Figure S1: Population of energy bins of $(H_2O)_{32}$ in the original MCTBP method. The X-axis defines energy bins and Y-axis represents the frequency of the structures.
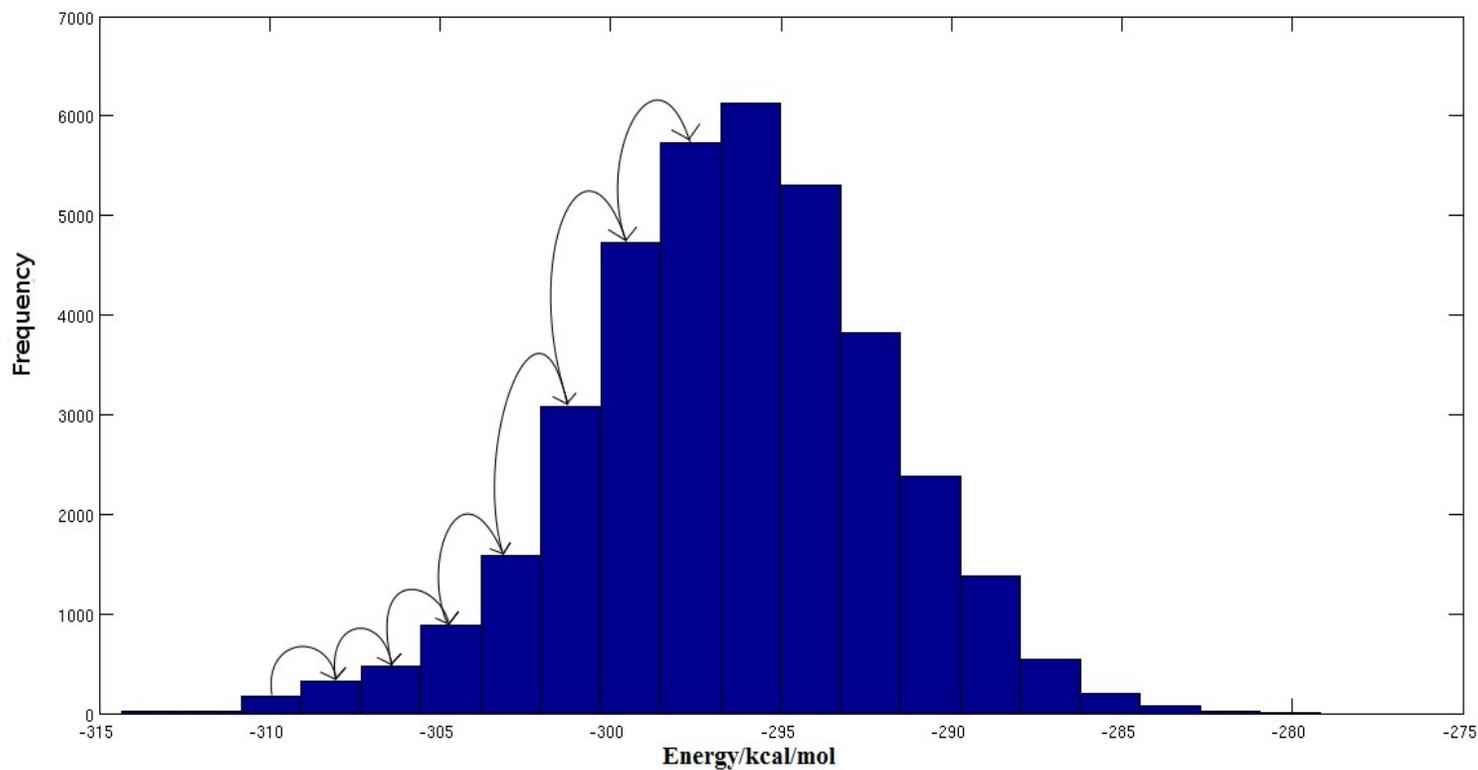
Figure S2: Variation in energy and effective temperature in the original MCTBP method for $(H_2O)_{33}$ with occasional lowering of effective temperature.
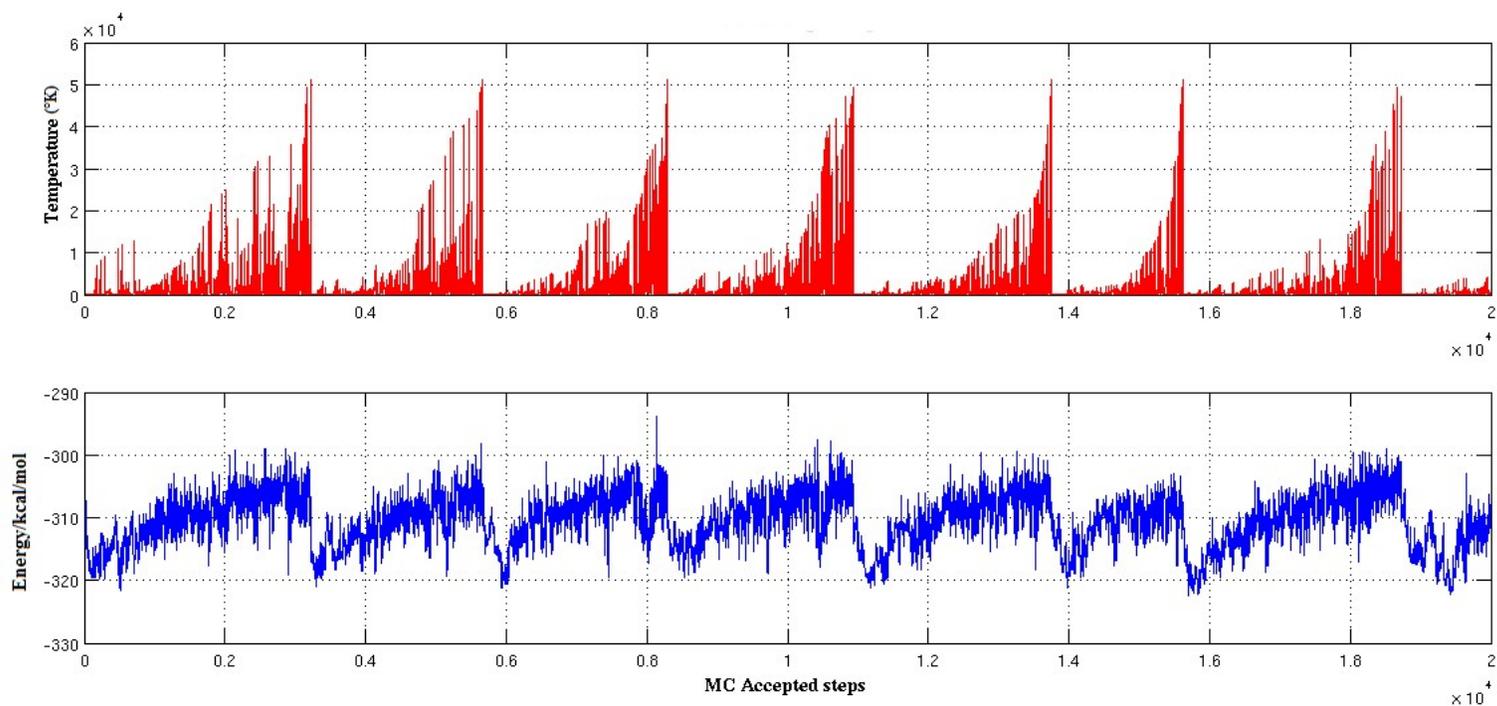
Figure S3. Graphical representation of undirected and directed graph of $(H_2O)_4$.

Water Tetramer   Undirected Graph   Directed Graph
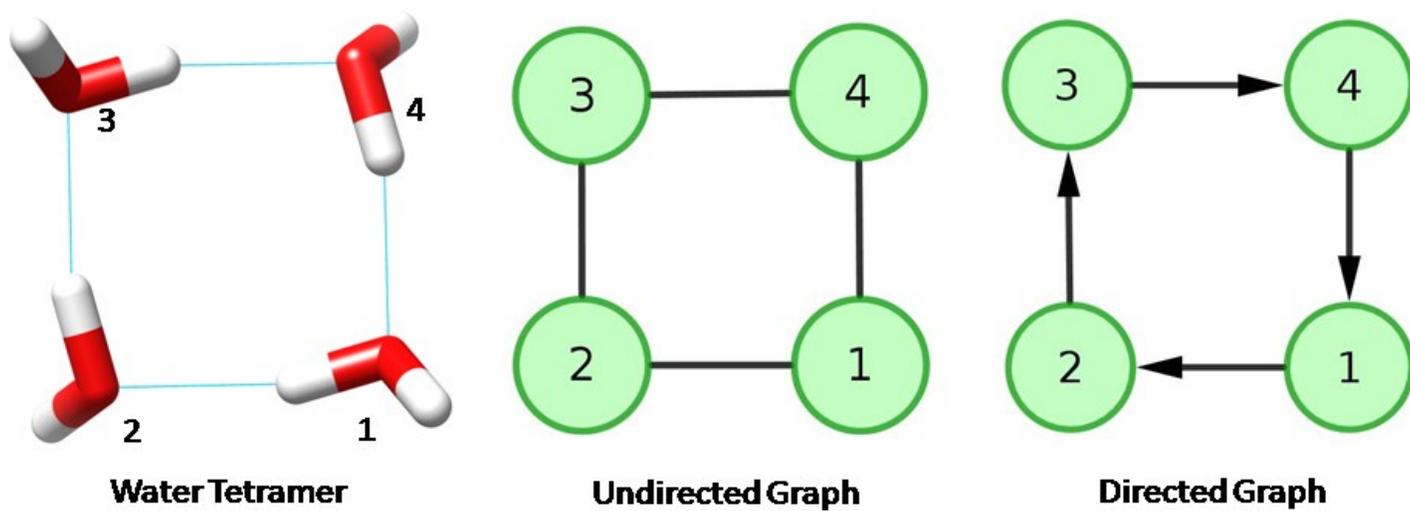
Figure S4. The decomposition analysis of polarized charges on oxygen atom into the contribution of each surrounded molecule by adapting the CDRK approach for the most stable structure. (a) w15 in structure 1 for $(H_2O)_{32}$ and (b) w6 in structure 11 for $(H_2O)_{33}$ molecules were analyzed (see Figure 6). □Absolute values of ΔQ by surrounded water molecules on oxygen atom were shown. The water molecule belonging to the first, second and third solvation shells were indicated by blue, red, and black colors, respectively.

(a)
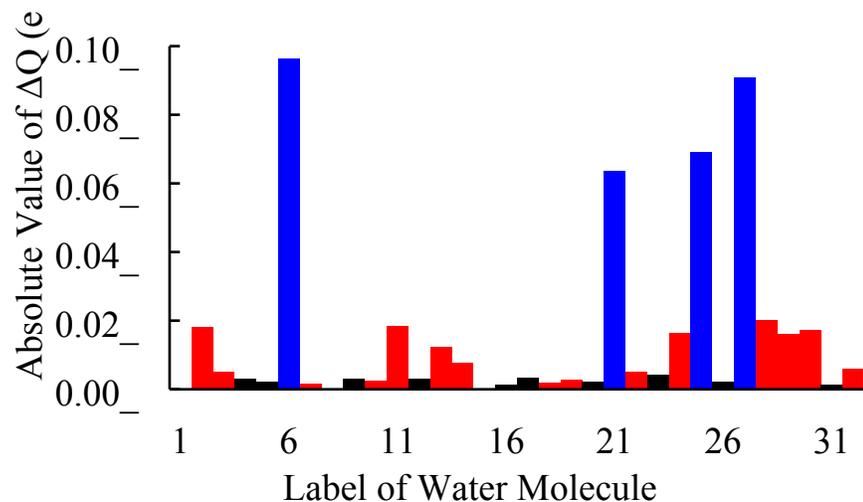
(b)
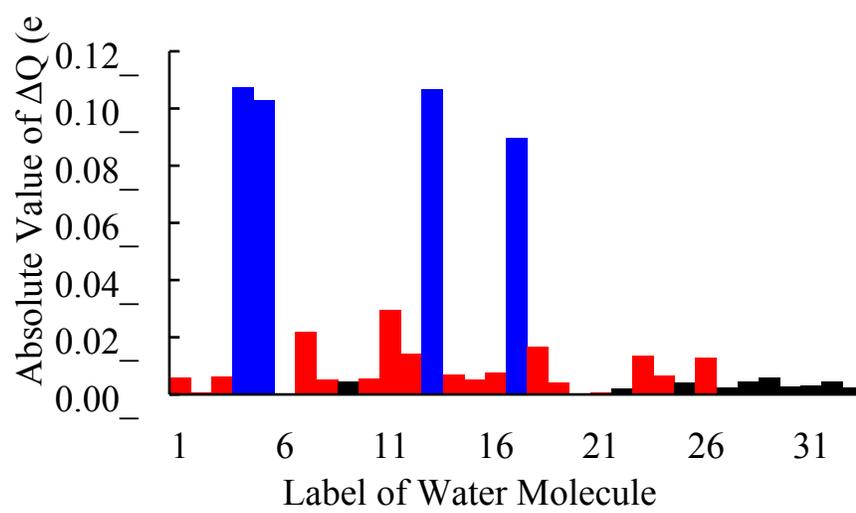
Table ST1. Total energies by the quantum mechanical calculation E_{QM}, sum of atomic energies by QTAIM method E_{QTAIM}, and their difference DE for $(H_2O)_{32}$ clusters. The wave functions are constructed using M06-2x/6-311G(d,p) and M06-2x/6-311+G(d,p) level of theory. The structure numbers with reference to figure number 4 are also given.

Structure No.	M062x / 6-311G(d,p) Level			M062x / 6-311+G(d,p) Level		
	EQM (hartree)	EQTAIM (hartree)	ΔE (kcal/mol)	EQM (hartree)	EQTAIM (hartree)	ΔE (kcal/mol)
1. (6(a))	-2445.94906	-2445.94880	-0.16	-2446.06671	-2446.06700	0.18
2. (6(b))	-2445.93454	-2445.93562	0.67	-2446.05758	-2446.05718	-0.25
3. (6(c))	-2445.93676	-2445.93660	-0.10	-2446.05899	-2446.05946	0.29
4.	-2445.94407	-2445.94356	-0.31	-2446.06258	-2446.06218	-0.25
5.	-2445.93643	-2445.93607	-0.23	-2446.05857	-2446.05826	-0.19
6.	-2445.93246	-2445.93207	-0.25	-2446.05625	-2446.05591	-0.21
7.	-2445.93175	-2445.93132	-0.27	-2446.05539	-2446.05516	-0.15
8.	-2445.93304	-2445.93288	-0.10	-2446.05677	-2446.05641	-0.23
9.	-2445.93043	-2445.93018	-0.16	-2446.05482	-2446.05477	-0.03
10.	-2445.93280	-2445.93240	-0.25	-2446.05621	-2446.05589	-0.20
11. Structure T	-2445.94856	-2445.94815	-0.26	-2446.06659	-2446.06625	-0.22
12. Structure H	-2445.94409	-2445.94478	0.43	-2446.06208	-2446.06198	-0.07

[a] $\Delta E = E_{QM} - E_{QTAIM}$

Table ST2. Total energies by the quantum mechanical calculation E_{QM}, sum of atomic energies by QTAIM method E_{QTAIM}, and their difference DE for $(H_2O)_{33}$ clusters. The wave functions are constructed using M06-2x/6-311G(d,p) and M06-2x/6-311+G(d,p) level of theory. The structure numbers with reference to figure number 5 are also given.

Structure	M062x / 6-311G(d,p) Level			M062x / 6-311+G(d,p) Level		
	EQM (hartree)	EQTAIM (hartree)	ΔE (kcal/mol)	EQM (hartree)	EQTAIM (hartree)	ΔE (kcal/mol)
1. (7(a))	-2522.37349	-2522.37306	-0.27	-2522.49901	-2522.49864	-0.23
2. (7(b))	-2522.37023	-2522.37134	0.70	-2522.49682	-2522.49647	-0.22
3. (7(c))	-2522.37006	-2522.36967	-0.25	-2522.49692	-2522.49666	-0.16
4. (7(d))	-2522.37842	-2522.37947	0.66	-2522.50090	-2522.50118	0.17
5. (7(e))	-2522.37137	-2522.37076	-0.39	-2522.49645	-2522.49580	-0.41
6.	-2522.36144	-2522.36136	-0.05	-2522.49165	-2522.49137	-0.18
7.	-2522.36828	-2522.36797	-0.19	-2522.49508	-2522.49485	-0.14
8.	-2522.37307	-2522.37272	-0.22	-2522.49698	-2522.49657	-0.26
9.	-2522.36827	-2522.37095	1.68	-2522.49495	-2522.49491	-0.02
10.	-2522.36686	-2522.36820	0.84	-2522.49353	-2522.49353	0.00
11.Structure T33	-2522.38608	-2522.38685	0.49	-2522.50452	-2522.50550	0.61
12.Structure H33	-2522.37749	-2522.37889	0.88	-2522.49951	-2522.50074	0.77

[a]$\Delta E = E_{QM} - E_{QTAIM}$

Table ST3.Hydrogen bond network of the lowest energy structures of $(H_2O)_{32}$. N_{HB} represents number of different HB networks (directed graph) for each structure.

Structure	N_{HB}
1[a].	7
2[b].	193
3[c].	66
4.	14
5.	12
6.	57
7.	43
8.	20
9.	10
10.	7
11[d].	2
12[e].	7

a) This structure is depicted in Figure 6(a).
b) This structure is depicted in Figure 6(b).
c) This structure is depicted in Figure 6(c).
d) This is T structure.
e) This is H structure.

Table ST4.Hydrogen bond network of lowest energy unique oxygen frames of $(H_2O)_{33}$. The structure numbers with reference to figure number 4 are also given. N_{HB} represents number of different HB networks (directed graph) for each structure.

Structure	N_{HB}
1[a].	12
2[b].	6
3[c].	4
4[d].	11
5[e].	2
6.	24
7.	13
8.	16
9.	3
10.	6
11[f].	8
12[g].	1

a) This structure is depicted in Figure 7(a).
b) This structure is depicted in Figure 7(b).
c) This structure is depicted in Figure 7(c).
d) This structure is depicted in Figure 7(d).
e) This structure is depicted in Figure 7(e).
f) This is T33 structure.
g) This is H33 structure.

The coordinates of the three structures in figure 6 and coordinates of 5 structures in figure 7 are given below.

Coordinate Figure 6(a)

96
Energy   -317.459209670007
O   -3.8048469977   2.7056331788   0.8952304031
H   -4.0767909600   3.5519277945   1.2125793575
H   -3.8614327997   2.1108840212   1.6259491867
O   -1.0735695713   2.2161502117   0.0457972539
H   -1.9711071067   2.3509977659   0.3048743923
H   -0.8386407067   1.3455152206   0.3245114353
O   -3.3647061124   -1.0103209490   0.3459640368
H   -4.1723135655   -1.1130259776   -0.1316344692
H   -2.7083491380   -0.7554287380   -0.2826089001
O   -3.5186521565   0.6999685080   2.6984583693
H   -2.7239360737   0.7281090433   3.2069000199
H   -3.4252630863   -0.0141738048   2.0884110819
O   -4.8943894596   1.8705669160   -1.6922662682
H   -5.0811457394   0.9454425987   -1.7043304168
H   -4.6018441324   2.0768972563   -0.8189258556
O   -1.3246486906   -0.7924395071   -1.6474127037
H   -0.4451190503   -0.4944131828   -1.4786336295
H   -1.2584678062   -1.6949189658   -1.9157955855
O   -0.0439352546   -0.0931474026   1.4598096250
H   -0.2813379452   0.2471182040   2.3075936385
H   -0.4187506625   -0.9573085312   1.3996647348
O   -5.3628306936   -1.0666624688   -1.7451694400
H   -4.8863024957   -1.5035926068   -2.4328404261
H   -6.2468037274   -1.3960783806   -1.7760771512
O   -0.8292836081   0.9777637996   3.9598259679
H   -0.4365792803   0.4079239129   4.6016548147
H   -0.3866830303   1.8086470873   4.0277681859
O   -1.3404117463   -2.6108122197   1.4566852258
H   -0.9800527916   -3.1883703529   0.8028913129
H   -2.2165252800   -2.3979657204   1.1774006076
O   -0.6195295986   3.2440696467   -2.5838429324
H   -0.7572838718   2.8005327272   -1.7621512534
H   -1.4542679112   3.2654063440   -3.0238828726
O   -3.2781655058   2.7975049727   -3.7297502710
H   -3.7560544572   3.3505037715   -4.3269880233
H   -3.8821245838   2.5481810584   -3.0486119062
O   1.0707463434   3.7477656663   1.0176494775
H   1.1472021884   3.7068045599   1.9575192268
H   0.2623226781   3.3159281912   0.7921588421
O   -2.1386719877   0.1434056675   -4.1836385720
H   -1.9187788239   0.0286291225   -3.2729510321
H   -2.5117810120   1.0064787980   -4.2659360908
O   1.3662027212   0.0669087882   -1.6859066669
H   1.4352733348   0.5020698467   -2.5206177292
H   1.7718158637   0.6341764511   -1.0498533426
O   1.2336920296   3.1024879992   3.9070054614
H   1.8537524076   2.4005741554   4.0241401603

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H    1.4363523776     3.7549782900     4.5582071643
O   -3.7676215561    -2.2380453189    -3.6999338896
H   -3.0954707537    -2.8220269725    -3.3867930569
H   -3.3273447111    -1.5303673896    -4.1429087221
O    1.4245557616     5.1294396192    -1.6164435886
H    0.6564574861     4.7460071446    -2.0087228648
H    1.3515866616     4.9911090629    -0.6856274834
O   -1.2267901451    -3.4853791115    -2.6334700080
H   -1.0004588520    -4.0742297168    -1.9313962481
H   -0.5099155564    -3.5066022463    -3.2470813318
O    0.6760482855    -1.0195279322     5.4025223059
H    0.5504568506    -1.8069108098     4.8974149414
H    0.6116100905    -1.2669144593     6.3111069631
O    2.8959201021     2.0047697549    -0.2577142380
H    2.3842461520     2.6770967431     0.1630524951
H    3.3610621199     2.4210130122    -0.9657134670
O    0.2534347132    -4.2326610983    -0.1738476166
H    0.6761607422    -4.7300245457     0.5079226964
H    0.9196976697    -3.6935523493    -0.5692384153
O    0.1300659900    -3.2627984902     3.8661100424
H    0.7886457011    -3.7881074929     3.4404321480
H   -0.5287169763    -3.0750934327     3.2167640108
O    2.8397739277    -0.2210118530     1.5766984770
H    3.1725254897     0.4546442171     1.0078015382
H    1.9010155986    -0.2201974226     1.4786648596
O    1.5244285799     1.8614398784    -3.8528595832
H    2.3123488085     2.3627168771    -3.7158138315
H    0.8050978466     2.4049068487    -3.5734219292
O    2.7131542773     0.7960943183     4.2808949307
H    2.1874193389     0.1577727488     4.7358969114
H    2.9700807516     0.4022608899     3.4625047599
O    2.0947647148    -2.6440884541    -1.6381617222
H    2.0261206893    -2.9272828179    -2.5359185959
H    1.9064330661    -1.7192383748    -1.6302893086
O    0.4560294402    -0.5004221892    -5.2838033406
H   -0.4466907386    -0.2920493224    -5.1033719647
H    0.9643883621     0.2532171296    -5.0298792621
O    1.0766636773    -3.0384273739    -4.3579531884
H    1.3566524482    -3.5754516707    -5.0818935498
H    0.9217769057    -2.1744758543    -4.7050501688
O    3.5306117468     3.6624833787    -2.6294335004
H    4.2952117463     4.1195079642    -2.9415133348
H    2.9169573744     4.3216966244    -2.3470425266
O    2.0128055271    -4.7903611262     2.1525748127
H    2.4878760812    -5.5481331087     2.4541839062
H    2.6524962957    -4.1900242893     1.8043365940
O    3.6099744250    -2.9433938889     0.8762150953
H    3.5061251325    -2.0603490732     1.1929573122
H    3.3730559629    -2.9335219191    -0.0373770679
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Coordinates Figure 6(b).

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96
Energy    -316.853667005944
O     3.6309697125      -2.6651772485      3.1141607811
H     2.8152756232      -2.2415933730      3.3288659446
H     4.1337294229      -2.7058812255      3.9119416494
O     2.5380254790       0.5738630412     -2.6154473183
H     2.2170379460       1.4421160718     -2.4311048852
H     3.4727028511       0.6475866292     -2.7241740245
O    -1.7244665214       1.4484462969      1.5464615312
H    -2.0150036260       2.0698026849      2.1948309352
H    -0.8102428160       1.2865555472      1.7163581341
O     6.7403205965      -1.1832275006     -3.5993574746
H     6.4298313762      -1.8601447606     -3.0194799692
H     6.4905793132      -1.4387882473     -4.4729686297
O     3.0194758714      -5.0604216394      1.5430658491
H     2.0767536039      -5.0229713302      1.5156677708
H     3.3049828234      -4.3281891846      2.0657510953
O    -1.3084852087      -2.8295924592      2.8168813567
H    -1.7987165794      -2.3117619515      2.1984937578
H    -1.8905076294      -3.0161372161      3.5361375068
O     4.2496116587      -5.4559754290     -0.9249591858
H     4.7698946899      -6.2422730159     -0.8811399400
H     3.8570371913      -5.3426782448     -0.0741199003
O     0.9797096479       0.7879458884      1.6560866404
H     1.1440538559       0.2082286655      0.9295899942
H     1.5920734990       1.5018737519      1.5773721330
O    -2.7045701162      -1.2525707097      1.0453501063
H    -2.5688460229      -0.3367877503      1.2291951388
H    -2.5276405344      -1.3738679914      0.1261867114
O    -1.5328739566      -1.4056983456     -1.6267135765
H    -0.8790212779      -2.0794698706     -1.5298267315
H    -1.8023590960      -1.4172539854     -2.5312149203
O     2.0854205814      -4.8730781062     -2.8399663056
H     2.4646718888      -4.3696498760     -3.5425379510
H     2.8032625996      -5.1928894535     -2.3171833745
O    -0.0083021805       3.0022162037     -5.8418003402
H    -0.6634633377       2.6317451100     -5.2722448286
H    -0.4590957292       3.5876321909     -6.4291262740
O     1.1927664211      -1.3934751225      3.5709555631
H     0.4075654164      -1.8781069993      3.3722855346
H     1.1348660254      -0.5779659238      3.0992875177
O     2.8487719638       2.8331864674      0.8324833096
H     3.1351767560       3.5961616644      1.3086341237
H     3.6278511428       2.3781325103      0.5552830516
O     4.3319207144      -1.3553983553      0.5741087068
H     4.3586104950      -1.7826073536      1.4153331605
H     3.4206060219      -1.2372842300      0.3586254389
O     1.3092935257       2.8837663984     -1.6457922794
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H     0.4521049225      2.5153761736     -1.5029819333
H     1.6966840713      3.0076112485     -0.7940473221
O     5.0873681655     -2.8018300618     -1.8233334763
H     4.9360864536     -2.2846861912     -1.0483789519
H     4.9803792907     -3.7052375550     -1.5717649252
O     5.0440836822      1.4148056069      0.0263013090
H     5.2404852261      1.4227320623     -0.8968682631
H     4.9986979263      0.5085730084      0.2862264226
O     4.7938492837      3.0519062562     -4.8877934295
H     5.3089226948      3.8047224297     -5.1303746409
H     3.9317777025      3.3707530542     -4.6732060058
O     5.2942305779      1.0935305244     -2.8466146515
H     5.8724602679      0.3979653365     -3.1162773095
H     5.3539250525      1.7667189122     -3.5055019093
O     3.5200141589     -2.7861601235     -4.2707070809
H     4.1131950949     -2.5933523279     -4.9791137333
H     3.9849896600     -2.6028774516     -3.4700300551
O     1.7823257771     -0.9322015339     -0.4220406238
H     1.3475300472     -1.7357572839     -0.6589568199
H     1.9913792121     -0.4888532119     -1.2286491911
O     0.4946183668     -3.3393751098     -1.1137405390
H     0.3561408968     -3.9047382263     -0.3707284322
H     0.9540040546     -3.8499026390     -1.7612008743
O    -1.4813248016     -1.1231292835     -4.5070949800
H    -1.8460798811     -1.6125213705     -5.2270446805
H    -0.5427140421     -1.1725602271     -4.5933786868
O     2.2378873135      3.9550041385     -4.2316827221
H     1.9286829364      3.7835467478     -3.3565407505
H     1.5450654262      3.6987973875     -4.8192492182
O    -1.8607543529      1.7758199457     -4.1628900727
H    -1.7540151613      1.8896523134     -3.2320155424
H    -1.8874714433      0.8457030005     -4.3211528903
O     5.4263838916     -1.6836041460     -6.1602047744
H     5.7970840941     -2.0633523195     -6.9407501854
H     5.1051938609     -0.8291884674     -6.4003906744
O     1.3070664850     -1.0071185315     -4.5747771901
H     1.6317372394     -0.3928241615     -3.9359424837
H     1.9027420171     -1.7392721240     -4.5742959941
O    -1.1690914388      1.4569460222     -1.3121420020
H    -1.0885436883      0.5175195669     -1.3553675631
H    -1.5996265574      1.6550350934     -0.4958830446
O     4.4606650751      0.8137710782     -6.8223282138
H     4.6506293509      1.5234457156     -6.2297457833
H     3.5301917004      0.8333102432     -6.9795413625
O     1.6055051242      0.7295820976     -6.8872515541
H     1.4302602759      0.0876721409     -6.2178344160
H     1.1172918215      1.5034207005     -6.6555188595
O     0.0708556729     -4.8259484922      1.3450281410
H    -0.4455826979     -5.6159452208      1.3363660428
H    -0.3722345745     -4.2184281381      1.9155266127
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Coordinates Figure 6(c).

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96
Energy    -316.732596776585
O      1.7839649926      6.5950534232      3.4289318935
H      2.0635806991      7.4958869081      3.4634651120
H      2.4738503473      6.0817570860      3.8181150401
O     -2.7866179454      4.2798100199      2.7481773844
H     -2.2793619003      4.0709399891      1.9800998695
H     -2.2221268632      4.7755773340      3.3195293272
O      2.2637182483      0.5465461296      2.6018848042
H      1.3595723139      0.8138947779      2.5580295461
H      2.3426759856     -0.0211601961      3.3517872362
O      0.3320529164     -3.2998423435     -0.9733647866
H     -0.3368887887     -3.6253192579     -0.3924515164
H      0.0798754174     -2.4224023675     -1.2129144716
O      2.0268094005     -1.1624508407      4.7812951561
H      2.3740498635     -0.8100486757      5.5851080878
H      1.0983212473     -1.2712063944      4.9115273830
O     -2.4840940309     -0.1200501966      3.0900590345
H     -3.2044946127      0.4581966160      3.2837910135
H     -2.6952909282     -0.5542589178      2.2790491017
O      3.7051729056      4.7928716470      4.3033718165
H      3.4624439731      4.2476310505      5.0345857464
H      3.8976575734      4.2125101607      3.5843386796
O     -4.0570136545      2.1345012479      3.9374591906
H     -4.9872140352      2.2945139365      3.9387419051
H     -3.6553449508      2.8727637285      3.5079138307
O      2.8327755945     -3.2135582140      0.1934924070
H      3.4278576581     -3.8429186936     -0.1815558277
H      1.9941898498     -3.3557913395     -0.2156801005
O     -1.6039276720     -0.3915288709      7.6386057363
H     -0.8178795187     -0.0495914058      8.0336823423
H     -2.0583567781     -0.8729896243      8.3113376179
O     -0.0394788707     -0.3209950771     -0.9066553290
H     -0.2140341016      0.4740837152     -1.3844195381
H      0.8343880295     -0.2421485985     -0.5587784432
O      3.5980153433      2.9474172972      2.0048664157
H      4.0611521408      2.7727864347      1.2011955734
H      3.2469351326      2.1226159253      2.3003724845
O     -0.2894367129      2.4369192784     -2.0186364529
H      0.5535945893      2.8612628800     -2.0290856326
H     -0.7180771254      2.6651498463     -2.8279921588
O      0.7107884085      0.7430687581      8.6676283943
H      1.5079957550      0.4888097144      8.2309463138
H      0.7130985482      1.6860148299      8.7091714195
O      4.1877550590      1.9136696470     -0.7272679938
H      3.7596935723      1.0805081488     -0.6111485055
H      4.9800661766      1.7463412420     -1.2121625718
O     -0.8479740639      3.4294647486      0.6877451022
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H      -0.0665742916      3.9561457322      0.7415966706
H      -0.9094987005      3.1257404711     -0.2037955511
O       2.4762180217      3.0306179985      6.3164676840
H       1.7002185163      2.8852029045      5.7992079117
H       2.1917989932      3.4156914661      7.1299187857
O       2.1011823204      3.7929004945     -1.6161483237
H       2.8421942063      3.2446190798     -1.4132509865
H       1.9796968305      4.3687825684     -0.8782597368
O       1.5997136796      4.7839998933      1.1183102467
H       1.5513754096      5.5463510116      1.6727132031
H       2.2126444451      4.1919187007      1.5240616388
O       3.1357203682      0.4029612085      6.9860140833
H       4.0138439605      0.2493616929      7.2961505043
H       3.1074910425      1.2963477202      6.6827945259
O      -2.3709482802      2.0396511075      6.2803925526
H      -3.0316785384      1.9554231766      5.6116477316
H      -2.3427930367      1.2153293985      6.7392819253
O      -1.6208897689     -4.0429136583      1.0540393799
H      -2.1808461008     -4.8005785531      0.9968443839
H      -1.2233362012     -4.0633827103      1.9098493079
O      -0.6923850418      5.3663956757      4.5230794408
H      -0.2748578285      4.5253093321      4.6185951088
H      -0.0363625156      5.9589180229      4.1922771324
O      -0.3138593857      1.4684469277      2.5720709254
H      -0.5578524871      2.0674934391      1.8846925015
H      -1.0371790338      0.8720422822      2.6815635717
O      -0.3974623877     -4.0535652319      3.5266754739
H       0.5422874863     -4.0670353077      3.4396859032
H      -0.6047861258     -3.3507449043      4.1216031239
O      -0.8326256634     -1.4913863678      5.0284055712
H      -1.3838553545     -1.0362110592      4.4120941887
H      -1.1523274133     -1.2749062304      5.8896869395
O      -1.4684476267      4.6354734062      7.3332974089
H      -1.9647164934      3.8715968259      7.0861370641
H      -1.3354478098      5.1389734750      6.5461016369
O       2.7424608489     -0.3507805537      0.0670643565
H       2.6496101454     -0.1441125051      0.9833315220
H       2.9678883633     -1.2659538994      0.0168783304
O       0.8197114023      3.7201589757      8.6153300669
H       0.0455462481      4.0873158443      8.2194227522
H       0.9664075284      4.1964279792      9.4169075972
O       2.4102140323     -3.5968514700      3.1441289846
H       2.6128192572     -3.3916799498      2.2453886305
H       2.5533681798     -2.8075383392      3.6414921573
O      -2.4308130306     -1.2932108954      0.6115197084
H      -1.6883999583     -0.9303360791      0.1554241572
H      -2.2788522810     -2.2221517915      0.6811989468
O       0.0663267198      2.7263534885      4.9646453189
H       0.0073709630      2.2686639287      4.1412845597
H      -0.6670251559      2.4418340847      5.4862986419
```

Coordinates Figure 7(a).

```
99
Energy    -325.768527792549
O      0.0102969424      4.8652819401     -4.5734691602
H      0.2671410555      5.6395275370     -5.0482884010
H     -0.7482409121      4.5162927837     -5.0135888553
O     -2.9164382896      3.3878785899      1.6241601595
H     -3.0600070536      4.2900223130      1.3866666505
H     -2.7866295407      3.3707846302      2.5588985931
O     -1.7227739996     -1.2807044529     -3.1589569184
H     -1.8433607119     -1.0596040978     -4.0686007673
H     -1.6928146170     -2.2228441078     -3.1104413537
O     -3.4143021690      5.9761945758      0.7839725516
H     -2.7166852385      6.4801454488      0.3963611612
H     -4.1443375738      6.0197551165      0.1872906924
O     -3.6287307775      5.4811960206     -5.5714625064
H     -3.5166117497      4.9309834865     -6.3301284045
H     -3.5690618811      4.9177983139     -4.8165445633
O     -5.1854650049      1.9341367169      0.4249422213
H     -4.8161180661      1.2611876859     -0.1242398018
H     -4.4626421846      2.3524060759      0.8647789727
O      0.3942463398      7.1921092334     -6.2873496517
H      0.2160390964      6.8746939369     -7.1581930142
H      1.1710539917      7.7249770786     -6.3465120188
O     -4.2900183114      8.6361466223     -7.3692522083
H     -3.6296081729      8.6975154809     -6.6977086384
H     -5.0521727763      8.2522957103     -6.9659440097
O     -7.7652711740      4.5488754337     -5.7351794373
H     -8.6538220102      4.4704378593     -6.0437299396
H     -7.7226867268      4.0902016187     -4.9113570351
O     -5.9678392978      8.1223513922     -3.0760519515
H     -6.0492088526      7.7642903096     -3.9455631421
H     -6.5587756779      8.8568120562     -3.0287213928
O      0.6716546364      1.9613879961     -4.5864393641
H      0.7293331015      1.5198436288     -3.7542193089
H      0.8917951074      2.8657154102     -4.4295682218
O     -1.3233789795      2.3401531389     -0.5809515313
H     -1.6564253113      2.5576147039      0.2750093689
H     -1.1768006560      3.1569922163     -1.0305815690
O     -2.2902951806      7.9415812407     -5.3737782857
H     -2.6347068806      7.0646995340     -5.4315494499
H     -1.3780813153      7.8909103080     -5.6107946871
O     -5.4372863435      5.9106255108     -1.2955083245
H     -5.7899293925      6.6600690074     -1.7481182884
H     -6.1672410371      5.3472303293     -1.0939383150
O      0.3901663759      0.5344746151     -2.1847670130
H     -0.2112973558     -0.1589584914     -2.4044721799
H     -0.0028861932      1.0205953990     -1.4776074020
O     -1.0340870882      4.8517818319     -1.9617140228
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H     -1.0258792268      5.6923725023      -1.5325073012
H     -0.5193754295      4.9434011435      -2.7475615043
O     -6.0145574654      6.8916593089      -5.5804741043
H     -5.2188068680      6.3840579680      -5.5810393846
H     -6.7235071993      6.2848541376      -5.7220940640
O     -3.3277535356      0.5170453646      -1.4872533917
H     -2.6247202961      1.1086144165      -1.2712238222
H     -2.9359371689     -0.2213871808      -1.9255178835
O     -3.6543528091      4.4504579044      -2.9543008549
H     -2.7925988320      4.4958151016      -2.5719381190
H     -4.2172589504      4.9865095201      -2.4188909228
O     -0.9564053662      3.2816611152      -8.2486152593
H     -1.1451861947      3.1583066779      -7.3320870624
H     -0.4968126574      2.5094310292      -8.5372563693
O      0.3409842526      0.6433952809      -7.1226825885
H      1.0425503347      0.0658331664      -7.3778403643
H      0.6220434802      1.0798893213      -6.3344205017
O     -5.9027107032      2.9589026642      -7.4759537214
H     -6.4957304511      3.4936477010      -6.9727104618
H     -5.2863565116      3.5465828200      -7.8829156349
O     -3.1424606991      7.0823748537      -9.3746277712
H     -3.3653766536      7.4131856557     -10.2300523117
H     -3.5383669950      7.6653261587      -8.7466911224
O     -2.0949340700     -0.6349373983      -5.8717078505
H     -1.3899689601     -0.2896612126      -6.3958137592
H     -2.8521122866     -0.1001270763      -6.0492959188
O     -1.7784772472      2.8372782273      -5.6411038179
H     -1.1800959637      2.2698607165      -5.1819135936
H     -2.6011525382      2.3776876164      -5.6945854977
O     -3.0545856520      8.7322263121      -2.7244156369
H     -2.7587065379      8.5873481999      -3.6089179470
H     -3.9848113122      8.5724185327      -2.7199268914
O     -0.3917992138      6.1333500962      -8.6899792540
H     -0.4784908859      5.1941710267      -8.6538450118
H     -1.2257118542      6.4720246507      -8.9741758555
O     -3.5891551733      4.4688363705      -8.2771533556
H     -3.5324667209      5.2748698089      -8.7649801381
H     -2.8550661705      3.9385335640      -8.5431810297
O     -7.5590716923      3.0349306502      -3.3962311012
H     -6.7848407358      2.4962646577      -3.4320616539
H     -7.6256176620      3.3557489829      -2.5110612387
O     -1.4951509361      7.4690419172      -0.8304793379
H     -2.0268607761      7.9313872045      -1.4584920251
H     -0.8909028281      8.0986552965      -0.4708271856
O     -4.9079063635      1.9707153892      -3.3017893155
H     -4.5393594086      1.3720127118      -2.6720221361
H     -4.4601367003      2.7937720048      -3.1879535121
O     -4.1561496936      1.3944994032      -5.8915591135
H     -4.5636582548      1.4489796510      -5.0419432419
H     -4.7756845458      1.7431521604      -6.5124425776
O     -7.1397250829      3.7281257615      -0.5493532948
H     -7.8168179079      3.7191447521       0.1081747288
H     -6.4891438772      3.1006993284      -0.2773999533
```

Coordinates Figure 7(b).

```
99
Energy    -325.72034733038
O      -0.1075827694      7.9698723211      -3.5012454272
H       0.5930139679      7.3611759784      -3.6730925343
H       0.0559734061      8.7298917052      -4.0365008497
O      -1.7917933518     -2.1568478326      -1.1040246185
H      -2.5484936172     -1.6144122800      -0.9489542030
H      -1.3985102639     -2.3210161387      -0.2618514570
O       2.0671164410      2.0183843216      -1.5893505201
H       1.8488925666      1.9060654360      -0.6779552916
H       2.3844647335      2.9020937977      -1.6854029906
O      -2.0212829196      3.0220283087       3.5206206008
H      -1.7153877666      2.4556841536       4.2109545109
H      -1.8612885980      2.5697510172       2.7077703547
O      -0.3322773089      5.1076733756      -0.0299075909
H      -0.3688272470      5.0186695561       0.9090390935
H      -1.1527591551      4.7833209225      -0.3652931605
O      -0.8980588849      7.8180191903       3.3566213809
H      -1.1400759098      8.2798737557       4.1433847342
H      -1.6001261130      7.9475041011       2.7391963093
O       2.2333128502      4.8463964931      -1.2189994841
H       2.8139469787      5.2267188469      -0.5793922843
H       1.3664618789      4.8697800415      -0.8463051626
O       2.0464647037      1.5914922667       4.7101771819
H       2.2535017778      2.3652539379       4.2108706826
H       2.6021606899      0.9016268428       4.3843457501
O       3.3570631238      6.0872292644       1.2238345949
H       4.2088645395      6.4788301924       1.3332033082
H       2.7231639928      6.7701043109       1.3746060002
O      -0.3172535260      5.0723249229       2.8207967718
H      -0.9711655926      4.5201776908       3.2188054365
H      -0.4616226929      5.9448115912       3.1506497866
O      -2.8253828544      4.7068486063      -1.2994168924
H      -2.7725675576      5.2114414538      -2.0953283553
H      -3.5243629057      5.0807339213      -0.7870546052
O       1.4593712213      8.1290212037       1.5605093542
H       0.9336082553      8.2602126726       0.7876959510
H       0.8637079186      8.0995901006       2.2920812878
O      -4.6501207108      0.5524446818       1.9282652252
H      -4.0171418301      0.1178709373       2.4772295695
H      -4.5096861191      0.2366796858       1.0499435035
O      -1.9026869839     -0.4912625873       2.9248100096
H      -1.7200562409      0.1787164421       2.2855506210
H      -1.5498687426     -0.1865483682       3.7455090941
O       2.4868736968     -0.9107038897      -1.6794279129
H       1.7478366594     -1.1410938204      -2.2194493858
H       2.6484545316      0.0087426141      -1.8186694817
O       1.6102340520      5.8565627535      -3.8599061423
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H      1.0949202794      5.1423458224     -4.1993532592
H      1.9830944978      5.5589731089     -3.0454775417
O     -0.3359023639      3.8139619428     -4.8183061836
H     -0.3375794820      3.0028576295     -4.3356205361
H     -0.3330312758      3.5847636270     -5.7339143656
O     -0.6077833611     -2.5309696123      1.5690131643
H     -1.0840783992     -1.9543774338      2.1448281957
H     -0.6458715381     -3.3916195186      1.9546418504
O     -2.3694332419      1.9761393092     -1.4194917990
H     -1.6813706327      1.8700677331     -2.0568277548
H     -2.6438124181      2.8781408711     -1.4640754730
O     -0.1662962308      1.5231053740     -3.1457175902
H      0.6089988285      1.6860011069     -2.6326279244
H     -0.1668585264      0.6019374980     -3.3514550011
O     -0.6544649734      1.0159669176      5.1365049389
H     -0.7544919227      0.8637651047      6.0626300232
H      0.2614576397      1.1882862517      4.9872726773
O      3.5477315844     -0.5350471984      3.3862624483
H      3.1257806524     -0.9042064583      2.6269487411
H      4.4754970899     -0.6648575331      3.2710283480
O     -4.5827700313      5.6390677929      0.7404766734
H     -5.4627472780      5.9707445151      0.6597979810
H     -4.6210761876      4.9113620698      1.3403562221
O      1.4502246334      1.6046244797      1.0888287465
H      1.7329783171      0.7461621967      1.3608054314
H      1.8170853802      2.2187923324      1.7045311870
O      2.1930604371      3.7850913713      2.7172322202
H      1.3785727976      4.2512459024      2.8181692906
H      2.7997944572      4.3837161580      2.3117687228
O     -4.6959333445      3.4710561146      2.5109211141
H     -4.8597387439      2.5822489756      2.2387665352
H     -3.9418642405      3.4465061322      3.0780679547
O     -3.9904173117     -0.2070625150     -0.8728239511
H     -3.5371099959      0.5733991889     -1.1489950216
H     -4.7232484721     -0.3163996499     -1.4575310020
O     -1.3068003525      1.6074013370      1.1866406305
H     -0.3773257118      1.6698399335      1.0347960784
H     -1.7259925317      1.7034503600      0.3464436559
O      1.9730549834     -1.1818726383      1.1089742305
H      1.1806016576     -1.6840555911      1.2124559312
H      2.2112708840     -1.2357751245      0.1972581778
O     -2.1974977366      5.8928402538     -3.7306187209
H     -1.6889707799      6.6868752033     -3.6883423999
H     -1.6574310111      5.2472324821     -4.1576983285
O     -0.4646197747      7.8473120950     -0.6026646475
H     -0.3886307112      8.0640396025     -1.5181608538
H     -0.3536295788      6.9124366787     -0.5350807268
O     -0.0596252743     -1.3729725816     -3.1233621189
H     -0.1241560627     -2.0049309054     -3.8214616163
H     -0.6610917468     -1.6495618896     -2.4505955239
O     -2.6918250743      7.9457210685      1.2692284883
H     -3.2423538561      7.1963643940      1.1071757532
H     -2.1186088382      8.0274891620      0.5238322316
```

Coordinates Figure 7(c).

```
99
Energy   -325.358848563249
O     -3.0813706735     -0.7144253992     -0.9873970384
H     -2.9894703837     -1.4850416388     -0.4501974460
H     -2.4084463917     -0.1115364901     -0.7143103703
O      1.3883509940      1.3820677628      1.6522266063
H      1.8633856565      1.9251789569      1.0437442694
H      0.5188915551      1.7436292511      1.7169724812
O     -1.0570143426      2.6461988996      1.7913654492
H     -0.8471112075      3.4996148351      2.1356042746
H     -1.7295621679      2.2871338758      2.3478096832
O      2.8900786011      2.7481101587     -2.4789701454
H      2.0301866401      2.8885675152     -2.8419246887
H      3.0594608031      1.8211721464     -2.5335049521
O     -0.1353922455      5.0272246854      3.0175094692
H      0.4057421480      4.7652895397      3.7451371223
H     -0.8909981685      5.4589436195      3.3829638510
O      0.3936382365     -1.7719842665      4.4261569319
H      0.6694491219     -1.0600797736      4.9811333300
H      0.4543705898     -2.5588184266      4.9439233269
O      0.2216650682     -2.7585171139     -0.2103412919
H      0.8117384886     -2.4323551542      0.4501965107
H      0.2340068410     -2.1335916111     -0.9175854157
O      0.0534112344      3.1220947300     -2.9122611429
H     -0.2981319288      2.6170912171     -2.1965326256
H     -0.4881421439      2.9409862319     -3.6637916508
O      1.5099661365      4.1099021390      5.0551504022
H      1.0315553168      3.7145414097      5.7662702482
H      2.1079690170      3.4545336176      4.7330275838
O      4.8791667836      1.9559043208      1.7465550222
H      5.7604834582      2.2739881024      1.6326160870
H      4.3180457697      2.5262675276      1.2458480479
O     -1.9781405525     -0.4867862439     -3.7259476908
H     -1.1072082663     -0.6462898533     -3.3989706189
H     -2.5739344266     -0.6974783643     -3.0248649966
O     -3.0757208173      5.5853237658     -1.1228022417
H     -3.4460863021      6.4029865091     -1.4145821245
H     -2.1386103961      5.6701692503     -1.1969895466
O     -2.2829374324     -1.2820310929      3.2015772533
H     -2.3339848207     -1.8125057909      2.4225591451
H     -1.4338504247     -1.4401281209      3.5822805985
O     -2.6025515681      3.1670644059      5.4431100602
H     -2.6634965110      4.0060537507      5.0150200611
H     -2.8423735727      2.5172805719      4.8019042982
O     -5.3866143935      2.1963638846      1.6360720835
H     -5.4156770661      1.7945690917      0.7824944599
H     -6.2656204600      2.1690609719      1.9788275943
O     -0.3474071202      5.6785036049     -1.5662912005
```

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H      0.2673355917      5.7142471063     -0.8509645238
H     -0.0871233940      4.9534784931     -2.1116987758
O     -1.4046942776      1.7209686297     -0.8237286169
H     -2.1851099244      2.0957060293     -1.1997628623
H     -1.2983631435      2.1137269297      0.0279245178
O      2.9029081335      1.8084249612      3.9781450540
H      2.3410069979      1.5990515889      3.2492360344
H      3.7866827937      1.8131451877      3.6467864513
O      1.3693416484      0.3290428940      5.9519258983
H      0.7920752695      1.0005407694      6.2786254315
H      2.0472616507      0.7681224131      5.4635488918
O     -3.5139875558      2.9914393911     -2.2316656025
H     -3.2206819176      2.9264311098     -3.1264416527
H     -3.5013438220      3.9083254001     -2.0079724276
O      0.3538008863     -0.4446230805     -1.9751088431
H     -0.0185535990      0.2840333753     -1.5046937490
H      1.2749499463     -0.2629062474     -2.0717621196
O     -2.1366719681      2.1251609614     -4.6094374917
H     -2.3277887003      2.1890903913     -5.5315361180
H     -2.1240419530      1.2053384089     -4.3981428899
O      1.3948666436      5.7512902032      0.7934671421
H      1.8430587722      6.5637103709      0.9666021792
H      0.8543001307      5.5738396491      1.5465790860
O      3.2179118145     -0.1245382343     -2.0954883152
H      3.6674829083     -0.7112542881     -2.6824538660
H      3.5707657925     -0.2796843777     -1.2339187019
O     -5.2817059106      1.1359947223     -0.8783274579
H     -4.8956356273      1.7763987432     -1.4542709278
H     -4.7402629029      0.3645110275     -0.9286348329
O      2.9072536321      3.3138627575      0.2199131973
H      2.5176686473      4.1561634833      0.3920511680
H      2.9671106427      3.2292850899     -0.7182457501
O      4.1879565158     -0.6439355618      0.4640814931
H      3.5664727568     -1.1144856218      0.9962647628
H      4.4697077984      0.1009854890      0.9706259599
O     -2.8045039848      5.6616867279      3.8235990554
H     -3.2981316650      5.4289462385      3.0535068323
H     -3.2169596663      6.4280709906      4.1888577674
O     -2.3146568295     -2.9028554638      0.7279997086
H     -2.6924819045     -3.7677875287      0.7236190934
H     -1.4268134680     -2.9930949941      0.4206408846
O     -3.0998191322      1.4262821514      3.2087042518
H     -2.9320212002      0.4979896145      3.2402522153
H     -3.9148332788      1.5390734296      2.7462017951
O     -4.1982608000      4.8922444775      1.5477364805
H     -3.8171574444      5.0286641762      0.6950769047
H     -4.5646702619      4.0224079454      1.5450968427
O      1.7120414425     -1.4200297276      1.8320865229
H      1.4103847237     -1.6694510494      2.6909640941
H      1.5162994508     -0.5021517944      1.7317688954
O     -0.2619574514      2.6301065691      6.8256635412
H     -1.0858270708      2.7728194284      6.3877704674
H     -0.4191049654      2.7575236401      7.7475897872
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Coordinates Figure 7(d).

```
99
Energy   -325.172022710616
O      -4.2939445040      6.0926533948      0.5845768013
H      -4.6744846586      5.7027066510      1.3552967127
H      -3.9082562512      5.3894273836      0.0869864045
O      -5.1101365164      2.1622563544     -1.6944471503
H      -4.8032427645      1.2703954218     -1.7302068479
H      -5.6851945189      2.2215591757     -0.9483439917
O      -3.2003668269      4.1750296972     -1.1178376731
H      -3.2232682965      4.6772538217     -1.9166648793
H      -3.7495298877      3.4199576763     -1.2562740483
O      -4.5884591685      0.1565113861      2.0805906469
H      -3.7734911994      0.4459871538      1.7025569931
H      -4.6924438889     -0.7501020857      1.8395146327
O      -1.4028004057     -0.3154428222      4.6012001568
H      -1.1851191204     -0.7629778352      5.4032012318
H      -2.2622784132      0.0554247330      4.7221681902
O      -2.1482217787      2.3273275035     -4.9753692799
H      -3.0100092603      2.6589661895     -4.7798786850
H      -2.1068002474      2.2147495012     -5.9115791411
O      -5.2103876759      7.6114878969     -1.6494159729
H      -5.1023192678      7.1747785312     -0.8196662497
H      -6.1389832018      7.6606280593     -1.8111999272
O      -0.6467480099      6.0384065656      2.4855387143
H       0.1696935912      6.0044968499      2.0131493651
H      -1.1178603754      6.7884918985      2.1594964063
O      -0.1471483411      7.7630346867     -1.1020907570
H       0.4964301524      7.2552887853     -0.6342454018
H      -0.8618700465      7.9124930142     -0.5039991701
O       3.3544514081      3.6831371952     -0.2088034871
H       4.2981861972      3.6796477032     -0.2239997140
H       3.0686549863      3.2892100256     -1.0175186683
O       0.9388654505     -0.1991605168     -2.2765472574
H       0.0984857914     -0.1450744978     -2.7028278989
H       1.3917234107     -0.9322871833     -2.6616750450
O      -3.7567774016     -2.3521018316      0.7708566762
H      -4.0119460624     -3.2608018496      0.7764857014
H      -2.9171323261     -2.3034474478      1.1992342575
O      -2.2424974081      1.0558820469      0.7132449801
H      -2.1167436697      1.9784710645      0.8678216793
H      -1.3876590655      0.6568317994      0.7430570919
O      -1.1642117167      4.6429506783      5.1137232212
H      -0.9680629270      5.2632444318      4.4298813055
H      -0.6500541995      3.8716324103      4.9359913135
O      -4.5744222550      3.4243258843     -4.3017148669
H      -4.4196273525      4.3316389211     -4.0926693089
H      -4.9835263893      3.0373870815     -3.5442251810
O      -0.1113382138      3.7938808791     -3.4941202168
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H     -0.7392845518      3.3195854963     -4.0152782931
H     -0.2839695875      4.7117945344     -3.6301767649
O     -2.2516355467      7.9550271321      0.9919056905
H     -3.0009352852      7.4021973780      0.8376085135
H     -2.5860032598      8.8068445867      1.2231711450
O      1.2478814812      5.6974934136      0.3396829573
H      0.6708512739      5.0461020653     -0.0258357224
H      2.1237107728      5.3519458030      0.2733628636
O     -1.3202419762     -1.9840174804      2.1325910012
H     -1.3853820685     -1.5068067931      2.9443207483
H     -0.6545522748     -1.5555191370      1.6186602225
O      0.3448832961     -0.1759208693      0.5506733826
H      0.9079801528      0.4990197481      0.8945564253
H      0.5693896237     -0.2784253679     -0.3603525175
O     -3.8469984028      3.7942592804      5.3775162630
H     -2.9656307730      4.1257797293      5.3129891597
H     -4.1613049816      4.0248207954      6.2371273473
O     -2.0251109663      3.5193388893      2.1414773850
H     -1.5870667631      3.0528182180      2.8352743245
H     -1.6239153309      4.3722967758      2.0926577154
O     -0.4253222459      3.6782847484     -0.6406013819
H     -0.2397001946      3.5275583496     -1.5536755634
H     -1.3528983690      3.8402744870     -0.5754836848
O      1.2840097941      2.3398489004      1.3492912896
H      0.6436073010      2.7535084784      0.7928302806
H      2.1211112530      2.7127395805      1.1232555796
O     -6.2564235262      2.2398647581      0.9081290996
H     -5.9736876453      2.9747732141      1.4285601105
H     -5.9121036309      1.4651592026      1.3230430257
O     -0.7661725191      6.6868577430     -3.5846435806
H     -0.5464944421      7.0587467646     -2.7454066938
H     -0.3967476131      7.2576045331     -4.2393586290
O      2.2921896056      2.4401979638     -2.4855488937
H      1.9334047564      1.5740078078     -2.3766154290
H      1.6582611927      2.9364188610     -2.9782740125
O     -0.1629929761      2.1875323478      3.8503477591
H     -0.3788174105      1.3000905085      4.0885603731
H      0.5034737777      2.1351248927      3.1840490432
O     -4.7454024545      4.1244387764      2.6043142992
H     -4.8243615064      4.1589967818      3.5442343312
H     -3.8779917081      3.8031421897      2.4165763051
O     -3.8948347306      0.8607494393      4.7971929482
H     -3.9420612788      1.7919998581      4.9435512915
H     -4.3462925736      0.6903900827      3.9859950934
O     -3.5585436736     -0.2515038449     -1.3844036462
H     -3.1044879148      0.2622553626     -0.7357409459
H     -3.8023961320     -1.0619462553     -0.9665549510
O     -1.5431647261     -0.0932399871     -3.4617727507
H     -2.2683380238     -0.2463953565     -2.8773537442
H     -1.7601900957      0.6729916159     -3.9683964509
O     -3.5402078259      5.9477483339     -3.2836278905
H     -2.7089175842      6.3147343836     -3.5388850698
H     -4.0421364115      6.6511249217     -2.9038812319
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Coordinates Figure 7(e).

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99
Energy    -325.018870577002
O      0.8874397435      5.0257846925     -3.3104845796
H      0.8918667357      5.5810044446     -4.0737603376
H      1.0247548019      4.1433870703     -3.6160945681
O     -4.1298730105      3.6682373238      1.4123862540
H     -4.1591951681      4.5821757030      1.1784304797
H     -4.2455170695      3.6238907439      2.3480882827
O     -2.0305234299     -1.1841745206     -2.8954751896
H     -2.0037010072     -2.1197677449     -2.7737199830
H     -1.9480615557     -1.0288115113     -3.8228051356
O     -4.2859489593      6.3048775440      0.5640238633
H     -4.8819976433      6.3927136827     -0.1625359987
H     -3.5013796652      6.7742947527      0.3295521997
O     -3.2509052714      5.4175385838     -5.5492953203
H     -4.0866567775      5.3158155799     -5.9759688543
H     -3.3942777278      5.2575436587     -4.6302064145
O     -6.0737073406      2.3090400396     -0.3614337360
H     -5.5930195484      1.6102017317     -0.7754901572
H     -5.4838209333      2.7180594231      0.2514411489
O      0.9387006132      6.8208161162     -5.6630523859
H      0.9536424153      6.3678901272     -6.4910096584
H      1.7115145147      7.3620187618     -5.6359078819
O     -3.1327148281      8.7723162970     -7.6238697072
H     -2.5876600894      8.7371541655     -6.8540922001
H     -3.0351615224      9.6384661069     -7.9860109963
O     -5.7161702963      4.8849100685     -6.7552176964
H     -5.5742284906      4.2472214233     -7.4364549309
H     -6.3034916293      4.4891541031     -6.1312711267
O     -5.7972692770      8.4414059380     -3.8194406531
H     -6.3893661744      9.1731735231     -3.7500438263
H     -5.7840402544      8.1884277741     -4.7286741191
O      0.5175019807      2.2669963522     -4.1525736007
H     -0.3185902207      2.5148336484     -4.5136898695
H      0.3395029006      1.8001802259     -3.3517755702
O     -2.0468090712      2.5628496621     -0.3237209607
H     -2.5807185459      2.7872307812      0.4215791402
H     -1.7539204246      3.3763143263     -0.7023631862
O     -1.7666210935      7.8570727530     -5.3657441897
H     -2.2417478576      7.0422571824     -5.4005090876
H     -0.8490600042      7.6374177248     -5.3924232109
O     -5.7803736206      6.2649166955     -1.9215246529
H     -5.9289328734      6.9843240515     -2.5141979682
H     -6.5506377288      5.7205803395     -1.9571559476
O     -0.1499197746      0.7859635133     -1.8102881288
H     -0.6899338731      0.0456022487     -2.0364040847
H     -0.5957993285      1.2451720968     -1.1166042279
O     -1.2925632818      5.0666115465     -1.5483743443
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H    -0.5243724865    5.0863199168    -2.0964372387
H    -1.3363483971    5.9026519481    -1.1124870139
O    -5.7301072371    7.8064506236    -6.5415241375
H    -4.9710763730    8.1187765475    -7.0075746912
H    -5.8435256340    6.9012058378    -6.7834881825
O    -3.8359109696    0.7638449398    -1.6610860996
H    -3.3899284759   -0.0084330557    -1.9702216153
H    -3.1761339435    1.3282276656    -1.2908903827
O    -3.6607826645    4.7510091680    -2.9647733249
H    -4.3186745448    5.2514005558    -2.5090703658
H    -2.8734559158    4.8027098682    -2.4467751759
O    -0.0163676336    2.7875411677    -8.0517376456
H    -0.5074900526    2.9012705498    -7.2537759602
H     0.4930045378    1.9998750372    -7.9468543208
O     0.9545082183    0.5284961711    -6.3179737767
H     1.7046856648   -0.0438728017    -6.2954790713
H     1.0239286172    1.0963419272    -5.5672338353
O    -4.8433089247    2.7293385006    -8.5785225345
H    -4.0281084811    2.9572085368    -8.9961371144
H    -5.3903563665    2.3433830983    -9.2438464992
O    -2.1207995101    6.1209677879    -8.3966989019
H    -2.3308685816    5.8318247379    -7.5231167730
H    -2.4808984557    6.9885168112    -8.4892510255
O    -1.7396230743   -0.6853012189    -5.6388172097
H    -2.4193000105   -0.1386803147    -5.9995432879
H    -0.9191937070   -0.3426791807    -5.9556519399
O    -1.6475949164    3.0605137411    -5.8174754229
H    -2.0701545733    3.9002883162    -5.7332112348
H    -2.3315501710    2.4256602290    -5.9590546660
O    -2.9849793102    8.8909993193    -2.9267766548
H    -2.5051305848    8.6730483143    -3.7097970978
H    -3.9000605433    8.7797692578    -3.1295885487
O     0.7252910982    5.5960409677    -8.1281962827
H     0.7516747283    4.6547473815    -8.1926070172
H    -0.1182374496    5.8667057733    -8.4538933907
O    -2.4078798764    3.5065426252    -9.6715254939
H    -2.3109473235    4.4341979481    -9.5268253342
H    -1.6188817260    3.0983284877    -9.3525872700
O    -7.1315081676    3.4903695687    -4.7299077716
H    -6.4730808009    2.8851249757    -4.4281945976
H    -7.5369406225    3.8561486720    -3.9600320504
O    -1.9962654272    7.7086304385    -0.6020283895
H    -1.4822012903    8.3468747311    -0.1337755303
H    -2.3279592814    8.1402954790    -1.3730815226
O    -4.7598350411    2.2599957954    -3.8242647283
H    -4.3361238077    3.0684804293    -3.5840568152
H    -4.5957042261    1.6491297956    -3.1237061941
O    -3.7770611460    1.3385305475    -6.2578014172
H    -4.2885806833    1.5543530666    -5.4944883378
H    -4.2664885592    1.6399538394    -7.0064557168
O    -7.6662963675    4.1245073837    -1.8459024309
H    -7.1312052034    3.4794744213    -1.4117499488
H    -8.5081489293    4.1102115510    -1.4193366712
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