

Supporting Information:

Using dispersion-corrected DFT to understand supramolecular binding thermodynamics

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Table S1: Contributions to ΔG_a and final ΔG_a values on the PW6B95-D3/def2-QZVP(-g,-f)/COSMO-RS//TPSS-D3/def2-TZVP/HF-3c(freq.) for all 8 complexes including Cl⁻ counter ions for **2a**, **2b**, **3a** and **3b**. All values are given kcal mol⁻¹.

	ΔE	$\Delta E_{disp}^{(2)}$	$\Delta E_{disp}^{(3)}$	ΔG_{RRHO}^T	$\Delta \delta G_{solv}^T$	ΔG_a
1	-32.58	-20.51	1.73	15.42	8.45	-6.98
2	-26.24	-18.01	1.77	15.94	6.56	-1.96
3	-27.75	-17.40	1.64	20.33	-3.20	-8.99
4	-38.99	-22.94	2.35	21.64	12.15	-2.86
5	-38.37	-23.34	3.75	17.58	1.48	-15.57
6	-46.30	-23.90	3.86	18.52	5.52	-18.39
7	-52.94	-43.95	4.50	18.26	11.8	-18.44
8	-45.80	-36.61	3.91	16.02	11.1	-14.80

Coordinates (in Å) and SCF energies (in a.u.) of the optimized complexes, the host and the guest molecules on the TPSS-D3(BJ)/def2-TZVP (including COSMO in case of chloride counterions) level of theory.

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1
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Energy = -2293.019434660
C   -3.6642303   -2.4521942   -3.7502499
C   -3.2048814   -2.9458462   -2.5515376
C   -3.2184958   -2.1403428   -1.3781824
C   -3.7367305   -0.7959762   -1.4636097
C   -4.2119949   -0.3265451   -2.7196384
C   -4.1707919   -1.1295120   -3.8355132
C   -2.7007073   -2.5921677   -0.1560789
C   -2.6396816   -1.7677535    0.9709244
C   -3.1566178   -0.4164600    0.8856001
C   -3.7066696    0.0208951   -0.3226450
C   -3.0334026    0.4589315    2.0158294
C   -2.3972706    0.0108306    3.1341404
C   -1.8730245   -1.3275795    3.2099057
C   -2.0071110   -2.2053058    2.1788869
C   -1.9627382    0.7084218    4.4240144
C   -0.4488475    0.8308025    4.2511352
C    0.0729472   -0.4733931    4.2941694
C   -1.1114762   -1.4122626    4.5272063
C    1.3984608   -0.7503087    3.9578135
C    2.2097517    0.3525103    3.6977003
C    1.6949544    1.6615575    3.6515598
C    0.3441920    1.9175156    3.8871498
C    2.8062512    2.5444748    3.0730918
C    2.9239747    2.0567023    1.6276475
C    3.4656574    0.7255828    1.7051266
C    3.6483741    0.4242151    3.1876240
C    4.0455785    1.8398405    3.6981545
C   -2.0108326   -0.4965381    5.4087888
C    2.5329377    2.5940703    0.4385109
C    2.6392633    1.8023123   -0.7538902
C    3.1916494    0.4651130   -0.6729982
C    3.6196303   -0.0453761    0.5948258
C    2.1655693    2.2647062   -1.9845859
C    2.1732543    1.4578254   -3.1328778
C    2.7187625    0.1241565   -3.0500382
C    3.2286093   -0.3263174   -1.8242186
C    1.6124163    1.8905522   -4.3668063
C    1.5785029    1.0550270   -5.4583235
C    2.1177902   -0.2552368   -5.3772665
C    2.6774927   -0.7066239   -4.2052015
O    1.8849868   -2.0466814    3.8808749
O   -0.2417919    3.1577788    3.7574157
H    2.7213595    3.6246267    3.2120976
H    4.2885184   -0.4193293    3.4391905
H    4.0571468    1.9058893    4.7893309
H    4.9905544    2.1933857    3.2745450
H   -3.0206192   -0.8974770    5.5403134
H   -1.5552600   -0.2645532    6.3753233
H   -2.4982145    1.6184013    4.6895387
H   -0.8679457   -2.4102215    4.8874825
H    4.0106285   -1.0578350    0.6507991
H    2.1085049    3.5931310    0.3664674
H   -3.4149644    1.4743379    1.9391471
H   -1.5993234   -3.2116366    2.2257355
H    1.7424038    3.2652524   -2.0469122
H    3.6318607   -1.3349995   -1.7580980
H    1.1896166    2.8900986   -4.4267888
H    1.1264657    1.3936020   -6.3855120
H    2.0842813   -0.9028322   -6.2487680
H    3.0839710   -1.7126697   -4.1382944
H   -2.3000625   -3.6021312   -0.0930108
H   -4.0879239    1.0377021   -0.3925049
H   -2.8090956   -3.9562284   -2.4853447
H   -4.5912088    0.6898571   -2.7881972

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H	-4.5172635	-0.7472126	-4.7907600
H	-3.6393889	-3.0746101	-4.6402031
H	0.4403310	3.7956982	3.4936781
H	1.7084769	-2.3684570	2.9709703
C	-0.0395379	-1.6488245	-2.3066129
C	0.0948196	-1.0670552	-1.0199381
C	-0.3418297	0.2433535	-0.8043393
C	-0.9061153	0.9729622	-1.8509311
C	-1.0445110	0.3930941	-3.1376947
C	-0.6065226	-0.9180987	-3.3503571
H	-0.2408083	0.6916694	0.1760905
H	-0.7069082	-1.3679119	-4.3286152
C	-1.6211406	1.1344404	-4.2094319
C	-1.3343928	2.3095009	-1.6055645
C	0.6700750	-1.7825286	0.0694730
C	0.4038709	-2.9815185	-2.5387935
N	-1.6717357	3.3992827	-1.3845204
N	-2.0899483	1.7358828	-5.0867513
N	0.7671745	-4.0693264	-2.7274835
N	1.1309503	-2.3181126	0.9908103

2
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Energy = -2432.383782221

C	-0.5387245	-1.0939244	-3.3942733
C	-0.0212031	-1.9551172	-2.4341782
C	0.1561509	-1.5278976	-1.1086726
C	-0.1729336	-0.2236990	-0.7497963
C	-0.6988926	0.6106328	-1.7193776
C	-0.8933254	0.1985158	-3.0391980
F	0.3299407	-3.1875905	-2.8219233
N	0.6650957	-2.4129891	-0.0575683
N	-1.0678272	1.9819548	-1.3370778
H	-1.3068706	0.8890799	-3.7609821
C	-2.8290906	-2.5676035	-0.2224696
C	-3.3322106	-2.1021519	-1.4456941
C	-3.7923636	-0.7374665	-1.5400330
C	-3.7424774	0.0782307	-0.4006555
C	-3.2071077	-0.3731909	0.8084765
C	-2.7234678	-1.7371611	0.8963039
C	-4.2383970	-0.2529211	-2.8026434
C	-4.2354790	-1.0650491	-3.9115480
C	-3.7963153	-2.4123568	-3.8151978
C	-3.3593442	-2.9161972	-2.6139868
C	-3.0648597	0.4997165	1.9371285
C	-2.4333488	0.0423246	3.0531941
C	-1.9171741	-1.2992180	3.1250606
C	-2.0764936	-2.1782627	2.0977591
C	-1.1460346	-1.3861534	4.4390124
C	0.0404091	-0.4477769	4.2075769
C	-0.4803930	0.8561282	4.1632708
C	-1.9927230	0.7362722	4.3418865
C	-2.0408837	-0.4699333	5.3250119
C	1.3652834	-0.7225982	3.8692594
C	2.1726687	0.3762541	3.5833927
C	1.6558560	1.6842013	3.5364535
C	0.3081227	1.9411288	3.7861035
C	2.7648294	2.5701091	2.9606178
C	2.8881077	2.0916526	1.5136276
C	3.4328386	0.7620831	1.5832296
C	3.6095101	0.4506126	3.0659591
C	4.0052657	1.8647024	3.5837915
C	3.6001268	0.0053337	0.4649014
C	3.1815743	0.5279327	-0.8021373
C	2.6181886	1.8614860	-0.8712041
C	2.5004348	2.6386123	0.3283968
C	3.2396539	-0.2441193	-1.9648881
C	2.7292677	0.2153075	-3.1872129
C	2.1611374	1.5402029	-3.2538297
C	2.1449139	2.3337714	-2.0979915
C	2.7163028	-0.5950813	-4.3583815
C	2.1582593	-0.1373803	-5.5270446
C	1.5847726	1.1609770	-5.5886806
C	1.5920392	1.9781037	-4.4839022
O	1.8540307	-2.0231011	3.8166038
O	-0.2781619	3.1813826	3.6691121

H	2.6767356	3.6490352	3.1067455
H	4.2522783	-0.3921588	3.3145159
H	4.0159356	1.9255466	4.6753810
H	4.9500390	2.2213991	3.1619553
H	-3.0512970	-0.8688465	5.4586870
H	-1.5815213	-0.2410026	6.2906372
H	-2.5255146	1.6470240	4.6100962
H	-0.9043172	-2.3851173	4.7981183
H	3.9978793	-1.0053136	0.5125766
H	2.0635117	3.6324331	0.2660512
H	-3.4220854	1.5233619	1.8590618
H	-1.6844962	-3.1917494	2.1429783
H	1.7077731	3.3291101	-2.1483006
H	3.6604607	-1.2468340	-1.9121176
H	1.1509012	2.9707816	-4.5275502
H	1.1427035	1.5072548	-6.5186770
H	2.1503844	-0.7688709	-6.4110487
H	3.1474013	-1.5919908	-4.3056862
H	-2.4618350	-3.5899947	-0.1579421
H	-4.0884608	1.1076124	-0.4728068
H	-3.0120385	-3.9437968	-2.5391212
H	-4.5712237	0.7796151	-2.8746655
H	-4.5741145	-0.6794559	-4.8691236
H	-3.8049372	-3.0431276	-4.6997112
H	0.3676296	3.7923877	3.2804161
H	1.7036535	-2.3456057	2.9064708
H	-0.0322399	0.1154498	0.2679749
H	-0.6541680	-1.4539276	-4.4086042
O	1.0905598	-1.8637403	0.9700142
O	0.6262101	-3.6302864	-0.2353275
O	-1.5383126	2.7090137	-2.2206764
O	-0.8861728	2.3240247	-0.1659033

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Energy = -1691.414670609

C	0.7067218	-1.2764684	3.3439290
C	1.4404377	-0.0921804	3.3506365
C	0.8088319	1.1652771	3.3608330
C	-0.5793037	1.2835123	3.3664607
C	-1.3097239	0.0977604	3.4256856
C	-0.6801397	-1.1555512	3.4140339
O	1.2697088	-2.5359960	3.2851672
O	-1.2542072	2.4876825	3.3297378
C	2.9419915	0.1745197	3.2171108
C	1.9186742	2.2119962	3.2325301
C	3.1200605	0.7455791	1.8119202
C	2.4745776	2.0305518	1.8214493
C	3.0392528	1.4928894	4.0433016
H	1.6773400	3.2367652	3.5242663
H	3.6213696	-0.6345822	3.4952228
H	2.7725449	1.3511110	5.0940953
H	4.0129720	1.9826064	3.9451171
C	-1.7881710	-2.2062114	3.3594567
C	-2.8145891	-0.1629929	3.3791876
C	-2.4149761	-2.0328035	1.9772602
C	-3.0608032	-0.7479540	1.9898533
C	-2.8676642	-1.4772517	4.2171958
H	-3.8450556	-1.9677486	4.1735344
H	-2.5506841	-1.3281575	5.2534968
H	-3.4558163	0.6652515	3.6767149
H	-1.5045577	-3.2196497	3.6390709
C	3.6749437	1.0350372	-0.5193639
C	3.0242575	2.3297208	-0.5099894
C	2.4215439	2.8042785	0.7028232
C	3.7025040	0.2540694	0.6841734
H	4.1942779	-0.7164142	0.6666591
H	1.9371553	3.7786291	0.6995601
C	-3.0850617	-2.3532791	-0.3185799
C	-3.7009426	-0.2654417	0.8897087
C	-2.4176935	-2.8165637	0.8643024
C	-3.7370377	-1.0587919	-0.3054838
H	-4.1879818	0.7071606	0.8905616
H	-1.9278407	-3.7875796	0.8459774
C	4.2595236	0.5795737	-1.7034235

C	3.0006362	3.0839081	-1.6855330
C	4.2336622	1.3359898	-2.8839494
C	3.5854529	2.6252686	-2.8747427
H	2.5108291	4.0559776	-1.6797689
H	4.7475298	-0.3933930	-1.7114299
C	3.5627156	3.3878714	-4.0785117
C	4.8254768	0.8765616	-4.0962930
C	4.7828420	1.6405788	-5.2353260
C	4.1440887	2.9108632	-5.2263140
H	3.0724558	4.3584407	-4.0691995
H	4.1186385	3.5021384	-6.1372969
H	5.2369684	1.2778257	-6.1530811
H	5.3123165	-0.0957942	-4.1006111
C	-3.1226112	-3.1178631	-1.4873588
C	-4.3840768	-0.6153354	-1.4616598
C	-4.4203281	-1.3827255	-2.6348298
C	-3.7704424	-2.6712633	-2.6481333
C	-5.0770272	-0.9360665	-3.8183348
C	-3.8111178	-3.4449919	-3.8444328
C	-5.0944295	-1.7106232	-4.9510646
C	-4.4538461	-2.9800380	-4.9642709
H	-2.6320333	-4.0895828	-1.4980951
H	-4.8736170	0.3569318	-1.4523841
H	-3.3199481	-4.4152357	-3.8518071
H	-5.5658221	0.0353522	-3.8054160
H	-5.5984401	-1.3573040	-5.8463003
H	-4.4765677	-3.5804277	-5.8694609
H	-0.6006837	3.2003884	3.2510347
H	2.2309392	-2.4358058	3.2003775

TCNB (D2h symmetry)

16

Energy = -601.5479652445

C	1.2137350	-0.7087544	0.0000000
C	1.2137350	0.7087544	0.0000000
C	0.0000000	1.4025501	0.0000000
C	-1.2137350	0.7087544	0.0000000
C	-1.2137350	-0.7087544	0.0000000
C	0.0000000	-1.4025501	0.0000000
H	0.0000000	2.4862684	0.0000000
H	0.0000000	-2.4862684	0.0000000
C	-2.4409641	-1.4355860	0.0000000
C	-2.4409641	1.4355860	0.0000000
C	2.4409641	1.4355860	0.0000000
C	2.4409641	-1.4355860	0.0000000
N	-3.4311888	2.0429765	0.0000000
N	-3.4311888	-2.0429765	0.0000000
N	3.4311888	-2.0429765	0.0000000
N	3.4311888	2.0429765	0.0000000

FDNB (Cs symmetry)

16

Energy = -740.9253977026

C	-1.1811175	1.1674476	0.0000000
C	-1.2008820	-0.2371868	0.0000000
C	-0.0013999	-0.9424447	0.0000000
C	1.1904262	-0.2365406	0.0000000
C	1.2287143	1.1569854	0.0000000
C	0.0312628	1.8574467	0.0000000
N	-2.4566295	-1.0280515	0.0000000
H	-0.0136258	-2.0251312	0.0000000
H	0.0082427	2.9417221	0.0000000
F	-2.2990655	1.8946441	0.0000000
O	-2.3352210	-2.2545073	0.0000000
O	-3.5224708	-0.4159992	0.0000000
H	2.1850495	1.6661247	0.0000000
N	2.4643962	-0.9913560	0.0000000
O	2.3955045	-2.2207084	0.0000000
O	3.5068160	-0.3324450	0.0000000

3

128

Energy = -3728.607672560

C	0.6955865	4.2671008	-1.4320680
C	-0.6195209	3.9926303	-1.0438932
C	-1.5055325	5.0561156	-0.8276842

C	-1.0863114	6.3749689	-1.0010853
C	0.2316906	6.6434603	-1.3803024
C	1.1192931	5.5868179	-1.5922263
C	-1.1277678	2.5928510	-0.8513404
N	-0.1236724	1.6864310	-0.1773898
C	-0.8382344	0.4587674	0.3620270
C	0.0908788	-0.6821818	0.6680697
C	0.2921261	-1.6964644	-0.2923302
C	1.1765405	-2.7980121	0.0151588
C	1.8216305	-2.8557049	1.2686531
C	1.6123698	-1.8491578	2.2341184
C	0.7422249	-0.7364861	1.9187959
C	-0.3312899	-1.6711205	-1.5789422
C	-0.1174510	-2.6647755	-2.4991540
C	0.7502478	-3.7458451	-2.1993484
C	1.3769975	-3.8028873	-0.9822476
C	2.2383821	-1.8726088	3.5175557
C	2.0499798	-0.8615930	4.4237607
C	1.2161226	0.2402973	4.1040741
C	0.5779362	0.2951513	2.8923113
C	2.7356771	-4.0191369	1.5394070
N	1.9303863	-5.2758349	1.7910031
C	2.7345817	-6.5539195	1.6759604
C	1.8143394	-7.7387908	1.5677207
C	1.3072909	-8.3609730	2.7153185
C	0.4273170	-9.4367182	2.5972830
C	0.0472451	-9.8973996	1.3339859
C	0.5501662	-9.2808636	0.1862273
C	1.4311678	-8.2053542	0.3038551
D	1.3336322	3.3005717	1.8583906
C	2.6971001	3.5268982	1.4616766
C	3.3904584	2.1895638	1.4284401
D	2.7737043	1.4269282	0.3754634
C	3.4076587	0.2862786	-0.0220707
C	4.3620041	-0.3958428	0.7306486
C	4.9530441	-1.5597001	0.2256672
C	4.5942946	-2.0357351	-1.0316907
C	3.6398610	-1.3522883	-1.7940345
C	3.0417391	-0.1987154	-1.2944592
D	2.0970722	0.5336956	-1.9692502
C	2.1324476	0.4246730	-3.4116162
C	1.4474278	1.6438907	-3.9897177
D	0.0314437	1.6686207	-3.7540754
C	-0.6729016	0.7866021	-4.6359989
C	-2.1593639	0.9893344	-4.4866967
D	-2.6016823	0.4939623	-3.2152664
C	-4.0317068	0.4860948	-3.1586608
C	-4.4850826	0.0069072	-1.7945760
D	-4.2804152	0.9802461	-0.7493417
C	-5.1743726	2.0159323	-0.6577798
C	-6.2546848	2.2323585	-1.5130564
C	-7.1104914	3.3240407	-1.3128766
C	-6.8898976	4.2009598	-0.2577720
C	-5.8139448	3.9889544	0.6142292
C	-4.9590925	2.9052011	0.4229742
D	-3.8925159	2.6047249	1.2267909
C	-3.7269631	3.3800975	2.4306111
C	-2.5180656	2.8108976	3.1392396
D	-1.3114756	3.1134499	2.4197624
C	-0.5509802	4.1621663	3.0382602
C	0.6162644	4.5123171	2.1454599
H	1.6528513	-0.5116443	-3.7187582
H	3.1790425	0.4169986	-3.7349318
H	1.8744021	2.5364230	-3.5231914
H	1.6427953	1.6748974	-5.0720745
H	-0.4171106	-0.2612631	-4.4283289
H	-0.3923906	1.0094256	-5.6765242
H	-2.4149549	2.0553725	-4.5806302
H	-2.6673970	0.4378303	-5.2920578
H	-4.4280307	-0.2007152	-3.9228510
H	-4.4166645	1.4929483	-3.3717594
H	-5.5394312	-0.2886024	-1.8284637
H	-3.8907397	-0.8565675	-1.4865123
H	-6.4458465	1.5569870	-2.3386746
H	-7.9441757	3.4750595	-1.9920862
H	-7.5466940	5.0507367	-0.0979089

H	-5.6511591	4.6687069	1.4430778
H	-4.6234862	3.2826573	3.0560708
H	-3.5709523	4.4370062	2.1819238
H	-2.6048477	1.7202167	3.1968397
H	-2.4657712	3.2086359	4.1591303
H	-0.1943964	3.8175679	4.0192569
H	-1.1717235	5.0577117	3.1820507
H	0.2819393	4.9785564	1.2117333
H	1.2700503	5.2139926	2.6798925
H	3.1899559	4.1718538	2.2016571
H	2.7407771	4.0020744	0.4737150
H	4.4546458	2.3265402	1.2043599
H	3.2738020	1.6686708	2.3857077
H	4.6405753	-0.0287610	1.7120957
H	5.6902604	-2.0861431	0.8247362
H	5.0473393	-2.9389830	-1.4296319
H	3.3547767	-1.7308324	-2.7688797
H	1.5913373	-7.9888646	3.6957921
H	0.0386770	-9.9165322	3.4909510
H	-0.6367371	-10.7366003	1.2445636
H	0.2617419	-9.6390673	-0.7977154
H	1.8316680	-7.7327209	-0.5903259
H	3.3671698	-6.5942991	2.5639201
H	3.3635841	-6.4553089	0.7885530
H	1.5245810	-5.2260177	2.7875865
H	3.3854405	-4.2165149	0.6850757
H	3.3668156	-3.8780474	2.4129079
H	2.0692185	-4.6183028	-0.7988877
H	0.9283363	-4.5188682	-2.9406702
H	-0.6088441	-2.6223147	-3.4667387
H	-0.9816557	-0.8493475	-1.8562125
H	-0.0374406	1.1589486	2.6672063
H	1.0856968	1.0445133	4.8223332
H	2.5393624	-0.9049136	5.3923264
H	2.8621553	-2.7119876	3.7969218
H	-1.5731586	0.1912828	-0.3937742
H	-1.3829408	0.8007089	1.2399849
H	0.3594121	2.1938797	0.5966690
H	0.6165875	1.3928221	-0.8392765
H	-2.0083556	2.5937806	-0.2086487
H	-1.3742026	2.1051021	-1.7973645
H	-2.5242507	4.8477914	-0.5098014
H	-1.7827501	7.1902760	-0.8258625
H	0.5640853	7.6705928	-1.5035130
H	2.1511115	5.7625795	-1.8835786
H	1.4260210	3.4778021	-1.5943747
H	1.1460040	-5.3098535	1.1324984
Cl	1.1421425	-5.1822698	4.6879023
Cl	4.0768320	3.6725439	-2.3933784

4

192

Energy = -5264.994313646

C	4.1255184	-4.7040361	4.0552123
C	2.8875377	-5.3723559	3.9043324
C	2.7264458	-6.6387476	4.4653432
C	3.7684945	-7.2412984	5.1792740
C	4.9769241	-6.5786936	5.3364030
C	5.1553061	-5.3107409	4.7713321
O	1.9357730	-4.6988731	3.1844356
C	0.6846193	-5.3643329	2.9481676
C	-0.2518194	-5.3339339	4.1440073
O	-0.8326222	-4.0360213	4.2403193
C	-1.7088260	-3.9345323	5.3674539
C	-2.3869978	-2.5837847	5.3569489
O	-1.4162991	-1.5820660	5.6232859
C	-1.9792789	-0.2771814	5.8446698
C	-2.5851168	0.3533665	4.6115262
O	-1.5616850	0.4508224	3.5885314
C	-1.8572240	1.3416732	2.5800787
C	-0.8177672	2.1714270	2.1239119
C	-1.0655692	3.0887657	1.1015501
C	-2.3358378	3.1852167	0.5291673
C	-3.3610085	2.3611049	0.9826122
C	-3.1211886	1.4427292	2.0064589

D	0.3968314	2.0075770	2.7196207
C	1.2393652	3.1708937	2.7983727
C	2.2376039	2.9263277	3.9002964
D	3.0279257	1.7693601	3.5406925
C	4.1947473	1.6096431	4.3500322
C	5.1547411	0.7005584	3.6187854
D	4.5678012	-0.5993283	3.4750205
C	5.4083820	-1.5166210	2.7680447
C	5.4979520	-2.8285106	3.5153875
D	4.2199303	-3.4737495	3.4522115
N	1.2338462	-0.6079853	3.5862304
C	1.2012372	-1.4640090	2.3315538
C	0.5684864	-0.7828452	1.1514571
C	-0.7614743	-1.0758981	0.7919172
C	-1.3525361	-0.4281553	-0.3616314
C	-0.6134533	0.5323764	-1.0780232
C	0.7175113	0.8267993	-0.7133883
C	1.3262601	0.1368875	0.3954913
C	-2.6863457	-0.7856802	-0.7299213
C	-3.4071215	-1.6959290	-0.0062255
C	-2.8433727	-2.3005268	1.1464831
C	-1.5650490	-1.9990009	1.5304410
C	2.6859798	0.4276464	0.7083373
C	3.4081776	1.3417842	-0.0146555
C	2.8043827	2.0317840	-1.0931802
C	1.4974731	1.7827721	-1.4262471
C	-1.2549611	1.2928262	-2.2037259
N	-0.9123932	0.7812493	-3.5921585
C	-1.7919800	1.4852122	-4.5974413
C	-1.2975451	1.3768232	-6.0109699
C	-0.7144583	0.2100905	-6.5092717
C	-0.2702544	0.1541055	-7.8304883
C	-0.4143124	1.2612142	-8.6670451
C	-1.0005242	2.4307309	-8.1744343
C	-1.4349211	2.4900989	-6.8508596
C	1.6476401	-1.4640220	4.7619601
C	2.1377329	-0.6630522	5.9355268
C	1.5326181	0.5340914	6.3239897
C	2.0094170	1.2394562	7.4291234
C	3.0921167	0.7501454	8.1601562
C	3.7003515	-0.4489403	7.7782723
C	3.2280226	-1.1486381	6.6688166
D	1.1656032	-1.1024961	-3.1241397
C	0.9328193	-2.1692318	-2.3060039
C	-0.3600754	-2.7227347	-2.3483119
C	-0.6664293	-3.8170504	-1.5449201
C	0.2977404	-4.3586382	-0.6923434
C	1.5718351	-3.8029254	-0.6344884
C	1.8871010	-2.7091297	-1.4442311
D	-1.2686651	-2.1342248	-3.1964706
C	-2.1897079	-3.0531876	-3.8302015
C	-2.7951847	-2.3760818	-5.0394181
D	-3.5215565	-1.1733351	-4.7288392
C	-4.7782061	-1.4134660	-4.1126804
C	-5.4983159	-0.0941494	-3.9427474
D	-4.8228781	0.6765914	-2.9425787
C	-5.5494589	1.8271911	-2.5170858
C	-5.4749909	3.0070737	-3.4722056
D	-4.1521693	3.5524746	-3.3966976
C	-3.9237674	4.7230592	-4.0708314
C	-2.6587807	5.3200051	-3.8550995
C	-2.3660148	6.5404487	-4.4588973
C	-3.3001716	7.1615296	-5.2961101
C	-4.5291792	6.5616677	-5.5305630
C	-4.8425601	5.3451231	-4.9138902
D	-1.8183850	4.6208043	-3.0267807
C	-0.5328343	5.1738311	-2.7137558
C	0.4941254	5.0585891	-3.8277535
D	0.6979113	3.6900555	-4.1727354
C	1.8899220	3.5447316	-4.9581712
C	1.9762170	2.1552600	-5.5477470
D	1.9123570	1.1967482	-4.4888823
C	2.4079298	-0.1046974	-4.8831522
C	2.4981318	-0.9690652	-3.6518135
Cl	0.5369954	-2.8753316	-5.9789929
Cl	-0.7243873	2.9939497	5.7681818

H	-5.7005129	2.7049358	-4.5038903
H	-6.2061567	3.7679525	-3.1634517
H	-5.1152840	2.1148350	-1.5561201
H	-6.6086466	1.5655881	-2.3640009
H	-5.5190589	0.4416394	-4.9026762
H	-6.5350226	-0.2834694	-3.6212285
H	-4.6591062	-1.8947899	-3.1303777
H	-5.3906930	-2.0742928	-4.7490152
H	-1.9880469	-2.1045638	-5.7228279
H	-3.4619305	-3.0931606	-5.5435270
H	-2.9503437	-3.3589315	-3.0995007
H	-1.6188680	-3.9202303	-4.1796364
H	-1.6582970	-4.2518352	-1.5853381
H	0.0450475	-5.2268690	-0.0917545
H	2.3242059	-4.2144612	0.0320394
H	2.8802217	-2.2738148	-1.4116492
H	2.8633187	-1.9589299	-3.9457974
H	3.1499386	-0.5157463	-2.8936757
H	3.4148356	0.0145926	-5.3109911
H	1.7507430	-0.5887113	-5.6172870
H	1.1760982	1.9815390	-6.2751478
H	2.9426887	2.0689030	-6.0676838
H	2.7623507	3.7492815	-4.3180493
H	1.8830650	4.2728584	-5.7841549
H	0.1937585	5.6178670	-4.7245842
H	1.4319041	5.4982230	-3.4487946
H	-0.1993544	4.5971433	-1.8481270
H	-0.6331973	6.2247698	-2.4122379
H	-1.4121481	7.0223306	-4.2794663
H	-3.0512536	8.1110643	-5.7593029
H	-5.2565190	7.0302106	-6.1859298
H	-5.8092918	4.8888022	-5.0928591
H	-3.4292575	-0.2283974	4.2192633
H	-2.8985917	1.3690402	4.8761211
H	-1.1714002	0.3646105	6.1984727
H	-2.7560917	-0.3342343	6.6234456
H	-2.8734517	-2.4203808	4.3840532
H	-3.1659856	-2.5742607	6.1378077
H	-1.1364262	-4.0643933	6.2982967
H	-2.4747238	-4.7254941	5.3123530
H	-1.0446892	-6.0875897	3.9974753
H	0.2841014	-5.5778009	5.0726500
H	0.8665333	-6.3969046	2.6260877
H	0.2330535	-4.8145721	2.1199809
H	1.7895030	-7.1711214	4.3517412
H	3.6186435	-8.2270541	5.6082639
H	5.7900609	-7.0345195	5.8922708
H	6.1057238	-4.8040181	4.8910411
H	6.2576928	-3.4717895	3.0484366
H	5.7750459	-2.6428587	4.5615142
H	5.0089171	-1.6783740	1.7570460
H	6.4241817	-1.1093211	2.6756097
H	5.3814290	1.1192903	2.6271997
H	6.0905438	0.6246714	4.1943563
H	3.9350264	1.2050772	5.3355160
H	4.6836782	2.5859828	4.4889082
H	2.9016637	3.7997005	3.9833623
H	1.7011240	2.7755308	4.8452091
H	0.6246253	4.0362794	3.0690336
H	1.7405300	3.3254906	1.8347299
H	-0.2599974	3.7277795	0.7569382
H	-2.5176368	3.8989625	-0.2689835
H	-4.3567153	2.4346439	0.5560793
H	-3.9212854	0.8023703	2.3597898
H	-0.5403373	-0.6806172	-5.9009179
H	0.1900925	-0.7707072	-8.1682793
H	-0.0680255	1.2192242	-9.6963198
H	-1.1102682	3.3002426	-8.8173061
H	-1.8721810	3.4072316	-6.4614737
H	-1.8267230	2.5274929	-4.2841443
H	-2.7802427	1.0406963	-4.4735333
H	0.0926895	0.9466323	-3.8107015
H	-1.0424372	-0.2495434	-3.6235225
H	-2.3402608	1.2688892	-2.1430119
H	-0.9571892	2.3396349	-2.2009569
H	-3.1455326	-0.3362583	-1.6006531

H	-4.4206912	-1.9455099	-0.3088125
H	-3.4259845	-3.0128106	1.7248910
H	-1.1686562	-2.4741387	2.4185328
H	3.1579656	-0.0620884	1.5513550
H	4.4419193	1.5477851	0.2478484
H	3.3819256	2.7498168	-1.6683221
H	1.0713972	2.3073399	-2.2726639
H	0.6695273	-2.3680988	2.6145567
H	2.2358649	-1.7480179	2.1404589
H	1.8911110	0.1935285	3.4751075
H	0.2963014	-0.1851174	3.7368994
H	2.4351048	-2.1219338	4.3941252
H	0.7653183	-2.0568029	5.0112890
H	3.7097465	-2.0743998	6.3623107
H	4.5468922	-0.8354372	8.3399001
H	3.4645075	1.2976462	9.0219089
H	1.5089611	2.1690070	7.6883733
H	0.6987553	0.9877803	5.7828188

ADMPA (C2 symmetry)

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Energy = -2192.120573862

C	-0.0788926	-6.7673882	-0.9349392
C	0.5139114	-6.0317399	0.0984901
C	0.1701534	-6.3092351	1.4277501
C	-0.7577692	-7.3085919	1.7222883
C	-1.3462353	-8.0390363	0.6874567
C	-1.0050296	-7.7678771	-0.6400771
C	1.4866171	-4.9251044	-0.2039219
N	0.7462731	-3.6178975	-0.3948413
C	1.6423606	-2.3984388	-0.3863277
C	0.8170341	-1.1519581	-0.2066712
C	0.5575075	-0.2844044	-1.2887279
C	-0.2699022	0.8841095	-1.0740007
C	-0.8039027	1.1489159	0.2068338
C	-0.5431108	0.2821926	1.2892400
C	0.2837425	-0.8866794	1.0743788
C	1.0766427	-0.5113753	-2.6006496
C	0.8221679	0.3531683	-3.6332932
C	0.0090160	1.4960257	-3.4260172
C	-0.5235709	1.7458141	-2.1873404
C	-1.0610586	0.5100149	2.6014840
C	-0.8063466	-0.3543337	3.6342533
C	0.0063735	-1.4974919	3.4268945
C	0.5373610	-1.7483953	2.1877479
C	-1.6339619	2.3923728	0.3852896
N	-0.7434208	3.6158936	0.3963932
C	-1.4902209	4.9194661	0.2049168
C	-0.5236254	6.0311629	-0.0985028
C	-0.1867882	6.3138376	-1.4284289
C	0.7352406	7.3182908	-1.7241980
C	1.3244546	8.0488810	-0.6899083
C	0.9900672	7.7726215	0.6383181
C	0.0698599	6.7670521	0.9344019
H	0.6370957	-5.7489569	2.2349777
H	-1.0157998	-7.5199566	2.7559043
H	-2.0665954	-8.8196796	0.9149443
H	-1.4600674	-8.3365982	-1.4459213
H	0.1751983	-6.5420167	-1.9667457
H	2.1904667	-4.7746499	0.6176041
H	2.0407817	-5.0973152	-1.1276616
H	0.0372710	-3.5213334	0.3387066
H	2.1952108	-2.4186313	-1.3218242
H	2.3568018	-2.5289635	0.4284179
H	1.6701366	-1.3945346	-2.7984347
H	1.2313268	0.1549349	-4.6192072
H	-0.2025979	2.1665867	-4.2534313
H	-1.1726381	2.6075839	-2.0697751
H	-1.6536220	1.3937829	2.7994236
H	-1.2143540	-0.1552829	4.6204804
H	0.2183961	-2.1676957	4.2544902
H	1.1866420	-2.6100022	2.0701439
H	-2.3470452	2.5202262	-0.4310498
H	-2.1891529	2.4097272	1.3194873
H	-0.2352099	3.6571712	1.3461762
H	-0.0327387	3.5232926	-0.3360221

H	-2.0450323	5.0892407	1.1287338
H	-2.1935329	4.7650089	-0.6163026
H	-0.1787739	6.5377100	1.9666806
H	1.4456229	8.3414644	1.4437814
H	2.0401947	8.8334949	-0.9183220
H	0.9879524	7.5335990	-2.7583169
H	-0.6544230	5.7534452	-2.2351693
H	0.2362332	-3.6570989	-1.3438693
Cl	0.3719187	3.7936449	3.1792283
Cl	-0.3746132	-3.7880705	-3.1754194

DB24c8

64

Energy = -1536.448460434

O	2.7853559	-0.8381745	-1.7023883
C	2.3723689	-1.1667348	-3.0424587
H	1.2961332	-1.3625772	-3.0440520
H	2.9120924	-2.0544112	-3.4013161
C	2.7198477	0.0121206	-3.9327302
H	3.7998516	0.1867245	-3.9140142
H	2.4226702	-0.2388332	-4.9622543
O	2.1393877	1.2565985	-3.5330632
C	0.7291977	1.4125434	-3.7614577
H	0.3828323	0.7206805	-4.5411631
H	0.5983676	2.4376077	-4.1259308
C	-0.1100297	1.2492459	-2.5029224
H	0.4595757	1.6213994	-1.6402644
H	-1.0317555	1.8451122	-2.5969332
O	-0.4607724	-0.1249862	-2.3081052
C	-1.0853427	-0.3431278	-1.0372776
H	-1.8870701	0.3956029	-0.8873043
H	-0.3588762	-0.2400506	-0.2222752
C	-1.6746297	-1.7474952	-1.0745334
H	-2.3341071	-1.8522580	-1.9458278
H	-0.8849485	-2.4988065	-1.1212770
O	-2.4094136	-2.0459641	0.1364399
C	-3.5536338	-1.2833215	0.3122105
C	-4.7235755	-1.5713398	-0.3828435
H	-4.7190290	-2.3919734	-1.0952807
C	-5.8806467	-0.8158436	-0.1645542
H	-6.7907322	-1.0474931	-0.7096443
C	-5.8533956	0.2291245	0.7574532
H	-6.7450029	0.8231813	0.9370887
C	-4.6839403	0.5260213	1.4653552
H	-4.6794009	1.3433111	2.1781487
C	-3.5249728	-0.2282541	1.2485532
O	-2.3324405	-0.0253269	1.8769403
C	-2.1994013	1.1518517	2.6933015
H	-2.8906088	1.1042567	3.5453059
H	-2.4376053	2.0410259	2.0962295
C	-0.7733932	1.1845968	3.2151934
H	-0.5522957	0.2439264	3.7276168
H	-0.6928566	2.0118825	3.9373294
O	0.2243782	1.3122258	2.2047013
C	0.2824298	2.6042776	1.5937573
H	0.1211708	3.3867362	2.3507353
H	-0.4926419	2.7069976	0.8188652
C	1.6492823	2.7719217	0.9612703
H	1.8769740	1.9138689	0.3223192
H	1.6543184	3.6839858	0.3488538
O	2.6444852	2.9057384	1.9962322
C	3.7634480	2.0139467	1.9019777
H	4.4133763	2.2998427	2.7334571
H	4.3094916	2.1692390	0.9603085
C	3.4000736	0.5413667	2.0413995
H	4.2269359	-0.0194603	2.4962717
H	2.4986143	0.4419943	2.6544537
O	3.1556005	0.0192932	0.7158386
C	2.6161055	-1.2329965	0.6138171
C	2.2661930	-2.0438881	1.6915311
H	2.4196263	-1.6934220	2.7057113
C	1.7005333	-3.3070819	1.4710624
H	1.4260806	-3.9230362	2.3225435
C	1.4942511	-3.7621598	0.1745721
H	1.0548888	-4.7390689	-0.0051739
C	1.8505171	-2.9572293	-0.9164381

H	1.6889491	-3.3166362	-1.9266302
C	2.4071141	-1.6962974	-0.7087308

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Energy = -5122.250476908

C	-1.3132289	-0.8639830	0.0186431
C	-0.1146932	-1.8267342	-0.0049245
C	1.1913715	-1.0203948	0.0826393
C	1.2865169	-0.0572800	-1.1127218
C	0.0837814	0.9033654	-1.0985720
C	-1.2268721	0.0998433	-1.1767691
C	0.1010599	1.7140077	0.2110327
C	0.0100632	0.7440018	1.3956943
C	1.2067510	-0.2128380	1.3928178
C	-1.2947525	-0.0565097	1.3287690
N	0.0263684	1.5393998	2.6842887
O	2.9606131	2.4641007	2.8869648
C	3.5807086	2.7539918	1.8615619
N	3.4800501	3.9394961	1.1694267
C	4.3040364	3.9654139	-0.0193504
C	5.1288971	2.6502603	0.0878109
N	4.5054597	1.9574669	1.2151292
N	4.9284717	2.0231436	-1.1994627
C	4.0267322	2.7055457	-1.9933101
N	3.5758800	3.7958719	-1.2698748
C	2.7359100	5.0803947	1.6630526
N	1.4213706	5.2344443	1.0799811
C	0.2726590	4.9900981	1.7981854
N	-0.7979889	5.3704290	1.0206538
C	-0.3957747	5.9481281	-0.2510275
C	1.1610743	5.8476104	-0.2114669
N	1.4742430	5.0189209	-1.3625357
C	0.3518530	4.6864066	-2.0984073
N	-0.7536456	5.1693477	-1.4231187
C	-2.1491904	5.3894724	1.5364091
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C	-3.2925771	3.1903571	1.6803186
N	-4.2756901	2.5158881	0.9830682
C	-4.7478748	3.2805888	-0.1710797
C	-3.7597386	4.4814349	-0.2284407
N	-2.9947136	4.2202350	-1.4406107
C	-3.5404224	3.1937556	-2.1918139
N	-4.5613792	2.6318135	-1.4496423
C	-5.0982001	1.5026954	1.6260931
N	-4.9987250	0.1939180	1.0189462
C	-4.6153661	-0.9098547	1.7651323
N	-4.8895557	-2.0354413	1.0140485
C	-5.5578992	-1.7288067	-0.2331861
C	-5.7498442	-0.1845499	-0.1711983
N	-5.1952920	0.2781452	-1.4257331
C	-4.6622096	-0.7486059	-2.1820801
N	-4.7616220	-1.9120603	-1.4398684
C	-4.6721073	-3.3772263	1.5149335
N	-3.5106840	-4.0427018	0.9583476
C	-2.3924794	-4.3291152	1.7213564
N	-1.5762832	-5.1569466	0.9726881
C	-2.1790006	-5.5472223	-0.2889540
C	-3.5302786	-4.7686116	-0.2986022
N	-3.4337899	-3.9455408	-1.4903972
C	-2.2674536	-4.1624961	-2.1976681
N	-1.5039383	-5.0615058	-1.4792784
O	-2.1792129	-3.9435945	2.8646444
O	-4.1429659	-0.8887978	2.8953067
O	-2.7671768	2.8254023	2.7343891
O	0.2140186	4.5315847	2.9381094
C	5.1587871	0.8512808	1.8978413
N	4.9247701	-0.4372162	1.2845444
C	4.3630387	-1.4786618	2.0069221
N	4.5294458	-2.6337961	1.2691942
C	5.2983158	-2.4222325	0.0606421
C	5.6825820	-0.9147320	0.1351038
N	4.5516778	-2.5094004	-1.1876751
C	4.6395688	-1.3461457	-1.9316846
N	5.2582980	-0.3917458	-1.1464299
O	3.8378802	-1.3915949	3.1103011

C	4.1131987	-3.9337317	1.7542765
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C	1.7242302	-4.5896120	1.8333720
N	0.8542528	-5.3160263	1.0414801
C	1.4685813	-5.7796786	-0.1889454
C	2.9062517	-5.1789647	-0.1221035
N	0.9246283	-5.2123025	-1.4102681
C	1.8370337	-4.4260148	-2.0863066
N	2.9824243	-4.3595385	-1.3174533
O	1.4989424	-4.1742431	2.9637867
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O	-1.9783844	-3.6706960	-3.2838983
C	-4.5475703	-3.2117400	-2.0486484
C	-5.4334405	1.5991897	-1.9705583
C	-2.0746731	5.1806914	-2.0200055
C	2.8140585	4.8610831	-1.8936398
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O	1.6730677	-3.9075883	-3.1861387
O	4.2636683	-1.1962679	-3.0891979
O	3.7068454	2.4144308	-3.1405747
O	0.3410705	4.0937619	-3.1719840
O	-3.1998345	2.8627343	-3.3220562
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H	-5.5621081	-3.9792648	1.3023933
H	-4.7542061	1.4042760	2.6568249
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H	3.3249013	5.9813417	1.4663707
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H	-0.4779856	-6.8841274	1.3408728
H	-0.4315235	-5.6191997	2.6155880
H	-2.2926365	-6.6356124	-0.3353530
H	-4.4142961	-5.4130704	-0.3523033
H	-4.3305181	-3.0402843	-3.1040361
H	-5.4580427	-3.8126703	-1.9383786
H	-6.4951532	-2.2904686	-0.3100798
H	-6.7953479	0.1293187	-0.0777309
H	-6.4711829	1.8821937	-1.7651422
H	-5.2593727	1.5429960	-3.0457780
H	-5.7945991	3.5684922	-0.0313126
H	-4.2452177	5.4609677	-0.2804703
H	-2.4946354	6.1881527	-1.9212327
H	-1.9616151	4.9179620	-3.0728967
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H	3.3522350	5.8082939	-1.7734158
H	2.7206225	4.6089559	-2.9510029
H	4.9111582	4.8757286	-0.0449067
H	6.1950470	2.8049837	0.2817981
H	6.7423977	1.0372070	-1.4142411
H	5.5672211	0.8474925	-2.7583426
H	6.7531671	-0.7362346	0.2840199
H	6.1587625	-3.0997074	0.0342159
H	5.0288318	-4.4850326	-1.6515198
H	4.0745026	-3.5816853	-2.8760546
H	3.7027694	-5.9307800	-0.1251137
H	1.4456663	-6.8737570	-0.2366626
H	-0.2591554	-5.3911695	-3.0807008
H	-0.3768216	-6.7526360	-1.9153640
H	2.2226070	0.5123252	-1.0614253
H	1.3027131	-0.6272459	-2.0493799
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H	2.1369858	0.3587403	1.4736686
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H	-1.3662184	-0.7218489	2.1957391
H	-2.1495165	0.6265267	1.3637340
H	2.0469646	-1.7033399	0.0763026
H	0.1484897	1.5973630	-1.9434643
H	0.8986867	2.0852892	2.7687006
H	-0.0356446	0.9032275	3.5362152
H	-0.7748794	2.1895323	2.7247833
H	-2.2458259	-1.4352696	-0.0336161
Cl	-0.1462150	-0.1154479	5.2562067

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N	1.0130609	-5.1535116	-1.3134302
C	1.9844368	-4.4844520	-2.0519783
N	2.9087791	-4.2024391	1.2007904
C	1.7083486	-4.3181688	1.9007793
N	0.8659073	-5.1198085	1.1406016
C	4.0870358	-3.6759795	1.8565745
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C	4.5028287	-1.2449113	1.9811958
N	5.1735742	-0.2878792	1.2372009
C	5.8056434	-0.8344583	0.0533590
C	5.3861366	-2.3440422	0.0860637
N	5.2957927	-0.3717513	-1.2172737
C	4.7105034	-1.3880326	-1.9690996
N	4.6811099	-2.5251706	-1.1641479
C	5.4258555	1.0336230	1.7676749
N	4.7053154	2.1013116	1.1099379
C	3.6868174	2.7908402	1.7532456
N	3.3658351	3.8842477	0.9638391
C	4.2079641	4.0002990	-0.2106368
C	5.1350181	2.7413850	-0.1156270
N	4.8544043	2.0241241	-1.3387940
C	3.9763192	2.7060081	-2.1792171
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C	2.5204544	4.9474894	1.4660784
N	1.2350988	5.0499318	0.8169629
C	0.0589267	4.8848349	1.5448525
N	-0.9871443	5.2755246	0.7171491
C	-0.5375147	5.8090201	-0.5495964
C	1.0222836	5.7163022	-0.4514260
N	1.3936039	4.9743101	-1.6335514
C	0.2985180	4.6159035	-2.4156316
N	-0.8419418	5.0239520	-1.7280829
C	5.6291619	0.9013601	-1.8202402
O	3.6763052	2.3962990	-3.3132279
C	2.7451524	4.8516670	-2.1330335
O	-0.0282175	4.5075928	2.6958045
C	-2.3480074	5.3425378	1.2071747
N	-3.2455856	4.3456222	0.6680880
C	-3.7055524	3.2860371	1.4442246
N	-4.6370356	2.5930596	0.6747973
C	-4.9491001	3.2709193	-0.5692861
C	-3.9001816	4.4322467	-0.6156842
N	-3.0923850	4.1030144	-1.7740225
C	-3.6213168	3.0478040	-2.5145462
N	-4.6912476	2.5390181	-1.7864026
O	0.3341509	4.0873266	-3.5076886
C	-2.1370501	5.0085403	-2.3725440
O	-3.3847405	3.0374900	2.5884030
C	-5.4846530	1.5876819	1.2811119
N	-5.3020352	0.2525254	0.7577254
C	-4.7923137	-0.7661657	1.5579036
N	-4.9398165	-1.9528588	0.8472157
C	-5.6289598	-1.7767143	-0.4108999
C	-5.9235957	-0.2390969	-0.4540140
N	-5.3267535	0.1822442	-1.7009837
C	-4.7472566	-0.8655616	-2.4101039
N	-4.8467206	-2.0005999	-1.6090778
O	-3.2475746	2.6740796	-3.6074850

C	-5.5239885	1.4793467	-2.3101465
O	-4.3396160	-0.6458115	2.6783726
C	-4.6670792	-3.2349416	1.4572624
N	-3.4965115	-3.9133989	0.9418288
C	-2.4235931	-4.2062593	1.7799177
N	-1.5718737	-5.0457704	1.0669292
C	-2.1089398	-5.4440398	-0.2133181
C	-3.4862854	-4.7020946	-0.2742575
N	-3.4172653	-3.9719300	-1.5185513
C	-2.2226510	-4.1706318	-2.2036178
N	-1.4114346	-4.9575403	-1.3871409
O	-4.2838453	-0.8106498	-3.5308042
C	-4.5400584	-3.3098231	-2.1434470
O	-2.2757484	-3.8330540	2.9252026
C	-0.3898419	-5.6084895	1.6762766
O	-1.9536803	-3.7703592	-3.3175932
C	-0.2231467	-5.5836516	-1.9269827
O	3.9698648	-1.0720263	3.0649686
C	4.3453754	-3.8190616	-1.7272261
O	4.3354519	-1.3079774	-3.1202560
O	1.4618299	-3.8347499	2.9873692
O	1.8847286	-4.0948832	-3.1971031
N	1.3871121	0.2565495	3.8350052
C	0.2851569	-0.4887704	3.1610986
C	0.1310828	-0.1989687	1.6602334
C	1.4376075	-0.4406105	0.8766977
C	1.2168760	-0.2020096	-0.6269770
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C	-1.1752061	-0.9184295	-0.3878668
C	-0.9455346	-1.1588569	1.1120135
C	0.7613455	1.2508310	-0.8486786
C	-0.5542100	1.4948796	-0.0899495
C	-1.6324367	0.5320820	-0.6165723
C	-0.3306473	1.2518562	1.4135744
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H	-5.5477783	-3.8822948	1.3293230
H	-5.2193369	1.5511259	2.3416263
H	-6.5381567	1.8812210	1.1559584
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H	2.3234670	4.7316196	2.5198585
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H	4.8844864	-4.4325871	1.8253118
H	3.8051486	-3.4577982	2.8905886
H	-0.4126720	-6.7027746	1.5700765
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H	-2.2007962	-6.5401886	-0.2597501
H	-4.3503409	-5.3842080	-0.2865882
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H	-5.4271588	-3.9542616	-2.0514449
H	-6.5376126	-2.3977708	-0.4322517
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H	-6.5780545	1.7701485	-2.1976394
H	-5.2639326	1.3698487	-3.3666207
H	-5.9919602	3.6225782	-0.5548362
H	-4.3535120	5.4273783	-0.7413917
H	-2.5518680	6.0286829	-2.3676717
H	-1.9765028	4.6639807	-3.3982221
H	-0.9083615	6.8376765	-0.6761373
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H	2.6679033	4.5631192	-3.1850547
H	4.7564314	4.9536644	-0.1838769
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H	6.6976775	1.1050218	-1.6557690
H	5.4148146	0.8080922	-2.8887157
H	6.8938419	-0.6801719	0.1056230
H	6.2400722	-3.0354239	0.1424993
H	5.1706765	-4.5181332	-1.5279559
H	4.2178025	-3.6694385	-2.8031545
H	3.7344783	-5.8242281	0.1567827
H	1.4793306	-6.7460115	-0.0280140
H	-0.1643588	-5.2990624	-2.9814476
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H	0.4252431	1.9556013	1.7864960
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H	2.1538435	-0.3758734	-1.1689761
H	-0.6386376	-0.2314689	3.6876949
H	0.4837762	-1.5498900	3.3299577
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H	2.3076948	-0.1032137	3.5590600
H	1.3719333	1.2561079	3.6215396
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Cl	1.2172602	0.0080928	6.7077124

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O	-2.6473548	3.3335087	3.0729633
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O	3.8226821	-1.8480090	3.0715691
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N	5.0912955	-1.2187314	-1.2312438
N	4.1211074	-3.2283345	-1.2258791
N	2.2269163	-4.7592666	-1.2296428
N	0.0508476	-5.2539445	-1.2236610
N	-2.3250295	-4.7177893	-1.2277165
N	-4.0551066	-3.3077940	-1.2199434
N	-5.0988924	-1.1169987	1.2208872
N	-5.1243759	1.1145597	1.2318312
N	-4.0552323	3.3036254	1.2196205
N	-2.3299099	4.7192040	1.2308087
N	0.0475660	5.2499620	1.2230530
N	2.2256923	4.7647619	1.2329715
N	4.1147878	3.2270268	1.2217923
N	5.0970345	1.2230308	1.2302286
N	5.0827584	-1.2131194	1.2205126
N	4.1322283	-3.2323568	1.2268225
N	2.2270215	-4.7501010	1.2223885
N	0.0555258	-5.2641367	1.2292544
N	-2.3160950	-4.7092719	1.2245460
N	-4.0635868	-3.3216105	1.2324385
C	-5.8132173	-0.7814199	0.0005751
C	-5.8131102	0.7780316	-0.0008083
C	-2.9670601	-3.7359140	-1.9568409
C	-1.2576753	-5.5229062	-1.7865734
C	-4.2387923	4.0694040	-0.0016512
C	-3.0245612	5.0480098	-0.0008025
C	1.0582768	-4.6598212	-1.9594503
C	3.5192859	-4.4201322	-1.7905659
C	0.5360598	5.8671337	0.0017432

C	2.0557848	5.5169401	0.0028568
C	4.2844277	-2.0698067	-1.9610907
C	5.6318675	0.0034004	-1.7910742
C	4.9039725	3.2328720	0.0015957
C	5.5763544	1.8258696	-0.0003517
C	4.2853814	2.0757520	-1.9589322
C	5.5762607	-1.8220045	-0.0027816
C	4.9048159	-3.2294441	-0.0025997
C	-5.0808330	-2.4548821	-1.7882580
C	-4.7530263	-0.0033486	-1.9579710
C	2.0580306	-5.5148338	-0.0011575
C	0.5387623	-5.8669513	-0.0002116
C	-5.0770844	2.4467683	-1.7906950
C	-2.9656548	3.7342096	-1.9592427
C	-3.0224851	-5.0500481	0.0016041
C	-4.2375705	-4.0725580	0.0020516
C	-1.2583128	5.5211044	-1.7867758
C	1.0601936	4.6612966	-1.9571212
C	-5.0774750	-2.4502222	1.7905950
C	-4.7546110	-0.0000218	1.9586388
C	3.5204344	4.4273467	-1.7861842
C	-2.9659593	-3.7371526	1.9607727
C	-1.2562214	-5.5221383	1.7880007
C	-5.0813889	2.4514648	1.7882654
C	-2.9689169	3.7340294	1.9578040
C	1.0609554	-4.6594864	1.9582462
C	3.5210485	-4.4209045	1.7867867
C	-1.2597866	5.5215113	1.7878163
C	1.0561636	4.6590197	1.9600528
C	4.2859694	-2.0695176	1.9563747
C	5.6376304	0.0001023	1.7882849
C	3.5173592	4.4194056	1.7907839
C	4.2844078	2.0699950	1.9583202
H	-6.8135499	-1.2266705	0.0109542
H	5.4005397	-0.0025206	2.8531339
H	3.3706693	4.2319487	2.8554508
H	4.2019744	5.2620272	1.6423223
H	6.7232308	-0.0053725	1.6388762
H	4.1977407	-5.2694422	1.6358897
H	-1.4970708	6.5801203	1.6344221
H	-1.2059392	5.2946281	2.8534859
H	3.3728204	-4.2377166	2.8519792
H	-1.5028540	-6.5786405	1.6347479
H	-6.0572317	2.9266289	1.6381585
H	-4.8667394	2.3521511	2.8531962
H	-1.2048948	-5.2945291	2.8536453
H	3.3719872	4.2468567	-2.8518051
H	-4.8634116	-2.3445174	2.8550429
H	-6.0598216	-2.9126553	1.6427943
H	4.1940010	5.2779892	-1.6332669
H	-5.2115254	-4.5730652	-0.0044229
H	-1.5078180	6.5769507	-1.6335696
H	-3.3026188	-6.1086633	0.0063926
H	-1.2074665	5.2933441	-2.8524115
H	0.3310416	-6.9421187	-0.0044607
H	-6.0600371	2.9081155	-1.6436022
H	2.7177122	-6.3890172	0.0021401
H	-4.8623710	2.3407674	-2.8549790
H	5.6160205	-4.0620436	-0.0073510
H	-6.0569140	-2.9296439	-1.6384044
H	6.6709088	-1.8509792	0.0012313
H	-4.8660859	-2.3553648	-2.8531519
H	6.6709627	1.8555599	-0.0090159
H	5.3923506	0.0060111	-2.8553963
H	5.6146557	4.0658877	0.0125784
H	6.7179155	0.0083120	-1.6442281
H	2.7143359	6.3919967	-0.0027361
H	4.2012985	-5.2646055	-1.6406797
H	0.3270117	6.9420527	0.0090016
H	3.3717985	-4.2351597	-2.8555559
H	-3.3056922	6.1063713	-0.0086736
H	-1.2047837	-5.2962885	-2.8523454
H	-5.2131956	4.5690764	0.0056945
H	-1.4970379	-6.5809830	-1.6327148
H	-6.8134628	1.2232984	-0.0121765

AdNH3+

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Energy = -907.2464224537

C	-1.3072296	-0.9597523	-0.5989042
C	-0.1061042	-1.9210646	-0.6561530
C	1.2026832	-1.1191111	-0.5384323
C	1.2954660	-0.1078824	-1.6954370
C	0.0936969	0.8528119	-1.6388559
C	-1.2157657	0.0517129	-1.7557725
C	0.1095724	1.6094216	-0.2967558
C	0.0170479	0.5882542	0.8421750
C	1.2185895	-0.3638507	0.8043736
C	-1.2919506	-0.2044504	0.7438873
N	0.0316226	1.3231386	2.1666225
H	2.2332381	0.4585596	-1.6258758
H	1.3005372	-0.6398740	-2.6550258
H	1.1566565	-1.0657087	1.6446341
H	2.1488343	0.2100414	0.9072542
H	1.0345070	2.1924055	-0.1983104
H	-0.7374229	2.3053533	-0.2411403
H	-0.1184561	-2.4747987	-1.6033489
H	-0.1722722	-2.6546303	0.1575662
H	-2.0765648	0.7323895	-1.7293924
H	-1.2421052	-0.4781630	-2.7161668
H	-1.3596303	-0.9058153	1.5842181
H	-2.1461992	0.4825766	0.8038874
H	2.0604817	-1.8003229	-0.5698136
H	0.1595122	1.5804353	-2.4556062
H	0.8898128	1.8722719	2.2712602
H	-0.0313350	0.6429162	2.9872403
H	-0.7545278	1.9764481	2.2311916
H	-2.2417883	-1.5271810	-0.6736103
Cl	-0.1509063	-0.6561312	4.5042909

AdCH2NH3+

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Energy = -946.5784259382

N	1.1720864	0.1259264	2.8160129
C	0.1250377	-0.6711350	2.0890331
C	-0.0291813	-0.2686616	0.6221660
C	1.2800939	-0.4881916	-0.1662033
C	1.0675221	-0.1378802	-1.6501620
C	-0.0296457	-1.0425593	-2.2379838
C	-1.3433815	-0.8227366	-1.4671994
C	-1.1284849	-1.1690199	0.0156372
C	0.6393232	1.3357382	-1.7698658
C	-0.6765769	1.5551570	-1.0020914
C	-1.7731283	0.6498204	-1.5901726
C	-0.4652738	1.2059015	0.4823009
H	0.2748052	-2.0954176	-2.1689816
H	-0.1755242	-0.8095684	-3.3008074
H	-2.0634826	-1.0301823	0.5751371
H	-0.8348915	-2.2224791	0.1186123
H	1.5988376	-1.5344069	-0.0645047
H	2.0835416	0.1437688	0.2379813
H	-1.9408957	0.9041309	-2.6448833
H	-2.7192690	0.8108985	-1.0565721
H	1.4238023	1.9889307	-1.3648052
H	0.5029051	1.5995823	-2.8266397
H	-1.3930010	1.3692034	1.0470800
H	0.2996233	1.8753245	0.9008034
H	-2.1262954	-1.4725099	-1.8769504
H	2.0074933	-0.2950627	-2.1928357
H	-0.8081617	-0.5199204	2.6369501
H	0.4225509	-1.7187061	2.1787625
H	1.2408241	-0.1860455	3.8363199
H	2.0937490	0.0104564	2.3872778
H	0.9545590	1.1255634	2.8052951
H	-0.9809827	2.6057364	-1.0824502
Cl	1.3014214	-0.8216556	5.7137389

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Energy = -4981.013156181

C	1.6204057	3.0636280	1.7085800
C	2.2892456	2.7262102	0.5027992

C	3.1937701	1.5730684	0.5023097
C	3.3627676	0.8424912	1.7076625
C	2.7427078	1.2647037	2.9432624
C	1.8833606	2.3601331	2.9436732
C	3.4157153	-0.5954721	1.7070146
C	2.8283961	-1.0632761	2.9421996
C	2.0520825	-2.2190120	2.9416455
C	1.8415732	-2.9387608	1.7059045
C	2.4836812	-2.5519190	0.5004788
C	0.4904929	-3.4336290	1.7056801
C	-0.2491853	-3.5527111	0.4999841
C	-1.6586807	-3.1516127	0.5001051
C	-2.2244545	-2.6606931	1.7059051
C	-1.4745192	-2.6390254	2.9414518
C	-0.1354094	-3.0202284	2.9413181
C	-3.1125764	-1.5285067	1.7064253
C	-2.9123073	-0.8059349	2.9422208
C	-2.9635777	0.5854206	2.9428224
C	-3.2164626	1.2924121	1.7076710
C	-3.5089777	0.6030477	0.5016779
C	-3.4550123	-0.8614313	0.5010530
C	-1.8862294	3.0192680	0.5028042
C	-0.5100656	3.5230365	0.5030790
C	0.2364879	3.4576012	1.7087396
C	-0.3572338	2.9980640	2.9439636
C	-1.6646320	2.5193600	2.9437281
C	-2.4142523	2.4869850	1.7082410
C	3.3010215	-1.3354442	0.5010280
C	3.4190770	-0.5934227	-0.7041243
C	1.8419679	-2.9411524	-0.7051411
C	2.8284264	-1.0614557	-1.9393768
C	2.0524762	-2.2167001	-1.9398733
C	0.4925259	-3.4353499	-0.7054167
C	-0.1356411	-3.0181224	-1.9403580
C	-1.4741672	-2.6370970	-1.9402435
C	-2.2275708	-2.6610265	-0.7051331
C	-3.1146503	-1.5302325	-0.7046860
C	-2.9123980	-0.8034959	-1.9394680
C	-2.9636312	0.5872659	-1.9388333
C	-3.2188096	1.2961122	-0.7034583
C	-2.4175446	2.4892043	-0.7029214
C	-1.6643288	2.5217390	-1.9379737
C	-0.3574939	3.0002057	-1.9377145
C	0.2382814	3.4615251	-0.7024123
C	1.6205063	3.0680419	-0.7025370
C	1.8837498	2.3621119	-1.9378939
C	2.7427064	1.2671457	-1.9384055
C	3.3661830	0.8427997	-0.7035132
C	0.8314024	-2.2700162	-2.7188891
C	-1.9025134	-1.4918859	-2.7187161
C	-2.0072134	1.3487697	-2.7174580
C	0.6619828	2.3260212	-2.7168837
C	2.4163175	0.0895491	-2.7178348
C	2.4165193	0.0867405	3.7221198
C	0.8314051	-2.2732345	3.7210880
C	-1.9029633	-1.4949671	3.7214457
C	-2.0076702	1.3461693	3.7226788
C	0.6619802	2.3236302	3.7231210
C	0.4246110	-1.1625842	4.4662695
C	-0.9720608	-0.7650611	4.4664601
C	-1.0255558	0.6860761	4.4670735
C	0.3380580	1.1853380	4.4672781
C	1.2342418	0.0428060	4.4667481
C	0.3382367	1.1888294	-3.4635848
C	-1.0254025	0.6895638	-3.4638603
C	-0.9719020	-0.7615899	-3.4645350
C	0.4247986	-1.1591200	-3.4646196
C	1.2344520	0.0462840	-3.4639797
C	-0.9857617	6.8317666	-0.3864666
C	-1.8100210	6.9622570	0.7469049
C	-3.1154757	6.4850694	0.7474516
C	-3.6619019	5.8532740	-0.3853257
C	-2.8910760	5.8737800	-1.5607590
C	-1.5888111	6.3496990	-1.5612665
C	-4.8366282	4.9621330	-0.3166261
C	-5.1210004	4.2766524	0.8764840

C	-5.8945240	3.1239517	0.8769354
C	-6.4215738	2.6003358	-0.3156920
C	-6.3063728	3.3995822	-1.4691313
C	-5.5330675	4.5520837	-1.4695498
C	-6.8012609	1.1755587	-0.3834477
C	-6.5306904	0.4540939	-1.5592130
C	-6.4791011	-0.9313864	-1.5598296
C	-6.6951547	-1.6720623	-0.3846779
C	-7.1251241	-0.9582002	0.7495559
C	-7.1768629	0.4307495	0.7501756
C	-6.2110170	-3.0649330	-0.3180295
C	-5.6485373	-3.5498642	0.8747981
C	-4.7920243	-4.6423259	0.8742417
C	-4.4558979	-5.3033464	-0.3192686
C	-5.1792517	-4.9444151	-1.4727381
C	-6.0356552	-3.8522476	-1.4721351
C	-2.4479504	-6.0699507	-1.5624704
C	-1.1144075	-6.4494200	-1.5625158
C	-0.4776925	-6.8848621	-0.3872329
C	-1.2902886	-7.0741172	0.7462692
C	-2.6272656	-6.6941064	0.7461864
C	0.9965642	-6.8543192	-0.3195012
C	1.6307054	-6.4696850	0.8739263
C	2.9341824	-5.9922439	0.8744054
C	3.6674540	-5.8760702	-0.3185667
C	3.1034219	-6.4525424	-1.4727347
C	1.8001473	-6.9296403	-1.4732483
C	4.8125723	-4.9469904	-0.3855903
C	5.0169659	-4.2023587	-1.5602995
C	5.7902044	-3.0515494	-1.5597249
C	6.4018874	-2.5818038	-0.3843748
C	6.3308878	-3.4139615	0.7485024
C	5.5556364	-4.5676248	0.7478962
C	-3.2185061	-6.1052691	-0.3872087
C	6.8290032	-1.1704814	-0.3162820
C	6.6585380	-0.4482531	0.8768937
C	6.6068333	0.9389694	0.8768505
C	6.7232596	1.6719383	-0.3162729
C	7.0982939	0.9571494	-1.4699526
C	7.1499322	-0.4297437	-1.4699283
C	6.1928001	3.0477768	-0.3840571
C	5.5491961	3.4720218	-1.5596701
C	4.6929153	4.5624953	-1.5601328
C	4.4330296	5.2890209	-0.3850370
C	5.2012712	4.9648605	0.7488113
C	6.0597385	3.8716890	0.7492916
C	3.2223545	6.1308353	-0.3179505
C	2.6176395	6.6649625	-1.4718619
C	1.2827723	7.0447906	-1.4723234
C	0.4867655	6.9096303	-0.3188060
C	1.1472441	6.5718792	0.8745443
C	2.4823113	6.1916367	0.8749535
H	-1.4074906	7.3958210	1.6581117
H	-3.7021955	6.5573132	1.6589872
H	-3.2683760	5.3888629	-2.4555296
H	-0.9881831	6.2213929	-2.4561378
H	-4.6152355	4.5646364	1.7926653
H	-5.9691444	2.5472968	1.7934678
H	-6.7791244	3.0812620	-2.3939690
H	-5.4181894	5.1100157	-2.3945612
H	-6.2256340	0.9866021	-2.4544707
H	-6.1354110	-1.4388484	-2.4556187
H	-7.3727269	-1.4946499	1.6612835
H	-7.4634103	0.9465485	1.6624185
H	-5.7670022	-2.9816225	1.7919170
H	-4.2679811	-4.8934307	1.7909735
H	-5.0223581	-5.4911606	-2.3982534
H	-6.5295394	-3.5688398	-2.3972756
H	-2.8593999	-5.6141950	-2.4574308
H	-0.5247911	-6.2784765	-2.4575785
H	-0.8571654	-7.4757711	1.6580704
H	-3.2071908	-6.8084271	1.6577555
H	1.0531154	-6.4073793	1.7907358
H	3.3343844	-5.5719425	1.7915921
H	3.6725084	-6.4717723	-2.3978810
H	1.3783448	-7.3107818	-2.3989331

H	4.4561375	-4.4518721	-2.4554403
H	5.8094938	-2.4370875	-2.4542562
H	6.8474600	-3.1272274	1.6602496
H	5.4847904	-5.1548694	1.6591739
H	6.4205720	-0.9781674	1.7937762
H	6.3299985	1.4497022	1.7937016
H	7.2926276	1.4922008	-2.3952160
H	7.3839828	-0.9488649	-2.3950677
H	5.6150529	2.8616550	-2.4547434
H	4.1157675	4.7704984	-2.4554879
H	5.0866887	5.5447786	1.6603435
H	6.5955548	3.6234220	1.6612333
H	3.1839737	6.7266858	-2.3968280
H	0.8343359	7.3951599	-2.3976671
H	0.5754535	6.4664912	1.7910415
H	2.9121612	5.8009851	1.7918040

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Energy = -5212.209930092

C	-3.2077386	6.5964936	-0.2865241
C	-2.5399948	6.7901966	-1.5093939
C	-1.1920873	7.1129059	-1.5563741
C	-0.4293423	7.2329181	-0.3818623
C	-1.1270011	7.1744280	0.8377976
C	-2.4810703	6.8787458	0.8838665
C	1.0443164	7.1970093	-0.4044401
C	1.7142850	6.6197251	-1.4967267
C	3.0492496	6.2545108	-1.4117570
C	3.7768239	6.4384179	-0.2250125
C	3.1526195	7.1494827	0.8145231
C	1.8198029	7.5264231	0.7231500
C	5.0217171	5.6759581	-0.0288698
C	5.2448423	5.0436566	1.2051865
C	6.1552817	4.0034103	1.3194640
C	6.8874492	3.5556451	0.2069962
C	6.7881120	4.3032755	-0.9800282
C	5.8709962	5.3386551	-1.0971128
C	7.4877566	2.2100323	0.2393324
C	7.4154419	1.4042642	-0.9090157
C	7.5608799	0.0272954	-0.8274954
C	7.7844070	-0.6057169	0.4063965
C	8.0336128	0.2157560	1.5204935
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C	6.8179565	-2.4932052	1.6926049
C	6.1366874	-3.7013554	1.7010829
C	6.0859282	-4.5108527	0.5546558
C	6.8852235	-4.1386210	-0.5406608
C	7.5672778	-2.9297511	-0.5488880
C	5.0350563	-5.5376404	0.4479940
C	4.3590906	-5.6985669	-0.7728164
C	3.1392704	-6.3558757	-0.8335297
C	2.5418458	-6.8831052	0.3233456
C	3.2899278	-6.8533698	1.5133701
C	4.5101499	-6.1944129	1.5746009
C	1.1080546	-7.2204765	0.3053466
C	0.3117422	-6.9099257	1.4200138
C	-1.0718787	-6.8768282	1.3242104
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C	-0.9311437	-7.6005153	-0.9640698
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C	-3.1235691	-6.7399862	-0.0672715
C	-3.5183834	-6.1512011	-1.2796615
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C	-5.2079412	-5.9652236	0.9150751
C	-4.0320171	-6.6971969	1.0046983
C	7.4767730	-2.0409700	0.5370790
C	-6.5007772	-4.1407745	-0.2479487
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C	-7.6747113	-2.4008857	-1.4765927
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C	-7.2977763	2.6811878	-0.4412291
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C	-4.5142368	5.9127921	-0.2430618
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H	-2.9626972	6.8023672	1.8534860
H	1.1565232	6.3400594	-2.3843148
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H	4.6007591	5.2776225	2.0475958
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H	7.3601856	-0.5753464	-1.7080218
H	8.2887963	-0.2365723	2.4748596
H	8.0345445	2.1977340	2.3300774
H	6.7234549	-1.8300084	2.5469835
H	5.5260312	-3.9561172	2.5620097
H	6.9300680	-4.7821373	-1.4150111
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H	4.7309898	-5.1929047	-1.6589276
H	2.5841310	-6.3515894	-1.7666594
H	2.8887825	-7.3161159	2.4108027
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H	0.7851945	-6.5721773	2.3370585
H	-1.6516097	-6.5131344	2.1675453
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C	-3.9772097	-0.7957605	0.8726307
C	-2.2433294	-1.3618393	-2.8022478
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C	-1.2309523	-2.4882707	2.4226690

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C	-2.5996773	0.7683497	2.8125570
C	0.2279295	-1.5905110	-3.1265478
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C	1.1791079	-2.4050194	2.5446228
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C	-0.1920104	0.9162067	3.4786625
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C	1.3702549	0.6157885	-3.3149949
C	2.6270149	-2.2808876	-1.6853809
C	2.5352194	-2.8952149	0.5588443
C	2.4528066	-2.4022326	1.8571456
C	2.3190961	-0.4531896	3.1268936
C	1.0071774	1.6212227	3.1899345
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C	-1.3948850	2.6609545	2.1688935
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C	3.3420332	-2.2042647	-0.4271793
C	3.1720804	-1.1976897	2.2233017
C	2.2748774	0.9367441	3.0587429
C	1.0144804	2.7449122	2.2911757
C	-1.2839621	3.4065996	-0.5538168
C	-0.1782743	3.1892718	1.6589446
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C	2.4801615	2.2962738	-1.9113385
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C	3.9445090	-0.5225053	1.2731179
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C	3.1953699	2.3911596	-0.6540355
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10CPP

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Energy = -2311.901220836

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C	-3.6640433	5.8622010	-0.0401203
C	-2.8988963	5.8893865	-1.2189658
C	-1.5947442	6.3657066	-1.2191051
C	-4.8254930	4.9525266	0.0416772
C	-5.0347640	4.2155746	1.2202064
C	-5.8092625	3.0632802	1.2199839
C	-6.4124798	2.5915461	0.0412298
C	-6.3544347	3.4293447	-1.0880692
C	-5.5790367	4.5826464	-1.0878814
C	-6.8162987	1.1726310	-0.0408352
C	-6.5531536	0.4540243	-1.2198861
C	-6.5012870	-0.9334217	-1.2201523
C	-6.7098856	-1.6701275	-0.0413402
C	-7.1549401	-0.9589301	1.0886065
C	-7.2069310	0.4297770	1.0888516
C	-6.2013169	-3.0549977	0.0402492
C	-5.5647705	-3.4808632	1.2189543
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C	-5.2222164	-4.9784694	-1.0892104
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C	-2.4532802	-6.0850808	-1.2198480
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C	-0.4823311	-6.8921293	-0.0410376
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C	6.3544301	-3.4293149	1.0881139
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C	6.5530337	-0.4540203	1.2198507
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C	7.5965847	0.2890182	0.4435493
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C	7.7456924	-0.9365143	-1.6570504
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C	4.7982176	-0.0870384	-5.8905128
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H	-6.9762283	-2.3344763	0.1348196
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H	-7.8979908	1.7645022	-2.4708650
H	-6.9200756	1.8942823	1.7057683
H	-5.9398419	1.9033721	3.9426391
H	-6.8908609	-2.2634689	4.3823822
H	-7.8911202	-2.2699796	2.1447099
H	-4.6593484	-2.2408597	4.9156971
H	-2.6178028	-2.1656674	6.2318205
H	-3.6465478	1.7793911	7.6054867
H	-5.6830614	1.7106899	6.2549659

C70
70

Energy = -2669.029078010

C	-2.4169652	0.0000000	3.2195260
C	-1.2348879	0.0000000	3.9653920
C	-0.3816013	-1.1744482	3.9653920
C	0.9990453	-0.7258489	3.9653920
C	-2.7860770	-1.1642712	2.4410551
C	-0.7468833	-2.2986705	3.2195260
C	-2.7860770	1.1642712	2.4410551
C	-0.3816013	1.1744482	3.9653920
C	0.9990453	0.7258489	3.9653920
C	-0.7468833	2.2986705	3.2195260
C	1.9553659	-1.4206565	3.2195260
C	-1.9682329	-2.2899371	2.4410551
C	0.2463426	-3.0094963	2.4410551
C	1.9553659	1.4206565	3.2195260
C	1.5696422	-2.5795302	2.4410551
C	2.9383251	-0.6956998	2.4410551
C	-3.3936684	-0.7191006	1.2063603
C	-1.9682329	2.2899371	2.4410551
C	-3.3936684	0.7191006	1.2063603
C	-1.7326065	-3.0053562	1.2063603
C	-0.3647959	-3.4497847	1.2063603
C	2.3228587	-2.5765128	1.2063603
C	3.1682121	-1.4129837	1.2063603
C	2.9383251	0.6956998	2.4410551
C	-3.2515324	-1.4551686	0.0000000
C	-2.3887264	-2.6427193	0.0000000
C	0.3791688	-3.5420629	0.0000000
C	1.7752183	-3.0884590	0.0000000
C	3.4858717	-0.7339466	0.0000000
C	3.1682121	1.4129837	1.2063603
C	-3.3936684	-0.7191006	-1.2063603
C	-3.2515324	1.4551686	0.0000000
C	-1.7326065	-3.0053562	-1.2063603
C	-0.3647959	-3.4497847	-1.2063603

C	2.3228587	-2.5765128	-1.2063603
C	3.1682121	-1.4129837	-1.2063603
C	3.4858717	0.7339466	0.0000000
C	-2.7860770	-1.1642712	-2.4410551
C	-3.3936684	0.7191006	-1.2063603
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C	-2.4169652	0.0000000	-3.2195260
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C	-0.3647959	3.4497847	-1.2063603
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C	-0.7468833	2.2986705	-3.2195260
C	0.9990453	0.7258489	-3.9653920
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