
F	0.1757	-2.3779	1.2072
F	-0.1576	-2.3542	3.8967
F	-0.2901	0.0280	5.2325
F	-0.0850	2.3744	3.8435
F	0.2480	2.3272	1.1542
Cl	0.7865	-0.0862	-3.4525

SCF = -0.454611**11-Br**

C	0.0059	-0.0163	1.1099
C	0.0223	0.0256	3.8909
C	0.0391	-1.2293	1.7870
C	-0.0195	1.2198	1.7861
C	-0.0111	1.2363	3.1869
C	0.0469	-1.1885	3.1759
I	0.0769	-3.0847	0.7330
F	0.0783	-2.3185	3.8738
F	0.0305	0.0332	5.2227
F	-0.0347	2.3932	3.8437
F	-0.0512	2.3667	1.1097
F	-0.0029	0.0034	-0.2185
Br	0.1237	-5.3837	-0.5729

SCF = -0.443513**11-DMF**

C	0.0912	0.3606	1.9442
C	0.6057	-0.1840	4.6245
C	0.2153	-0.9699	2.3380
C	0.2175	1.4249	2.8547
C	0.4768	1.1474	4.2047
C	0.4728	-1.2226	3.6839
F	0.5985	-2.4753	4.1025
F	0.8516	-0.4580	5.9021
F	0.5992	2.1387	5.0783
F	0.0932	2.6837	2.4446
F	-0.1545	0.6443	0.6696
I	0.0204	-2.5301	0.9509
O	-0.1559	-4.0743	-0.3299
C	-0.3452	-4.5856	-1.4465
H	-0.3190	-5.6866	-1.5216
N	-0.5822	-3.8588	-2.5782
C	-0.6401	-2.3833	-2.6015
H	0.1362	-1.9676	-3.2654
H	-0.4681	-1.9560	-1.5838
H	-1.6292	-2.0318	-2.9398
C	-0.7993	-4.5340	-3.8773
H	-0.0376	-4.2145	-4.6129
H	-1.7952	-4.2792	-4.2855
H	-0.7427	-5.6315	-3.7904

SCF = -0.399964**11-NH3**

C	0.0072	-0.0119	1.1113
C	0.0204	0.0288	3.8958
C	0.0378	-1.2247	1.7935
C	-0.0170	1.2224	1.7867
C	-0.0102	1.2394	3.1888
C	0.0439	-1.1853	3.1847
I	0.0737	-3.0595	0.7542
F	0.0727	-2.3212	3.8717
F	0.0270	0.0337	5.2254
F	-0.0327	2.3940	3.8426
F	-0.0460	2.3646	1.1066
F	0.0002	-0.0076	-0.2165
N	0.1079	-4.8193	-0.2431
H	1.0587	-5.1490	-0.4604
H	-0.3797	-4.7867	-1.1492
H	-0.3340	-5.5925	0.2735

SCF = -0.340619

12-Cl

C	0.5787	-0.2999	1.0253
C	-0.0001	0.5671	3.6328
C	0.2576	-1.1975	2.0329
C	0.6009	1.0451	1.3634
C	0.3161	1.5160	2.6604
C	-0.0382	-0.7987	3.3514
I	1.0175	-0.9576	-0.9494
Cl	1.5234	-1.7153	-3.2269
I	-0.5155	-2.1884	4.8319
I	0.3630	3.5504	3.1187
F	-0.2736	0.9768	4.8651
F	0.2202	-2.4947	1.7706
F	0.9004	1.9493	0.4438

SCF = -0.266761**13-Cl**

C	0.0004	-0.0038	1.0562
I	-0.0023	-0.0189	-1.1577
Cl	-0.0082	-0.0346	-3.5826
Br	-0.9074	-1.5762	1.8077
Br	1.8221	0.0026	1.7931
Br	-0.9102	1.5771	1.7861

SCF = -0.119491**14-Cl**

C	0.0002	-0.0013	0.9872
I	-0.0006	-0.0211	-1.1960
Cl	-0.0014	-0.0438	-3.6357
F	-0.6063	-1.0466	1.5882
F	1.2129	0.0022	1.5796
F	-0.6049	1.0532	1.5730

SCF = -0.406773**15-Cl**

C	-0.0002	-0.0043	1.0856
I	0.0000	-0.0160	-1.1255
Cl	0.0001	-0.0292	-3.6377
C	-0.7263	-1.2577	1.5708
H	-0.2322	-2.1641	1.2036
H	-1.7572	-1.2819	1.2005
H	-0.7594	-1.3110	2.6628
C	1.4505	-0.0026	1.5641
H	1.9854	-0.8859	1.1977
H	1.5182	0.0034	2.6558
H	1.9865	0.8759	1.1880
C	-0.7249	1.2550	1.5573
H	-0.2291	2.1569	1.1814
H	-0.7589	1.3194	2.6487
H	-1.7554	1.2769	1.1858

SCF = -0.150151**16-Cl**

C	-0.0007	-0.0044	1.1822
I	-0.0010	-0.0151	-1.0869
Cl	-0.0010	-0.0269	-3.5011
C	-0.6958	-1.2049	1.5783
N	-1.2531	-2.1673	1.9008
C	1.3883	-0.0034	1.5721
N	2.5018	-0.0026	1.8899
C	-0.6943	1.2007	1.5668
N	-1.2502	2.1668	1.8805

SCF = -0.004529**17-Cl**

I	0.1137	-1.3403	-1.5498
Cl	0.9802	-2.4695	-3.5328
N	-0.5684	-0.4510	0.0117
C	0.0895	-0.3863	1.2662
C	-1.8054	0.2388	0.0822
O	1.1621	-0.8724	1.5402
O	-2.6060	0.3706	-0.8142
C	-2.0087	0.8197	1.4930
H	-2.1342	1.9124	1.4305
H	-2.9380	0.4200	1.9291
C	-0.7629	0.4088	2.2714
H	-0.1880	1.2704	2.6465
H	-0.9919	-0.2219	3.1451

SCF = -0.305630**18-Cl**

I	-0.0028	-0.0179	-0.9740
Cl	-0.0059	0.1003	-3.4765
C	-0.0002	-0.0608	1.1388
H	0.0010	0.9290	1.5704
C	0.0000	-1.1582	1.8792
H	0.0014	-1.1536	2.9589
H	-0.0011	-2.1543	1.4615

SCF = -0.088731

19-Cl

I	-0.0025	-0.0497	-0.9637
Cl	-0.0064	0.0057	-3.4379
C	-0.0004	-0.0535	1.1510
H	0.0000	0.9390	1.5811
C	0.0004	-1.1572	1.8952
H	0.0000	-2.1618	1.4604
C	0.0019	-1.1337	3.3253
N	0.0030	-1.1254	4.4854

SCF = -0.058008**20-Cl**

I	-0.0849	-0.0391	-0.9495
Cl	0.1261	0.1861	-3.4319
C	-0.3026	-0.2106	1.1401
H	-0.8833	0.5952	1.5493
C	0.2160	-1.2078	1.8434
H	0.7981	-2.0133	1.3813
N	0.1964	-1.3574	3.2933
C	-0.3512	-2.6938	3.6857
H	0.2371	-3.4805	3.1877
H	-1.4086	-2.8403	3.4210
H	-0.2365	-2.8286	4.7704
C	-0.5110	-0.2658	4.0233
H	-0.0267	0.6916	3.7652
H	-0.3972	-0.4183	5.1052
H	-1.5815	-0.1786	3.7856

SCF = -0.093086**21-Cl**

I	0.0289	-0.0540	-0.9001
Cl	0.2850	-0.1356	-3.3768
C	-0.1805	0.0124	1.1232
H	-0.4102	0.0852	3.3427
C	-0.3046	0.0518	2.3220

SCF = -0.035101**22-Cl**

I	0.0254	-0.0550	-0.8751
Cl	0.2828	-0.1350	-3.3204
C	-0.1865	0.0133	1.1576
C	-0.3111	0.0545	2.3637
C	-0.4503	0.0996	3.7281
N	-0.5686	0.1383	4.8844

SCF = -0.002065**23-Cl**

I	0.0239	-0.0530	-0.8492
Cl	0.2778	-0.1344	-3.2982
C	-0.1897	0.0155	1.2104
N	-0.3089	0.0537	2.3600

SCF = -0.089712**24-Cl**

C	-0.8045	0.5117	1.5953
C	1.0065	-0.4961	3.4905
C	-1.0225	-0.7461	2.1615
C	0.3093	1.2759	1.9640
C	1.2054	0.7519	2.9164
C	-0.1170	-1.2459	3.1066
C	-0.3133	-2.5742	3.7289
C	-0.3055	-5.0523	5.1616
C	0.2805	-3.7270	3.1894
C	-0.9956	-2.7140	4.9488
C	-0.9918	-3.9285	5.6510
C	0.2843	-4.9418	3.8917
C	-0.1011	-6.2533	6.0017
C	0.3404	-8.4997	7.6160
C	-1.0016	-7.3260	5.9659
C	1.0250	-6.2893	6.8399
C	1.2314	-7.4086	7.6345
C	-0.7761	-8.4432	6.7729
I	2.3373	-4.6288	6.8356
I	2.3267	-1.3220	4.9240
F	0.5510	-9.5666	8.3833
F	2.2875	-7.4698	8.4368
F	-1.6271	-9.4631	6.7423
F	0.8855	-6.0017	3.3606
F	0.8781	-3.6557	2.0042
F	-1.6299	-1.6644	5.4617
F	-1.6225	-4.0106	6.8183
F	-1.6603	0.9899	0.6984
F	0.5127	2.4742	1.4216
F	2.2589	1.4828	3.2608
Cl	3.7442	-2.5278	6.6462
I	-2.7006	-1.8712	1.5916
I	-2.6836	-7.2665	4.7114

SCF = -0.683017

25-Cl

C	0.2997	-1.3122	0.4490
C	-0.3303	1.4136	0.1921
C	1.3543	-0.3849	0.3974
C	-1.0544	-0.9438	0.3739
C	-1.3308	0.4284	0.2502
C	1.0004	0.9694	0.2730
C	2.7634	-0.8224	0.3362
C	5.4420	-1.6559	0.1941
C	3.3444	-1.0974	-0.9161
C	3.5187	-0.9639	1.5089
C	4.8505	-1.3788	1.4322
C	4.6686	-1.5085	-0.9739
C	-2.1255	-1.9569	0.2885
C	-4.1602	-3.8841	0.1005
C	-2.7629	-2.4214	1.4477
C	-2.5027	-2.4543	-0.9731
C	-3.5092	-3.4063	-1.0536
C	-3.7742	-3.3800	1.3482
C	-0.6559	2.8279	-0.0805
C	-1.2737	5.5135	-0.6246
C	-0.7451	3.2683	-1.4145
C	-0.8745	3.7263	0.9734
C	-1.1815	5.0608	0.6969
C	-1.0510	4.5973	-1.6712
I	2.6536	-0.5542	3.3762
I	2.1177	-0.8513	-2.6086
I	-1.4785	-1.6861	-2.6437
I	-2.2014	-1.6805	3.3289
I	-0.3978	1.8337	-2.9150
I	-0.7418	3.0710	2.9624
Cl	0.1258	-0.3657	-4.2434
F	0.5971	-2.5988	0.5688
F	-2.5980	0.8122	0.1794
F	1.9703	1.8722	0.2239
F	-3.8764	-3.8853	-2.2360
F	-5.1240	-4.7973	0.0100
F	-4.3776	-3.8197	2.4465
F	5.5654	-1.5126	2.5434
F	6.7109	-2.0510	0.1253
F	5.2310	-1.7718	-2.1472
F	-1.5663	6.7855	-0.8838
F	-1.3885	5.9114	1.6956
F	-1.1388	5.0281	-2.9237

SCF = -0.749886**26-Cl**

H	-1.4338	0.9111	-2.1382
C	-1.3373	1.6313	-1.3151
C	-1.0856	3.4671	0.8211
C	-1.1393	1.2373	-0.0099
C	-1.4113	3.0138	-1.5506
C	-1.2861	3.9167	-0.4896
C	-1.0065	2.0914	1.0937
H	-1.5672	3.3757	-2.5674
H	-1.3453	4.9890	-0.6849
H	-0.9902	4.1857	1.6357
C	-0.7988	1.5014	2.4267
C	-0.4103	0.2183	4.8832
C	-0.7468	0.0999	2.5042
C	-0.6540	2.2626	3.5958
C	-0.4600	1.6138	4.8204
C	-0.5552	-0.5443	3.7134
H	-0.6911	3.3494	3.5579
H	-0.3472	2.2025	5.7303
H	-0.5151	-1.6313	3.7714
H	-0.2590	-0.2792	5.8398
I	-0.9892	-0.8419	0.6153
Cl	-1.2841	-1.6693	-1.6188

SCF = 0.131956**27-Cl**

H	-0.2260	0.1395	0.1411
C	-0.1698	0.1120	1.2301
C	-0.0240	0.0768	4.0383
C	-0.1622	-1.0882	1.9156
C	-0.1041	1.3197	1.9441
C	-0.0317	1.2955	3.3414
C	-0.0898	-1.1232	3.3187
H	-0.1106	2.2633	1.3948
H	0.0327	0.0647	5.1287
C	-0.0878	-2.4511	3.9544
C	-0.0969	-5.0953	4.9710
C	-0.1573	-3.5895	3.1372
C	-0.0210	-2.6803	5.3370
C	-0.0260	-3.9945	5.8335
C	-0.1646	-4.8923	3.5825
H	0.0348	-1.8280	6.0215
H	-0.2207	-5.7499	2.8953
H	-0.1012	-6.1211	5.3516
I	-0.2535	-3.0261	1.0410
Cl	-0.3448	-5.2997	0.3168
C	0.0400	2.5715	4.1392
C	0.0475	-4.1863	7.3287
F	1.1426	2.6778	4.9012
F	-0.9708	2.7272	5.0120
F	0.0299	3.7154	3.4371
F	-0.9652	-3.6111	7.9981
F	0.0402	-5.4548	7.7644
F	1.1503	-3.6611	7.8878

SCF = -0.380608

28-Cl			
H	-0.1684	0.1493	0.1578
C	-0.1318	0.1256	1.2478
C	-0.0368	0.0879	4.0642
C	-0.1270	-1.0744	1.9367
C	-0.0890	1.3325	1.9603
C	-0.0418	1.3061	3.3633
C	-0.0800	-1.1106	3.3403
H	-0.0922	2.2857	1.4296
H	0.0001	0.0873	5.1539
C	-0.0790	-2.4401	3.9747
C	-0.0859	-5.0913	4.9803
C	-0.1244	-3.5774	3.1536
C	-0.0356	-2.6689	5.3576
C	-0.0394	-3.9873	5.8481
C	-0.1297	-4.8839	3.5940
H	0.0010	-1.8268	6.0534
H	-0.1664	-5.7380	2.9013
H	-0.0882	-6.1096	5.3778
I	-0.1867	-3.0107	1.0591
Cl	-0.2468	-5.2828	0.3249
C	0.0021	2.5394	4.0956
N	0.0375	3.5330	4.6850
C	0.0053	-4.2063	7.2660
N	0.0413	-4.3827	8.4073

SCF = 0.238836

29-Cl			
H	0.0170	0.1471	0.1507
C	-0.0177	0.1082	1.2401
C	-0.1054	0.0347	4.0452
C	-0.0114	-1.1063	1.9050
C	-0.0718	1.3030	1.9618
C	-0.1113	1.2828	3.3763
C	-0.0505	-1.1494	3.3057
H	-0.0681	2.2470	1.4227
H	-0.1252	-0.0082	5.1310
C	-0.0338	-2.4910	3.9309
C	0.0066	-5.1457	4.9042
C	0.0183	-3.6137	3.0927
C	-0.0696	-2.7300	5.3056
C	-0.0423	-4.0565	5.8137
C	0.0427	-4.9242	3.5279
H	-0.1014	-1.8809	5.9865
H	0.0859	-5.7668	2.8247
H	0.0313	-6.1714	5.2681
I	0.0528	-3.0237	1.0114
Cl	0.1066	-5.2979	0.2168
N	-0.0234	2.4961	4.1202
N	0.0655	-4.2829	7.2061
C	-0.4507	3.7394	3.4207
H	0.1409	3.8643	2.4960
H	-0.2319	4.6126	4.0572
H	-1.5199	3.7565	3.1581
C	-0.5280	2.4572	5.5208
H	0.0213	1.6858	6.0886
H	-1.6070	2.2511	5.5979
H	-0.3205	3.4217	6.0131
C	-0.3951	-3.2014	8.1171
H	0.1421	-2.2644	7.8846
H	-0.1409	-3.4621	9.1585
H	-1.4789	-3.0111	8.0604
C	-0.2900	-5.6356	7.7121
H	0.3135	-6.4001	7.1893
H	-1.3561	-5.8853	7.5890
H	-0.0348	-5.7093	8.7825

SCF = 0.128992

30-Cl

H	1.4139	-0.5100	1.4207
C	0.5656	-0.0629	1.9430
C	-1.6025	1.1150	3.2690
C	-0.5747	-0.8095	2.2245
C	0.6318	1.2822	2.3249
C	-0.4551	1.8669	2.9918
C	-1.6561	-0.2305	2.8787
H	1.5262	1.8661	2.0997
H	-2.4585	1.5571	3.7813
C	0.5704	-2.8276	4.4115
C	-0.1904	-5.4537	5.0881
C	-0.1466	-3.6368	3.5407
C	0.9106	-3.3577	5.6610
C	0.5299	-4.6680	5.9962
C	-0.5406	-4.9312	3.8337
H	1.4752	-2.7417	6.3673
H	-1.1025	-5.5554	3.1227
H	-0.4908	-6.4774	5.3318
I	-0.6810	-2.8358	1.5839
Cl	-0.8785	-5.0117	0.6121
C	-0.3542	3.3145	3.3980
C	0.9166	-5.2008	7.3523
F	0.6640	3.5742	4.2378
F	-1.4201	3.8347	4.0272
F	-0.1494	4.1598	2.3731
F	0.4228	-4.4832	8.3756
F	0.5332	-6.4562	7.6281
F	2.2418	-5.2141	7.5723
H	-2.5572	-0.8088	3.0925
H	0.8698	-1.8083	4.1509

SCF = -0.382904**31-Cl**

H	1.6260	-0.1801	2.7042
C	0.5686	0.0917	2.6878
C	-2.1400	0.8155	2.6342
C	-0.3882	-0.7942	2.2018
C	0.1814	1.3518	3.1590
C	-1.1765	1.7085	3.1308
C	-1.7342	-0.4408	2.1695
H	0.9253	2.0515	3.5406
H	-3.1918	1.1011	2.6084
C	1.1728	-4.7069	3.5363
C	-0.3669	-3.7051	5.6767
C	0.3296	-3.6155	3.3951
C	1.2438	-5.3182	4.7947
C	0.4767	-4.8158	5.8592
C	-0.4454	-3.0922	4.4217
H	1.8947	-6.1844	4.9415
H	-1.1022	-2.2299	4.2748
H	-0.9616	-3.3221	6.5095
I	0.2117	-2.6820	1.4307
Cl	0.8812	-4.6875	0.3118
H	-2.4851	-1.1313	1.7796
H	1.7698	-5.1049	2.7022
C	-1.5836	2.9979	3.6134
N	-1.9116	4.0354	4.0033
C	0.5531	-5.4417	7.1478
N	0.6147	-5.9449	8.1862

SCF = 0.236592

32-Cl

H	1.7998	-0.1564	2.7625
C	0.7432	0.1201	2.7571
C	-1.9554	0.8494	2.7467
C	-0.2145	-0.7655	2.2691
C	0.3714	1.3706	3.2488
C	-0.9904	1.7613	3.2412
C	-1.5570	-0.3956	2.2618
H	1.1378	2.0465	3.6174
H	-3.0072	1.1189	2.7205
C	1.3501	-4.6999	3.5232
C	-0.1727	-3.7566	5.6931
C	0.5069	-3.6016	3.4076
C	1.4300	-5.3430	4.7561
C	0.6747	-4.8827	5.8660
C	-0.2551	-3.1126	4.4607
H	2.0901	-6.2034	4.8538
H	-0.9071	-2.2429	4.3413
H	-0.7607	-3.3757	6.5255
I	0.3654	-2.6309	1.4755
Cl	1.0147	-4.6272	0.2800
H	-2.3169	-1.0786	1.8757
H	1.9394	-5.0722	2.6742
N	-1.3637	3.0838	3.6003
N	0.8618	-5.4502	7.1491
C	-2.7864	3.3124	3.9714
H	-2.9680	4.3940	4.0842
H	-3.0861	2.8076	4.9030
H	-3.4435	2.9623	3.1549
C	-0.4324	3.8374	4.4827
H	0.5737	3.8604	4.0263
H	-0.3470	3.4161	5.4966
H	-0.7686	4.8842	4.5647
C	1.4287	-6.8240	7.2135
H	2.3955	-6.8540	6.6790
H	0.7672	-7.5938	6.7842
H	1.6381	-7.0891	8.2633
C	-0.2150	-5.2396	8.1537
H	0.1172	-5.6172	9.1353
H	-1.1633	-5.7361	7.8921
H	-0.4053	-4.1583	8.2765

SCF = 0.126035**33-Cl**

I	-1.3804	1.1630	-3.4356
Cl	-2.0836	1.9085	-5.6087
C	-0.7547	0.4675	-1.4794
C	0.0917	-0.3278	1.0661
N	-0.9437	-0.8036	-1.0470
C	-0.1188	1.3885	-0.6161
C	0.3034	1.0063	0.6437
C	-0.5305	-1.2225	0.2170
H	0.0291	2.4144	-0.9761
H	0.7952	1.7129	1.3152
H	0.4184	-0.6470	2.0571
C	-1.6079	-1.7901	-1.9315
H	-1.0467	-1.8984	-2.8866
H	-2.6248	-1.4379	-2.2153
H	-1.6996	-2.7825	-1.4664
H	-0.7129	-2.2626	0.5056

SCF = 0.024468**34-Cl**

I	-1.4534	1.1841	-3.3917
Cl	-2.2550	1.8387	-5.5738
C	-0.7557	0.5691	-1.4649
C	0.1164	-0.3371	1.0233
C	-0.9308	-0.7554	-1.0927
C	-0.1364	1.4572	-0.5847
C	0.3014	1.0014	0.6652
N	-0.4960	-1.1986	0.1430
H	-1.4156	-1.4800	-1.7649
H	0.0047	2.5057	-0.8737
H	0.7886	1.6792	1.3698
H	0.4502	-0.7168	1.9946
H	-0.1757	-3.2896	-0.1934
C	-0.6932	-2.6169	0.5198
H	-0.3053	-2.8444	1.5286
H	-1.7699	-2.8806	0.5118

SCF = 0.039391

35-Cl

I	-1.4378	1.0461	-3.3894
Cl	-2.2670	1.6672	-5.5710
C	-0.7055	0.4984	-1.4633
N	0.2558	-0.2197	1.0651
C	-0.7982	-0.8219	-1.0031
C	-0.1160	1.4491	-0.6175
C	0.3613	1.0908	0.6386
C	-0.3197	-1.1776	0.2545
H	-1.2547	-1.5879	-1.6430
H	-0.0298	2.4912	-0.9512
H	0.8247	1.8196	1.3129
H	-0.3849	-2.2055	0.6283
H	1.8526	-0.3779	2.4855
C	0.7680	-0.5870	2.4044
H	0.2464	-0.0178	3.1985
H	0.6241	-1.6612	2.6228

SCF = 0.043038**36-Cl**

N	-0.3786	0.5832	-0.1680
C	-0.5928	1.8583	-0.6464
N	-0.3283	2.7146	0.4013
C	0.0215	0.6374	1.1836
H	0.2459	-0.2343	1.7718
C	0.0531	1.9765	1.5413
H	0.3086	2.4282	2.4830
I	-1.2196	2.4068	-2.6410
H	0.2434	4.5778	-0.4541
C	-0.4308	4.1773	0.3326
H	-0.1707	4.6488	1.2933
H	-1.4621	4.4822	0.0545
H	0.1217	-0.6291	-1.8443
C	-0.5443	-0.6444	-0.9556
H	-0.3177	-1.5431	-0.3605
H	-1.5844	-0.7238	-1.3374
Cl	-1.9150	3.0155	-4.8567

SCF = 0.003256**37-Cl**

N	-0.3104	0.5877	-0.2080
C	-0.5647	1.8638	-0.6640
N	-0.3833	2.7184	0.4028
C	0.0467	0.6344	1.1542
C	-0.0235	1.9780	1.5462
I	-1.1449	2.4252	-2.6918
H	-0.6298	4.4965	-0.7446
C	-0.5361	4.1772	0.3229
H	0.3379	4.7042	0.7467
H	-1.4554	4.5159	0.8388
H	0.5798	-1.0337	-1.2799
C	-0.4180	-0.6190	-1.0387
H	-1.0311	-1.3984	-0.5510
H	-0.9086	-0.3731	-2.0129
Cl	-1.7803	3.0398	-4.9123
C	0.4201	-0.5536	1.9832
C	0.2278	2.5614	2.9007
F	1.3562	-0.3003	2.9071
F	0.9225	-1.5970	1.3047
F	-0.6123	-1.0690	2.6653
F	1.5218	2.8228	3.1330
F	-0.3952	3.7228	3.1544
F	-0.1554	1.7724	3.9129

SCF = -0.492167**38-Cl**

N	0.0819	-0.9779	-0.8889
C	-0.4904	0.1459	-1.4479
N	-0.5383	1.1096	-0.4621
C	0.4004	-0.7265	0.4655
C	0.0083	0.5935	0.7353
I	-1.1852	0.3583	-3.4988
H	-2.1448	2.4172	-0.9530
C	-1.0784	2.4638	-0.6413
H	-0.5298	2.9956	-1.4492
H	-1.0096	3.0638	0.2821
H	0.9788	-2.0685	-2.4820
C	0.3193	-2.2393	-1.6031
H	0.7880	-3.0007	-0.9565
H	-0.6378	-2.6491	-1.9938
Cl	-1.9489	0.5916	-5.7520
C	1.0014	-1.6694	1.3351
N	1.4914	-2.4343	2.0493
C	0.1132	1.3207	1.9464
N	0.2013	1.9087	2.9372

SCF = 0.125138

39-Cl

N	-0.3478	0.5873	-0.1900
C	-0.4939	1.8666	-0.6811
N	-0.2910	2.7177	0.3837
C	-0.0498	0.6274	1.1982
C	-0.0139	1.9717	1.5602
I	-0.9512	2.4281	-2.7208
H	-0.5860	4.5158	-0.7219
C	-0.3514	4.1831	0.3164
H	0.6162	4.6319	0.6018
H	-1.1404	4.5769	0.9810
H	-0.7169	-0.3961	-2.0444
C	-0.4804	-0.6414	-0.9825
H	0.4597	-1.2206	-0.9736
H	-1.2971	-1.2754	-0.5949
Cl	-1.4587	3.0514	-4.9850
C	0.1637	-0.5823	2.0124
H	1.0121	-1.1805	1.6425
H	-0.7243	-1.2348	2.0172
H	0.3824	-0.3313	3.0621
C	0.2486	2.5971	2.8686
H	1.1306	3.2571	2.8375
H	0.4404	1.8427	3.6475
H	-0.6059	3.2024	3.2120

SCF = -0.028023**40-Cl**

N	-0.0163	-0.9906	-0.9652
C	-0.5235	0.1537	-1.5493
N	-0.5083	1.1408	-0.5837
C	0.3324	-0.7215	0.3834
C	0.0074	0.6130	0.6281
I	-1.2109	0.3600	-3.5893
H	-2.0936	2.4907	-1.0342
C	-1.0201	2.5064	-0.7554
H	-0.4759	3.0228	-1.5721
H	-0.9058	3.0841	0.1796
H	0.8996	-2.1395	-2.5078
C	0.2060	-2.2693	-1.6520
H	0.6362	-3.0132	-0.9574
H	-0.7489	-2.6598	-2.0590
Cl	-1.9741	0.5894	-5.8538
O	0.9285	-1.6730	1.1443
O	0.0464	1.3726	1.7511
C	1.4072	1.6806	2.1965
H	1.9553	0.7546	2.3942
H	1.2137	2.2411	3.1188
H	1.9120	2.2972	1.4487
C	0.1010	-2.1214	2.2665
H	-0.1458	-1.2734	2.9123
H	0.7743	-2.8281	2.7659
H	-0.7970	-2.6176	1.8902

SCF = -0.104757**7.7 PM7****1-Cl**

H	2.6827	0.0929	-1.4578
C	2.0982	0.0928	-0.5378
C	0.6042	0.1378	1.8175
C	1.6647	-1.0968	0.0432
C	1.7799	1.3080	0.0667
C	1.0335	1.3333	1.2436
C	0.9183	-1.0817	1.2193
H	2.1150	2.2396	-0.3815
H	0.5739	-2.0062	1.6826
H	0.0222	0.1565	2.7351
I	2.1476	-2.9558	-0.8752
Cl	2.9548	-6.0569	-2.4058
H	0.7873	2.2810	1.7118

SCF = -0.037254**2-Cl**

H	0.3628	0.2044	0.0860
C	0.2215	0.1758	1.1680
C	-0.1456	0.1320	3.9398
C	0.3349	-1.0195	1.8782
C	-0.0765	1.3546	1.8439
C	-0.2604	1.3339	3.2314
C	0.1525	-1.0451	3.2610
H	-0.1671	2.2927	1.2983
H	0.2395	-1.9762	3.8241
H	-0.2897	0.1222	5.0192
I	0.7914	-2.8237	0.8409
Cl	1.5285	-5.7410	-0.8370
C	-0.5644	2.5357	3.9225
N	-0.8126	3.5168	4.4866

SCF = 0.005927**3-Cl**

H	0.3652	0.1911	0.0774
C	0.2243	0.1634	1.1598
C	-0.1412	0.1162	3.9354
C	0.3384	-1.0332	1.8699
C	-0.0729	1.3431	1.8321
C	-0.2547	1.3141	3.2199
C	0.1564	-1.0581	3.2539
H	-0.1637	2.2834	1.2826
H	0.2439	-1.9899	3.8163
H	-0.2849	0.1041	5.0187
I	0.7944	-2.8378	0.8321
Cl	1.5212	-5.7180	-0.8244
N	-0.5644	2.5397	3.9247
O	-0.6604	3.5784	3.2856
O	-0.7205	2.4983	5.1374

SCF = -0.054047

4-Cl			
H	0.3622	0.1885	0.0783
C	0.2213	0.1558	1.1591
C	-0.1471	0.1178	3.9234
C	0.3374	-1.0380	1.8668
C	-0.0804	1.3337	1.8394
C	-0.2666	1.3201	3.2233
C	0.1545	-1.0625	3.2471
H	-0.1705	2.2663	1.2899
H	0.2428	-1.9904	3.8129
H	-0.2892	0.1014	5.0001
I	0.7978	-2.8390	0.8307
Cl	1.5756	-5.8515	-0.9030
C	-0.5748	2.5865	3.9516
H	-1.1640	2.4091	4.8604
H	0.3530	3.0923	4.2565
H	-1.1433	3.2919	3.3321

SCF = -0.052011

5-Cl			
H	1.3954	0.1052	0.2910
C	0.8104	0.1036	1.2129
C	-0.6759	0.1499	3.5700
C	0.3822	-1.0873	1.7908
C	0.4941	1.3216	1.8063
C	-0.2555	1.3639	2.9964
C	-0.3552	-1.0639	2.9702
H	0.8449	2.2355	1.3397
H	-0.6946	-1.9882	3.4420
H	-1.2471	0.1406	4.4917
I	0.8503	-2.9448	0.8672
Cl	1.5612	-6.0673	-0.7361
N	-0.4739	2.5950	3.6675
C	-1.6173	2.6157	4.6007
C	-0.4583	3.7961	2.8095
H	-2.5688	2.3071	4.1398
H	-1.7428	3.6247	5.0229
H	-1.3969	1.9432	5.4496
H	-1.1547	3.7391	1.9582
H	-0.7034	4.6897	3.4041
H	0.5664	3.9450	2.4231

SCF = -0.034630**6-Cl**

H	0.2768	0.2206	0.0849
C	0.2011	0.1365	1.1710
C	0.0025	-0.0555	3.9612
C	0.3592	-1.0940	1.8112
C	-0.0570	1.2791	1.9178
C	-0.1535	1.1668	3.3127
C	0.2615	-1.1933	3.1943
H	-0.1836	2.2464	1.4422
H	0.3837	-2.1513	3.7032
H	-0.0727	-0.1376	5.0377
I	0.7544	-2.8378	0.6558
Cl	1.4165	-5.8035	-1.1906
O	-0.4091	2.3605	3.9244
C	-0.5243	2.3471	5.3384
H	0.4127	2.0250	5.8032
H	-1.3633	1.7200	5.6557
H	-0.7243	3.4012	5.5679

SCF = -0.101190**7-Cl**

H	0.9523	0.4185	0.5558
C	0.4192	0.1573	1.4708
C	-0.9576	-0.4713	3.8180
C	0.2617	-1.1714	1.8605
C	-0.1116	1.1757	2.2607
C	-0.7948	0.8576	3.4324
C	-0.4273	-1.4908	3.0291
H	0.0134	2.2128	1.9499
H	-0.5608	-2.5273	3.3411
H	-1.4968	-0.7273	4.7299
I	1.0847	-2.7276	0.6617
Cl	2.4906	-5.2867	-1.2813
S	-1.5047	2.1558	4.4199
C	-0.1347	2.5371	5.5665
H	-0.4613	3.3383	6.2363
H	0.7570	2.8739	5.0288
H	0.1372	1.6663	6.1710

SCF = -0.040691

8-Cl

H	0.5243	0.2044	0.1069
C	0.3152	0.1585	1.1768
C	-0.2260	0.0789	3.9183
C	0.3436	-1.0538	1.8662
C	0.0154	1.3330	1.8604
C	-0.2549	1.2915	3.2305
C	0.0742	-1.0965	3.2333
H	-0.0066	2.2799	1.3204
H	0.0937	-2.0393	3.7825
H	-0.4345	0.0302	4.9868
I	0.8024	-2.8535	0.8218
Cl	1.5435	-5.7696	-0.8554
C	-0.5726	2.5755	3.9282
F	-0.8236	2.4893	5.2355
F	0.3988	3.4898	3.8534
F	-1.6451	3.2073	3.4424

SCF = -0.298538**9-Cl**

H	0.3589	0.2077	0.0877
C	0.2191	0.1771	1.1697
C	-0.1458	0.1339	3.9452
C	0.3341	-1.0171	1.8793
C	-0.0799	1.3600	1.8459
C	-0.2566	1.3141	3.2223
C	0.1535	-1.0445	3.2611
H	-0.1698	2.2925	1.2924
H	0.2417	-1.9749	3.8246
H	-0.2869	0.1130	5.0240
I	0.7910	-2.8207	0.8402
Cl	1.5375	-5.7695	-0.8586
Br	-0.6653	2.9274	4.1518

SCF = -0.034928**10-Cl**

C	0.2169	-0.0228	1.1321
C	-0.1281	0.0049	3.9312
C	0.1141	-1.2237	1.8439
C	0.1467	1.1922	1.8240
C	-0.0251	1.2096	3.2177
C	-0.0578	-1.2137	3.2377
I	0.4864	-0.0443	-1.0532
Cl	0.8439	-0.0724	-3.9603
C	0.1800	-2.4842	1.1830
N	0.2318	-3.5137	0.6580
C	-0.1621	-2.4378	3.9600
N	-0.2471	-3.4300	4.5486
C	-0.3020	0.0189	5.3418
N	-0.4435	0.0302	6.4902
C	-0.0963	2.4478	3.9198
N	-0.1543	3.4515	4.4919
C	0.2464	2.4394	1.1425
N	0.3258	3.4584	0.6008

SCF = 0.230339**11-I**

C	0.0020	0.0655	1.1500
C	0.0227	0.0988	3.9262
C	0.0375	-1.1521	1.8305
C	-0.0231	1.2878	1.8328
C	-0.0127	1.3070	3.2283
C	0.0473	-1.1132	3.2252
I	0.0753	-3.0032	0.7782
F	0.0804	-2.2238	3.9366
F	0.0328	0.1017	5.2444
F	-0.0361	2.4520	3.8792
F	-0.0564	2.4213	1.1605
F	-0.0093	0.1080	-0.1686
I	0.1465	-6.4651	-1.1902

SCF = -0.382553**11-F**

C	0.0040	0.0087	1.1298
C	0.0228	0.0525	3.9035
C	0.0371	-1.1801	1.8185
C	-0.0204	1.2412	1.8029
C	-0.0108	1.2576	3.1991
C	0.0465	-1.1587	3.1926
I	0.0784	-3.3096	0.6123
F	0.0781	-2.2750	3.9020
F	0.0320	0.0658	5.2241
F	-0.0334	2.4071	3.8500
F	-0.0521	2.3800	1.1348
F	-0.0062	0.0423	-0.1928
F	0.1126	-5.0535	-0.3752

SCF = -0.404415**11-OCH2**

C	1.3841	0.5606	0.0000
C	-0.2553	2.8042	-0.0000
C	0.0000	0.3793	-0.0000
C	1.9539	1.8392	0.0000
C	1.1315	2.9681	-0.0000
C	-0.8080	1.5174	-0.0000
F	-2.1227	1.4160	-0.0000
F	-1.0445	3.8587	-0.0000
F	1.6586	4.1736	-0.0000
F	3.2640	1.9759	0.0000
F	2.2026	-0.4742	0.0000
I	-0.8386	-1.5549	0.0000
O	-1.3309	-4.4949	0.0000
C	-0.2501	-5.0124	0.0000
H	-0.1399	-6.1093	0.0000
H	0.6758	-4.4103	0.0000

SCF = -413.008337**11-OMe**

C	0.0506	0.2084	1.2445
C	-0.0224	0.1479	4.0170
C	0.0723	-1.0058	1.8895
C	-0.0077	1.4142	1.9623
C	-0.0442	1.3782	3.3574
C	0.0362	-1.0362	3.2638
I	0.1735	-3.0673	0.6077
F	0.0549	-2.1773	3.9322
F	-0.0569	0.1119	5.3367
F	-0.0992	2.5022	4.0496
F	-0.0283	2.5767	1.3359
F	0.0835	0.2926	-0.0755
O	0.2654	-4.9804	-0.5107
C	0.2996	-4.8867	-1.8845
H	0.3430	-5.9203	-2.2561
H	1.1904	-4.3456	-2.2286
H	-0.6042	-4.4034	-2.2772

SCF = -0.356264**11-Cl**

C	0.2132	-0.0236	1.1651
C	-0.1327	0.0065	3.9726
C	0.1144	-1.2080	1.8935
C	0.1354	1.1761	1.8705
C	-0.0357	1.2027	3.2603
C	-0.0570	-1.2047	3.2835
I	0.4760	-0.0465	-0.9686
F	0.1791	-2.3827	1.2957
F	-0.1471	-2.3424	3.9441
F	-0.2938	0.0206	5.2806
F	-0.1056	2.3543	3.8988
F	0.2208	2.3378	1.2501
Cl	0.8792	-0.0801	-4.2258

SCF = -0.390346**11-Br**

C	0.0006	0.0593	1.1467
C	0.0252	0.0884	3.9225
C	0.0372	-1.1589	1.8250
C	-0.0238	1.2808	1.8313
C	-0.0114	1.2977	3.2268
C	0.0490	-1.1224	3.2192
I	0.0740	-3.0151	0.7658
F	0.0833	-2.2339	3.9292
F	0.0372	0.0895	5.2409
F	-0.0341	2.4419	3.8797
F	-0.0583	2.4157	1.1611
F	-0.0126	0.1044	-0.1718
Br	0.1380	-6.1901	-1.0481

SCF = -0.381859

11-DMF

C	-1.6423	1.1873	-0.0497
C	-3.5991	-0.7764	0.1369
C	-1.2482	-0.1516	-0.0381
C	-2.9911	1.5535	0.0300
C	-3.9762	0.5680	0.1237
C	-2.2448	-1.1240	0.0563
F	-1.9416	-2.4073	0.0728
F	-4.5161	-1.7178	0.2251
F	-5.2464	0.9033	0.1990
F	-3.3298	2.8265	0.0165
F	-0.7504	2.1558	-0.1365
I	0.7914	-0.6836	-0.1584
O	3.7367	-1.2096	-0.1411
C	4.8042	-0.7808	0.2230
H	5.5858	-1.4255	0.6733
N	5.1484	0.5477	0.0256
C	4.1465	1.4851	-0.4811
H	3.4757	1.8465	0.3172
H	3.5231	0.9838	-1.2483
H	4.6324	2.3508	-0.9589
C	6.2814	1.1359	0.7356
H	5.9645	1.6569	1.6568
H	6.7954	1.8685	0.0858
H	7.0225	0.3664	1.0102

SCF = -413.037975**11-NH3**

C	0.0033	0.2624	1.2615
C	0.0139	0.2986	4.0407
C	0.0331	-0.9518	1.9478
C	-0.0211	1.4856	1.9427
C	-0.0158	1.5058	3.3391
C	0.0380	-0.9149	3.3424
I	0.0698	-2.7953	0.9042
F	0.0656	-2.0274	4.0505
F	0.0192	0.3003	5.3578
F	-0.0386	2.6507	3.9873
F	-0.0490	2.6153	1.2661
F	-0.0029	0.2966	-0.0571
N	0.1247	-5.6877	-0.7339
H	1.0710	-5.9451	-0.9094
H	-0.3629	-5.5825	-1.5964
H	-0.3182	-6.3856	-0.1776

SCF = -0.288542**12-Cl**

C	0.5631	-0.2769	1.0954
C	-0.0142	0.5877	3.6956
C	0.2460	-1.1830	2.1053
C	0.5821	1.0759	1.4288
C	0.2976	1.5341	2.7197
C	-0.0463	-0.7776	3.4120
I	1.0066	-0.9415	-0.9031
Cl	1.6896	-1.9610	-3.9735
I	-0.5213	-2.1811	4.9104
I	0.3372	3.5897	3.1821
F	-0.2869	0.9960	4.9234
F	0.2184	-2.4733	1.8263
F	0.8785	1.9636	0.4975

SCF = -0.193284**13-Cl**

C	0.0003	-0.0040	1.1802
I	-0.0024	-0.0191	-1.2775
Cl	-0.0054	-0.0358	-3.8495
Br	-0.9272	-1.5851	1.8946
Br	1.8386	-0.0081	1.8817
Br	-0.9096	1.5983	1.8734

SCF = -0.061355**14-Cl**

C	0.0001	-0.0015	1.1208
I	-0.0004	-0.0205	-1.1397
Cl	-0.0007	-0.0445	-4.0884
F	-0.6059	-1.0493	1.6770
F	1.2149	0.0042	1.6674
F	-0.6080	1.0543	1.6592

SCF = -0.340070**15-Cl**

C	-0.0005	-0.0042	1.1401
I	0.0082	-0.0088	-1.0809
Cl	0.0227	-0.0160	-4.7325
C	-0.7256	-1.2570	1.6318
H	-0.2352	-2.1781	1.2931
H	-1.7659	-1.2951	1.2853
H	-0.7495	-1.2888	2.7260
C	1.4451	-0.0027	1.6376
H	1.9995	-0.8868	1.2991
H	1.4801	-0.0004	2.7320
H	1.9989	0.8804	1.2955
C	-0.7266	1.2500	1.6266
H	-0.2368	2.1701	1.2842
H	-0.7505	1.2863	2.7207
H	-1.7669	1.2859	1.2800

SCF = -0.115875**16-Cl**

C	-0.0006	-0.0011	1.7515
I	-0.0013	-0.0186	-1.6430
Cl	-0.0017	-0.0298	-3.9939
C	-0.6971	-1.2074	1.8052
N	-1.2788	-2.2150	1.8389
C	1.3926	-0.0019	1.7975
N	2.5562	-0.0027	1.8249
C	-0.6967	1.2057	1.7902
N	-1.2783	2.2137	1.8114

SCF = 0.036609**17-Cl**

I	0.1793	-1.4267	-1.7012
Cl	1.1435	-2.6843	-3.9087
N	-0.5959	-0.4154	0.0740
C	0.0600	-0.3567	1.3058
C	-1.8158	0.2621	0.1342
O	1.1289	-0.8411	1.5803
O	-2.6152	0.3940	-0.7582
C	-2.0298	0.8473	1.5411
H	-2.1584	1.9379	1.4741
H	-2.9604	0.4487	1.9717
C	-0.7833	0.4361	2.3196
H	-0.2045	1.2933	2.6945
H	-1.0065	-0.1959	3.1920

SCF = -0.223866**18-Cl**

I	-0.0027	-0.0425	-0.8096
Cl	-0.0070	0.1971	-4.3975
C	-0.0000	-0.0612	1.3068
H	0.0011	0.9349	1.7237
C	0.0002	-1.1804	2.0220
H	0.0016	-1.1844	3.1007
H	-0.0008	-2.1791	1.6123

SCF = -0.051204**19-Cl**

I	-0.0026	-0.0342	-0.8278
Cl	-0.0071	0.0566	-4.2547
C	-0.0000	-0.0484	1.2868
H	0.0011	0.9448	1.7182
C	0.0002	-1.1770	2.0058
H	-0.0009	-2.1799	1.5622
C	0.0020	-1.1530	3.4234
N	0.0034	-1.1454	4.5827

SCF = -0.010622**20-Cl**

I	-0.0236	0.0826	-0.8391
Cl	0.2512	0.1567	-4.4670
C	-0.2600	-0.1014	1.2509
H	-0.6756	0.7843	1.6908
C	0.0932	-1.2180	1.9005
H	0.5042	-2.0985	1.3863
N	0.1067	-1.3642	3.3096
C	-0.2956	-2.7139	3.7552
H	0.3108	-3.4713	3.2299
H	-1.3596	-2.9370	3.5819
H	-0.0857	-2.8182	4.8316
C	-0.5769	-0.3081	4.0759
H	-0.0760	0.6564	3.8744
H	-0.4763	-0.5064	5.1540
H	-1.6466	-0.2044	3.8351

SCF = -0.053376**21-Cl**

I	0.0069	-0.0480	-0.6879
Cl	0.3684	-0.1664	-4.1847
C	-0.2010	0.0197	1.3202
H	-0.4305	0.0943	3.5405
C	-0.3253	0.0601	2.5231

SCF = 0.021921**22-Cl**

I	0.0095	-0.0483	-0.7138
Cl	0.3546	-0.1587	-4.0382
C	-0.1989	0.0183	1.2975
C	-0.3242	0.0585	2.5074
C	-0.4650	0.1036	3.8652
N	-0.5843	0.1423	5.0203

SCF = 0.062891

23-Cl

I	-0.0004	-0.0452	-0.6297
Cl	0.3409	-0.1548	-3.9396
C	-0.2100	0.0222	1.4220
N	-0.3273	0.0597	2.5702

SCF = -0.029341**24-Cl**

C	-1.0417	0.2967	1.5445
C	0.9791	-0.3358	3.3797
C	-1.0782	-0.9204	2.2191
C	-0.0032	1.2016	1.7793
C	0.9996	0.8779	2.6957
C	-0.0668	-1.2339	3.1358
C	-0.0962	-2.5141	3.8517
C	-0.0884	-4.9748	5.2744
C	0.5360	-3.6468	3.3315
C	-0.7412	-2.6367	5.0855
C	-0.7373	-3.8474	5.7855
C	0.5398	-4.8575	4.0315
C	-0.0509	-6.2337	6.0267
C	0.0278	-8.6240	7.4606
C	-1.0582	-7.1895	5.8436
C	0.9983	-6.4652	6.9242
C	1.0264	-7.6633	7.6348
C	-1.0140	-8.3812	6.5618
I	2.5363	-4.9979	7.1992
I	2.5237	-0.8224	4.7839
F	0.0624	-9.7548	8.1370
F	1.9922	-7.9317	8.4932
F	-1.9421	-9.3100	6.4205
F	1.1447	-5.9033	3.5049
F	1.1373	-3.5786	2.1607
F	-1.3672	-1.5976	5.6005
F	-1.3599	-3.9224	6.9447
F	-1.9739	0.6334	0.6718
F	0.0241	2.3521	1.1365
F	1.9620	1.7601	2.8884
Cl	4.5423	-2.2701	7.0875
I	-2.6579	-2.2769	1.8509
I	-2.6429	-6.8397	4.4882

SCF = -0.600931**ZPE = 0.146967****H₂₉₈ = -0.420868****G₂₉₈ = -0.516916****25-Cl**

C	0.3049	-1.3267	0.2475
C	-0.3220	1.3861	-0.0040
C	1.3498	-0.3988	0.1998
C	-1.0406	-0.9534	0.1766
C	-1.3219	0.4103	0.0492
C	1.0043	0.9499	0.0718
C	2.7491	-0.8232	0.2701
C	5.4156	-1.6318	0.4070
C	3.4406	-1.1267	-0.9090
C	3.3849	-0.9225	1.5147
C	4.7157	-1.3265	1.5769
C	4.7718	-1.5294	-0.8282
C	-2.1112	-1.9508	0.2231
C	-4.1514	-3.8513	0.3143
C	-2.6611	-2.3251	1.4561
C	-2.5767	-2.5227	-0.9672
C	-3.5958	-3.4706	-0.9092
C	-3.6791	-3.2740	1.4957
C	-0.6500	2.8059	-0.1441
C	-1.2752	5.5118	-0.4085
C	-0.7677	3.3664	-1.4219
C	-0.8434	3.5920	0.9993
C	-1.1552	4.9418	0.8614
C	-1.0802	4.7186	-1.5415
I	2.3413	-0.4644	3.2956
I	2.4649	-0.9733	-2.8051
I	-1.7334	-1.9474	-2.8457
I	-1.9587	-1.4620	3.2540
I	-0.4713	2.1615	-3.1630
I	-0.6659	2.7464	2.9290
Cl	0.1573	-0.4581	-5.3135
F	0.6000	-2.6038	0.3733
F	-2.5805	0.7920	-0.0144
F	1.9673	1.8471	0.0296
F	-4.0699	-4.0393	-2.0018
F	-5.1154	-4.7489	0.3598
F	-4.2259	-3.6561	2.6353
F	5.3538	-1.4336	2.7281
F	6.6753	-2.0136	0.4740
F	5.4678	-1.8266	-1.9095
F	-1.5706	6.7904	-0.5311
F	-1.3458	5.7195	1.9115
F	-1.2025	5.2950	-2.7224

SCF = -0.675125

26-Cl

H	-1.4279	0.8755	-2.1045
C	-1.3290	1.5881	-1.2661
C	-1.0834	3.4400	0.8330
C	-1.1309	1.1705	0.0349
C	-1.4053	2.9616	-1.5187
C	-1.2835	3.8774	-0.4780
C	-1.0046	2.0762	1.1050
H	-1.5615	3.3093	-2.5405
H	-1.3442	4.9464	-0.6837
H	-0.9900	4.1684	1.6358
C	-0.7969	1.5167	2.4436
C	-0.4079	0.2485	4.9051
C	-0.7414	0.1205	2.5455
C	-0.6533	2.2777	3.6046
C	-0.4595	1.6399	4.8294
C	-0.5502	-0.5258	3.7506
H	-0.6913	3.3652	3.5612
H	-0.3474	2.2361	5.7356
H	-0.5074	-1.6108	3.8268
H	-0.2560	-0.2369	5.8679
I	-0.9841	-0.8515	0.6484
Cl	-1.3575	-1.4922	-2.1012

SCF = 0.161068**27-Cl**

H	-0.2248	0.1850	0.1587
C	-0.1692	0.1434	1.2462
C	-0.0247	0.0870	4.0521
C	-0.1603	-1.0502	1.9376
C	-0.1046	1.3384	1.9701
C	-0.0332	1.3003	3.3611
C	-0.0889	-1.1077	3.3345
H	-0.1114	2.2858	1.4265
H	0.0317	0.0712	5.1441
C	-0.0874	-2.4397	3.9428
C	-0.0952	-5.0622	4.9332
C	-0.1573	-3.5503	3.0800
C	-0.0212	-2.6652	5.3151
C	-0.0257	-3.9765	5.7989
C	-0.1621	-4.8471	3.5510
H	0.0339	-1.8213	6.0071
H	-0.2170	-5.7217	2.8764
H	-0.0993	-6.0929	5.3009
I	-0.2516	-3.0053	1.0301
Cl	-0.3394	-5.7361	0.5285
C	0.0375	2.5669	4.1703
C	0.0474	-4.1691	7.2902
F	1.1370	2.6515	4.9197
F	-0.9726	2.6984	5.0306
F	0.0258	3.6984	3.4688
F	-0.9632	-3.5953	7.9442
F	0.0406	-5.4320	7.7096
F	1.1453	-3.6431	7.8347

SCF = -0.342216**28-Cl**

H	-0.1672	0.1991	0.1750
C	-0.1308	0.1592	1.2636
C	-0.0363	0.0970	4.0772
C	-0.1258	-1.0349	1.9570
C	-0.0878	1.3514	1.9882
C	-0.0409	1.3138	3.3863
C	-0.0792	-1.0952	3.3550
H	-0.0906	2.3110	1.4681
H	0.0007	0.0927	5.1684
C	-0.0794	-2.4297	3.9601
C	-0.0869	-5.0590	4.9360
C	-0.1260	-3.5381	3.0930
C	-0.0363	-2.6574	5.3325
C	-0.0403	-3.9733	5.8131
C	-0.1303	-4.8392	3.5566
H	0.0005	-1.8251	6.0368
H	-0.1669	-5.7097	2.8749
H	-0.0896	-6.0819	5.3220
I	-0.1870	-2.9873	1.0446
Cl	-0.2467	-5.7194	0.5209
C	0.0028	2.5332	4.1171
N	0.0383	3.5264	4.7093
C	0.0039	-4.1988	7.2174
N	0.0399	-4.3790	8.3596

SCF = 0.266266

29-Cl

H	-0.0105	0.1852	0.1633
C	-0.0410	0.1342	1.2524
C	-0.1230	0.0464	4.0567
C	-0.0244	-1.0715	1.9262
C	-0.1017	1.3176	1.9788
C	-0.1343	1.2955	3.3921
C	-0.0643	-1.1315	3.3268
H	-0.1149	2.2613	1.4430
H	-0.1507	0.0020	5.1413
C	-0.0449	-2.4754	3.9303
C	-0.0038	-5.1051	4.8814
C	0.0116	-3.5698	3.0511
C	-0.0824	-2.7062	5.2968
C	-0.0533	-4.0306	5.7973
C	0.0342	-4.8748	3.5122
H	-0.1234	-1.8645	5.9794
H	0.0781	-5.7354	2.8179
H	0.0133	-6.1339	5.2323
I	0.0545	-3.0001	1.0219
Cl	0.1020	-5.8602	0.4325
N	-0.0641	2.4819	4.1226
N	0.0400	-4.2608	7.1699
C	-0.4473	3.7291	3.4438
H	0.2611	3.9313	2.6187
H	-0.3694	4.5829	4.1387
H	-1.4719	3.7041	3.0373
C	-0.4682	2.4391	5.5367
H	0.2410	1.8034	6.1001
H	-1.4911	2.0539	5.6831
H	-0.4096	3.4460	5.9835
C	-0.3904	-3.1867	8.0771
H	0.2882	-2.3203	7.9670
H	-0.3110	-3.5151	9.1271
H	-1.4268	-2.8566	7.8959
C	-0.2876	-5.6082	7.6606
H	0.4436	-6.3333	7.2543
H	-1.3049	-5.9336	7.3852
H	-0.1942	-5.6513	8.7583

SCF = 0.155215**30-Cl**

H	1.0495	-0.0050	0.6310
C	0.4247	0.1976	1.5022
C	-1.1514	0.7848	3.7377
C	-0.2937	-0.8010	2.1448
C	0.3550	1.5053	1.9831
C	-0.4311	1.7919	3.0999
C	-1.0823	-0.5225	3.2519
H	0.9201	2.2950	1.4815
H	-1.7714	0.9932	4.6132
C	0.8956	-2.9489	4.2356
C	-0.5577	-5.1981	5.0474
C	0.0142	-3.5837	3.3622
C	1.0341	-3.4368	5.5312
C	0.3016	-4.5573	5.9322
C	-0.7081	-4.7042	3.7470
H	1.7204	-2.9412	6.2224
H	-1.3739	-5.2423	3.0550
H	-1.1186	-6.0922	5.3347
I	-0.1860	-2.8274	1.3852
Cl	-0.0521	-5.5919	0.9012
C	-0.4734	3.2133	3.5895
C	0.4748	-5.0416	7.3467
F	0.7232	3.6812	3.9466
F	-1.2471	3.4345	4.6499
F	-0.9145	4.0731	2.6706
F	0.1514	-4.1192	8.2553
F	-0.2500	-6.1052	7.6855
F	1.7288	-5.3825	7.6424
H	-1.6522	-1.2994	3.7663
H	1.4838	-2.0798	3.9381

SCF = -0.345991

31-Cl

H	1.1087	-0.8875	3.4656
C	0.2308	-0.3361	3.1204
C	-2.0048	1.1150	2.2749
C	-0.6442	-0.8621	2.1792
C	-0.0135	0.9288	3.6523
C	-1.1326	1.6521	3.2269
C	-1.7570	-0.1524	1.7492
H	0.6632	1.3540	4.3964
H	-2.8757	1.6860	1.9481
C	1.2634	-4.4546	3.4295
C	-0.3689	-3.7602	5.5991
C	0.1805	-3.6003	3.2660
C	1.5367	-4.9673	4.6994
C	0.7272	-4.6132	5.7801
C	-0.6475	-3.2562	4.3332
H	2.3769	-5.6522	4.8385
H	-1.5120	-2.6014	4.2099
H	-1.0042	-3.4979	6.4467
I	-0.2629	-2.8214	1.3391
Cl	0.3758	-5.4833	0.6837
H	-2.4529	-0.5553	1.0110
H	1.8983	-4.7692	2.5863
C	-1.3856	2.9433	3.7659
N	-1.5918	3.9942	4.2034
C	1.0117	-5.1205	7.0787
N	1.2429	-5.5264	8.1371

SCF = 0.261939**32-Cl**

H	1.3134	-0.7475	3.4617
C	0.3962	-0.2361	3.1529
C	-1.9392	1.0978	2.4128
C	-0.4937	-0.8203	2.2564
C	0.1267	1.0131	3.6888
C	-1.0445	1.7163	3.3178
C	-1.6579	-0.1550	1.8888
H	0.8311	1.4481	4.3912
H	-2.8532	1.6005	2.1134
C	1.2146	-4.6594	3.4292
C	-0.2029	-3.7628	5.6663
C	0.2892	-3.6243	3.3150
C	1.4408	-5.2450	4.6657
C	0.7449	-4.8040	5.8134
C	-0.4271	-3.1866	4.4267
H	2.1597	-6.0578	4.7292
H	-1.1699	-2.3885	4.3527
H	-0.7656	-3.4040	6.5211
I	-0.0683	-2.7404	1.4344
Cl	0.6818	-5.4532	0.4130
H	-2.3743	-0.5964	1.1913
H	1.7620	-5.0499	2.5517
N	-1.2546	3.0204	3.7468
N	1.0632	-5.3058	7.0730
C	-2.6040	3.5889	3.6221
H	-2.6213	4.6249	4.0030
H	-3.3679	3.0066	4.1643
H	-2.8860	3.6422	2.5537
C	-0.5179	3.4930	4.9277
H	0.5666	3.4984	4.7083
H	-0.6981	2.8737	5.8226
H	-0.7958	4.5346	5.1641
C	1.7360	-6.6129	7.1376
H	2.7395	-6.5314	6.6786
H	1.1729	-7.4121	6.6248
H	1.8923	-6.9159	8.1858
C	0.1059	-5.0865	8.1668
H	0.4832	-5.5355	9.1013
H	-0.8922	-5.5070	7.9571
H	0.0039	-4.0025	8.3576

SCF = 0.148981

33-Cl

I	-1.4802	1.2917	-3.7433
Cl	-2.1931	2.0575	-5.9426
C	-0.7366	0.4459	-1.4160
C	0.0950	-0.3665	1.1044
N	-0.9247	-0.8135	-1.0049
C	-0.1080	1.3647	-0.5533
C	0.3077	0.9709	0.6981
C	-0.5214	-1.2489	0.2457
H	0.0369	2.3867	-0.9054
H	0.7964	1.6658	1.3820
H	0.4186	-0.6917	2.0916
C	-1.5792	-1.7811	-1.8960
H	-1.0032	-1.8898	-2.8370
H	-2.5983	-1.4340	-2.1605
H	-1.6698	-2.7787	-1.4379
H	-0.7061	-2.2903	0.5171

SCF = 0.097368**34-Cl**

I	-1.5021	1.2321	-3.5274
Cl	-2.3515	1.9808	-5.8724
C	-0.7440	0.5360	-1.4190
C	0.1203	-0.3520	1.0397
C	-0.9201	-0.7802	-1.0533
C	-0.1311	1.4378	-0.5621
C	0.3060	0.9855	0.6833
N	-0.4848	-1.2100	0.1748
H	-1.4006	-1.5194	-1.7065
H	0.0095	2.4842	-0.8514
H	0.7931	1.6624	1.3874
H	0.4544	-0.7312	2.0108
H	-0.1567	-3.2861	-0.1572
C	-0.6769	-2.6136	0.5549
H	-0.2866	-2.8344	1.5647
H	-1.7545	-2.8759	0.5502

SCF = 0.118722**35-Cl**

I	-1.4637	1.0748	-3.4685
Cl	-2.3764	1.7649	-5.8951
C	-0.6890	0.4906	-1.4149
N	0.2544	-0.2220	1.0931
C	-0.7222	-0.8401	-0.9965
C	-0.1709	1.4567	-0.5513
C	0.2998	1.0887	0.7003
C	-0.2460	-1.1855	0.2596
H	-1.1224	-1.6210	-1.6526
H	-0.1310	2.5095	-0.8521
H	0.7156	1.8188	1.4041
H	-0.2541	-2.2203	0.6208
H	1.8642	-0.7979	2.3578
C	0.7741	-0.5998	2.4110
H	0.6069	0.2002	3.1579
H	0.2803	-1.5116	2.7986

SCF = 0.120886**36-Cl**

N	-0.3644	0.5817	-0.1248
C	-0.5796	1.8471	-0.6031
N	-0.3157	2.6924	0.4420
C	0.0370	0.6266	1.2269
H	0.2576	-0.2500	1.7974
C	0.0678	1.9596	1.5848
H	0.3193	2.4224	2.5150
I	-1.3557	2.5270	-3.0683
H	0.2703	4.5474	-0.3784
C	-0.4129	4.1400	0.3931
H	-0.1499	4.5974	1.3617
H	-1.4447	4.4496	0.1334
H	0.1522	-0.6374	-1.7693
C	-0.5232	-0.6411	-0.8908
H	-0.2934	-1.5329	-0.2839
H	-1.5637	-0.7333	-1.2605
Cl	-2.0509	3.1354	-5.2778

SCF = 0.072721

37-Cl

N	-0.3040	0.5752	-0.1250
C	-0.5473	1.8458	-0.6031
N	-0.3460	2.6871	0.4712
C	0.0559	0.6172	1.2316
C	0.0099	1.9535	1.6144
I	-1.3926	2.6657	-3.5482
H	-0.5311	4.4604	-0.6454
C	-0.4786	4.1326	0.4122
H	0.3865	4.6431	0.8743
H	-1.4067	4.4719	0.9116
H	0.5800	-1.0394	-1.1815
C	-0.4171	-0.6329	-0.9239
H	-1.0018	-1.4147	-0.4049
H	-0.9390	-0.4047	-1.8749
Cl	-2.0148	3.2734	-5.7150
C	0.4111	-0.5726	2.0523
C	0.2733	2.5457	2.9543
F	1.1980	-0.2914	3.0876
F	1.0693	-1.5252	1.3911
F	-0.6485	-1.1916	2.5722
F	1.5243	2.9803	3.1035
F	-0.4890	3.5976	3.2545
F	0.0718	1.6994	3.9610

SCF = -0.421378**38-Cl**

N	0.1047	-0.9743	-0.8052
C	-0.4674	0.1379	-1.3845
N	-0.5105	1.0924	-0.3911
C	0.4215	-0.7259	0.5454
C	0.0303	0.5883	0.8087
I	-1.4421	0.4238	-4.2995
H	-2.1055	2.3939	-0.8525
C	-1.0395	2.4360	-0.5512
H	-0.4801	2.9756	-1.3416
H	-0.9696	3.0243	0.3809
H	1.0244	-2.0746	-2.3526
C	0.3506	-2.2336	-1.4868
H	0.8171	-2.9822	-0.8221
H	-0.6018	-2.6556	-1.8657
Cl	-2.1791	0.6376	-6.5084
C	1.0159	-1.6598	1.4113
N	1.5052	-2.4228	2.1312
C	0.1303	1.3152	2.0074
N	0.2163	1.9067	2.9985

SCF = 0.184456**39-Cl**

N	1.4869	1.1086	-0.0002
C	0.6858	-0.0000	-0.0003
N	1.4869	-1.1086	-0.0004
C	2.8279	0.7000	0.0001
C	2.8279	-0.7000	0.0000
I	-1.4349	0.0000	-0.0001
H	0.4193	-2.7090	0.9038
C	1.0249	-2.4871	-0.0001
H	1.8789	-3.1963	-0.0031
H	0.4141	-2.7079	-0.9008
H	0.4184	2.7090	0.9031
C	1.0249	2.4871	-0.0003
H	1.8789	3.1963	-0.0024
H	0.4149	2.7080	-0.9015
Cl	-4.3440	-0.0000	0.0003
C	3.9616	1.6320	0.0004
H	3.9746	2.2863	0.8924
H	3.9753	2.2862	-0.8916
H	4.9343	1.1035	0.0008
C	3.9616	-1.6320	0.0003
H	3.9771	-2.2831	0.8945
H	4.9343	-1.1035	-0.0042
H	3.9728	-2.2894	-0.8894

SCF = -758.109334**40-Cl**

N	-0.0117	-0.9824	-0.9406
C	-0.5172	0.1510	-1.5304
N	-0.4978	1.1298	-0.5663
C	0.3358	-0.7151	0.4028
C	0.0169	0.6088	0.6422
I	-1.3780	0.4074	-4.0725
H	-2.1326	2.4694	-0.5820
C	-1.0318	2.4724	-0.6986
H	-0.7851	2.8863	-1.6948
H	-0.6095	3.1436	0.0718
H	1.2113	-2.2040	-2.1570
C	0.2547	-2.2463	-1.6014
H	0.3239	-3.0695	-0.8666
H	-0.5564	-2.4835	-2.3158
Cl	-2.1415	0.6353	-6.3259
O	0.9477	-1.6514	1.1511
O	0.0352	1.3589	1.7594
C	1.3687	1.5903	2.2363
H	1.8770	0.6410	2.4371
H	1.1911	2.1481	3.1638
H	1.9337	2.1884	1.5164
C	0.1610	-2.0382	2.2872
H	-0.0617	-1.1697	2.9164
H	0.8266	-2.7407	2.8034
H	-0.7605	-2.5300	1.9643

SCF = -0.040583

7.8 GFN2-xTB

OCH2

O	2.8299	-5.5750	-2.1692
C	2.8330	-5.2064	-3.3029
H	2.8331	-5.9033	-4.1580
H	2.8360	-4.1398	-3.5846

SCF = -7.175648**ZPE = 0.025548****H₂₉₈ = -7.146273****G₂₉₈ = -7.171730****SCF_{DFT} = -114.528691****Cl**

Cl	0.0000	0.0000	0.0000
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SCF = -4.785134**ZPE = 0.000000****H₂₉₈ = -4.782773****G₂₉₈ = -4.800168****1**

H	2.6896	0.0647	-1.4432
C	2.1060	0.0804	-0.5356
C	0.6059	0.1153	1.7970
C	1.6681	-1.0984	0.0391
C	1.7860	1.2842	0.0689
C	1.0372	1.3042	1.2334
C	0.9197	-1.0946	1.2015
H	2.1254	2.2078	-0.3756
H	0.5835	-2.0214	1.6407
H	0.0217	0.1240	2.7050
I	2.1532	-2.9464	-0.8796
H	0.7902	2.2452	1.7012

SCF = -19.188037**ZPE = 0.087485****H₂₉₈ = -19.093565****G₂₉₈ = -19.132361****SCF_{DFT} = -529.369533****1-OCH2**

H	2.6882	0.1268	-1.3919
C	2.1003	0.1361	-0.4865
C	0.5924	0.1550	1.8393
C	1.6520	-1.0487	0.0687
C	1.7885	1.3354	0.1306
C	1.0353	1.3475	1.2924
C	0.8993	-1.0490	1.2291
H	2.1372	2.2620	-0.3008
H	0.5546	-1.9790	1.6553
H	0.0050	0.1575	2.7454
I	2.1239	-2.8870	-0.8650
H	0.7940	2.2848	1.7710
O	2.7964	-5.5610	-2.2869
C	2.8783	-5.4107	-3.4674
H	3.1106	-6.2408	-4.1547
H	2.7285	-4.4347	-3.9556

SCF = -26.366456**ZPE = 0.113945****H₂₉₈ = -26.240631****G₂₉₈ = -26.290931****SCF_{DFT} = -643.902300****1-Cl**

H	2.6980	0.0318	-1.4434
C	2.1106	0.0536	-0.5360
C	0.6082	0.0989	1.7837
C	1.6766	-1.1393	0.0217
C	1.7966	1.2613	0.0603
C	1.0438	1.2886	1.2231
C	0.9235	-1.1076	1.1855
H	2.1401	2.1875	-0.3829
H	0.5838	-2.0363	1.6226
H	0.0196	0.1132	2.6923
I	2.1605	-2.9974	-0.8978
Cl	2.8235	-5.5429	-2.1580
H	0.7976	2.2331	1.6904

SCF = -23.984788**ZPE = 0.087612****H₂₉₈ = -23.887877****G₂₉₈ = -23.932079****SCF_{DFT} = -989.660419**

2

H	0.3580	0.1804	0.0968
C	0.2184	0.1663	1.1667
C	-0.1387	0.1129	3.9260
C	0.3324	-1.0193	1.8748
C	-0.0763	1.3350	1.8411
C	-0.2562	1.3131	3.2245
C	0.1560	-1.0542	3.2487
H	-0.1681	2.2660	1.3020
H	0.2474	-1.9839	3.7889
H	-0.2788	0.1003	4.9965
I	0.7837	-2.8069	0.8404
C	-0.5581	2.5096	3.9168
N	-0.8026	3.4784	4.4777

SCF = -23.705695**ZPE = 0.085926****H₂₉₈ = -23.610873****G₂₉₈ = -23.654014****SCF_{DFT} = -621.639599****2-Cl**

H	0.3692	0.1548	0.0934
C	0.2261	0.1469	1.1648
C	-0.1359	0.0948	3.9154
C	0.3436	-1.0549	1.8553
C	-0.0686	1.3168	1.8293
C	-0.2529	1.3013	3.2163
C	0.1593	-1.0653	3.2340
H	-0.1597	2.2512	1.2915
H	0.2506	-1.9992	3.7704
H	-0.2790	0.0859	4.9877
I	0.7999	-2.8518	0.8171
Cl	1.4151	-5.2720	-0.5803
C	-0.5534	2.4904	3.9034
N	-0.7996	3.4638	4.4645

SCF = -28.514823**ZPE = 0.086085****H₂₉₈ = -28.417525****G₂₉₈ = -28.465992****SCF_{DFT} = -1081.943256****2-OCH2**

H	0.3385	0.2695	0.1354
C	0.2013	0.2390	1.2056
C	-0.1486	0.1427	3.9629
C	0.3116	-0.9615	1.8902
C	-0.0848	1.3985	1.8983
C	-0.2613	1.3554	3.2819
C	0.1378	-1.0135	3.2646
H	-0.1729	2.3391	1.3753
H	0.2257	-1.9532	3.7883
H	-0.2859	0.1137	5.0336
I	0.7480	-2.7321	0.8319
C	-0.5545	2.5416	3.9937
N	-0.7917	3.5034	4.5702
O	1.3762	-5.2754	-0.7112
C	1.4830	-5.1463	-1.8927
H	1.7091	-5.9928	-2.5609
H	1.3638	-4.1756	-2.3994

SCF = -30.885211**ZPE = 0.112454****H₂₉₈ = -30.759008****G₂₉₈ = -30.813296****SCF_{DFT} = -736.173371****3**

H	0.3710	0.1752	0.0911
C	0.2263	0.1611	1.1600
C	-0.1436	0.1019	3.9210
C	0.3305	-1.0271	1.8687
C	-0.0652	1.3295	1.8358
C	-0.2486	1.2930	3.2128
C	0.1480	-1.0655	3.2436
H	-0.1533	2.2702	1.3140
H	0.2324	-1.9970	3.7809
H	-0.2916	0.1060	4.9902
I	0.7769	-2.8099	0.8352
N	-0.5539	2.5143	3.9204
O	-0.6359	3.5325	3.2692
O	-0.7083	2.4422	5.1197

SCF = -29.644447**ZPE = 0.089623****H₂₉₈ = -29.545208****G₂₉₈ = -29.590213****SCF_{DFT} = -733.930604**

3-Cl

H	0.3667	0.1470	0.0858
C	0.2254	0.1415	1.1569
C	-0.1308	0.0856	3.9120
C	0.3439	-1.0602	1.8513
C	-0.0679	1.3093	1.8216
C	-0.2479	1.2862	3.2070
C	0.1629	-1.0734	3.2323
H	-0.1634	2.2489	1.2983
H	0.2559	-2.0077	3.7667
H	-0.2743	0.0925	4.9821
I	0.7958	-2.8459	0.8199
Cl	1.4133	-5.2669	-0.5792
N	-0.5497	2.4826	3.8982
O	-0.6460	3.5228	3.2529
O	-0.7028	2.4323	5.1155

SCF = -34.463682**ZPE = 0.089604****H₂₉₈ = -34.362089****G₂₉₈ = -34.412662****SCF_{DFT} = -1194.234679****3-OCH2**

H	0.3315	0.2726	0.1205
C	0.1977	0.2401	1.1905
C	-0.1432	0.1314	3.9520
C	0.3117	-0.9635	1.8730
C	-0.0878	1.3961	1.8882
C	-0.2570	1.3359	3.2669
C	0.1425	-1.0219	3.2496
H	-0.1823	2.3459	1.3845
H	0.2337	-1.9636	3.7681
H	-0.2800	0.1163	5.0225
I	0.7468	-2.7245	0.8108
N	-0.5552	2.5417	3.9972
O	-0.6466	3.5728	3.3656
O	-0.6964	2.4510	5.1980
O	1.3637	-5.2364	-0.7076
C	1.4858	-5.1581	-1.8925
H	1.7081	-6.0351	-2.5209
H	1.3854	-4.2082	-2.4406

SCF = -36.824870**ZPE = 0.116221****H₂₉₈ = -36.694221****G₂₉₈ = -36.750174****SCF_{DFT} = -848.464403****4**

H	0.3809	0.1645	0.0923
C	0.2308	0.1453	1.1610
C	-0.1588	0.1025	3.8999
C	0.3330	-1.0402	1.8643
C	-0.0686	1.3113	1.8423
C	-0.2677	1.3081	3.2176
C	0.1400	-1.0718	3.2325
H	-0.1492	2.2376	1.2921
H	0.2193	-2.0002	3.7771
H	-0.3104	0.0771	4.9693
I	0.7885	-2.8340	0.8304
C	-0.5688	2.5788	3.9503
H	-1.1567	2.3822	4.8437
H	0.3612	3.0584	4.2574
H	-1.1112	3.2744	3.3144

SCF = -22.359294**ZPE = 0.114606****H₂₉₈ = -22.235754****G₂₉₈ = -22.279069****SCF_{DFT} = -568.694661****4-OCH2**

H	0.3549	0.2084	0.1132
C	0.2120	0.1829	1.1830
C	-0.1588	0.1250	3.9227
C	0.3179	-1.0093	1.8753
C	-0.0808	1.3459	1.8722
C	-0.2706	1.3350	3.2485
C	0.1336	-1.0448	3.2453
H	-0.1637	2.2759	1.3282
H	0.2154	-1.9771	3.7832
H	-0.3031	0.0941	4.9931
I	0.7621	-2.7962	0.8346
C	-0.5652	2.6013	3.9923
H	-1.1764	2.4026	4.8696
H	0.3659	3.0598	4.3276
H	-1.0813	3.3152	3.3549
O	1.4267	-5.4025	-0.7375
C	1.5161	-5.1720	-1.9043
H	1.7568	-5.9524	-2.6451
H	1.3652	-4.1656	-2.3261

SCF = -29.537513**ZPE = 0.141045****H₂₉₈ = -29.382622****G₂₉₈ = -29.437469****SCF_{DFT} = -683.227292**

4-Cl

H	0.3869	0.1428	0.0882
C	0.2365	0.1260	1.1587
C	-0.1520	0.0851	3.8889
C	0.3467	-1.0742	1.8428
C	-0.0645	1.2943	1.8338
C	-0.2633	1.2913	3.2088
C	0.1490	-1.0837	3.2145
H	-0.1483	2.2246	1.2855
H	0.2308	-2.0156	3.7564
H	-0.3047	0.0619	4.9610
I	0.8116	-2.8729	0.8039
Cl	1.4549	-5.3408	-0.6211
C	-0.5662	2.5653	3.9449
H	-1.1557	2.3665	4.8383
H	0.3609	3.0522	4.2544
H	-1.1139	3.2594	3.3096

SCF = -27.154445**ZPE = 0.114735****H₂₉₈ = -27.028444****G₂₉₈ = -27.077337****SCF_{DFT} = -1028.984399****5**

H	1.3338	0.0853	0.2687
C	0.7523	0.0951	1.1781
C	-0.7429	0.1389	3.5025
C	0.3689	-1.0894	1.7777
C	0.3899	1.3018	1.7400
C	-0.3652	1.3600	2.9220
C	-0.3795	-1.0668	2.9391
H	0.7043	2.2043	1.2434
H	-0.6859	-1.9881	3.4110
H	-1.3285	0.1174	4.4061
I	0.9249	-2.9435	0.9116
N	-0.7025	2.5573	3.4952
C	-1.5749	2.5906	4.6430
C	-0.4025	3.7946	2.8179
H	-2.5522	2.1450	4.4252
H	-1.7318	3.6220	4.9490
H	-1.1264	2.0554	5.4843
H	-0.8902	3.8515	1.8381
H	-0.7500	4.6306	3.4199
H	0.6760	3.9067	2.6786

SCF = -28.956859**ZPE = 0.158324****H₂₉₈ = -28.786779****G₂₉₈ = -28.836075****SCF_{DFT} = -663.368828****5-Cl**

H	1.3411	0.0665	0.2763
C	0.7772	0.0767	1.1988
C	-0.6649	0.1318	3.5412
C	0.3794	-1.1206	1.7670
C	0.4611	1.2877	1.7851
C	-0.2679	1.3470	2.9761
C	-0.3432	-1.0734	2.9461
H	0.7943	2.1895	1.2948
H	-0.6673	-1.9953	3.4088
H	-1.2335	0.1076	4.4581
I	0.8525	-2.9795	0.8457
Cl	1.4940	-5.5495	-0.4330
N	-0.5450	2.5696	3.6037
C	-1.5931	2.5896	4.5972
C	-0.4366	3.7702	2.8083
H	-2.5608	2.2425	4.2073
H	-1.7153	3.6071	4.9671
H	-1.3139	1.9618	5.4440
H	-1.0833	3.7562	1.9192
H	-0.7100	4.6295	3.4200
H	0.5956	3.9096	2.4857

SCF = -33.746643**ZPE = 0.158588****H₂₉₈ = -33.574199****G₂₉₈ = -33.628384****SCF_{DFT} = -1123.655214****5-OCH2**

H	1.3026	0.1200	0.2782
C	0.7266	0.1281	1.1915
C	-0.7521	0.1699	3.5241
C	0.3314	-1.0592	1.7783
C	0.3852	1.3344	1.7677
C	-0.3606	1.3912	2.9548
C	-0.4090	-1.0345	2.9451
H	0.7097	2.2374	1.2781
H	-0.7257	-1.9565	3.4092
H	-1.3325	0.1468	4.4312
I	0.8515	-2.9100	0.8922
N	-0.6704	2.5895	3.5484
C	-1.5727	2.6219	4.6734
C	-0.4009	3.8254	2.8550
H	-2.5582	2.2115	4.4232
H	-1.7044	3.6502	5.0016
H	-1.1599	2.0542	5.5108
H	-0.9267	3.8820	1.8945
H	-0.7224	4.6626	3.4700
H	0.6710	3.9363	2.6738
O	1.6118	-5.6308	-0.5383
C	1.5936	-5.4301	-1.7137
H	1.8280	-6.2148	-2.4526
H	1.3418	-4.4489	-2.1469

SCF = -36.134465
 ZPE = 0.184781
 H₂₉₈ = -35.933058
 G₂₉₈ = -35.993618

SCF_{DFT} = -777.901227

6			
H	0.2823	0.1634	0.0856
C	0.2065	0.1017	1.1601
C	0.0105	-0.0531	3.9272
C	0.3661	-1.1112	1.8094
C	-0.0514	1.2359	1.8988
C	-0.1528	1.1734	3.2910
C	0.2696	-1.1925	3.1835
H	-0.1797	2.1919	1.4167
H	0.3945	-2.1388	3.6872
H	-0.0607	-0.1407	4.9996
I	0.7626	-2.8586	0.6816
O	-0.4093	2.3495	3.9183
C	-0.5251	2.3572	5.3215
H	0.4030	2.0333	5.8030
H	-1.3522	1.7251	5.6598
H	-0.7289	3.3915	5.5933

SCF = -26.421687
 ZPE = 0.118781
 H₂₉₈ = -26.293265
 G₂₉₈ = -26.337831

SCF_{DFT} = -643.925421

6-Cl			
H	0.2961	0.1398	0.0812
C	0.2144	0.0816	1.1572
C	0.0045	-0.0643	3.9145
C	0.3681	-1.1444	1.7881
C	-0.0408	1.2226	1.8893
C	-0.1479	1.1586	3.2770
C	0.2606	-1.2023	3.1656
H	-0.1620	2.1817	1.4073
H	0.3784	-2.1519	3.6684
H	-0.0724	-0.1503	4.9888
I	0.7629	-2.9057	0.6602
Cl	1.3036	-5.3219	-0.8718
O	-0.4044	2.3560	3.9149
C	-0.5194	2.3430	5.3106
H	0.4059	2.0046	5.7918
H	-1.3491	1.7088	5.6445
H	-0.7178	3.3741	5.6036

SCF = -31.217526
 ZPE = 0.118854

H₂₉₈ = -31.086682
 G₂₉₈ = -31.136636

SCF_{DFT} = -1104.214818

6-OCH2			
H	0.2829	0.1814	0.1109
C	0.2024	0.1184	1.1853
C	-0.0054	-0.0383	3.9498
C	0.3461	-1.0997	1.8294
C	-0.0448	1.2549	1.9243
C	-0.1519	1.1908	3.3155
C	0.2430	-1.1785	3.2037
H	-0.1601	2.2134	1.4438
H	0.3550	-2.1276	3.7056
H	-0.0815	-0.1269	5.0219
I	0.7252	-2.8479	0.7057
O	-0.3972	2.3707	3.9450
C	-0.5173	2.3753	5.3471
H	0.4052	2.0387	5.8310
H	-1.3529	1.7517	5.6812
H	-0.7098	3.4110	5.6221
O	1.2862	-5.3915	-0.9913
C	1.3494	-5.1146	-2.1498
H	1.5462	-5.8696	-2.9288
H	1.2159	-4.0876	-2.5249

SCF = -33.600005
 ZPE = 0.145231
 H₂₉₈ = -33.440233
 G₂₉₈ = -33.496168

SCF_{DFT} = -758.458051

7			
H	1.6286	0.2683	1.3726
C	0.8503	-0.0367	2.0551
C	-1.1449	-0.8119	3.8084
C	0.2864	-1.2944	1.9616
C	0.4158	0.8427	3.0316
C	-0.5851	0.4608	3.9151
C	-0.7129	-1.6889	2.8361
H	0.8695	1.8189	3.0868
H	-1.1523	-2.6715	2.7617
H	-1.9224	-1.1040	4.4974
I	0.9570	-2.6328	0.4646
S	-1.2221	1.4882	5.1982
C	-0.2793	3.0311	5.0389
H	-0.6553	3.6824	5.8219
H	-0.4620	3.4810	4.0674
H	0.7781	2.8397	5.1964

SCF = -25.596423

ZPE = 0.115379
H₂₉₈ = -25.470633
G₂₉₈ = -25.517153

SCF_{DFT} = -966.890604

7-Cl

H	1.0936	0.4294	0.7798
C	0.4794	0.1476	1.6235
C	-1.0964	-0.5856	3.7793
C	0.2648	-1.1975	1.8912
C	-0.0866	1.1236	2.4202
C	-0.8636	0.7530	3.5069
C	-0.5324	-1.5534	2.9697
H	0.0737	2.1713	2.2039
H	-0.7070	-2.5995	3.1782
H	-1.7146	-0.8595	4.6226
I	1.1600	-2.6923	0.6691
Cl	2.3960	-4.7137	-0.9742
S	-1.5624	2.0101	4.5708
C	-0.0246	2.5573	5.3827
H	-0.2937	3.3569	6.0653
H	0.6728	2.9197	4.6331
H	0.4072	1.7233	5.9291

SCF = -30.395290
ZPE = 0.115203
H₂₉₈ = -30.267098
G₂₉₈ = -30.319721

SCF_{DFT} = -1427.183174

7-OCH2

H	1.8647	0.1704	1.6146
C	1.0094	-0.0987	2.2158
C	-1.1798	-0.7821	3.7608
C	0.4365	-1.3506	2.0963
C	0.4888	0.8201	3.1105
C	-0.6096	0.4834	3.8894
C	-0.6605	-1.6964	2.8688
H	0.9529	1.7903	3.1854
H	-1.1078	-2.6743	2.7770
H	-2.0336	-1.0385	4.3692
I	1.2420	-2.7476	0.7322
S	-1.3637	1.5641	5.0633
C	-0.3587	3.0737	4.9834
H	-0.7962	3.7521	5.7093
H	-0.4182	3.5096	3.9903
H	0.6682	2.8520	5.2593
O	2.4075	-4.7493	-1.3253
C	2.1245	-4.4340	-2.4404
H	2.4450	-5.0174	-3.3192
H	1.5243	-3.5399	-2.6726

SCF = -32.774900
ZPE = 0.141841
H₂₉₈ = -32.617744
G₂₉₈ = -32.675672

SCF_{DFT} = -1081.423433

8

H	0.5150	0.1761	0.1196
C	0.3089	0.1498	1.1780
C	-0.2215	0.0733	3.9086
C	0.3376	-1.0482	1.8726
C	0.0127	1.3179	1.8548
C	-0.2521	1.2765	3.2187
C	0.0750	-1.0959	3.2308
H	-0.0141	2.2598	1.3287
H	0.1000	-2.0344	3.7620
H	-0.4279	0.0477	4.9673
I	0.7896	-2.8328	0.8405
C	-0.5678	2.5667	3.9223
F	-0.8342	2.4099	5.2244
F	0.4490	3.4445	3.8426
F	-1.6345	3.1854	3.3847

SCF = -35.036798
ZPE = 0.090785
H₂₉₈ = -34.935125
G₂₉₈ = -34.983241

SCF_{DFT} = -866.541419

8-Cl

H	0.5401	0.1538	0.1188
C	0.3248	0.1317	1.1771
C	-0.2251	0.0520	3.8954
C	0.3501	-1.0838	1.8505
C	0.0291	1.3009	1.8459
C	-0.2470	1.2621	3.2107
C	0.0727	-1.1095	3.2113
H	0.0089	2.2476	1.3245
H	0.0919	-2.0536	3.7359
H	-0.4401	0.0273	4.9539
I	0.8083	-2.8804	0.8117
Cl	1.4235	-5.2886	-0.5789
C	-0.5634	2.5417	3.9091
F	-0.8141	2.4043	5.2228
F	0.4361	3.4511	3.8232
F	-1.6481	3.1691	3.3960

SCF = -39.847827
ZPE = 0.090831
H₂₉₈ = -39.743790
G₂₉₈ = -39.797087

SCF_{DFT} = -1326.841150

8-OCH2

H	0.5141	0.2686	0.1466
C	0.3025	0.2230	1.2035
C	-0.2412	0.0963	3.9279
C	0.3180	-0.9919	1.8698
C	0.0142	1.3802	1.9012
C	-0.2571	1.3141	3.2629
C	0.0478	-1.0602	3.2263
H	-0.0012	2.3335	1.3950
H	0.0620	-2.0103	3.7373
H	-0.4526	0.0515	4.9850
I	0.7585	-2.7572	0.8115
C	-0.5666	2.5912	3.9895
F	-0.8053	2.4177	5.2953
F	0.4408	3.4801	3.9009
F	-1.6497	3.2109	3.4832
O	1.3951	-5.2867	-0.7070
C	1.4963	-5.1850	-1.8919
H	1.7297	-6.0451	-2.5397
H	1.3643	-4.2284	-2.4213

SCF = -42.216746

ZPE = 0.117339

H₂₉₈ = -42.083690

G₂₉₈ = -42.142781

SCF_{DFT} = -981.074809

9

H	0.3548	0.1725	0.0957
C	0.2172	0.1568	1.1656
C	-0.1371	0.1155	3.9226
C	0.3313	-1.0267	1.8745
C	-0.0761	1.3294	1.8383
C	-0.2510	1.2992	3.2121
C	0.1563	-1.0556	3.2474
H	-0.1676	2.2582	1.2968
H	0.2466	-1.9815	3.7939
H	-0.2757	0.1057	4.9926
I	0.7796	-2.8177	0.8445
Br	-0.6547	2.9117	4.1394

SCF = -22.766981

ZPE = 0.077382

H₂₉₈ = -22.681092

G₂₉₈ = -22.724374

SCF_{DFT} = -3102.870986

9-OCH2

H	0.3209	0.2527	0.1345
C	0.1935	0.2208	1.2056
C	-0.1345	0.1380	3.9633
C	0.3090	-0.9771	1.8907
C	-0.0871	1.3847	1.8984
C	-0.2487	1.3329	3.2728
C	0.1462	-1.0227	3.2652
H	-0.1788	2.3228	1.3731
H	0.2370	-1.9582	3.7954
H	-0.2628	0.1120	5.0344
I	0.7380	-2.7515	0.8350
Br	-0.6347	2.9344	4.2301
O	1.3750	-5.2978	-0.7072
C	1.4862	-5.1514	-1.8862
H	1.7286	-5.9854	-2.5644
H	1.3535	-4.1762	-2.3807

SCF = -29.946372

ZPE = 0.103901

H₂₉₈ = -29.829099

G₂₉₈ = -29.883589

SCF_{DFT} = -3217.404156

9-Cl

H	0.3540	0.1463	0.0902
C	0.2188	0.1342	1.1621
C	-0.1267	0.0956	3.9129
C	0.3449	-1.0633	1.8525
C	-0.0767	1.3100	1.8272
C	-0.2459	1.2740	3.1992
C	0.1693	-1.0693	3.2293
H	-0.1741	2.2412	1.2875
H	0.2657	-1.9980	3.7732
H	-0.2627	0.0884	4.9850
I	0.8015	-2.8677	0.8143
Cl	1.4186	-5.2895	-0.5821
Br	-0.6553	2.8969	4.1343

SCF = -27.574508

ZPE = 0.077557

H₂₉₈ = -27.486105

G₂₉₈ = -27.534690

SCF_{DFT} = -3563.168055

10

C	0.2295	-0.0235	1.1347
C	-0.1343	0.0056	3.9261
C	0.1326	-1.2247	1.8439
C	0.1446	1.1922	1.8203
C	-0.0369	1.2079	3.2129
C	-0.0489	-1.2113	3.2366
I	0.5013	-0.0453	-0.9521
C	0.2140	-2.4782	1.1850
N	0.2778	-3.4960	0.6667
C	-0.1457	-2.4361	3.9455
N	-0.2241	-3.4224	4.5193
C	-0.3175	0.0203	5.3319
N	-0.4654	0.0321	6.4660
C	-0.1216	2.4472	3.8977
N	-0.1902	3.4453	4.4521
C	0.2382	2.4317	1.1370
N	0.3121	3.4385	0.5988

SCF = -41.745965**ZPE = 0.079141****H₂₉₈ = -41.649967****G₂₉₈ = -41.710242****SCF_{DFT} = -990.670765****10-OCH2**

C	0.2055	-0.2372	1.0296
C	-0.1112	0.0391	3.8178
C	0.1195	-1.3686	1.8473
C	0.1327	1.0328	1.6124
C	-0.0249	1.1743	3.0000
C	-0.0383	-1.2341	3.2359
I	0.4410	-0.4305	-1.0472
C	0.1893	-2.6723	1.2942
N	0.2440	-3.7305	0.8623
C	-0.1242	-2.3909	4.0514
N	-0.1935	-3.3235	4.7102
C	-0.2705	0.1777	5.2188
N	-0.3993	0.2906	6.3500
C	-0.0970	2.4692	3.5726
N	-0.1549	3.5151	4.0326
C	0.2165	2.1997	0.8119
N	0.2834	3.1459	0.1715
O	0.7572	-0.4466	-3.8739
C	0.8044	0.6060	-4.4391
H	0.9251	0.6761	-5.5301
H	0.7311	1.5692	-3.9114

SCF = -48.931087**ZPE = 0.106046****H₂₉₈ = -48.803600****G₂₉₈ = -48.873867****SCF_{DFT} = -1105.210110****10-Cl**

C	0.2258	-0.0232	1.1023
C	-0.1300	0.0051	3.9182
C	0.1346	-1.2188	1.8299
C	0.1359	1.1868	1.8059
C	-0.0401	1.2102	3.1990
C	-0.0414	-1.2142	3.2232
I	0.4879	-0.0444	-1.0173
Cl	0.8165	-0.0716	-3.7336
C	0.2185	-2.4690	1.1747
N	0.2797	-3.5107	0.6996
C	-0.1301	-2.4312	3.9338
N	-0.2028	-3.4169	4.5151
C	-0.3064	0.0191	5.3160
N	-0.4502	0.0304	6.4543
C	-0.1276	2.4412	3.8852
N	-0.1992	3.4384	4.4468
C	0.2212	2.4236	1.1260
N	0.2836	3.4556	0.6303

SCF = -46.591291**ZPE = 0.078501****H₂₉₈ = -46.493372****G₂₉₈ = -46.559951****SCF_{DFT} = -1451.007808****11**

C	0.2163	-0.0250	1.1655
C	-0.1317	0.0092	3.9384
C	0.1054	-1.2131	1.8761
C	0.1517	1.1804	1.8524
C	-0.0214	1.2053	3.2332
C	-0.0680	-1.2039	3.2570
I	0.4763	-0.0505	-0.9075
F	0.1653	-2.3753	1.2324
F	-0.1728	-2.3506	3.9249
F	-0.2973	0.0255	5.2576
F	-0.0814	2.3681	3.8781
F	0.2563	2.3264	1.1858

SCF = -40.273980**ZPE = 0.046778****H₂₉₈ = -40.215471****G₂₉₈ = -40.265017****SCF_{DFT} = -1025.700673**

11-I

C	0.0060	0.0039	1.1262
C	0.0215	0.0300	3.8851
C	0.0382	-1.2069	1.7989
C	-0.0183	1.2177	1.7970
C	-0.0103	1.2319	3.1871
C	0.0451	-1.1665	3.1839
I	0.0731	-3.0431	0.7500
F	0.0756	-2.3168	3.8790
F	0.0290	0.0424	5.2324
F	-0.0333	2.4025	3.8534
F	-0.0492	2.3820	1.1194
F	-0.0023	0.0137	-0.2181
I	0.1318	-5.7061	-0.7613

SCF = -44.395871**11-F**

C	0.0075	-0.0007	1.1285
C	0.0191	0.0307	3.8833
C	0.0363	-1.2199	1.7948
C	-0.0153	1.2140	1.7970
C	-0.0096	1.2338	3.1871
C	0.0414	-1.1661	3.1834
I	0.0763	-3.0798	0.7445
F	0.0689	-2.3102	3.8893
F	0.0247	0.0450	5.2327
F	-0.0316	2.4072	3.8530
F	-0.0432	2.3792	1.1169
F	0.0012	0.0179	-0.2159
F	0.1131	-5.0725	-0.3932

SCF = -45.274458**11-OCH2**

C	0.0003	-0.1297	1.1065
C	-0.0003	-0.0943	3.8776
C	-0.0003	-1.3323	1.7994
C	0.0006	1.0875	1.7785
C	0.0003	1.1053	3.1708
C	-0.0006	-1.3019	3.1869
F	-0.0011	-2.4456	3.8694
F	-0.0005	-0.0821	5.2108
F	0.0006	2.2662	3.8240
F	0.0012	2.2330	1.0960
F	0.0006	-0.1415	-0.2271
I	-0.0005	-3.1452	0.7665
O	-0.0013	-5.5248	-0.8218
C	-0.0001	-5.3684	-2.0072
H	-0.0001	-6.2173	-2.7074
H	0.0011	-4.3724	-2.4753

SCF = -47.458283**ZPE = 0.073648****H₂₉₈ = -47.368350****G₂₉₈ = -47.427876****SCF_{DFT} = -1140.236384****11-OMe**

C	0.0600	0.1627	1.2406
C	-0.0220	0.1264	3.9897
C	0.0933	-1.0751	1.8704
C	-0.0119	1.3619	1.9356
C	-0.0537	1.3461	3.3245
C	0.0503	-1.0516	3.2586
I	0.1955	-2.9942	0.6807
F	0.0789	-2.2095	3.9438
F	-0.0623	0.1086	5.3404
F	-0.1241	2.5021	4.0193
F	-0.0420	2.5458	1.2847
F	0.0985	0.2228	-0.1040
O	0.2954	-4.9444	-0.4695
C	0.2886	-4.8368	-1.8326
H	0.3539	-5.8440	-2.2748
H	1.1403	-4.2483	-2.2216
H	-0.6322	-4.3633	-2.2215

SCF = -48.235221**11-Cl**

C	0.2187	-0.0258	1.1276
C	-0.1276	0.0102	3.9205
C	0.1038	-1.1995	1.8593
C	0.1551	1.1665	1.8351
C	-0.0153	1.2010	3.2123
C	-0.0673	-1.1985	3.2368
I	0.4840	-0.0534	-1.0141
F	0.1580	-2.3828	1.2288
F	-0.1759	-2.3540	3.9206
F	-0.2933	0.0275	5.2569
F	-0.0733	2.3739	3.8723
F	0.2603	2.3332	1.1806
Cl	0.8188	-0.0883	-3.7165

SCF = -45.105452**ZPE = 0.046549****H₂₉₈ = -45.044786****G₂₉₈ = -45.099774****SCF_{DFT} = -1486.013541**

11-Br

C	0.0058	0.0047	1.1261
C	0.0216	0.0288	3.8848
C	0.0387	-1.2079	1.7972
C	-0.0190	1.2179	1.7977
C	-0.0109	1.2316	3.1880
C	0.0458	-1.1671	3.1828
I	0.0735	-3.0481	0.7480
F	0.0769	-2.3174	3.8779
F	0.0293	0.0402	5.2321
F	-0.0344	2.4017	3.8551
F	-0.0506	2.3826	1.1208
F	-0.0027	0.0162	-0.2181
Br	0.1302	-5.5258	-0.6642

SCF = -44.663426**11-DMF**

C	0.0916	0.5840	2.2081
C	0.6839	-0.0419	4.8391
C	0.2409	-0.7481	2.5661
C	0.2333	1.6042	3.1414
C	0.5312	1.2899	4.4642
C	0.5375	-1.0461	3.8885
F	0.6858	-2.3189	4.2578
F	0.9699	-0.3489	6.1064
F	0.6699	2.2610	5.3685
F	0.0858	2.8799	2.7753
F	-0.1939	0.8940	0.9404
I	0.0201	-2.2622	1.1514
O	-0.2529	-4.3170	-0.5960
C	-0.4510	-4.7537	-1.7149
H	-0.4994	-5.8421	-1.8928
N	-0.6305	-4.0462	-2.8292
C	-0.6052	-2.6027	-2.8187
H	0.1924	-2.2350	-3.4667
H	-0.4276	-2.2664	-1.8002
H	-1.5593	-2.2063	-3.1703
C	-0.8584	-4.6620	-4.1106
H	-0.0737	-4.3714	-4.8134
H	-1.8209	-4.3420	-4.5167
H	-0.8600	-5.7454	-4.0126

SCF = -57.271877**ZPE = 0.146854****H₂₉₈ = -57.104950****G₂₉₈ = -57.172727****11-NH3**

C	0.1960	-0.0261	1.2836
C	-0.1426	0.0104	4.0604
C	0.0958	-1.2085	2.0012
C	0.1246	1.1748	1.9733
C	-0.0434	1.2049	3.3528
C	-0.0726	-1.2022	3.3810
I	0.4516	-0.0492	-0.7902
F	0.1620	-2.3751	1.3561
F	-0.1670	-2.3515	4.0538
F	-0.3039	0.0279	5.3840
F	-0.1099	2.3715	3.9985
F	0.2189	2.3241	1.3012
N	0.7893	-0.0888	-3.5581
H	1.7634	0.0608	-3.7852
H	0.2346	0.6442	-3.9801
H	0.4959	-0.9829	-3.9286

SCF = -44.714155**ZPE = 0.082172****H₂₉₈ = -44.616322****G₂₉₈ = -44.673968****12**

C	0.5649	-0.2794	1.0920
C	-0.0085	0.5786	3.6682
C	0.2455	-1.1920	2.0874
C	0.5919	1.0709	1.4108
C	0.3075	1.5153	2.6943
C	-0.0436	-0.7783	3.3800
I	0.9974	-0.9264	-0.8507
I	-0.5228	-2.1730	4.8651
I	0.3543	3.5569	3.1520
F	-0.2833	0.9898	4.9028
F	0.2158	-2.4895	1.7965
F	0.8964	1.9572	0.4670

SCF = -38.449249**ZPE = 0.042514****H₂₉₈ = -38.393484****G₂₉₈ = -38.448695****SCF_{DFT} = -1421.299171**

12-Cl

C	0.5728	-0.2887	1.0580
C	-0.0057	0.5723	3.6537
C	0.2510	-1.1861	2.0633
C	0.5952	1.0547	1.3968
C	0.3117	1.4999	2.6763
C	-0.0383	-0.7788	3.3541
I	1.0210	-0.9586	-0.9630
Cl	1.5788	-1.7939	-3.4831
I	-0.5238	-2.1750	4.8567
I	0.3562	3.5526	3.1531
F	-0.2838	0.9861	4.9012
F	0.2149	-2.4971	1.7901
F	0.9005	1.9652	0.4628

SCF = -43.282051**ZPE = 0.042373****H₂₉₈ = -43.224008****G₂₉₈ = -43.284698****SCF_{DFT} = -1881.611054****12-OCH2**

C	0.5204	-0.4158	1.0136
C	0.0428	0.6020	3.5550
C	0.2296	-1.2601	2.0747
C	0.5663	0.9492	1.2540
C	0.3307	1.4744	2.5156
C	-0.0114	-0.7688	3.3495
I	0.8815	-1.1777	-0.8988
I	-0.4481	-2.0682	4.9330
I	0.4071	3.5410	2.8478
F	-0.1860	1.0900	4.7730
F	0.1807	-2.5741	1.8643
F	0.8440	1.7761	0.2457
O	1.3975	-2.1029	-3.5723
C	1.5895	-1.2849	-4.4223
H	1.7959	-1.5654	-5.4664
H	1.5737	-0.2028	-4.2219

SCF = -45.632880**ZPE = 0.069333****H₂₉₈ = -45.545684****G₂₉₈ = -45.610944****SCF_{DFT} = -1535.834483****13**

C	-0.0011	-0.0040	1.1556
I	-0.0038	-0.0160	-1.0141
Br	-0.9344	-1.5672	1.8268
Br	1.8237	-0.0258	1.8149
Br	-0.8903	1.5920	1.8092

SCF = -18.156262**ZPE = 0.005705****H₂₉₈ = -18.142251****G₂₉₈ = -18.186809****SCF_{DFT} = -8058.046574****13-OCH2**

C	0.0004	0.0289	0.9519
I	0.0014	-0.2678	-1.1755
Br	-0.9373	-1.4352	1.8307
Br	1.8311	0.1006	1.6156
Br	-0.8933	1.7045	1.3887
O	-0.0005	-0.6250	-3.9457
C	-0.0021	0.3025	-4.7017
H	-0.0054	0.1597	-5.7924
H	-0.0005	1.3484	-4.3622

SCF = -25.343253**ZPE = 0.032678****H₂₉₈ = -25.297745****G₂₉₈ = -25.352452****SCF_{DFT} = -8172.582582****13-Cl**

C	-0.0001	-0.0037	1.1724
I	-0.0025	-0.0182	-1.2651
Cl	-0.0047	-0.0333	-3.8483
Br	-0.9311	-1.5685	1.8914
Br	1.8250	-0.0219	1.8798
Br	-0.8923	1.5917	1.8728

SCF = -23.008001**ZPE = 0.005954****H₂₉₈ = -22.991269****G₂₉₈ = -23.041526****SCF_{DFT} = -8518.363696****14**

C	-0.0003	-0.0020	1.1430
I	0.0063	-0.0198	-1.0126
F	-0.6274	-1.0651	1.6139
F	1.2351	-0.0064	1.6110
F	-0.6130	1.0772	1.5963

SCF = -20.139653**ZPE = 0.012849****H₂₉₈ = -20.120922****G₂₉₈ = -20.157154**

SCF_{DFT} = -635.408207

14-Cl

C	-0.0005	-0.0028	1.0863
I	0.0008	-0.0191	-1.1505
Cl	0.0017	-0.0385	-3.8834
F	-0.6287	-1.0727	1.6221
F	1.2432	-0.0060	1.6152
F	-0.6166	1.0817	1.6068

SCF = -24.970571

ZPE = 0.012690

H₂₉₈ = -24.949572

G₂₉₈ = -24.991718

SCF_{DFT} = -1095.717206

14-OCH2

C	-0.0001	0.0606	0.9077
I	0.0001	-0.2566	-1.2123
F	-0.6246	-0.9247	1.5403
F	1.2381	0.1274	1.3823
F	-0.6140	1.1964	1.2212
O	-0.0006	-0.6519	-4.0441
C	0.0039	0.2786	-4.7950
H	0.0030	0.1449	-5.8875
H	0.0095	1.3231	-4.4498

SCF = -27.324206

ZPE = 0.039578

H₂₉₈ = -27.274136

G₂₉₈ = -27.321141

SCF_{DFT} = -749.943249

15

C	0.0033	-0.0003	1.1612
I	0.0135	0.0013	-1.0536
C	-0.7227	-1.2539	1.6153
H	-0.2195	-2.1510	1.2596
H	-1.7489	-1.2676	1.2533
H	-0.7444	-1.2836	2.7051
C	1.4485	-0.0009	1.6262
H	1.9761	-0.8838	1.2706
H	1.4768	-0.0017	2.7162
H	1.9764	0.8824	1.2719
C	-0.7223	1.2529	1.6171
H	-0.2187	2.1503	1.2628
H	-0.7439	1.2810	2.7070
H	-1.7485	1.2674	1.2551

SCF = -16.974358

ZPE = 0.120113

H₂₉₈ = -16.846400

G₂₉₈ = -16.885818

SCF_{DFT} = -455.552568

15-Cl

C	-0.0002	-0.0041	1.1136
I	-0.0003	-0.0176	-1.1002
Cl	-0.0005	-0.0357	-4.0256
C	-0.7222	-1.2503	1.5974
H	-0.2211	-2.1471	1.2354
H	-1.7474	-1.2648	1.2299
H	-0.7481	-1.2883	2.6910
C	1.4426	-0.0019	1.5897
H	1.9658	-0.8859	1.2275
H	1.4943	0.0048	2.6830
H	1.9667	0.8770	1.2167
C	-0.7209	1.2486	1.5820
H	-0.2189	2.1404	1.2090
H	-0.7467	1.3001	2.6750
H	-1.7461	1.2597	1.2144

SCF = -21.766707

ZPE = 0.120118

H₂₉₈ = -21.636405

G₂₉₈ = -21.681564

SCF_{DFT} = -915.833572

15-OCH2

C	-0.0003	-0.0444	1.0103
I	-0.0010	-0.3176	-1.1763
C	-0.7242	-1.2303	1.6239
H	-0.2240	-2.1650	1.3774
H	-1.7524	-1.2873	1.2714
H	-0.7400	-1.1268	2.7095
C	1.4461	0.0107	1.4705
H	1.9719	-0.9090	1.2212
H	1.4802	0.1415	2.5527
H	1.9732	0.8439	1.0092
C	-0.7224	1.2559	1.3186
H	-0.2194	2.1031	0.8560
H	-0.7403	1.4163	2.3971
H	-1.7499	1.2281	0.9607
O	0.0021	-0.7176	-4.2918
C	0.0013	0.3465	-4.8307
H	0.0065	0.4541	-5.9283
H	-0.0046	1.2963	-4.2731

SCF = -24.152160

ZPE = 0.146549

H₂₉₈ = -23.992852

G₂₉₈ = -24.044058**SCF_{DFT} = -570.083699**

16			
C	-0.0009	-0.0048	1.1418
I	0.0023	-0.0156	-1.0741
C	-0.6902	-1.1948	1.5967
N	-1.2328	-2.1319	1.9530
C	1.3754	-0.0027	1.5935
N	2.4590	-0.0013	1.9473
C	-0.6897	1.1900	1.5844
N	-1.2324	2.1307	1.9310

SCF = -20.985616**ZPE = 0.031862****H₂₉₈ = -20.944489****G₂₉₈ = -20.988596****SCF_{DFT} = -614.327992**

16-OCH2			
C	0.0009	-0.0272	1.0660
I	0.0109	-0.3028	-1.1367
C	-0.6922	-1.1529	1.6470
N	-1.2431	-2.0481	2.0903
C	1.3754	0.0272	1.5054
N	2.4671	0.0710	1.8337
C	-0.6861	1.2122	1.3431
N	-1.2307	2.1955	1.5390
O	0.0222	-0.5943	-3.9003
C	0.0047	0.3448	-4.6412
H	0.0094	0.2194	-5.7337
H	-0.0171	1.3855	-4.2860

SCF = -28.172456**ZPE = 0.058831****H₂₉₈ = -28.099825****G₂₉₈ = -28.154158****SCF_{DFT} = -728.869175**

16-Cl			
C	-0.0005	-0.0036	1.4023
I	0.0003	-0.0145	-1.2692
Cl	-0.0003	-0.0257	-3.7827
C	-0.6902	-1.1986	1.6739
N	-1.2580	-2.1764	1.8843
C	1.3803	-0.0018	1.6690
N	2.5117	-0.0027	1.8753
C	-0.6907	1.1934	1.6638
N	-1.2587	2.1728	1.8659

SCF = -25.851806**ZPE = 0.032209****H₂₉₈ = -25.807863****G₂₉₈ = -25.857773****SCF_{DFT} = -1074.688164**

17			
I	0.0895	-1.3315	-1.5148
N	-0.6221	-0.3895	0.1271
C	0.0667	-0.3760	1.3207
C	-1.8267	0.2800	0.1238
O	1.1243	-0.9081	1.4934
O	-2.5468	0.3650	-0.8279
C	-2.0142	0.8457	1.5156
H	-2.1231	1.9285	1.4449
H	-2.9404	0.4506	1.9347
C	-0.7728	0.4182	2.2989
H	-0.1859	1.2624	2.6626
H	-1.0055	-0.2125	3.1577

SCF = -25.488585**ZPE = 0.078450****H₂₉₈ = -25.401500****G₂₉₈ = -25.444297****SCF_{DFT} = -657.805390**

17-Cl			
I	0.1805	-1.4282	-1.7068
Cl	1.0979	-2.6243	-3.8094
N	-0.6174	-0.3874	0.1226
C	0.0491	-0.3526	1.2958
C	-1.8039	0.2559	0.1414
O	1.1250	-0.8522	1.5292
O	-2.5801	0.3646	-0.7791
C	-2.0275	0.8458	1.5450
H	-2.1486	1.9264	1.4580
H	-2.9500	0.4346	1.9573
C	-0.7858	0.4378	2.3188
H	-0.1981	1.2854	2.6738
H	-0.9993	-0.2066	3.1727

SCF = -30.330931**ZPE = 0.078964****H₂₉₈ = -30.241049****G₂₉₈ = -30.289256****SCF_{DFT} = -1118.135961**

17-OCH2

I	0.4244	-1.2697	-1.4892
N	-0.4429	-0.3767	0.1076
C	0.0870	-0.4339	1.3716
C	-1.6099	0.3323	-0.0079
O	1.1003	-1.0082	1.6563
O	-2.2081	0.4846	-1.0374
C	-1.9598	0.8535	1.3727
H	-2.0226	1.9417	1.3353
H	-2.9439	0.4776	1.6546
C	-0.8416	0.3483	2.2824
H	-0.2779	1.1531	2.7554
H	-1.1988	-0.3114	3.0739
O	1.4636	-2.4134	-3.7514
C	0.8705	-2.2278	-4.7746
H	1.2187	-2.6513	-5.7281
H	-0.0499	-1.6291	-4.8270

SCF = -32.675901**ZPE = 0.105731****H₂₉₈ = -32.557205****G₂₉₈ = -32.609513****SCF_{DFT} = -772.345395****18**

I	-0.0010	0.0064	-0.8257
C	0.0010	-0.0624	1.2807
H	0.0051	0.9167	1.7283
C	-0.0007	-1.1834	1.9669
H	0.0011	-1.1640	3.0446
H	-0.0054	-2.1534	1.5002

SCF = -9.578465**ZPE = 0.040758****H₂₉₈ = -9.532995****G₂₉₈ = -9.565176****SCF_{DFT} = -375.664867****18-OCH2**

I	-0.0010	-0.3326	-1.1150
C	0.0015	-0.0492	0.9702
H	0.0049	0.9888	1.2573
C	-0.0009	-1.0401	1.8346
H	0.0006	-0.8465	2.8952
H	-0.0044	-2.0733	1.5319
O	-0.0067	-0.6453	-4.2053
C	-0.0039	0.4161	-4.7495
H	-0.0075	0.5181	-5.8472
H	0.0026	1.3690	-4.1969

SCF = -16.756888**ZPE = 0.067241****H₂₉₈ = -16.680052****G₂₉₈ = -16.724848****SCF_{DFT} = -490.197617****18-Cl**

I	-0.0026	-0.0064	-0.9033
Cl	-0.0066	0.1120	-3.8573
C	0.0003	-0.0607	1.2178
H	0.0018	0.9104	1.6924
C	0.0004	-1.1694	1.9314
H	0.0013	-1.1607	3.0135
H	-0.0021	-2.1406	1.4638

SCF = -14.373054**ZPE = 0.040937****H₂₉₈ = -14.325145****G₂₉₈ = -14.363377****SCF_{DFT} = -835.953134****19**

I	-0.0023	-0.0350	-0.8354
C	0.0015	-0.0586	1.2554
H	0.0048	0.9205	1.7063
C	-0.0007	-1.1789	1.9703
H	-0.0046	-2.1634	1.5223
C	0.0018	-1.1419	3.3791
N	0.0033	-1.1252	4.5250

SCF = -14.096079**ZPE = 0.039641****H₂₉₈ = -14.049981****G₂₉₈ = -14.087016****SCF_{DFT} = -467.933516****19-Cl**

I	-0.0030	-0.0335	-0.8987
Cl	-0.0074	0.0106	-3.7649
C	0.0002	-0.0518	1.2100
H	0.0022	0.9142	1.6960
C	-0.0001	-1.1708	1.9431
H	-0.0020	-2.1479	1.4767
C	0.0021	-1.1451	3.3413
N	0.0040	-1.1122	4.4931

SCF = -18.907980**ZPE = 0.039841****H₂₉₈ = -18.859419****G₂₉₈ = -18.901928**

SCF_{DFT} = -928.240286

19-OCH2

I	-0.0083	-0.3622	-1.0502
C	-0.0022	-0.1280	1.0239
H	-0.0014	0.8964	1.3604
C	0.0005	-1.1519	1.8728
H	-0.0003	-2.1826	1.5448
C	0.0046	-0.9461	3.2657
N	0.0079	-0.7878	4.4014
O	-0.0168	-0.6407	-4.0522
C	-0.0035	0.3651	-4.6949
H	-0.0049	0.3606	-5.7965
H	0.0110	1.3660	-4.2355

SCF = -21.276307

ZPE = 0.066210

H₂₉₈ = -21.198811

G₂₉₈ = -21.247453

SCF_{DFT} = -582.468113

20

I	0.0392	0.0068	-0.8779
C	-0.2838	-0.1002	1.2035
H	-0.6356	0.8204	1.6271
C	-0.0104	-1.2142	1.8818
H	0.3385	-2.0904	1.3525
N	-0.0708	-1.3762	3.2387
C	-0.2458	-2.7097	3.7606
H	0.2744	-3.4243	3.1258
H	-1.3038	-2.9968	3.8165
H	0.1798	-2.7626	4.7638
C	-0.6144	-0.3159	4.0504
H	-0.1060	0.6184	3.8144
H	-0.4391	-0.5488	5.0995
H	-1.6922	-0.1801	3.8957

SCF = -19.352139

ZPE = 0.112505

H₂₉₈ = -19.230652

G₂₉₈ = -19.273535

SCF_{DFT} = -509.669535

20-Cl

I	-0.0328	-0.0151	-0.9264
Cl	0.2778	0.1476	-3.8813
C	-0.2796	-0.1172	1.1831
H	-0.6987	0.7675	1.6327
C	0.0767	-1.1872	1.8762
H	0.4897	-2.0442	1.3608
N	0.0553	-1.3573	3.2692
C	-0.2781	-2.6883	3.7184
H	0.2681	-3.4178	3.1228
H	-1.3541	-2.9094	3.6378
H	0.0175	-2.7998	4.7645
C	-0.5730	-0.3172	4.0445
H	-0.1152	0.6387	3.7950
H	-0.4062	-0.5171	5.1045
H	-1.6574	-0.2446	3.8683

SCF = -24.139611

ZPE = 0.112594

H₂₉₈ = -24.015868

G₂₉₈ = -24.063871

SCF_{DFT} = -969.953493

20-OCH2

I	0.0457	-0.3843	-1.0930
C	-0.2610	-0.2744	0.9888
H	-0.6005	0.6860	1.3261
C	0.0013	-1.3182	1.7732
H	0.3376	-2.2462	1.3313
N	-0.0510	-1.3473	3.1426
C	-0.2570	-2.6221	3.7859
H	0.2517	-3.4032	3.2242
H	-1.3211	-2.8822	3.8610
H	0.1622	-2.5895	4.7927
C	-0.5847	-0.2082	3.8470
H	-0.0691	0.6940	3.5197
H	-0.4092	-0.3386	4.9138
H	-1.6621	-0.0788	3.6813
O	0.4492	-0.5215	-4.2481
C	0.2207	0.5689	-4.6731
H	0.2815	0.8110	-5.7476
H	-0.0672	1.4125	-4.0257

SCF = -26.529656

ZPE = 0.138881

H₂₉₈ = -26.376854

G₂₉₈ = -26.431376

SCF_{DFT} = -624.201804

21

I	0.0000	0.0000	-0.5548
C	-0.0000	-0.0000	1.4630
H	0.0000	0.0000	3.7098
C	-0.0000	0.0000	2.6604

SCF = -8.511802**ZPE = 0.017915****H₂₉₈ = -8.489066****G₂₉₈ = -8.519072****SCF_{DFT} = -374.405451****21-Cl**

I	0.0218	-0.0534	-0.8307
Cl	0.3216	-0.1523	-3.7317
C	-0.1897	0.0162	1.2134
H	-0.4218	0.0923	3.4527
C	-0.3134	0.0569	2.4074

SCF = -13.314043**ZPE = 0.018136****H₂₉₈ = -13.288798****G₂₉₈ = -13.324668****SCF_{DFT} = -834.711369****21-OCH2**

I	0.0423	-0.4114	-0.9874
C	-0.1672	-0.0032	0.9800
H	-0.4005	0.4486	3.1688
C	-0.2916	0.2377	2.1467
O	0.3400	-0.8291	-3.9510
C	0.3005	0.1796	-4.5869
H	0.3998	0.1899	-5.6840
H	0.1624	1.1707	-4.1258

SCF = -15.691704**ZPE = 0.044458****H₂₉₈ = -15.638068****G₂₉₈ = -15.680867****SCF_{DFT} = -488.941514****22**

I	0.0000	-0.0000	-1.2783
C	-0.0000	0.0000	0.7246
C	-0.0000	0.0000	1.9345
C	-0.0000	0.0000	3.2953
N	0.0000	-0.0000	4.4441

SCF = -13.031866**ZPE = 0.017493****H₂₉₈ = -13.007785****G₂₉₈ = -13.042763****SCF_{DFT} = -466.674402****22-OCH2**

I	0.0137	-0.4057	-0.9039
C	-0.1829	-0.1107	1.0693
C	-0.3016	0.0689	2.2607
C	-0.4349	0.2726	3.5984
N	-0.5467	0.4464	4.7293
O	0.2973	-0.7302	-3.7923
C	0.2939	0.2231	-4.5113
H	0.4038	0.1357	-5.6031
H	0.1813	1.2529	-4.1369

SCF = -20.214010**ZPE = 0.044112****H₂₉₈ = -20.158993****G₂₉₈ = -20.206172****SCF_{DFT} = -581.212696****22-Cl**

I	0.0202	-0.0513	-0.8098
Cl	0.3093	-0.1457	-3.6059
C	-0.1903	0.0164	1.2210
C	-0.3157	0.0565	2.4319
C	-0.4559	0.1008	3.7761
N	-0.5758	0.1389	4.9250

SCF = -17.853840**ZPE = 0.017860****H₂₉₈ = -17.827140****G₂₉₈ = -17.867471****SCF_{DFT} = -927.000558****23**

I	0.0000	0.0000	-0.5247
C	-0.0000	-0.0000	1.4847
N	0.0000	0.0000	2.6249

SCF = -8.815840**ZPE = 0.008126****H₂₉₈ = -8.803473****G₂₉₈ = -8.832437****SCF_{DFT} = -390.505903**

23-OCH2

I	0.0060	-0.2633	-0.8655
C	-0.1763	0.1423	1.0949
N	-0.2797	0.3761	2.2074
O	0.2755	-0.7451	-3.7486
C	0.2914	0.1704	-4.5151
H	0.3999	0.0254	-5.6009
H	0.1993	1.2199	-4.1936

SCF = -15.997931**ZPE = 0.034729****H₂₉₈ = -15.954638****G₂₉₈ = -15.996206****SCF_{DFT} = -505.044807****23-Cl**

I	0.0115	-0.0493	-0.7328
Cl	0.3057	-0.1450	-3.5773
C	-0.1981	0.0189	1.2952
N	-0.3161	0.0574	2.4378

SCF = -13.633288**ZPE = 0.008468****H₂₉₈ = -13.618294****G₂₉₈ = -13.653112****SCF_{DFT} = -850.831061****24**

C	4.9720	2.0625	0.3033
C	3.5831	-0.2991	-0.1432
C	3.5835	2.0647	0.3031
C	5.6741	0.8824	0.0807
C	4.9716	-0.2975	-0.1425
C	2.8833	0.8830	0.0797
C	1.4028	0.8831	0.0795
C	-1.4028	0.8831	0.0793
C	0.6946	1.1021	-1.0979
C	0.6944	0.6642	1.2569
C	-0.6946	0.6641	1.2567
C	-0.6945	1.1023	-1.0980
C	-2.8833	0.8829	0.0795
C	-5.6741	0.8822	0.0804
C	-3.5835	2.0646	0.3031
C	-3.5832	-0.2991	-0.1438
C	-4.9716	-0.2975	-0.1430
C	-4.9720	2.0624	0.3032
I	-2.5738	-2.1096	-0.4862
I	2.5731	-2.1093	-0.4853
F	-7.0049	0.8819	0.0809
F	-5.6390	-1.4277	-0.3564
F	-5.6398	3.1922	0.5171
F	-1.3658	1.3129	-2.2298
F	1.3661	1.3129	-2.2296
F	1.3658	0.4536	2.3887
F	-1.3661	0.4535	2.3885
F	5.6397	3.1924	0.5169
F	7.0048	0.8821	0.0811
F	5.6391	-1.4276	-0.3557
I	2.5750	3.8758	0.6449
I	-2.5746	3.8755	0.6446

SCF = -101.064955**ZPE = 0.130808****H₂₉₈ = -100.902051****G₂₉₈ = -100.995873****SCF_{DFT} = -2875.469219**

24-OCH2

C	-0.9954	0.4596	1.6162
C	1.0601	-0.4467	3.2518
C	-1.1110	-0.7662	2.2579
C	0.1449	1.2377	1.7871
C	1.1693	0.7770	2.6076
C	-0.0845	-1.2215	3.0762
C	-0.1769	-2.5243	3.7729
C	-0.1180	-4.9450	5.1894
C	0.3186	-3.6806	3.1792
C	-0.6835	-2.6008	5.0662
C	-0.6543	-3.7990	5.7674
C	0.3478	-4.8788	3.8803
C	0.0374	-6.1860	5.9814
C	0.3862	-8.5034	7.4881
C	-0.9530	-7.1603	5.9989
C	1.2054	-6.3688	6.7187
C	1.3741	-7.5244	7.4672
C	-0.7777	-8.3147	6.7502
I	2.7122	-4.9088	6.7049
I	2.6208	-1.1164	4.4839
F	0.5519	-9.6124	8.2082
F	2.4901	-7.7016	8.1728
F	-1.7254	-9.2497	6.7685
F	0.8547	-5.9751	3.3148
F	0.7972	-3.6187	1.9358
F	-1.1700	-1.4993	5.6397
F	-1.1125	-3.8557	7.0186
F	-1.9779	0.8980	0.8319
F	0.2535	2.4137	1.1698
F	2.2626	1.5197	2.7737
O	4.4381	-2.5488	6.3178
C	5.4943	-2.2535	6.7973
H	6.0242	-2.9128	7.4997
H	5.9992	-1.3049	6.5648
I	-2.7266	-6.9158	4.9000
I	-2.8508	-1.9085	1.9725

SCF = -108.253947**ZPE = 0.157874****H₂₉₈ = -108.059595****G₂₉₈ = -108.161941****SCF_{DFT} = -2990.006711****24-Cl**

C	-0.8757	0.4290	1.5887
C	0.9841	-0.4754	3.4629
C	-1.0391	-0.8108	2.1861
C	0.2149	1.2229	1.9224
C	1.1344	0.7630	2.8565
C	-0.1160	-1.2604	3.1166
C	-0.2556	-2.5784	3.7748
C	-0.2478	-5.0100	5.1808
C	0.3552	-3.7071	3.2396
C	-0.9205	-2.6991	4.9900
C	-0.9167	-3.8999	5.6843
C	0.3591	-4.9078	3.9339
C	-0.1002	-6.2374	5.9942
C	0.2458	-8.5097	7.5496
C	-1.0188	-7.2724	5.9224
C	1.0028	-6.3238	6.8442
C	1.1606	-7.4664	7.6144
C	-0.8478	-8.4079	6.6984
I	2.3986	-4.7082	6.9309
I	2.3871	-1.1994	4.9027
F	0.4070	-9.6120	8.2989
F	2.2086	-7.5783	8.4386
F	-1.7327	-9.4136	6.6342
F	0.9741	-5.9781	3.4184
F	0.9665	-3.6170	2.0532
F	-1.5456	-1.6321	5.5000
F	-1.5380	-3.9932	6.8652
F	-1.7650	0.8708	0.6873
F	0.3688	2.4229	1.3405
F	2.1794	1.5382	3.1681
Cl	4.0785	-2.4157	6.8379
I	-2.7050	-1.9850	1.6536
I	-2.6889	-7.1556	4.6440

SCF = -105.925445**ZPE = 0.130862****H₂₉₈ = -105.760420****G₂₉₈ = -105.857621****SCF_{DFT} = -3335.803078**

	25		
C	0.3042	-1.3217	0.2323
C	-0.3198	1.3745	-0.0191
C	1.3398	-0.3962	0.1834
C	-1.0322	-0.9474	0.1601
C	-1.3163	0.4073	0.0347
C	0.9998	0.9454	0.0574
C	2.7535	-0.8240	0.2624
C	5.4223	-1.6316	0.4114
C	3.3957	-1.3330	-0.8634
C	3.4512	-0.7205	1.4631
C	4.7784	-1.1227	1.5345
C	4.7229	-1.7340	-0.7866
C	-2.1134	-1.9553	0.2144
C	-4.1531	-3.8594	0.3168
C	-2.5139	-2.4884	1.4369
C	-2.7371	-2.3780	-0.9566
C	-3.7513	-3.3250	-0.9029
C	-3.5284	-3.4354	1.4850
C	-0.6517	2.8097	-0.1532
C	-1.2779	5.5190	-0.4063
C	-0.5662	3.4359	-1.3940
C	-1.0516	3.5436	0.9605
C	-1.3625	4.8909	0.8319
C	-0.8782	4.7834	-1.5171
I	2.5327	0.0242	3.2013
I	2.4014	-1.4989	-2.7083
I	-2.1661	-1.6230	-2.8337
I	-1.6229	-1.8785	3.2407
I	0.0157	2.3778	-3.1148
I	-1.1845	2.6596	2.8633
F	0.6040	-2.6166	0.3530
F	-2.5919	0.7932	-0.0365
F	1.9758	1.8545	0.0079
F	-4.3449	-3.7287	-2.0224
F	-5.1252	-4.7672	0.3655
F	-3.9106	-3.9426	2.6534
F	5.4428	-1.0246	2.6823
F	6.6943	-2.0166	0.4824
F	5.3352	-2.2186	-1.8631
F	-1.5763	6.8104	-0.5269
F	-1.7427	5.5909	1.8969
F	-0.7974	5.3796	-2.7031

SCF = -131.008753

ZPE = 0.171811

H₂₉₈ = -130.794366G₂₉₈ = -130.909500SCF_{DFT} = -3899.257673

	25-OCH2		
C	0.3115	-1.2925	0.2658
C	-0.3129	1.4068	0.0594
C	1.3464	-0.3660	0.2370
C	-1.0246	-0.9182	0.1963
C	-1.3091	0.4385	0.0971
C	1.0061	0.9769	0.1322
C	2.7610	-0.7956	0.2965
C	5.4299	-1.6060	0.4058
C	3.4591	-1.0675	-0.8768
C	3.4021	-0.9305	1.5247
C	4.7300	-1.3339	1.5766
C	4.7867	-1.4703	-0.8199
C	-2.0993	-1.9359	0.1891
C	-4.1059	-3.8699	0.1504
C	-2.6632	-2.3789	1.3806
C	-2.5407	-2.4585	-1.0243
C	-3.5401	-3.4213	-1.0381
C	-3.6632	-3.3420	1.3589
C	-0.6371	2.8430	-0.0918
C	-1.2268	5.5493	-0.4025
C	-0.7629	3.3872	-1.3679
C	-0.8079	3.6518	1.0264
C	-1.1021	4.9997	0.8693
C	-1.0569	4.7352	-1.5171
I	2.3948	-0.5320	3.3264
I	2.5396	-0.8818	-2.7579
I	-1.7237	-1.7789	-2.8330
I	-2.0312	-1.6095	3.2333
I	-0.5346	2.1766	-3.0662
I	-0.6330	2.8683	2.9705
F	0.6139	-2.5908	0.3544
F	-2.5846	0.8246	0.0251
F	1.9841	1.8861	0.0910
F	-3.9627	-3.9225	-2.1975
F	-5.0645	-4.7955	0.1336
F	-4.2051	-3.7673	2.4982
F	5.3421	-1.4628	2.7505
F	6.7030	-1.9926	0.4576
F	5.4529	-1.7299	-1.9424
F	-1.5077	6.8437	-0.5495
F	-1.2665	5.7761	1.9383
F	-1.1770	5.2572	-2.7366
O	-0.4109	-0.1326	-4.9224
C	-0.0713	-0.3004	-6.0576
H	-0.1683	-1.2727	-6.5617
H	0.3583	0.5074	-6.6673

SCF = -138.198177

ZPE = 0.198696

H₂₉₈ = -137.952365G₂₉₈ = -138.076701SCF_{DFT} = -4013.794609

25-Cl

C	0.2989	-1.3074	0.3911
C	-0.3244	1.3869	0.1356
C	1.3354	-0.3843	0.3376
C	-1.0371	-0.9353	0.3150
C	-1.3192	0.4194	0.1941
C	0.9938	0.9565	0.2162
C	2.7505	-0.8192	0.3259
C	5.4049	-1.6375	0.2616
C	3.3546	-1.1018	-0.9004
C	3.4669	-0.9443	1.5073
C	4.7918	-1.3526	1.4756
C	4.6807	-1.5096	-0.9172
C	-2.1154	-1.9491	0.2792
C	-4.1367	-3.8522	0.1695
C	-2.7212	-2.3860	1.4482
C	-2.5142	-2.4599	-0.9573
C	-3.5248	-3.4096	-0.9967
C	-3.7301	-3.3359	1.3939
C	-0.6529	2.8130	-0.0885
C	-1.2648	5.4834	-0.5508
C	-0.7448	3.2815	-1.4003
C	-0.8655	3.6713	0.9805
C	-1.1712	5.0042	0.7501
C	-1.0509	4.6174	-1.6160
I	2.5732	-0.5218	3.3669
I	2.2241	-0.8941	-2.6827
I	-1.5602	-1.7665	-2.7199
I	-2.1331	-1.6276	3.3228
I	-0.4162	1.9348	-3.0054
I	-0.7322	2.9831	2.9663
Cl	0.1402	-0.4095	-4.7423
F	0.5999	-2.6077	0.5009
F	-2.5988	0.8057	0.1113
F	1.9734	1.8676	0.1551
F	-3.9237	-3.9130	-2.1692
F	-5.1129	-4.7704	0.1228
F	-4.3198	-3.7629	2.5181
F	5.4902	-1.4756	2.6118
F	6.6863	-2.0321	0.2367
F	5.2803	-1.7860	-2.0796
F	-1.5602	6.7734	-0.7678
F	-1.3781	5.8390	1.7768
F	-1.1437	5.0889	-2.8635

SCF = -135.877556**ZPE = 0.171959****H₂₉₈ = -135.661080****G₂₉₈ = -135.779129****SCF_{DFT} = -4359.601785****26**

H	-1.4182	0.8963	-2.0642
C	-1.3263	1.6136	-1.2645
C	-1.0870	3.4643	0.8143
C	-1.1290	1.2233	0.0392
C	-1.4045	2.9757	-1.5222
C	-1.2849	3.8897	-0.4860
C	-1.0026	2.1045	1.1170
H	-1.5588	3.3129	-2.5347
H	-1.3470	4.9461	-0.6955
H	-0.9960	4.1874	1.6093
C	-0.7975	1.5407	2.4392
C	-0.4090	0.2385	4.8967
C	-0.7384	0.1490	2.5583
C	-0.6514	2.2670	3.6220
C	-0.4603	1.6228	4.8300
C	-0.5497	-0.5220	3.7436
H	-0.6890	3.3443	3.5864
H	-0.3499	2.2056	5.7310
H	-0.5110	-1.5986	3.7865
H	-0.2597	-0.2590	5.8417
I	-0.9785	-0.8328	0.6579

SCF = -33.107717**ZPE = 0.153856****H₂₉₈ = -32.942567****G₂₉₈ = -32.990513****SCF_{DFT} = -759.582896****26-Cl**

H	-1.4189	0.8733	-2.0445
C	-1.3283	1.6076	-1.2587
C	-1.0862	3.4475	0.8146
C	-1.1311	1.1975	0.0385
C	-1.4053	2.9658	-1.5198
C	-1.2841	3.8788	-0.4830
C	-1.0045	2.0859	1.1071
H	-1.5597	3.3064	-2.5316
H	-1.3445	4.9369	-0.6887
H	-0.9939	4.1705	1.6100
C	-0.7982	1.5304	2.4373
C	-0.4118	0.2366	4.8752
C	-0.7460	0.1396	2.5166
C	-0.6523	2.2699	3.6100
C	-0.4610	1.6222	4.8154
C	-0.5552	-0.5111	3.7186
H	-0.6878	3.3481	3.5830
H	-0.3488	2.2014	5.7197
H	-0.5196	-1.5899	3.7461
H	-0.2620	-0.2589	5.8222
I	-0.9885	-0.8412	0.6203
Cl	-1.3253	-1.5162	-1.8739

SCF = -38.082501

ZPE = 0.155689

H₂₉₈ = -37.913617

G₂₉₈ = -37.965804

SCF_{DFT} = -1220.039775

26-OCH2

H	-1.3815	1.4455	-2.1630
C	-1.3122	2.0779	-1.2942
C	-1.1274	3.6887	0.9795
C	-1.1175	1.5458	-0.0414
C	-1.4160	3.4575	-1.3996
C	-1.3236	4.2528	-0.2670
C	-1.0178	2.3053	1.1278
H	-1.5690	3.9042	-2.3690
H	-1.4054	5.3245	-0.3576
H	-1.0576	4.3209	1.8502
C	-0.8112	1.6058	2.3855
C	-0.4152	0.0535	4.6839
C	-0.7257	0.2107	2.3389
C	-0.6901	2.2057	3.6387
C	-0.4948	1.4357	4.7702
C	-0.5315	-0.5755	3.4532
H	-0.7496	3.2790	3.7243
H	-0.4035	1.9173	5.7310
H	-0.4711	-1.6492	3.3741
H	-0.2627	-0.5400	5.5711
I	-0.9300	-0.5422	0.3566
O	-1.2475	-0.9200	-2.3272
C	-1.2665	-1.9723	-2.9052
H	-1.1582	-2.9364	-2.3905
H	-1.3951	-2.0238	-3.9943

SCF = -40.308095

ZPE = 0.181517

H₂₉₈ = -40.110937

G₂₉₈ = -40.168145

SCF_{DFT} = -874.132410

27

H	-0.0612	0.1623	0.1877
C	-0.0588	0.1506	1.2661
C	-0.0530	0.1143	4.0689
C	-0.0647	-1.0250	1.9826
C	-0.0497	1.3403	1.9795
C	-0.0465	1.3098	3.3705
C	-0.0620	-1.0990	3.3802
H	-0.0441	2.2843	1.4555
H	-0.0502	0.1231	5.1485
C	-0.0687	-2.4156	3.9936
C	-0.0827	-5.0571	4.9600
C	-0.0776	-3.5331	3.1512
C	-0.0669	-2.6688	5.3655
C	-0.0739	-3.9726	5.8316
C	-0.0846	-4.8379	3.5902
H	-0.0600	-1.8479	6.0668
H	-0.0913	-5.6710	2.9054
H	-0.0880	-6.0656	5.3457
I	-0.0790	-2.9728	1.0778
C	-0.0424	2.6330	4.1149
C	-0.0718	-4.2543	7.3234
F	1.0001	3.3833	3.7492
F	0.0208	2.4684	5.4356
F	-1.1495	3.3316	3.8468
F	-0.0659	-3.1362	8.0479
F	-1.1501	-4.9598	7.6759
F	1.0023	-4.9683	7.6713

SCF = -64.772267

ZPE = 0.160159

H₂₉₈ = -64.592838

G₂₉₈ = -64.658713

SCF_{DFT} = -1433.906680

27-OCH2

H	-0.0610	0.4040	0.2670
C	-0.0588	0.3526	1.3440
C	-0.0534	0.2024	4.1413
C	-0.0641	-0.8591	2.0028
C	-0.0505	1.5120	2.1027
C	-0.0475	1.4251	3.4916
C	-0.0616	-0.9765	3.3971
H	-0.0456	2.4775	1.6206
H	-0.0509	0.1695	5.2197
C	-0.0678	-2.3207	3.9529
C	-0.0809	-4.9944	4.8168
C	-0.0760	-3.4023	3.0657
C	-0.0662	-2.6242	5.3146
C	-0.0726	-3.9445	5.7300
C	-0.0826	-4.7220	3.4578
H	-0.0598	-1.8318	6.0470
H	-0.0890	-5.5200	2.7347
H	-0.0859	-6.0158	5.1652
I	-0.0772	-2.7537	1.0394
C	-0.0426	2.7149	4.2860
C	-0.0707	-4.2847	7.2067
F	1.0100	3.4746	3.9642
F	0.0039	2.5027	5.6018
F	-1.1407	3.4369	4.0349
F	-0.0641	-3.1991	7.9800
F	-1.1492	-5.0052	7.5339
F	1.0028	-5.0148	7.5289
O	-0.0925	-5.3471	0.3887
C	-0.0948	-5.8109	-0.7207
H	-0.1019	-6.8969	-0.8809
H	-0.0898	-5.1909	-1.6265

SCF = -71.978718**ZPE = 0.188028****H₂₉₈ = -71.767211****G₂₉₈ = -71.841562****SCF_{DFT} = -1548.458508****27-Cl**

H	-0.0641	0.1205	0.2046
C	-0.0611	0.1268	1.2834
C	-0.0540	0.1022	4.0785
C	-0.0659	-1.0662	1.9802
C	-0.0526	1.3191	1.9833
C	-0.0486	1.2948	3.3762
C	-0.0625	-1.1002	3.3737
H	-0.0483	2.2645	1.4636
H	-0.0509	0.1169	5.1566
C	-0.0683	-2.4257	3.9767
C	-0.0807	-5.0545	4.9494
C	-0.0767	-3.5321	3.1258
C	-0.0662	-2.6679	5.3501
C	-0.0724	-3.9692	5.8209
C	-0.0828	-4.8299	3.5845
H	-0.0598	-1.8464	6.0484
H	-0.0891	-5.6474	2.8792
H	-0.0853	-6.0610	5.3373
I	-0.0790	-3.0152	1.0662
Cl	-0.0940	-5.5185	0.5027
C	-0.0427	2.6117	4.1045
C	-0.0704	-4.2470	7.3010
F	1.0115	3.3706	3.7590
F	-0.0002	2.4803	5.4355
F	-1.1366	3.3421	3.8255
F	-0.0623	-3.1356	8.0464
F	-1.1483	-4.9548	7.6775
F	1.0012	-4.9670	7.6723

SCF = -69.777490**ZPE = 0.162032****H₂₉₈ = -69.594284****G₂₉₈ = -69.664107****SCF_{DFT} = -1894.380180**

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H	-0.1634	0.1615	0.1860
C	-0.1278	0.1524	1.2638
C	-0.0360	0.1122	4.0639
C	-0.1240	-1.0246	1.9792
C	-0.0844	1.3423	1.9728
C	-0.0387	1.3179	3.3680
C	-0.0790	-1.0983	3.3769
H	-0.0860	2.2851	1.4474
H	-0.0001	0.1231	5.1427
C	-0.0810	-2.4165	3.9890
C	-0.0941	-5.0640	4.9476
C	-0.1279	-3.5317	3.1434
C	-0.0398	-2.6728	5.3572
C	-0.0463	-3.9824	5.8292
C	-0.1356	-4.8377	3.5811
H	-0.0024	-1.8557	6.0616
H	-0.1727	-5.6670	2.8926
H	-0.0987	-6.0737	5.3288
I	-0.1874	-2.9710	1.0692
C	0.0057	2.5398	4.0946
N	0.0410	3.5185	4.6837
C	-0.0035	-4.2159	7.2316
N	0.0311	-4.3974	8.3594

SCF = -42.119531**ZPE = 0.150491****H₂₉₈ = -41.953823****G₂₉₈ = -42.010245****SCF_{DFT} = -944.093642****28-OCH2**

H	-0.1445	0.4357	0.2917
C	-0.1144	0.3781	1.3682
C	-0.0367	0.2014	4.1620
C	-0.1118	-0.8399	2.0165
C	-0.0775	1.5318	2.1322
C	-0.0389	1.4394	3.5251
C	-0.0735	-0.9693	3.4104
H	-0.0786	2.5002	1.6563
H	-0.0064	0.1622	5.2399
C	-0.0757	-2.3195	3.9536
C	-0.0873	-5.0066	4.7863
C	-0.1155	-3.3916	3.0541
C	-0.0411	-2.6378	5.3088
C	-0.0469	-3.9679	5.7186
C	-0.1222	-4.7157	3.4329
H	-0.0095	-1.8556	6.0516
H	-0.1536	-5.5039	2.6996
H	-0.0914	-6.0323	5.1211
I	-0.1645	-2.7253	1.0311
C	-0.0010	2.6239	4.3096
N	0.0294	3.5737	4.9452
C	-0.0110	-4.2675	7.1076
N	0.0179	-4.5042	8.2256
O	-0.2170	-5.3317	0.3498
C	-0.2525	-5.7942	-0.7588
H	-0.2716	-6.8796	-0.9217
H	-0.2680	-5.1729	-1.6638

SCF = -49.323418**ZPE = 0.178236****H₂₉₈ = -49.125674****G₂₉₈ = -49.191101****SCF_{DFT} = -1058.646790**

28-Cl

H	-0.1596	0.1222	0.2017
C	-0.1254	0.1308	1.2805
C	-0.0377	0.1024	4.0739
C	-0.1215	-1.0630	1.9773
C	-0.0854	1.3238	1.9763
C	-0.0416	1.3054	3.3735
C	-0.0780	-1.0976	3.3716
H	-0.0876	2.2684	1.4542
H	-0.0034	0.1212	5.1524
C	-0.0791	-2.4251	3.9730
C	-0.0887	-5.0613	4.9369
C	-0.1228	-3.5300	3.1190
C	-0.0397	-2.6713	5.3424
C	-0.0445	-3.9790	5.8188
C	-0.1281	-4.8292	3.5749
H	-0.0052	-1.8542	6.0463
H	-0.1628	-5.6431	2.8664
H	-0.0919	-6.0699	5.3201
I	-0.1799	-3.0111	1.0589
Cl	-0.2356	-5.5254	0.4908
C	-0.0007	2.5265	4.0898
N	0.0326	3.5130	4.6710
C	-0.0040	-4.2082	7.2164
N	0.0290	-4.3890	8.3467

SCF = -47.115839**ZPE = 0.152376****H₂₉₈ = -46.946333****G₂₉₈ = -47.006979****SCF_{DFT} = -1404.574749****29**

H	0.0236	0.1609	0.1993
C	-0.0500	0.1366	1.2746
C	-0.2390	0.0603	4.0505
C	-0.0426	-1.0583	1.9643
C	-0.1534	1.3097	1.9857
C	-0.2512	1.3099	3.3965
C	-0.1359	-1.1343	3.3588
H	-0.1581	2.2342	1.4365
H	-0.3114	0.0164	5.1226
C	-0.1165	-2.4605	3.9600
C	-0.0594	-5.1035	4.8927
C	-0.0058	-3.5568	3.0969
C	-0.1985	-2.7300	5.3152
C	-0.1732	-4.0452	5.8238
C	0.0236	-4.8628	3.5407
H	-0.2841	-1.8966	5.9897
H	0.1099	-5.6855	2.8494
H	-0.0352	-6.1256	5.2259
I	0.1111	-2.9813	1.0398
N	-0.3524	2.4630	4.0906
N	-0.2546	-4.2855	7.1495
C	-0.3632	3.7354	3.4044
H	0.5613	3.8863	2.8416
H	-0.4496	4.5386	4.1301
H	-1.2120	3.8056	2.7197
C	-0.4521	2.4514	5.5317
H	0.4314	1.9929	5.9838
H	-1.3439	1.9110	5.8602
H	-0.5247	3.4710	5.8985
C	-0.3699	-3.1967	8.0919
H	0.4971	-2.5331	8.0345
H	-0.4206	-3.5943	9.1011
H	-1.2783	-2.6154	7.9127
C	-0.2284	-5.6401	7.6539
H	0.7060	-6.1405	7.3883
H	-1.0670	-6.2214	7.2627
H	-0.3058	-5.6257	8.7370

SCF = -52.672618**ZPE = 0.296239****H₂₉₈ = -52.355675****G₂₉₈ = -52.423146****SCF_{DFT} = -1027.602817**

29-Cl

H	0.0186	0.1305	0.2076
C	-0.0381	0.1107	1.2859
C	-0.1908	0.0487	4.0527
C	-0.0280	-1.0981	1.9510
C	-0.1231	1.2907	1.9953
C	-0.1975	1.2878	3.3994
C	-0.1049	-1.1412	3.3418
H	-0.1311	2.2174	1.4474
H	-0.2529	0.0069	5.1261
C	-0.0903	-2.4739	3.9355
C	-0.0534	-5.0993	4.8872
C	-0.0020	-3.5647	3.0703
C	-0.1594	-2.7323	5.2983
C	-0.1400	-4.0385	5.8068
C	0.0160	-4.8605	3.5316
H	-0.2288	-1.8955	5.9710
H	0.0825	-5.6756	2.8277
H	-0.0403	-6.1213	5.2237
I	0.0931	-3.0238	1.0256
Cl	0.2166	-5.5825	0.4175
N	-0.2528	2.4615	4.1078
N	-0.1893	-4.2723	7.1544
C	-0.3994	3.7178	3.4143
H	0.4568	3.8982	2.7593
H	-0.4416	4.5281	4.1380
H	-1.3144	3.7479	2.8119
C	-0.4587	2.4371	5.5346
H	0.3636	1.9171	6.0335
H	-1.4010	1.9457	5.8044
H	-0.4862	3.4556	5.9141
C	-0.3714	-3.1811	8.0785
H	0.4588	-2.4717	8.0117
H	-0.3994	-3.5668	9.0945
H	-1.3083	-2.6444	7.8917
C	-0.2514	-5.6238	7.6547
H	0.6334	-6.1902	7.3522
H	-1.1430	-6.1479	7.2942
H	-0.2828	-5.6071	8.7413

SCF = -57.620913**ZPE = 0.297200****H₂₉₈ = -57.300800****G₂₉₈ = -57.373845****SCF_{DFT} = -1488.040604****29-OCH2**

H	-0.0263	0.3503	0.2425
C	-0.0888	0.2965	1.3178
C	-0.2498	0.1442	4.0898
C	-0.0785	-0.9231	1.9651
C	-0.1805	1.4502	2.0620
C	-0.2638	1.4101	3.4717
C	-0.1583	-1.0278	3.3585
H	-0.1868	2.3907	1.5405
H	-0.3118	0.0714	5.1609
C	-0.1378	-2.3725	3.9208
C	-0.0821	-5.0358	4.7868
C	-0.0403	-3.4458	3.0284
C	-0.2072	-2.6750	5.2704
C	-0.1820	-4.0015	5.7442
C	-0.0118	-4.7612	3.4400
H	-0.2826	-1.8593	5.9671
H	0.0642	-5.5601	2.7220
H	-0.0587	-6.0659	5.0949
I	0.0560	-2.8101	1.0037
N	-0.3537	2.5457	4.2015
N	-0.2511	-4.2743	7.0672
C	-0.3705	3.8366	3.5521
H	0.5495	4.0049	2.9864
H	-0.4525	4.6187	4.3013
H	-1.2244	3.9255	2.8756
C	-0.4336	2.4922	5.6423
H	0.4529	2.0142	6.0686
H	-1.3242	1.9475	5.9680
H	-0.4938	3.5010	6.0401
C	-0.3518	-3.2082	8.0362
H	0.5173	-2.5465	7.9858
H	-0.3942	-3.6296	9.0362
H	-1.2592	-2.6183	7.8802
C	-0.2247	-5.6405	7.5376
H	0.7054	-6.1378	7.2504
H	-1.0690	-6.2098	7.1403
H	-0.2916	-5.6525	8.6215
O	0.2077	-5.4926	0.3167
C	0.2916	-5.9139	-0.8029
H	0.3494	-6.9909	-1.0099
H	0.3158	-5.2585	-1.6845

SCF = -59.867917**ZPE = 0.323601****H₂₉₈ = -59.519131****G₂₉₈ = -59.596168****SCF_{DFT} = -1142.149108**

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H	1.5111	-0.1833	1.4634
C	0.6166	0.1521	1.9641
C	-1.7151	1.0280	3.2291
C	-0.4537	-0.6935	2.1903
C	0.5113	1.4664	2.3927
C	-0.6506	1.8959	3.0200
C	-1.6250	-0.2877	2.8038
H	1.3280	2.1531	2.2274
H	-2.6169	1.3780	3.7088
C	1.3695	-3.4824	4.0158
C	-0.6803	-4.7804	5.4028
C	0.0950	-3.6032	3.4922
C	1.6110	-4.0181	5.2707
C	0.5885	-4.6641	5.9545
C	-0.9371	-4.2473	4.1489
H	2.5959	-3.9439	5.7070
H	-1.9170	-4.3474	3.7093
H	-1.4640	-5.2932	5.9400
I	-0.2971	-2.7558	1.5331
C	-0.7518	3.3234	3.5213
C	0.8611	-5.2151	7.3405
F	-0.3804	3.3917	4.8080
F	-1.9991	3.7884	3.4451
F	0.0354	4.1523	2.8370
F	0.7040	-4.2540	8.2622
F	0.0316	-6.2082	7.6579
F	2.1085	-5.6723	7.4555
H	-2.4544	-0.9612	2.9505
H	2.1639	-2.9932	3.4747

SCF = -65.768450**ZPE = 0.180436****H₂₉₈ = -65.567101****G₂₉₈ = -65.637982****SCF_{DFT} = -1435.098478****30-OCH2**

H	0.9786	0.1505	0.7185
C	0.3569	0.3883	1.5676
C	-1.2650	0.9890	3.7545
C	-0.4278	-0.5788	2.1703
C	0.3310	1.6785	2.0737
C	-0.4777	1.9702	3.1629
C	-1.2482	-0.2997	3.2505
H	0.9333	2.4504	1.6197
H	-1.8952	1.2343	4.5957
C	0.9487	-2.9416	4.1174
C	-0.6395	-5.0684	4.9835
C	-0.0554	-3.4699	3.3262
C	1.1531	-3.4930	5.3714
C	0.3589	-4.5505	5.7973
C	-0.8565	-4.5207	3.7288
H	1.9277	-3.1017	6.0134
H	-1.6254	-4.9158	3.0852
H	-1.2503	-5.8894	5.3270
I	-0.3860	-2.5842	1.4006
C	-0.4971	3.3632	3.7541
C	0.6233	-5.1667	7.1549
F	0.1981	3.3980	4.9016
F	-1.7410	3.7591	4.0400
F	0.0387	4.2719	2.9400
F	0.9895	-4.2474	8.0522
F	-0.4479	-5.7971	7.6391
F	1.6148	-6.0655	7.0836
H	-1.8649	-1.0641	3.6979
H	1.5653	-2.1234	3.7793
O	-0.2440	-5.1902	0.8419
C	-0.1037	-5.7560	-0.2095
H	-0.0419	-6.8508	-0.2609
H	-0.0308	-5.2250	-1.1674

SCF = -72.973232**ZPE = 0.208308****H₂₉₈ = -72.739873****G₂₉₈ = -72.818274****SCF_{DFT} = -1549.646652**

30-Cl

H	1.0082	-0.1114	0.6586
C	0.4049	0.1168	1.5244
C	-1.1691	0.6730	3.7429
C	-0.3182	-0.8904	2.1396
C	0.3554	1.4090	2.0197
C	-0.4298	1.6792	3.1310
C	-1.1146	-0.6129	3.2384
H	0.9205	2.1984	1.5489
H	-1.7825	0.9019	4.6010
C	0.9541	-2.9517	4.0994
C	-0.6040	-5.0266	5.1107
C	0.0012	-3.5782	3.3176
C	1.1308	-3.3705	5.4061
C	0.3455	-4.4013	5.9076
C	-0.7758	-4.6118	3.8010
H	1.8734	-2.9012	6.0328
H	-1.4891	-5.1020	3.1578
H	-1.2059	-5.8283	5.5094
I	-0.2496	-2.9175	1.3035
Cl	-0.1092	-5.4367	0.8320
C	-0.5056	3.0657	3.7086
C	0.5671	-4.8530	7.3267
F	-0.0567	3.1026	4.9773
F	-1.7677	3.5272	3.7473
F	0.2107	3.9655	3.0254
F	0.7505	-3.8180	8.1626
F	-0.4561	-5.5639	7.8149
F	1.6610	-5.6263	7.4404
H	-1.6906	-1.3988	3.7047
H	1.5551	-2.1491	3.7001

SCF = -70.765016**ZPE = 0.182422****H₂₉₈ = -70.559932****G₂₉₈ = -70.633264****SCF_{DFT} = -1895.557869****31**

H	1.5764	-0.3293	2.1399
C	0.5895	0.0453	2.3621
C	-1.9751	1.0173	2.9020
C	-0.5399	-0.7362	2.1902
C	0.4251	1.3391	2.8247
C	-0.8544	1.8259	3.0947
C	-1.8219	-0.2784	2.4406
H	1.2863	1.9738	2.9690
H	-2.9621	1.4041	3.1060
C	1.3451	-3.8223	3.8592
C	-0.8408	-4.6526	5.3907
C	0.0424	-3.6709	3.4166
C	1.5511	-4.3952	5.1021
C	0.4610	-4.8099	5.8680
C	-1.0580	-4.0814	4.1491
H	2.5553	-4.5274	5.4752
H	-2.0625	-3.9705	3.7720
H	-1.6783	-4.9832	5.9862
I	-0.2898	-2.7683	1.4716
H	-2.6873	-0.9017	2.2784
H	2.1864	-3.5129	3.2591
C	-1.0177	3.1575	3.5637
N	-1.1486	4.2272	3.9453
C	0.6784	-5.4026	7.1412
N	0.8529	-5.8755	8.1673

SCF = -43.114981**ZPE = 5.000000****H₂₉₈ = -42.927384****G₂₉₈ = -42.988907****SCF_{DFT} = -945.286823**

31-Cl

H	1.1789	-1.0015	3.3060
C	0.2925	-0.4370	3.0526
C	-1.9842	1.0084	2.3735
C	-0.6331	-0.9615	2.1641
C	0.0815	0.8051	3.6187
C	-1.0623	1.5304	3.2812
C	-1.7618	-0.2368	1.8161
H	0.7943	1.2209	4.3153
H	-2.8637	1.5788	2.1145
C	1.2985	-4.3250	3.4585
C	-0.4837	-3.7285	5.5171
C	0.1470	-3.5991	3.2212
C	1.5699	-4.7530	4.7445
C	0.6788	-4.4553	5.7764
C	-0.7485	-3.2960	4.2315
H	2.4658	-5.3175	4.9538
H	-1.6444	-2.7311	4.0210
H	-1.1735	-3.5120	6.3189
I	-0.2893	-2.9231	1.2439
Cl	0.2241	-5.3862	0.6823
H	-2.4657	-0.6535	1.1107
H	1.9614	-4.5703	2.6440
C	-1.2856	2.8019	3.8617
N	-1.4674	3.8295	4.3346
C	0.9542	-4.8925	7.0953
N	1.1786	-5.2393	8.1635

SCF = -48.103610**ZPE = 0.172668****H₂₉₈ = -47.912256****G₂₉₈ = -47.976645****SCF_{DFT} = -1405.753266****31-OCH2**

H	1.2588	-0.5759	3.3539
C	0.3401	-0.0654	3.1071
C	-2.0293	1.2522	2.4404
C	-0.5597	-0.6087	2.2041
C	0.0414	1.1502	3.6942
C	-1.1423	1.8106	3.3609
C	-1.7367	0.0328	1.8557
H	0.7244	1.5932	4.4028
H	-2.9401	1.7720	2.1856
C	1.4019	-4.1971	3.3777
C	-0.5021	-3.9301	5.4045
C	0.2382	-3.4739	3.1926
C	1.6125	-4.8005	4.6051
C	0.6630	-4.6676	5.6185
C	-0.7224	-3.3284	4.1785
H	2.5110	-5.3725	4.7801
H	-1.6253	-2.7627	4.0065
H	-1.2333	-3.8352	6.1927
I	-0.1012	-2.5064	1.3067
H	-2.4156	-0.4052	1.1402
H	2.1258	-4.2987	2.5854
C	-1.4440	3.0611	3.9628
N	-1.6885	4.0656	4.4513
C	0.8826	-5.2886	6.8771
N	1.0609	-5.7874	7.8904
O	0.4957	-5.0298	0.5975
C	0.3725	-5.5977	-0.4542
H	0.6410	-6.6564	-0.5646
H	-0.0089	-5.1033	-1.3574

SCF = -50.317569**ZPE = 0.198406****H₂₉₈ = -50.098007****G₂₉₈ = -50.167799****SCF_{DFT} = -1059.836172**

32

H	1.5803	-0.2081	2.3719
C	0.5860	0.1490	2.5906
C	-1.9783	1.0700	3.1337
C	-0.5181	-0.6770	2.4286
C	0.4042	1.4341	3.0397
C	-0.8835	1.9444	3.3239
C	-1.8024	-0.2162	2.6855
H	1.2753	2.0532	3.1642
H	-2.9822	1.4026	3.3319
C	1.3582	-3.9041	4.0126
C	-0.8268	-4.9100	5.4027
C	0.0650	-3.7122	3.5450
C	1.5540	-4.5898	5.1863
C	0.4708	-5.1216	5.9232
C	-1.0286	-4.2257	4.2292
H	2.5646	-4.7203	5.5320
H	-2.0302	-4.0898	3.8519
H	-1.6899	-5.2928	5.9186
I	-0.2423	-2.6733	1.6935
H	-2.6586	-0.8562	2.5397
H	2.2058	-3.5194	3.4672
N	-1.0601	3.2102	3.7518
N	0.6668	-5.8050	7.0683
C	-2.3866	3.7220	4.0120
H	-2.3190	4.7520	4.3495
H	-2.8834	3.1421	4.7936
H	-3.0017	3.7007	3.1088
C	0.0691	4.0974	3.9154
H	0.5914	4.2499	2.9675
H	0.7746	3.7016	4.6499
H	-0.2767	5.0644	4.2688
C	2.0028	-6.0355	7.5695
H	2.5115	-5.0908	7.7767
H	2.5980	-6.6102	6.8555
H	1.9510	-6.5996	8.4961
C	-0.4515	-6.3615	7.7954
H	-0.0905	-6.8651	8.6873
H	-0.9921	-7.0923	7.1886
H	-1.1447	-5.5767	8.1075

SCF = -53.669167**ZPE = 0.316715****H₂₉₈ = -53.330156****G₂₉₈ = -53.402564****SCF_{DFT} = -1028.799261****32-Cl**

H	1.2407	-0.9889	3.3640
C	0.3339	-0.4445	3.1388
C	-1.9763	0.9559	2.5654
C	-0.5810	-0.9722	2.2445
C	0.0973	0.7658	3.7553
C	-1.0693	1.5010	3.4877
C	-1.7311	-0.2583	1.9578
H	0.8337	1.1382	4.4477
H	-2.8827	1.4795	2.3113
C	1.2867	-4.4657	3.4306
C	-0.4651	-3.8828	5.4945
C	0.1804	-3.6708	3.2059
C	1.5203	-4.9687	4.6922
C	0.6512	-4.6932	5.7618
C	-0.6973	-3.3784	4.2322
H	2.3905	-5.5858	4.8374
H	-1.5627	-2.7575	4.0533
H	-1.1736	-3.6478	6.2709
I	-0.1992	-2.8728	1.2722
Cl	0.3255	-5.3411	0.5198
H	-2.4427	-0.6574	1.2490
H	1.9484	-4.7115	2.6155
N	-1.3220	2.6906	4.1219
N	0.8963	-5.1784	7.0177
C	-2.4576	3.4891	3.7291
H	-2.5060	4.3792	4.3519
H	-3.3846	2.9298	3.8739
H	-2.3978	3.8043	2.6808
C	-0.2876	3.3197	4.9072
H	0.6157	3.5112	4.3169
H	-0.0202	2.6935	5.7620
H	-0.6517	4.2696	5.2909
C	1.9365	-6.1589	7.2196
H	2.9180	-5.7304	7.0009
H	1.7902	-7.0410	6.5875
H	1.9353	-6.4798	8.2582
C	-0.0646	-4.9734	8.0738
H	0.3187	-5.3981	8.9985
H	-1.0281	-5.4461	7.8508
H	-0.2283	-3.9059	8.2391

SCF = -58.609379**ZPE = 0.317779****H₂₉₈ = -58.267356****G₂₉₈ = -58.343174****SCF_{DFT} = -1489.219903**

32-OCH2

H	1.5787	-0.3417	3.0986
C	0.5833	0.0645	3.0007
C	-1.9759	1.1055	2.7383
C	-0.3946	-0.6313	2.3032
C	0.2766	1.2724	3.5793
C	-1.0124	1.8392	3.4648
C	-1.6716	-0.1054	2.1636
H	1.0515	1.7859	4.1214
H	-2.9744	1.4875	2.6168
C	1.4660	-4.3007	3.4959
C	-0.5237	-4.1035	5.4241
C	0.3249	-3.5502	3.2692
C	1.6091	-4.9570	4.6958
C	0.6201	-4.8843	5.7009
C	-0.6751	-3.4512	4.2228
H	2.5032	-5.5349	4.8518
H	-1.5607	-2.8620	4.0380
H	-1.3086	-4.0067	6.1538
I	0.0833	-2.5089	1.4190
H	-2.4254	-0.6413	1.6070
H	2.2302	-4.3789	2.7398
N	-1.3099	3.0320	4.0246
N	0.7620	-5.5333	6.8779
C	-2.6270	3.6072	3.8748
H	-2.6676	4.5615	4.3918
H	-3.3905	2.9557	4.3073
H	-2.8646	3.7813	2.8221
C	-0.3030	3.7809	4.7408
H	0.5379	4.0349	4.0900
H	0.0708	3.2149	5.5979
H	-0.7337	4.7065	5.1114
C	1.9398	-6.3273	7.1427
H	2.8439	-5.7150	7.0964
H	2.0312	-7.1489	6.4272
H	1.8737	-6.7539	8.1394
C	-0.2740	-5.4704	7.8830
H	0.0154	-6.0702	8.7409
H	-1.2194	-5.8626	7.4992
H	-0.4291	-4.4434	8.2245
O	0.7199	-5.0708	0.5792
C	0.5368	-5.5628	-0.4984
H	0.8243	-6.6006	-0.7152
H	0.0751	-5.0150	-1.3320

SCF = -60.862578**ZPE = 0.343892****H₂₉₈ = -60.491894****G₂₉₈ = -60.573441****SCF_{DFT} = -1143.340737****33**

I	-1.3639	1.0883	-3.3512
C	-0.7415	0.4625	-1.4463
C	0.0813	-0.3340	1.0504
N	-0.9458	-0.8085	-1.0442
C	-0.1162	1.3744	-0.6046
C	0.3012	0.9820	0.6540
C	-0.5419	-1.1951	0.1782
H	0.0367	2.3860	-0.9475
H	0.7872	1.6856	1.3118
H	0.3895	-0.6850	2.0220
C	-1.5942	-1.7691	-1.9066
H	-1.0275	-1.8935	-2.8319
H	-2.5994	-1.4301	-2.1662
H	-1.6675	-2.7332	-1.4088
H	-0.7299	-2.2234	0.4500

SCF = -22.719824**ZPE = 0.114956****H₂₉₈ = -22.596392****G₂₉₈ = -22.638318****SCF_{DFT} = -585.089063****33-OCH2**

I	-1.2838	0.9000	-3.5084
C	-0.7299	0.4078	-1.5489
C	0.0009	-0.2231	1.0281
N	-0.9431	-0.8328	-1.0666
C	-0.1374	1.3719	-0.7405
C	0.2333	1.0662	0.5540
C	-0.5865	-1.1413	0.1920
H	0.0247	2.3582	-1.1461
H	0.6929	1.8115	1.1836
H	0.2728	-0.5077	2.0312
C	-1.5565	-1.8440	-1.8957
H	-0.9549	-2.0171	-2.7904
H	-2.5499	-1.5218	-2.2145
H	-1.6476	-2.7775	-1.3454
H	-0.7833	-2.1508	0.5207
O	-2.0411	1.3910	-6.0635
C	-2.0754	2.3589	-6.7700
H	-2.4363	2.3012	-7.8060
H	-1.7533	3.3552	-6.4353

SCF = -29.914169**ZPE = 0.142098****H₂₉₈ = -29.759081****G₂₉₈ = -29.810958****SCF_{DFT} = -699.633965**

33-Cl

I	-1.4386	1.1288	-3.4034
Cl	-1.4305	1.7124	-5.9552
C	-1.0159	0.5209	-1.3361
C	0.2689	-0.3844	0.9478
N	-1.0315	-0.7880	-0.9895
C	-0.3360	1.4132	-0.5013
C	0.2674	0.9887	0.6559
C	-0.3739	-1.2391	0.0986
H	-0.3207	2.4515	-0.7932
H	0.7478	1.6859	1.3238
H	0.7700	-0.7660	1.8215
C	-1.7542	-1.7103	-1.8298
H	-1.2501	-1.8072	-2.7948
H	-2.7566	-1.3265	-2.0202
H	-1.8191	-2.6860	-1.3535
H	-0.3931	-2.3050	0.2712

SCF = -27.658978**ZPE = 0.114909****H₂₉₈ = -27.533088****G₂₉₈ = -27.580853****SCF_{DFT} = -1045.509940****34-Cl**

I	-1.4599	1.1681	-3.3890
Cl	-1.8360	1.7197	-5.9850
C	-0.9007	0.5965	-1.3731
C	0.1270	-0.3650	1.0002
C	-0.9342	-0.7414	-1.0423
C	-0.3023	1.4791	-0.4593
C	0.2566	0.9766	0.7020
N	-0.4854	-1.2019	0.1320
H	-1.3471	-1.4614	-1.7336
H	-0.2792	2.5341	-0.6793
H	0.7611	1.6234	1.4025
H	0.4853	-0.7920	1.9223
H	-1.0103	-3.1614	-0.3514
C	-0.6670	-2.5861	0.5057
H	0.2745	-3.0050	0.8612
H	-1.4079	-2.6673	1.3037

SCF = -27.644197**ZPE = 0.114140****H₂₉₈ = -27.518653****G₂₉₈ = -27.567588****SCF_{DFT} = -1045.496722****34**

I	-1.3809	1.1424	-3.3433
C	-0.7295	0.5424	-1.4411
C	0.0836	-0.3510	1.0192
C	-0.8815	-0.7790	-1.0500
C	-0.1426	1.4432	-0.5507
C	0.2635	0.9806	0.6896
N	-0.4782	-1.1992	0.1535
H	-1.3318	-1.5087	-1.7081
H	-0.0092	2.4780	-0.8267
H	0.7207	1.6488	1.4022
H	0.3897	-0.7401	1.9787
H	-0.3352	-3.2368	-0.2960
C	-0.6795	-2.5868	0.5080
H	-0.1360	-2.8321	1.4176
H	-1.7413	-2.7801	0.6730

SCF = -22.720455**ZPE = 0.114646****H₂₉₈ = -22.596913****G₂₉₈ = -22.640979****SCF_{DFT} = -585.090046****34-OCH2**

I	-1.3293	0.9132	-3.5017
C	-0.7190	0.4503	-1.5516
C	0.0445	-0.2832	0.9825
C	-0.8672	-0.8437	-1.0787
C	-0.1604	1.4060	-0.7003
C	0.2212	1.0272	0.5748
N	-0.4909	-1.1873	0.1575
H	-1.2942	-1.6164	-1.7020
H	-0.0310	2.4225	-1.0381
H	0.6555	1.7413	1.2561
H	0.3316	-0.6105	1.9701
H	-0.1461	-3.2341	-0.0864
C	-0.6782	-2.5572	0.5829
H	-0.3053	-2.6975	1.5947
H	-1.7378	-2.8154	0.5591
O	-2.1578	1.3282	-6.0937
C	-2.3058	2.2945	-6.7859
H	-2.6542	2.2122	-7.8249
H	-2.1063	3.3174	-6.4350

SCF = -29.911704**ZPE = 0.141663****H₂₉₈ = -29.756599****G₂₉₈ = -29.809987****SCF_{DFT} = -699.632759**

35

I	-1.4208	1.0109	-3.3128
C	-0.7006	0.4850	-1.4250
N	0.2461	-0.2109	1.0785
C	-0.7233	-0.8431	-0.9905
C	-0.1823	1.4508	-0.5574
C	0.2802	1.0690	0.6793
C	-0.2437	-1.1532	0.2602
H	-1.1132	-1.6252	-1.6230
H	-0.1428	2.4894	-0.8464
H	0.6876	1.7933	1.3699
H	-0.2478	-2.1716	0.6208
H	1.8442	-0.7581	2.3076
C	0.7693	-0.5752	2.3755
H	0.6022	0.2272	3.0920
H	0.2882	-1.4807	2.7399

SCF = -22.723651**ZPE = 5.000000****H₂₉₈ = -22.600966****G₂₉₈ = -22.641940****SCF_{DFT} = -585.092920****35-OCH2**

I	-1.2456	0.8137	-3.4577
C	-0.6125	0.3933	-1.5190
N	0.2197	-0.1808	1.0604
C	-0.6627	-0.9099	-1.0136
C	-0.1232	1.3958	-0.6752
C	0.2820	1.0777	0.5973
C	-0.2418	-1.1613	0.2688
H	-1.0314	-1.7184	-1.6252
H	-0.0632	2.4170	-1.0169
H	0.6651	1.8318	1.2690
H	-0.2692	-2.1589	0.6819
H	1.7603	-0.6635	2.3870
C	0.6835	-0.4809	2.3962
H	0.4812	0.3545	3.0642
H	0.1857	-1.3691	2.7800
O	-2.1006	1.1671	-6.0567
C	-2.3427	2.0886	-6.7825
H	-2.6881	1.9357	-7.8146
H	-2.2380	3.1382	-6.4711

SCF = -29.914622**ZPE = 5.000000****H₂₉₈ = -29.760381****G₂₉₈ = -29.811772****SCF_{DFT} = -699.635399****35-Cl**

I	-1.6095	1.0479	-3.2604
Cl	-1.4952	1.5197	-5.9101
C	-1.0445	0.5419	-1.2903
N	0.2595	-0.2125	1.0649
C	-0.9395	-0.8081	-0.8939
C	-0.3934	1.4816	-0.4633
C	0.2268	1.0919	0.6825
C	-0.3074	-1.1500	0.2609
H	-1.3850	-1.5739	-1.5087
H	-0.4077	2.5244	-0.7381
H	0.6992	1.7962	1.3502
H	-0.2471	-2.1722	0.6025
H	2.0035	-0.7321	2.1012
C	0.9335	-0.5953	2.2804
H	0.8046	0.1767	3.0382
H	0.5219	-1.5304	2.6564

SCF = -27.649664**ZPE = 0.114567****H₂₉₈ = -27.523776****G₂₉₈ = -27.572535****SCF_{DFT} = -1045.495653****36**

N	-0.3798	0.5931	-0.1574
C	-0.5758	1.8433	-0.5949
N	-0.3253	2.7039	0.3998
C	0.0046	0.6640	1.1477
H	0.2240	-0.2073	1.7308
C	0.0386	1.9798	1.4951
H	0.2922	2.4384	2.4293
I	-1.1731	2.3648	-2.5109
H	0.2521	4.5234	-0.4429
C	-0.4245	4.1364	0.3209
H	-0.1585	4.5674	1.2831
H	-1.4430	4.4340	0.0658
H	0.1250	-0.6020	-1.7918
C	-0.5466	-0.6073	-0.9316
H	-0.3199	-1.4695	-0.3090
H	-1.5732	-0.6879	-1.2928

SCF = -24.054183**ZPE = 0.125504****H₂₉₈ = -23.918947****G₂₉₈ = -23.963636****SCF_{DFT} = -602.352911**

36-OCH2

N	-0.3738	0.5810	-0.1550
C	-0.5568	1.8077	-0.6572
N	-0.3428	2.7068	0.3106
C	-0.0363	0.7058	1.1601
H	0.1628	-0.1398	1.7859
C	-0.0169	2.0342	1.4513
H	0.2016	2.5350	2.3720
I	-1.0881	2.2301	-2.6168
H	0.2542	4.4831	-0.6029
C	-0.4442	4.1326	0.1588
H	-0.2097	4.6124	1.1059
H	-1.4554	4.4107	-0.1428
H	0.1866	-0.6714	-1.7257
C	-0.5132	-0.6475	-0.8887
H	-0.3083	-1.4861	-0.2275
H	-1.5264	-0.7410	-1.2832
O	-1.8058	2.5608	-5.1959
C	-1.9446	3.4611	-5.9752
H	-2.2625	3.2801	-7.0110
H	-1.7658	4.5133	-5.7114

SCF = -31.248635**ZPE = 0.152572****H₂₉₈ = -31.081754****G₂₉₈ = -31.136612****SCF_{DFT} = -716.898993****36-Cl**

N	-0.3670	0.5990	-0.1145
C	-0.5689	1.8383	-0.5759
N	-0.3133	2.6771	0.4345
C	0.0190	0.6527	1.1964
H	0.2358	-0.2234	1.7720
C	0.0529	1.9649	1.5430
H	0.3044	2.4310	2.4732
I	-1.2671	2.4468	-2.8100
H	0.2511	4.4737	-0.4423
C	-0.4179	4.1061	0.3360
H	-0.1556	4.5596	1.2894
H	-1.4361	4.3852	0.0642
H	0.1265	-0.5587	-1.7673
C	-0.5388	-0.5883	-0.9042
H	-0.3173	-1.4656	-0.3004
H	-1.5639	-0.6438	-1.2710
Cl	-1.9937	3.0774	-5.1258

SCF = -28.993703**ZPE = 5.000000****H₂₉₈ = -28.858591****G₂₉₈ = -28.904737****SCF_{DFT} = -1062.780078****37**

N	-0.3329	0.5907	-0.1791
C	-0.5460	1.8463	-0.6012
N	-0.3496	2.7043	0.4115
C	0.0234	0.6513	1.1415
C	-0.0119	1.9711	1.5172
I	-1.0963	2.3794	-2.5241
H	-0.3963	4.4706	-0.6854
C	-0.4488	4.1410	0.3510
H	0.3705	4.5961	0.9079
H	-1.3926	4.4787	0.7848
H	0.5029	-0.9830	-1.2749
C	-0.4751	-0.6124	-0.9603
H	-0.9647	-1.3865	-0.3693
H	-1.0787	-0.4088	-1.8433
C	0.4192	-0.5741	1.9467
C	0.2126	2.5975	2.8824
F	1.2381	-0.2546	2.9323
F	1.0522	-1.4528	1.1660
F	-0.6539	-1.1815	2.4464
F	1.4582	3.0515	2.9975
F	-0.6108	3.6347	3.0524
F	-0.0282	1.7340	3.8517

SCF = -55.692334**ZPE = 0.132318****H₂₉₈ = -55.542766****G₂₉₈ = -55.604305****SCF_{DFT} = -1276.654285**

37-OCH2

N	-0.3266	0.6115	-0.2040
C	-0.5952	1.8477	-0.6458
N	-0.4213	2.7236	0.3567
C	0.0352	0.7015	1.1124
C	-0.0309	2.0243	1.4689
I	-1.1833	2.3097	-2.5826
H	-0.8588	4.4112	-0.7650
C	-0.6136	4.1492	0.2621
H	0.2940	4.6757	0.5587
H	-1.4266	4.4691	0.9153
H	0.6073	-0.9714	-1.1939
C	-0.3974	-0.6095	-0.9656
H	-0.9228	-1.3762	-0.3956
H	-0.9326	-0.4301	-1.8960
C	0.4303	-0.5198	1.9101
C	0.2643	2.6113	2.8352
F	0.8947	-0.2084	3.1045
F	1.3766	-1.2045	1.2589
F	-0.6147	-1.3391	2.0592
F	1.5558	2.4850	3.1289
F	-0.0360	3.9068	2.9000
F	-0.4491	1.9903	3.7686
O	-2.0655	2.7470	-5.0079
C	-1.7594	3.3921	-5.9735
H	-2.3588	3.3569	-6.8931
H	-0.8775	4.0466	-6.0017

SCF = -62.893624**ZPE = 0.159641****H₂₉₈ = -62.712327****G₂₉₈ = -62.782850****SCF_{DFT} = -1391.202097****38**

N	0.0676	-0.9763	-0.8731
C	-0.4930	0.1250	-1.3923
N	-0.5407	1.0902	-0.4635
C	0.3907	-0.7108	0.4314
C	0.0067	0.5938	0.6900
I	-1.1823	0.3079	-3.3381
H	-2.1253	2.3668	-0.9217
C	-1.0716	2.4159	-0.6406
H	-0.5248	2.9405	-1.4264
H	-0.9757	2.9695	0.2923
H	0.9399	-2.0640	-2.4244
C	0.2925	-2.2207	-1.5596
H	0.7687	-2.9257	-0.8796
H	-0.6550	-2.6394	-1.9040
C	1.0014	-1.6433	1.2953
N	1.4963	-2.4055	1.9883
C	0.1254	1.3328	1.8853
N	0.2175	1.9392	2.8496

SCF = -33.055947**ZPE = 0.122135****H₂₉₈ = -32.920177****G₂₉₈ = -32.973551****SCF_{DFT} = -786.849195****38-OCH2**

N	0.0816	-0.9918	-0.9029
C	-0.4336	0.1030	-1.4776
N	-0.5274	1.0775	-0.5614
C	0.3251	-0.7121	0.4182
C	-0.0601	0.5975	0.6342
I	-1.0150	0.3022	-3.4623
H	-2.0612	2.3546	-1.1608
C	-1.0339	2.4033	-0.7956
H	-0.4219	2.9145	-1.5408
H	-1.0102	2.9675	0.1355
H	0.1120	-2.2170	-2.5807
C	0.3459	-2.2643	-1.5190
H	1.3969	-2.5284	-1.3907
H	-0.2625	-3.0399	-1.0500
C	0.8705	-1.6462	1.3205
N	1.3139	-2.4161	2.0398
C	-0.0107	1.3558	1.8205
N	0.0241	1.9825	2.7760
O	-1.8059	0.3668	-5.9881
C	-1.8818	1.1534	-6.8910
H	-2.2724	0.8579	-7.8739
H	-1.5716	2.2036	-6.7976

SCF = -40.253379**ZPE = 5.000000****H₂₉₈ = -40.086909****G₂₉₈ = -40.148505****SCF_{DFT} = -901.398233**

39

N	-0.3494	0.5975	-0.1744
C	-0.5475	1.8475	-0.6109
N	-0.3341	2.6989	0.4000
C	0.0012	0.6505	1.1549
C	0.0106	1.9723	1.5162
I	-1.0972	2.3802	-2.5449
H	-0.7160	4.4739	-0.6173
C	-0.4344	4.1323	0.3763
H	0.5246	4.5765	0.6455
H	-1.1874	4.4643	1.0921
H	0.4861	-1.1507	-0.9292
C	-0.4684	-0.6230	-0.9238
H	-1.2218	-1.2668	-0.4683
H	-0.7598	-0.4085	-1.9496
C	0.2894	-0.5724	1.9362
H	1.1218	-1.1230	1.4997
H	-0.5769	-1.2325	1.9549
H	0.5465	-0.3142	2.9580
C	0.3122	2.6237	2.8099
H	1.1566	3.3049	2.7124
H	0.5574	1.8778	3.5587
H	-0.5436	3.1980	3.1625

SCF = -30.407459**ZPE = 0.180027****H₂₉₈ = -30.214165****G₂₉₈ = -30.266160****SCF_{DFT} = -681.016240****39-Cl**

N	-0.3390	0.6029	-0.1343
C	-0.5422	1.8424	-0.5924
N	-0.3240	2.6736	0.4318
C	0.0135	0.6417	1.1992
C	0.0229	1.9572	1.5588
I	-1.1788	2.4600	-2.8347
H	-0.7200	4.3731	-0.6489
C	-0.4356	4.1026	0.3652
H	0.5183	4.5712	0.6116
H	-1.1958	4.4585	1.0621
H	0.4793	-1.1301	-0.9529
C	-0.4690	-0.5919	-0.9182
H	-1.2320	-1.2454	-0.4932
H	-0.7590	-0.3054	-1.9264
Cl	-1.8438	3.1054	-5.1779
C	0.3008	-0.5905	1.9748
H	1.1321	-1.1382	1.5317
H	-0.5681	-1.2480	1.9872
H	0.5589	-0.3386	2.9989
C	0.3238	2.6195	2.8524
H	1.1667	3.3022	2.7475
H	0.5706	1.8780	3.6060
H	-0.5348	3.1943	3.1984

SCF = -35.339704**ZPE = 5.000000****H₂₉₈ = -35.143488****G₂₉₈ = -35.201634****SCF_{DFT} = -1141.438841****39-OCH2**

N	-0.3207	0.5568	-0.1858
C	-0.5088	1.7885	-0.6738
N	-0.3218	2.6700	0.3155
C	-0.0050	0.6528	1.1505
C	-0.0057	1.9844	1.4666
I	-1.0097	2.2440	-2.6407
H	-0.6873	4.3932	-0.7829
C	-0.4263	4.1002	0.2316
H	0.5244	4.5609	0.5024
H	-1.1966	4.4589	0.9153
H	0.5298	-1.2138	-0.8698
C	-0.4232	-0.6845	-0.9021
H	-1.1891	-1.3144	-0.4481
H	-0.6890	-0.4949	-1.9398
C	0.2630	-0.5442	1.9790
H	1.1068	-1.1074	1.5823
H	-0.6035	-1.2040	1.9959
H	0.4930	-0.2522	2.9983
C	0.2610	2.6821	2.7446
H	1.1058	3.3625	2.6444
H	0.4891	1.9633	3.5246
H	-0.6055	3.2648	3.0548
O	-1.6904	2.6122	-5.2490
C	-1.8249	3.5218	-6.0174
H	-2.1217	3.3540	-7.0620
H	-1.6632	4.5721	-5.7347

SCF = -37.600052**ZPE = 0.207144****H₂₉₈ = -37.375090****G₂₉₈ = -37.437054****SCF_{DFT} = -795.561265**

40			
N	-0.1334	-1.1239	-1.0358
C	-0.4649	0.0698	-1.5534
N	-0.4912	0.9817	-0.5831
C	0.0610	-0.9719	0.3158
C	-0.1607	0.3573	0.6139
I	-0.8519	0.4197	-3.5569
H	-1.7163	2.4692	-1.3705
C	-0.8561	2.3690	-0.7090
H	-0.0281	2.9509	-1.1177
H	-1.1185	2.7456	0.2788
H	0.7901	-2.2952	-2.4965
C	-0.0045	-2.3671	-1.7529
H	0.2385	-3.1480	-1.0358
H	-0.9411	-2.6118	-2.2548
O	0.3658	-2.0424	1.0345
O	-0.1619	1.0191	1.7770
C	1.0269	1.7555	2.1058
H	1.8897	1.0903	2.1773
H	0.8255	2.2019	3.0759
H	1.2281	2.5388	1.3731
C	0.4789	-1.8882	2.4477
H	1.3828	-1.3336	2.7059
H	0.5478	-2.8994	2.8415
H	-0.3958	-1.3837	2.8590

SCF = -38.513492

ZPE = 0.187119

H₂₉₈ = -38.310776

G₂₉₈ = -38.367960

SCF_{DFT} = -831.458619

40-OCH2			
N	-0.1252	-1.1290	-1.0554
C	-0.4454	0.0574	-1.5939
N	-0.4782	0.9765	-0.6313
C	0.0545	-0.9652	0.2967
C	-0.1655	0.3652	0.5777
I	-0.8128	0.3710	-3.6067
H	-1.6754	2.4532	-1.4722
C	-0.8356	2.3622	-0.7840
H	0.0054	2.9369	-1.1765
H	-1.1247	2.7530	0.1905
H	0.8028	-2.3092	-2.5043
C	0.0043	-2.3762	-1.7645
H	0.2398	-3.1548	-1.0428
H	-0.9293	-2.6185	-2.2728
O	0.3480	-2.0327	1.0316
O	-0.1754	1.0435	1.7355
C	1.0149	1.7748	2.0599
H	1.8732	1.1049	2.1463
H	0.8126	2.2382	3.0218
H	1.2268	2.5452	1.3162
C	0.4424	-1.8581	2.4417
H	1.3414	-1.2971	2.7045
H	0.5078	-2.8628	2.8522
H	-0.4383	-1.3486	2.8343
O	-1.2675	0.5702	-6.2681
C	-1.4986	1.4396	-7.0604
H	-1.6479	1.2204	-8.1267
H	-1.5754	2.4997	-6.7797

SCF = -45.707166

ZPE = 0.214273

H₂₉₈ = -45.472757

G₂₉₈ = -45.539856

SCF_{DFT} = -946.003328

7.9 ONIOM(DFT:AM1) (Link Atom = F)

1-Cl			
H	2.7181	0.0338	-1.4693
C	2.1191	0.0442	-0.5471
C	0.6030	0.0882	1.7884
C	1.6812	-1.1494	0.0145
C	1.8018	1.2640	0.0548
C	1.0423	1.2863	1.2247
C	0.9245	-1.1272	1.1804
H	2.1483	2.2071	-0.3899
H	0.5749	-2.0681	1.6298
H	0.0047	0.1048	2.7098
I	2.1944	-3.1194	-0.9624
Cl	2.7790	-5.3635	-2.0725
H	0.7910	2.2437	1.7003

SCF = -857.742791

2-Cl			
H	0.3762	0.1561	0.0636
C	0.2313	0.1369	1.1539
C	-0.1372	0.0950	3.9201
C	0.3466	-1.0607	1.8519
C	-0.0678	1.3215	1.8249
C	-0.2538	1.3040	3.2162
C	0.1626	-1.0785	3.2305
H	-0.1591	2.2683	1.2741
H	0.2530	-2.0233	3.7867
H	-0.2828	0.0816	5.0095
I	0.8354	-2.9914	0.7400
Cl	1.3784	-5.1418	-0.4955
C	-0.5589	2.5048	3.9092
N	-0.8093	3.4903	4.4777

SCF = -857.703032

3-Cl			
H	0.3743	0.1405	0.0532
C	0.2319	0.1233	1.1442
C	-0.1296	0.0777	3.9187
C	0.3495	-1.0735	1.8441
C	-0.0658	1.3107	1.8075
C	-0.2471	1.2843	3.2032
C	0.1690	-1.0911	3.2236
H	-0.1596	2.2594	1.2565
H	0.2617	-2.0361	3.7798
H	-0.2731	0.0668	5.0104
I	0.8401	-3.0217	0.7251
Cl	1.3768	-5.1566	-0.4979
N	-0.5634	2.5328	3.9230
O	-0.6643	3.5676	3.3104
O	-0.7193	2.5106	5.1195

SCF = -857.755432**4-Cl**

H	0.3834	0.1353	0.0563
C	0.2360	0.1154	1.1461
C	-0.1428	0.0855	3.9029
C	0.3501	-1.0810	1.8440
C	-0.0666	1.2999	1.8190
C	-0.2578	1.2936	3.2056
C	0.1602	-1.0935	3.2208
H	-0.1575	2.2439	1.2634
H	0.2473	-2.0356	3.7817
H	-0.2938	0.0716	4.9916
I	0.8383	-2.9926	0.7473
Cl	1.3945	-5.1698	-0.5019
C	-0.5634	2.5497	3.9273
H	-1.1984	2.3515	4.8257
H	0.3833	3.0372	4.2722
H	-1.1042	3.2712	3.2666

SCF = -857.754629**5-Cl**

H	1.3588	0.0659	0.2494
C	0.7874	0.0733	1.1900
C	-0.6552	0.1251	3.5661
C	0.3754	-1.1211	1.7633
C	0.4869	1.2981	1.7848
C	-0.2409	1.3488	2.9946
C	-0.3416	-1.0860	2.9506
H	0.8329	2.2188	1.2947
H	-0.6753	-2.0230	3.4217
H	-1.2254	0.1048	4.5053
I	0.8518	-3.0896	0.7752
Cl	1.3904	-5.3382	-0.3551
N	-0.4845	2.5911	3.6573
C	-1.5917	2.5848	4.5849
C	-0.4392	3.7591	2.8090
H	-2.5402	2.1731	4.1438
H	-1.7920	3.6274	4.9477
H	-1.3093	1.9573	5.4718
H	-1.0796	3.6674	1.8896
H	-0.7722	4.6624	3.3851
H	0.6237	3.9249	2.4880

SCF = -857.726537

6-Cl

H	0.3009	0.1305	0.0509
C	0.2171	0.0744	1.1465
C	0.0023	-0.0594	3.9305
C	0.3685	-1.1456	1.7966
C	-0.0418	1.2392	1.8674
C	-0.1479	1.1613	3.2661
C	0.2614	-1.2096	3.1781
H	-0.1637	2.2089	1.3685
H	0.3800	-2.1713	3.6990
H	-0.0797	-0.1253	5.0226
I	0.7882	-3.0174	0.6048
Cl	1.2637	-5.1466	-0.7501
O	-0.4075	2.3745	3.8994
C	-0.5162	2.3188	5.3113
H	0.4379	1.9619	5.7713
H	-1.3622	1.6573	5.6207
H	-0.7203	3.3786	5.6078

SCF = -857.803798**7-Cl**

H	1.2291	0.4197	0.8725
C	0.5834	0.0961	1.7019
C	-1.0435	-0.7046	3.8142
C	0.2871	-1.2520	1.8720
C	0.0611	1.0485	2.5765
C	-0.7541	0.6530	3.6416
C	-0.5313	-1.6486	2.9236
H	0.2875	2.1150	2.4312
H	-0.7752	-2.7119	3.0637
H	-1.6790	-1.0202	4.6549
I	1.1419	-2.7964	0.4472
Cl	2.1097	-4.5374	-1.1536
S	-1.4880	1.7747	4.7010
C	-0.1478	2.7244	5.3173
H	-0.6007	3.5297	5.9388
H	0.4493	3.1841	4.4987
H	0.5369	2.1168	5.9495

SCF = -857.745920**8-Cl**

H	0.5465	0.1411	0.0763
C	0.3305	0.1108	1.1543
C	-0.2189	0.0454	3.8903
C	0.3563	-1.0998	1.8393
C	0.0311	1.2950	1.8264
C	-0.2437	1.2585	3.1975
C	0.0825	-1.1302	3.2023
H	0.0078	2.2575	1.2954
H	0.1018	-2.0846	3.7489
H	-0.4362	0.0258	4.9683
I	0.8465	-3.0346	0.7297
Cl	1.3898	-5.1850	-0.5003
C	-0.5680	2.5529	3.9162
F	-0.8253	2.4409	5.2634
F	0.4208	3.5105	3.8620
F	-1.6736	3.2213	3.4380

SCF = -858.003139**9-Cl**

H	0.3610	0.1463	0.0613
C	0.2235	0.1270	1.1524
C	-0.1286	0.0990	3.9173
C	0.3469	-1.0675	1.8520
C	-0.0756	1.3144	1.8231
C	-0.2515	1.2969	3.2090
C	0.1709	-1.0790	3.2304
H	-0.1713	2.2546	1.2614
H	0.2666	-2.0194	3.7929
H	-0.2661	0.0803	5.0080
I	0.8332	-2.9927	0.7461
Cl	1.3777	-5.1529	-0.4930
Br	-0.6553	2.8919	4.1245

SCF = -857.741467

10-Cl

C	0.2168	-0.0227	1.1372
C	-0.1310	0.0051	3.9357
C	0.1237	-1.2207	1.8460
C	0.1357	1.1891	1.8235
C	-0.0380	1.2155	3.2224
C	-0.0501	-1.2192	3.2451
I	0.5213	-0.0464	-1.2666
Cl	0.8271	-0.0711	-3.6893
C	0.2028	-2.4701	1.1682
N	0.2662	-3.4958	0.6228
C	-0.1446	-2.4414	3.9679
N	-0.2213	-3.4429	4.5553
C	-0.3055	0.0191	5.3461
N	-0.4483	0.0306	6.5009
C	-0.1202	2.4518	3.9223
N	-0.1868	3.4648	4.4909
C	0.2272	2.4249	1.1226
N	0.3008	3.4397	0.5584

SCF = -857.502353**11-Cl**

C	0.2156	-0.0258	1.1406
C	-0.1311	0.0110	3.9555
C	0.1030	-1.2201	1.8499
C	0.1563	1.1866	1.8249
C	-0.0173	1.2229	3.2371
C	-0.0714	-1.2193	3.2624
I	0.5100	-0.0568	-1.2226
F	0.1545	-2.4227	1.2296
F	-0.1799	-2.3829	3.9458
F	-0.2964	0.0286	5.2998
F	-0.0739	2.4040	3.8961
F	0.2607	2.3726	1.1799
Cl	0.8161	-0.0881	-3.6787

SCF = -858.102058**12-Cl**

C	0.5676	-0.2793	1.0811
C	-0.0130	0.5828	3.6880
C	0.2465	-1.2049	2.0733
C	0.5977	1.0787	1.3963
C	0.3087	1.5394	2.7045
C	-0.0506	-0.7954	3.3966
I	1.0584	-1.0130	-1.1332
Cl	1.5656	-1.7799	-3.4326
I	-0.5180	-2.1516	4.8368
I	0.3552	3.5208	3.1556
F	-0.2942	1.0000	4.9497
F	0.2171	-2.5238	1.7694
F	0.9095	1.9788	0.4344

SCF = -857.896235**13-Cl**

C	0.0017	-0.0045	1.2847
I	-0.0052	-0.0166	-1.1767
Cl	-0.0107	-0.0300	-3.6287
Br	-0.9210	-1.5626	1.7554
Br	1.8173	-0.0205	1.7371
Br	-0.8879	1.5804	1.7311

SCF = -857.805928**14-Cl**

C	0.0003	-0.0040	1.1184
I	-0.0004	-0.0190	-1.4302
Cl	-0.0011	-0.0333	-3.8755
F	-0.6280	-1.0750	1.7013
F	1.2452	-0.0072	1.6944
F	-0.6161	1.0811	1.6880

SCF = -858.079047**15-Cl**

C	-0.0006	-0.0039	1.1583
I	0.0091	-0.0120	-1.2213
Cl	0.0205	-0.0219	-3.7907
C	-0.7194	-1.2440	1.5798
H	-0.1974	-2.1560	1.2000
H	-1.7674	-1.2485	1.1923
H	-0.7699	-1.3218	2.6978
C	1.4313	-0.0029	1.5844
H	1.9607	-0.9109	1.2053
H	1.5204	0.0007	2.7027
H	1.9611	0.9025	1.1994
C	-0.7188	1.2392	1.5716
H	-0.1958	2.1485	1.1867
H	-0.7701	1.3239	2.6892
H	-1.7665	1.2422	1.1833

SCF = -857.818910**16-Cl**

C	-0.0013	-0.0027	1.5525
I	0.0012	-0.0159	-1.3484
Cl	0.0031	-0.0273	-3.7197
C	-0.6984	-1.2124	1.7009
N	-1.2789	-2.2197	1.8117
C	1.3953	-0.0005	1.6973
N	2.5581	0.0012	1.8051
C	-0.7011	1.2067	1.6906
N	-1.2839	2.2135	1.7928

SCF = -857.693323**17-Cl**

I	0.3449	-1.6579	-2.0910
Cl	1.1753	-2.7746	-4.0217
N	-0.6103	-0.3909	0.1092
C	0.0130	-0.3536	1.3421
C	-1.7995	0.3103	0.1746
O	1.1022	-0.8761	1.6575
O	-2.6260	0.4895	-0.7439
C	-2.0376	0.8983	1.5904
H	-2.1209	2.0075	1.5256
H	-2.9872	0.4927	2.0089
C	-0.8170	0.4511	2.3767
H	-0.2144	1.3089	2.7540
H	-1.0807	-0.2060	3.2369

SCF = -857.923424**18-Cl**

I	-0.0038	0.0021	-1.0191
Cl	-0.0057	0.1092	-3.6365
C	-0.0020	-0.0556	1.1989
H	-0.0045	0.9434	1.6381
C	0.0017	-1.1668	1.9098
H	0.0025	-1.1809	3.0106
H	0.0042	-2.1668	1.4566

SCF = -857.747690**19-Cl**

I	-0.0047	-0.0387	-1.0453
Cl	-0.0054	-0.0194	-3.5987
C	-0.0041	-0.0227	1.2140
H	-0.0105	0.9833	1.6356
C	0.0032	-1.1364	1.9369
H	0.0096	-2.1380	1.4724
C	0.0038	-1.1653	3.3580
N	0.0042	-1.1994	4.5237

SCF = -857.716977**20-Cl**

I	-0.0634	-0.0227	-1.0257
Cl	0.2424	0.1902	-3.6075
C	-0.3501	-0.1835	1.1700
H	-0.9360	0.6391	1.5777
C	0.1592	-1.1884	1.8766
H	0.7437	-1.9948	1.3924
N	0.1229	-1.3683	3.2915
C	-0.3282	-2.6801	3.6960
H	0.2294	-3.4590	3.1137
H	-1.4302	-2.8425	3.5386
H	-0.1075	-2.8182	4.7877
C	-0.5062	-0.3034	4.0341
H	-0.0211	0.6674	3.7520
H	-0.3534	-0.4823	5.1311
H	-1.6113	-0.2149	3.8420

SCF = -857.742777**21-Cl**

I	0.0285	-0.0563	-0.9261
Cl	0.3037	-0.1436	-3.5166
C	-0.1875	0.0175	1.1717
H	-0.4166	0.0874	3.4167
C	-0.3094	0.0548	2.3654

SCF = -0.128955**22-Cl**

I	0.0352	-0.0569	-0.9586
Cl	0.2947	-0.1423	-3.4666
C	-0.1896	0.0190	1.2226
C	-0.3145	0.0573	2.4220
C	-0.4564	0.1008	3.7793
N	-0.5777	0.1377	4.9397

SCF = -0.130141**23-Cl**

I	0.0285	-0.0558	-0.8912
Cl	0.2904	-0.1400	-3.4145
C	-0.1973	0.0194	1.2853
N	-0.3185	0.0582	2.4432

SCF = -0.129991

24-Cl

C	-0.8817	0.4580	1.5708
C	0.9897	-0.4678	3.4608
C	-1.0583	-0.8020	2.1693
C	0.2342	1.2613	1.9168
C	1.1721	0.7859	2.8708
C	-0.1154	-1.2473	3.1091
C	-0.2687	-2.5616	3.7551
C	-0.2612	-5.0356	5.1855
C	0.3367	-3.7081	3.2028
C	-0.9509	-2.6832	4.9823
C	-0.9472	-3.9145	5.6942
C	0.3404	-4.9395	3.9148
C	-0.1000	-6.2503	6.0020
C	0.2648	-8.5330	7.5809
C	-1.0383	-7.2913	5.9221
C	1.0082	-6.3291	6.8496
C	1.1981	-7.4649	7.6416
C	-0.8541	-8.4374	6.7154
I	2.4232	-4.6282	6.8929
I	2.4136	-1.2718	4.9525
F	0.4353	-9.6384	8.3410
F	2.2527	-7.5900	8.4779
F	-1.7209	-9.4778	6.6866
F	0.9576	-6.0030	3.3532
F	0.9506	-3.6613	1.9994
F	-1.6017	-1.6302	5.5254
F	-1.5946	-3.9721	6.8794
F	-1.7531	0.9475	0.6567
F	0.3974	2.4722	1.3372
F	2.2235	1.5784	3.1767
Cl	3.9429	-2.4718	6.7442
I	-2.6492	-1.9678	1.6893
I	-2.6337	-7.1333	4.6770

SCF = -1255.752252**25-Cl**

C	0.3063	-1.3400	0.3939
C	-0.3277	1.4027	0.1302
C	1.3512	-0.3894	0.3355
C	-1.0493	-0.9466	0.3118
C	-1.3512	0.4293	0.1915
C	1.0185	0.9793	0.2150
C	2.7597	-0.8224	0.3219
C	5.4392	-1.6462	0.2632
C	3.3694	-1.1029	-0.9085
C	3.4649	-0.9460	1.5293
C	4.8091	-1.3595	1.4997
C	4.7060	-1.5142	-0.9451
C	-2.1225	-1.9557	0.2743
C	-4.1629	-3.8762	0.1706
C	-2.7235	-2.3819	1.4691
C	-2.5230	-2.4719	-0.9657
C	-3.5405	-3.4304	-1.0247
C	-3.7470	-3.3454	1.4169
C	-0.6546	2.8219	-0.0948
C	-1.2731	5.5178	-0.5542
C	-0.7509	3.2938	-1.4114
C	-0.8623	3.6734	1.0015
C	-1.1726	5.0260	0.7709
C	-1.0592	4.6380	-1.6475
I	2.5472	-0.5307	3.2914
I	2.1880	-0.8798	-2.6759
I	-1.5311	-1.7453	-2.7119
I	-2.1159	-1.6111	3.2456
I	-0.4150	1.9016	-2.9905
I	-0.7147	2.9523	2.8929
Cl	0.1388	-0.4000	-4.5442
F	0.6090	-2.6501	0.5222
F	-2.6424	0.8209	0.1253
F	2.0062	1.8998	0.1714
F	-3.9627	-3.9586	-2.1949
F	-5.1471	-4.8020	0.1254
F	-4.3657	-3.7970	2.5330
F	5.5428	-1.4981	2.6288
F	6.7314	-2.0430	0.2398
F	5.3392	-1.7961	-2.1054
F	-1.5714	6.8185	-0.7710
F	-1.3841	5.8972	1.7851
F	-1.1635	5.1422	-2.8970

SCF = -1653.262792

26-Cl

H	-1.4202	0.8521	-2.0932
C	-1.3254	1.5876	-1.2668
C	-1.0869	3.4504	0.8188
C	-1.1294	1.1589	0.0390
C	-1.4030	2.9582	-1.5314
C	-1.2850	3.8810	-0.4950
C	-1.0061	2.0864	1.1020
H	-1.5583	3.2993	-2.5662
H	-1.3478	4.9595	-0.7090
H	-0.9945	4.1869	1.6308
C	-0.7995	1.5302	2.4348
C	-0.4099	0.2185	4.8700
C	-0.7460	0.1276	2.5016
C	-0.6561	2.2751	3.6073
C	-0.4620	1.6104	4.8209
C	-0.5536	-0.5343	3.6974
H	-0.6949	3.3737	3.5834
H	-0.3494	2.1955	5.7463
H	-0.5119	-1.6326	3.7432
H	-0.2561	-0.2935	5.8316
I	-0.9995	-0.7008	0.6014
Cl	-1.3178	-1.4893	-1.7324

SCF = -957.394698**27-Cl**

H	-0.0014	0.1141	0.1438
C	-0.0097	0.0996	1.2443
C	-0.0286	0.0919	4.0622
C	-0.0407	-1.0860	1.9499
C	0.0117	1.3081	1.9521
C	0.0013	1.2941	3.3476
C	-0.0494	-1.1113	3.3545
H	0.0413	2.2681	1.4114
H	-0.0308	0.1096	5.1637
C	-0.0804	-2.4393	3.9571
C	-0.1430	-5.0724	4.9254
C	-0.1009	-3.5420	3.0690
C	-0.0905	-2.6769	5.3323
C	-0.1210	-3.9919	5.8050
C	-0.1328	-4.8453	3.5453
H	-0.0794	-1.8370	6.0463
H	-0.1502	-5.7062	2.8425
H	-0.1731	-6.1054	5.3107
I	-0.0813	-3.0392	1.1845
Cl	-0.1336	-5.4054	0.5043
C	0.0054	2.6150	4.1122
C	-0.1132	-4.2424	7.3132
F	0.6523	3.6415	3.4689
F	0.6051	2.5557	5.3465
F	-1.2484	3.1145	4.3698
F	-0.7344	-3.2652	8.0510
F	-0.7308	-5.4066	7.6965
F	1.1466	-4.3288	7.8532

SCF = -957.884494**28-Cl**

H	-0.1577	0.1246	0.1602
C	-0.1242	0.1112	1.2603
C	-0.0379	0.1001	4.0773
C	-0.1206	-1.0754	1.9649
C	-0.0843	1.3198	1.9650
C	-0.0417	1.3112	3.3655
C	-0.0777	-1.1012	3.3688
H	-0.0867	2.2761	1.4191
H	-0.0041	0.1110	5.1772
C	-0.0791	-2.4308	3.9707
C	-0.0884	-5.0680	4.9332
C	-0.1241	-3.5314	3.0811
C	-0.0392	-2.6690	5.3442
C	-0.0440	-3.9885	5.8229
C	-0.1286	-4.8357	3.5560
H	-0.0040	-1.8273	6.0534
H	-0.1641	-5.6940	2.8506
H	-0.0920	-6.1031	5.3104
I	-0.1769	-3.0254	1.1997
Cl	-0.2412	-5.3936	0.5138
C	-0.0020	2.5410	4.0789
N	0.0303	3.5471	4.6620
C	-0.0033	-4.2247	7.2255
N	0.0298	-4.4182	8.3720

SCF = -957.287804

29-Cl

H	-0.0060	0.1218	0.1761
C	-0.0420	0.0943	1.2762
C	-0.1410	0.0552	4.0815
C	-0.0356	-1.1036	1.9594
C	-0.0987	1.2943	1.9844
C	-0.1387	1.3019	3.4001
C	-0.0853	-1.1339	3.3620
H	-0.1073	2.2347	1.4137
H	-0.1782	0.0198	5.1798
C	-0.0737	-2.4735	3.9542
C	-0.0461	-5.1169	4.8796
C	-0.0142	-3.5569	3.0445
C	-0.1182	-2.7213	5.3186
C	-0.0962	-4.0538	5.8185
C	-0.0012	-4.8640	3.5153
H	-0.1648	-1.8681	6.0111
H	0.0429	-5.7127	2.7994
H	-0.0380	-6.1658	5.2121
I	0.0410	-3.0298	1.1838
Cl	0.1259	-5.4132	0.4390
N	-0.1052	2.5086	4.1218
N	-0.0757	-4.3016	7.1881
C	-0.3510	3.7284	3.3971
H	0.4696	3.8776	2.6445
H	-0.3374	4.5991	4.1042
H	-1.3378	3.7182	2.8584
C	-0.5501	2.4768	5.4913
H	0.2046	1.9156	6.1060
H	-1.5506	1.9770	5.6057
H	-0.6238	3.5198	5.8971
C	-0.3606	-3.2286	8.1000
H	0.4475	-2.4509	8.0255
H	-0.3828	-3.6125	9.1537
H	-1.3495	-2.7429	7.8746
C	-0.2401	-5.6503	7.6569
H	0.6139	-6.2803	7.2864
H	-1.2043	-6.1015	7.2947
H	-0.2324	-5.6715	8.7782

SCF = -957.369274**30-Cl**

H	1.5574	-0.5331	1.6853
C	0.6377	-0.1163	2.1247
C	-1.6895	0.9787	3.2194
C	-0.5038	-0.8965	2.2750
C	0.6228	1.2212	2.5249
C	-0.5423	1.7609	3.0741
C	-1.6661	-0.3579	2.8142
H	1.5184	1.8514	2.4039
H	-2.6063	1.4176	3.6446
C	0.9558	-2.9584	4.0986
C	-0.4673	-5.1178	5.1566
C	-0.0692	-3.5535	3.3555
C	1.2674	-3.4385	5.3691
C	0.5529	-4.5176	5.8940
C	-0.7795	-4.6350	3.8843
H	2.0716	-2.9673	5.9578
H	-1.5713	-5.1377	3.2982
H	-1.0275	-5.9713	5.5737
I	-0.4932	-2.8961	1.5792
Cl	-0.4811	-5.2437	0.8290
C	-0.5564	3.2153	3.5334
C	0.9058	-5.0539	7.2807
F	-0.1763	3.3907	4.8427
F	-1.7838	3.8265	3.4550
F	0.2806	4.0444	2.8271
F	1.3743	-4.1008	8.1512
F	-0.1443	-5.6374	7.9453
F	1.8836	-6.0178	7.2714
H	-2.5766	-0.9667	2.9271
H	1.5198	-2.0997	3.6944

SCF = -957.889007

31-Cl

H	1.6640	-0.3113	2.4980
C	0.6073	-0.0189	2.6004
C	-2.0672	0.7567	2.8564
C	-0.4149	-0.8967	2.2600
C	0.3005	1.2565	3.0775
C	-1.0402	1.6448	3.2072
C	-1.7468	-0.5159	2.3828
H	1.1068	1.9550	3.3490
H	-3.1199	1.0639	2.9523
C	1.3290	-4.3386	3.5530
C	-0.6653	-3.8837	5.4625
C	0.2178	-3.5529	3.2336
C	1.4475	-4.8958	4.8261
C	0.4515	-4.6689	5.7844
C	-0.7785	-3.3303	4.1899
H	2.3232	-5.5184	5.0696
H	-1.6578	-2.7072	3.9504
H	-1.4535	-3.7059	6.2108
I	0.0477	-2.7977	1.4551
Cl	0.6082	-5.0368	0.5829
H	-2.5608	-1.2032	2.1035
H	2.1088	-4.5517	2.7985
C	-1.3602	2.9422	3.6938
N	-1.6223	4.0032	4.0925
C	0.5701	-5.2350	7.0839
N	0.6674	-5.6976	8.1466

SCF = -957.292270**32-Cl**

H	1.7488	-0.2989	2.7267
C	0.6894	-0.0149	2.8319
C	-1.9795	0.7424	3.0986
C	-0.3197	-0.8845	2.4368
C	0.3827	1.2322	3.3652
C	-0.9663	1.6396	3.5230
C	-1.6490	-0.5000	2.5699
H	1.2098	1.8926	3.6643
H	-3.0425	1.0120	3.1822
C	1.3999	-4.4337	3.5461
C	-0.5146	-3.9851	5.5255
C	0.3223	-3.5787	3.2875
C	1.5324	-5.0577	4.7763
C	0.5808	-4.8463	5.8098
C	-0.6307	-3.3701	4.2905
H	2.3914	-5.7281	4.9296
H	-1.4877	-2.6972	4.1092
H	-1.2894	-3.7912	6.2820
I	0.1434	-2.7327	1.5664
Cl	0.7139	-4.9319	0.5089
H	-2.4622	-1.1721	2.2514
H	2.1463	-4.6454	2.7574
N	-1.2901	2.8584	4.1405
N	0.7403	-5.4199	7.0666
C	-2.6306	3.3572	3.9733
H	-2.7205	4.3761	4.4337
H	-3.3444	2.6701	4.5028
H	-2.9313	3.4241	2.8921
C	-0.2480	3.8444	4.2634
H	0.2339	4.0844	3.2764
H	0.5403	3.4570	4.9638
H	-0.6661	4.7905	4.6973
C	1.7292	-6.4486	7.2435
H	2.7513	-6.0157	7.0675
H	1.5724	-7.3032	6.5298
H	1.6900	-6.8444	8.2922
C	-0.3462	-5.3589	8.0057
H	-0.0759	-5.9115	8.9436
H	-1.2872	-5.8064	7.5832
H	-0.5468	-4.2860	8.2737

SCF = -957.375266

33-Cl

I	-1.5032	1.2806	-3.8268
Cl	-2.1840	2.0276	-5.9738
C	-0.7393	0.4395	-1.4202
C	0.1021	-0.3618	1.1118
N	-0.9374	-0.8294	-1.0055
C	-0.0974	1.3646	-0.5526
C	0.3218	0.9754	0.7018
C	-0.5249	-1.2437	0.2505
H	0.0475	2.3903	-0.9225
H	0.8208	1.6752	1.3891
H	0.4253	-0.7012	2.1054
C	-1.5923	-1.7778	-1.8860
H	-0.9959	-1.8775	-2.8322
H	-2.6183	-1.3991	-2.1407
H	-1.6760	-2.7795	-1.3895
H	-0.7146	-2.2945	0.5329

SCF = -857.637751**34-Cl**

I	-1.5512	1.2563	-3.6592
Cl	-2.3597	1.9018	-5.8314
C	-0.7326	0.5594	-1.4159
C	0.1172	-0.3605	1.0503
C	-0.9060	-0.7637	-1.0477
C	-0.1220	1.4484	-0.5387
C	0.3091	0.9837	0.7112
N	-0.4844	-1.2286	0.1810
H	-1.3860	-1.5055	-1.7129
H	0.0215	2.5038	-0.8208
H	0.7971	1.6479	1.4395
H	0.4448	-0.7596	2.0274
H	-0.1389	-3.2714	-0.1955
C	-0.6780	-2.6179	0.5422
H	-0.2815	-2.8196	1.5717
H	-1.7749	-2.8586	0.5154

SCF = -857.612333**35-Cl**

I	-1.5398	1.1114	-3.6603
Cl	-2.3793	1.7131	-5.8352
C	-0.6841	0.4864	-1.4172
N	0.2660	-0.2248	1.1228
C	-0.7117	-0.8442	-0.9881
C	-0.1686	1.4532	-0.5482
C	0.3014	1.0868	0.7103
C	-0.2355	-1.1847	0.2754
H	-1.1093	-1.6361	-1.6418
H	-0.1287	2.5122	-0.8474
H	0.7171	1.8181	1.4276
H	-0.2386	-2.2238	0.6528
H	1.8848	-0.7863	2.3507
C	0.7805	-0.5931	2.4242
H	0.5985	0.2386	3.1557
H	0.2666	-1.5209	2.7909

SCF = -857.610005**36-Cl**

N	-0.3424	0.5754	-0.1349
C	-0.5915	1.8518	-0.6015
N	-0.3495	2.7076	0.4556
C	0.0583	0.6288	1.2208
H	0.3065	-0.2625	1.7937
C	0.0540	1.9667	1.5913
H	0.2976	2.4378	2.5416
I	-1.3824	2.5471	-3.2148
H	-0.8217	4.4536	-0.5870
C	-0.4781	4.1285	0.4310
H	0.5118	4.6081	0.6589
H	-1.2278	4.4598	1.1990
H	0.5284	-1.1552	-0.9362
C	-0.4639	-0.6313	-0.8869
H	-1.2115	-1.3138	-0.4002
H	-0.8066	-0.3881	-1.9279
Cl	-2.0310	3.1177	-5.4051

SCF = -857.635397

37-Cl

N	-0.3470	0.5744	-0.1415
C	-0.5744	1.8566	-0.6094
N	-0.3455	2.7112	0.4544
C	0.0316	0.6212	1.2197
C	0.0234	1.9655	1.5973
I	-1.3270	2.6047	-3.4141
H	-0.5804	4.4660	-0.6499
C	-0.4747	4.1366	0.4178
H	0.4356	4.6105	0.8759
H	-1.3820	4.4528	1.0017
H	0.5606	-1.0470	-1.1183
C	-0.4613	-0.6248	-0.9152
H	-1.0625	-1.3854	-0.3467
H	-0.9696	-0.3851	-1.8867
Cl	-1.8915	3.1688	-5.6154
C	0.3487	-0.6354	2.0086
C	0.3386	2.6316	2.9235
F	0.9178	-0.4209	3.2338
F	1.2209	-1.4809	1.3660
F	-0.7561	-1.4121	2.2583
F	1.5114	3.3460	2.9062
F	-0.6101	3.5442	3.3179
F	0.4570	1.7779	3.9858

SCF = -858.118077**38-Cl**

N	0.0668	-0.9916	-0.8314
C	-0.4775	0.1466	-1.3998
N	-0.4949	1.1210	-0.4174
C	0.3976	-0.7367	0.5229
C	0.0433	0.5963	0.7840
I	-1.4138	0.4217	-4.2138
H	-1.3446	2.5920	-1.6259
C	-0.9782	2.4579	-0.5730
H	-0.1523	3.1913	-0.3686
H	-1.8226	2.6471	0.1433
H	-0.0837	-2.1539	-2.5556
C	0.2716	-2.2422	-1.4940
H	1.3633	-2.5070	-1.4864
H	-0.3061	-3.0525	-0.9729
Cl	-2.1450	0.6201	-6.4305
C	0.9720	-1.6704	1.4071
N	1.4462	-2.4307	2.1487
C	0.1799	1.3091	1.9910
N	0.2987	1.8849	2.9947

SCF = -857.523123**39-Cl**

N	-0.3596	0.5793	-0.1513
C	-0.5702	1.8583	-0.6207
N	-0.3331	2.7121	0.4354
C	0.0171	0.6204	1.2193
C	0.0338	1.9671	1.5898
I	-1.2767	2.5607	-3.2394
H	-0.7398	4.4610	-0.6296
C	-0.4343	4.1348	0.3999
H	0.5569	4.5961	0.6593
H	-1.1999	4.4832	1.1448
H	0.4876	-1.1711	-0.9328
C	-0.4926	-0.6225	-0.9088
H	-1.2667	-1.2878	-0.4391
H	-0.8044	-0.3695	-1.9571
Cl	-1.8548	3.1373	-5.4492
C	0.3162	-0.5734	2.0231
H	1.1705	-1.1442	1.5776
H	-0.5737	-1.2520	2.0664
H	0.5901	-0.2777	3.0657
C	0.3554	2.5741	2.8893
H	1.2288	3.2687	2.7940
H	0.6110	1.7799	3.6331
H	-0.5169	3.1595	3.2773

SCF = -857.660941**40-Cl**

N	-0.0486	-1.0315	-0.7687
C	-0.4995	0.1278	-1.3742
N	-0.3954	1.1462	-0.4436
C	0.3564	-0.7395	0.5625
C	0.1204	0.6205	0.7726
I	-1.4473	0.3671	-4.0555
H	-1.4807	2.5777	-1.5085
C	-0.7644	2.5096	-0.6471
H	0.1481	3.1243	-0.8778
H	-1.2483	2.9117	0.2830
H	0.9662	-2.8387	-1.0455
C	0.0262	-2.3208	-1.3760
H	-0.8591	-2.9419	-1.0693
H	0.0266	-2.2076	-2.4926
Cl	-2.2260	0.5531	-6.2667
O	0.9535	-1.6397	1.4013
O	0.2458	1.3380	1.9301
C	1.4527	2.1115	1.9933
H	2.3451	1.4471	1.9087
H	1.3993	2.5872	3.0041
H	1.4568	2.8830	1.1863
C	0.0197	-2.4851	2.0885
H	-0.6845	-1.8712	2.6984
H	0.6756	-3.1132	2.7413
H	-0.5388	-3.1155	1.3555

SCF = -857.741196

7.10 ONIOM(DFT:AM1) (Link Atom = Cl) SCF = -1218.104231

1-Cl

H	2.7249	0.0359	-1.4623
C	2.1225	0.0488	-0.5421
C	0.5976	0.0979	1.7887
C	1.6782	-1.1432	0.0197
C	1.8065	1.2691	0.0589
C	1.0430	1.2940	1.2259
C	0.9169	-1.1192	1.1831
H	2.1579	2.2105	-0.3855
H	0.5626	-2.0590	1.6317
H	-0.0039	0.1160	2.7080
I	2.1814	-3.0756	-0.9349
Cl	2.8013	-5.4832	-2.1301
H	0.7934	2.2525	1.7005

SCF = -1218.093830

2-Cl

H	0.3746	0.1603	0.0651
C	0.2304	0.1407	1.1557
C	-0.1368	0.0982	3.9224
C	0.3465	-1.0571	1.8541
C	-0.0690	1.3247	1.8276
C	-0.2543	1.3066	3.2186
C	0.1632	-1.0756	3.2332
H	-0.1609	2.2711	1.2760
H	0.2541	-2.0204	3.7897
H	-0.2818	0.0837	5.0120
I	0.8222	-2.9415	0.7670
Cl	1.3981	-5.2278	-0.5504
C	-0.5603	2.5075	3.9118
N	-0.8113	3.4925	4.4803

SCF = -1218.052729

3-Cl

H	0.3635	0.1437	0.0524
C	0.2257	0.1254	1.1443
C	-0.1247	0.0784	3.9204
C	0.3488	-1.0719	1.8437
C	-0.0719	1.3117	1.8099
C	-0.2475	1.2842	3.2057
C	0.1736	-1.0902	3.2246
H	-0.1698	2.2601	1.2585
H	0.2702	-2.0351	3.7809
H	-0.2638	0.0661	5.0128
I	0.8269	-2.9653	0.7509
Cl	1.3973	-5.2209	-0.5489
N	-0.5638	2.5331	3.9276
O	-0.6689	3.5665	3.3145
O	-0.7146	2.5088	5.1242

4-Cl

H	0.3702	0.1450	0.0568
C	0.2283	0.1236	1.1475
C	-0.1366	0.0885	3.9069
C	0.3494	-1.0732	1.8447
C	-0.0748	1.3056	1.8240
C	-0.2590	1.2969	3.2114
C	0.1667	-1.0891	3.2229
H	-0.1712	2.2496	1.2691
H	0.2595	-2.0318	3.7823
H	-0.2819	0.0721	4.9964
I	0.8271	-2.9438	0.7645
Cl	1.4223	-5.2750	-0.5862
C	-0.5656	2.5514	3.9360
H	-1.1952	2.3498	4.8375
H	0.3816	3.0412	4.2762
H	-1.1122	3.2715	3.2786

SCF = -1218.105666

5-Cl

H	1.3527	0.0712	0.2459
C	0.7830	0.0787	1.1879
C	-0.6561	0.1287	3.5673
C	0.3757	-1.1162	1.7652
C	0.4790	1.3026	1.7816
C	-0.2465	1.3532	2.9931
C	-0.3399	-1.0824	2.9543
H	0.8209	2.2235	1.2887
H	-0.6698	-2.0202	3.4272
H	-1.2250	0.1076	4.5074
I	0.8479	-3.0468	0.7997
Cl	1.4247	-5.4621	-0.4183
N	-0.4917	2.5937	3.6535
C	-1.5886	2.5883	4.5926
C	-0.4433	3.7644	2.8095
H	-2.5407	2.1745	4.1612
H	-1.7862	3.6314	4.9548
H	-1.2968	1.9628	5.4781
H	-1.0842	3.6761	1.8901
H	-0.7747	4.6661	3.3888
H	0.6199	3.9291	2.4889

SCF = -1218.077708

6-Cl

H	0.2929	0.1416	0.0514
C	0.2120	0.0838	1.1475
C	0.0055	-0.0558	3.9325
C	0.3663	-1.1375	1.7963
C	-0.0461	1.2461	1.8715
C	-0.1484	1.1659	3.2707
C	0.2638	-1.2047	3.1787
H	-0.1703	2.2163	1.3740
H	0.3853	-2.1674	3.6976
H	-0.0730	-0.1243	5.0248
I	0.7732	-2.9704	0.6258
Cl	1.2904	-5.2553	-0.8233
O	-0.4081	2.3764	3.9060
C	-0.5167	2.3187	5.3186
H	0.4384	1.9633	5.7774
H	-1.3618	1.6554	5.6265
H	-0.7228	3.3782	5.6151

SCF = -1218.154735**7-Cl**

H	1.6189	0.2938	1.2880
C	0.8501	-0.0298	2.0055
C	-1.0931	-0.8232	3.8325
C	0.3163	-1.3099	1.9306
C	0.4180	0.8603	2.9911
C	-0.5563	0.4689	3.9108
C	-0.6556	-1.7041	2.8454
H	0.8501	1.8703	3.0374
H	-1.0853	-2.7158	2.7951
H	-1.8612	-1.1361	4.5552
I	1.0098	-2.7158	0.3644
Cl	1.8783	-4.4488	-1.5737
S	-1.1774	1.4458	5.1628
C	-0.3386	2.9762	5.0321
H	-0.7428	3.6124	5.8530
H	-0.5260	3.4789	4.0569
H	0.7612	2.8680	5.1641

SCF = -1218.096960**8-Cl**

H	0.5496	0.1461	0.0781
C	0.3323	0.1148	1.1562
C	-0.2209	0.0474	3.8918
C	0.3565	-1.0967	1.8408
C	0.0326	1.2982	1.8295
C	-0.2441	1.2606	3.1999
C	0.0807	-1.1284	3.2039
H	0.0107	2.2608	1.2982
H	0.0984	-2.0833	3.7502
H	-0.4396	0.0260	4.9696
I	0.8338	-2.9837	0.7556
Cl	1.4087	-5.2664	-0.5565
C	-0.5693	2.5554	3.9195
F	-0.8284	2.4409	5.2658
F	0.4208	3.5113	3.8665
F	-1.6739	3.2229	3.4389

SCF = -1218.352705**9-Cl**

H	0.3457	0.1527	0.0618
C	0.2148	0.1326	1.1541
C	-0.1209	0.1025	3.9214
C	0.3465	-1.0619	1.8533
C	-0.0848	1.3181	1.8276
C	-0.2526	1.3002	3.2144
C	0.1789	-1.0747	3.2335
H	-0.1871	2.2577	1.2657
H	0.2812	-2.0150	3.7955
H	-0.2518	0.0821	5.0130
I	0.8203	-2.9429	0.7699
Cl	1.3982	-5.2449	-0.5566
Br	-0.6571	2.8925	4.1319

SCF = -1218.091604

10-Cl

C	0.2231	-0.0228	1.1272
C	-0.1308	0.0054	3.9275
C	0.1357	-1.2210	1.8392
C	0.1352	1.1896	1.8148
C	-0.0418	1.2149	3.2133
C	-0.0413	-1.2182	3.2378
I	0.5008	-0.0458	-1.1591
Cl	0.8027	-0.0741	-3.6940
C	0.2234	-2.4733	1.1672
N	0.2936	-3.5038	0.6318
C	-0.1308	-2.4410	3.9602
N	-0.2037	-3.4428	4.5474
C	-0.3104	0.0196	5.3373
N	-0.4576	0.0312	6.4915
C	-0.1319	2.4519	3.9109
N	-0.2051	3.4653	4.4778
C	0.2224	2.4281	1.1178
N	0.2922	3.4472	0.5609

SCF = -1217.847167**11-Cl**

C	0.2214	-0.0245	1.1323
C	-0.1333	0.0100	3.9514
C	0.1094	-1.2198	1.8451
C	0.1574	1.1879	1.8217
C	-0.0199	1.2215	3.2332
C	-0.0685	-1.2188	3.2569
I	0.5009	-0.0537	-1.1351
F	0.1647	-2.4238	1.2291
F	-0.1761	-2.3837	3.9374
F	-0.3026	0.0264	5.2944
F	-0.0807	2.4028	3.8908
F	0.2604	2.3764	1.1822
Cl	0.8131	-0.0907	-3.7191

SCF = -1218.448512**12-Cl**

C	0.5696	-0.2839	1.0732
C	-0.0128	0.5827	3.6834
C	0.2532	-1.2080	2.0723
C	0.5930	1.0768	1.3894
C	0.3033	1.5377	2.6970
C	-0.0440	-0.7959	3.3944
I	1.0403	-0.9892	-1.0490
Cl	1.5772	-1.7891	-3.4693
I	-0.5032	-2.1505	4.8377
I	0.3409	3.5198	3.1434
F	-0.2944	1.0012	4.9438
F	0.2286	-2.5280	1.7753
F	0.8988	1.9789	0.4283

SCF = -1218.242721**13-Cl**

C	0.0007	-0.0035	1.2378
I	-0.0031	-0.0168	-1.0970
Cl	-0.0068	-0.0320	-3.6661
Br	-0.9217	-1.5609	1.7530
Br	1.8140	-0.0197	1.7411
Br	-0.8888	1.5791	1.7341

SCF = -1218.150292**14-Cl**

C	-0.0005	-0.0025	1.0933
I	0.0002	-0.0189	-1.3336
Cl	0.0021	-0.0398	-3.8847
F	-0.6296	-1.0716	1.6805
F	1.2430	-0.0069	1.6742
F	-0.6153	1.0823	1.6666

SCF = -1218.421031**15-Cl**

C	-0.0004	-0.0042	1.1378
I	0.0015	-0.0167	-1.1493
Cl	0.0029	-0.0319	-3.9447
C	-0.7166	-1.2423	1.5897
H	-0.1988	-2.1596	1.2177
H	-1.7692	-1.2520	1.2158
H	-0.7492	-1.2966	2.7087
C	1.4321	-0.0013	1.5833
H	1.9656	-0.9104	1.2135
H	1.5004	0.0054	2.7020
H	1.9654	0.9034	1.2026
C	-0.7171	1.2390	1.5751
H	-0.1982	2.1522	1.1946
H	-0.7522	1.3050	2.6933
H	-1.7689	1.2450	1.1988

SCF = -1218.169082**16-Cl**

C	-0.0014	-0.0035	1.4582
I	0.0018	-0.0158	-1.2436
Cl	0.0044	-0.0263	-3.6867
C	-0.7011	-1.2098	1.6720
N	-1.2810	-2.2098	1.8298
C	1.3937	-0.0043	1.6679
N	2.5502	-0.0050	1.8219
C	-0.6977	1.2070	1.6583
N	-1.2749	2.2103	1.8048

SCF = -1218.029124**17-Cl**

I	0.3149	-1.6191	-2.0323
Cl	1.1608	-2.7778	-4.0041
N	-0.5997	-0.3778	0.0987
C	0.0284	-0.3383	1.3300
C	-1.8002	0.3047	0.1692
O	1.1260	-0.8458	1.6370
O	-2.6298	0.4748	-0.7470
C	-2.0410	0.8815	1.5879
H	-2.1412	1.9896	1.5288
H	-2.9829	0.4594	2.0077
C	-0.8110	0.4491	2.3686
H	-0.2203	1.3144	2.7478
H	-1.0622	-0.2156	3.2268

SCF = -1218.259303**18-Cl**

I	-0.0030	0.0016	-0.9637
Cl	-0.0064	0.1145	-3.8096
C	0.0005	-0.0550	1.2253
H	0.0030	0.9437	1.6652
C	-0.0004	-1.1696	1.9321
H	0.0014	-1.1820	3.0325
H	-0.0029	-2.1687	1.4766

SCF = -1218.100583**19-Cl**

I	-0.0032	-0.0376	-0.9913
Cl	-0.0072	-0.0091	-3.7124
C	0.0001	-0.0270	1.2225
H	0.0019	0.9786	1.6466
C	0.0000	-1.1407	1.9465
H	-0.0018	-2.1438	1.4845
C	0.0022	-1.1632	3.3675
N	0.0040	-1.1938	4.5328

SCF = -1218.067304**20-Cl**

I	-0.0615	-0.0162	-0.9834
Cl	0.2669	0.1963	-3.7886
C	-0.3396	-0.1636	1.1826
H	-0.8875	0.6819	1.5962
C	0.1346	-1.1933	1.8817
H	0.6795	-2.0211	1.3862
N	0.1051	-1.3685	3.2929
C	-0.3148	-2.6861	3.7110
H	0.2468	-3.4589	3.1242
H	-1.4163	-2.8669	3.5726
H	-0.0728	-2.8130	4.7995
C	-0.5215	-0.3071	4.0421
H	-0.0325	0.6643	3.7680
H	-0.3705	-0.4940	5.1379
H	-1.6257	-0.2152	3.8473

SCF = -1218.095289**21-Cl**

I	0.0294	-0.0567	-0.9121
Cl	0.3150	-0.1490	-3.6532
C	-0.1910	0.0152	1.2135
H	-0.4214	0.0935	3.4571
C	-0.3135	0.0567	2.4058

SCF = -0.128390**22-Cl**

I	0.0319	-0.0555	-0.9285
Cl	0.3064	-0.1485	-3.5551
C	-0.1937	0.0193	1.2379
C	-0.3180	0.0584	2.4360
C	-0.4580	0.1024	3.7939
N	-0.5769	0.1396	4.9542

SCF = -0.134781**23-Cl**

I	0.0239	-0.0529	-0.8542
Cl	0.2990	-0.1414	-3.5031
C	-0.2002	0.0194	1.3114
N	-0.3196	0.0569	2.4688

SCF = -0.133439

24-Cl

C	-0.9076	0.4378	1.5613
C	0.9844	-0.4495	3.4487
C	-1.0656	-0.8192	2.1708
C	0.2003	1.2576	1.8947
C	1.1491	0.8021	2.8474
C	-0.1125	-1.2454	3.1094
C	-0.2486	-2.5563	3.7655
C	-0.2411	-5.0293	5.1950
C	0.3632	-3.7005	3.2157
C	-0.9277	-2.6762	4.9944
C	-0.9238	-3.9076	5.7063
C	0.3668	-4.9319	3.9274
C	-0.0969	-6.2512	6.0034
C	0.2310	-8.5505	7.5666
C	-1.0462	-7.2812	5.9085
C	1.0037	-6.3495	6.8581
C	1.1760	-7.4938	7.6430
C	-0.8805	-8.4355	6.6938
I	2.4418	-4.6747	6.9337
I	2.4270	-1.2097	4.9363
F	0.3838	-9.6635	8.3190
F	2.2226	-7.6376	8.4855
F	-1.7583	-9.4658	6.6504
F	0.9861	-5.9948	3.3676
F	0.9794	-3.6522	2.0137
F	-1.5781	-1.6231	5.5373
F	-1.5705	-3.9655	6.8917
F	-1.7895	0.9092	0.6482
F	0.3458	2.4654	1.3046
F	2.1920	1.6097	3.1409
Cl	4.0800	-2.4207	6.8331
I	-2.6442	-2.0084	1.7086
I	-2.6301	-7.0957	4.6529

SCF = -1976.468284**25-Cl**

C	0.3080	-1.3432	0.3532
C	-0.3256	1.3995	0.0946
C	1.3524	-0.3922	0.2992
C	-1.0471	-0.9488	0.2754
C	-1.3492	0.4264	0.1511
C	1.0206	0.9761	0.1746
C	2.7604	-0.8236	0.3126
C	5.4422	-1.6467	0.3084
C	3.3947	-1.1124	-0.9002
C	3.4443	-0.9387	1.5341
C	4.7888	-1.3514	1.5313
C	4.7315	-1.5236	-0.9139
C	-2.1216	-1.9557	0.2648
C	-4.1671	-3.8751	0.2154
C	-2.7064	-2.3660	1.4742
C	-2.5429	-2.4882	-0.9582
C	-3.5619	-3.4456	-0.9945
C	-3.7318	-3.3283	1.4487
C	-0.6538	2.8213	-0.1036
C	-1.2790	5.5257	-0.5106
C	-0.7570	3.3202	-1.4063
C	-0.8581	3.6530	1.0097
C	-1.1716	5.0087	0.8050
C	-1.0683	4.6669	-1.6208
I	2.4949	-0.5124	3.2764
I	2.2465	-0.9019	-2.7317
I	-1.5727	-1.7871	-2.7701
I	-2.0724	-1.5738	3.2317
I	-0.4220	1.9507	-3.0580
I	-0.7007	2.8979	2.8869
Cl	0.1452	-0.4114	-4.7789
F	0.6107	-2.6535	0.4793
F	-2.6402	0.8178	0.0829
F	2.0084	1.8961	0.1289
F	-4.0000	-3.9865	-2.1524
F	-5.1530	-4.7996	0.1971
F	-4.3348	-3.7648	2.5791
F	5.5021	-1.4815	2.6741
F	6.7346	-2.0428	0.3120
F	5.3835	-1.8128	-2.0614
F	-1.5806	6.8295	-0.7011
F	-1.3799	5.8609	1.8357
F	-1.1781	5.1913	-2.8610

SCF = -2734.354351

26-Cl

H	-1.4283	0.8830	-2.1248
C	-1.3325	1.6150	-1.2986
C	-1.0844	3.4450	0.8293
C	-1.1355	1.2075	0.0040
C	-1.4070	2.9931	-1.5369
C	-1.2835	3.8926	-0.4787
C	-1.0052	2.0725	1.1004
H	-1.5635	3.3561	-2.5638
H	-1.3436	4.9751	-0.6743
H	-0.9897	4.1729	1.6487
C	-0.7993	1.5045	2.4281
C	-0.4093	0.2346	4.8950
C	-0.7430	0.1081	2.5326
C	-0.6558	2.2672	3.5929
C	-0.4618	1.6256	4.8182
C	-0.5519	-0.5379	3.7353
H	-0.6942	3.3654	3.5537
H	-0.3494	2.2283	5.7322
H	-0.5105	-1.6351	3.7964
H	-0.2558	-0.2588	5.8662
I	-0.9949	-0.8424	0.5819
Cl	-1.3142	-1.5712	-1.8031

SCF = -1678.083063**27-Cl**

H	0.0129	0.1620	0.1335
C	0.0006	0.1327	1.2334
C	-0.0290	0.0750	4.0482
C	-0.0330	-1.0604	1.9232
C	0.0192	1.3296	1.9605
C	0.0033	1.2894	3.3557
C	-0.0469	-1.1212	3.3232
H	0.0506	2.2990	1.4371
H	-0.0354	0.0780	5.1498
C	-0.0798	-2.4437	3.9374
C	-0.1457	-5.0801	4.9509
C	-0.0993	-3.5763	3.1100
C	-0.0933	-2.6696	5.3199
C	-0.1254	-3.9793	5.8083
C	-0.1324	-4.8778	3.5648
H	-0.0836	-1.8230	6.0258
H	-0.1482	-5.7379	2.8650
H	-0.1769	-6.1050	5.3565
I	-0.0736	-3.0638	1.0373
Cl	-0.1305	-5.4778	0.4180
C	0.0036	2.5954	4.1449
C	-0.1210	-4.2061	7.3206
F	0.6441	3.6372	3.5200
F	0.6069	2.5157	5.3765
F	-1.2515	3.0845	4.4159
F	-0.7441	-3.2175	8.0415
F	-0.7393	-5.3643	7.7206
F	1.1376	-4.2838	7.8646

SCF = -1678.573130**28-Cl**

H	-0.1553	0.1734	0.1530
C	-0.1227	0.1455	1.2525
C	-0.0393	0.0850	4.0667
C	-0.1196	-1.0481	1.9420
C	-0.0836	1.3427	1.9762
C	-0.0423	1.3080	3.3767
C	-0.0784	-1.1095	3.3412
H	-0.0854	2.3085	1.4475
H	-0.0065	0.0816	5.1666
C	-0.0796	-2.4334	3.9551
C	-0.0884	-5.0742	4.9639
C	-0.1237	-3.5647	3.1272
C	-0.0389	-2.6598	5.3360
C	-0.0434	-3.9739	5.8309
C	-0.1295	-4.8670	3.5805
H	-0.0032	-1.8115	6.0372
H	-0.1654	-5.7247	2.8783
H	-0.0915	-6.1012	5.3620
I	-0.1797	-3.0494	1.0566
Cl	-0.2428	-5.4660	0.4327
C	-0.0032	2.5246	4.1125
N	0.0286	3.5201	4.7136
C	-0.0013	-4.1875	7.2372
N	0.0332	-4.3627	8.3865

SCF = -1677.976280

29-Cl

H	-0.0205	0.1686	0.1590
C	-0.0509	0.1257	1.2584
C	-0.1346	0.0351	4.0605
C	-0.0414	-1.0787	1.9259
C	-0.1042	1.3139	1.9872
C	-0.1368	1.2934	3.4026
C	-0.0829	-1.1474	3.3233
H	-0.1166	2.2645	1.4338
H	-0.1639	-0.0145	5.1584
C	-0.0688	-2.4810	3.9273
C	-0.0376	-5.1292	4.9011
C	-0.0146	-3.5977	3.0816
C	-0.1075	-2.7181	5.2999
C	-0.0833	-4.0442	5.8167
C	0.0017	-4.9022	3.5288
H	-0.1502	-1.8576	5.9834
H	0.0426	-5.7507	2.8163
H	-0.0283	-6.1713	5.2535
I	0.0341	-3.0596	1.0259
Cl	0.1114	-5.4929	0.3447
N	-0.0987	2.4863	4.1505
N	-0.0507	-4.2689	7.1931
C	-0.3212	3.7221	3.4453
H	0.5011	3.8665	2.6938
H	-0.2871	4.5800	4.1674
H	-1.3091	3.7428	2.9089
C	-0.5862	2.4306	5.5053
H	0.1551	1.8678	6.1345
H	-1.5844	1.9193	5.5821
H	-0.6832	3.4665	5.9243
C	-0.3631	-3.1842	8.0830
H	0.4341	-2.3960	8.0017
H	-0.3876	-3.5497	9.1432
H	-1.3574	-2.7177	7.8418
C	-0.2341	-5.6092	7.6809
H	0.6116	-6.2546	7.3186
H	-1.2046	-6.0542	7.3283
H	-0.2233	-5.6140	8.8025

SCF = -1678.056244**30-Cl**

H	1.3521	-0.7259	1.5710
C	0.5258	-0.1718	2.0422
C	-1.5715	1.2643	3.2156
C	-0.6914	-0.7815	2.3107
C	0.7036	1.1751	2.3694
C	-0.3464	1.8838	2.9575
C	-1.7432	-0.0828	2.8868
H	1.6604	1.6795	2.1593
H	-2.3959	1.8388	3.6674
C	0.0062	-2.7454	4.5838
C	0.2252	-5.5286	4.9145
C	-0.3178	-3.6340	3.5688
C	0.4548	-3.2740	5.7965
C	0.5628	-4.6592	5.9531
C	-0.2256	-5.0097	3.6963
H	0.7170	-2.5993	6.6281
H	-0.5108	-5.6873	2.8532
H	0.3058	-6.6203	5.0489
I	-1.0127	-2.8667	1.6734
Cl	-1.3867	-5.2518	0.8981
C	-0.1493	3.3482	3.3360
C	1.0731	-5.2239	7.2780
F	0.3196	3.5344	4.6148
F	-1.2912	4.1096	3.2830
F	0.7476	4.0261	2.5473
F	0.7345	-4.4746	8.3778
F	0.6186	-6.4857	7.5696
F	2.4410	-5.3285	7.3451
H	-2.7122	-0.5667	3.0831
H	-0.0797	-1.6526	4.4611

SCF = -1678.578675

31-Cl

H	1.6395	0.0747	2.6406
C	0.5512	0.2388	2.6653
C	-2.2133	0.6818	2.7096
C	-0.3347	-0.7497	2.2606
C	0.0547	1.4679	3.1040
C	-1.3303	1.6881	3.1276
C	-1.7069	-0.5439	2.2726
H	0.7462	2.2617	3.4258
H	-3.2996	0.8594	2.7224
C	0.8778	-4.8925	3.4461
C	0.0399	-3.4900	5.7315
C	0.4547	-3.5755	3.3840
C	0.8802	-5.5262	4.6915
C	0.4616	-4.8256	5.8314
C	0.0350	-2.8515	4.4902
H	1.2121	-6.5739	4.7676
H	-0.2967	-1.8023	4.4152
H	-0.2878	-2.9417	6.6286
I	0.4619	-2.6320	1.4416
Cl	1.3835	-4.7841	0.4506
H	-2.4044	-1.3270	1.9375
H	1.2103	-5.4330	2.5244
C	-1.8410	2.9377	3.5747
N	-2.2587	3.9599	3.9409
C	0.4631	-5.4694	7.0996
N	0.4642	-5.9959	8.1368

SCF = -1677.981766**32-Cl**

H	1.8588	0.0760	2.8394
C	0.7724	0.2496	2.8906
C	-1.9759	0.7225	3.0062
C	-0.1245	-0.7114	2.4491
C	0.3061	1.4568	3.4019
C	-1.0856	1.7189	3.4824
C	-1.4906	-0.4787	2.4984
H	1.0412	2.2010	3.7416
H	-3.0641	0.8803	3.0297
C	1.1308	-4.8850	3.4454
C	0.2248	-3.6283	5.7816
C	0.6551	-3.5834	3.4347
C	1.1575	-5.5755	4.6503
C	0.7143	-4.9621	5.8537
C	0.1999	-2.9402	4.5746
H	1.5343	-6.6092	4.6452
H	-0.1799	-1.9044	4.5461
H	-0.1406	-3.1108	6.6809
I	0.6286	-2.5550	1.5446
Cl	1.5286	-4.6962	0.4203
H	-2.2067	-1.2322	2.1344
H	1.4791	-5.3687	2.4985
N	-1.5680	2.8959	4.0787
N	0.8062	-5.6264	7.0755
C	-2.9422	3.2521	3.8349
H	-3.1634	4.2550	4.2860
H	-3.6083	2.4930	4.3270
H	-3.1879	3.2896	2.7385
C	-0.6430	3.9875	4.2443
H	-0.1378	4.2722	3.2812
H	0.1437	3.6891	4.9887
H	-1.1805	4.8863	4.6461
C	1.0920	-7.0357	7.0783
H	2.1161	-7.2070	6.6482
H	0.3444	-7.6157	6.4708
H	1.0821	-7.4274	8.1292
C	0.1246	-5.0782	8.2164
H	0.2349	-5.7641	9.0970
H	-0.9710	-4.9246	8.0158
H	0.5839	-4.0875	8.4823

SCF = -1678.063692

33-Cl

I	-1.4411	1.2051	-3.6249
Cl	-2.1439	1.9666	-5.8562
C	-0.7457	0.4529	-1.4401
C	0.0956	-0.3498	1.0877
N	-0.9454	-0.8189	-1.0309
C	-0.1060	1.3775	-0.5750
C	0.3142	0.9863	0.6804
C	-0.5316	-1.2309	0.2239
H	0.0393	2.4052	-0.9422
H	0.8128	1.6881	1.3666
H	0.4186	-0.6927	2.0807
C	-1.5999	-1.7726	-1.9084
H	-1.0059	-1.8731	-2.8566
H	-2.6291	-1.3994	-2.1603
H	-1.6771	-2.7728	-1.4076
H	-0.7209	-2.2828	0.5046

SCF = -1217.976999**34-Cl**

I	-1.5068	1.2201	-3.5336
Cl	-2.3408	1.8861	-5.7930
C	-0.7400	0.5653	-1.4271
C	0.1138	-0.3570	1.0397
C	-0.9110	-0.7607	-1.0569
C	-0.1288	1.4534	-0.5473
C	0.3035	0.9871	0.7014
N	-0.4879	-1.2245	0.1694
H	-1.3914	-1.5019	-1.7242
H	0.0140	2.5101	-0.8276
H	0.7915	1.6527	1.4289
H	0.4424	-0.7579	2.0160
H	-0.1418	-3.2667	-0.2128
C	-0.6809	-2.6156	0.5271
H	-0.2831	-2.8183	1.5559
H	-1.7780	-2.8562	0.5008

SCF = -1217.955001**35-Cl**

I	-1.4949	1.0711	-3.5350
Cl	-2.3684	1.6862	-5.7956
C	-0.6883	0.4899	-1.4299
N	0.2627	-0.2197	1.1109
C	-0.7156	-0.8409	-0.9994
C	-0.1715	1.4574	-0.5616
C	0.2984	1.0907	0.6972
C	-0.2390	-1.1795	0.2648
H	-1.1135	-1.6345	-1.6521
H	-0.1306	2.5170	-0.8610
H	0.7144	1.8243	1.4126
H	-0.2433	-2.2193	0.6413
H	1.8799	-0.7813	2.3411
C	0.7756	-0.5871	2.4141
H	0.5933	0.2458	3.1441
H	0.2602	-1.5142	2.7809

SCF = -1217.952898**36-Cl**

N	-0.3500	0.5809	-0.1669
C	-0.5850	1.8561	-0.6341
N	-0.3489	2.7180	0.4152
C	0.0381	0.6385	1.1914
H	0.2748	-0.2531	1.7697
C	0.0388	1.9790	1.5565
H	0.2765	2.4540	2.5070
I	-1.3081	2.4733	-2.9223
H	-0.7831	4.4693	-0.6437
C	-0.4697	4.1416	0.3840
H	0.5173	4.6127	0.6397
H	-1.2396	4.4746	1.1311
H	0.5145	-1.1668	-0.9347
C	-0.4720	-0.6302	-0.9158
H	-1.2424	-1.2954	-0.4406
H	-0.7855	-0.3910	-1.9677
Cl	-2.0256	3.0704	-5.1715

SCF = -1217.972152

37-Cl

N	-0.3467	0.5762	-0.1482
C	-0.5724	1.8586	-0.6141
N	-0.3443	2.7128	0.4494
C	0.0305	0.6217	1.2134
C	0.0228	1.9658	1.5921
I	-1.3128	2.5894	-3.3386
H	-0.5765	4.4691	-0.6540
C	-0.4729	4.1385	0.4136
H	0.4371	4.6111	0.8737
H	-1.3810	4.4543	0.9963
H	0.5613	-1.0447	-1.1255
C	-0.4609	-0.6226	-0.9232
H	-1.0629	-1.3831	-0.3555
H	-0.9682	-0.3821	-1.8951
Cl	-1.8973	3.1675	-5.5685
C	0.3464	-0.6359	2.0016
C	0.3366	2.6309	2.9194
F	0.9136	-0.4222	3.2278
F	1.2196	-1.4804	1.3592
F	-0.7590	-1.4126	2.2485
F	1.5097	3.3449	2.9037
F	-0.6125	3.5434	3.3130
F	0.4534	1.7760	3.9807

SCF = -1218.452659**38-Cl**

N	0.0686	-0.9901	-0.8392
C	-0.4738	0.1485	-1.4069
N	-0.4954	1.1222	-0.4249
C	0.3944	-0.7364	0.5166
C	0.0386	0.5962	0.7780
I	-1.3941	0.4123	-4.1377
H	-1.3378	2.5960	-1.6362
C	-0.9785	2.4594	-0.5810
H	-0.1542	3.1924	-0.3690
H	-1.8279	2.6461	0.1300
H	-0.0708	-2.1495	-2.5669
C	0.2768	-2.2399	-1.5028
H	1.3681	-2.5055	-1.4876
H	-0.3058	-3.0501	-0.9870
Cl	-2.1468	0.6140	-6.3854
C	0.9659	-1.6712	1.4016
N	1.4377	-2.4323	2.1438
C	0.1703	1.3080	1.9861
N	0.2854	1.8828	2.9907

SCF = -1217.857773**39-Cl**

N	-0.3488	0.5803	-0.1791
C	-0.5560	1.8574	-0.6456
N	-0.3323	2.7165	0.4048
C	0.0134	0.6254	1.1945
C	0.0237	1.9739	1.5631
I	-1.2099	2.4885	-2.9388
H	-0.7272	4.4694	-0.6671
C	-0.4358	4.1412	0.3667
H	0.5522	4.6006	0.6409
H	-1.2130	4.4849	1.1017
H	0.5115	-1.1695	-0.9449
C	-0.4714	-0.6252	-0.9364
H	-1.2500	-1.2880	-0.4708
H	-0.7715	-0.3782	-1.9902
Cl	-1.8574	3.1098	-5.2065
C	0.3054	-0.5671	2.0033
H	1.1665	-1.1365	1.5688
H	-0.5837	-1.2474	2.0371
H	0.5661	-0.2685	3.0485
C	0.3298	2.5848	2.8648
H	1.2041	3.2794	2.7780
H	0.5768	1.7920	3.6132
H	-0.5476	3.1706	3.2410

SCF = -1217.997955**40-Cl**

N	-0.0471	-1.0559	-0.8412
C	-0.5017	0.1116	-1.4186
N	-0.4157	1.1140	-0.4744
C	0.3568	-0.7843	0.4944
C	0.1095	0.5705	0.7295
I	-1.3384	0.3741	-3.7576
H	-1.5845	2.5482	-1.4524
C	-0.7995	2.4791	-0.6525
H	0.0930	3.0900	-0.9589
H	-1.2047	2.8798	0.3152
H	1.1714	-2.5555	-1.6563
C	0.0850	-2.3238	-1.4877
H	-0.3594	-3.1223	-0.8347
H	-0.4504	-2.2975	-2.4743
Cl	-2.1531	0.6330	-6.0328
O	0.9491	-1.7080	1.3091
O	0.2182	1.2633	1.9027
C	1.3964	2.0803	1.9780
H	2.3123	1.4523	1.8717
H	1.3305	2.5279	3.0010
H	1.3647	2.8712	1.1904
C	0.0173	-2.4025	2.1531
H	-0.5375	-1.6772	2.7945
H	0.6769	-3.0639	2.7685
H	-0.6891	-3.0044	1.5333

SCF = -1218.077421

7.11 ONIOM(DFT:AM1) (Link Atom = Br) SCF = -3332.033865

1-Cl

H	2.7196	0.0342	-1.4662
C	2.1199	0.0468	-0.5443
C	0.6016	0.0958	1.7905
C	1.6810	-1.1459	0.0205
C	1.8017	1.2674	0.0548
C	1.0412	1.2924	1.2240
C	0.9232	-1.1215	1.1864
H	2.1487	2.2091	-0.3926
H	0.5732	-2.0613	1.6380
H	0.0025	0.1137	2.7114
I	2.1821	-3.0742	-0.9345
Cl	2.7983	-5.4630	-2.1234
H	0.7892	2.2511	1.6970

SCF = -3332.023256

2-Cl

H	0.3773	0.1591	0.0650
C	0.2322	0.1394	1.1555
C	-0.1370	0.0968	3.9216
C	0.3475	-1.0590	1.8533
C	-0.0676	1.3233	1.8271
C	-0.2541	1.3053	3.2179
C	0.1633	-1.0769	3.2325
H	-0.1589	2.2698	1.2755
H	0.2538	-2.0217	3.7891
H	-0.2828	0.0822	5.0111
I	0.8216	-2.9407	0.7668
Cl	1.3925	-5.2117	-0.5429
C	-0.5607	2.5060	3.9109
N	-0.8123	3.4910	4.4793

SCF = -3331.982290

3-Cl

H	0.3777	0.1447	0.0540
C	0.2338	0.1253	1.1451
C	-0.1320	0.0760	3.9188
C	0.3495	-1.0737	1.8431
C	-0.0640	1.3117	1.8103
C	-0.2474	1.2831	3.2051
C	0.1667	-1.0926	3.2231
H	-0.1560	2.2610	1.2596
H	0.2576	-2.0383	3.7789
H	-0.2770	0.0628	5.0105
I	0.8268	-2.9649	0.7509
Cl	1.3933	-5.2056	-0.5415
N	-0.5640	2.5319	3.9267
O	-0.6626	3.5665	3.3144
O	-0.7213	2.5069	5.1224

4-Cl

H	0.3948	0.1493	0.0592
C	0.2429	0.1254	1.1485
C	-0.1478	0.0847	3.9042
C	0.3521	-1.0743	1.8430
C	-0.0612	1.3071	1.8254
C	-0.2586	1.2956	3.2109
C	0.1566	-1.0923	3.2197
H	-0.1483	2.2529	1.2722
H	0.2399	-2.0369	3.7775
H	-0.3034	0.0660	4.9922
I	0.8267	-2.9420	0.7638
Cl	1.4143	-5.2582	-0.5769
C	-0.5672	2.5493	3.9360
H	-1.2064	2.3478	4.8307
H	0.3786	3.0344	4.2868
H	-1.1045	3.2734	3.2753

SCF = -3332.035119

5-Cl

H	1.3525	0.0691	0.2468
C	0.7845	0.0768	1.1898
C	-0.6495	0.1280	3.5718
C	0.3787	-1.1184	1.7681
C	0.4809	1.3011	1.7828
C	-0.2433	1.3523	2.9951
C	-0.3336	-1.0835	2.9592
H	0.8214	2.2217	1.2886
H	-0.6616	-2.0209	3.4341
H	-1.2160	0.1074	4.5134
I	0.8423	-3.0441	0.7970
Cl	1.4054	-5.4392	-0.4222
N	-0.4907	2.5939	3.6532
C	-1.5885	2.5878	4.5914
C	-0.4464	3.7623	2.8057
H	-2.5390	2.1698	4.1604
H	-1.7897	3.6314	4.9505
H	-1.2955	1.9658	5.4788
H	-1.0869	3.6690	1.8865
H	-0.7810	4.6646	3.3821
H	0.6162	3.9296	2.4846

SCF = -3332.007136

6-Cl

H	0.3052	0.1423	0.0511
C	0.2177	0.0834	1.1465
C	-0.0052	-0.0580	3.9301
C	0.3626	-1.1397	1.7943
C	-0.0383	1.2463	1.8704
C	-0.1483	1.1654	3.2689
C	0.2511	-1.2072	3.1762
H	-0.1545	2.2177	1.3733
H	0.3645	-2.1711	3.6949
H	-0.0903	-0.1274	5.0218
I	0.7750	-2.9714	0.6303
Cl	1.2958	-5.2424	-0.8033
O	-0.4034	2.3768	3.9047
C	-0.5136	2.3187	5.3170
H	0.4386	1.9566	5.7766
H	-1.3633	1.6607	5.6237
H	-0.7129	3.3792	5.6145

SCF = -3332.084181**7-Cl**

H	1.6230	0.2877	1.2916
C	0.8494	-0.0328	2.0053
C	-1.1055	-0.8180	3.8228
C	0.3121	-1.3115	1.9282
C	0.4153	0.8597	2.9877
C	-0.5647	0.4723	3.9030
C	-0.6660	-1.7010	2.8384
H	0.8503	1.8684	3.0352
H	-1.0992	-2.7111	2.7867
H	-1.8780	-1.1279	4.5421
I	1.0132	-2.7170	0.3696
Cl	1.8850	-4.4398	-1.5500
S	-1.1889	1.4531	5.1505
C	-0.3260	2.9715	5.0377
H	-0.7244	3.6066	5.8623
H	-0.5008	3.4857	4.0662
H	0.7714	2.8450	5.1739

SCF = -3332.026429**8-Cl**

H	0.5610	0.1468	0.0799
C	0.3389	0.1145	1.1570
C	-0.2259	0.0455	3.8900
C	0.3571	-1.0983	1.8398
C	0.0392	1.2980	1.8303
C	-0.2435	1.2596	3.1994
C	0.0758	-1.1302	3.2021
H	0.0219	2.2611	1.3000
H	0.0892	-2.0856	3.7477
H	-0.4490	0.0236	4.9669
I	0.8316	-2.9831	0.7551
Cl	1.4021	-5.2521	-0.5485
C	-0.5691	2.5542	3.9188
F	-0.8342	2.4390	5.2639
F	0.4230	3.5083	3.8711
F	-1.6704	3.2244	3.4343

SCF = -3332.282276**9-Cl**

H	0.3528	0.1524	0.0620
C	0.2190	0.1316	1.1539
C	-0.1241	0.1004	3.9201
C	0.3479	-1.0638	1.8525
C	-0.0814	1.3171	1.8271
C	-0.2531	1.2986	3.2134
C	0.1766	-1.0765	3.2323
H	-0.1815	2.2571	1.2654
H	0.2766	-2.0171	3.7943
H	-0.2580	0.0796	5.0113
I	0.8206	-2.9417	0.7696
Cl	1.3950	-5.2295	-0.5471
Br	-0.6591	2.8909	4.1307

SCF = -3332.021130

10-Cl

C	0.2210	-0.0228	1.1266
C	-0.1301	0.0050	3.9272
C	0.1306	-1.2211	1.8381
C	0.1366	1.1894	1.8148
C	-0.0388	1.2147	3.2134
C	-0.0449	-1.2186	3.2369
I	0.5035	-0.0455	-1.1647
Cl	0.8090	-0.0708	-3.6820
C	0.2138	-2.4732	1.1652
N	0.2803	-3.5030	0.6281
C	-0.1370	-2.4414	3.9588
N	-0.2120	-3.4428	4.5466
C	-0.3075	0.0191	5.3374
N	-0.4527	0.0305	6.4918
C	-0.1248	2.4516	3.9117
N	-0.1948	3.4644	4.4802
C	0.2261	2.4279	1.1180
N	0.2977	3.4470	0.5614

SCF = -3331.777091**11-Cl**

C	0.2213	-0.0247	1.1311
C	-0.1331	0.0100	3.9504
C	0.1101	-1.2198	1.8442
C	0.1567	1.1876	1.8204
C	-0.0205	1.2214	3.2319
C	-0.0677	-1.2189	3.2560
I	0.5016	-0.0538	-1.1381
F	0.1660	-2.4238	1.2282
F	-0.1746	-2.3838	3.9368
F	-0.3023	0.0265	5.2935
F	-0.0820	2.4028	3.8895
F	0.2588	2.3761	1.1807
Cl	0.8117	-0.0897	-3.7044

SCF = -3332.378246**12-Cl**

C	0.5690	-0.2848	1.0721
C	-0.0119	0.5824	3.6826
C	0.2506	-1.2083	2.0710
C	0.5945	1.0758	1.3889
C	0.3057	1.5371	2.6965
C	-0.0457	-0.7961	3.3932
I	1.0413	-0.9895	-1.0529
Cl	1.5750	-1.7838	-3.4568
I	-0.5074	-2.1503	4.8366
I	0.3468	3.5192	3.1434
F	-0.2925	1.0011	4.9432
F	0.2233	-2.5283	1.7739
F	0.9017	1.9780	0.4281

SCF = -3332.172441**13-Cl**

C	0.0004	-0.0033	1.2393
I	-0.0027	-0.0165	-1.1048
Cl	-0.0062	-0.0324	-3.6538
Br	-0.9202	-1.5621	1.7504
Br	1.8139	-0.0174	1.7390
Br	-0.8910	1.5780	1.7328

SCF = -3332.080194**14-Cl**

C	-0.0004	-0.0027	1.0990
I	0.0004	-0.0194	-1.3565
Cl	0.0015	-0.0388	-3.8808
F	-0.6294	-1.0720	1.6852
F	1.2433	-0.0069	1.6786
F	-0.6155	1.0824	1.6708

SCF = -3332.351323**15-Cl**

C	-0.0004	-0.0040	1.1353
I	0.0009	-0.0181	-1.1518
Cl	0.0026	-0.0355	-3.9161
C	-0.7152	-1.2425	1.5884
H	-0.1965	-2.1596	1.2173
H	-1.7678	-1.2537	1.2146
H	-0.7481	-1.2962	2.7075
C	1.4320	0.0004	1.5809
H	1.9664	-0.9083	1.2115
H	1.5007	0.0077	2.6997
H	1.9644	0.9055	1.1998
C	-0.7182	1.2385	1.5725
H	-0.2004	2.1520	1.1915
H	-0.7532	1.3052	2.6908
H	-1.7701	1.2434	1.1967

SCF = -3332.098206**16-Cl**

C	-0.0017	-0.0025	1.5850
I	0.0022	-0.0156	-1.3868
Cl	0.0051	-0.0284	-3.7760
C	-0.6998	-1.2120	1.7169
N	-1.2815	-2.2200	1.8156
C	1.3949	-0.0013	1.7141
N	2.5590	-0.0004	1.8104
C	-0.7008	1.2074	1.7067
N	-1.2834	2.2157	1.7967

SCF = -3331.963324**17-Cl**

I	0.3511	-1.6651	-2.1133
Cl	1.1815	-2.8085	-4.0576
N	-0.6029	-0.3718	0.1095
C	0.0260	-0.3241	1.3389
C	-1.8061	0.3036	0.1833
O	1.1281	-0.8239	1.6470
O	-2.6411	0.4677	-0.7306
C	-2.0489	0.8839	1.6016
H	-2.1561	1.9912	1.5396
H	-2.9873	0.4574	2.0245
C	-0.8147	0.4611	2.3801
H	-0.2281	1.3307	2.7556
H	-1.0594	-0.2029	3.2406

SCF = -3332.193409**18-Cl**

I	-0.0030	0.0003	-0.9654
Cl	-0.0064	0.1127	-3.7880
C	0.0003	-0.0553	1.2194
H	0.0024	0.9433	1.6600
C	-0.0002	-1.1686	1.9286
H	0.0016	-1.1794	3.0289
H	-0.0023	-2.1685	1.4748

SCF = -3332.029901**19-Cl**

I	-0.0031	-0.0385	-0.9920
Cl	-0.0072	-0.0092	-3.6955
C	0.0001	-0.0281	1.2184
H	0.0018	0.9774	1.6433
C	0.0000	-1.1409	1.9440
H	-0.0017	-2.1445	1.4832
C	0.0022	-1.1618	3.3650
N	0.0040	-1.1909	4.5304

SCF = -3331.996838**20-Cl**

I	-0.0617	-0.0175	-0.9826
Cl	0.2659	0.1967	-3.7646
C	-0.3411	-0.1664	1.1792
H	-0.8931	0.6763	1.5935
C	0.1364	-1.1934	1.8800
H	0.6854	-2.0195	1.3861
N	0.1062	-1.3684	3.2915
C	-0.3161	-2.6853	3.7093
H	0.2441	-3.4588	3.1222
H	-1.4180	-2.8641	3.5708
H	-0.0745	-2.8130	4.7977
C	-0.5199	-0.3062	4.0401
H	-0.0320	0.6651	3.7640
H	-0.3670	-0.4917	5.1360
H	-1.6245	-0.2152	3.8471

SCF = -3332.024632**21-Cl**

I	0.0181	-0.0621	-0.9148
Cl	0.3251	-0.1438	-3.6393
C	-0.2038	0.0092	1.2085
H	-0.4076	0.0999	3.4546
C	-0.3131	0.0567	2.4021

SCF = -0.110084**22-Cl**

I	0.0323	-0.0550	-0.9293
Cl	0.3052	-0.1483	-3.5427
C	-0.1931	0.0191	1.2349
C	-0.3178	0.0582	2.4332
C	-0.4577	0.1022	3.7910
N	-0.5771	0.1394	4.9513

SCF = -0.115745**23-Cl**

I	0.0239	-0.0522	-0.8563
Cl	0.2978	-0.1413	-3.4919
C	-0.1999	0.0193	1.3068
N	-0.3187	0.0560	2.4643

SCF = -0.114416

24-Cl

C	-0.9044	0.4391	1.5619
C	0.9866	-0.4509	3.4509
C	-1.0642	-0.8176	2.1716
C	0.2045	1.2571	1.8956
C	1.1523	0.8005	2.8488
C	-0.1120	-1.2450	3.1103
C	-0.2501	-2.5563	3.7654
C	-0.2427	-5.0294	5.1948
C	0.3604	-3.7008	3.2149
C	-0.9295	-2.6764	4.9942
C	-0.9257	-3.9078	5.7060
C	0.3641	-4.9323	3.9266
C	-0.0963	-6.2508	6.0038
C	0.2355	-8.5495	7.5665
C	-1.0448	-7.2815	5.9102
C	1.0061	-6.3470	6.8574
C	1.1795	-7.4919	7.6416
C	-0.8773	-8.4357	6.6953
I	2.4318	-4.6773	6.9329
I	2.4193	-1.2107	4.9317
F	0.3904	-9.6622	8.3188
F	2.2271	-7.6355	8.4831
F	-1.7545	-9.4665	6.6534
F	0.9826	-5.9954	3.3663
F	0.9757	-3.6528	2.0125
F	-1.5797	-1.6233	5.5373
F	-1.5723	-3.9658	6.8914
F	-1.7854	0.9116	0.6484
F	0.3522	2.4646	1.3053
F	2.1960	1.6072	3.1419
Cl	4.0615	-2.4234	6.8288
I	-2.6444	-2.0045	1.7091
I	-2.6305	-7.0974	4.6567

SCF = -6204.324415**25-Cl**

C	0.3076	-1.3428	0.3539
C	-0.3261	1.3999	0.0952
C	1.3519	-0.3919	0.2995
C	-1.0476	-0.9485	0.2761
C	-1.3498	0.4268	0.1523
C	1.0201	0.9765	0.1753
C	2.7599	-0.8235	0.3116
C	5.4410	-1.6473	0.3066
C	3.3927	-1.1120	-0.9029
C	3.4440	-0.9390	1.5327
C	4.7884	-1.3520	1.5298
C	4.7299	-1.5237	-0.9154
C	-2.1218	-1.9558	0.2642
C	-4.1654	-3.8762	0.2138
C	-2.7066	-2.3666	1.4731
C	-2.5413	-2.4877	-0.9605
C	-3.5601	-3.4462	-0.9957
C	-3.7313	-3.3296	1.4475
C	-0.6540	2.8217	-0.1043
C	-1.2779	5.5256	-0.5125
C	-0.7565	3.3188	-1.4085
C	-0.8582	3.6538	1.0085
C	-1.1710	5.0096	0.8034
C	-1.0673	4.6662	-1.6222
I	2.4951	-0.5127	3.2754
I	2.2523	-0.9020	-2.7223
I	-1.5773	-1.7891	-2.7595
I	-2.0738	-1.5740	3.2310
I	-0.4241	1.9565	-3.0483
I	-0.7014	2.8994	2.8860
Cl	0.1444	-0.4090	-4.7705
F	0.6103	-2.6531	0.4802
F	-2.6408	0.8182	0.0847
F	2.0080	1.8965	0.1298
F	-3.9982	-3.9879	-2.1533
F	-5.1506	-4.8016	0.1947
F	-4.3345	-3.7666	2.5775
F	5.5020	-1.4825	2.6724
F	6.7332	-2.0439	0.3094
F	5.3826	-1.8131	-2.0625
F	-1.5788	6.8294	-0.7040
F	-1.3792	5.8623	1.8336
F	-1.1769	5.1911	-2.8623

SCF = -9076.136855

26-Cl

H	-1.4287	0.8761	-2.1238
C	-1.3325	1.6087	-1.2970
C	-1.0842	3.4404	0.8274
C	-1.1351	1.1971	0.0050
C	-1.4073	2.9862	-1.5371
C	-1.2836	3.8874	-0.4809
C	-1.0051	2.0688	1.0987
H	-1.5641	3.3474	-2.5646
H	-1.3436	4.9697	-0.6774
H	-0.9892	4.1689	1.6462
C	-0.7991	1.5035	2.4282
C	-0.4096	0.2346	4.8954
C	-0.7433	0.1065	2.5331
C	-0.6553	2.2667	3.5922
C	-0.4615	1.6255	4.8178
C	-0.5525	-0.5388	3.7362
H	-0.6932	3.3650	3.5523
H	-0.3487	2.2286	5.7316
H	-0.5115	-1.6360	3.7981
H	-0.2564	-0.2584	5.8668
I	-0.9936	-0.8279	0.5881
Cl	-1.3152	-1.5188	-1.8020

SCF = -5905.931215**27-Cl**

H	0.0100	0.1614	0.1318
C	-0.0019	0.1320	1.2317
C	-0.0306	0.0749	4.0470
C	-0.0344	-1.0610	1.9216
C	0.0158	1.3290	1.9588
C	0.0002	1.2892	3.3539
C	-0.0476	-1.1211	3.3223
H	0.0462	2.2983	1.4351
H	-0.0368	0.0783	5.1486
C	-0.0793	-2.4450	3.9349
C	-0.1426	-5.0795	4.9471
C	-0.1004	-3.5758	3.1018
C	-0.0898	-2.6703	5.3168
C	-0.1205	-3.9801	5.8055
C	-0.1323	-4.8762	3.5613
H	-0.0787	-1.8239	6.0228
H	-0.1496	-5.7375	2.8616
H	-0.1726	-6.1049	5.3515
I	-0.0777	-3.0582	1.0536
Cl	-0.1393	-5.4759	0.4704
C	-0.0014	2.5954	4.1430
C	-0.1125	-4.2069	7.3176
F	0.6348	3.6388	3.5165
F	0.6047	2.5174	5.3732
F	-1.2574	3.0809	4.4165
F	-0.7390	-3.2214	8.0397
F	-0.7245	-5.3681	7.7188
F	1.1474	-4.2786	7.8596

SCF = -5906.421284**28-Cl**

H	-0.1513	0.1747	0.1517
C	-0.1199	0.1461	1.2513
C	-0.0399	0.0847	4.0660
C	-0.1178	-1.0478	1.9403
C	-0.0818	1.3430	1.9758
C	-0.0426	1.3078	3.3762
C	-0.0778	-1.1094	3.3402
H	-0.0831	2.3089	1.4473
H	-0.0086	0.0809	5.1660
C	-0.0792	-2.4350	3.9518
C	-0.0867	-5.0742	4.9580
C	-0.1232	-3.5640	3.1175
C	-0.0387	-2.6612	5.3319
C	-0.0428	-3.9756	5.8264
C	-0.1279	-4.8655	3.5750
H	-0.0036	-1.8134	6.0336
H	-0.1636	-5.7240	2.8725
H	-0.0892	-6.1018	5.3544
I	-0.1814	-3.0426	1.0717
Cl	-0.2512	-5.4628	0.4841
C	-0.0058	2.5242	4.1125
N	0.0239	3.5195	4.7140
C	-0.0016	-4.1902	7.2326
N	0.0320	-4.3665	8.3818

SCF = -5905.824445

29-Cl

H	-0.0274	0.1692	0.1562
C	-0.0561	0.1260	1.2557
C	-0.1361	0.0351	4.0584
C	-0.0439	-1.0784	1.9231
C	-0.1093	1.3140	1.9849
C	-0.1387	1.2936	3.4005
C	-0.0846	-1.1470	3.3212
H	-0.1234	2.2646	1.4316
H	-0.1651	-0.0149	5.1564
C	-0.0696	-2.4821	3.9237
C	-0.0374	-5.1280	4.8973
C	-0.0119	-3.5973	3.0729
C	-0.1108	-2.7181	5.2958
C	-0.0858	-4.0440	5.8132
C	0.0047	-4.9006	3.5254
H	-0.1562	-1.8578	5.9792
H	0.0484	-5.7504	2.8130
H	-0.0280	-6.1703	5.2490
I	0.0412	-3.0539	1.0408
Cl	0.1334	-5.4933	0.4071
N	-0.0976	2.4868	4.1467
N	-0.0545	-4.2684	7.1899
C	-0.3363	3.7210	3.4442
H	0.4806	3.8746	2.6886
H	-0.3080	4.5790	4.1665
H	-1.3270	3.7313	2.9128
C	-0.5586	2.4305	5.5104
H	0.1913	1.8616	6.1240
H	-1.5585	1.9254	5.6054
H	-0.6406	3.4660	5.9334
C	-0.3745	-3.1850	8.0786
H	0.4213	-2.3949	8.0020
H	-0.4041	-3.5510	9.1385
H	-1.3685	-2.7206	7.8322
C	-0.2346	-5.6093	7.6772
H	0.6121	-6.2527	7.3135
H	-1.2046	-6.0564	7.3256
H	-0.2224	-5.6146	8.7988

SCF = -5905.904470**30-Cl**

H	1.4508	-0.5511	1.5339
C	0.5776	-0.1069	2.0360
C	-1.6407	1.0520	3.2874
C	-0.5787	-0.8437	2.2557
C	0.6315	1.2265	2.4486
C	-0.4786	1.7969	3.0760
C	-1.6886	-0.2807	2.8698
H	1.5372	1.8294	2.2757
H	-2.5134	1.5170	3.7731
C	0.7276	-2.8583	4.1865
C	-0.3124	-5.2958	5.1088
C	-0.1488	-3.6130	3.4164
C	1.0851	-3.3370	5.4483
C	0.5619	-4.5512	5.9016
C	-0.6756	-4.8238	3.8430
H	1.7744	-2.7575	6.0843
H	-1.3438	-5.4287	3.1990
H	-0.7186	-6.2539	5.4740
I	-0.6964	-2.8939	1.4975
Cl	-0.8244	-5.2863	0.7623
C	-0.4147	3.2459	3.5477
C	0.9707	-5.0761	7.2772
F	0.0625	3.3949	4.8282
F	-1.6247	3.8955	3.5625
F	0.3960	4.0566	2.7913
F	1.2189	-4.0937	8.2040
F	0.0356	-5.8832	7.8760
F	2.1177	-5.8311	7.2649
H	-2.6092	-0.8621	3.0316
H	1.1348	-1.8972	3.8292

SCF = -5906.425938

31-Cl

H	1.6494	-0.2172	2.5565
C	0.5836	0.0483	2.6303
C	-2.1203	0.7512	2.8067
C	-0.4071	-0.8373	2.2304
C	0.2260	1.3015	3.1317
C	-1.1287	1.6523	3.2212
C	-1.7517	-0.4998	2.3091
H	1.0032	2.0121	3.4523
H	-3.1829	1.0313	2.8706
C	1.2499	-4.5721	3.5138
C	-0.4974	-3.7107	5.5382
C	0.2928	-3.5945	3.2817
C	1.3371	-5.1268	4.7937
C	0.4665	-4.6958	5.8039
C	-0.5871	-3.1537	4.2623
H	2.0888	-5.9056	4.9987
H	-1.3409	-2.3749	4.0557
H	-1.1848	-3.3768	6.3310
I	0.1588	-2.7535	1.3400
Cl	0.8391	-4.9986	0.4484
H	-2.5345	-1.1993	1.9773
H	1.9158	-4.9370	2.7075
C	-1.4988	2.9269	3.7319
N	-1.8017	3.9693	4.1503
C	0.5566	-5.2607	7.1062
N	0.6306	-5.7224	8.1713

SCF = -5905.829038**32-Cl**

H	1.7873	-0.1569	2.7812
C	0.7155	0.0867	2.8527
C	-1.9922	0.7380	3.0255
C	-0.2484	-0.8025	2.4011
C	0.3386	1.3082	3.4023
C	-1.0308	1.6602	3.5124
C	-1.5951	-0.4788	2.4803
H	1.1269	1.9920	3.7498
H	-3.0669	0.9671	3.0705
C	1.3057	-4.7200	3.4724
C	-0.1984	-3.7591	5.6316
C	0.4755	-3.6156	3.3385
C	1.3960	-5.3503	4.7070
C	0.6550	-4.8803	5.8246
C	-0.2830	-3.1318	4.3956
H	2.0558	-6.2267	4.7926
H	-0.9463	-2.2576	4.2762
H	-0.8073	-3.3634	6.4577
I	0.3566	-2.6612	1.4504
Cl	1.0994	-4.8659	0.3992
H	-2.3656	-1.1730	2.1093
H	1.8676	-5.1207	2.6016
N	-1.4255	2.8505	4.1463
N	0.8001	-5.4649	7.0820
C	-2.7736	3.3072	3.9256
H	-2.9203	4.3121	4.4016
H	-3.4865	2.5849	4.4073
H	-3.0264	3.3874	2.8331
C	-0.4260	3.8711	4.3307
H	0.0849	4.1509	3.3692
H	0.3480	3.4969	5.0538
H	-0.8958	4.7912	4.7677
C	1.4734	-6.7323	7.1806
H	2.5465	-6.6059	6.8717
H	0.9987	-7.5117	6.5239
H	1.4537	-7.0959	8.2415
C	-0.1412	-5.1270	8.1151
H	0.0716	-5.7255	9.0395
H	-1.2019	-5.3221	7.7969
H	-0.0364	-4.0374	8.3696

SCF = -5905.910764

33-Cl

I	-1.3085	1.2104	-3.7517
Cl	-1.8867	1.9717	-5.9855
C	-0.7062	0.4334	-1.4627
C	0.0255	-0.3281	1.1148
N	-0.9733	-0.8124	-1.0207
C	-0.0491	1.3552	-0.6036
C	0.3162	0.9853	0.6736
C	-0.6149	-1.2053	0.2597
H	0.1526	2.3631	-0.9972
H	0.8261	1.6840	1.3544
H	0.3045	-0.6523	2.1271
C	-1.6426	-1.7819	-1.8668
H	-1.8693	-1.3172	-2.8657
H	-2.6004	-2.1046	-1.3792
H	-0.9766	-2.6731	-2.0123
H	-0.8631	-2.2396	0.5576

SCF = -3331.908192**34-Cl**

I	-1.5098	1.2238	-3.5440
Cl	-2.3386	1.8829	-5.7885
C	-0.7400	0.5654	-1.4264
C	0.1143	-0.3573	1.0398
C	-0.9116	-0.7602	-1.0564
C	-0.1279	1.4532	-0.5471
C	0.3047	0.9867	0.7015
N	-0.4883	-1.2244	0.1698
H	-1.3929	-1.5011	-1.7233
H	0.0153	2.5096	-0.8275
H	0.7935	1.6519	1.4288
H	0.4433	-0.7584	2.0159
H	-0.1440	-3.2669	-0.2127
C	-0.6818	-2.6153	0.5278
H	-0.2829	-2.8184	1.5561
H	-1.7790	-2.8553	0.5028

SCF = -3331.885214**35-Cl**

I	-1.4974	1.0751	-3.5447
Cl	-2.3621	1.6862	-5.7916
C	-0.6901	0.4897	-1.4289
N	0.2625	-0.2200	1.1113
C	-0.7171	-0.8411	-0.9985
C	-0.1735	1.4572	-0.5606
C	0.2974	1.0906	0.6979
C	-0.2396	-1.1799	0.2654
H	-1.1153	-1.6346	-1.6510
H	-0.1332	2.5168	-0.8599
H	0.7136	1.8240	1.4132
H	-0.2432	-2.2197	0.6418
H	1.8816	-0.7810	2.3392
C	0.7773	-0.5875	2.4136
H	0.5955	0.2451	3.1442
H	0.2629	-1.5150	2.7809

SCF = -3331.883083**36-Cl**

N	-0.3364	0.5741	-0.1236
C	-0.5834	1.8512	-0.5919
N	-0.3431	2.7055	0.4680
C	0.0603	0.6262	1.2334
H	0.3056	-0.2656	1.8067
C	0.0561	1.9636	1.6046
H	0.2972	2.4337	2.5560
I	-1.4179	2.5664	-3.2983
H	-0.8029	4.4527	-0.5769
C	-0.4701	4.1262	0.4441
H	0.5174	4.6053	0.6828
H	-1.2274	4.4579	1.2045
H	0.5349	-1.1600	-0.9171
C	-0.4555	-0.6317	-0.8766
H	-1.2103	-1.3119	-0.3977
H	-0.7876	-0.3868	-1.9206
Cl	-2.0868	3.1252	-5.5001

SCF = -3331.904900

37-Cl

N	-0.3461	0.5742	-0.1339
C	-0.5762	1.8570	-0.6005
N	-0.3464	2.7099	0.4652
C	0.0346	0.6193	1.2267
C	0.0252	1.9630	1.6065
I	-1.3471	2.6255	-3.4953
H	-0.5832	4.4658	-0.6361
C	-0.4775	4.1350	0.4310
H	0.4319	4.6097	0.8901
H	-1.3853	4.4494	1.0150
H	0.5620	-1.0438	-1.1161
C	-0.4601	-0.6239	-0.9091
H	-1.0579	-1.3870	-0.3403
H	-0.9718	-0.3835	-1.8785
Cl	-1.9064	3.1858	-5.7127
C	0.3549	-0.6377	2.0133
C	0.3411	2.6270	2.9333
F	0.9276	-0.4244	3.2372
F	1.2260	-1.4820	1.3674
F	-0.7484	-1.4158	2.2655
F	1.5140	3.3415	2.9166
F	-0.6071	3.5394	3.3297
F	0.4600	1.7721	3.9945

SCF = -3332.388138**38-Cl**

N	0.0674	-0.9884	-0.8215
C	-0.4789	0.1507	-1.3879
N	-0.4944	1.1230	-0.4026
C	0.4007	-0.7359	0.5325
C	0.0463	0.5963	0.7968
I	-1.4360	0.4189	-4.3037
H	-1.3493	2.5945	-1.6059
C	-0.9779	2.4599	-0.5549
H	-0.1511	3.1934	-0.3542
H	-1.8188	2.6493	0.1655
H	-0.0870	-2.1473	-2.5471
C	0.2714	-2.2375	-1.4868
H	1.3632	-2.5017	-1.4830
H	-0.3040	-3.0494	-0.9659
Cl	-2.1534	0.5929	-6.5406
C	0.9773	-1.6708	1.4141
N	1.4536	-2.4323	2.1532
C	0.1852	1.3066	2.0050
N	0.3063	1.8807	3.0094

SCF = -3331.793147**39-Cl**

N	-0.3518	0.5772	-0.1433
C	-0.5675	1.8559	-0.6139
N	-0.3349	2.7092	0.4446
C	0.0224	0.6188	1.2280
C	0.0330	1.9650	1.5993
I	-1.3005	2.5818	-3.3270
H	-0.7478	4.4565	-0.6194
C	-0.4419	4.1312	0.4102
H	0.5468	4.5971	0.6706
H	-1.2096	4.4767	1.1544
H	0.5029	-1.1701	-0.9239
C	-0.4790	-0.6244	-0.9015
H	-1.2518	-1.2931	-0.4344
H	-0.7892	-0.3717	-1.9501
Cl	-1.8795	3.1589	-5.5508
C	0.3248	-0.5742	2.0318
H	1.1823	-1.1413	1.5876
H	-0.5623	-1.2565	2.0731
H	0.5956	-0.2780	3.0750
C	0.3500	2.5723	2.8998
H	1.2204	3.2709	2.8065
H	0.6080	1.7788	3.6435
H	-0.5255	3.1536	3.2870

SCF = -3331.930390**40-Cl**

N	-0.0414	-1.0258	-0.7649
C	-0.4951	0.1346	-1.3685
N	-0.3915	1.1501	-0.4334
C	0.3633	-0.7371	0.5671
C	0.1251	0.6217	0.7812
I	-1.5116	0.3725	-4.1378
H	-1.4600	2.5850	-1.5088
C	-0.7625	2.5132	-0.6326
H	0.1515	3.1346	-0.8377
H	-1.2688	2.9056	0.2897
H	0.9770	-2.8303	-1.0472
C	0.0363	-2.3127	-1.3759
H	-0.8478	-2.9370	-1.0720
H	0.0368	-2.1957	-2.4921
Cl	-2.3256	0.5483	-6.3512
O	0.9615	-1.6388	1.4038
O	0.2499	1.3362	1.9410
C	1.4621	2.1006	2.0112
H	2.3498	1.4294	1.9307
H	1.4070	2.5760	3.0219
H	1.4766	2.8727	1.2048
C	0.0285	-2.4888	2.0861
H	-0.6794	-1.8787	2.6957
H	0.6841	-3.1169	2.7391
H	-0.5261	-3.1188	1.3498

SCF = -3332.010813

7.12 ONIOM(DFT:AM1) (Link Atom = I)

SCF = -1055.631130

1-Cl

H	2.7167	0.0356	-1.4669
C	2.1182	0.0491	-0.5442
C	0.6027	0.0990	1.7929
C	1.6802	-1.1419	0.0230
C	1.8000	1.2701	0.0546
C	1.0411	1.2952	1.2247
C	0.9242	-1.1187	1.1894
H	2.1458	2.2118	-0.3937
H	0.5756	-2.0587	1.6418
H	0.0049	0.1178	2.7146
I	2.1858	-3.0931	-0.9420
Cl	2.7980	-5.4757	-2.1296
H	0.7892	2.2541	1.6972

SCF = -1055.620219

2-Cl

H	0.3891	0.1658	0.0679
C	0.2377	0.1447	1.1575
C	-0.1476	0.0968	3.9219
C	0.3443	-1.0542	1.8544
C	-0.0612	1.3283	1.8303
C	-0.2553	1.3073	3.2201
C	0.1520	-1.0766	3.2317
H	-0.1457	2.2766	1.2810
H	0.2356	-2.0234	3.7859
H	-0.2997	0.0807	5.0105
I	0.8301	-2.9615	0.7533
Cl	1.4043	-5.2220	-0.5503
C	-0.5597	2.5078	3.9145
N	-0.8093	3.4925	4.4842

SCF = -1055.579395

3-Cl

H	0.3699	0.1469	0.0545
C	0.2280	0.1282	1.1458
C	-0.1319	0.0783	3.9210
C	0.3452	-1.0691	1.8448
C	-0.0682	1.3147	1.8118
C	-0.2482	1.2857	3.2073
C	0.1653	-1.0902	3.2244
H	-0.1613	2.2643	1.2619
H	0.2575	-2.0364	3.7790
H	-0.2745	0.0653	5.0129
I	0.8346	-2.9901	0.7352
Cl	1.4033	-5.2165	-0.5518
N	-0.5618	2.5344	3.9299
O	-0.6610	3.5695	3.3184
O	-0.7160	2.5096	5.1261

4-Cl

H	0.3702	0.1459	0.0568
C	0.2284	0.1247	1.1474
C	-0.1356	0.0893	3.9074
C	0.3511	-1.0709	1.8454
C	-0.0762	1.3065	1.8241
C	-0.2601	1.2974	3.2116
C	0.1693	-1.0880	3.2233
H	-0.1742	2.2504	1.2695
H	0.2641	-2.0305	3.7824
H	-0.2805	0.0731	4.9969
I	0.8344	-2.9598	0.7553
Cl	1.4235	-5.2697	-0.5810
C	-0.5687	2.5514	3.9363
H	-1.1979	2.3488	4.8378
H	0.3776	3.0430	4.2764
H	-1.1167	3.2706	3.2790

SCF = -1055.632059

5-Cl

H	1.3528	0.0702	0.2478
C	0.7843	0.0784	1.1904
C	-0.6517	0.1294	3.5718
C	0.3774	-1.1153	1.7693
C	0.4806	1.3028	1.7837
C	-0.2442	1.3536	2.9957
C	-0.3358	-1.0822	2.9591
H	0.8216	2.2235	1.2901
H	-0.6643	-2.0199	3.4330
H	-1.2190	0.1090	4.5129
I	0.8487	-3.0622	0.7888
Cl	1.4129	-5.4507	-0.4274
N	-0.4909	2.5952	3.6545
C	-1.5896	2.5892	4.5918
C	-0.4457	3.7638	2.8074
H	-2.5400	2.1723	4.1597
H	-1.7902	3.6327	4.9515
H	-1.2978	1.9663	5.4790
H	-1.0861	3.6714	1.8880
H	-0.7798	4.6662	3.3841
H	0.6171	3.9306	2.4866

SCF = -1055.604060

6-Cl

H	0.2968	0.1417	0.0517
C	0.2125	0.0841	1.1474
C	-0.0017	-0.0555	3.9322
C	0.3621	-1.1366	1.7971
C	-0.0444	1.2471	1.8713
C	-0.1499	1.1668	3.2701
C	0.2554	-1.2051	3.1785
H	-0.1646	2.2179	1.3740
H	0.3731	-2.1683	3.6972
H	-0.0833	-0.1238	5.0243
I	0.7793	-2.9882	0.6183
Cl	1.3001	-5.2534	-0.8115
O	-0.4064	2.3783	3.9054
C	-0.5134	2.3211	5.3179
H	0.4408	1.9619	5.7755
H	-1.3606	1.6610	5.6268
H	-0.7150	3.3813	5.6150

SCF = -1055.681126**7-Cl**

H	1.6188	0.2925	1.2901
C	0.8488	-0.0300	2.0066
C	-1.0977	-0.8219	3.8311
C	0.3069	-1.3058	1.9262
C	0.4228	0.8575	2.9974
C	-0.5532	0.4666	3.9156
C	-0.6659	-1.7002	2.8389
H	0.8607	1.8646	3.0491
H	-1.1013	-2.7090	2.7833
H	-1.8670	-1.1337	4.5529
I	1.0003	-2.7180	0.3323
Cl	1.8491	-4.4209	-1.6027
S	-1.1671	1.4410	5.1735
C	-0.3249	2.9697	5.0445
H	-0.7269	3.6057	5.8666
H	-0.5118	3.4742	4.0702
H	0.7748	2.8586	5.1754

SCF = -1055.623412**8-Cl**

H	0.5551	0.1491	0.0798
C	0.3342	0.1172	1.1570
C	-0.2270	0.0475	3.8914
C	0.3533	-1.0942	1.8410
C	0.0355	1.3007	1.8311
C	-0.2450	1.2617	3.2008
C	0.0737	-1.1283	3.2028
H	0.0176	2.2642	1.3015
H	0.0880	-2.0839	3.7475
H	-0.4486	0.0258	4.9686
I	0.8396	-3.0054	0.7418
Cl	1.4133	-5.2638	-0.5554
C	-0.5677	2.5563	3.9214
F	-0.8306	2.4410	5.2670
F	0.4253	3.5094	3.8725
F	-1.6691	3.2284	3.4393

SCF = -1055.879407**9-Cl**

H	0.3672	0.1570	0.0651
C	0.2262	0.1358	1.1560
C	-0.1342	0.1019	3.9205
C	0.3453	-1.0596	1.8547
C	-0.0731	1.3217	1.8292
C	-0.2533	1.3016	3.2146
C	0.1656	-1.0755	3.2327
H	-0.1656	2.2632	1.2687
H	0.2583	-2.0176	3.7932
H	-0.2749	0.0803	5.0109
I	0.8265	-2.9625	0.7597
Cl	1.4007	-5.2419	-0.5516
Br	-0.6573	2.8945	4.1319

SCF = -1055.618173

10-Cl

C	0.2198	-0.0231	1.1362
C	-0.1310	0.0056	3.9342
C	0.1335	-1.2212	1.8461
C	0.1321	1.1893	1.8212
C	-0.0435	1.2156	3.2199
C	-0.0420	-1.2188	3.2451
I	0.5103	-0.0473	-1.2275
Cl	0.8142	-0.0732	-3.7192
C	0.2211	-2.4718	1.1714
N	0.2915	-3.4993	0.6303
C	-0.1304	-2.4410	3.9685
N	-0.2024	-3.4421	4.5571
C	-0.3086	0.0201	5.3443
N	-0.4541	0.0319	6.4987
C	-0.1334	2.4524	3.9180
N	-0.2066	3.4654	4.4857
C	0.2181	2.4258	1.1207
N	0.2873	3.4422	0.5589

SCF = -1055.375757**11-Cl**

C	0.2201	-0.0242	1.1412
C	-0.1337	0.0097	3.9563
C	0.1090	-1.2197	1.8503
C	0.1563	1.1881	1.8271
C	-0.0209	1.2220	3.2389
C	-0.0688	-1.2196	3.2623
I	0.5072	-0.0538	-1.1842
F	0.1647	-2.4221	1.2307
F	-0.1762	-2.3842	3.9437
F	-0.3029	0.0259	5.2998
F	-0.0823	2.4027	3.8978
F	0.2589	2.3752	1.1846
Cl	0.8148	-0.0899	-3.7282

SCF = -1055.976427**12-Cl**

C	0.5677	-0.2811	1.0817
C	-0.0132	0.5842	3.6883
C	0.2485	-1.2062	2.0766
C	0.5955	1.0783	1.3955
C	0.3062	1.5398	2.7032
C	-0.0484	-0.7944	3.3990
I	1.0501	-1.0039	-1.0962
Cl	1.5765	-1.7927	-3.4786
I	-0.5127	-2.1489	4.8413
I	0.3492	3.5217	3.1508
F	-0.2945	1.0028	4.9491
F	0.2207	-2.5255	1.7760
F	0.9048	1.9783	0.4332

SCF = -1055.770637**13-Cl**

C	-0.0000	-0.0029	1.2729
I	-0.0021	-0.0169	-1.1440
Cl	-0.0043	-0.0334	-3.6681
Br	-0.9225	-1.5621	1.7570
Br	1.8143	-0.0184	1.7462
Br	-0.8910	1.5799	1.7388

SCF = -1055.679465**14-Cl**

C	-0.0004	-0.0026	1.1183
I	0.0008	-0.0202	-1.3992
Cl	0.0015	-0.0391	-3.9038
F	-0.6299	-1.0728	1.7009
F	1.2443	-0.0063	1.6943
F	-0.6164	1.0835	1.6858

SCF = -1055.952098**15-Cl**

C	-0.0003	-0.0039	1.1517
I	-0.0004	-0.0167	-1.1791
Cl	-0.0010	-0.0320	-3.9253
C	-0.7157	-1.2438	1.5917
H	-0.1960	-2.1584	1.2153
H	-1.7672	-1.2521	1.2139
H	-0.7533	-1.3073	2.7105
C	1.4335	-0.0002	1.5842
H	1.9649	-0.9088	1.2095
H	1.5133	0.0063	2.7025
H	1.9633	0.9050	1.1991
C	-0.7182	1.2394	1.5778
H	-0.1990	2.1508	1.1930
H	-0.7578	1.3142	2.6958
H	-1.7690	1.2424	1.1982

SCF = -1055.696419**16-Cl**

C	-0.0015	-0.0028	1.5688
I	0.0014	-0.0153	-1.3674
Cl	0.0038	-0.0270	-3.7491
C	-0.7002	-1.2117	1.7094
N	-1.2821	-2.2189	1.8144
C	1.3952	-0.0025	1.7058
N	2.5586	-0.0023	1.8077
C	-0.6998	1.2076	1.6985
N	-1.2814	2.2158	1.7946

SCF = -1055.565411**17-Cl**

I	0.3472	-1.6605	-2.1025
Cl	1.1740	-2.8002	-4.0394
N	-0.6016	-0.3734	0.1074
C	0.0256	-0.3282	1.3379
C	-1.8034	0.3049	0.1796
O	1.1259	-0.8309	1.6473
O	-2.6364	0.4717	-0.7354
C	-2.0469	0.8847	1.5979
H	-2.1514	1.9922	1.5366
H	-2.9869	0.4600	2.0190
C	-0.8149	0.4583	2.3781
H	-0.2267	1.3262	2.7550
H	-1.0626	-0.2057	3.2377

SCF = -1055.795522**18-Cl**

I	-0.0030	0.0022	-0.9745
Cl	-0.0061	0.1120	-3.7991
C	0.0003	-0.0537	1.2275
H	0.0025	0.9454	1.6656
C	-0.0003	-1.1693	1.9320
H	0.0015	-1.1846	3.0324
H	-0.0024	-2.1674	1.4743

SCF = -1055.626663**19-Cl**

I	-0.0048	-0.0370	-1.0104
Cl	-0.0093	-0.0135	-3.7049
C	-0.0010	-0.0235	1.2274
H	-0.0012	0.9826	1.6490
C	0.0013	-1.1388	1.9483
H	0.0015	-2.1404	1.4832
C	0.0037	-1.1659	3.3694
N	0.0058	-1.1999	4.5347

SCF = -1055.593765**20-Cl**

I	-0.0601	-0.0183	-0.9950
Cl	0.2714	0.1893	-3.7773
C	-0.3446	-0.1634	1.1839
H	-0.8974	0.6799	1.5942
C	0.1351	-1.1905	1.8821
H	0.6847	-2.0149	1.3863
N	0.1068	-1.3681	3.2937
C	-0.3165	-2.6855	3.7089
H	0.2427	-3.4582	3.1198
H	-1.4186	-2.8632	3.5707
H	-0.0743	-2.8158	4.7969
C	-0.5189	-0.3072	4.0444
H	-0.0313	0.6646	3.7693
H	-0.3652	-0.4943	5.1399
H	-1.6237	-0.2159	3.8525

SCF = -1055.621367**21-Cl**

I	0.0278	-0.0563	-0.9142
Cl	0.3160	-0.1495	-3.6495
C	-0.1918	0.0163	1.2128
H	-0.4200	0.0928	3.4567
C	-0.3134	0.0566	2.4052

SCF = -0.084518**22-Cl**

I	0.0343	-0.0529	-0.9455
Cl	0.3023	-0.1457	-3.5525
C	-0.1906	0.0220	1.2414
C	-0.3159	0.0589	2.4399
C	-0.4579	0.0994	3.7975
N	-0.5804	0.1340	4.9576

SCF = -0.089301**23-Cl**

I	0.0232	-0.0564	-0.8672
Cl	0.3000	-0.1398	-3.4982
C	-0.2015	0.0191	1.3154
N	-0.3186	0.0590	2.4729

SCF = -0.088030

24-Cl

C	-0.9116	0.4341	1.5590
C	0.9836	-0.4455	3.4455
C	-1.0673	-0.8215	2.1720
C	0.1959	1.2562	1.8882
C	1.1466	0.8045	2.8409
C	-0.1121	-1.2443	3.1102
C	-0.2451	-2.5543	3.7686
C	-0.2374	-5.0276	5.1981
C	0.3671	-3.6984	3.2190
C	-0.9226	-2.6740	4.9984
C	-0.9187	-3.9054	5.7102
C	0.3708	-4.9299	3.9307
C	-0.0963	-6.2513	6.0043
C	0.2271	-8.5558	7.5616
C	-1.0477	-7.2793	5.9067
C	1.0033	-6.3545	6.8593
C	1.1740	-7.5010	7.6409
C	-0.8844	-8.4359	6.6892
I	2.4449	-4.6761	6.9440
I	2.4313	-1.2011	4.9390
F	0.3776	-9.6712	8.3108
F	2.2206	-7.6487	8.4827
F	-1.7645	-9.4640	6.6434
F	0.9900	-5.9928	3.3706
F	0.9831	-3.6501	2.0169
F	-1.5721	-1.6207	5.5419
F	-1.5644	-3.9631	6.8962
F	-1.7956	0.9021	0.6461
F	0.3391	2.4623	1.2942
F	2.1892	1.6136	3.1308
Cl	4.0840	-2.4130	6.8471
I	-2.6454	-2.0136	1.7154
I	-2.6313	-7.0874	4.6516

SCF = -1651.517021**25-Cl**

C	0.3085	-1.3436	0.3439
C	-0.3253	1.3992	0.0866
C	1.3527	-0.3925	0.2907
C	-1.0466	-0.9491	0.2670
C	-1.3489	0.4261	0.1423
C	1.0210	0.9759	0.1660
C	2.7606	-0.8240	0.3088
C	5.4416	-1.6490	0.3162
C	3.3990	-1.1139	-0.9019
C	3.4395	-0.9384	1.5330
C	4.7838	-1.3520	1.5362
C	4.7358	-1.5263	-0.9090
C	-2.1212	-1.9558	0.2617
C	-4.1672	-3.8747	0.2252
C	-2.7023	-2.3620	1.4742
C	-2.5460	-2.4919	-0.9589
C	-3.5658	-3.4495	-0.9880
C	-3.7280	-3.3242	1.4554
C	-0.6540	2.8215	-0.1068
C	-1.2817	5.5267	-0.5029
C	-0.7580	3.3247	-1.4081
C	-0.8582	3.6487	1.0097
C	-1.1728	5.0050	0.8106
C	-1.0708	4.6723	-1.6165
I	2.4836	-0.5097	3.2713
I	2.2655	-0.9040	-2.7355
I	-1.5880	-1.8020	-2.7705
I	-2.0625	-1.5645	3.2273
I	-0.4218	1.9686	-3.0623
I	-0.6989	2.8868	2.8840
Cl	0.1580	-0.4039	-4.8158
F	0.6111	-2.6540	0.4694
F	-2.6399	0.8172	0.0739
F	2.0087	1.8959	0.1207
F	-4.0083	-3.9945	-2.1422
F	-5.1534	-4.7990	0.2128
F	-4.3275	-3.7567	2.5890
F	5.4924	-1.4814	2.6820
F	6.7336	-2.0462	0.3251
F	5.3928	-1.8172	-2.0531
F	-1.5846	6.8308	-0.6885
F	-1.3810	5.8531	1.8447
F	-1.1821	5.2019	-2.8544

SCF = -2246.926412

26-Cl

H	-1.4332	0.8966	-2.1434
C	-1.3359	1.6219	-1.3117
C	-1.0838	3.4323	0.8321
C	-1.1379	1.2029	-0.0133
C	-1.4095	3.0021	-1.5383
C	-1.2838	3.8913	-0.4722
C	-1.0055	2.0580	1.0940
H	-1.5669	3.3741	-2.5618
H	-1.3427	4.9757	-0.6577
H	-0.9879	4.1558	1.6553
C	-0.7991	1.4908	2.4252
C	-0.4082	0.2413	4.9076
C	-0.7418	0.0952	2.5508
C	-0.6546	2.2623	3.5847
C	-0.4603	1.6312	4.8158
C	-0.5513	-0.5432	3.7552
H	-0.6919	3.3603	3.5388
H	-0.3471	2.2432	5.7237
H	-0.5103	-1.6398	3.8245
H	-0.2545	-0.2423	5.8837
I	-0.9960	-0.8300	0.5647
Cl	-1.3112	-1.5785	-1.8233

SCF = -1353.108273**27-Cl**

H	0.0199	0.1860	0.1241
C	0.0051	0.1493	1.2236
C	-0.0311	0.0651	4.0395
C	-0.0289	-1.0454	1.9063
C	0.0206	1.3398	1.9622
C	0.0009	1.2856	3.3567
C	-0.0458	-1.1267	3.3063
H	0.0520	2.3142	1.4482
H	-0.0401	0.0625	5.1410
C	-0.0786	-2.4523	3.9205
C	-0.1437	-5.0825	4.9600
C	-0.0991	-3.5966	3.1046
C	-0.0909	-2.6680	5.3048
C	-0.1227	-3.9732	5.8058
C	-0.1318	-4.8932	3.5720
H	-0.0807	-1.8169	6.0054
H	-0.1484	-5.7595	2.8801
H	-0.1744	-6.1033	5.3756
I	-0.0742	-3.0855	1.0498
Cl	-0.1385	-5.5011	0.4038
C	-0.0041	2.5842	4.1581
C	-0.1163	-4.1843	7.3205
F	0.6296	3.6352	3.5418
F	0.6017	2.4963	5.3878
F	-1.2614	3.0640	4.4359
F	-0.7404	-3.1893	8.0315
F	-0.7320	-5.3394	7.7332
F	1.1431	-4.2539	7.8639

SCF = -1353.598249**28-Cl**

H	-0.1505	0.2006	0.1458
C	-0.1195	0.1647	1.2450
C	-0.0404	0.0760	4.0605
C	-0.1173	-1.0309	1.9268
C	-0.0817	1.3551	1.9810
C	-0.0429	1.3053	3.3810
C	-0.0781	-1.1137	3.3260
H	-0.0828	2.3262	1.4622
H	-0.0096	0.0663	5.1604
C	-0.0797	-2.4411	3.9392
C	-0.0875	-5.0762	4.9725
C	-0.1244	-3.5836	3.1221
C	-0.0381	-2.6580	5.3218
C	-0.0421	-3.9679	5.8285
C	-0.1297	-4.8814	3.5872
H	-0.0019	-1.8056	6.0180
H	-0.1661	-5.7448	2.8924
H	-0.0901	-6.0995	5.3800
I	-0.1807	-3.0681	1.0694
Cl	-0.2524	-5.4866	0.4198
C	-0.0063	2.5147	4.1289
N	0.0233	3.5043	4.7397
C	0.0008	-4.1678	7.2369
N	0.0360	-4.3320	8.3878

SCF = -1353.001396

29-Cl

H	-0.0370	0.1929	0.1478
C	-0.0632	0.1420	1.2469
C	-0.1357	0.0236	4.0502
C	-0.0498	-1.0638	1.9070
C	-0.1149	1.3236	1.9880
C	-0.1409	1.2880	3.4028
C	-0.0864	-1.1542	3.3044
H	-0.1314	2.2793	1.4438
H	-0.1598	-0.0314	5.1481
C	-0.0692	-2.4916	3.9077
C	-0.0341	-5.1348	4.9055
C	-0.0125	-3.6197	3.0726
C	-0.1085	-2.7196	5.2819
C	-0.0825	-4.0415	5.8105
C	0.0059	-4.9196	3.5312
H	-0.1536	-1.8555	5.9606
H	0.0488	-5.7737	2.8255
H	-0.0232	-6.1736	5.2671
I	0.0329	-3.0780	1.0328
Cl	0.1223	-5.5151	0.3374
N	-0.0985	2.4729	4.1637
N	-0.0517	-4.2537	7.1887
C	-0.2980	3.7187	3.4695
H	0.5266	3.8546	2.7190
H	-0.2471	4.5687	4.2000
H	-1.2856	3.7634	2.9341
C	-0.6050	2.4081	5.5112
H	0.1304	1.8461	6.1481
H	-1.6012	1.8906	5.5711
H	-0.7143	3.4411	5.9343
C	-0.3603	-3.1609	8.0698
H	0.4380	-2.3747	7.9805
H	-0.3837	-3.5173	9.1332
H	-1.3543	-2.6949	7.8264
C	-0.2327	-5.5897	7.6889
H	0.6154	-6.2366	7.3349
H	-1.2013	-6.0402	7.3378
H	-0.2251	-5.5840	8.8105

SCF = -1353.081321**33-Cl**

I	-1.4992	1.2755	-3.8144
Cl	-2.1762	2.0295	-5.9861
C	-0.7415	0.4400	-1.4192
C	0.1032	-0.3616	1.1109
N	-0.9388	-0.8292	-1.0053
C	-0.0992	1.3653	-0.5526
C	0.3218	0.9757	0.7012
C	-0.5245	-1.2436	0.2500
H	0.0448	2.3913	-0.9224
H	0.8214	1.6757	1.3880
H	0.4279	-0.7014	2.1039
C	-1.5946	-1.7777	-1.8852
H	-0.9997	-1.8766	-2.8325
H	-2.6213	-1.3998	-2.1378
H	-1.6766	-2.7797	-1.3888
H	-0.7134	-2.2946	0.5323

SCF = -1055.509418**34-Cl**

I	-1.5359	1.2495	-3.6206
Cl	-2.3613	1.8973	-5.8386
C	-0.7330	0.5630	-1.4159
C	0.1152	-0.3608	1.0494
C	-0.9055	-0.7616	-1.0501
C	-0.1240	1.4511	-0.5363
C	0.3061	0.9840	0.7130
N	-0.4847	-1.2278	0.1776
H	-1.3842	-1.5022	-1.7181
H	0.0189	2.5073	-0.8161
H	0.7928	1.6477	1.4428
H	0.4420	-0.7618	2.0261
H	-0.1374	-3.2697	-0.2034
C	-0.6778	-2.6184	0.5353
H	-0.2821	-2.8218	1.5648
H	-1.7746	-2.8597	0.5070

SCF = -1055.484741

35-Cl

I	-1.5272	1.0965	-3.6224
Cl	-2.3849	1.6991	-5.8438
C	-0.6859	0.4874	-1.4185
N	0.2660	-0.2225	1.1205
C	-0.7142	-0.8430	-0.9890
C	-0.1692	1.4549	-0.5513
C	0.3017	1.0885	0.7072
C	-0.2369	-1.1825	0.2746
H	-1.1129	-1.6354	-1.6419
H	-0.1287	2.5138	-0.8512
H	0.7186	1.8206	1.4233
H	-0.2405	-2.2217	0.6521
H	1.8853	-0.7845	2.3476
C	0.7812	-0.5903	2.4222
H	0.6004	0.2422	3.1530
H	0.2666	-1.5174	2.7898

SCF = -1055.482464**36-Cl**

N	-0.3372	0.5746	-0.1285
C	-0.5819	1.8517	-0.5970
N	-0.3425	2.7065	0.4624
C	0.0571	0.6269	1.2291
H	0.3007	-0.2650	1.8031
C	0.0538	1.9645	1.5999
H	0.2940	2.4347	2.5515
I	-1.4091	2.5597	-3.2644
H	-0.7994	4.4538	-0.5840
C	-0.4692	4.1273	0.4380
H	0.5179	4.6060	0.6790
H	-1.2284	4.4591	1.1965
H	0.5329	-1.1603	-0.9213
C	-0.4572	-0.6314	-0.8813
H	-1.2127	-1.3106	-0.4021
H	-0.7888	-0.3866	-1.9255
Cl	-2.0797	3.1210	-5.4582

SCF = -1055.507188**37-Cl**

N	-0.3479	0.5746	-0.1356
C	-0.5755	1.8576	-0.6023
N	-0.3442	2.7104	0.4632
C	0.0327	0.6191	1.2251
C	0.0258	1.9629	1.6046
I	-1.3448	2.6256	-3.4812
H	-0.5787	4.4664	-0.6384
C	-0.4727	4.1357	0.4287
H	0.4380	4.6088	0.8869
H	-1.3794	4.4519	1.0134
H	0.5576	-1.0458	-1.1162
C	-0.4638	-0.6235	-0.9106
H	-1.0641	-1.3849	-0.3425
H	-0.9736	-0.3819	-1.8808
Cl	-1.9020	3.1846	-5.6892
C	0.3504	-0.6384	2.0119
C	0.3430	2.6266	2.9314
F	0.9224	-0.4260	3.2362
F	1.2206	-1.4840	1.3667
F	-0.7544	-1.4147	2.2632
F	1.5170	3.3394	2.9144
F	-0.6038	3.5404	3.3280
F	0.4609	1.7716	3.9926

SCF = -1055.990229**38-Cl**

N	0.0670	-0.9891	-0.8258
C	-0.4784	0.1509	-1.3909
N	-0.4937	1.1221	-0.4046
C	0.4001	-0.7383	0.5286
C	0.0463	0.5937	0.7944
I	-1.4353	0.4266	-4.2828
H	-1.3459	2.5962	-1.6069
C	-0.9768	2.4594	-0.5553
H	-0.1504	3.1923	-0.3513
H	-1.8193	2.6474	0.1634
H	-0.0852	-2.1454	-2.5534
C	0.2714	-2.2373	-1.4926
H	1.3630	-2.5022	-1.4874
H	-0.3055	-3.0496	-0.9738
Cl	-2.1550	0.6102	-6.5082
C	0.9759	-1.6747	1.4092
N	1.4514	-2.4374	2.1475
C	0.1851	1.3027	2.0034
N	0.3059	1.8756	3.0085

SCF = -1055.395242

39-Cl

N	-0.3514	0.5782	-0.1474
C	-0.5678	1.8568	-0.6168
N	-0.3366	2.7101	0.4417
C	0.0222	0.6194	1.2240
C	0.0315	1.9656	1.5961
I	-1.2934	2.5749	-3.2929
H	-0.7492	4.4579	-0.6220
C	-0.4444	4.1321	0.4079
H	0.5437	4.5983	0.6699
H	-1.2134	4.4765	1.1513
H	0.5060	-1.1675	-0.9286
C	-0.4767	-0.6232	-0.9064
H	-1.2489	-1.2929	-0.4400
H	-0.7866	-0.3703	-1.9551
Cl	-1.8738	3.1504	-5.5102
C	0.3253	-0.5737	2.0274
H	1.1836	-1.1398	1.5833
H	-0.5612	-1.2569	2.0677
H	0.5952	-0.2778	3.0709
C	0.3472	2.5726	2.8971
H	1.2175	3.2714	2.8047
H	0.6049	1.7788	3.6406
H	-0.5288	3.1534	3.2838

SCF = -1055.532696**40-Cl**

N	-0.0336	-1.0254	-0.7708
C	-0.4961	0.1326	-1.3714
N	-0.3993	1.1475	-0.4355
C	0.3698	-0.7360	0.5614
C	0.1219	0.6207	0.7779
I	-1.5139	0.3669	-4.0912
H	-1.4825	2.5759	-1.5054
C	-0.7807	2.5082	-0.6322
H	0.1282	3.1360	-0.8407
H	-1.2857	2.8961	0.2928
H	0.9958	-2.8234	-1.0541
C	0.0528	-2.3109	-1.3841
H	-0.8284	-2.9407	-1.0832
H	0.0552	-2.1921	-2.5002
Cl	-2.3431	0.5456	-6.2918
O	0.9751	-1.6346	1.3962
O	0.2418	1.3342	1.9387
C	1.4467	2.1100	2.0086
H	2.3408	1.4478	1.9247
H	1.3889	2.5822	3.0208
H	1.4520	2.8844	1.2043
C	0.0489	-2.4929	2.0774
H	-0.6627	-1.8893	2.6892
H	0.7098	-3.1178	2.7283
H	-0.5021	-3.1252	1.3403

SCF = -1055.613061