

# A global optimization perspective on molecular clusters

## Electronic Supplemental Material

J. M. C. Marques<sup>1</sup>, F. B. Pereira<sup>2</sup>, J. L. Llanio-Trujillo<sup>1</sup>, P. E. Abreu<sup>1</sup>,  
M. Albertí<sup>3</sup>, A. Aguilar<sup>3</sup>, F. Pirani<sup>4</sup> and M. Bartolomei<sup>5</sup>

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<sup>1</sup>CQC, Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal

<sup>2</sup>Instituto Superior de Engenharia de Coimbra, Quinta da Nora, 3030-199 Coimbra, Portugal, and Centro de Informática e Sistemas da Universidade de Coimbra (CISUC), 3030-290 Coimbra, Portugal

<sup>3</sup>IQTCUB, Departament de Química Física, Universitat de Barcelona, 08028-Barcelona, Spain

<sup>4</sup>Dipartimento di Chimica, Biologia e Biotecnologie, Università di Perugia, 06123-Perugia, Italy

<sup>5</sup> Consejo Superior de Investigaciones Científicas (IFF-CSIC), Instituto de Física Fundamental, Serrano 123, Madrid 28006, Spain

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3.4.2	n=2	54
3.4.3	n=3	54
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3.4.6	n=6	55
3.4.7	n=7	55
3.4.8	n=8	56
3.4.9	n=9	56
3.4.10	n=10	57
3.4.11	n=11	57
3.4.12	n=12	58
3.4.13	n=13	59
3.4.14	n=14	59
3.4.15	n=15	60
3.4.16	n=16	61
3.4.17	n=17	62
3.4.18	n=18	63
3.4.19	n=19	64
3.4.20	n=20	65
3.4.21	n=21	66
3.4.22	n=22	67
3.4.23	n=23	68
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3.5.5	n=5	76
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3.5.7	n=7	78
3.5.8	n=8	78
3.5.9	n=9	79
3.5.10	n=10	80

#### 4 References

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# 1 Figures

## 1.1 Figure S1

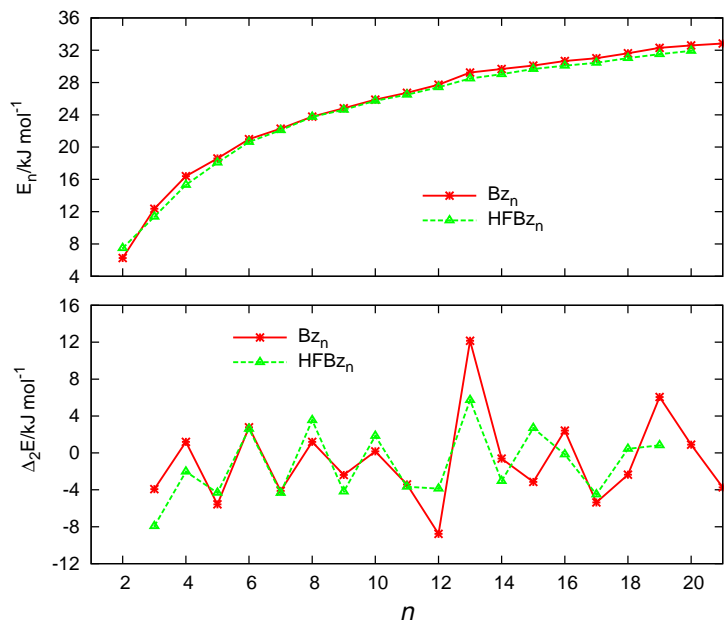


Figure S1: Average binding energy,  $E_n$  (top), and second energy difference,  $\Delta_2 E$  (bottom). In top panel,  $E_n = -E_{GM,n}/n$ , where  $E_{GM,n}$  is the global minimum energy for the cluster size  $n$ ; in bottom panel,  $\Delta_2 E = E_{GM,n+1} + E_{GM,n-1} - 2E_{GM,n}$ . Values for  $(HFBz)_n$  are from this work, while those for  $Bz_n$  were taken from Ref. [1].

## 1.2 Figure S2

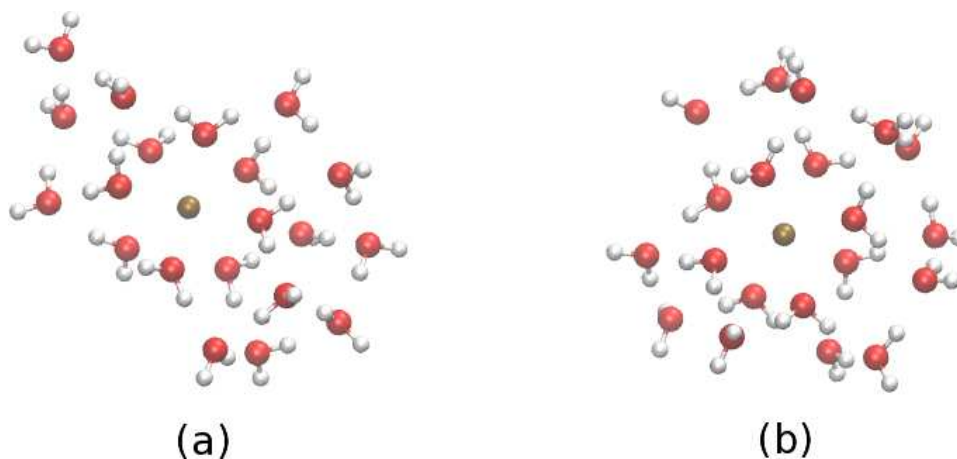


Figure S2: Comparison between the  $\text{Ca}^{2+}-(\text{H}_2\text{O})_{20}$  global minimum obtained by the EA in this work (left) and the corresponding lowest-energy structure of González *et al.* [2] (right). Colours for the atoms: H (white), O (red), and  $\text{Ca}^{2+}$  (brown). The best superposition between the two structures leads to a RMSD of 1.6 Å.

### 1.3 Figure S3

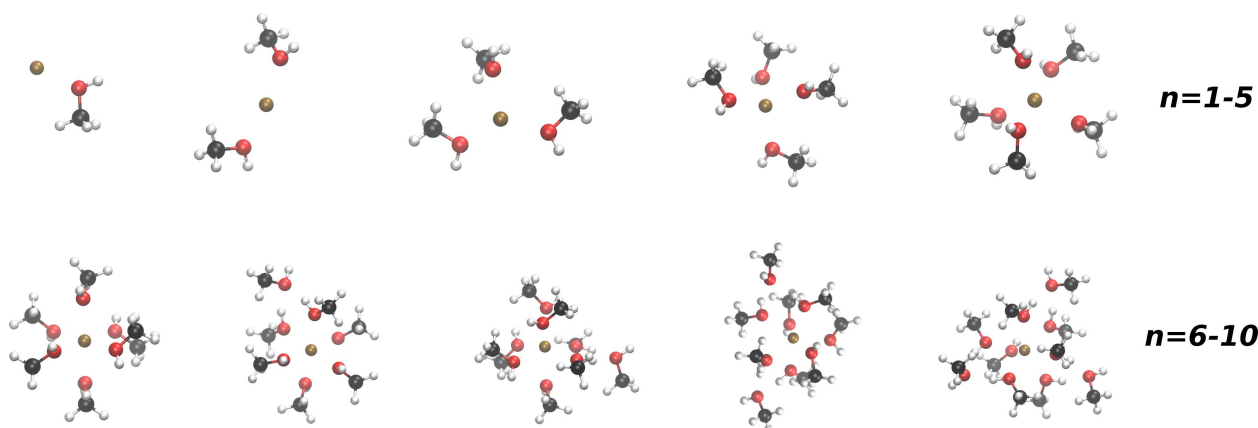


Figure S3: Global minimum structures of the clusters  $\text{Ca}^{2+}-(\text{CH}_3\text{OH})_n$  ( $n = 1 - 10$ ) obtained with the EA. Colours for the atoms: H (white), C (black), O (red), and  $\text{Ca}^{2+}$  (brown).

## 2 Tables

### 2.1 Table S1

Table S1: RMSD between the geometries of the EA optimized structures and MP2/TZV optimized structures for  $\text{K}^+(\text{C}_6\text{H}_6)_n$  and  $\text{K}^+(\text{C}_6\text{F}_6)_n$ . Entries for  $n = 3$  refer to global minimum (s1) and low energy minima (s2 and s3).

$n$	$(\text{C}_6\text{H}_6)_n + \text{K}^+$	$(\text{C}_6\text{F}_6)_n + \text{K}^+$
1	0.10	0.10
2	0.27	1.61
3 (s1)	0.18	1.60
3 (s2)	0.17	2.08
3 (s3)	0.70	2.30
4	0.04	-

## 3 Coordinates and energies of minima

All geometries shown in this section, corresponds to a XYZ file, so the first number is the number of atoms (we shall call it  $N$ ), the second line contains a comment (in this case the energy of the system) and  $N$  lines, each containing the symbol of the atom followed by its cartesian coordinates in Å. The energies are in kJ/mol in subsections 3.1, 3.4 and 3.5. We used atomic units (Hartree) in subsections 3.2 and 3.3.

### 3.1 (HFBZ)<sub>n</sub>      n = 2 – 20

#### 3.1.1 n=2

```
24
-14.96065762
C -4.54263636 -2.53445457 1.34246221
C -5.67446078 -1.72964404 1.40037168
C -5.60737850 -0.47822959 2.00172124
C -4.40847181 -0.03162568 2.54516134
C -3.27664740 -0.83643621 2.48725187
C -3.34372967 -2.08785065 1.88590231
F -4.60655715 -3.72733342 0.76924773
F -6.81729522 -2.15533580 0.88235950
F -6.68629216 0.28895750 2.05692354
```

F	-4.34455103	1.16125318	3.11837582
F	-2.13381296	-0.41074444	3.00526405
F	-2.26481602	-2.85503774	1.83070001
C	-1.24168683	-2.85873719	-1.82696160
C	-2.37351138	-2.05392679	-1.76905302
C	-2.30642955	-0.80251204	-1.16770405
C	-1.10752316	-0.35590768	-0.62426366
C	0.02430139	-1.16071808	-0.68217224
C	-0.04278044	-2.41213283	-1.28352121
F	-1.30560720	-4.05161633	-2.40017552
F	-3.51634554	-2.47961898	-2.28706548
F	-3.38534335	-0.03532509	-1.11250259
F	-1.04360280	0.83697146	-0.05104974
F	1.16713555	-0.73502589	-0.16415978
F	1.03613335	-3.17931979	-1.33872267

### 3.1.2 n=3

36

-34.13079656

C	-3.82404331	-1.28494790	1.07332459
C	-2.89808538	-0.46648793	0.43706583
C	-1.53795267	-0.71811811	0.57447288
C	-1.10377788	-1.78820825	1.34813868
C	-2.02973580	-2.60666822	1.98439744
C	-3.38986851	-2.35503804	1.84699039
F	-5.12055611	-1.04510762	0.94235944
F	-3.31192713	0.55355079	-0.30041413
F	-0.65528162	0.06208033	-0.03204193
F	0.19273492	-2.02804853	1.47910383
F	-1.61589406	-3.62670694	2.72187739
F	-4.27253957	-3.13523648	2.45350520
C	-0.81298334	-5.12984942	-4.04291695
C	-0.59356734	-4.00057966	-4.82311335
C	-1.00957580	-2.75309546	-4.37269182
C	-1.64500027	-2.63488102	-3.14207387
C	-1.86441627	-3.76415078	-2.36187746
C	-1.44840780	-5.01163498	-2.81229900
F	-0.41644370	-6.31898846	-4.47224821
F	0.01213099	-4.11324028	-5.99616825
F	-0.80041711	-1.67661704	-5.11641544
F	-2.04153991	-1.44574198	-2.71274260
F	-2.47011460	-3.65149017	-1.18882256
F	-1.65756650	-6.08811340	-2.06857537
C	2.01694552	-1.44556981	-1.50684299
C	2.63958955	-0.51258739	-0.68589340
C	3.38789243	-0.93719005	0.40585512
C	3.51355127	-2.29477513	0.67665405
C	2.89090724	-3.22775754	-0.14429554
C	2.14260436	-2.80315488	-1.23604406
F	1.30364207	-1.04085247	-2.54752677
F	2.51982264	0.78149711	-0.94400552
F	3.98142897	-0.04782289	1.18842679
F	4.22685472	-2.69949246	1.71733783
F	3.01067415	-4.52184204	0.11381658
F	1.54906782	-3.69252205	-2.01861573

### 3.1.3 n=4

48

-61.24166107

C	1.86170329	-0.90134385	-2.52909041
C	2.37617295	-1.99753769	-1.84660961
C	3.07751936	-1.81150689	-0.66100209
C	3.26439611	-0.52928226	-0.15787537
C	2.74992645	0.56691158	-0.84035616
C	2.04858004	0.38088079	-2.02596368
F	1.19316146	-1.07864846	-3.65923888
F	2.19805025	-3.21979104	-2.32618204
F	3.56793849	-2.85645564	-0.01042605
F	3.93293794	-0.35197765	0.97227311
F	2.92804915	1.78916494	-0.36078374
F	1.55816091	1.42582954	-2.67653973
C	-3.12019865	0.93420950	-0.05248691
C	-1.89295158	0.35837971	-0.35970779
C	-1.32722670	-0.57361637	0.50255558
C	-1.98874889	-0.92978266	1.67203982
C	-3.21599597	-0.35395286	1.97926071
C	-3.78172085	0.57804322	1.11699734
F	-3.65947884	1.82261048	-0.87440007
F	-1.26235628	0.69786990	-1.47447981
F	-0.15735122	-1.12252716	0.20969672
F	-1.44946871	-1.81818364	2.49395299
F	-3.84659126	-0.69344306	3.09403272
F	-4.95159633	1.12695400	1.40985620
C	2.43789610	4.04448819	3.40197029
C	1.25704752	4.76898290	3.51512531
C	0.04103951	4.16783173	3.21164351
C	0.00588006	2.84218584	2.79500670
C	1.18672864	2.11769112	2.68185169
C	2.40273665	2.71884230	2.98533349
F	3.59703272	4.61749781	3.69125035
F	1.29053812	6.03261841	3.91227058
F	-1.08460652	4.85845761	3.31950873
F	-1.15325656	2.26917622	2.50572665
F	1.15323804	0.85405562	2.28470642
F	3.52838268	2.02821641	2.87746827
C	-0.80147216	3.99855706	-2.58349551
C	0.01175760	4.31130714	-3.66652125
C	1.32823880	4.70483276	-3.45634447
C	1.83149024	4.78560830	-2.16314195
C	1.01826048	4.47285822	-1.08011622
C	-0.29822072	4.07933260	-1.29029300
F	-2.05637356	3.62343762	-2.78381661
F	-0.46793107	4.23431727	-4.89923857
F	2.10345154	5.00296233	-4.48874070
F	3.08639164	5.16072774	-1.96282085
F	1.49794915	4.54984809	0.15260111
F	-1.07343346	3.78120303	-0.25789677

### 3.1.4 n=5

	60		
	-90.38238890		
C	3.81284438	-3.92087792	0.52229800
C	3.11848474	-3.58848821	1.67965782
C	2.28885388	-2.47332299	1.69634958
C	2.15358267	-1.69054748	0.55568151
C	2.84794231	-2.02293719	-0.60167832
C	3.67757317	-3.13810241	-0.61837007
F	4.60367205	-4.98387292	0.50636390
F	3.24741282	-4.33463212	2.76697906

F	1.62695430	-2.15647190	2.79960491
F	1.36275500	-0.62755247	0.57161561
F	2.71901422	-1.27679328	-1.68899955
F	4.33947275	-3.45495350	-1.72162541
C	-0.44043989	-3.06491969	-2.81923550
C	-1.18363695	-2.08427168	-3.46583246
C	-1.96588525	-1.20459708	-2.72663043
C	-2.00493648	-1.30557048	-1.34083145
C	-1.26173942	-2.28621849	-0.69423450
C	-0.47949112	-3.16589309	-1.43343652
F	0.30522316	-3.90345539	-3.52383835
F	-1.14642784	-1.98800291	-4.78680500
F	-2.67433919	-0.26979261	-3.34300013
F	-2.75059953	-0.46703478	-0.63622860
F	-1.29894853	-2.38248726	0.62673805
F	0.22896281	-4.10069756	-0.81706682
C	0.58646799	0.40361929	4.59951303
C	0.32119380	0.97120944	3.35871851
C	-0.84501088	0.64077953	2.67831999
C	-1.74594137	-0.25724053	3.23871598
C	-1.48066718	-0.82483068	4.47951049
C	-0.31446250	-0.49440077	5.15990901
F	1.69811305	0.71857744	5.24810173
F	1.17996576	1.82722393	2.82451761
F	-1.09788398	1.18183587	1.49553039
F	-2.85758643	-0.57219868	2.59012728
F	-2.33943914	-1.68084516	5.01371139
F	-0.06158940	-1.03545710	6.34269861
C	5.93910258	3.15797492	1.31139519
C	5.91713532	1.89906639	0.72252614
C	5.23907249	0.85461032	1.34018442
C	4.58297692	1.06906277	2.54671175
C	4.60494418	2.32797130	3.13558080
C	5.28300701	3.37242738	2.51792252
F	6.58544030	4.15358783	0.72264808
F	6.54253271	1.69462248	-0.42756144
F	5.21813216	-0.34544650	0.77884395
F	3.93663920	0.07344987	3.13545886
F	3.97954679	2.53241522	4.28566838
F	5.30394734	4.57248420	3.07926299
C	-0.64412996	2.69151344	-1.36899242
C	0.54610191	1.97887856	-1.45616835
C	1.66178034	2.39924298	-0.74152521
C	1.58722691	3.53224228	0.06029386
C	0.39699505	4.24487715	0.14746979
C	-0.71868339	3.82451273	-0.56717335
F	-1.70763145	2.29083160	-2.05019673
F	0.61719108	0.89887625	-2.22047326
F	2.79637101	1.71992251	-0.82462582
F	2.65072841	3.93292412	0.74149817
F	0.32590588	5.32487947	0.91177470
F	-1.85327405	4.50383321	-0.48407274

### 3.1.5 n=6

72

-123.85359975

C	-0.07879649	2.84231017	1.90164758
C	-1.05661661	1.85598306	1.95756380
C	-1.40503768	1.29119920	3.17894884
C	-0.77563861	1.71274245	4.34441764

C	0.20218151	2.69906957	4.28850142
C	0.55060258	3.26385343	3.06711639
F	0.25334218	3.38068851	0.73740820
F	-1.65658674	1.45414330	0.84662666
F	-2.33714647	0.35098110	3.23225108
F	-1.10777728	1.17436411	5.50865702
F	0.80215164	3.10090932	5.39943856
F	1.48271137	4.20407152	3.01381415
C	-6.49059890	0.72740440	2.38555525
C	-5.55146733	1.62783760	2.87479132
C	-4.82896808	2.42525602	1.99486056
C	-5.04560040	2.32224123	0.62569373
C	-5.98473197	1.42180802	0.13645765
C	-6.70723122	0.62438961	1.01638841
F	-7.17931242	-0.03272215	3.22430550
F	-5.34495199	1.72605063	4.17990675
F	-3.93373923	3.28359559	2.46122574
F	-4.35688688	3.08236777	-0.21305653
F	-6.19124731	1.32359500	-1.16865778
F	-7.60246008	-0.23394996	0.55002324
C	-4.48388827	-1.81893228	5.19203140
C	-4.67170438	-2.68760674	4.12327989
C	-3.58637052	-3.36361785	3.57810209
C	-2.31322055	-3.17095451	4.10167580
C	-2.12540444	-2.30228005	5.17042732
C	-3.21073830	-1.62626894	5.71560512
F	-5.51843719	-1.17453321	5.71172268
F	-5.88528935	-2.87127315	3.62418186
F	-3.76540656	-4.19168334	2.55931278
F	-1.27867162	-3.81535358	3.58198452
F	-0.91181947	-2.11861364	5.66952534
F	-3.03170225	-0.79820346	6.73439442
C	-4.23173693	-2.64438710	-0.48526399
C	-3.35331470	-1.91543182	0.30789336
C	-2.02262384	-2.30416937	0.40940393
C	-1.57035522	-3.42186220	-0.28224285
C	-2.44877745	-4.15081748	-1.07540020
C	-3.77946831	-3.76207993	-1.17691077
F	-5.50018446	-2.27385268	-0.58204102
F	-3.78440465	-0.85001947	0.96719500
F	-1.18526627	-1.60929143	1.16548260
F	-0.30190769	-3.79239661	-0.18546582
F	-2.01768750	-5.21622982	-1.73470184
F	-4.61682588	-4.45695786	-1.93298944
C	2.82945367	-3.18103346	0.65137989
C	2.55214732	-1.84777572	0.37276727
C	1.99485458	-1.03436561	1.35253675
C	1.71486820	-1.55421323	2.61091885
C	1.99217456	-2.88747097	2.88953147
C	2.54946729	-3.70088108	1.90976199
F	3.36067711	-3.95641219	-0.28254203
F	2.81902797	-1.35222412	-0.82674263
F	1.73051179	0.23656473	1.08694876
F	1.18364476	-0.77883449	3.54484077
F	1.72529391	-3.38302256	4.08904138
F	2.81381008	-4.97181141	2.17534998
C	0.20881855	1.51906556	-2.10910045
C	-0.58385280	0.37816632	-2.15515534
C	-1.92792928	0.47897260	-2.49494343
C	-2.47933441	1.72067813	-2.78867664
C	-1.68666307	2.86157737	-2.74262176



C	-0.34258659	2.76077109	-2.40283367
F	1.49002367	1.42299885	-1.78520961
F	-0.05826305	-0.80546466	-1.87516639
F	-2.68354466	-0.60859166	-2.53884533
F	-3.76053954	1.81674484	-3.11256749
F	-2.21225281	4.04520834	-3.02261071
F	0.41302879	3.84833535	-2.35893177

### 3.1.6 n=7

84

-154.71093685

C	0.60011543	0.92160912	-4.52074990
C	-0.60817891	0.81754276	-3.84156291
C	-1.00721587	-0.40611274	-3.31659036
C	-0.19795847	-1.52570187	-3.47080480
C	1.01033587	-1.42163550	-4.14999179
C	1.40937282	-0.19798000	-4.67496434
F	0.98050639	2.08801371	-5.02117346
F	-1.37959671	1.88474589	-3.69455025
F	-2.15902462	-0.50531419	-2.66915414
F	-0.57834943	-2.69210645	-2.97038125
F	1.78175367	-2.48883863	-4.29700446
F	2.56118158	-0.09877855	-5.32240056
C	1.78725249	1.66076829	4.70019683
C	1.07702420	0.78121043	3.89146092
C	1.42445537	-0.56419875	3.85505815
C	2.48211482	-1.03005007	4.62739128
C	3.19234311	-0.15049222	5.43612718
C	2.84491194	1.19491696	5.47252996
F	1.45609142	2.94324551	4.73491267
F	0.06883674	1.22524755	3.15524781
F	0.74742897	-1.40263885	3.08412919
F	2.81327589	-2.31252730	4.59267543
F	4.20053057	-0.59452934	6.17234030
F	3.52193833	2.03335706	6.24345892
C	-1.20536314	-5.16949269	5.21590478
C	-1.82576377	-4.06336709	4.64696788
C	-1.50596780	-2.78424409	5.08712051
C	-0.56577120	-2.61124670	6.09621004
C	0.05462943	-3.71737231	6.66514695
C	-0.26516654	-4.99649530	6.22499432
F	-1.51018383	-6.38878973	4.79635770
F	-2.72198248	-4.22824790	3.68508066
F	-2.09736582	-1.72982787	4.54478038
F	-0.26095051	-1.39194967	6.51575712
F	0.95084814	-3.55249149	7.62703416
F	0.32623148	-6.05091152	6.76733445
C	4.60544577	-0.62342848	-1.71909162
C	3.50385462	-0.15115875	-1.01513264
C	3.56047901	-0.03672053	0.36901223
C	4.71869454	-0.39455203	1.04919811
C	5.82028569	-0.86682175	0.34523913
C	5.76366130	-0.98125998	-1.03890574
F	4.55149295	-0.73252182	-3.03848861
F	2.39980806	0.18993987	-1.66347946
F	2.51038527	0.41347144	1.04006239
F	4.77264736	-0.28545868	2.36859509
F	6.92433225	-1.20792037	0.99358594
F	6.81375504	-1.43145194	-1.70995591
C	2.18397062	3.74391000	-1.64401469

C	0.87763769	4.21887763	-1.64409878
C	0.22192416	4.44956922	-0.44036268
C	0.87254356	4.20529318	0.76345751
C	2.17887650	3.73032554	0.76354160
C	2.83459003	3.49963395	-0.44019450
F	2.80903062	3.52400255	-2.79142978
F	0.25743347	4.45173393	-2.79159403
F	-1.02334007	4.90233297	-0.44044284
F	0.24748356	4.42520063	1.91087259
F	2.79908072	3.49746924	1.91103684
F	4.07985425	3.04687020	-0.44011434
C	-1.03939307	0.46740574	0.22541927
C	-2.20640184	1.05667864	0.69759297
C	-3.19430060	0.27202517	1.28114624
C	-3.01519060	-1.10190118	1.39252582
C	-1.84818183	-1.69117408	0.92035212
C	-0.86028307	-0.90652062	0.33679885
F	-0.09769310	1.21533457	-0.33083993
F	-2.37715507	2.36633291	0.59143420
F	-4.30675380	0.83375062	1.73124667
F	-3.95689057	-1.84983001	1.94878502
F	-1.67742860	-3.00082835	1.02651089
F	0.25217013	-1.46824606	-0.11330158
C	1.25363401	-4.94994930	-1.02186389
C	0.33177510	-5.65032785	-0.25261359
C	0.31713639	-5.49350847	1.12845587
C	1.22435658	-4.63631053	1.74027501
C	2.14621549	-3.93593198	0.97102470
C	2.16085421	-4.09275136	-0.41004475
F	1.26760638	-5.09941722	-2.33833067
F	-0.53301619	-6.46743289	-0.83579113
F	-0.56162727	-6.16114558	1.86174511
F	1.21038421	-4.48684261	3.05674179
F	3.01100678	-3.11882694	1.55420224
F	3.03961787	-3.42511425	-1.14333399

### 3.1.7 n=8

96

-189.90249245			
C	-3.54578641	6.13826209	-0.82938358
C	-4.64332340	6.33587220	0.00035300
C	-4.56459202	7.23961231	1.05354559
C	-3.38832366	7.94574231	1.27700160
C	-2.29078666	7.74813220	0.44726502
C	-2.36951804	6.84439209	-0.60592757
F	-3.62081194	5.27680265	-1.83331558
F	-5.76457805	5.66278494	-0.21263111
F	-5.61082114	7.42798449	1.84449348
F	-3.31329812	8.80720175	2.28093360
F	-1.16953202	8.42121946	0.66024913
F	-1.32328893	6.65601990	-1.39687546
C	-3.10425382	0.39727332	-2.59893309
C	-2.75306018	0.17957758	-1.27176634
C	-3.39101657	0.88645338	-0.25909775
C	-4.38016662	1.81102493	-0.57359592
C	-4.73136026	2.02872067	-1.90076267
C	-4.09340386	1.32184486	-2.91343126
F	-2.49615352	-0.27652444	-3.56424718
F	-1.81018391	-0.70173903	-0.97195633
F	-3.05624060	0.67893452	1.00602634

F	-4.98826691	2.48482268	0.39171817
F	-5.67423653	2.91003728	-2.20057268
F	-4.42817983	1.52936372	-4.17855535
C	-4.36130525	-2.20562900	2.09674317
C	-3.58764003	-2.88174072	3.03291361
C	-2.74381322	-3.90859707	2.62587334
C	-2.67365161	-4.25934171	1.28266264
C	-3.44731683	-3.58322999	0.34649220
C	-4.29114364	-2.55637364	0.75353247
F	-5.16566626	-1.22680410	2.48471977
F	-3.65450329	-2.54742053	4.31329636
F	-2.00631546	-4.55310178	3.51827949
F	-1.86929060	-5.23816661	0.89468604
F	-3.38045357	-3.91755018	-0.93389054
F	-5.02864140	-1.91186893	-0.13887368
C	0.36460347	-1.11935811	3.85523776
C	0.00300931	-0.69206451	2.58292890
C	0.54741864	0.47559877	2.06106647
C	1.45342214	1.21596844	2.81151290
C	1.81501630	0.78867485	4.08382176
C	1.27060697	-0.37898843	4.60568419
F	-0.15432647	-2.23239678	4.35270866
F	-0.86061092	-1.39778479	1.86756909
F	0.20272836	0.88291716	0.84823575
F	1.97235208	2.32900711	2.31404200
F	2.67863653	1.49439513	4.79918157
F	1.61529725	-0.78630682	5.81851491
C	1.71119387	4.82289611	0.19038408
C	0.37894598	4.56526465	0.49178345
C	-0.37396314	3.74056332	-0.33595746
C	0.20537563	3.17349345	-1.46509775
C	1.53762353	3.43112491	-1.76649712
C	2.29053265	4.25582624	-0.93875621
F	2.42890235	5.60901608	0.97939016
F	-0.17331325	5.10579698	1.56809903
F	-1.64393084	3.49497568	-0.04864797
F	-0.51233284	2.38737348	-2.25410383
F	2.08988275	2.89059258	-2.84281270
F	3.56050035	4.50141388	-1.22606570
C	-3.56624037	3.68216052	3.11286233
C	-4.90895608	3.63410337	3.46909966
C	-5.40522318	2.53621691	4.16229785
C	-4.55877457	1.48638761	4.49925871
C	-3.21605886	1.53444476	4.14302139
C	-2.71979176	2.63233122	3.44982320
F	-3.09316580	4.72867949	2.45209067
F	-5.71582768	4.63481176	3.14791186
F	-6.68516934	2.49040634	4.50188171
F	-5.03184913	0.43986865	5.16003038
F	-2.40918725	0.53373637	4.46420919
F	-1.43984559	2.67814179	3.11023933
C	1.74390241	-0.96404684	-1.48140770
C	1.01404146	-1.16485585	-2.64720302
C	0.27975059	-2.33312297	-2.81491790
C	0.27532067	-3.30058110	-1.81683744
C	1.00518161	-3.09977209	-0.65104211
C	1.73947249	-1.93150497	-0.48332724
F	2.44385162	0.14956286	-1.32151646
F	1.01824941	-0.24266769	-3.59860828
F	-0.41599067	-2.52454451	-3.92621439
F	-0.42462854	-4.41419080	-1.97672868

F	1.00097366	-4.02196025	0.30036314
F	2.43521375	-1.74008343	0.62796925
C	-1.20445571	6.66992031	4.77280641
C	-0.15066962	7.34923322	4.17266572
C	1.09138989	6.73714093	4.05104896
C	1.27966331	5.44573573	4.52957289
C	0.22587723	4.76642282	5.12971359
C	-1.01618228	5.37851511	5.25133035
F	-2.38842235	7.25336004	4.88874500
F	-0.33011278	8.58022920	3.71651911
F	2.09591337	7.38469718	3.47896376
F	2.46362995	4.86229600	4.41363431
F	0.40532038	3.53542684	5.58586020
F	-2.02070577	4.73095886	5.82341555

### 3.1.8 n=9

	108		
	-221.54537288		
C	-0.73170249	-4.03463723	3.22578886
C	-1.83666497	-3.74898751	2.43233934
C	-3.04795046	-3.40969294	3.02380031
C	-3.15427348	-3.35604810	4.40871080
C	-2.04931100	-3.64169782	5.20216033
C	-0.83802550	-3.98099239	4.61069936
F	0.42293104	-4.35806247	2.66201746
F	-1.73533891	-3.80011664	1.11221074
F	-4.10125793	-3.13739683	2.26744312
F	-4.30890701	-3.03262285	4.97248221
F	-2.15063706	-3.59056869	6.52228893
F	0.21528197	-4.25328850	5.36705655
C	3.44319760	2.35618335	-0.84206522
C	3.52254546	3.71541501	-0.56225598
C	3.25714407	4.64688873	-1.55929072
C	2.91239482	4.21913078	-2.83613469
C	2.83304696	2.85989912	-3.11594393
C	3.09844835	1.92842540	-2.11890919
F	3.69617965	1.46826451	0.10831412
F	3.85116600	4.12318620	0.65485201
F	3.33278256	5.94257875	-1.29256206
F	2.65941276	5.10704962	-3.78651403
F	2.50442641	2.45212793	-4.33305192
F	3.02280986	0.63273538	-2.38563785
C	1.59210309	1.99184993	3.15563898
C	2.84639575	1.46639587	3.44329842
C	2.96039136	0.17616313	3.94774258
C	1.82009430	-0.58861556	4.16452729
C	0.56580164	-0.06316151	3.87686785
C	0.45180603	1.22707124	3.37242369
F	1.48341590	3.22172520	2.67479121
F	3.93336530	2.19538112	3.23666254
F	4.15604809	-0.32472689	4.22195446
F	1.92878149	-1.81849084	4.64537506
F	-0.52116791	-0.79214676	4.08350373
F	-0.74385070	1.72796126	3.09821180
C	-3.83448308	-2.87828531	-3.93920079
C	-3.94312185	-3.06899547	-2.56663849
C	-5.15803225	-2.84833873	-1.92831038
C	-6.26430386	-2.43697182	-2.66254456
C	-6.15566508	-2.24626166	-4.03510685
C	-4.94075469	-2.46691841	-4.67343497

F	-2.67641433	-3.08861402	-4.54769014
F	-2.88861322	-3.46111898	-1.86673038
F	-5.26159236	-3.03013353	-0.61991291
F	-7.42237260	-2.22664312	-2.05405520
F	-7.21017371	-1.85413816	-4.73501497
F	-4.83719458	-2.28512361	-5.98183244
C	-0.00334834	-0.13082193	-1.82434558
C	-0.11359118	-1.23483385	-2.66166523
C	0.26541306	-2.49253486	-2.20701878
C	0.75466014	-2.64622395	-0.91505268
C	0.86490298	-1.54221203	-0.07773303
C	0.48589874	-0.28451102	-0.53237948
F	-0.36461732	1.06805538	-2.25770293
F	-0.57994934	-1.08835789	-3.89319904
F	0.16032387	-3.54493621	-3.00519524
F	1.11592911	-3.84510126	-0.48169533
F	1.33126114	-1.68868799	1.15380078
F	0.59098792	0.76789033	0.26579698
C	-3.46319495	1.57694817	-4.01644412
C	-2.51284048	1.32343109	-4.99861288
C	-1.45402795	2.20450696	-5.18510890
C	-1.34556989	3.33909992	-4.38943616
C	-2.29592436	3.59261701	-3.40726740
C	-3.35473689	2.71154113	-3.22077138
F	-4.47248637	0.73710162	-3.83865418
F	-2.61620479	0.24191892	-5.75707707
F	-0.54810084	1.96284135	-6.12136303
F	-0.33627846	4.17894647	-4.56722610
F	-2.19256004	4.67412917	-2.64880321
F	-4.26066400	2.95320675	-2.28451725
C	-2.04572396	0.27327232	7.06975577
C	-3.42163362	0.07585932	7.06891678
C	-4.26290511	1.04796891	6.54031043
C	-3.72826694	2.21749149	6.01254307
C	-2.35235728	2.41490449	6.01338206
C	-1.51108579	1.44279491	6.54198841
F	-1.24378657	-0.65334973	7.57362944
F	-3.93128460	-1.03894703	7.57199068
F	-5.57449347	0.85978461	6.53951066
F	-4.53020432	3.14411354	5.50866940
F	-1.84270630	3.52971085	5.51030816
F	-0.19949742	1.63097921	6.54278819
C	-0.54543031	4.25387284	0.23571111
C	-0.18059053	5.38483227	0.95676776
C	-0.97678429	5.82612223	2.00724295
C	-2.13781783	5.13645276	2.33666148
C	-2.50265761	4.00549332	1.61560483
C	-1.70646385	3.56420336	0.56512964
F	0.21350338	3.83320738	-0.76562844
F	0.92612735	6.04225593	0.64277676
F	-0.62900011	6.90421134	2.69459150
F	-2.89675152	5.55711821	3.33800103
F	-3.60937549	3.34806966	1.92959583
F	-2.05424803	2.48611425	-0.12221890
C	-5.95721458	0.66405611	1.16843370
C	-5.25898852	0.40556726	-0.00534817
C	-3.93050363	0.00047203	0.05108937
C	-3.30024480	-0.14613435	1.28130879
C	-3.99847086	0.11235450	2.45509066
C	-5.32695575	0.51744973	2.39865312
F	-7.22355572	1.05020275	1.11466044

F	-5.85974441	0.54530894	-1.17803112
F	-3.26491839	-0.24593293	-1.06782031
F	-2.03390366	-0.53228099	1.33508205
F	-3.39771497	-0.02738718	3.62777361
F	-5.99254099	0.76385469	3.51756280

### 3.1.9 n=10

120  
-257.38142004

C	-1.57454472	-5.27512027	5.09757670
C	-0.54042995	-4.35290756	5.20816764
C	0.62446073	-4.52298028	4.46907062
C	0.75523665	-5.61526571	3.61938266
C	-0.27887812	-6.53747842	3.50879172
C	-1.44376880	-6.36740570	4.24788873
F	-2.68495275	-5.11302359	5.80209024
F	-0.66506622	-3.31170994	6.01810220
F	1.61023249	-3.64387935	4.57449164
F	1.86564468	-5.77736239	2.91486911
F	-0.15424185	-7.57867604	2.69885715
F	-2.42954057	-7.24650663	4.14246772
C	-0.32737899	3.97495241	-1.42542162
C	0.60197765	2.95145357	-1.28103898
C	0.98136428	2.53115620	-0.01156061
C	0.43139428	3.13435768	1.11353513
C	-0.49796236	4.15785653	0.96915248
C	-0.87734900	4.57815389	-0.30032589
F	-0.68903343	4.37560532	-2.63550592
F	1.12623411	2.37645436	-2.35349026
F	1.86727518	1.55550409	0.12607241
F	0.79304871	2.73370478	2.32361942
F	-1.02221882	4.73285574	2.04160376
F	-1.76325989	5.55380601	-0.43795890
C	5.65103048	-4.08920645	2.10294741
C	6.62154318	-3.87968380	1.13016513
C	7.55156068	-2.85827550	1.28492943
C	7.51106548	-2.04638986	2.41247601
C	6.54055278	-2.25591252	3.38525829
C	5.61053529	-3.27732081	3.23049399
F	4.76450756	-5.06282881	1.95544391
F	6.66016322	-4.65357830	0.05535517
F	8.47670365	-2.65854765	0.35762297
F	8.39758841	-1.07276751	2.55997952
F	6.50193274	-1.48201802	4.46006826
F	4.68539231	-3.47704866	4.15780045
C	2.42743134	-0.47760042	2.47540441
C	1.10511065	-0.75844826	2.79896660
C	0.46069508	-1.84092596	2.21148890
C	1.13860019	-2.64255581	1.30044902
C	2.46092088	-2.36170797	0.97688683
C	3.10533645	-1.27923027	1.56436452
F	3.04172232	0.55423543	3.03538838
F	0.45889706	0.00566888	3.66738681
F	-0.79980950	-2.10864467	2.51992514
F	0.52430921	-3.67439166	0.74046504
F	3.10713447	-3.12582511	0.10846662
F	4.36584103	-1.01151156	1.25592829
C	-3.07420127	0.75121647	1.81870460
C	-3.77619166	-0.34810331	1.33828239
C	-4.10814920	-1.38994881	2.19649075

C	-3.73811633	-1.33247452	3.53512133
C	-3.03612593	-0.23315475	4.01554355
C	-2.70416840	0.80869075	3.15733518
F	-2.75776139	1.74433773	1.00066021
F	-4.12892539	-0.40291061	0.06227465
F	-4.77732281	-2.43787736	1.73852741
F	-4.05455621	-2.32559578	4.35316573
F	-2.68339220	-0.17834745	5.29155128
F	-2.03499479	1.85661931	3.61529852
C	2.64676161	-5.16671146	-2.41724531
C	3.80429328	-5.73949943	-1.90330526
C	3.72289234	-6.65466792	-0.86023289
C	2.48395973	-6.99704843	-0.33110057
C	1.32642806	-6.42426045	-0.84504061
C	1.40782900	-5.50909196	-1.88811299
F	2.72433060	-4.29435079	-3.41152424
F	4.98528141	-5.41314994	-2.40766992
F	4.82631148	-7.20067909	-0.37031862
F	2.40639074	-7.86940909	0.66317837
F	0.14543993	-6.75060994	-0.34067595
F	0.30440985	-4.96308080	-2.37802726
C	-3.03539465	-6.22530953	0.18807439
C	-2.65296701	-4.92340586	0.48956391
C	-2.55660193	-3.97534035	-0.52238717
C	-2.84266450	-4.32917850	-1.83582777
C	-3.22509214	-5.63108217	-2.13731729
C	-3.32145721	-6.57914769	-1.12536621
F	-3.12725865	-7.12904272	1.15267172
F	-2.38028117	-4.58609703	1.74155667
F	-2.19205210	-2.73429833	-0.23499174
F	-2.75080050	-3.42544531	-2.80042509
F	-3.49777797	-5.96839100	-3.38931004
F	-3.68600705	-7.82018971	-1.41276163
C	4.90179084	2.93775265	1.19004387
C	5.80745818	1.88345323	1.17217217
C	6.27073157	1.38567056	-0.04016014
C	5.82833760	1.94218731	-1.23462074
C	4.92267026	2.99648672	-1.21674904
C	4.45939688	3.49426939	-0.00441673
F	4.46017507	3.41226605	2.34565333
F	6.22917144	1.35295382	2.31074539
F	7.13406059	0.38065774	-0.05719638
F	6.26995337	1.46767390	-2.39023020
F	4.50095700	3.52698613	-2.35532226
F	3.59606785	4.49928221	0.01261951
C	-1.70974310	0.34011138	-2.58991635
C	-1.90131013	0.12657634	-3.94999166
C	-1.15146894	-0.83682210	-4.61464275
C	-0.21006071	-1.58668551	-3.91921852
C	-0.01849368	-1.37315047	-2.55914320
C	-0.76833487	-0.40975202	-1.89449212
F	-2.42449648	1.25843816	-1.95633589
F	-2.79867514	0.84135046	-4.61290544
F	-1.33408056	-1.04037476	-5.91113698
F	0.50469267	-2.50501229	-4.55279898
F	0.87887133	-2.08792458	-1.89622943
F	-0.58572324	-0.20619936	-0.59799788
C	4.06059931	-1.16339071	-5.09554523
C	3.46624595	-0.57816906	-3.98362810
C	3.95207358	-0.85283125	-2.71056422
C	5.03225457	-1.71271507	-2.54941747

C	5.62660793	-2.29793672	-3.66133461
C	5.14078030	-2.02327453	-4.93439849
F	3.59751480	-0.90159135	-6.30906676
F	2.43659303	0.24149388	-4.13721262
F	3.38550517	-0.29496766	-1.65062721
F	5.49533907	-1.97451443	-1.33589594
F	6.65626084	-3.11759966	-3.50775009
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### 3.1.10 n=11

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C	3.59853887	0.60442472	2.26856343
F	5.02202198	-0.21209094	0.58435665
F	3.65275830	-2.55538564	0.51073273
F	1.52825770	-2.93855900	2.15724651
F	0.77302079	-0.97843764	3.87738421
F	2.14228447	1.36485707	3.95100813
F	4.26678506	1.74803042	2.30449435
C	-0.80599780	-5.28095499	-1.44502624
C	0.35588433	-4.51948766	-1.49295767
C	0.58545088	-3.66877248	-2.56801224
C	-0.34686469	-3.57952463	-3.59513537
C	-1.50874682	-4.34099196	-3.54720393
C	-1.73831338	-5.19170714	-2.47214937
F	-1.02484669	-6.09188182	-0.42027090
F	1.24460167	-4.60454439	-0.51389306
F	1.69301712	-2.94290238	-2.61370296
F	-0.12801580	-2.76859779	-4.61989071
F	-2.39746416	-4.25593522	-4.52626854
F	-2.84587961	-5.91757724	-2.42645864
C	-1.70791706	-3.36494385	3.40451563
C	-2.03724822	-2.66102452	2.25206669
C	-2.70142457	-1.44365735	2.34717916
C	-3.03626977	-0.93020951	3.59474056
C	-2.70693861	-1.63412884	4.74718950
C	-2.04276226	-2.85149601	4.65207704
F	-1.07480989	-4.52536642	3.31387657
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F	-3.01536009	-0.77264497	1.24860513
F	-3.66937694	0.23021306	3.68537963
F	-3.02611027	-1.14471864	5.93640259
F	-1.72882674	-3.52250838	5.75065106
C	-5.49051326	3.19792284	-1.35021309
C	-6.35613522	4.28543980	-1.33994273
C	-6.80076589	4.80842398	-0.13124486
C	-6.37977461	4.24389120	1.06718266
C	-5.51415264	3.15637424	1.05691231
C	-5.06952197	2.63339006	-0.15178557
F	-5.06666874	2.69938639	-2.50235800
F	-6.75744640	4.82358084	-2.48229742
F	-7.62592159	5.84510147	-0.12145463
F	-6.80361912	4.74242765	2.21932757
F	-5.11284146	2.61823319	2.19926699
F	-4.24436627	1.59671256	-0.16157580



C	-1.41370699	1.78609514	-2.12361307
C	-2.03677247	0.54449249	-2.17169900
C	-1.45942887	-0.54795778	-1.53499953
C	-0.25901978	-0.39880540	-0.85021413
C	0.36404570	0.84279726	-0.80212820
C	-0.21329790	1.93524753	-1.43882767
F	-1.96402499	2.82745632	-2.73052135
F	-3.18102876	0.40229371	-2.82444528
F	-2.05336716	-1.73151774	-1.58083753
F	0.29129822	-1.44016657	-0.24330585
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C	-5.31894253	-2.05160071	-1.89980218
C	-6.14605127	-0.93448677	-1.90670085
C	-6.76324281	-0.51942926	-0.73240902
C	-6.55332562	-1.22148568	0.44878148
C	-5.72621688	-2.33859962	0.45568015
C	-5.10902533	-2.75365713	-0.71861168
F	-4.73061178	-2.44726081	-3.01915051
F	-6.34616341	-0.26525601	-3.03262535
F	-7.55168570	0.54546161	-0.73898519
F	-7.14165636	-0.82582558	1.56812981
F	-5.52610473	-3.00783038	1.58160465
F	-4.32058244	-3.81854800	-0.71203551
C	3.65360687	0.56010806	-3.02564426
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C	4.55908517	2.77712906	-3.27320513
C	3.36912303	3.19815793	-3.85534277
C	2.32140281	2.30016186	-4.02263116
C	2.46364473	0.98113693	-3.60778191
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F	5.83563380	1.05679267	-2.30345221
F	5.55782636	3.63314543	-3.11373717
F	3.23355751	4.45548575	-4.25077847
F	1.18709610	2.70147332	-4.57753482
F	1.46490355	0.12512056	-3.76724986
C	2.94340581	4.49610216	0.22539823
C	3.44823032	5.70556263	-0.23769740
C	3.01502079	6.90054191	0.32489788
C	2.07698675	6.88606072	1.35058881
C	1.57216224	5.67660024	1.81368444
C	2.00537177	4.48162096	1.25108915
F	3.35633595	3.35700980	-0.31086474
F	4.34238533	5.71939065	-1.21540712
F	3.49624566	8.05346229	-0.11654886
F	1.66405661	8.02515308	1.88685177
F	0.67800723	5.66277222	2.79139416
F	1.52414690	3.32870058	1.69253590
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C	-2.50969586	5.96964685	-2.02322158
C	-1.15548309	5.97985231	-1.70991171
C	-0.20700015	5.98251622	-2.72604776
C	-0.61272998	5.97497468	-4.05549367
C	-1.96694274	5.96476922	-4.36880354
F	-4.20628504	5.95237719	-3.65134485
F	-3.41379252	5.96710773	-1.05460223
F	-0.76872040	5.98704130	-0.44261501
F	1.08385920	5.99224434	-2.42737040
F	0.29136669	5.97751380	-5.02411302
F	-2.35370543	5.95758022	-5.63610024
C	-1.33980889	2.49648486	4.15740288

C	-1.86749387	3.60116157	4.81568697
C	-2.42206247	4.64588410	4.08550348
C	-2.44894609	4.58592994	2.69703590
C	-1.92126112	3.48125323	2.03875182
C	-1.36669251	2.43653069	2.76893530
F	-0.81117709	1.50062107	4.85340891
F	-1.84187872	3.65833283	6.13920349
F	-2.92507912	5.69891916	4.71301397
F	-2.97757790	5.58179373	2.00102988
F	-1.94687626	3.42408197	0.71523529
F	-0.86367586	1.38349564	2.14142481
C	-4.39521619	-0.13476596	-5.92809625
C	-3.03941151	-0.43015489	-6.00957668
C	-2.10065216	0.59360437	-5.95659268
C	-2.51769749	1.91275256	-5.82212826
C	-3.87350217	2.20814150	-5.74064784
C	-4.81226152	1.18438224	-5.79363183
F	-5.29007971	-1.11061910	-5.97859956
F	-2.64185179	-1.68758806	-6.13775135
F	-0.80822892	0.31202434	-6.03426405
F	-1.62283397	2.88860571	-5.77162495
F	-4.27106189	3.46557467	-5.61247317
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-329.02843962

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C	-0.44407505	-5.83620581	-0.87757075
C	-0.97225465	-6.90547596	-1.59156491
C	-0.17189019	-7.99999198	-1.89752380
F	1.91955982	-9.06856467	-1.78114646
F	2.95122757	-6.98001082	-0.38653609
F	1.38795716	-4.84216799	0.21108072
F	-1.20698101	-4.79287900	-0.58591283
F	-2.23864876	-6.88143285	-1.98052320
F	-0.67537835	-9.01927568	-2.57814001
C	5.67388482	1.13268864	1.03458303
C	6.20954138	2.13288205	0.23159786
C	6.95089334	1.79704945	-0.89524427
C	7.15658874	0.46102344	-1.21910123
C	6.62093218	-0.53916998	-0.41611606
C	5.87958022	-0.20333738	0.71072607
F	4.96720882	1.45278798	2.10871808
F	6.01348096	3.40641756	0.54028585
F	7.46150892	2.75048562	-1.66069133
F	7.86326474	0.14092409	-2.29323628
F	6.81699261	-1.81270549	-0.72480405
F	5.36896464	-1.15677355	1.47617313
C	3.00419615	-2.03156615	-3.09266978
C	2.68359000	-3.38395177	-3.07356931
C	3.66244868	-4.33410594	-3.34040672
C	4.96191350	-3.93187448	-3.62634459
C	5.28251965	-2.57948886	-3.64544506
C	4.30366098	-1.62933469	-3.37860765
F	2.07114327	-1.12584103	-2.83831767
F	1.44491873	-3.76739067	-2.80100966
F	3.35683029	-5.62326996	-3.32219917

F	5.89496638	-4.83759960	-3.88069670
F	6.52119092	-2.19604996	-3.91800471
F	4.60927937	-0.34017067	-3.39681520
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C	-4.47145823	1.73352943	0.22302713
C	-3.45424379	1.28104250	1.05530701
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C	-2.10772315	3.18036361	0.44226469
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F	-5.27642229	3.34077291	-1.29298730
F	-5.59803127	1.04393625	0.11855181
F	-3.61119966	0.16010987	1.74418501
F	-1.30275908	1.57312014	1.95827911
F	-0.98115010	3.86995679	0.54674000
F	-2.96798171	4.75378318	-1.07889320
C	3.60236401	5.23463892	2.23482670
C	3.73796656	5.11840400	3.61330462
C	3.13879902	4.05832311	4.28366736
C	2.40402892	3.11447713	3.57555217
C	2.26842636	3.23071205	2.19707424
C	2.86759391	4.29079295	1.52671151
F	4.17349466	6.24512255	1.59580145
F	4.43836060	6.01808649	4.28831594
F	3.26806240	3.94752196	5.59770392
F	1.83289826	2.10399350	4.21457741
F	1.56803232	2.33102956	1.52206293
F	2.73833052	4.40159409	0.21267495
C	4.97481931	0.36455979	5.44875574
C	3.84251780	0.02739984	6.18109205
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C	4.12101134	-2.27919692	5.54975178
C	5.25331285	-1.94203696	4.81741547
C	5.68021683	-0.62015861	4.76691745
F	5.38177191	1.62459623	5.40060569
F	3.17010196	0.96603794	6.83104290
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F	3.71405874	-3.53923335	5.59790183
F	5.92572869	-2.88067507	4.16746462
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C	-0.66452150	-1.44506259	2.75290286
C	0.56515661	-1.00121639	3.22512347
C	1.65099893	-0.91434812	2.36166542
C	1.50716315	-1.27132604	1.02598677
C	0.27748504	-1.71517224	0.55376616
C	-0.80835728	-1.80204052	1.41722420
F	-1.69958366	-1.52787538	3.57595148
F	0.70228731	-0.66093199	4.49831723
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F	-1.98055015	-2.22513770	0.96707906
C	2.54048592	3.78663460	-3.62466974
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C	0.45193519	2.98383845	-2.73594388
C	1.14211849	2.11490773	-1.89882629
C	2.53148551	2.08184045	-1.92463043
C	3.23066922	2.91770388	-2.78755215
F	3.20698387	4.58338856	-4.44721717
F	0.49320025	4.64797730	-4.39681520
F	-0.87248141	3.01535990	-2.71134604
F	0.47562055	1.31815377	-1.07627886

F	3.18940417	1.25356504	-1.12668084
F	4.55508583	2.88618243	-2.81214999
C	-5.27400618	-3.01703518	1.94479724
C	-4.49350665	-3.18235040	3.08303771
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C	-4.31467759	-5.01164073	0.99728728
C	-5.18459165	-3.93168035	0.90192203
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F	-2.87958001	-4.41989782	4.26343273
F	-2.70495025	-6.20638994	2.22645395
F	-4.22946236	-5.88348769	0.00318371
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C	-2.24230340	-0.65068307	-2.63090171
C	-1.26964605	-0.87507218	-3.59821097
C	-1.09123941	-2.15033702	-4.12168982
C	-1.88549012	-3.20121275	-3.67785940
C	-2.85814747	-2.97682365	-2.71055013
C	-3.03655411	-1.70155881	-2.18707129
F	-2.41238226	0.56491856	-2.13189616
F	-0.51253755	0.12663013	-4.02129472
F	-0.16405205	-2.36423634	-5.04377911
F	-1.71541127	-4.41681438	-4.17686494
F	-3.61525598	-3.97852596	-2.28746638
F	-3.96374148	-1.48765949	-1.26498199
C	5.62386567	-6.54354866	2.35775316
C	4.57646788	-5.73466883	2.78292525
C	4.13051733	-4.69396385	1.97656262
C	4.73196456	-4.46213869	0.74502790
C	5.77936235	-5.27101852	0.31985581
C	6.22531290	-6.31172350	1.12621844
F	6.04897197	-7.53557691	3.12637872
F	4.00314036	-5.95563093	3.95684687
F	3.13208351	-3.92289770	2.38185868
F	4.30685826	-3.47011044	-0.02359766
F	6.35268987	-5.05005642	-0.85406581
F	7.22374672	-7.08278965	0.72092238
C	0.64853133	-6.78274327	3.54692601
C	0.41108456	-5.43074447	3.76559990
C	0.64162301	-4.87865364	5.02027403
C	1.10960823	-5.67856161	6.05627428
C	1.34705500	-7.03056041	5.83760039
C	1.11651654	-7.58265124	4.58292626
F	0.42878421	-7.30902984	2.35095180
F	-0.03500912	-4.66823574	2.77807696
F	0.41527645	-3.58985835	5.22872531
F	1.32935535	-5.15227504	7.25224849
F	1.79314867	-7.79306914	6.82512333
F	1.34286310	-8.87144653	4.37447498

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C	5.73069469	-1.44626545	5.21886502
C	4.47098209	-1.57733562	4.64611310
C	3.48043085	-0.64263750	4.92415467

F	2.80536200	1.31409313	6.03996905
F	5.26589791	1.57010616	7.15869777
F	7.20067937	-0.25555430	6.61563531
F	6.67492491	-2.33722780	4.95384413
F	4.21438900	-2.59324083	3.83511541
F	2.27960754	-0.76758037	4.37817787
C	-2.96450298	-1.11898068	-4.96664314
C	-2.48330261	-1.71160560	-3.80503137
C	-1.91727547	-0.92651607	-2.80733044
C	-1.83244869	0.45119837	-2.97124128
C	-2.31364906	1.04382329	-4.13285305
C	-2.87967620	0.25873377	-5.13055399
F	-3.50405625	-1.86732510	-5.91768655
F	-2.56415077	-3.02487079	-3.64876627
F	-1.45857035	-1.49143685	-1.70002193
F	-1.29289542	1.19954279	-2.02019787
F	-2.23280090	2.35708848	-4.28911816
F	-3.33838132	0.82365454	-6.23786250
C	5.71891702	-4.71342869	1.47376863
C	4.37631141	-5.07261525	1.45151583
C	3.70151667	-5.16477392	0.23977400
C	4.36932754	-4.89774604	-0.94971505
C	5.71193315	-4.53855948	-0.92746226
C	6.38672789	-4.44640081	0.28427958
F	6.36216618	-4.62557474	2.62881532
F	3.73971935	-5.32715653	2.58535002
F	2.42167545	-5.50716915	0.21856148
F	3.72607838	-4.98559999	-2.10476175
F	6.34852521	-4.28401820	-2.06129644
F	7.66656911	-4.10400557	0.30549209
C	6.19589490	2.21717144	0.91209760
C	6.27314514	2.16173637	-0.47464656
C	6.43311434	0.93759486	-1.11343200
C	6.51583330	-0.23111160	-0.36547329
C	6.43858306	-0.17567653	1.02127087
C	6.27861386	1.04846499	1.66005631
F	6.04340887	3.38403833	1.52102317
F	6.19429803	3.27575969	-1.18763735
F	6.50675327	0.88475128	-2.43534836
F	6.66831933	-1.39797848	-0.97439886
F	6.51743016	-1.28969984	1.73426166
F	6.20497493	1.10130856	2.98197267
C	0.80516399	0.58597179	0.58227859
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C	2.29502525	-1.22961175	1.11173990
C	1.21391918	-1.99271363	1.53723328
C	-0.07156449	-1.46647281	1.48524931
C	-0.27594208	-0.17713010	1.00777197
F	0.61032301	1.81499868	0.12714065
F	3.12119630	0.78711785	0.22867843
F	3.52041487	-1.73125176	1.16129372
F	1.40876016	-3.22174053	1.99237122
F	-1.10211313	-2.19385970	1.89083344
F	-1.50133170	0.32450991	0.95821816
C	-3.95447783	-3.29466373	0.48258867
C	-4.05608728	-4.32328520	1.41195049
C	-4.37746060	-4.03661547	2.73357793
C	-4.59722448	-2.72132426	3.12584355
C	-4.49561503	-1.69270279	2.19648173
C	-4.17424171	-1.97937252	0.87485429
F	-3.64813903	-3.56789989	-0.77722053

F	-3.84660787	-5.57705663	1.03805711
F	-4.47431999	-5.01715074	3.61949375
F	-4.90356328	-2.44808810	4.38565275
F	-4.70509444	-0.43893136	2.57037511
F	-4.07738232	-0.99883725	-0.01106153
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C	1.95909402	4.19094692	3.00276798
C	3.09861990	3.49023526	3.38044957
C	4.04472670	4.09263318	4.20152088
C	3.85130762	5.39574277	4.64491061
C	2.71178175	6.09645444	4.26722902
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F	1.05725804	3.61670804	2.22010443
F	3.28299698	2.24804369	2.95778751
F	5.13093976	3.42468050	4.56152238
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F	2.52740467	7.33864601	4.68989107
C	-3.78552051	2.87712629	1.93642641
C	-4.39916557	2.48801562	0.75146539
C	-3.87214360	2.89246640	-0.46952882
C	-2.73147657	3.68602784	-0.50556200
C	-2.11783151	4.07513851	0.67939902
C	-2.64485348	3.67068774	1.90039323
F	-4.28787155	2.49160700	3.10031600
F	-5.48647487	1.73157588	0.78578876
F	-4.45710186	2.52154595	-1.59909504
F	-2.22912553	4.07154713	-1.66945159
F	-1.03052221	4.83157825	0.64507566
F	-2.05989522	4.04160818	3.02995945
C	-1.57559076	2.82660325	6.67226612
C	-0.55944530	2.58572200	5.75491960
C	-0.68846817	1.55701080	4.82903310
C	-1.83363650	0.76918086	4.82049311
C	-2.84978195	1.01006212	5.73783963
C	-2.72075908	2.03877331	6.66372613
F	-1.45262515	3.80718745	7.55485026
F	0.53216279	3.33668570	5.76304153
F	0.28017431	1.32739031	3.95457088
F	-1.95660210	-0.21140333	3.93790897
F	-3.94139004	0.25909841	5.72971770
F	-3.68940157	2.26839380	7.53818835
C	1.83646154	-0.63084445	-4.83605663
C	2.73667098	-0.96842680	-5.83992969
C	4.00252561	-1.43790941	-5.50923715
C	4.36817081	-1.56980966	-4.17467154
C	3.46796138	-1.23222731	-3.17079848
C	2.20210674	-0.76274470	-3.50149103
F	0.62981621	-0.18332142	-5.15125633
F	2.38815191	-0.84270476	-7.11207320
F	4.86065188	-1.75971039	-6.46618095
F	5.57481615	-2.01733269	-3.85947184
F	3.81648044	-1.35794935	-1.89865498
F	1.34398047	-0.44094372	-2.54454722
C	0.26375895	-3.03410367	5.78802476
C	-0.65911023	-3.60795542	4.92136066
C	-0.35472530	-4.79782049	4.27041491
C	0.87252879	-5.41383382	4.48613326
C	1.79539797	-4.83998207	5.35279736
C	1.49101304	-3.65011700	6.00374311
F	-0.02636566	-1.89989904	6.40853119
F	-1.82896154	-3.02077600	4.71571798

F	-1.23445200	-5.34484570	3.44426580
F	1.16265340	-6.54803845	3.86562683
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F	2.37073974	-3.10309179	6.82989222
C	1.71415022	5.21720453	-1.06481773
C	2.54034893	4.10188147	-1.13931708
C	2.44276508	3.23576000	-2.22212382
C	1.51898252	3.48496158	-3.23043120
C	0.69278380	4.60028464	-3.15593185
C	0.79036765	5.46640612	-2.07312512
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F	3.42092574	3.86431718	-0.17818839
F	3.23034049	2.17257628	-2.29314046
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F	-0.18779301	4.83784894	-4.11706054
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C	-1.26034611	-5.98911650	-1.78568743
C	-0.53378684	-4.95174673	-1.21290861
C	0.35274690	-4.21336401	-1.98815588
C	0.51272137	-4.51235107	-3.33618197
C	-0.21383790	-5.54972084	-3.90896080
C	-1.10037164	-6.28810356	-3.13371353
F	-2.10541491	-6.69297230	-1.04672437
F	-0.68626171	-4.66672792	0.07205690
F	1.04534083	-3.22448941	-1.44215343
F	1.35779017	-3.80849527	-4.07514504
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C	3.91269345	2.29987677	-2.17980651
C	2.79833666	2.55428145	-1.38882823
F	0.82875991	3.78130784	-1.00839679
F	1.23308676	5.20744523	-3.28303644
F	3.40966542	4.71055379	-4.82800778
F	5.18191724	2.78752495	-4.09833947
F	4.77759039	1.36138756	-1.82369982
F	2.60101172	1.85827901	-0.27872848
C	3.10747458	-1.67766544	-2.03500323
C	3.12801340	-2.55620223	-0.95803932
C	4.22873698	-3.38023292	-0.75422454
C	5.30892174	-3.32572682	-1.62737367
C	5.28838293	-2.44719002	-2.70433757
C	4.18765935	-1.62315933	-2.90815235
F	2.05825180	-0.89217221	-2.22930352
F	2.09836927	-2.60817578	-0.12572183
F	4.24831564	-4.21769970	0.27239324
F	6.35814453	-4.11122005	-1.43307338
F	6.31802705	-2.39521647	-3.53665506
F	4.16808069	-0.78569255	-3.93477013
C	1.15718107	-5.43877848	2.79091249
C	2.23053382	-5.95677699	3.50623858
C	2.00265351	-6.78889789	4.59610317
C	0.70142045	-7.10302027	4.97064167

C	-0.37193230	-6.58502176	4.25531558
C	-0.14405199	-5.75290086	3.16545099
F	1.37437757	-4.64558083	1.75202663
F	3.47090576	-5.65736236	3.14923860
F	3.02582895	-7.28268090	5.27798905
F	0.48422394	-7.89621792	6.00952753
F	-1.61230425	-6.88443639	4.61231556
F	-1.16722743	-5.25911785	2.48356511
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C	1.20173078	3.22143166	4.40505344
C	0.80624315	4.39129980	3.76696449
C	1.52951005	4.86890508	2.68025495
C	2.64826458	4.17664222	2.23163435
C	3.04375221	3.00677407	2.86972330
F	2.69749120	1.41402308	4.56465752
F	0.51228191	2.76618676	5.44092650
F	-0.26021161	5.05120062	4.19461287
F	1.15250416	5.98405079	2.07203026
F	3.33771345	4.63188711	1.19576129
F	4.11020697	2.34687325	2.44207492
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C	5.76808637	-2.55093574	3.46897739
C	4.46719276	-2.60789184	3.95538385
C	3.46493256	-1.85989267	3.34864570
C	3.76356597	-1.05493741	2.25550110
C	5.06445959	-0.99798132	1.76909465
F	7.30675256	-1.69167306	1.91216255
F	6.72344630	-3.26395337	4.04734920
F	4.18251991	-3.37521689	4.99742590
F	2.22489979	-1.91420009	3.81231595
F	2.80820605	-0.34191978	1.67712930
F	5.34913244	-0.23065627	0.72705260
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C	-0.63561735	1.18754700	-4.59162059
C	0.52392500	0.43722084	-4.74856529
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C	-1.95150182	-0.69527838	-5.31257556
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C	-2.11553814	4.77705832	0.33421182



C	-2.71928787	3.61941397	-0.14276331
F	-3.53237127	2.36617908	-1.95876224
F	-2.81713955	4.33488045	-3.68618578
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F	-1.17385472	6.88846820	-0.09553126
F	-1.88908644	4.91976683	1.63189228
F	-3.06834472	2.65862227	0.70027679
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C	-0.17614168	-4.61681940	-2.41239582
C	0.47887093	-5.51610758	-1.57908994
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C	-1.64463171	-6.34119579	-0.80042092
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C	-4.63482720	-1.43225199	-1.79461185
C	-5.36549964	-2.49177821	-2.31960898
C	-6.24737945	-3.19703858	-1.50901953
F	-7.23921951	-3.51505639	0.59921964
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F	-4.08951974	-0.06799089	0.04142917
F	-3.79419450	-0.75996835	-2.56726445
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C	-1.23641062	-1.50092311	6.34796225
C	-0.53603372	-0.38760646	6.79758174
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F	1.39863941	-3.97749260	6.32734764
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C	-0.33357950	-0.10866713	2.19888427
C	-0.60703639	-1.44895543	1.95200657
C	-0.85025392	-1.88090678	0.65338318
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C	-0.30334014	0.79966982	1.14713858
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F	-1.05185782	-1.38433781	-1.63623023
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C	-4.76765814	0.45813732	4.87435581
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C	-4.24074193	-4.61805696	2.29801384
C	-4.08725478	-3.88350334	3.46807029
C	-4.59069938	-4.37358906	4.66742825
C	-5.24763113	-5.59822841	4.69672976
F	-6.02732332	-7.50013222	3.55462800
F	-5.04396924	-6.54287140	1.21197991
F	-3.76083245	-4.15088187	1.15472371
F	-3.46104974	-2.71615315	3.44011559
F	-4.44440382	-3.67341397	5.78276368
F	-5.72754061	-6.06540351	5.84001989

### 3.1.14 n=15

	180		
	-445.18845565		
C	-0.92417383	9.44339978	0.20077181
C	0.14081177	9.71744990	1.05094956
C	1.15198943	8.77932120	1.22297787
C	1.09818148	7.56714238	0.54482843
C	0.03319588	7.29309227	-0.30534932
C	-0.97798177	8.23122097	-0.47737763
F	-1.88806145	10.33762932	0.03677531
F	0.19212359	10.87291821	1.69738653
F	2.16718886	9.04055997	2.03341133
F	2.06206910	6.67291284	0.70882492
F	-0.01811594	6.13762396	-0.95178629
F	-1.99318121	7.96998220	-1.28781110
C	0.52787193	2.92815943	-4.00863456
C	1.63692804	2.84591103	-4.84249892
C	2.90570188	3.10929188	-4.33950498
C	3.06541962	3.45492111	-3.00264668
C	1.95636352	3.53716951	-2.16878232
C	0.68758968	3.27378866	-2.67177626
F	-0.68156023	2.67710343	-4.48807736
F	1.48470559	2.51645161	-6.11682442
F	3.96291160	3.03088845	-5.13438768
F	4.27485179	3.70597711	-2.52320387
F	2.10858596	3.86662893	-0.89445681
F	-0.36962004	3.35219209	-1.87689356
C	-1.38666878	3.96959542	1.83846512
C	-0.11359179	3.44993864	1.63516284
C	0.03977114	2.17175855	1.11085862
C	-1.07994292	1.41323524	0.78985669
C	-2.35301991	1.93289202	0.99315897
C	-2.50638284	3.21107211	1.51746318
F	-1.53288174	5.18798185	2.33824202
F	0.95375818	4.17296132	1.94114148
F	1.25333407	1.67639480	0.91706036
F	-0.93372996	0.19484881	0.29007978
F	-3.42036988	1.20986935	0.68718033
F	-3.71994577	3.70643586	1.71126145
C	1.03350069	0.64955837	6.32336568
C	1.46463534	-0.48436984	7.00191541

C	1.69542205	-1.66515748	6.30575632
C	1.49507413	-1.71201691	4.93104750
C	1.06393948	-0.57808871	4.25249777
C	0.83315276	0.60269893	4.94865686
F	0.81350345	1.77512157	6.98693885
F	1.65561797	-0.43972574	8.31231734
F	2.10640193	-2.74607658	6.95258508
F	1.71507137	-2.83758012	4.26747433
F	0.87295684	-0.62273281	2.94209585
F	0.42217288	1.68361804	4.30182811
C	-1.41982001	-4.81921300	1.60858606
C	-1.24020097	-4.43794428	2.93315058
C	-1.64260164	-3.17565976	3.35371085
C	-2.22462133	-2.29464397	2.44970661
C	-2.40424037	-2.67591269	1.12514209
C	-2.00183970	-3.93819721	0.70458182
F	-1.03625069	-6.02244480	1.20767649
F	-0.68540949	-5.27773098	3.79488452
F	-1.47137947	-2.81221467	4.61635436
F	-2.60819065	-1.09141217	2.85061618
F	-2.95903185	-1.83612598	0.26340815
F	-2.17306187	-4.30164230	-0.55806169
C	-6.56145496	-0.33126904	1.19962262
C	-6.89191041	1.00251792	0.99007180
C	-6.61308418	1.94961834	1.96854825
C	-6.00380251	1.56293180	3.15657553
C	-5.67334707	0.22914484	3.36612635
C	-5.95217330	-0.71795558	2.38764990
F	-6.82722867	-1.23408292	0.26693184
F	-7.47269136	1.37113886	-0.14237368
F	-6.92809142	3.22105316	1.76879355
F	-5.73802880	2.46574569	4.08926631
F	-5.09256612	-0.13947609	4.49857183
F	-5.63716605	-1.98939039	2.58740459
C	0.35134222	6.82622606	4.89709999
C	0.24595101	8.07988882	5.48813500
C	0.06525129	8.18750387	6.86215321
C	-0.01005722	7.04145616	7.64513642
C	0.09533399	5.78779340	7.05410142
C	0.27603371	5.68017835	5.68008320
F	0.52358939	6.72362090	3.58735812
F	0.31773382	9.17233994	4.74179831
F	-0.03521307	9.38256015	7.42555839
F	-0.18230439	7.14406132	8.95487829
F	0.02355118	4.69534228	7.80043811
F	0.37649807	4.48512207	5.11667802
C	-3.49016331	7.54441545	3.17471762
C	-3.87570812	7.19840348	4.46457456
C	-5.06381478	6.50769942	4.67311689
C	-5.86637663	6.16300734	3.59180228
C	-5.48083183	6.50901932	2.30194534
C	-4.29272516	7.19972337	2.09340302
F	-2.35763861	8.20280947	2.97590669
F	-3.11070470	7.52696096	5.49532207
F	-5.43133606	6.17786288	5.90267533
F	-6.99890133	5.50461332	3.79061321
F	-6.24583524	6.18046184	1.27119784
F	-3.92520388	7.52955991	0.86384457
C	-6.74281050	7.97056418	-1.52770656
C	-6.01057374	7.62487305	-2.65749723
C	-4.92065341	8.39693470	-3.04240494

C	-4.56296986	9.51468748	-2.29752197
C	-5.29520662	9.86037861	-1.16773129
C	-6.38512694	9.08831696	-0.78282359
F	-7.78174984	7.23463310	-1.16078534
F	-6.35150706	6.55941128	-3.36755101
F	-4.22264740	8.06740401	-4.11937993
F	-3.52403052	10.25061856	-2.66444318
F	-4.95427330	10.92584037	-0.45767752
F	-7.08313296	9.41784765	0.29415140
C	-1.91578281	-0.66592549	-3.23769738
C	-2.17167012	-2.00480295	-3.50977978
C	-3.41677764	-2.54817962	-3.21548656
C	-4.40599784	-1.75267884	-2.64911095
C	-4.15011053	-0.41380138	-2.37702856
C	-2.90500301	0.12957530	-2.67132177
F	-0.72892685	-0.14794561	-3.51821557
F	-1.22873920	-2.76311042	-4.04966100
F	-3.66070268	-3.82446697	-3.47484960
F	-5.59285380	-2.27065872	-2.36859276
F	-5.09304144	0.34450609	-1.83714733
F	-2.66107797	1.40586264	-2.41195873
C	-0.25559080	9.31696857	-4.08814679
C	-1.12303575	8.98654797	-5.12277789
C	-0.97946610	7.77570572	-5.79016701
C	0.03154850	6.89528407	-5.42292505
C	0.89899344	7.22570467	-4.38829395
C	0.75542379	8.43654692	-3.72090483
F	-0.39242557	10.47116398	-3.45196296
F	-2.08676396	9.82576934	-5.47285800
F	-1.80635955	7.46073168	-6.77643096
F	0.16838326	5.74108866	-6.05910888
F	1.86272165	6.38648330	-4.03821384
F	1.58231724	8.75152096	-2.73464088
C	3.32812959	-1.69599658	0.94709141
C	4.10169948	-0.75396665	0.27905755
C	3.65203294	-0.20767926	-0.91740788
C	2.42879651	-0.60342180	-1.44583945
C	1.65522663	-1.54545173	-0.77780559
C	2.10489317	-2.09173912	0.41865984
F	3.75674132	-2.21674298	2.08758948
F	5.26771809	-0.37672132	0.78275114
F	4.38943982	0.69031247	-1.55421236
F	2.00018479	-0.08267540	-2.58633752
F	0.48920801	-1.92269705	-1.28149918
F	1.36748628	-2.98973085	1.05546432
C	-2.66110309	1.34771088	7.85025776
C	-2.86899563	2.68594251	8.16333410
C	-2.95412255	3.63201792	7.14851679
C	-2.83135693	3.23986170	5.82062314
C	-2.62346440	1.90163007	5.50754680
C	-2.53833748	0.95555466	6.52236411
F	-2.57995495	0.44587396	8.81758698
F	-2.98602142	3.05977730	9.42910390
F	-3.15229649	4.90768963	7.44695737
F	-2.91250508	4.14169862	4.85329393
F	-2.50643861	1.52779528	4.24177700
F	-2.34016354	-0.32011705	6.22392353
C	3.79099647	2.77074520	3.01586163
C	4.21479713	3.36015357	1.83049637
C	4.42585216	4.73287773	1.77354378
C	4.21310654	5.51619352	2.90195643

C	3.78930589	4.92678515	4.08732168
C	3.57825085	3.55406099	4.14427428
F	3.58980784	1.46223687	3.07017338
F	4.41759724	2.61349983	0.75485657
F	4.82984090	5.29473231	0.64359222
F	4.41429517	6.82470184	2.84764467
F	3.58650578	5.67343889	5.16296148
F	3.17426211	2.99220640	5.27422584
C	-3.55187969	4.44881455	-4.40374287
C	-4.70991745	3.68134506	-4.35858597
C	-5.33154897	3.43224964	-3.14051981
C	-4.79514275	3.95062371	-1.96761056
C	-3.63710499	4.71809320	-2.01276746
C	-3.01547347	4.96718862	-3.23083361
F	-2.95931004	4.68627063	-5.56481844
F	-5.22124936	3.18720947	-5.47661565
F	-6.43545054	2.70065797	-3.09747392
F	-5.38771240	3.71316763	-0.80653498
F	-3.12577308	5.21222879	-0.89473778
F	-1.91157190	5.69878029	-3.27387950

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C	1.96633144	-1.71854219	0.78353303
C	1.64575816	-2.34065432	-0.41745353
C	0.42133003	-2.08900458	-1.02535826
C	-0.48252482	-1.21524271	-0.43227643
F	-1.02354104	0.23975435	1.33403029
F	1.36807541	-0.25178096	2.52142130
F	3.13351976	-1.95842776	1.36301931
F	2.50734766	-3.17353925	-0.98277369
F	0.11573121	-2.68200394	-2.17016470
F	-1.64971314	-0.97535715	-1.01176270
C	-0.90695257	5.07822724	2.55098114
C	-1.01163339	5.12151412	1.16560459
C	-0.17644163	4.33513531	0.38060615
C	0.76343093	3.50546964	0.98098425
C	0.86811175	3.46218277	2.36636079
C	0.03292000	4.24856157	3.15135924
F	-1.70306484	5.82781169	3.29927860
F	-1.90753283	5.91236185	0.59328937
F	-0.27622881	4.37639860	-0.94000654
F	1.55954320	2.75588520	0.23268679
F	1.76401120	2.67133503	2.93867602
F	0.13270718	4.20729828	4.47197192
C	-4.59692840	0.01171308	-6.24275458
C	-4.55277630	1.37595898	-5.98010710
C	-5.43421068	1.93598824	-5.06271945
C	-6.35979716	1.13177160	-4.40797928
C	-6.40394927	-0.23247431	-4.67062676
C	-5.52251489	-0.79250357	-5.58801441
F	-3.75673591	-0.52214075	-7.11722433
F	-3.67049573	2.14257502	-6.60420766
F	-5.39212261	3.23645811	-4.81235027
F	-7.19998966	1.66562542	-3.53350954
F	-7.28622984	-0.99909035	-4.04652620
F	-5.56460296	-2.09297343	-5.83838359

C	0.82909938	1.72850445	-5.95294955
C	1.57131138	2.42728158	-5.00799883
C	1.21546264	2.37218840	-3.66542822
C	0.11740190	1.61831807	-3.26780832
C	-0.62481011	0.91954094	-4.21275904
C	-0.26896137	0.97463413	-5.55532965
F	1.16828353	1.78100583	-7.23272234
F	2.61801046	3.14589352	-5.38699565
F	1.92297757	3.03829896	-2.76465225
F	-0.22178226	1.56581669	-1.98803553
F	-1.67150919	0.20092900	-3.83376222
F	-0.97647630	0.30852357	-6.45610562
C	1.97187984	-6.22331556	-2.18325339
C	2.97561355	-7.12894029	-2.50645994
C	3.20540618	-8.23165383	-1.69197996
C	2.43146510	-8.42874263	-0.55429342
C	1.42773139	-7.52311790	-0.23108687
C	1.19793876	-6.42040436	-1.04556686
F	1.75281863	-5.17217809	-2.95961857
F	3.71336331	-6.94109123	-3.59092234
F	4.16221715	-9.09494223	-2.00007718
F	2.65052631	-9.47988010	0.22207175
F	0.68998163	-7.71096696	0.85337552
F	0.24112779	-5.55711596	-0.73746964
C	-2.81856566	-5.11819646	-2.05503614
C	-3.45035504	-3.88048706	-2.02313590
C	-3.28909002	-2.99045191	-3.07859336
C	-2.49603563	-3.33812615	-4.16595107
C	-1.86424625	-4.57583555	-4.19785131
C	-2.02551127	-5.46587070	-3.14239385
F	-2.97227260	-5.96661314	-1.04896259
F	-4.20631634	-3.54905503	-0.98665338
F	-3.89134439	-1.81060320	-3.04818440
F	-2.34232869	-2.48970947	-5.17202462
F	-1.10828495	-4.90726758	-5.23433382
F	-1.42325691	-6.64571941	-3.17280281
C	0.81829188	-4.69561623	3.56720237
C	1.83919745	-5.42522510	2.96927034
C	2.18207865	-6.67711328	3.46663129
C	1.50405427	-7.19939258	4.56192427
C	0.48314871	-6.46978371	5.15985630
C	0.14026751	-5.21789553	4.66249536
F	0.49143301	-3.50228732	3.09312425
F	2.48551865	-4.92739716	1.92521243
F	3.15525871	-7.37261424	2.89665150
F	1.83091315	-8.39272149	5.03600239
F	-0.16317249	-6.96761165	6.20391421
F	-0.83291256	-4.52239457	5.23247514
C	2.67048805	6.42513836	-3.25381319
C	2.32642847	6.44873593	-1.90727461
C	3.12941728	5.80437526	-0.97337538
C	4.27646566	5.13641702	-1.38601475
C	4.62052524	5.11281945	-2.73255333
C	3.81753643	5.75718012	-3.66645255
F	1.90507683	7.03934988	-4.14404380
F	1.23304184	7.08544188	-1.51391489
F	2.80144186	5.82686969	0.31021494
F	5.04187688	4.52220550	-0.49578414
F	5.71391187	4.47611350	-3.12591305
F	4.14551185	5.73468569	-4.95004288
C	6.03658653	1.43225722	0.36873423

C	4.69866528	1.10443275	0.18272921
C	4.19540098	0.94080405	-1.10261515
C	5.03005792	1.10499981	-2.20195449
C	6.36797916	1.43282428	-2.01594947
C	6.87124346	1.59645298	-0.73060511
F	6.51633081	1.58823659	1.59394300
F	3.90303373	0.94791286	1.23062837
F	2.92002515	0.62830479	-1.27992477
F	4.55031363	0.94902044	-3.42716326
F	7.16361071	1.58934417	-3.06384862
F	8.14661929	1.90895224	-0.55329549
C	-3.87764665	1.73169679	1.40639765
C	-4.89791880	0.92361219	1.89439766
C	-5.63849150	0.13569545	1.02095692
C	-5.35879205	0.15586330	-0.34048383
C	-4.33851989	0.96394790	-0.82848384
C	-3.59794719	1.75186464	0.04495690
F	-3.17170368	2.48276437	2.23896157
F	-5.16455210	0.90437168	3.19214847
F	-6.61106777	-0.63461265	1.48614381
F	-6.06473502	-0.59520428	-1.17304775
F	-4.07188659	0.98318841	-2.12623464
F	-2.62537092	2.52217273	-0.42022999
C	3.84418436	-2.59974056	-4.15414861
C	4.30713038	-3.72013053	-4.83422750
C	3.50957681	-4.32741015	-5.79718087
C	2.24907721	-3.81429980	-6.08005535
C	1.78613118	-2.69390983	-5.39997645
C	2.58368476	-2.08663021	-4.43702308
F	4.60441228	-2.02085207	-3.23623668
F	5.50866242	-4.20925579	-4.56460200
F	3.95088093	-5.39542390	-6.44546730
F	1.48884929	-4.39318829	-6.99796727
F	0.58459914	-2.20478457	-5.66960195
F	2.14238064	-1.01861646	-3.78873665
C	-1.81475119	0.75476490	4.84349475
C	-2.67701025	1.60490946	5.52603671
C	-3.65305347	1.07845429	6.36409638
C	-3.76683765	-0.29814545	6.51961408
C	-2.90457859	-1.14829002	5.83707211
C	-1.92853536	-0.62183484	4.99901245
F	-0.88435818	1.25657089	4.04463288
F	-2.56856724	2.91711729	5.37780920
F	-4.47500347	1.88885613	7.01473073
F	-4.69723065	-0.79995145	7.31847594
F	-3.01302159	-2.46049785	5.98529962
F	-1.10658536	-1.43223668	4.34837809
C	-1.88922746	6.84657237	-3.20997968
C	-1.78789712	5.50608930	-3.56344439
C	-2.75453139	4.60094433	-3.14096338
C	-3.82249600	5.03628242	-2.36501765
C	-3.92382634	6.37676549	-2.01155294
C	-2.95719207	7.28191047	-2.43403395
F	-0.96782260	7.70939398	-3.61268632
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228

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C	1.50605304	-0.99429399	-9.39641301
C	1.15302801	-0.27558269	-8.26019700
C	1.73153970	-0.58469703	-7.03468789
C	2.66307641	-1.61252267	-6.94539481
F	3.90406459	-3.31097542	-7.99647094
F	2.77408560	-2.70719728	-10.39019880
F	0.95458573	-0.69963019	-10.56463177
F	0.26506486	0.70415875	-8.34533688
F	1.39504384	0.10038061	-5.95160903
F	3.21454371	-1.90718647	-5.77717606

### 3.1.19 n=20

240

-638.37417354

C	-1.88935683	5.46752077	0.66375964
C	-1.22277385	4.45649849	1.34610932
C	-0.06963777	4.74702420	2.06585331
C	0.41691534	6.04857219	2.10324763
C	-0.24966763	7.05959448	1.42089795
C	-1.40280372	6.76906876	0.70115396
F	-2.98855284	5.19060870	-0.02232235
F	-1.68654844	3.21582761	1.31047838
F	0.56578366	3.78326539	2.71630437
F	1.51611135	6.32548427	2.78932963
F	0.21410695	8.30026536	1.45652889
F	-2.03822514	7.73282757	0.05070290
C	-7.27428273	2.51741650	4.29727129
C	-5.90033193	2.72748075	4.31250888
C	-5.30103329	3.47934277	3.30866422
C	-6.07568547	4.02114054	2.28958198
C	-7.44963628	3.81107629	2.27434439
C	-8.04893491	3.05921427	3.27818905
F	-7.84556877	1.80072875	5.25414725
F	-5.16189688	2.21103713	5.28391010
F	-3.99131221	3.67958690	3.32318948
F	-5.50439944	4.73782829	1.33270601
F	-8.18807133	4.32751992	1.30294317
F	-9.35865599	2.85897015	3.26366379
C	-6.28209686	-1.63730359	-4.70782957
C	-5.45258268	-0.52873987	-4.83068194
C	-4.17794187	-0.67048953	-5.36673912
C	-3.73281525	-1.92080290	-5.77994392
C	-4.56232944	-3.02936662	-5.65709154
C	-5.83697024	-2.88761696	-5.12103436

F	-7.49711584	-1.50220853	-4.19685123
F	-5.87686577	0.66309555	-4.43681286
F	-3.38720598	0.38625083	-5.48384837
F	-2.51779627	-2.05589796	-6.29092226
F	-4.13804634	-4.22120203	-6.05096063
F	-6.62770613	-3.94435732	-5.00392511
C	-5.97031603	-2.27496005	-0.52085416
C	-6.29966575	-0.92712076	-0.43743949
C	-6.73539227	-0.39151447	0.76897161
C	-6.84176908	-1.20374747	1.89196803
C	-6.51241937	-2.55158676	1.80855336
C	-6.07669285	-3.08719305	0.60214226
F	-5.55496986	-2.78553329	-1.67082077
F	-6.19827278	-0.15286376	-1.50789091
F	-7.04934548	0.89331576	0.84848680
F	-7.25711525	-0.69317423	3.04193464
F	-6.61381234	-3.32584376	2.87900478
F	-5.76273964	-4.37202328	0.52262707
C	2.48976205	-6.42524500	0.54991939
C	3.79310264	-6.19403502	0.12571984
C	4.22051039	-6.68121743	-1.10396929
C	3.34457755	-7.39960983	-1.90945887
C	2.04123696	-7.63081981	-1.48525932
C	1.61382921	-7.14363740	-0.25557019
F	2.08232581	-5.96086179	1.72208176
F	4.62807816	-5.50925047	0.89351323
F	5.46292215	-6.46081609	-1.50833827
F	3.75201379	-7.86399304	-3.08162123
F	1.20626144	-8.31560436	-2.25305270
F	0.37141746	-7.36403873	0.14879880
C	4.07698919	3.28001242	-1.12387779
C	4.37522454	2.08755387	-1.77287569
C	3.35721723	1.19649459	-2.09198999
C	2.04097458	1.49789388	-1.76210639
C	1.74273923	2.69035243	-1.11310849
C	2.76074654	3.58141171	-0.79399420
F	5.04735945	4.12940440	-0.81968130
F	5.62988818	1.80023258	-2.08733761
F	3.64151062	0.05978133	-2.71064840
F	1.07060432	0.64850190	-2.06630288
F	0.48807559	2.97767372	-0.79864658
F	2.47645316	4.71812497	-0.17533578
C	2.71288144	-1.65309050	6.92426216
C	1.46797666	-1.38942150	6.36498516
C	0.42218829	-0.95425493	7.17066262
C	0.62130469	-0.78275736	8.53561708
C	1.86620946	-1.04642635	9.09489408
C	2.91199784	-1.48159292	8.28921662
F	3.70976403	-2.06790159	6.15629241
F	1.27815154	-1.55288965	5.06388360
F	-0.76451943	-0.70291199	6.63753081
F	-0.37557790	-0.36794627	9.30358683
F	2.05603459	-0.88295820	10.39599563
F	4.09870555	-1.73293586	8.82234842
C	3.41054439	2.25697936	5.53738418
C	3.57640264	1.68695548	4.28053741
C	3.84420794	2.49424189	3.18111555
C	3.94615497	3.87155219	3.33854047
C	3.78029672	4.44157607	4.59538725
C	3.51249143	3.63428966	5.69480910
F	3.15526597	1.48747616	6.58539106

F	3.47922890	0.37407599	4.13045284
F	4.00231261	1.95086561	1.98302411
F	4.20143340	4.64105539	2.29053359
F	3.87747046	5.75445556	4.74547182
F	3.35438675	4.17766594	6.89290055
C	-2.42881037	-5.56592269	2.34039602
C	-2.35849234	-4.24905367	2.77972661
C	-1.40437928	-3.88042009	3.72096887
C	-0.52058425	-4.82865553	4.22288054
C	-0.59090227	-6.14552455	3.78354996
C	-1.54501533	-6.51415813	2.84230770
F	-3.33828332	-5.91733499	1.44318423
F	-3.20093452	-3.34515821	2.30130749
F	-1.33734850	-2.62511233	4.13976154
F	0.38888871	-4.47724322	5.12009234
F	0.25153990	-7.04942000	4.26196908
F	-1.61204612	-7.76946589	2.42351503
C	-0.71248985	0.54447047	-7.59576434
C	-0.23994026	1.48854397	-6.69159505
C	0.91952134	1.23762091	-5.96713259
C	1.60643334	0.04262434	-6.14683942
C	1.13388375	-0.90144916	-7.05100870
C	-0.02557785	-0.65052610	-7.77547117
F	-1.81771150	0.78363419	-8.28634850
F	-0.89470316	2.62764746	-6.52027822
F	1.36998009	2.13756067	-5.10523159
F	2.71165499	-0.19653938	-5.45625525
F	1.78864665	-2.04055265	-7.22232554
F	-0.47603660	-1.55046587	-8.63737216
C	-4.22726405	-2.35225617	6.17338188
C	-4.88871243	-1.17234782	6.49338552
C	-4.65447976	-0.55387448	7.71599961
C	-3.75879869	-1.11530947	8.61861006
C	-3.09735031	-2.29521782	8.29860642
C	-3.33158299	-2.91369117	7.07599233
F	-4.45052400	-2.94181585	5.00796563
F	-5.74249925	-0.63715775	5.63301332
F	-5.28500662	0.57087528	8.02104366
F	-3.53553874	-0.52574979	9.78402631
F	-2.24356349	-2.83040789	9.15897862
F	-2.70105612	-4.03844092	6.77094828
C	-0.56523870	5.91911577	-6.04978890
C	-1.57536608	6.27883893	-5.16528795
C	-1.37291423	6.16341474	-3.79494130
C	-0.16033501	5.68826738	-3.30909559
C	0.84979237	5.32854421	-4.19359654
C	0.64734053	5.44396841	-5.56394319
F	-0.75819777	6.02913219	-7.35603690
F	-2.73123089	6.73176210	-5.62838384
F	-2.33581997	6.50632149	-2.95178918
F	0.03262407	5.57825096	-2.00284759
F	2.00565719	4.87562104	-3.73050065
F	1.61024627	5.10106166	-6.40709531
C	-0.27175430	-4.81727909	-7.14883497
C	0.77995091	-5.15419650	-7.99293378
C	1.97729642	-5.61790516	-7.46048899
C	2.12293671	-5.74469641	-6.08394537
C	1.07123150	-5.40777900	-5.23984656
C	-0.12611400	-4.94407034	-5.77229135
F	-1.41309899	-4.37525987	-7.65635046
F	0.64114610	-5.03334440	-9.30508799

F	2.97983630	-5.93907228	-8.26512770
F	3.26428140	-6.18671563	-5.57642988
F	1.21003631	-5.52863110	-3.92769235
F	-1.12865389	-4.62290322	-4.96765264
C	-2.74479129	-6.81474614	-2.02335966
C	-2.96525900	-7.95340032	-1.25722609
C	-4.25761039	-8.29528961	-0.87630742
C	-5.32949408	-7.49852473	-1.26152233
C	-5.10902637	-6.35987055	-2.02765591
C	-3.81667498	-6.01798126	-2.40857457
F	-1.51290264	-6.48883040	-2.38647115
F	-1.94353159	-8.71290871	-0.89001937
F	-4.46777163	-9.38071375	-0.14598921
F	-6.56138273	-7.82444047	-0.89841084
F	-6.13075378	-5.60036216	-2.39486262
F	-3.60651374	-4.93255712	-3.13889278
C	3.52201724	-3.11516490	2.95798598
C	4.85510246	-2.73126297	3.04518186
C	5.37768157	-1.82223481	2.13263690
C	4.56717548	-1.29710859	1.13289605
C	3.23409027	-1.68101052	1.04570017
C	2.71151115	-2.59003868	1.95824513
F	3.02386196	-3.98166873	3.82783258
F	5.62771305	-3.23181158	3.99814809
F	6.64844745	-1.45627959	2.21575653
F	5.06533076	-0.43060476	0.26304945
F	2.46147967	-1.18046191	0.09273394
F	1.44074527	-2.95599389	1.87512550
C	-0.69519023	-1.83377652	-3.04349118
C	-1.82571161	-2.15059572	-2.29941658
C	-1.73424644	-3.05358014	-1.24660478
C	-0.51225989	-3.63974536	-0.93786757
C	0.61826148	-3.32292616	-1.68194217
C	0.52679632	-2.41994174	-2.73475398
F	-0.78235310	-0.97303501	-4.04705850
F	-2.99054601	-1.59186268	-2.59369345
F	-2.81191797	-3.35558862	-0.53731433
F	-0.42509703	-4.50048687	0.06569974
F	1.78309589	-3.88165920	-1.38766530
F	1.60446785	-2.11793326	-3.44404443
C	-2.02625624	2.98753644	7.86023332
C	-3.16300913	3.69368388	7.48440269
C	-3.09404953	4.62456952	6.45442407
C	-1.88833704	4.84930771	5.80027609
C	-0.75158415	4.14316028	6.17610672
C	-0.82054375	3.21227464	7.20608534
F	-2.09196641	2.10019133	8.84202835
F	-4.31233104	3.47947508	8.10793649
F	-4.17766126	5.29770583	6.09616284
F	-1.82262687	5.73665283	4.81848106
F	0.39773776	4.35736908	5.55257292
F	0.26306799	2.53913833	7.56434657
C	4.77508384	-3.25959755	-3.49132851
C	4.87609481	-2.67624386	-4.74894342
C	5.76208931	-1.62593156	-4.95874633
C	6.54707282	-1.15897294	-3.91093434
C	6.44606184	-1.74232663	-2.65331943
C	5.56006735	-2.79263893	-2.44351651
F	3.93054166	-4.26077907	-3.29131661
F	4.12784154	-3.12134243	-5.74775519
F	5.85837820	-1.06984861	-6.15757001

F	7.39161499	-0.15779142	-4.11094624
F	7.19431512	-1.29722806	-1.65450765
F	5.46377846	-3.34872188	-1.24469284
C	-2.89336872	2.08113347	-1.75029523
C	-2.66561777	2.52763774	-3.04677640
C	-3.65437284	3.23315347	-3.72262433
C	-4.87087885	3.49216493	-3.10199109
C	-5.09862980	3.04566066	-1.80550991
C	-4.10987473	2.34014493	-1.12966198
F	-1.95088062	1.40861877	-1.10604309
F	-1.50602567	2.28075404	-3.63839728
F	-3.43726883	3.65878447	-4.95849735
F	-5.81336695	4.16467963	-3.74624323
F	-6.25822190	3.29254436	-1.21388904
F	-4.32697874	1.91451393	0.10621103
C	-1.97875497	0.77302793	3.89866877
C	-2.81776455	0.21439381	2.94154243
C	-2.29245006	-0.24269332	1.73851480
C	-0.92812598	-0.14114633	1.49261351
C	-0.08911639	0.41748780	2.44973985
C	-0.61443088	0.87457492	3.65276748
F	-2.47947387	1.20873989	5.04542783
F	-4.11827086	0.11758679	3.17591908
F	-3.09223746	-0.77521230	0.82613240
F	-0.42740707	-0.57685829	0.34585446
F	1.21138992	0.51429481	2.21536320
F	0.18535652	1.40709390	4.56514989

### 3.2 $K^+(Bz)_n$ $n = 1 - 4$ (MP2/TZV)

#### 3.2.1 $n=1$

13

-830.4616153832			
C	-0.915782	1.099496	3.073245
C	-0.026648	0.095555	3.467546
C	1.344932	0.250483	3.246885
C	1.827381	1.409362	2.631927
C	0.938249	2.413304	2.237623
C	-0.433330	2.258372	2.458284
H	-1.969031	0.998949	3.282244
H	-0.394434	-0.778928	3.980516
H	2.034510	-0.504545	3.589723
H	2.888868	1.547738	2.500695
H	1.314277	3.325619	1.802415
H	-1.114673	3.051234	2.193207
K	0.182980	0.001121	0.276829

#### 3.2.2 $n=2$

25

-1062.0853868996			
C	-0.422688	1.135151	3.190394
C	-0.764623	-0.200433	3.428168
C	-1.883627	-0.752812	2.812040
C	-2.668300	0.027888	1.956633
C	-2.325041	1.363312	1.717855
C	-1.205996	1.915599	2.334103
H	0.418896	1.577261	3.705431
H	-0.186282	-0.791741	4.119920
H	-2.170063	-1.768963	3.029808
H	-3.561963	-0.388374	1.512369

H	-2.952105	1.978145	1.092208
H	-0.968196	2.955930	2.181879
C	2.933485	0.242599	-1.117740
C	2.771910	1.413742	-0.369839
C	2.803709	1.362735	1.027403
C	2.997830	0.141637	1.676790
C	3.160744	-1.029170	0.929411
C	3.127639	-0.978717	-0.468181
H	2.951678	0.289345	-2.197594
H	2.665163	2.365025	-0.873202
H	2.720686	2.274305	1.602319
H	3.066049	0.107041	2.754991
H	3.354245	-1.967598	1.431010
H	3.296497	-1.877004	-1.045378
K	0.084003	-0.233984	0.340720

### 3.2.3 n=3 (s1)

37

-1293.7121683519

C	2.374867	-1.841714	-0.891465
C	1.611406	-2.730201	-0.130410
C	1.651843	-2.668392	1.264985
C	2.453912	-1.715928	1.898574
C	3.217624	-0.827656	1.137519
C	3.179325	-0.891283	-0.257856
H	2.378625	-1.918977	-1.969489
H	1.021274	-3.492577	-0.619269
H	1.093480	-3.382877	1.853425
H	2.518223	-1.696584	2.977281
H	3.870036	-0.118274	1.627005
H	3.802088	-0.231597	-0.845649
C	-0.777307	1.604084	-2.193158
C	-0.268194	0.401168	-2.689544
C	-0.913569	-0.803284	-2.399246
C	-2.068340	-0.805673	-1.612845
C	-2.575877	0.396966	-1.114180
C	-1.930355	1.601396	-1.404240
H	-0.301672	2.539509	-2.452520
H	0.601073	0.408091	-3.332027
H	-0.545967	-1.728299	-2.820360
H	-2.591426	-1.732407	-1.422954
H	-3.491008	0.398454	-0.538862
H	-2.348103	2.535602	-1.056588
C	0.709944	2.510925	2.558489
C	-0.552720	2.813554	2.042065
C	-1.641020	1.985504	2.327419
C	-1.467552	0.854714	3.129383
C	-0.204331	0.550567	3.643546
C	0.884030	1.378453	3.357949
H	1.542696	3.174426	2.371925
H	-0.694567	3.710927	1.456353
H	-2.626098	2.244148	1.965702
H	-2.317316	0.237308	3.384774
H	-0.078939	-0.302241	4.295815
H	1.851124	1.168522	3.792433
K	0.205140	0.101028	0.481407

### 3.2.4 n=3 (s2)

37



-1293.7114261518

C	-2.685020	0.471072	-0.915969
C	-2.841461	-0.728503	-0.216953
C	-2.841464	-0.728499	1.179938
C	-2.685013	0.471067	1.878966
C	-2.533829	1.671312	1.179941
C	-2.533829	1.671317	-0.216947
H	-2.729314	0.476753	-1.996034
H	-3.001946	-1.650667	-0.757282
H	-3.001949	-1.650664	1.720267
H	-2.729209	0.476735	2.959036
H	-2.456542	2.604141	1.720272
H	-2.456540	2.604149	-0.757271
C	1.970270	2.418177	1.878979
C	1.009641	3.153451	1.179950
C	1.009633	3.153460	-0.216940
C	1.970280	2.418201	-0.915960
C	2.934160	1.687182	-0.216945
C	2.934154	1.687182	1.179944
H	1.997342	2.453688	2.959042
H	0.291268	3.753525	1.720282
H	0.291244	3.753518	-0.757264
H	1.997294	2.453676	-1.996030
H	3.703382	1.153862	-0.757288
H	3.703408	1.153874	1.720254
C	1.328703	-2.587050	-0.915968
C	0.213681	-3.056289	-0.216952
C	0.213680	-3.056290	1.179938
C	1.328685	-2.587044	1.878975
C	2.445761	-2.122727	1.179951
C	2.445772	-2.122726	-0.216938
H	1.345935	-2.628241	-1.996033
H	-0.632806	-3.455787	-0.757286
H	-0.632811	-3.455792	1.720263
H	1.345873	-2.628150	2.959045
H	3.324621	-1.800633	1.720286
H	3.324637	-1.800625	-0.757260
K	0.204660	0.100733	0.481488

### 3.2.5 n=3 (s3)

37

-1293.7035526959

C	-2.372122	-1.136760	0.487296
C	-1.587458	-2.029229	1.222167
C	-0.630541	-2.812654	0.571950
C	-0.451451	-2.698289	-0.809757
C	-1.234682	-1.802291	-1.543284
C	-2.195001	-1.020495	-0.894488
H	-3.142570	-0.564492	0.985538
H	-1.763588	-2.158746	2.278896
H	-0.055762	-3.534684	1.135551
H	0.260557	-3.333168	-1.318415
H	-1.126251	-1.743859	-2.617214
H	-2.829433	-0.359687	-1.468584
C	-2.010553	-2.266328	4.965999
C	-3.258285	-1.841780	4.503235
C	-4.011293	-2.670072	3.669006
C	-3.517851	-3.921333	3.297751
C	-2.272160	-4.346530	3.760808
C	-1.517692	-3.519624	4.595109

H	-1.447244	-1.644574	5.648910
H	-3.656356	-0.886827	4.819033
H	-4.987724	-2.352751	3.330339
H	-4.113028	-4.572931	2.673895
H	-1.902588	-5.326617	3.493133
H	-0.567975	-3.863824	4.981995
C	1.338218	2.099235	2.741398
C	2.343977	1.130537	2.792476
C	2.025906	-0.190399	3.121982
C	0.701269	-0.543694	3.391063
C	-0.304698	0.425233	3.340083
C	0.014114	1.747195	3.019665
H	1.590584	3.128538	2.528458
H	3.373284	1.411596	2.619185
H	2.809684	-0.931153	3.198284
H	0.451868	-1.554992	3.679403
H	-1.320136	0.151585	3.589197
H	-0.757469	2.504500	3.017052
K	0.553791	0.148004	0.281096

### 3.2.6 n=4

49

-1525.3302228285

K	0.022566	0.001496	0.000979
C	2.238427	1.729757	-1.770501
C	1.195712	2.645994	-1.619072
C	-0.018039	2.435126	-2.273362
C	-0.201275	1.291474	-3.053430
C	0.840634	0.376358	-3.204562
C	2.055619	0.587278	-2.549579
H	3.191899	1.911048	-1.294696
H	1.353701	3.555742	-1.058156
H	-0.810929	3.164759	-2.186835
H	-1.121269	1.154608	-3.603318
H	0.710733	-0.488815	-3.839365
H	2.879170	-0.094069	-2.707023
C	2.114101	0.952919	2.400351
C	1.148999	0.236558	3.111021
C	-0.141911	0.748237	3.243292
C	-0.477789	1.960852	2.637698
C	0.486586	2.676268	1.927766
C	1.778790	2.164117	1.795207
H	3.124655	0.576035	2.328916
H	1.421466	-0.675250	3.622494
H	-0.877199	0.211815	3.826501
H	-1.461191	2.383718	2.784680
H	0.235985	3.633116	1.491857
H	2.539055	2.741507	1.289367
C	-3.011607	-1.227200	0.810891
C	-3.096883	0.100570	1.243713
C	-3.136102	1.140826	0.306548
C	-3.048221	0.855063	-1.060274
C	-2.962836	-0.474347	-1.493073
C	-2.923503	-1.513787	-0.557338
H	-3.018173	-2.031770	1.533638
H	-3.215806	0.316999	2.296152
H	-3.238796	2.165161	0.638103
H	-3.129778	1.654335	-1.783549
H	-2.931566	-0.698901	-2.550586
H	-2.908849	-2.540890	-0.894174

C	2.091526	-2.386747	0.998909
C	0.853891	-2.918489	1.366552
C	-0.061517	-3.298046	0.384814
C	0.272728	-3.176468	-0.965558
C	1.509117	-2.645322	-1.332946
C	2.425232	-2.265530	-0.350011
H	2.820154	-2.140480	1.757667
H	0.609275	-3.048719	2.411337
H	-0.996274	-3.758678	0.670366
H	-0.419953	-3.506407	-1.727042
H	1.786617	-2.599600	-2.376083
H	3.398116	-1.889033	-0.633046

### 3.3 $K^+(\text{HFBz})_n$ $n = 1 - 3$ (MP2/TZV)

#### 3.3.1 $n=1$

13

-1424.8978528008

C	-3.737664	3.781523	-1.622872
C	-2.858185	2.766934	-1.998147
C	-2.086487	2.157223	-1.019937
C	-2.132325	2.599129	0.293387
C	-3.004430	3.607672	0.683727
C	-3.781808	4.220714	-0.300735
F	-4.501326	4.362676	-2.540439
F	-2.795271	2.355193	-3.265033
F	-1.233039	1.161987	-1.327092
F	-1.344533	1.978101	1.199217
F	-3.056446	3.996233	1.927666
F	-4.617816	5.209500	0.036981
K	0.416540	-0.103784	0.569176

#### 3.3.2 $n=2$

25

-2250.9711865304

C	-3.368872	1.902988	1.995536
C	-4.466203	1.104614	2.319440
C	-4.602446	-0.162302	1.751701
C	-3.665889	-0.623451	0.828604
C	-2.572455	0.172654	0.517147
C	-2.432794	1.432672	1.082406
F	-3.221069	3.097212	2.547929
F	-5.363287	1.537992	3.190494
F	-5.630452	-0.930614	2.082843
F	-3.792825	-1.834847	0.283223
F	-1.627956	-0.271261	-0.318554
F	-1.341284	2.168616	0.767470
C	-2.879250	-2.678847	3.440231
C	-1.912040	-2.977952	2.480824
C	-0.918354	-2.047880	2.200769
C	-0.906856	-0.821046	2.849393
C	-1.860234	-0.517759	3.811259
C	-2.864626	-1.443084	4.087906
F	-3.831217	-3.556111	3.713459
F	-1.937217	-4.146530	1.842940
F	0.009420	-2.283399	1.265677
F	0.038020	0.071080	2.514942
F	-1.840962	0.666309	4.432594
F	-3.800923	-1.150122	4.978772
K	1.113035	0.063946	-0.094715

### 3.3.3 n=3 (s1)

37

-1425.0577693165

C	-1.232274	1.880909	-0.596750
C	-0.992144	2.150481	0.742420
C	-2.068468	2.254447	1.619982
C	-3.363855	2.020792	1.162912
C	-3.597366	1.746588	-0.184087
C	-2.519570	1.645463	-1.053800
F	-0.203359	1.791290	-1.470168
F	0.255791	2.355205	1.169428
F	-1.852522	2.527001	2.899043
F	-4.383294	2.094406	2.005523
F	-4.830642	1.529397	-0.621225
F	-2.703320	1.351422	-2.351447
C	-0.068124	-3.923579	1.162913
C	0.286094	-3.988702	-0.184087
C	-0.165231	-3.004743	-1.053799
C	-1.012781	-2.007636	-0.596746
C	-1.366298	-1.934463	0.742425
C	-0.918169	-2.918569	1.619986
F	0.377848	-4.843245	2.005523
F	1.090825	-4.948154	-0.621228
F	0.181286	-3.016854	-2.351447
F	-1.449631	-1.071760	-1.470163
F	-2.167562	-0.956083	1.169436
F	-1.262175	-2.867832	2.899048
C	2.358444	-0.216016	0.742418
C	2.986644	0.664126	1.619978
C	3.431985	1.902792	1.162906
C	3.311273	2.242117	-0.184093
C	2.684798	1.359279	-1.053805
C	2.245053	0.126726	-0.596753
F	1.911774	-1.399121	1.169429
F	3.114710	0.340837	2.899040
F	4.005457	2.748846	2.005515
F	3.739818	3.418760	-0.621234
F	2.522026	1.665429	-2.351452
F	1.652982	-0.719533	-1.470169
K	-0.000009	-0.000009	-3.919642

### 3.3.4 n=3 (s2)

37

-3077.201896695

C	-2.203785	-1.164493	0.000000
C	-1.002966	-1.877609	0.000000
C	0.195794	-1.176742	0.000000
C	0.208073	0.211076	0.000000
C	-0.982827	0.922881	0.000000
C	-2.194726	0.230393	0.000000
F	-3.354037	-1.815703	0.000000
F	-1.004652	-3.201565	0.000000
F	1.373492	-1.832801	0.000000
F	1.395409	0.855739	0.000000
F	-0.963849	2.251907	0.000000
F	-3.334428	0.903532	0.000000
C	-1.006065	-0.601357	-3.153110
C	0.294112	-1.072956	-2.991675

C	1.342003	-0.166596	-2.893926
C	1.108343	1.201367	-2.956244
C	-0.189877	1.675130	-3.122304
C	-1.247463	0.769994	-3.203837
F	-2.018139	-1.460016	-3.220606
F	0.529156	-2.380018	-2.892238
F	2.596306	-0.613097	-2.665630
F	2.129193	2.048965	-2.827705
F	-0.421891	2.978889	-3.176182
F	-2.490352	1.215364	-3.331919
C	1.108343	1.201367	2.956244
C	-0.189877	1.675130	3.122304
C	-1.247463	0.769994	3.203837
C	-1.006065	-0.601357	3.153110
C	0.294112	-1.072956	2.991675
C	1.342003	-0.166596	2.893926
F	2.129193	2.048965	2.827705
F	-0.421891	2.978889	3.176182
F	-2.490352	1.215364	3.331919
F	-2.018139	-1.460016	3.220606
F	0.529156	-2.380018	2.892238
F	2.596306	-0.613097	2.665630
K	4.180296	-0.590083	0.000000

### 3.3.5 n=3 (s3)

37

-3077.201677689

C	0.560930	-0.949308	-1.283173
C	0.283608	-2.155774	-0.637179
C	-0.283364	-2.155826	0.637222
C	-0.560860	-0.949411	1.283237
C	-0.279809	0.245041	0.635067
C	0.279702	0.245092	-0.634984
F	1.098005	-0.940311	-2.496118
F	0.550000	-3.300855	-1.243610
F	-0.549588	-3.300957	1.243634
F	-1.097939	-0.940513	2.496180
F	-0.522939	1.427663	1.237766
F	0.522668	1.427759	-1.237662
C	-3.445618	-1.291577	-0.171815
C	-3.751827	-0.275614	0.732874
C	-3.424853	1.042159	0.424791
C	-2.812602	1.335725	-0.787288
C	-2.519188	0.329474	-1.698578
C	-2.840404	-0.989445	-1.389960
F	-3.728675	-2.552203	0.127869
F	-4.330705	-0.564897	1.889244
F	-3.669809	2.022669	1.293200
F	-2.440738	2.607418	-1.050819
F	-1.897034	0.621436	-2.839967
F	-2.536091	-1.961462	-2.243841
C	3.751911	-0.275254	-0.732938
C	3.424718	1.042460	-0.424831
C	2.812425	1.335902	0.787256
C	2.519142	0.329580	1.698510
C	2.840576	-0.989280	1.389868
C	3.445840	-1.291289	0.171716
F	4.330849	-0.564417	-1.889307
F	3.669545	2.023031	-1.293207

F	2.440352	2.607529	1.050815
F	1.896933	0.621420	2.839901
F	2.536410	-1.961365	2.243724
F	3.729108	-2.551861	-0.127990
K	-0.000270	4.211753	0.000153

### 3.4 $\text{Ca}^{2+}(\text{H}_2\text{O})_n$ $n = 1 - 27$

#### 3.4.1 $n=1$

4			
-170.091026558086			
O	-2.14179718	-0.15310996	0.07242675
H	-2.60387750	-0.06663093	-0.76138029
H	-2.82756950	-0.36376879	0.70612242
Ca	0.20465800	0.10074000	0.48149700

#### 3.4.2 $n=2$

7			
-335.91580285			
O	0.49762654	2.43902836	0.92945298
H	0.57661654	3.15165539	0.29529660
H	0.56174751	2.86862192	1.78242947
O	-0.08831042	-2.23754831	0.03354067
H	0.59138063	-2.90086087	-0.08590614
H	-0.91111238	-2.71645631	-0.06583281
Ca	0.20465800	0.10074000	0.48149700

#### 3.4.3 $n=3$

10			
-493.64142000			
O	-1.88626144	-1.03196758	0.83633002
H	-2.04691929	-1.81326577	1.36547387
H	-2.74461862	-0.80269737	0.48011498
O	0.28370319	2.50376847	0.47238286
H	-0.17694661	3.10733489	1.05525537
H	0.78287589	3.07132423	-0.11493146
O	2.21653303	-1.16958077	0.13577881
H	3.08818993	-0.99452102	0.49046085
H	2.32536866	-1.96373463	-0.38738988
Ca	0.20465800	0.10074000	0.48149700

#### 3.4.4 $n=4$

13			
-642.74912377			
O	1.13709920	-1.71771144	1.76121374
H	1.81375278	-1.66972952	2.43654231
H	0.92145319	-2.64850107	1.70326140
O	0.11445927	-0.64992422	-1.80810003
H	0.78880175	-1.11831271	-2.30014215
H	-0.60979145	-0.55271575	-2.42635760
O	1.55899616	2.08502612	0.68707864
H	2.16716123	2.44627904	0.04220455
H	1.60375430	2.69224619	1.42566615
O	-1.99192206	0.68556946	1.28579646
H	-2.55248823	0.17912715	1.87359979
H	-2.49537813	1.47752636	1.09720355
Ca	0.20465800	0.10074000	0.48149700

### 3.4.5 n=5

16  
-778.37219156

O	0.82417177	0.03646784	-1.85757099
H	0.70009878	-0.68269264	-2.47696192
H	1.25292732	0.72253028	-2.36915484
O	0.55721209	-0.22002697	2.85467661
H	0.36858807	-1.00120626	3.37468711
H	0.92141924	0.40401562	3.48249428
O	-0.28075250	-2.27380474	0.32474730
H	0.33254558	-3.00869850	0.31949134
H	-1.14402939	-2.68115189	0.25366752
O	-2.04408180	0.99147294	0.40258403
H	-2.63125009	1.16604334	1.13810399
H	-2.54574746	1.24819310	-0.37114547
O	1.46658575	2.16770376	0.66549614
H	1.11338404	3.05690200	0.69388747
H	2.41478432	2.28408369	0.72554788
Ca	0.20465800	0.10074000	0.48149700

### 3.4.6 n=6

19  
-906.90284184

O	-0.43384487	2.28358617	-0.38645257
H	-0.33175775	3.13552407	0.03782454
H	-0.84327831	2.48237150	-1.22852125
O	1.02716719	1.15098935	2.51774225
H	1.90933458	1.47864654	2.69282077
H	0.54091846	1.32887464	3.32281989
O	0.84316089	-2.08210612	1.34944670
H	1.25259395	-2.28089141	2.19151558
H	0.74107415	-2.93404402	0.92516950
O	-1.99571299	-0.14008932	1.49451651
H	-2.32674917	-0.87681011	2.00821735
H	-2.72383569	0.48070713	1.46843735
O	2.40502899	0.34156931	-0.53152253
H	2.73606511	1.07829004	-1.04522349
H	3.13315173	-0.27922708	-0.50544326
O	-0.61785119	-0.94950935	-1.55474825
H	-0.13160250	-1.12739447	-2.35982596
H	-1.50001853	-1.27716668	-1.72982672
Ca	0.20465800	0.10074000	0.48149700

### 3.4.7 n=7

22  
-1000.78597290

O	1.70613435	-1.17486713	-1.01261629
H	2.27868626	-1.89645950	-0.75238604
H	1.84244656	-1.08862538	-1.95612694
O	-1.93006864	0.77187446	1.53340000
H	-2.44803095	1.54557566	1.31129078
H	-2.43342398	0.33526954	2.22059762
O	-1.39582838	-1.42701293	-0.63615229
H	-1.21258750	-2.06522414	-1.32560152
H	-2.33562493	-1.51097604	-0.47501985
O	-0.66086216	1.54132199	-1.31217228
H	-0.28006108	2.35533731	-1.64171835
H	-1.40547230	1.37360596	-1.88980373
O	0.89098612	0.97378339	2.70295215

H	1.76859005	1.10256360	3.06275490
H	0.30312462	1.31938159	3.37467513
O	0.45074359	-1.93112640	1.84260390
H	0.10475733	-2.80444536	1.65865142
H	0.84340066	-2.00683264	2.71227051
O	2.07873337	1.67174357	0.04801888
H	2.24479799	2.53920239	0.41702940
H	2.84260394	1.49415616	-0.50079392
Ca	0.20465800	0.10074000	0.48149700

### 3.4.8 n=8

25			
-1086.53586008			
O	0.80025035	2.17927656	-0.78905714
H	0.49521585	3.07528352	-0.64638094
H	1.42469264	2.25044620	-1.51102509
O	-1.77809287	0.65845307	-0.94923964
H	-1.79685183	1.26079612	-1.69292100
H	-2.68266948	0.35823319	-0.86069479
O	1.21341311	-1.75226247	1.83727987
H	2.06582734	-2.17470667	1.73163003
H	0.80081266	-2.22226127	2.56191289
O	1.96049938	1.14930868	1.93300553
H	2.39146550	1.99796709	1.83162444
H	2.37745035	0.75863177	2.70096025
O	-0.25628918	-1.92416469	-0.92443362
H	-0.80500963	-1.96517285	-1.70766744
H	0.03469384	-2.82576863	-0.78779451
O	2.32205407	-0.40334120	-0.76425102
H	2.41653478	-0.97552283	-1.52577096
H	3.21257928	-0.10871830	-0.57348094
O	-1.68582857	-1.00146051	1.70647325
H	-2.10274325	-1.84452195	1.52853909
H	-2.17850131	-0.64094509	2.44372031
O	-0.93874231	1.90011063	1.80219880
H	-1.77710513	2.32815178	1.62853369
H	-0.60186359	2.33994799	2.58276709
Ca	0.20465800	0.10074000	0.48149700

### 3.4.9 n=9

28			
-1161.40436609			
O	-1.53428426	-0.66577274	2.05039211
H	-2.08251093	-1.42463085	1.85086040
H	-1.76500563	-0.43283806	2.94969189
O	0.07573558	0.45045390	-1.96168750
H	-0.57622266	0.25185550	-2.63380368
H	0.80333067	0.84520257	-2.44232239
O	-0.60700999	-2.05448282	-0.41531936
H	-0.35054524	-2.61505582	-1.14758623
H	-1.36020527	-2.49837723	-0.02559428
O	2.40815667	1.63582897	-2.86798054
H	2.39247102	2.50098418	-3.27723772
H	3.05178074	1.14175996	-3.37579437
O	1.95099220	-1.44338778	1.25337621
H	2.89799264	-1.30510475	1.23608479
H	1.84631109	-2.35267235	1.53350913
O	2.21662765	1.39130733	-0.11792567
H	2.84168586	1.91530708	0.38303093



H	2.45105372	1.54781198	-1.03268341
O	0.80176062	1.24692549	2.60179090
H	0.58770951	2.14220991	2.86423891
H	1.29757854	0.89251559	3.33988929
O	-2.77872017	-2.93138733	1.06163147
H	-2.74085466	-3.75397443	1.54963524
H	-3.66612919	-2.90527106	0.70378488
O	-1.36553997	1.98299074	0.33513480
H	-1.35979088	2.70238969	-0.29626295
H	-2.17942292	2.10022316	0.82511656
Ca	0.20465800	0.10074000	0.48149700

### 3.4.10 n=10

31

-1236.78792627

O	0.58237363	-1.62819812	2.19093363
H	1.46166565	-1.97762609	2.33576685
H	0.01082081	-2.19379981	2.71021499
O	-0.55602396	1.27728272	2.50787804
H	-0.65347295	0.91502210	3.38850393
H	-0.73034076	2.21264196	2.61250958
O	-2.29398607	-2.95868243	-1.07642832
H	-2.35648362	-3.85742183	-0.75302060
H	-2.89748491	-2.92825232	-1.81878551
O	-2.07664555	-0.81931720	0.67927795
H	-2.32840990	-1.57937353	0.15472089
H	-2.87775239	-0.56954675	1.13979243
O	1.32930894	2.31029325	0.35187807
H	1.07163597	2.95290596	-0.30909437
H	2.04740086	2.72896625	0.82652313
O	0.17008607	-1.68287475	-1.20194445
H	-0.60653295	-2.23353867	-1.30125792
H	0.79723332	-2.03643253	-1.83274889
O	-0.94394275	1.34232242	-1.29645107
H	-0.66380352	2.21546215	-1.57100533
H	-1.69557740	1.14468619	-1.85521425
O	0.23397638	3.81571688	-1.69728523
H	-0.24844984	4.62373853	-1.52236534
H	0.72797774	3.99934165	-2.49633193
O	3.25969683	-2.33461016	2.19079465
H	3.53628642	-3.21342068	1.93113855
H	3.82661994	-2.11305967	2.92953993
O	2.60937929	-0.42002630	0.29858792
H	2.99685223	-1.08376485	0.86915507
H	3.34734323	-0.07541181	-0.20428493
Ca	0.20465800	0.10074000	0.48149700

### 3.4.11 n=11

34

-1309.31230943

O	-1.52601060	1.47212437	-0.71512513
H	-1.83957104	2.36785588	-0.59032159
H	-2.18273509	1.06443685	-1.27969120
O	0.41245679	-1.89303678	1.97033529
H	1.01567784	-2.63549723	1.93705077
H	-0.10666989	-2.04084798	2.76083536
O	1.37694733	1.54392443	-1.18521237
H	0.94004218	2.07316343	-1.85248366
H	2.31095614	1.67308485	-1.35006427

O	-1.45910759	2.38697647	3.80310843
H	-2.14422850	3.05489305	3.83008614
H	-1.17195084	2.30088429	4.71215197
O	0.35592086	2.27098705	1.70642395
H	0.87766681	3.06255747	1.57440708
H	-0.19501939	2.47017284	2.46340538
O	-3.24130889	-0.14694732	-2.18159405
H	-4.18076274	-0.16674092	-1.99920522
H	-3.18086285	-0.19952317	-3.13543528
O	1.56814552	-1.49192230	-0.88808504
H	2.50524072	-1.60910570	-0.73203485
H	1.38448608	-2.02779997	-1.65966482
O	-1.43060712	-1.47745686	-0.55218337
H	-2.11793966	-1.18262839	-1.14957870
H	-1.57309143	-2.42033456	-0.46905166
O	4.21759320	-1.50023092	-0.03567114
H	4.60144822	-2.26755712	0.38870705
H	4.91437218	-1.16402607	-0.59931675
O	-1.67687084	0.17044715	2.14366411
H	-2.53189592	-0.25908382	2.16947645
H	-1.73681570	0.86405626	2.80058423
O	2.54153181	0.21714496	1.37418525
H	3.24375914	-0.31968785	1.00687294
H	2.94558778	0.66510377	2.11735596
Ca	0.20465800	0.10074000	0.48149700

### 3.4.12 n=12

37

-1380.34430133

O	-0.15403168	2.35876587	1.49160645
H	0.04714343	3.25343209	1.21713976
H	-0.71792053	2.46388624	2.25790280
O	2.27141590	-1.95723289	-2.71600608
H	2.48090507	-1.62356148	-3.58836420
H	2.62149396	-2.84809326	-2.70935914
O	-1.86209805	2.15869987	3.67900967
H	-2.73877642	2.54241986	3.65839372
H	-1.54498660	2.33216416	4.56534002
O	-1.33849502	-0.26353625	2.41376069
H	-1.62025320	0.47338971	2.95577867
H	-1.66054926	-1.03783034	2.87525907
O	0.50292095	1.75539108	-1.36805022
H	-0.25593214	2.09709853	-1.84092338
H	1.25778316	2.08106515	-1.85830574
O	1.81774381	0.28680626	2.38175948
H	2.15770544	1.01549332	2.90105929
H	2.11779313	-0.49674565	2.84246311
O	0.59605528	-2.24064354	1.26405405
H	0.38350830	-3.10632831	0.91527806
H	1.18728611	-2.41544573	1.99625711
O	2.47469737	-0.31656602	-0.47789612
H	2.57978861	-0.86353650	-1.25636265
H	3.36834347	-0.15686863	-0.17437607
O	-1.97364517	2.44294932	-2.43394675
H	-2.21532063	2.19128547	-3.32528805
H	-2.32173763	3.32875921	-2.33194916
O	2.38294544	-2.24146795	3.39695496
H	3.25764121	-2.62013836	3.30893754
H	2.09801101	-2.49693867	4.27432496
O	-2.09809266	0.60139906	-0.35177168

H	-2.23052792	1.21804658	-1.07179791
H	-2.98036617	0.41271921	-0.03204619
O	-0.16353827	-1.37570745	-1.50147911
H	0.57701773	-1.67079201	-2.03132147
H	-0.93629768	-1.65577587	-1.99202533
Ca	0.20465800	0.10074000	0.48149700

### 3.4.13 n=13

40  
-1445.00873391

O	0.13766021	1.19729229	2.72077754
H	0.32489533	0.77971080	3.56149136
H	0.22529514	2.13467051	2.89361622
O	0.41755072	3.96555481	2.54302670
H	-0.29942170	4.53756139	2.81686979
H	1.21108196	4.43920609	2.79241324
O	-0.59597133	0.56399409	-3.80695404
H	-0.80303166	-0.14844396	-4.41175902
H	-0.61930427	1.35293356	-4.34848991
O	1.28122428	0.18955875	-1.76670518
H	2.19138496	0.42373727	-1.94836139
H	0.83292480	0.30061635	-2.60511129
O	3.97086220	0.90795409	-1.61519649
H	4.64766333	0.28878118	-1.88868537
H	4.31027879	1.76454074	-1.87459330
O	0.99613644	-1.58383986	2.17125910
H	1.29874793	-2.49098172	2.12941473
H	0.97001678	-1.38247151	3.10667322
O	-2.57866958	-3.16728098	0.50610301
H	-2.57317167	-3.93727026	1.07471298
H	-3.34391750	-3.28934872	-0.05579210
O	2.63471451	0.53817739	0.80346893
H	3.20198299	0.72749937	0.05607701
H	3.23692920	0.42082149	1.53817709
O	0.82131149	-0.57852748	4.77157440
H	1.60790447	-0.47129460	5.30636747
H	0.15543447	-0.89103633	5.38409137
O	-1.59694918	0.59928503	-1.19933864
H	-2.54036056	0.75404003	-1.15183195
H	-1.40094614	0.59738300	-2.13625390
O	-0.19467597	-2.14915675	-0.51507290
H	-0.97728320	-2.64276103	-0.26989591
H	0.20033354	-2.66074717	-1.22109963
O	-1.94550201	-0.64282511	1.50060191
H	-2.31003062	-1.49611829	1.26556859
H	-2.50818475	-0.32811488	2.20811631
O	0.24724325	2.56653847	0.13767423
H	0.34938924	3.16320366	0.87915105
H	0.03005483	3.13597139	-0.60043577
Ca	0.20465800	0.10074000	0.48149700

### 3.4.14 n=14

43  
-1509.64319726

O	0.41761345	2.55941763	0.82253415
H	0.73129655	3.26259209	0.25386939
H	0.25270557	2.98622694	1.66328990
O	-1.15909698	1.16486441	-1.33134731
H	-1.10212694	0.77200851	-2.20235229

H	-1.72766937	1.92599863	-1.44809989
O	2.40755791	0.18445809	1.64209000
H	3.21953384	0.43861425	1.20353469
H	2.65543853	0.07223616	2.55980044
O	-1.79578291	-0.87516715	4.81824078
H	-2.62689965	-0.52824221	5.14246150
H	-1.32895782	-1.15486988	5.60568712
O	-2.11425208	-0.74938847	0.76457626
H	-2.92691203	-0.68500714	0.26290917
H	-2.28181895	-1.44056381	1.40522359
O	-0.58516938	-0.25598086	-3.61558737
H	0.24393429	0.09485221	-3.94075545
H	-1.07645212	-0.48180797	-4.40544457
O	0.08749631	-1.61280959	-1.31578317
H	-0.14330640	-1.34086786	-2.20404486
H	0.05270325	-2.56904725	-1.34088275
O	-1.98232256	-2.67527353	2.72827629
H	-2.46934811	-3.47901452	2.91003866
H	-2.01251892	-2.18533255	3.55002871
O	-0.41807123	0.60233108	2.86360305
H	-0.37390761	1.49437031	3.20790901
H	-0.87504620	0.10549666	3.54224910
O	-0.19174010	3.33126550	3.41286658
H	0.46463816	3.68248712	4.01456582
H	-0.97200391	3.86230868	3.57227972
O	1.93893399	0.79660768	-4.02067118
H	2.00293589	1.63496967	-4.47814681
H	2.55794302	0.22647461	-4.47674916
O	4.47089026	0.94274123	-0.04448922
H	5.15305480	0.30845984	-0.26487451
H	4.93727445	1.77308241	0.05168949
O	0.46914679	-2.12023244	1.61106640
H	1.16591782	-2.74645676	1.80749515
H	-0.30787758	-2.48514327	2.03450970
O	1.93874883	0.76872946	-1.20981410
H	1.94821436	0.79463476	-2.16661624
H	2.85449712	0.88687389	-0.95746914
Ca	0.20465800	0.10074000	0.48149700

### 3.4.15 n=15

	46		
	-1571.11481441		
O	1.72193845	0.75861071	2.35777108
H	1.46917693	0.45655104	3.23018301
H	2.59360681	1.13555388	2.47751722
O	0.60355301	-0.39672131	4.59213155
H	-0.14008462	0.13754432	4.87104793
H	0.98532134	-0.72111271	5.40776271
O	-0.83882139	-1.83860642	-0.69017660
H	-1.50274264	-1.67129438	-1.35909085
H	-0.62020377	-2.76455251	-0.79534887
O	1.04922808	0.31940711	-1.86378856
H	0.69087384	0.73158082	-2.64987131
H	1.86327660	-0.08979973	-2.15722644
O	-0.13745947	-1.63823319	2.24507848
H	-0.61496191	-2.46287679	2.33555149
H	0.08321286	-1.38898764	3.14252564
O	-1.62573052	1.21281022	4.89483578
H	-2.39824498	0.82991676	5.31058215
H	-1.51305670	2.05790649	5.32997705

O	0.65579009	2.52352032	0.15639492
H	0.98797485	3.24769320	0.68692102
H	0.25908906	2.94627463	-0.60527306
O	-0.09800669	1.56744914	-4.06165916
H	-0.79790433	1.04721083	-4.45628101
H	0.40858665	1.89214324	-4.80608374
O	2.20732419	-1.36155508	0.24789269
H	2.74589544	-1.38274315	-0.54313392
H	2.65272972	-1.95015431	0.85731527
O	3.45099301	-1.07220755	-2.21266228
H	3.55345261	-1.81547583	-2.80704037
H	4.27680812	-0.59329754	-2.28270246
O	-2.17440041	-0.00721779	-5.04501260
H	-2.88243004	0.48567799	-5.45971589
H	-1.94181068	-0.67870738	-5.68628849
O	-2.76221000	-0.92921195	-2.48318845
H	-2.58787796	-0.67709538	-3.38998313
H	-3.64396140	-1.30118098	-2.50279762
O	-0.88689216	3.26432123	-2.02360999
H	-0.61568389	2.84717940	-2.84133231
H	-1.22353772	4.11964686	-2.29066589
O	-1.40679253	1.08759525	2.10985185
H	-2.19102647	1.50755444	1.75652137
H	-1.50583427	1.15467099	3.05954791
O	-1.77052794	0.98253080	-0.77013166
H	-1.68665067	1.82528763	-1.21617711
H	-2.28059146	0.44162409	-1.37302979
Ca	0.20465800	0.10074000	0.48149700

### 3.4.16 n=16

49

-1632.70493044

O	-1.34693864	-0.74330932	-1.30889731
H	-1.37072611	-0.64803138	-2.26104609
H	-1.94216816	-1.47015031	-1.12549879
O	1.88866191	-1.44894102	1.46714316
H	1.62500788	-2.19782221	2.00183423
H	2.65327642	-1.08993079	1.91737345
O	2.19248159	1.51544934	0.96233383
H	2.62738384	2.26881443	0.56291914
H	2.80605780	1.21075643	1.63085270
O	0.10609845	0.59326313	2.93441019
H	0.69201118	0.38692182	3.66266877
H	-0.62720589	1.05584243	3.34001610
O	1.67834706	-0.60597304	-1.38194857
H	2.45920376	-1.15765043	-1.42827227
H	1.63158804	-0.18373651	-2.23971365
O	3.66478847	0.13591612	2.85452409
H	3.20442766	0.10800260	3.69328495
H	4.59227323	0.15552966	3.09035952
O	0.67095678	-3.36074890	3.04484792
H	0.77088131	-4.30894956	2.96022156
H	0.85150105	-3.18182005	3.96768011
O	-2.21938148	1.99432981	3.60457133
H	-2.91530196	1.62322643	4.14698075
H	-2.17164388	2.91258987	3.87056117
O	0.13016273	1.99457693	-1.16046675
H	0.43468577	1.80688023	-2.04831060
H	-0.16058825	2.90592871	-1.19412414
O	1.88081869	-0.08762036	4.95813384

H	1.71335522	-0.97974024	5.26195800
H	1.99635005	0.42143458	5.76047204
O	1.34284500	-2.72149484	5.67432792
H	2.09823315	-3.19965969	6.01634859
H	0.65370485	-2.86596496	6.32274541
O	0.99119202	0.94832751	-3.55754009
H	1.45337958	1.29418497	-4.32108203
H	0.22313887	0.50775764	-3.92116569
O	-1.92943975	1.29767056	0.93699507
H	-2.17604475	1.59239369	1.81366791
H	-2.69829502	1.48092860	0.39707926
O	-2.88740575	-2.89728433	-0.39602525
H	-2.78192686	-3.76890444	-0.77731727
H	-3.82669684	-2.82073766	-0.22838315
O	-1.02758165	-1.84742100	1.39826411
H	-1.71521267	-2.35261778	0.96447752
H	-0.65265694	-2.45251534	2.03820421
O	-1.33582722	-0.44557373	-4.10679020
H	-2.05437870	0.03580070	-4.51690415
H	-1.23151790	-1.22816477	-4.64799428
Ca	0.20465800	0.10074000	0.48149700

### 3.4.17 n=17

	52		
	-1693.44191006		
O	1.41532293	-0.03238553	-1.70716196
H	2.33230701	-0.17276620	-1.94309518
H	0.97005965	0.10163317	-2.54382834
O	4.31427763	0.85708140	0.22595134
H	5.19292490	1.14996474	0.46767299
H	4.41967092	0.47604006	-0.64578875
O	-3.53853516	1.90281033	-0.35800034
H	-3.99304647	1.44003547	0.34591011
H	-4.20885446	2.46350509	-0.74854412
O	4.58480848	-3.20348078	-1.97134198
H	4.43914080	-3.73584118	-2.75339335
H	5.46982717	-3.43181312	-1.68702299
O	-1.44265866	2.34517677	3.74233714
H	-2.34348784	2.15027919	4.00070265
H	-1.19176412	3.08945430	4.28945130
O	1.80262195	1.99877767	0.47802651
H	1.74668862	2.95004220	0.56857089
H	2.73770488	1.82208973	0.37491339
O	-1.87621597	-0.83272859	1.53180976
H	-2.72947803	-0.41105001	1.63360396
H	-1.97518519	-1.68175363	1.96261434
O	-1.47514642	0.31356076	-1.32525396
H	-1.28956686	0.37752796	-2.26211011
H	-2.29220182	0.79842118	-1.20879854
O	2.38856121	-0.90833792	1.10413333
H	3.18579255	-0.39618049	0.96867861
H	2.63224190	-1.80098296	0.85911178
O	-0.32089997	0.44002239	-3.85958797
H	-0.27333168	1.26695538	-4.33932760
H	-0.54970795	-0.21001333	-4.52391582
O	4.11596321	-0.46784970	-2.19943267
H	4.57522333	-0.15236972	-2.97775365
H	4.31863649	-1.40266054	-2.16361038
O	-4.11420693	1.77428876	4.29011053
H	-4.27131038	1.26233710	5.08349254

H	-4.67772684	2.54224782	4.38453088
O	2.64419680	-3.42996580	0.01562744
H	2.81122330	-4.24702141	0.48547133
H	3.29606653	-3.41856757	-0.68520560
O	0.09405507	-2.31729191	-0.13060476
H	-0.55347101	-2.85561959	-0.58573584
H	0.90126361	-2.83041130	-0.16739994
O	0.43979362	0.43944992	2.93402107
H	-0.16072178	1.01973875	3.40186415
H	1.12405414	0.23726503	3.57209617
O	-4.31680205	0.43526033	1.86072954
H	-5.14674687	-0.04154319	1.85172795
H	-4.31302013	0.89460573	2.70050244
O	-1.14906511	2.11865696	1.00277968
H	-1.97690891	2.28778651	0.55300101
H	-1.31096385	2.37924805	1.90948366
Ca	0.20465800	0.10074000	0.48149700

### 3.4.18 n=18

55			
-1753.49813624			
O	0.10997735	2.59482839	0.68485491
H	0.56412051	3.16417070	0.06369924
H	-0.32544847	3.19696572	1.28823374
O	1.55617813	3.86886037	-1.36948879
H	1.11309734	4.38790021	-2.04068777
H	2.38569642	4.32354458	-1.22322637
O	-2.20155036	0.64072025	0.33476150
H	-2.86551392	0.31482289	-0.27283567
H	-2.69768386	1.12236718	0.99665182
O	0.52644564	-2.63387928	-3.43708398
H	0.22847495	-2.71962764	-4.34267313
H	0.57528240	-3.53368415	-3.11428809
O	-2.88747919	2.00306666	2.67228108
H	-2.44620376	2.85246188	2.67817802
H	-3.68617541	2.14402763	3.18065631
O	-0.74050161	-1.07439120	-1.51763574
H	-1.67422178	-1.03542401	-1.72470874
H	-0.36128908	-1.60521715	-2.21810179
O	-0.48143748	-2.10522130	1.38451110
H	-0.11454607	-2.92194863	1.04601712
H	-0.91188419	-2.35606621	2.20183814
O	2.20402809	0.64091967	1.84646947
H	2.12982444	1.08638640	2.69043880
H	3.09920645	0.30229101	1.83172690
O	-1.18191448	4.18600840	2.56118453
H	-1.51103198	5.06717233	2.38380694
H	-0.60562396	4.29289556	3.31795094
O	1.97787482	-1.54552920	-0.15506233
H	2.40297884	-1.45818829	-1.00822653
H	1.83955837	-2.48696046	-0.05110667
O	2.68098906	-1.02043708	-2.77280303
H	2.01581653	-1.58583414	-3.16536219
H	3.44407500	-1.11622710	-3.34267595
O	1.41453752	1.07821255	-1.43779696
H	1.61353464	1.99388467	-1.63318307
H	1.92356339	0.58023192	-2.07743669
O	-0.58058116	0.49383573	2.82426826
H	-0.00038696	0.87478019	3.48342456
H	-1.42027842	0.93238720	2.96142562

O	0.67660225	-5.18803908	-2.33986327
H	1.40516342	-5.71993183	-2.66005033
H	-0.09126510	-5.75190504	-2.43295429
O	1.40578415	1.72092078	4.30282349
H	1.77405706	1.41115427	5.13025977
H	1.17741825	2.63546597	4.46921801
O	0.55828749	4.34240327	4.72853680
H	0.13386357	4.48852612	5.57396182
H	1.24982578	5.00308855	4.68979722
O	1.05864398	-4.12618278	0.20928529
H	0.89318039	-4.54117097	-0.63725923
H	1.47378524	-4.81010879	0.73476981
O	-3.51647808	-0.66169351	-1.75978767
H	-3.88199589	-0.15507181	-2.48502019
H	-4.16522680	-1.34567375	-1.59387460
Ca	0.20465800	0.10074000	0.48149700

### 3.4.19 n=19

58

-1810.99492200

O	-0.35042676	2.47967897	0.94346105
H	0.00970420	3.02316528	1.64428866
H	-0.51308288	3.09106435	0.22514222
O	-2.73592540	-2.63620377	1.64449014
H	-3.34799579	-3.10996595	2.20765109
H	-2.85402850	-3.02757876	0.77897972
O	1.54524602	2.14125602	4.77171789
H	1.00489543	2.18269748	5.56072668
H	2.44364568	2.09242293	5.09840489
O	-0.47788196	3.89430384	-1.41667172
H	0.39811893	4.22872988	-1.60905854
H	-1.07059172	4.52302102	-1.82854655
O	0.29803289	1.28229852	-1.71802799
H	1.09532694	1.35058519	-2.24328045
H	-0.10484995	2.14839399	-1.77963213
O	1.00257044	4.00621290	2.80076574
H	1.20924058	3.44676962	3.54945907
H	0.66411161	4.81258673	3.18991596
O	-0.02347912	-2.18359593	1.48156597
H	-0.90451804	-2.50105809	1.67960442
H	0.41230110	-2.92812044	1.06682524
O	2.94414641	3.92304828	0.83724682
H	3.76864150	4.28001315	1.16742095
H	2.31310720	4.08935535	1.53750570
O	4.03217528	0.10683762	-1.41444951
H	4.95638912	-0.02804151	-1.62389500
H	3.72040187	0.71472931	-2.08489419
O	0.77625874	0.22392771	2.89585635
H	1.07007499	0.86966930	3.53844551
H	0.71902426	-0.59523300	3.38772112
O	2.21809454	4.38159137	-1.79172119
H	2.59522717	5.20218032	-2.10895262
H	2.52200586	4.31183680	-0.88673322
O	2.41877219	1.23663685	0.51688907
H	2.65688933	2.15296646	0.65785463
H	3.12964331	0.88351848	-0.01808821
O	1.26155599	-4.05913473	-0.09267893
H	1.93195189	-4.68104779	0.19020709
H	0.62808930	-4.59149278	-0.57387107
O	-0.72220993	-5.52649330	-1.39492538



H	-0.52925290	-5.74602923	-2.30640911
H	-0.93487427	-6.36535260	-0.98587775
O	-2.60201816	-3.51756819	-0.97617463
H	-2.00277299	-4.24514508	-1.14281230
H	-3.38444634	-3.72969559	-1.48513350
O	-2.06755734	0.05538226	1.47562111
H	-2.69595923	0.69789837	1.80503746
H	-2.50802770	-0.78770959	1.58245281
O	-1.23280492	-1.12008433	-1.15727698
H	-1.26395379	-0.82697478	-2.06796219
H	-1.73479839	-1.93505856	-1.15016652
O	1.79757256	-1.37080846	-0.70610273
H	2.65776029	-1.12926015	-1.04955944
H	1.80223092	-2.32796853	-0.69875904
O	2.66744130	1.91525236	-2.99398848
H	2.61472925	2.81015556	-2.65842818
H	2.78610879	2.01954598	-3.93806045
Ca	0.20465800	0.10074000	0.48149700

### 3.4.20 n=20

	61		
	-1870.70554467		
O	-0.40805357	1.83145419	-1.20398029
H	-0.63848926	2.70957603	-0.90061178
H	-1.00542600	1.66499862	-1.93313717
O	0.27851851	2.23811816	1.72365973
H	-0.13310886	3.05261043	1.43487562
H	0.97437215	2.51852518	2.31812641
O	2.51596060	2.25108443	3.42639952
H	3.41003875	2.49909908	3.19114645
H	2.43145871	2.50201124	4.34625070
O	4.00934551	-1.47073543	1.20828616
H	4.68504281	-2.09757231	1.46662645
H	4.49484949	-0.68692349	0.95107857
O	-5.15915837	-1.17928055	-0.67413509
H	-6.06033911	-1.50180076	-0.68335497
H	-4.93737249	-1.11329119	0.25467461
O	-4.16733233	-1.13243212	1.89524055
H	-4.64207470	-1.05008412	2.72232549
H	-3.74983838	-1.99247338	1.94276790
O	5.14112269	2.79674882	2.65443736
H	5.32474346	3.71299561	2.44705788
H	5.80652278	2.55881901	3.30008676
O	2.29535428	1.18450600	-0.37579312
H	2.26020230	1.80945036	-1.09997535
H	3.21734498	1.16609380	-0.11922899
O	-2.17069013	0.59275969	1.05042333
H	-2.65785447	1.39563875	0.86525545
H	-2.81872525	0.00191598	1.43407058
O	-3.62707591	2.80710716	0.29062973
H	-4.35864276	3.20803614	0.75998770
H	-4.03128955	2.38222365	-0.46588620
O	-1.17463071	4.07619216	0.17892859
H	-1.20172202	5.02151488	0.03107042
H	-2.09396556	3.81565997	0.23529729
O	-0.56649437	-1.80619657	1.86722276
H	-0.05925668	-2.07590099	2.63286006
H	-1.27482703	-2.44751121	1.81055369
O	1.84070161	-0.20396858	2.34086937
H	2.12650795	0.55749649	2.84556404

H	2.64574290	-0.69073204	2.16423166
O	-2.73633396	-3.45469827	1.58538831
H	-2.88344802	-4.35320398	1.88081336
H	-2.86227039	-3.49018373	0.63717324
O	1.68654679	-1.73945068	-0.28949243
H	2.56238309	-1.80762297	0.09063167
H	1.65943613	-2.42720803	-0.95468854
O	-1.10343757	-1.07269964	-1.28138091
H	-1.70282511	-1.81673309	-1.22324474
H	-1.46067543	-0.53116122	-1.98519074
O	-4.63257357	1.28981658	-1.79611403
H	-4.87169442	0.43529841	-1.43715590
H	-5.39798054	1.55962827	-2.30364219
O	-3.09547603	-2.97712117	-1.09501897
H	-3.86207438	-2.40408397	-1.08136726
H	-3.27634803	-3.60326076	-1.79606501
O	-2.20338298	0.80128850	-2.99416974
H	-3.08730282	0.99129011	-2.67981943
H	-2.26665941	0.87355275	-3.94653784
O	4.91853205	1.04656845	0.50275770
H	5.67983386	1.17320344	-0.06347031
H	5.05481369	1.65619502	1.22802578
Ca	0.20465800	0.10074000	0.48149700

### 3.4.21 n=21

64			
-1929.83610691			
O	4.14063033	2.35409487	-0.23257521
H	4.46565834	1.46691417	-0.38586650
H	4.91659267	2.85327600	0.02224171
O	4.65647719	-0.33934407	-0.50052370
H	4.62817788	-0.74198349	0.36741159
H	5.36968864	-0.79116685	-0.95154102
O	-1.07299184	1.09387707	-3.78200269
H	-0.11998875	1.13894052	-3.85936805
H	-1.37989485	0.94985861	-4.67715645
O	-2.09012947	1.10703746	0.55766182
H	-2.32814613	1.67200856	-0.17744821
H	-2.92669805	0.86438554	0.95452964
O	1.68497011	1.06835115	-3.68127308
H	1.99630950	1.88989428	-3.30131823
H	2.22938402	0.94180474	-4.45833841
O	-0.27877473	0.30608972	2.90988630
H	0.22008299	0.49684975	3.70423043
H	-1.10182794	-0.06582132	3.22689830
O	-2.20386004	2.65956902	-1.77443969
H	-2.69283315	3.42534561	-2.07564149
H	-1.95874500	2.20018712	-2.57763201
O	4.26864952	-1.40351541	2.02916131
H	4.12792473	-0.73575947	2.70037629
H	4.85665363	-2.03702119	2.44044298
O	3.54719239	0.66694169	3.73045789
H	2.80554376	0.66445247	4.33558774
H	4.22155223	1.17673227	4.17943829
O	0.29511598	2.25767475	-0.73272654
H	0.99664150	2.70774080	-1.20340002
H	-0.51109519	2.62592105	-1.09418087
O	1.22035310	0.79039607	5.21871872
H	1.03127582	1.64350945	5.60945950
H	1.13404869	0.17034929	5.94282131

O	-3.04292338	-2.34610582	-1.02703177
H	-3.14490440	-3.17540012	-1.49404554
H	-3.93647701	-2.08399355	-0.80546896
O	2.18532526	1.28958703	1.41982244
H	2.64491579	1.15297931	2.24828239
H	2.80434075	1.78142465	0.88024243
O	-2.64864872	-1.07559415	3.32576383
H	-3.37913934	-0.63951253	2.88707569
H	-3.04598409	-1.50691083	4.08228319
O	2.41969892	3.24750923	-2.17664236
H	2.61967900	4.14757700	-2.43377462
H	3.10836965	3.01746668	-1.55290839
O	-4.45709257	0.18904731	1.67465197
H	-4.90337401	-0.37976894	1.04734664
H	-5.13861585	0.78513879	1.98518696
O	1.62222908	-1.73521807	1.36455846
H	2.55201211	-1.72235135	1.59164649
H	1.34562916	-2.63530870	1.53648976
O	-1.29648506	-1.82839801	1.04311067
H	-1.78954855	-1.78972677	1.86263734
H	-1.92477453	-2.15751513	0.40033133
O	-0.95788399	-0.58406667	-1.61256263
H	-1.03698940	-0.10600976	-2.43805336
H	-1.71538989	-1.16910544	-1.60050124
O	1.98492699	-0.20211105	-1.22445859
H	1.92427353	0.08762814	-2.13473513
H	2.91947168	-0.35256728	-1.08226098
O	-5.58246371	-1.53020795	-0.20521630
H	-6.12845384	-1.13466331	-0.88467951
H	-6.12634515	-2.22531398	0.16525853
Ca	0.20465800	0.10074000	0.48149700

### 3.4.22 n=22

67

-1989.88036368

O	2.17110326	4.21679803	-0.09324051
H	1.49348504	4.50227802	0.51959368
H	2.88094451	4.84841906	0.02256670
O	-1.91463446	-0.11956124	-0.81678566
H	-2.14293569	0.16195282	-1.70270857
H	-2.65543169	-0.65759571	-0.53755568
O	0.02972116	-0.81796602	-3.59467214
H	0.26592675	-1.06491840	-4.48879320
H	-0.79237411	-0.33661110	-3.68788061
O	-0.28335854	-3.48520085	3.41613879
H	-0.68589331	-4.27332466	3.78090945
H	0.45785192	-3.80915906	2.90438771
O	0.58702401	-1.84772127	-1.05116388
H	0.37064105	-1.69106566	-1.97033115
H	0.89536853	-2.75360679	-1.02822678
O	1.06898867	3.61115058	-2.52745371
H	1.55871617	4.00947573	-3.24699181
H	1.49811835	3.93640728	-1.73607086
O	0.91816619	0.98410485	-1.72769655
H	1.06167741	1.86712941	-2.06814212
H	0.78666285	0.44470753	-2.50743267
O	1.86061330	-4.06775988	1.76309495
H	2.58802134	-4.61395561	2.06105263
H	1.73659628	-4.31259107	0.84608433
O	-1.63140691	3.22884793	-2.18205450

H	-0.73316966	3.47592222	-2.40195253
H	-2.14493514	4.01973235	-2.34643700
O	-1.18395788	-1.69220756	1.53258793
H	-0.98129376	-2.35613126	2.19165060
H	-2.08756619	-1.87655674	1.27619290
O	-0.09767377	0.74720065	2.86165569
H	-0.10704819	0.12056822	3.58517137
H	0.06836336	1.59268328	3.27857513
O	-2.21402089	0.80917561	-3.37739109
H	-2.95738717	0.88482428	-3.97565096
H	-2.05193771	1.70496269	-3.08154388
O	2.08899137	1.65762201	0.97365671
H	2.22678928	2.48897789	0.51968517
H	2.57273183	1.74936671	1.79451546
O	0.75184370	3.15326125	3.92974679
H	0.65138814	3.47942578	4.82403780
H	1.66289847	2.86375309	3.88080549
O	0.26548204	-1.17603191	4.83568479
H	-0.15163954	-1.20382568	5.69677022
H	0.05513961	-2.02172656	4.43972060
O	0.10781940	4.59800387	1.68810230
H	0.32224212	4.19541688	2.52963521
H	-0.36870391	5.39565007	1.91813944
O	1.86504364	-1.30854182	1.67961132
H	2.33319924	-1.05520056	2.47514859
H	1.94376473	-2.26198010	1.64815578
O	-0.80878518	2.37028504	0.34286446
H	-1.23373116	2.67561014	-0.45865193
H	-0.60396984	3.17090698	0.82586157
O	3.20432559	1.99559258	3.47688103
H	4.08837144	2.30054934	3.68107538
H	3.17808928	1.09744352	3.80683699
O	-3.75024496	-1.81089113	0.43016420
H	-4.12909862	-2.57735063	-0.00023185
H	-4.48167924	-1.41633014	0.90509215
O	2.87917675	-0.63453531	4.16445120
H	2.02531055	-0.82507943	4.55282791
H	3.50377910	-1.10808305	4.71386495
O	1.52096996	-4.47785820	-0.94525389
H	2.32455953	-4.61242673	-1.44761445
H	0.93645693	-5.17813773	-1.23539890
Ca	0.20465800	0.10074000	0.48149700

### 3.4.23 n=23

70			
-2047.50604895			
O	1.21315256	4.69875174	0.56601939
H	0.72141678	4.63815164	-0.25297668
H	1.71736847	5.50822619	0.48387046
O	0.58957865	0.46532494	-1.97051810
H	0.88282171	1.20211680	-2.50659393
H	0.79844410	-0.30936424	-2.49249791
O	2.46848826	-0.81565514	-0.05350146
H	3.18668565	-0.23887562	-0.31378767
H	2.70746197	-1.67178529	-0.40869684
O	-0.15980902	4.07160041	-1.73759840
H	0.42849944	3.64952973	-2.36368187
H	-0.71306644	4.63978559	-2.27360479
O	-2.06745776	-0.50384025	1.31012495
H	-2.68115311	0.05327596	1.78890524

H	-2.35745526	-1.39661064	1.49745756
O	-2.71467784	3.43662025	1.77640008
H	-3.25760261	4.21671451	1.66274864
H	-1.92701525	3.75462464	2.21763910
O	0.62210601	-1.71318521	2.12519077
H	1.05310554	-2.52984935	1.87313896
H	0.15457037	-1.92777924	2.93240255
O	-1.65409522	0.34585067	4.71128790
H	-2.43213866	0.61286089	4.22181372
H	-1.77446736	0.72820256	5.58051088
O	1.10744793	-2.09288248	-2.98922288
H	1.78117299	-2.58500318	-2.52002912
H	1.01425475	-2.55036590	-3.82483940
O	-0.03012400	1.25882409	2.66749269
H	-0.48017671	0.93678816	3.44850257
H	0.01200658	2.20737543	2.78876262
O	1.81472138	2.01062108	0.41415480
H	1.71869875	2.95698918	0.52091669
H	2.70712993	1.89525537	0.08776738
O	-0.40608435	-1.99264232	-0.70969887
H	-0.05074071	-2.15735524	-1.58310117
H	-0.73330633	-2.84399605	-0.41926192
O	4.21207213	1.26710003	-0.71550360
H	4.29568523	1.65276163	-1.58757298
H	5.09216868	1.32247014	-0.34321980
O	-2.66664053	-3.06050809	2.20441383
H	-3.52147241	-3.36424935	2.50975744
H	-2.16738355	-2.90360296	3.00588390
O	4.27795338	2.47098091	-3.23100327
H	4.73443609	3.31130383	-3.27237892
H	4.69813106	1.93619999	-3.90456922
O	1.49771033	2.63141169	-3.42276752
H	2.45348024	2.62071056	-3.37157787
H	1.30806097	2.67651049	-4.35990691
O	-1.13595946	-4.41159264	0.37989894
H	-1.73440183	-4.05532576	1.03653557
H	-1.61387517	-5.14481123	-0.00768087
O	-0.23095208	4.01999275	2.80481937
H	0.02312486	4.56446444	3.54995460
H	0.28852204	4.35554294	2.07421433
O	1.50132456	-4.15808977	1.11411401
H	0.60613150	-4.40165694	0.87845445
H	1.81365562	-4.88463968	1.65337792
O	-3.60631362	1.11688976	2.92834425
H	-3.39458115	1.97923200	2.57090020
H	-4.56044753	1.11650313	3.00489063
O	2.81349844	-3.30626303	-1.15514971
H	3.59959244	-3.83044341	-1.30851911
H	2.39191526	-3.72054968	-0.40224520
O	-1.17489229	2.08391520	-0.08247634
H	-1.81432275	2.53254187	0.47078112
H	-0.92112972	2.73736930	-0.73426872
O	-1.02193084	-2.28563209	4.26770171
H	-0.79271883	-2.72619098	5.08599306
H	-1.26735567	-1.39926308	4.53293301
Ca	0.20465800	0.10074000	0.48149700

### 3.4.24 n=24

73

-2106.09847826

O	1.25066373	-0.78091182	-4.95019370
H	1.64047549	-1.02498596	-5.78966117
H	0.35986827	-0.50782346	-5.16959562
O	3.88138843	-2.58918429	-0.41899570
H	3.17603423	-3.19640769	-0.64257165
H	4.63617712	-2.90465636	-0.91598909
O	-1.41179101	-0.13644410	-5.29776534
H	-1.75634120	0.23220710	-6.11116099
H	-1.62074583	0.51730201	-4.63054355
O	-2.16546740	-2.62268225	-4.34632149
H	-1.98590551	-1.78257984	-4.76847845
H	-2.50247854	-3.17755181	-5.04972343
O	-1.97389746	1.69186412	-3.30243220
H	-2.71905362	1.39048541	-2.78267823
H	-2.20465236	2.58520860	-3.55722394
O	2.18102089	-0.47762871	-0.90213251
H	2.43292940	-0.02088431	-1.70472685
H	2.86205457	-1.13877712	-0.77841132
O	0.69221932	-2.28395623	1.02309637
H	0.89713402	-2.96012679	0.37731439
H	0.98643238	-2.65116509	1.85665941
O	1.57041049	-3.96991522	-1.01783404
H	1.47078322	-4.91926384	-1.08884547
H	1.19184758	-3.62764306	-1.82763088
O	-2.65489014	1.76527239	3.03232599
H	-1.98219857	2.33909731	3.39898938
H	-3.43820042	1.95272424	3.54954724
O	-0.90869972	-1.26439362	-1.25534544
H	-1.81865591	-1.53147372	-1.38526452
H	-0.42042574	-1.74147740	-1.92632279
O	-0.32700318	3.05397249	3.85775330
H	-0.24855726	3.87048880	4.35108724
H	0.34340959	2.48223978	4.23178464
O	-3.46628211	-1.97529274	-2.00894633
H	-4.02656158	-2.69143717	-1.70985590
H	-3.14054591	-2.26523463	-2.86103826
O	2.12155313	0.20122403	2.06141768
H	2.09229864	0.65085612	2.90593303
H	2.85758768	-0.40589782	2.13814595
O	-3.95649265	0.70629290	-1.68449266
H	-3.93220010	-0.24070882	-1.82171012
H	-4.88807951	0.92610122	-1.69231883
O	1.84134423	-3.06075824	3.42038645
H	2.68050743	-2.71319515	3.11833343
H	2.04401349	-3.94460080	3.72694562
O	0.32458974	2.44833340	1.26874066
H	0.13901931	2.77600613	2.14875499
H	0.35984789	3.23371837	0.72270188
O	0.18013119	1.55897646	-1.56697008
H	-0.58784021	1.64485384	-2.13183823
H	0.92226815	1.54533194	-2.17135206
O	-0.80133608	-0.23931552	2.71529804
H	-0.46805095	-0.62185415	3.52697300
H	-1.54217355	0.30052734	2.99090748
O	1.64880043	1.26103441	4.58769589
H	2.30840928	1.46624877	5.25029249
H	1.27567727	0.42630976	4.87097118
O	3.99564206	-1.82934957	2.23224912
H	4.05187226	-2.13949543	1.32843569
H	4.90605090	-1.76331038	2.52039074
O	2.34800097	1.01950927	-3.19449131

H	3.01869299	1.55931394	-3.61283824
H	2.03947225	0.43845377	-3.88977223
O	0.35866239	-2.70722693	-3.16871046
H	0.81262291	-2.12087631	-3.77397389
H	-0.46540794	-2.91541528	-3.60893396
O	0.48673948	-1.21119109	4.94546944
H	0.12773907	-1.61621720	5.73496522
H	0.97719696	-1.91298691	4.51749150
O	-2.15105928	0.92205807	0.39506817
H	-2.86417924	0.91078344	-0.24333908
H	-2.53404145	1.32241380	1.17562628
Ca	0.20465800	0.10074000	0.48149700

### 3.4.25 n=25

	76		
	-2158.69193996		
O	-3.23683229	0.56152461	-2.50744265
H	-3.71365035	1.39115078	-2.53185531
H	-3.84648199	-0.05376680	-2.10004266
O	3.81100018	1.94604560	2.87460218
H	4.39994964	2.68765304	3.01384291
H	4.39311757	1.20770833	2.69507935
O	4.72088822	0.41313947	-0.71573497
H	5.32357236	1.02291759	-1.14137976
H	4.35006928	-0.09880401	-1.43451046
O	-5.64870044	1.52439982	0.23000915
H	-5.03874701	1.58030657	0.96557850
H	-6.50290719	1.72880840	0.61050750
O	-0.95443063	-0.21532683	-3.87829134
H	-1.79934533	0.03552512	-3.50489682
H	-0.96959311	0.14041353	-4.76680129
O	5.25859810	-0.23488846	1.93900372
H	5.17976430	-0.08962359	0.99618116
H	6.19004505	-0.40575268	2.07844195
O	-2.21829510	3.87568335	1.92394350
H	-2.25595427	4.71900239	2.37519266
H	-2.29200764	4.09676955	0.99554791
O	3.36669318	-0.82633792	-2.77284911
H	3.73545910	-0.83846468	-3.65607935
H	3.06506619	-1.72288774	-2.62638891
O	-5.09765944	-0.86947760	-1.02905659
H	-5.89379615	-1.21199836	-1.43535313
H	-5.38583208	-0.08747776	-0.55824474
O	0.96237050	0.23811445	-1.90003724
H	0.35123816	0.20588856	-2.63604659
H	1.80060500	-0.03627995	-2.27192656
O	-0.40782137	-2.81441183	-3.13080722
H	-0.59098208	-1.97049484	-3.54370829
H	-0.88647071	-3.45053476	-3.66228953
O	2.42692052	1.19329253	0.59084490
H	2.80814165	1.60895912	1.36422887
H	3.17891425	0.97607013	0.03989039
O	-1.08656667	-1.65484257	-0.72583393
H	-0.89140243	-2.16111393	-1.51439670
H	-1.88630864	-2.05002626	-0.37874078
O	1.78274671	-1.80250770	0.17007023
H	2.38050031	-2.09520943	0.85799999
H	1.93824503	-2.40657170	-0.55598622
O	1.01251114	-0.58268083	2.71797974
H	1.76815161	-1.16092661	2.82224057

H	1.09477201	0.05063716	3.43098218
O	-2.34344593	4.12049831	-0.80469447
H	-3.15954109	3.83894698	-1.21815373
H	-2.05480963	4.86821763	-1.32798781
O	3.30669781	-2.11136686	2.44845213
H	3.64378718	-2.83513305	2.97643346
H	4.05473384	-1.52386537	2.34114367
O	-1.93980409	-0.28917494	1.69829043
H	-2.55478025	0.39643281	1.95901511
H	-2.49267194	-1.04553450	1.50210590
O	-3.80835246	1.67018650	2.28042543
H	-4.10259709	1.64512948	3.19093257
H	-3.30784798	2.48325400	2.21225267
O	1.41345733	1.70378734	4.21040196
H	1.43725200	1.91853671	5.14289729
H	2.30964567	1.84990691	3.90753806
O	-4.57104775	2.92737032	-1.89648208
H	-5.25612676	3.36132672	-2.40498932
H	-5.03570847	2.52301611	-1.16380267
O	-1.43751780	1.51542238	-0.71228052
H	-1.61126211	2.45575844	-0.75484841
H	-2.06891183	1.12705531	-1.31787414
O	-0.08772335	2.12063167	1.92396850
H	-0.76626720	2.79400805	1.97268721
H	0.34512627	2.15394203	2.77705855
O	2.15127876	-3.21468201	-2.17554234
H	2.43705735	-4.11648414	-2.32153738
H	1.28197171	-3.17095551	-2.57381898
O	-3.40869668	-2.34052637	0.55869250
H	-4.08728573	-1.91779361	0.03234192
H	-3.82618225	-3.13256063	0.89724611
Ca	0.20465800	0.10074000	0.48149700

### 3.4.26 n=26

	79		
	-2214.00843167		
O	0.99262755	4.34670329	2.14599156
H	1.76776917	4.31341592	2.70659699
H	1.26230051	4.87500725	1.39472434
O	3.32293619	3.58978826	-0.94339618
H	3.77729717	3.24414834	-0.17507323
H	3.97775235	3.56425398	-1.64110301
O	-0.74664247	0.18868305	-1.82760762
H	-0.96802264	1.01784800	-2.25152663
H	-1.23084490	-0.47131193	-2.32377861
O	2.69168794	0.17446329	0.79252247
H	3.23836637	-0.54698704	1.10378302
H	3.20967136	0.96039424	0.96640959
O	2.63592137	-3.81277284	0.75502242
H	1.91124101	-4.07400548	1.32320101
H	2.97682179	-4.63661595	0.40674029
O	-4.03645631	-0.96198838	-0.97224797
H	-4.09084207	-0.01111846	-1.06774456
H	-4.92801436	-1.23252534	-0.75278268
O	2.73047339	-1.16400797	4.20585047
H	3.34668658	-1.39830102	3.51186265
H	2.94278636	-1.75790398	4.92587946
O	0.64156783	-1.41300723	2.41120320
H	0.43569776	-2.34755450	2.43288083
H	1.28826058	-1.29352898	3.10672061



O	4.26608480	2.40201550	1.34176063
H	3.95166708	2.85354060	2.12502151
H	5.20880759	2.31017237	1.47985337
O	4.14122599	-1.86767751	1.94546403
H	5.07612094	-2.04947727	1.84980157
H	3.70796178	-2.62476897	1.55135027
O	-0.73808497	4.32735936	-0.92055453
H	-1.22155830	4.39564007	-0.09725488
H	-0.03206715	4.96843475	-0.83813967
O	-1.71570311	4.16297483	1.66737474
H	-0.84902563	4.35246864	2.02680938
H	-2.31329761	4.70311315	2.18444576
O	0.60753246	1.64388471	2.39277717
H	0.71686018	2.58148229	2.23406598
H	0.97813233	1.50314734	3.26402900
O	1.61427685	5.63204024	-0.21906356
H	1.93103494	6.51714535	-0.39929752
H	2.30234006	5.05779865	-0.55528764
O	3.24703038	3.61078812	3.59184935
H	2.88863049	2.88660327	4.10501291
H	3.70143385	4.15738316	4.23292841
O	1.03157805	-1.99109544	-0.57511558
H	1.67909457	-2.59471060	-0.21096985
H	0.54988186	-2.51393738	-1.21608057
O	0.95284547	2.23512824	-0.54813340
H	0.33659918	2.95526439	-0.68183257
H	1.80562170	2.60282651	-0.78008537
O	-1.78480464	2.60118246	-2.78244094
H	-1.79489342	2.95114923	-3.67331270
H	-1.44183751	3.31689358	-2.24731277
O	-3.84152314	1.75832209	-1.16812477
H	-4.57125249	2.37777653	-1.16963866
H	-3.24731142	2.08582960	-1.84331533
O	-0.57214144	-3.62350324	-2.12842853
H	-1.21515509	-3.03636903	-2.52596832
H	-0.29154092	-4.19266239	-2.84505412
O	0.36246771	-4.16085137	2.25971923
H	0.16807438	-4.76612192	2.97532374
H	-0.34924399	-4.29315847	1.63346664
O	-1.75013122	-1.45202254	0.51423902
H	-1.74391531	-2.40776141	0.56673273
H	-2.59790224	-1.23859335	0.12441432
O	-2.34580283	-1.73199771	-2.99939121
H	-3.04998024	-1.55341543	-2.37611474
H	-2.77322218	-1.71508707	-3.85569592
O	2.00716290	1.43224896	4.75661638
H	1.64219562	1.45065038	5.64131480
H	2.35879415	0.54718693	4.66043074
O	-1.59434744	-4.20685381	0.35682127
H	-2.31464370	-4.83595585	0.31638676
H	-1.26278574	-4.16368316	-0.54008127
O	-1.79706416	1.57712999	0.67473083
H	-1.82413269	2.38980085	1.17976981
H	-2.56448895	1.62327314	0.10450190
Ca	0.20465800	0.10074000	0.48149700

### 3.4.27 n=27

	82		
	-2268.44840026		
O	-1.02961582	-0.52798788	-1.58037287

H	-1.98301987	-0.53754514	-1.66499200
H	-0.71663574	-1.02555124	-2.33582320
O	-3.38351671	2.11962971	-1.44987044
H	-3.61208597	1.21427086	-1.66037567
H	-3.75678685	2.63401595	-2.16562684
O	0.63169897	-4.55945758	1.94086107
H	1.54189209	-4.26318164	1.94059648
H	0.50573017	-4.94703713	2.80697017
O	1.77332046	-1.13916088	-0.99642606
H	2.70168865	-1.04018469	-1.20753559
H	1.55539295	-2.02622473	-1.28253154
O	0.13673388	1.61284132	2.45003250
H	0.88115655	2.00559032	2.90589886
H	-0.60305577	2.18107639	2.66462794
O	2.15878873	4.24872848	1.03621558
H	2.67254559	4.97746489	0.68803725
H	1.24827229	4.52218559	0.92480619
O	-0.42559554	-2.28571225	0.79337504
H	-1.07950555	-2.69407554	0.22603727
H	-0.08386030	-3.00613206	1.32294405
O	-2.17632158	0.06636313	1.22988423
H	-2.75645260	-0.69363750	1.18429853
H	-2.76666203	0.81330435	1.32891959
O	1.32768179	-3.68184613	-1.89175496
H	2.23457177	-3.90283097	-1.67974721
H	0.80871239	-4.36526537	-1.46767957
O	3.09389301	-3.37692449	1.72203252
H	3.81668894	-3.64944450	2.28730228
H	3.40410340	-3.55348220	0.83387268
O	3.93229552	0.68546087	3.12198143
H	4.42786535	0.50478494	3.92072906
H	3.46384151	1.49896504	3.30904517
O	-0.78946710	2.20241267	-0.41444200
H	-0.67942581	3.11285498	-0.14018530
H	-1.60515999	2.19956847	-0.91530928
O	-2.97706334	-2.86713868	-3.22520064
H	-2.08611375	-2.71159109	-3.53864088
H	-3.40351940	-3.34061130	-3.93947645
O	-0.30954742	-2.27288848	-3.62496930
H	0.10664593	-2.12484377	-4.47414353
H	0.28971476	-2.85910552	-3.16294610
O	-0.51879461	4.70696179	0.71850097
H	-0.91958385	5.53434547	0.45197657
H	-1.02021858	4.43391263	1.48677773
O	2.16032272	1.61904326	0.18407425
H	2.15711454	2.56085869	0.35496727
H	3.08635563	1.37689653	0.19175638
O	-3.97956766	-1.94763026	0.64491036
H	-4.73277775	-2.33099515	1.09428431
H	-3.50161347	-2.69899045	0.29384244
O	-1.89576000	3.47594847	2.75037193
H	-2.24844195	3.81452122	3.57330263
H	-2.65654303	3.11912455	2.29198683
O	-0.22957990	-5.49404743	-0.51418475
H	0.06144372	-5.33043563	0.38290357
H	-0.25895488	-6.44804161	-0.58673286
O	3.92616331	-3.77438897	-0.87048887
H	4.25658098	-2.90247205	-1.08685906
H	4.61385684	-4.37153434	-1.16498171
O	4.50004221	-1.12113973	-1.38635743
H	4.73349246	-0.48482173	-0.71046438

H	4.98814828	-0.83940461	-2.16005557
O	-2.28761735	-3.64849933	-0.67518243
H	-2.54778994	-3.51210921	-1.58619230
H	-1.74496860	-4.43674390	-0.69601154
O	4.80017665	0.85685862	0.51089406
H	5.56981188	1.42395156	0.46295427
H	4.64152649	0.74634629	1.44836308
O	-3.84615952	2.25899933	1.26012448
H	-3.80260698	2.32757265	0.30637824
H	-4.78259503	2.26152368	1.45840001
O	-3.73064266	-0.59816363	-1.76235474
H	-3.71545834	-1.30368691	-2.40906747
H	-4.00581732	-1.02312670	-0.95000241
O	1.94097958	-0.85313998	1.99847181
H	2.32766773	-1.72361904	1.90376434
H	2.59217817	-0.35355270	2.49099995
O	2.36802220	2.91266736	3.43457210
H	2.40010858	3.50587985	4.18510553
H	2.38771615	3.49000534	2.67133948
Ca	0.20465800	0.10074000	0.48149700

### 3.5 $\text{Ca}^{2+}(\text{CH}_3\text{OH})_n$ $n = 1 - 10$

#### 3.5.1 $n=1$

7			
-49.32339183			
C	2.08428155	-0.73996372	-1.96957857
O	2.06078150	0.12652180	-0.84339982
H	1.14054129	-1.29336748	-1.98622292
H	2.90886874	-1.46199018	-1.90048860
H	2.18271098	-0.18877834	-2.91571582
H	2.92210682	0.62980009	-0.83097913
Ca	0.20465800	0.10074000	0.48149700

#### 3.5.2 $n=2$

13			
-97.33672461			
C	-2.01363376	-2.08840331	-0.24221907
O	-0.62129073	-1.97780028	0.02003246
H	-2.44905613	-1.08736299	-0.16802957
H	-2.50794875	-2.73728825	0.49306366
H	-2.21674836	-2.48401139	-1.24765831
H	-0.22706627	-2.89169752	-0.04854984
C	0.88665399	3.03344907	-0.60799847
O	0.73441413	2.31799130	0.61846413
H	0.41513986	2.44838881	-1.40171459
H	1.94968884	3.16713445	-0.85538224
H	0.40509870	4.01783478	-0.57258711
H	0.90576979	2.95344451	1.36248843
Ca	0.20465800	0.10074000	0.48149700

#### 3.5.3 $n=3$

19			
-143.42063306			
C	2.76480822	0.47334660	-1.37303557
O	2.40379877	0.50828842	0.00103839
H	1.86398427	0.24446433	-1.95036352
H	3.51106224	-0.30793005	-1.56988936
H	3.16779466	1.43515371	-1.72117112

H	3.22679527	0.71737173	0.52476117
C	-1.82432174	-0.90433545	-1.77073951
O	-1.22604354	0.30219195	-1.29574251
H	-1.71796634	-1.66399797	-0.99214607
H	-1.31970678	-1.26142547	-2.68011515
H	-2.89205438	-0.77741292	-1.98522113
H	-1.55671056	1.04743835	-1.86319546
C	-2.29083263	-0.94013924	2.17675509
O	-0.86423906	-0.95808691	2.20582136
H	-2.59795592	-0.19508863	1.43698058
H	-2.71413087	-0.67380939	3.15291463
H	-2.69145444	-1.91637407	1.86727489
H	-0.59019899	-1.45689344	3.01682110
Ca	0.20465800	0.10074000	0.48149700

### 3.5.4 n=4

	25		
	-187.18646201		
C	2.75869612	0.64197294	-1.35349262
O	2.43834887	0.32630997	-0.00539673
H	1.82106077	0.71198399	-1.91306106
H	3.37797482	-0.14140129	-1.81050288
H	3.28987200	1.60057981	-1.44063865
H	3.29488720	0.26340093	0.50225389
C	0.43345322	-2.56663158	-1.26604863
O	-0.55484925	-1.76568792	-0.61719210
H	1.41013656	-2.29631172	-0.85663054
H	0.44297381	-2.37765703	-2.34924371
H	0.27224221	-3.63759276	-1.09511632
H	-1.43918514	-2.18948292	-0.77557002
C	0.13381432	3.19240531	-0.33079512
O	-0.69140325	2.02953627	-0.38636245
H	0.95390464	2.98407036	0.36255896
H	-0.42234498	4.06919675	0.02265081
H	0.56652292	3.41659107	-1.31660154
H	-1.53973890	2.28848548	-0.82783545
C	-0.57044738	1.25970942	3.36393923
O	-0.16544629	0.04268942	2.74507335
H	-0.65766593	2.01713478	2.57902795
H	0.17968134	1.60452093	4.08969944
H	-1.53980114	1.16328870	3.87066261
H	-0.12761509	-0.65142815	3.45674476
Ca	0.20465800	0.10074000	0.48149700

### 3.5.5 n=5

	31		
	-226.05415256		
C	-1.43790558	-2.47086449	1.45408247
O	-1.46880480	-1.05640237	1.58813528
H	-0.57495256	-2.72975470	0.83322309
H	-2.34503605	-2.84493859	0.96090650
H	-1.33493808	-2.97784029	2.42415597
H	-2.25622481	-0.82341782	2.15471496
C	-1.05952943	2.98644000	-0.02620492
O	-0.84711877	2.07697990	1.05408733
H	-0.97457460	2.42683554	-0.96120860
H	-0.30120840	3.78271797	-0.02415166
H	-2.05457699	3.44534379	0.01190478
H	-1.18992589	2.50560682	1.88203537

C	2.95236223	-1.40688368	1.26398168
O	1.74571082	-0.93124767	1.85904379
H	2.81420333	-1.39431376	0.17888004
H	3.18872659	-2.42872453	1.58487666
H	3.79915846	-0.74971537	1.50969748
H	1.78455076	-1.15028485	2.82451811
C	-1.81854900	-0.64504400	-1.87133893
O	-0.44176506	-0.80494190	-1.54414297
H	-2.27831665	-0.04184392	-1.08257450
H	-2.33392515	-1.61543358	-1.90370315
H	-1.95831801	-0.13412523	-2.83318034
H	-0.02065235	-1.31876304	-2.28465531
C	2.66744600	2.12721565	0.16392280
O	1.85967392	1.27075743	-0.64012491
H	2.29812728	2.06117306	1.19121225
H	2.60293773	3.17588467	-0.16154021
H	3.72039697	1.81764990	0.14730762
H	2.16487584	1.36017048	-1.58561658
Ca	0.20465800	0.10074000	0.48149700

### 3.5.6 n=6

37

-261.60479087

C	1.01652338	-1.62267450	-2.18253003
O	-0.10887339	-1.23597234	-1.40563137
H	1.90974840	-1.20241358	-1.71061025
H	0.94817940	-1.23138122	-3.20637491
H	1.12993708	-2.71497864	-2.23428302
H	-0.92149846	-1.62067528	-1.83803023
C	-0.61515370	2.03134590	2.98837216
O	0.51984174	1.39988290	2.39481748
H	-1.51335810	1.53297940	2.61492062
H	-0.66305158	3.09428571	2.71092243
H	-0.60559853	1.95115707	4.08182684
H	1.31944398	1.65297950	2.92709006
C	1.66405844	2.86918321	-0.39208844
O	1.75524266	1.46183540	-0.60978949
H	0.69491708	3.07044362	0.07369127
H	1.73575014	3.43140725	-1.33111179
H	2.45219328	3.21435223	0.29275615
H	2.51716224	1.30522926	-1.22345027
C	-1.59715808	1.84767788	-1.58985058
O	-1.61860182	1.36206931	-0.25123823
H	-0.67875473	1.48272126	-2.05966745
H	-1.57947666	2.94652594	-1.61300784
H	-2.45715407	1.49192750	-2.17256906
H	-2.47437271	1.66251005	0.15753819
C	1.89375148	-2.59787338	1.14885232
O	2.02655693	-1.17874689	1.17970377
H	0.87781760	-2.82751538	0.81534900
H	2.04244189	-3.04515716	2.14264434
H	2.60596381	-3.05239454	0.44815489
H	2.93754134	-0.96348210	1.52447310
C	-1.09494868	-1.59070090	2.93453521
O	-1.36451767	-1.23473498	1.57811687
H	-0.08085826	-1.26158664	3.17481548
H	-1.15541132	-2.67581374	3.09099481
H	-1.80066623	-1.09471449	3.61519716
H	-2.22503641	-1.65012271	1.30958063
Ca	0.20465800	0.10074000	0.48149700

### 3.5.7 n=7

43

-283.66814290

C	3.00793378	-1.50913567	0.31408755
O	2.37802343	-0.49274253	1.08206276
H	2.30888774	-1.81961937	-0.46828893
H	3.24875766	-2.38464425	0.93176728
H	3.93264522	-1.15554112	-0.16398046
H	3.01762920	-0.21153952	1.79421018
C	-1.63258727	-0.12670806	3.13965933
O	-0.29825668	0.20639872	2.75512187
H	-2.06881363	-0.74238999	2.34893265
H	-2.24519224	0.77886292	3.25700483
H	-1.66081464	-0.69675692	4.07582822
H	0.18170937	0.51756007	3.56724682
C	-0.17864807	-2.99280570	1.38239019
O	-0.43840914	-2.12996535	0.27587906
H	0.49538341	-2.46487121	2.06331471
H	0.29283524	-3.93077538	1.06471616
H	-1.10494720	-3.22467857	1.92783973
H	-0.85659659	-2.67783058	-0.43587190
C	1.83800664	0.78695964	-2.23711481
O	0.66509239	0.10626217	-1.80227963
H	2.39921718	1.08210826	-1.34530991
H	1.58340007	1.69766235	-2.79757180
H	2.47792602	0.15010294	-2.86211800
H	0.18021252	-0.19517153	-2.61697948
C	1.81733204	3.11230347	0.89089728
O	0.63232379	2.38148846	0.58401949
H	2.58982307	2.38873886	1.16620332
H	1.66772542	3.79928580	1.73675031
H	2.16775109	3.69008145	0.02591643
H	-0.08771434	3.03913559	0.37391773
C	-2.32843185	4.21015304	1.03284831
O	-1.70864911	3.64249481	-0.12165738
H	-2.28445556	3.47158066	1.83721583
H	-3.38108121	4.46201357	0.84818435
H	-1.79801810	5.11745468	1.35348125
H	-1.86633973	4.24781250	-0.89229045
C	-3.13093252	0.22862445	-0.33380149
O	-1.90733459	0.90234471	-0.06367852
H	-2.96604720	-0.84020800	-0.17168048
H	-3.44561144	0.37571181	-1.37579479
H	-3.94210008	0.56410251	0.32773741
H	-2.06529010	1.88503640	-0.14762049
Ca	0.20465800	0.10074000	0.48149700

### 3.5.8 n=8

49

-305.51932634

C	-2.41328915	2.17777717	1.35493940
O	-1.61669067	1.04098594	1.65951213
H	-2.04122132	2.60671177	0.41965384
H	-2.33715823	2.94071985	2.14117234
H	-3.47353067	1.91867158	1.22294862
H	-1.95830916	0.65198031	2.51232867
C	-2.86037951	-0.81383763	-0.70207991
O	-1.56903472	-1.28550918	-0.31578740
H	-2.77273956	0.24694508	-0.95040560

H	-3.58083113	-0.92267333	0.12145992
H	-3.24565842	-1.34325516	-1.58153538
H	-1.58409505	-2.27778911	-0.35925514
C	3.54274325	0.53494485	1.11792175
O	2.32553699	-0.02352928	1.61072165
H	3.41248727	0.72166025	0.04793941
H	4.39068434	-0.14525454	1.26395302
H	3.76426755	1.49360475	1.60905155
H	2.51235400	-0.39565810	2.50974669
C	1.02615454	2.98929575	1.97100196
O	0.87060036	2.38995346	0.68852379
H	0.91194938	2.20067441	2.72094830
H	0.25073462	3.74725614	2.15137920
H	2.01402795	3.45270728	2.09375433
H	1.01597209	3.10316950	0.01036706
C	1.03297084	1.32158139	-2.49592403
O	-0.10228546	1.02233106	-1.68712773
H	1.92510643	1.17385378	-1.88082063
H	1.02238116	2.36365958	-2.84771247
H	1.09145377	0.65653474	-3.36719061
H	-0.92044350	1.19697835	-2.23046295
C	-3.29095139	-1.18895447	3.79457071
O	-2.11201565	-0.39755790	3.94639916
H	-3.42537277	-1.39358548	2.72944760
H	-4.18309953	-0.66652009	4.16435337
H	-3.19149829	-2.14305843	4.33042069
H	-2.05854221	-0.09153473	4.88907704
C	0.33105594	-2.70936893	2.51469623
O	-0.14684150	-1.38597990	2.30419011
H	1.12008992	-2.89959745	1.78181718
H	-0.46610810	-3.44988922	2.36447397
H	0.74753196	-2.84274951	3.52312540
H	-0.82356382	-1.18103790	3.00968626
C	1.14435377	-2.17616871	-1.92253008
O	1.47120777	-1.53705533	-0.69273424
H	0.26661942	-1.67319781	-2.33855416
H	0.89030888	-3.23376175	-1.76439024
H	1.96578507	-2.11606464	-2.64885847
H	2.35256644	-1.88556791	-0.39728659
Ca	0.20465800	0.10074000	0.48149700

### 3.5.9 n=9

55			
-327.02249323			
C	-0.99538969	-3.03360117	-0.23826040
O	-0.98222155	-1.66136014	-0.60759650
H	-0.35248132	-3.15050457	0.63933909
H	-0.60161779	-3.66755637	-1.04391800
H	-2.00491148	-3.38479052	0.01903548
H	-1.56925974	-1.55781122	-1.40758925
C	2.75750470	1.89994665	-0.88505954
O	1.86680100	1.79175876	0.22589033
H	2.35370364	1.29699444	-1.70237202
H	3.75552392	1.51719349	-0.62704547
H	2.85489230	2.93442674	-1.23510420
H	2.07300467	2.53466882	0.85222923
C	-0.52656033	2.28969387	-2.13360020
O	-0.70883634	1.02028849	-1.50772354
H	-0.06074720	2.95621945	-1.40185349
H	-1.47998064	2.72306501	-2.45945232

H	0.14493340	2.20924515	-3.00074174
H	-1.32248065	0.49289557	-2.07949610
C	2.02760496	-1.55549187	-1.80876303
O	1.94602788	-1.23370949	-0.42385877
H	1.24298100	-0.99462836	-2.32566081
H	1.84990818	-2.62694773	-1.97823911
H	2.99958456	-1.28200011	-2.24023745
H	2.68682191	-1.71422274	0.03444007
C	2.86886713	-0.20488836	2.73170744
O	1.49499815	-0.41815266	2.41625305
H	3.34721234	0.22848324	1.84883912
H	3.38332968	-1.14505477	2.97911319
H	2.98413545	0.49123122	3.57250676
H	1.06360040	-0.85314484	3.20351108
C	-1.82111040	-1.23423151	-4.00143571
O	-2.38918674	-0.75152005	-2.78343374
H	-0.73363875	-1.16499760	-3.91751755
H	-2.14259010	-0.63805989	-4.86563209
H	-2.09874250	-2.28361218	-4.17190889
H	-3.37206910	-0.68042628	-2.90192060
C	-2.74331048	-0.68048700	2.04776454
O	-1.32316045	-0.70945792	2.12771379
H	-3.01403430	-0.29963687	1.05906085
H	-3.17184508	-0.01066945	2.80546508
H	-3.18467525	-1.67928517	2.17334882
H	-1.06661806	-1.11545660	3.00351640
C	-0.68215176	2.48323549	2.67654023
O	-0.83170869	2.07825433	1.31958768
H	0.13492515	1.90072532	3.11190282
H	-1.59454056	2.27850163	3.25419134
H	-0.44254178	3.55138834	2.76343870
H	-1.45957160	2.71182386	0.88378812
C	-0.27042106	-0.79110596	5.47250653
O	-0.02044882	-1.64141391	4.35439467
H	-0.35774079	0.23047698	5.09244384
H	0.54440496	-0.82712653	6.20781466
H	-1.21027138	-1.06016116	5.97313980
H	0.06888603	-2.56595683	4.69786478
Ca	0.20465800	0.10074000	0.48149700

### 3.5.10 n=10

61			
-347.63485031			
C	-0.28843597	2.47022934	-1.87641087
O	-0.13598461	2.25025604	-0.48070377
H	-0.21581953	1.50066513	-2.37825801
H	0.50380167	3.12313414	-2.26642948
H	-1.26156977	2.91879477	-2.12231536
H	-0.20287922	3.13568594	-0.02588114
C	1.43406896	-2.57204652	2.33748286
O	1.60781798	-1.23917327	1.85527183
H	0.58420598	-3.01409330	1.81123775
H	1.21853338	-2.57466495	3.41574589
H	2.31685558	-3.19518339	2.15159874
H	2.51869520	-0.93995750	2.11509547
C	3.02298139	1.13242393	-1.29149477
O	2.43295803	0.71053636	-0.06258490
H	2.26810292	1.02458248	-2.07585450
H	3.90008795	0.52692289	-1.55044073
H	3.31974465	2.19024484	-1.24398930



H	3.16576226	0.59474426	0.59408597
C	-2.17712180	-1.86107575	2.05849838
O	-1.33001157	-0.71690306	2.09633551
H	-2.01384976	-2.36222052	1.09954994
H	-3.23621829	-1.57269670	2.11738897
H	-1.95380063	-2.56784662	2.86863099
H	-1.45248827	-0.28887633	2.98599791
C	1.75749537	-2.37490086	-1.35088739
O	0.59157820	-1.58624400	-1.12468702
H	2.52324283	-2.04290612	-0.64414000
H	2.14759590	-2.24647499	-2.37124153
H	1.55979513	-3.44118010	-1.18125255
H	-0.09574892	-1.85569694	-1.79556254
C	5.05765996	-0.91545737	1.48900745
O	4.09151447	-0.01617859	2.03408585
H	4.54189358	-1.58673091	0.79777156
H	5.53743741	-1.52053210	2.26958631
H	5.83432092	-0.36638422	0.93886482
H	4.52167176	0.50304856	2.76245324
C	-3.05485746	0.52431874	-0.52199007
O	-1.82648547	-0.15446680	-0.75524907
H	-2.89075247	1.24276150	0.28595966
H	-3.84307491	-0.17369082	-0.20909480
H	-3.40176947	1.06832378	-1.41186794
H	-1.95002418	-0.76764178	-1.53398764
C	1.39506556	2.58398153	2.59607659
O	0.43685947	1.56304724	2.33678615
H	1.87290089	2.84380920	1.64705798
H	2.17394294	2.23055008	3.28635646
H	0.93207305	3.48537135	3.01921856
H	-0.10316314	1.44073147	3.16077515
C	-2.23190651	-3.20418848	-2.46072473
O	-1.56402906	-1.98588094	-2.78530187
H	-2.14311287	-3.34712990	-1.38026764
H	-1.78431609	-4.06783388	-2.97032892
H	-3.29776567	-3.15373823	-2.72099775
H	-1.63476079	-1.85972983	-3.76500334
C	-0.55307988	0.13473341	5.37170564
O	-1.27077633	0.83167485	4.36630469
H	0.21847030	-0.46271108	4.87703034
H	-1.20805732	-0.54344596	5.93583111
H	-0.06114532	0.81330806	6.08533297
H	-1.99801611	1.35425932	4.79893676
Ca	0.20465800	0.10074000	0.48149700

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