A Novel Salt Cocrystal of Chrysin with Berberine: Preparation, Characterization and Oral Bioavailability

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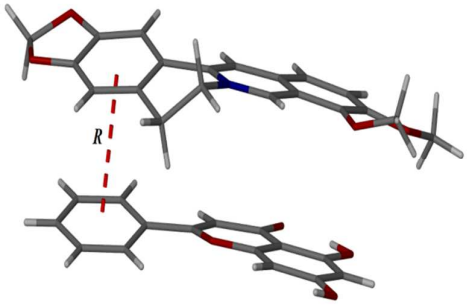
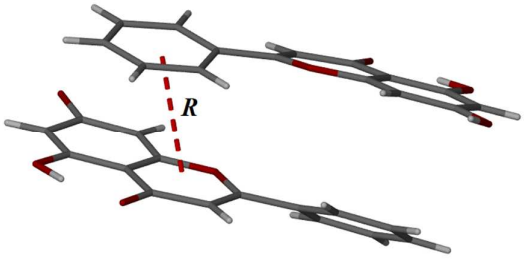
Supporting Information

Figure S1 Scheme of calculated models.

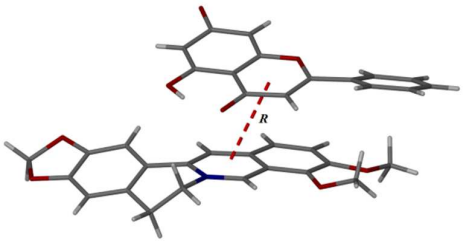
Table S1 Cartesian Coordinates and Energies



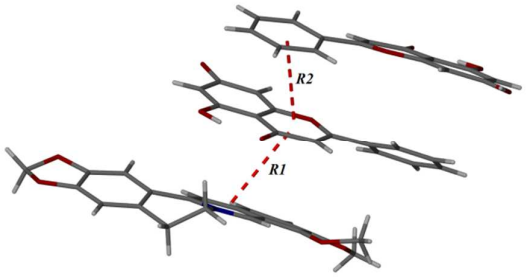
Ber^{+} -ChrH



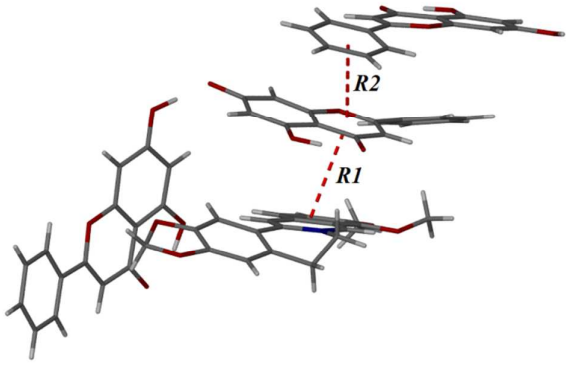
Chr^{-} -ChrH



Ber^{+} -Chr^{-}



[Ber^{+} -Chr^{-}] -ChrH



[Ber^{+} -Chr^{-}]-2ChrH

Figure S1 **Scheme of calculated models.**
R, R_1, R_2 is the central aromatic ring distance between monomers**.**

Table S1 Cartesian Coordinates and Energies

Berb^{+}-ChrH complex

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.530602	1.762031	0.328817
2	8	0	1.196418	1.025286	-3.277159
3	8	0	3.531411	1.423732	-2.187765
4	8	0	3.712545	2.185999	2.426122
5	6	0	-1.301637	1.631944	-0.784817
6	6	0	-0.764862	1.397102	-2.005015
7	1	0	-1.396419	1.328651	-2.880896
8	6	0	0.671409	1.304478	-2.189723
9	6	0	2.881524	1.611733	-1.040292
10	6	0	3.608329	1.842410	0.120696
11	1	0	4.689082	1.908392	0.077976
12	6	0	2.937637	2.002771	1.334450
13	6	0	1.541707	1.961013	1.413885
14	1	0	1.012444	2.124202	2.347369
15	6	0	0.832176	1.768533	0.232904
16	6	0	1.462984	1.572724	-0.996472
17	6	0	-2.736775	1.800638	-0.494249
18	6	0	-3.702172	1.287940	-1.368907
19	1	0	-3.400859	0.718641	-2.242492
20	6	0	-5.053525	1.477316	-1.107559
21	1	0	-5.793634	1.077071	-1.793172
22	6	0	-3.146780	2.496791	0.649149
23	1	0	-2.402605	2.916996	1.317208
24	6	0	-4.500773	2.673571	0.911097
25	1	0	-4.809745	3.224052	1.793568
26	6	0	-5.457140	2.163708	0.035626
27	1	0	-6.513189	2.302920	0.241006
28	1	0	2.849940	1.244005	-2.884175
29	1	0	3.173596	2.420881	3.190679
30	8	0	-6.078566	-1.207878	0.268569
31	8	0	-5.022914	-2.254444	-1.484027
32	8	0	4.147533	-1.078704	1.871313
33	8	0	5.780425	-1.225835	-0.465749
34	7	0	0.160567	-1.293026	1.618000
35	6	0	-6.294777	-2.035964	-0.876984
36	1	0	-6.720576	-2.993047	-0.556064

37	1	0	-6.949285	-1.519184	-1.579805
38	6	0	-4.099061	-1.871874	-0.561811
39	6	0	-2.737571	-2.011851	-0.608325
40	1	0	-2.266151	-2.537763	-1.429158
41	6	0	-4.745030	-1.231233	0.499419
42	6	0	-4.049072	-0.703989	1.560351
43	1	0	-4.557931	-0.200428	2.374122
44	6	0	-2.652448	-0.826922	1.532678
45	6	0	-2.000692	-1.458162	0.465010
46	6	0	-1.811107	-0.259297	2.643740
47	1	0	-2.386937	-0.192872	3.570164
48	1	0	-1.471840	0.751567	2.382955
49	6	0	-0.614690	-1.163930	2.871928
50	1	0	-0.940819	-2.167340	3.163437
51	1	0	0.062124	-0.774191	3.632922
52	6	0	-0.529529	-1.477531	0.424770
53	6	0	0.207290	-1.620152	-0.724055
54	1	0	-0.308413	-1.710598	-1.673052
55	6	0	1.488386	-1.243122	1.666674
56	1	0	1.943661	-1.082027	2.636456
57	6	0	2.278524	-1.391716	0.526698
58	6	0	1.620999	-1.592938	-0.721776
59	6	0	2.402304	-1.688206	-1.883472
60	1	0	1.930174	-1.818561	-2.850488
61	6	0	3.770889	-1.577196	-1.781095
62	1	0	4.365488	-1.636858	-2.684804
63	6	0	4.439048	-1.362200	-0.553185
64	6	0	3.694258	-1.272984	0.622331
65	6	0	5.446877	-0.540047	2.146209
66	1	0	5.609367	0.379468	1.582993
67	1	0	5.431991	-0.316228	3.211637
68	1	0	6.224051	-1.267858	1.917815
69	6	0	6.499440	-0.931445	-1.658740
70	1	0	6.037675	-0.090319	-2.186949
71	1	0	7.505399	-0.664582	-1.339333
72	1	0	6.552640	-1.806785	-2.313705

Zero-point correction=	0.573496 (Hartree/Particle)
Thermal correction to Energy=	0.609007
Thermal correction to Enthalpy=	0.609951
Thermal correction to Gibbs Free Energy=	0.508624
Sum of electronic and zero-point Energies=	-2005.614566
Sum of electronic and thermal Energies=	-2005.579056
Sum of electronic and thermal Enthalpies=	-2005.578112
Sum of electronic and thermal Free Energies=	-2005.679439

BSSE energy = 0.002927124581

Chr^{-} -ChrH complex

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.154036	-1.327162	0.877495
2	8	0	-3.131838	1.960242	2.291168
3	8	0	-5.267315	1.146509	1.049421
4	8	0	-4.956410	-2.875174	-1.428231
5	6	0	-0.523220	-0.406769	1.637341
6	6	0	-1.157398	0.666231	2.153171
7	1	0	-0.636159	1.373795	2.785347
8	6	0	-2.569294	0.920652	1.857908
9	6	0	-4.578087	0.054469	0.645749
10	6	0	-5.163712	-0.888429	-0.153986
11	1	0	-6.200327	-0.770583	-0.451342
12	6	0	-4.435125	-2.040446	-0.667253
13	6	0	-3.042501	-2.139180	-0.248575
14	1	0	-2.449375	-2.978158	-0.595905
15	6	0	-2.494676	-1.187378	0.560941
16	6	0	-3.204702	-0.060975	1.052242
17	6	0	0.911537	-0.727411	1.808285
18	6	0	1.830784	0.254156	2.197558
19	1	0	1.492694	1.273574	2.356535
20	6	0	3.178568	-0.055873	2.335917
21	1	0	3.882841	0.720909	2.618644
22	6	0	1.376979	-2.019370	1.537099
23	1	0	0.673735	-2.771184	1.197054
24	6	0	2.727772	-2.323688	1.666719
25	1	0	3.077107	-3.322492	1.424867
26	6	0	3.632154	-1.346920	2.074258
27	1	0	4.690293	-1.578829	2.146179
28	1	0	-4.635181	1.675474	1.602444
29	8	0	1.325380	1.418014	-1.057897
30	8	0	2.321092	-2.483427	-1.656833
31	8	0	4.744177	-1.910217	-1.064569
32	8	0	5.802683	2.544608	0.013583
33	6	0	0.366612	0.510455	-1.386914
34	6	0	0.655528	-0.797581	-1.598459
35	1	0	-0.142674	-1.506875	-1.777069
36	6	0	2.007516	-1.291204	-1.478010
37	6	0	4.360024	-0.643527	-0.910065

38	6	0	5.285045	0.325996	-0.543321
39	1	0	6.323926	0.063659	-0.389068
40	6	0	4.855506	1.641350	-0.356001
41	6	0	3.525848	2.018531	-0.529540
42	1	0	3.183990	3.036290	-0.375857
43	6	0	2.617556	1.032243	-0.901473
44	6	0	2.999746	-0.291709	-1.108910
45	6	0	-0.972398	1.115029	-1.450382
46	6	0	-2.004691	0.476777	-2.148175
47	1	0	-1.815938	-0.450149	-2.678504
48	6	0	-3.284805	1.011914	-2.140734
49	1	0	-4.089034	0.482072	-2.638781
50	6	0	-1.235128	2.310945	-0.771820
51	1	0	-0.441276	2.791120	-0.210477
52	6	0	-2.519204	2.840350	-0.764146
53	1	0	-2.729331	3.731084	-0.182340
54	6	0	-3.546344	2.188357	-1.441150
55	1	0	-4.561329	2.567041	-1.383509
56	1	0	3.918514	-2.415281	-1.319287
57	1	0	5.388319	3.409419	0.108329

Zero-point correction= 0.427414 (Hartree/Particle)
Thermal correction to Energy= 0.457208
Thermal correction to Enthalpy= 0.458152
Thermal correction to Gibbs Free Energy= 0.367721
Sum of electronic and zero-point Energies= -1755.448787
Sum of electronic and thermal Energies= -1755.418993
Sum of electronic and thermal Enthalpies= -1755.418049
Sum of electronic and thermal Free Energies= -1755.508479
BSSE energy = 0.002756795956

Berb^{+}-Chr^{-} complex

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.157554	0.701092	-1.251615
2	8	0	0.210279	4.063271	0.001387
3	8	0	-2.001268	3.086590	-0.956193
4	8	0	-1.858396	-1.401244	-2.418102
5	8	0	-7.444157	0.119775	0.396449
6	8	0	-6.503166	-1.271436	-1.168919
7	8	0	2.850256	-0.352161	1.581997
8	8	0	4.121320	-2.541993	0.374276

9	7	0	-1.155116	0.081716	1.387810
10	6	0	2.825942	1.698017	-0.631391
11	6	0	2.219615	2.833007	-0.223075
12	1	0	2.773983	3.630849	0.252412
13	6	0	0.784391	3.032004	-0.418191
14	6	0	-1.301974	1.989143	-1.332611
15	6	0	-1.951611	0.900962	-1.855630
16	1	0	-3.027205	0.935452	-1.990231
17	6	0	-1.253446	-0.334403	-2.154046
18	6	0	0.188617	-0.297119	-2.029519
19	1	0	0.759647	-1.187516	-2.268596
20	6	0	0.801342	0.796554	-1.488518
21	6	0	0.107175	1.962155	-1.081898
22	6	0	4.258053	1.366970	-0.461444
23	6	0	5.089177	2.146487	0.351927
24	1	0	4.686941	3.011288	0.868649
25	6	0	6.427486	1.813958	0.519660
26	1	0	7.057451	2.429648	1.153576
27	6	0	4.794689	0.239137	-1.091865
28	1	0	4.151218	-0.377642	-1.709103
29	6	0	6.136790	-0.088408	-0.924815
30	1	0	6.543880	-0.957161	-1.433686
31	6	0	6.959229	0.695486	-0.120001
32	1	0	8.005971	0.439518	0.008690
33	6	0	-7.644289	-0.475234	-0.886141
34	1	0	-7.738320	0.317394	-1.639896
35	1	0	-8.532728	-1.106932	-0.856570
36	6	0	-5.530588	-0.831560	-0.313482
37	6	0	-4.190745	-1.124572	-0.319973
38	1	0	-3.712204	-1.671689	-1.129433
39	6	0	-6.107433	0.012207	0.636242
40	6	0	-5.362109	0.627276	1.616453
41	1	0	-5.813941	1.314995	2.322119
42	6	0	-3.989333	0.345196	1.639963
43	6	0	-3.424908	-0.533980	0.709069
44	6	0	-3.054847	1.023041	2.610675
45	1	0	-3.491049	1.956792	2.974008
46	1	0	-2.853632	0.389725	3.484429
47	6	0	-1.754687	1.342237	1.887870
48	1	0	-1.938596	1.991292	1.025509
49	1	0	-1.018000	1.812086	2.540485
50	6	0	-1.992628	-0.851934	0.801490
51	6	0	-1.445217	-2.025039	0.345150
52	1	0	-2.091474	-2.760720	-0.114863

53	6	0	0.157404	-0.092247	1.473716
54	1	0	0.738562	0.706451	1.919878
55	6	0	0.770407	-1.249440	0.978136
56	6	0	-0.053080	-2.244840	0.385422
57	6	0	0.563611	-3.381180	-0.174238
58	1	0	-0.045727	-4.143902	-0.645288
59	6	0	1.933930	-3.481518	-0.168819
60	1	0	2.398629	-4.343126	-0.633894
61	6	0	2.763792	-2.483674	0.399874
62	6	0	2.186251	-1.377375	1.008721
63	6	0	4.089597	-0.577784	2.256944
64	1	0	4.051028	-1.511859	2.824679
65	1	0	4.202720	0.267585	2.936393
66	1	0	4.920513	-0.605010	1.550859
67	6	0	4.732985	-3.509386	-0.453912
68	1	0	4.560199	-4.526528	-0.083705
69	1	0	5.800690	-3.294676	-0.420720
70	1	0	4.374387	-3.430007	-1.486991
71	1	0	-1.338042	3.725675	-0.588064

Zero-point correction= 0.559674 (Hartree/Particle)
Thermal correction to Energy= 0.594972
Thermal correction to Enthalpy= 0.595916
Thermal correction to Gibbs Free Energy= 0.493894
Sum of electronic and zero-point Energies= -2005.175128
Sum of electronic and thermal Energies= -2005.139830
Sum of electronic and thermal Enthalpies= -2005.138886
Sum of electronic and thermal Free Energies= -2005.240908
BSSE energy = 0.003308579598

[Berb^{+}-Chr^{-}]-ChrH complex

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.279695	-0.132824	-1.112352
2	8	0	1.501961	-1.333990	2.576476
3	8	0	3.784026	-1.919120	1.586677
4	8	0	4.570479	-1.011610	-2.953075
5	6	0	-0.614692	-0.177031	-0.081148
6	6	0	-0.249366	-0.567546	1.167078
7	1	0	-1.002172	-0.663164	1.941092
8	6	0	1.100525	-0.998368	1.445655
9	6	0	3.332346	-1.480384	0.412704

10	6	0	4.172209	-1.479170	-0.695650
11	1	0	5.174898	-1.882895	-0.617722
12	6	0	3.694467	-1.000334	-1.916564
13	6	0	2.388228	-0.528910	-2.062410
14	1	0	1.997273	-0.192747	-3.017971
15	6	0	1.554620	-0.573984	-0.945777
16	6	0	1.997784	-1.016645	0.297312
17	6	0	-1.965382	0.215581	-0.500532
18	6	0	-2.900060	0.651713	0.446717
19	1	0	-2.626921	0.741847	1.492830
20	6	0	-4.202388	0.934584	0.054948
21	1	0	-4.937363	1.199478	0.807810
22	6	0	-2.346000	0.093209	-1.843779
23	1	0	-1.639986	-0.300797	-2.567974
24	6	0	-3.648787	0.384833	-2.229115
25	1	0	-3.954174	0.220736	-3.256688
26	6	0	-4.580480	0.799802	-1.279632
27	1	0	-5.613802	0.963383	-1.565261
28	1	0	3.015687	-1.820378	2.226524
29	1	0	4.115630	-0.776704	-3.769972
30	8	0	-2.128237	-2.922353	0.835869
31	8	0	-4.504624	-2.690871	-2.481107
32	8	0	-6.406711	-1.721328	-0.988063
33	8	0	-5.359317	-0.816983	3.527188
34	8	0	-4.413402	4.198718	-0.196225
35	8	0	-3.403394	4.338993	1.864664
36	8	0	5.586433	1.643693	-1.043959
37	8	0	6.748248	0.439783	1.280327
38	7	0	1.766543	2.855516	-1.032107
39	6	0	-1.664551	-3.275429	-0.382405
40	6	0	-2.433414	-3.246052	-1.489154
41	1	0	-2.050851	-3.572095	-2.448118
42	6	0	-3.819070	-2.770837	-1.430960
43	6	0	-5.582479	-1.834828	0.076325
44	6	0	-5.965122	-1.376362	1.307145
45	1	0	-6.952180	-0.944373	1.434362
46	6	0	-5.059605	-1.353585	2.446973
47	6	0	-3.753599	-1.963582	2.224401
48	1	0	-3.053954	-2.020088	3.051657
49	6	0	-3.414289	-2.431073	0.988120
50	6	0	-4.272768	-2.386354	-0.140739
51	6	0	-0.240864	-3.671544	-0.327481
52	6	0	0.552862	-3.678057	-1.481053
53	1	0	0.125612	-3.364939	-2.429023

54	6	0	1.889339	-4.053359	-1.414694
55	1	0	2.495816	-4.047377	-2.315656
56	6	0	0.340412	-4.022553	0.896694
57	1	0	-0.266108	-3.992469	1.794804
58	6	0	1.680045	-4.390429	0.960452
59	1	0	2.119506	-4.652143	1.917921
60	6	0	2.456664	-4.417319	-0.195046
61	1	0	3.505506	-4.692951	-0.141360
62	6	0	-4.669401	4.318021	1.206358
63	1	0	-5.193135	5.255634	1.397740
64	1	0	-5.246088	3.451692	1.545354
65	6	0	-2.491240	3.947589	0.937116
66	6	0	-1.162390	3.670199	1.109144
67	1	0	-0.702481	3.754871	2.085897
68	6	0	-3.107558	3.874079	-0.316452
69	6	0	-2.409990	3.544561	-1.454095
70	1	0	-2.901429	3.479827	-2.417625
71	6	0	-1.049098	3.248870	-1.302418
72	6	0	-0.435890	3.288359	-0.043875
73	6	0	-0.212794	2.835797	-2.483478
74	1	0	-0.625798	3.243618	-3.409678
75	1	0	-0.198204	1.742492	-2.573639
76	6	0	1.198010	3.364045	-2.300393
77	1	0	1.194775	4.457449	-2.242644
78	1	0	1.867021	3.049756	-3.102525
79	6	0	0.953675	2.837048	0.094174
80	6	0	1.488275	2.345024	1.260393
81	1	0	0.847390	2.248736	2.128925
82	6	0	3.030881	2.442380	-1.001890
83	1	0	3.587437	2.480500	-1.930106
84	6	0	3.626292	1.969918	0.167260
85	6	0	2.824315	1.896616	1.342606
86	6	0	3.379670	1.325095	2.501078
87	1	0	2.780699	1.225523	3.399033
88	6	0	4.670912	0.856788	2.461894
89	1	0	5.088689	0.398832	3.350937
90	6	0	5.481228	0.922343	1.302606
91	6	0	4.967445	1.487621	0.141136
92	6	0	6.740497	0.879987	-1.405473
93	1	0	6.572945	-0.181573	-1.223763
94	1	0	6.863902	1.052235	-2.473838
95	1	0	7.618125	1.220739	-0.856665
96	6	0	7.064514	-0.600960	2.199315
97	1	0	6.267619	-1.352376	2.218590

98	1	0	7.991922	-1.044554	1.838236
99	1	0	7.231633	-0.202145	3.205307
100	1	0	-5.908147	-2.085246	-1.763737

Zero-point correction= 0.780260 (Hartree/Particle)
Thermal correction to Energy= 0.831354
Thermal correction to Enthalpy= 0.832298
Thermal correction to Gibbs Free Energy= 0.696673
Sum of electronic and zero-point Energies= -2883.152080
Sum of electronic and thermal Energies= -2883.100986
Sum of electronic and thermal Enthalpies= -2883.100041
Sum of electronic and thermal Free Energies= -2883.235667
BSSE energy = 0.015063572203

[Berb^{+}-Chr^{-}]-2ChrH complex

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.121054	1.151665	-1.274968
2	8	0	0.333931	-2.675543	0.147119
3	8	0	2.731276	-2.859065	-0.865323
4	8	0	4.615551	1.118229	-2.596241
5	8	0	9.114311	-2.392572	0.323672
6	8	0	8.786162	-0.867555	-1.365495
7	8	0	0.056104	2.553989	1.511843
8	8	0	-0.186318	4.964874	0.080085
9	7	0	3.470146	0.388772	1.299585
10	6	0	-0.913147	0.603479	-0.603488
11	6	0	-0.886254	-0.666870	-0.141153
12	1	0	-1.764503	-1.097344	0.324012
13	6	0	0.294877	-1.500268	-0.309702
14	6	0	2.614022	-1.569144	-1.262414
15	6	0	3.675911	-0.925977	-1.843285
16	1	0	4.611539	-1.456844	-1.984484
17	6	0	3.606577	0.471228	-2.230673
18	6	0	2.310678	1.103149	-2.094677
19	1	0	2.192972	2.138501	-2.395660
20	6	0	1.284435	0.441833	-1.483285
21	6	0	1.381098	-0.888526	-1.003514
22	6	0	-2.040463	1.542261	-0.450394
23	6	0	-3.047696	1.292209	0.488611
24	1	0	-2.991143	0.408128	1.111313

25	6	0	-4.116797	2.166238	0.631882
26	1	0	-4.884587	1.953423	1.369662
27	6	0	-2.109371	2.698211	-1.231948
28	1	0	-1.329694	2.894430	-1.960413
29	6	0	-3.190224	3.566104	-1.100006
30	1	0	-3.260880	4.432902	-1.749748
31	6	0	-4.194849	3.305078	-0.171124
32	1	0	-5.044200	3.974400	-0.084372
33	6	0	9.742106	-1.738784	-0.779493
34	1	0	10.054277	-2.485492	-1.511754
35	1	0	10.598021	-1.156769	-0.413373
36	6	0	7.774514	-0.755776	-0.451420
37	6	0	6.677638	0.067597	-0.488334
38	1	0	6.448158	0.702973	-1.341143
39	6	0	7.971813	-1.691546	0.563778
40	6	0	7.057565	-1.875593	1.576629
41	1	0	7.196408	-2.643628	2.328890
42	6	0	5.929320	-1.044061	1.572223
43	6	0	5.763811	-0.071621	0.579484
44	6	0	4.813627	-1.204465	2.575257
45	1	0	4.820336	-2.212197	2.998034
46	1	0	4.907694	-0.496803	3.409268
47	6	0	3.489207	-0.982863	1.860316
48	1	0	3.376410	-1.686370	1.030182
49	1	0	2.642947	-1.060101	2.537916
50	6	0	4.611192	0.837744	0.656633
51	6	0	4.609948	2.103970	0.131952
52	1	0	5.494105	2.459860	-0.380841
53	6	0	2.365639	1.120309	1.391178
54	1	0	1.507807	0.667413	1.877961
55	6	0	2.297878	2.404292	0.830828
56	6	0	3.450578	2.906517	0.164569
57	6	0	3.370379	4.154989	-0.480369
58	1	0	4.237456	4.547546	-0.999034
59	6	0	2.173684	4.829487	-0.498508
60	1	0	2.106927	5.770667	-1.032187
61	6	0	1.012020	4.328447	0.136193
62	6	0	1.075237	3.134747	0.848474
63	6	0	-0.969200	3.366030	2.099162
64	1	0	-0.522574	4.232909	2.595136
65	1	0	-1.460411	2.732352	2.834818
66	1	0	-1.686169	3.694442	1.347731
67	6	0	-0.376086	5.951878	-0.913750
68	1	0	0.194445	6.861829	-0.695202

69	1	0	-1.440247	6.185192	-0.897989
70	1	0	-0.098091	5.572997	-1.904328
71	1	0	1.863791	-3.101370	-0.452743
72	8	0	-1.922746	-2.189565	2.607790
73	8	0	-4.441858	0.734075	3.912890
74	8	0	-2.422146	1.909376	5.018882
75	8	0	1.846115	-0.086176	4.431856
76	8	0	-3.003839	-1.266470	-2.438133
77	8	0	-4.210883	2.332089	-3.893146
78	8	0	-6.293493	2.199343	-2.326416
79	8	0	-6.770449	-1.626135	0.381451
80	6	0	-3.247030	-2.249626	2.341950
81	6	0	-4.127216	-1.301179	2.743947
82	1	0	-5.164901	-1.342777	2.432166
83	6	0	-3.679707	-0.167161	3.529272
84	6	0	-1.668233	0.914654	4.551890
85	6	0	-0.296088	0.935047	4.771043
86	1	0	0.133098	1.755259	5.337519
87	6	0	0.498158	-0.087349	4.247283
88	6	0	-0.034730	-1.135851	3.499003
89	1	0	0.574000	-1.930403	3.085136
90	6	0	-1.409342	-1.140524	3.305016
91	6	0	-2.249642	-0.140710	3.807364
92	6	0	-3.598246	-3.418161	1.518628
93	6	0	-4.884465	-3.966320	1.604610
94	1	0	-5.572875	-3.606152	2.364960
95	6	0	-5.265321	-4.988001	0.741406
96	1	0	-6.259723	-5.416733	0.815447
97	6	0	-2.672142	-3.934992	0.605298
98	1	0	-1.662751	-3.526296	0.550970
99	6	0	-3.066371	-4.958649	-0.254611
100	1	0	-2.354029	-5.350467	-0.973705
101	6	0	-4.358522	-5.475030	-0.201281
102	1	0	-4.656852	-6.268186	-0.878933
103	6	0	-2.216166	-0.588451	-3.305236
104	6	0	-2.595362	0.602168	-3.830076
105	1	0	-1.970816	1.117001	-4.547386
106	6	0	-3.840416	1.237052	-3.437690
107	6	0	-5.830675	1.016616	-1.917386
108	6	0	-6.535904	0.292280	-0.962496
109	1	0	-7.460972	0.680719	-0.555842
110	6	0	-6.047224	-0.948344	-0.546599
111	6	0	-4.860663	-1.481583	-1.049242
112	1	0	-4.484024	-2.452828	-0.749558

113	6	0	-4.168373	-0.731913	-1.987482
114	6	0	-4.618394	0.505947	-2.449219
115	6	0	-0.953204	-1.305563	-3.557134
116	6	0	0.110035	-0.675832	-4.213567
117	1	0	0.022775	0.357233	-4.533463
118	6	0	1.311694	-1.344910	-4.401541
119	1	0	2.144739	-0.832396	-4.870475
120	6	0	-0.791282	-2.616469	-3.091345
121	1	0	-1.601760	-3.096923	-2.555352
122	6	0	0.413474	-3.281008	-3.280190
123	1	0	0.541417	-4.284896	-2.888728
124	6	0	1.465957	-2.648430	-3.936206
125	1	0	2.421105	-3.151877	-4.043863
126	1	0	2.093864	0.655910	4.996065
127	1	0	-3.355823	1.718742	4.736598
128	1	0	-5.649480	2.536606	-3.000221
129	1	0	-6.386605	-2.508508	0.482757

Zero-point correction= 1.003134 (Hartree/Particle)
Thermal correction to Energy= 1.069996
Thermal correction to Enthalpy= 1.070940
Thermal correction to Gibbs Free Energy= 0.902414
Sum of electronic and zero-point Energies= -3761.191123
Sum of electronic and thermal Energies= -3761.124261
Sum of electronic and thermal Enthalpies= -3761.123317
Sum of electronic and thermal Free Energies= -3761.291843
BSSE energy = 0.008706030316