Supporting Information
An efficient implementation of the "Cluster-in-molecule" approach for local electron correlation calculations

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Contents

I. CARTESIAN COORDINATES

A. Alkanes

1. dodecane

C 0.09074600 7.04664200 0.00000000
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C 0.65625400 3.16015800 0.00000000
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H 1.49420500 5.66578800 0.87025800
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H 1.11824000 0.55914900 0.87103000
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C -0.58444900 -3.17458500 0.00000000
C 0.19253300 -4.49604900 0.00000000

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6. tetracontane

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C -21.12094900 0.45477600 0.00045100
C -22.40224600 -0.38646600 0.00123400
C -23.68164900 0.45825300 0.00072300
C -24.95690700 -0.38924400 0.00167700
H -25.00058000 -1.02705200 0.87872300
H 25.84435100 -0.23416000 0.00126000
H 25.00086200 1.02860900 -0.87422600
H 25.00060800 1.02704700 0.87875400
H 23.68091800 -1.10924900 -0.87006000
H 23.68059500 -1.11068900 0.87048200
H 22.40418900 1.03819800 0.87266600
H 22.40441100 1.03947300 -0.86929100
H 21.12005000 -1.10635600 -0.87106300
H 21.11981900 -1.10762100 0.87096900
H 19.84328200 1.04342500 -0.86966100
H 19.84306600 1.04218200 0.87233700
H 18.55985200 -1.10244100 -0.87131600
H 18.55957700 -1.10358400 0.87069500
H 17.28289900 1.04632400 0.87183100
H 17.28306500 1.04728400 -0.87017700
H 15.99960800 -1.09852700 -0.87148300
H 15.99943600 -1.09948000 0.87052700
H 14.72287500 1.05128300 -0.87044000
H 14.72271800 1.05035200 0.87156800
H 13.43944000 -1.09457100 -0.87166300
H 13.43922600 -1.09540600 0.87034500
H 12.16254800 1.05450300 0.87114700
H 12.16265500 1.05515700 -0.87086100
H 10.87919400 -1.09065300 -0.87174700
H 10.87908200 -1.09130200 0.87026200
H 9.60246100 1.05915800 -0.87103700
H 9.60236300 1.05853200 0.87097100
H 8.31902400 -1.08669600 -0.87184100
H 8.31886900 -1.08722600 0.87016700
H 7.04219200 1.06268400 0.87063500
H 7.04223900 1.06303300 -0.87137200
H 5.75877700 -1.08277800 -0.87183800
H 5.75872400 -1.08312100 0.87017000
H 4.48204500 1.06703500 -0.87146200
H 4.48200600 1.06671400 0.87054600
H 3.19860700 -1.07881900 -0.87184600
H 3.19851000 -1.07904400 0.87016200
H 1.92183400 1.07086700 0.87029600
H 1.92182200 1.07090900 -0.87171100
H 0.63836000 -1.07490100 -0.87175600
H 0.63836600 -1.07493700 0.87025200
H -0.63837200 1.07491200 -0.87171500
H -0.63835200 1.07489800 0.87029300
H -1.92181100 -1.07094200 -0.87167800
H -1.92184800 -1.07085900 0.87033100
H -3.19852400 1.07905300 0.87012900
H -3.19859500 1.07878700 -0.87187900
H -4.48205800 -1.06702300 -0.87150100
H -4.48199300 -1.06675100 0.87050700
H -5.75878900 1.08279100 -0.87179700
H -5.75870900 1.08308400 0.87021100
H -7.04222800 -1.06306300 -0.87133600
H -7.04220600 -1.06267200 0.87067200
H -8.31888100 1.08723900 0.87013400
H -8.31901100 1.08666700 -0.87187400
H -9.60247500 -1.05914300 -0.87107400
H -9.60235000 -1.05856400 0.87093400
H -10.87920500 1.09067000 -0.87170600
H -10.87906600 1.09127200 0.87030300
H -12.16264400 -1.05518200 -0.87082300
H -12.16256300 -1.05448400 0.87118500
H -13.43923700 1.09542700 0.87031100
H -13.43942600 1.09454700 -0.87169700
H -14.72288900 -1.05126200 -0.87047400
H -14.72270600 -1.05037500 0.87153400
H -15.99961800 1.09855100 -0.87144300
H -15.99942100 1.09945900 0.87056700
H -17.28305500 -1.04730100 -0.87013800
H -17.28291500 -1.04629600 0.87187100
H -18.55958900 1.10361400 0.87066200
H -18.55983700 1.10242800 -0.87134900
H -19.84329700 -1.04339000 -0.86969900
H -19.84305500 -1.04219600 0.87229900
H -21.12006000 1.10639200 -0.87102100
H -21.11980200 1.10761100 0.87101100
H -22.40439800 -1.03948500 -0.86924500
H -22.40420900 -1.03815000 0.87271300
H -23.68060500 1.11075000 0.87042400
H -23.68090400 1.10923100 -0.87011700
H -25.84435100 0.23418600 0.00130000
H -25.00089300 -1.02855600 -0.87425800

B. Alkenes

1. polyacetylene (n=6)

C 0.08043400 6.75908500 0.00000000
C 0.65103700 5.55867900 0.00000000
C -0.08043400 4.29671500 0.00000000
C 0.50051700 3.09363600 0.00000000
C -0.22289200 1.83328500 0.00000000
C 0.36099800 0.63007900 0.00000000
C -0.36099800 -0.63007900 0.00000000

C 0.22289200 -1.83328500 0.00000000
C -0.50051700 -3.09363600 0.00000000
C 0.08043400 -4.29671500 0.00000000
C -0.65103700 -5.55867900 0.00000000
C -0.08043400 -6.75908500 0.00000000
H 0.98738800 -6.87959300 0.00000000
H 1.15549000 -4.36514300 0.00000000
H 1.29833500 -1.89610700 0.00000000
H 1.43654400 0.56791300 0.00000000
H 1.57605900 3.02977300 0.00000000
H 0.66175600 7.66015100 0.00000000
H -0.98738800 6.87959300 0.00000000
H 1.72532500 5.48540300 0.00000000
H -1.15549000 4.36514300 0.00000000
H -1.29833500 1.89610700 0.00000000
H -1.43654400 -0.56791300 0.00000000
H -1.57605900 -3.02977300 0.00000000
H -1.72532500 -5.48540300 0.00000000
H -0.66175600 -7.66015100 0.00000000

2. polyacetylene (n=8)

C 0.29599500 9.22129800 0.00000000
C -0.33979400 8.05413000 0.00000000
C 0.32062800 6.75359200 0.00000000
C -0.32601200 5.58432200 0.00000000
C 0.32601300 4.28577400 0.00000000
C -0.32392900 3.11654800 0.00000000
C 0.32601300 1.81834000 0.00000000
C -0.32474200 0.64907200 0.00000000
C 0.32473100 -0.64907300 0.00000000
C -0.32602300 -1.81834100 0.00000000
C 0.32392200 -3.11654800 0.00000000
C -0.32601700 -4.28577500 0.00000000
C 0.32601300 -5.58432000 0.00000000
C -0.32062300 -6.75359200 0.00000000
C 0.33980400 -8.05412900 0.00000000
C -0.29598100 -9.22129800 0.00000000
H -1.36893100 -9.28275000 0.00000000
H -1.40135300 3.11512600 0.00000000
H -0.23507200 10.15304200 0.00000000
H 1.36894500 9.28274500 0.00000000
H -1.41657700 8.04067700 0.00000000
H 1.39788100 6.76201600 0.00000000
H -1.40351400 5.58070000 0.00000000
H 1.40334100 4.28818200 0.00000000
H 1.40339400 1.81941700 0.00000000
H -1.40214500 0.64821800 0.00000000
H 1.40213400 -0.64821700 0.00000000
H -1.40340400 -1.81941900 0.00000000
H 1.40134600 -3.11512300 0.00000000
H -1.40334500 -4.28818700 0.00000000
H 1.40351500 -5.58069400 0.00000000
H -1.39787700 -6.76202100 0.00000000
H 1.41658700 -8.04067200 0.00000000
H 0.23508900 -10.15304000 0.00000000

3. polyacetylene (n=12)

C -14.15692700 -0.25886500 0.00000000
C -12.98777700 0.37327900 0.00000000
C -11.68930100 -0.29116800 0.00000000
C -10.51803200 0.35187200 0.00000000
C -9.22150100 -0.30408700 0.00000000
C -8.05029000 0.34234500 0.00000000
C -6.75406700 -0.31137000 0.00000000
C -5.58284100 0.33605300 0.00000000
C -4.28666600 -0.31686100 0.00000000
C -3.11546000 0.33094300 0.00000000
C -1.81928000 -0.32166100 0.00000000
C -0.64809000 0.32628100 0.00000000
C 0.64809500 -0.32624300 0.00000000
C 1.81928600 0.32169700 0.00000000
C 3.11546300 -0.33091300 0.00000000
C 4.28667200 0.31688500 0.00000000
C 5.58284000 -0.33603700 0.00000000
C 6.75407100 0.31137900 0.00000000
C 8.05028600 -0.34234600 0.00000000
C 9.22150200 0.30407700 0.00000000
C 10.51802600 -0.35189400 0.00000000
C 11.68930000 0.29113800 0.00000000
C 12.98777000 -0.37331700 0.00000000
C 14.15692300 0.25882100 0.00000100
H 14.22172800 1.33157700 0.00000100
H 9.22715900 1.38139400 0.00000000
H 4.29030200 1.39427700 0.00000000
H -8.04570100 1.41976900 0.00000000
H -15.08701100 0.27510900 0.00000000
H -14.22172600 -1.33162100 0.00000000
H -12.97098800 1.45001900 0.00000000
H -11.70104100 -1.36839100 0.00000000
H -10.51113200 1.42936400 0.00000000
H -9.22714800 -1.38140400 0.00000000
H -6.75823200 -1.38874300 0.00000000
H -5.57905000 1.41346500 0.00000000
H -4.29029100 -1.39425300 0.00000000
H -3.11197700 1.40835100 0.00000000
H -1.82270300 -1.39906100 0.00000000
H -0.64470400 1.40368500 0.00000000
H 0.64470800 -1.40364700 0.00000000
H 1.82271200 1.39909700 0.00000000
H 3.11197400 -1.40832100 0.00000000
H 5.57904200 -1.41344900 0.00000000
H 6.75824400 1.38875200 0.00000000
H 8.04568800 -1.41977100 0.00000000
H 10.51111600 -1.42938600 0.00000000
H 11.70104900 1.36836200 0.00000100
H 12.97097500 -1.45005800 0.00000000
H 15.08700300 -0.27515900 0.00000100

4. polyacetylene (n=16)

C 0.03440700 19.09287600 0.00000000
C 0.64921100 17.91460700 0.00000000
C -0.03440700 16.62617800 0.00000000
C 0.59108500 15.44550300 0.00000000
C -0.08415000 14.15890300 0.00000000
C 0.54467400 12.97820300 0.00000000
C -0.12833900 11.69189100 0.00000000
C 0.50147100 10.51115700 0.00000000
C -0.17072800 9.22487700 0.00000000
C 0.45948600 8.04416500 0.00000000
C -0.21235900 6.75786000 0.00000000
C 0.41804400 5.57717800 0.00000000
C -0.25363500 4.29084200 0.00000000
C 0.37685900 3.11018400 0.00000000
C -0.29474300 1.82382800 0.00000000
C 0.33579000 0.64318100 0.00000000
C -0.33579000 -0.64318100 0.00000000
C 0.29474300 -1.82382800 0.00000000
C -0.37685900 -3.11018400 0.00000000
C 0.25363500 -4.29084200 0.00000000
C -0.41804400 -5.57717800 0.00000000
C 0.21235900 -6.75786000 0.00000000
C -0.45948600 -8.04416500 0.00000000
C 0.17072800 -9.22487700 0.00000000
C -0.50147100 -10.51115700 0.00000000
C 0.12833900 -11.69189100 0.00000000
C -0.54467400 -12.97820300 0.00000000
C 0.08415000 -14.15890300 0.00000000
C -0.59108500 -15.44550300 0.00000000
C 0.03440700 -16.62617800 0.00000000
C -0.64921100 -17.91460700 0.00000000
C -0.03440700 -19.09287600 0.00000000
H 1.03724300 -19.17323300 0.00000000
H 1.24793800 -9.24458400 0.00000000
H 1.33086200 -4.31018900 0.00000000
H 1.41302100 0.62389700 0.00000000
H 1.62190300 12.95751500 0.00000000
H 0.58211100 20.01486100 0.00000000
H -1.03724300 19.17323300 0.00000000
H 1.72556200 17.88186200 0.00000000
H -1.11133300 16.65396500 0.00000000
H 1.66834900 15.42252300 0.00000000
H -1.16125500 14.18064900 0.00000000
H -1.20552300 11.71215800 0.00000000
H 1.57870000 10.49127500 0.00000000
H -1.24793800 9.24458400 0.00000000
H 1.53671700 8.02462200 0.00000000
H -1.28958100 6.77732200 0.00000000
H 1.49527600 5.55779200 0.00000000
H -1.33086200 4.31018900 0.00000000
H 1.45409100 3.09087200 0.00000000
H -1.37197300 1.84312300 0.00000000
H -1.41302100 -0.62389700 0.00000000
H 1.37197300 -1.84312300 0.00000000
H -1.45409100 -3.09087200 0.00000000
H -1.49527600 -5.55779200 0.00000000
H 1.28958100 -6.77732200 0.00000000
H -1.53671700 -8.02462200 0.00000000
H -1.57870000 -10.49127500 0.00000000
H 1.20552300 -11.71215800 0.00000000
H -1.62190300 -12.95751500 0.00000000
H 1.16125500 -14.18064900 0.00000000
H -1.66834900 -15.42252300 0.00000000
H 1.11133300 -16.65396500 0.00000000
H -1.72556200 -17.88186200 0.00000000
H -0.58211100 -20.01486100 0.00000000

5. polyacetylene (n=20)

C -0.28657700 24.02513700 0.00000000
C 0.34761500 22.85706600 0.00000000
C -0.31450800 21.55743900 0.00000000
C 0.33058500 20.38731900 0.00000000
C -0.32304900 19.08969700 0.00000000
C 0.32546000 17.91965400 0.00000000
C -0.32590400 16.62234700 0.00000000
C 0.32362300 15.45230300 0.00000000
C -0.32690100 14.15503300 0.00000000
C 0.32304800 12.98502800 0.00000000
C -0.32710400 11.68773300 0.00000000
C 0.32304700 10.51776900 0.00000000
C -0.32691900 9.22043900 0.00000000
C 0.32333900 8.05050800 0.00000000
C -0.32652900 6.75315000 0.00000000
C 0.32378800 5.58324200 0.00000000
C -0.32602500 4.28586500 0.00000000
C 0.32432500 3.11597100 0.00000000
C -0.32546000 1.81858300 0.00000000
C 0.32490400 0.64869500 0.00000000
C -0.32490400 -0.64869500 0.00000000
C 0.32546000 -1.81858300 0.00000000
C -0.32432500 -3.11597100 0.00000000
C 0.32602500 -4.28586500 0.00000000
C -0.32378800 -5.58324200 0.00000000
C 0.32652900 -6.75315000 0.00000000
C -0.32333900 -8.05050800 0.00000000
C 0.32691900 -9.22043900 0.00000000
C -0.32304700 -10.51776900 0.00000000
C 0.32710400 -11.68773300 0.00000000
C -0.32304800 -12.98502800 0.00000000
C 0.32690100 -14.15503300 0.00000000
C -0.32362300 -15.45230300 0.00000000
C 0.32590400 -16.62234700 0.00000000
C -0.32546000 -17.91965400 0.00000000
C 0.32304900 -19.08969700 0.00000000
C -0.33058500 -20.38731900 0.00000000
C 0.31450800 -21.55743900 0.00000000
C -0.34761500 -22.85706600 0.00000000
C 0.28657700 -24.02513700 0.00000000
H 1.35936200 -24.08806500 0.00000000
H 1.40427300 -14.15670400 0.00000000
H 1.40344000 -4.28703300 0.00000000

H 1.40229400 0.64755200 0.00000000
H 1.40117900 5.58206200 0.00000000
H 1.40287100 17.91697300 0.00000000
H 0.24577700 24.95609000 0.00000000
H -1.35936200 24.08806500 0.00000000
H 1.42435600 22.84212300 0.00000000
H -1.39172700 21.56730000 0.00000000
H 1.40806500 20.38230100 0.00000000
H -1.40035200 19.09345200 0.00000000
H -1.40326200 16.62459100 0.00000000
H 1.40102000 15.45045200 0.00000000
H -1.40427300 14.15670400 0.00000000
H 1.40044200 12.98353300 0.00000000
H -1.40448600 11.68913800 0.00000000
H 1.40044000 10.51644700 0.00000000
H -1.40430600 9.22171400 0.00000000
H 1.40073000 8.04927800 0.00000000
H -1.40391700 6.75435400 0.00000000
H -1.40344000 4.28703300 0.00000000
H 1.40171600 3.11481700 0.00000000
H -1.40285000 1.81973000 0.00000000
H -1.40229400 -0.64755200 0.00000000
H 1.40285000 -1.81973000 0.00000000
H -1.40171600 -3.11481700 0.00000000
H -1.40117900 -5.58206200 0.00000000
H 1.40391700 -6.75435400 0.00000000
H -1.40073000 -8.04927800 0.00000000
H 1.40430600 -9.22171400 0.00000000
H -1.40044000 -10.51644700 0.00000000
H 1.40448600 -11.68913800 0.00000000
H -1.40044200 -12.98353300 0.00000000
H -1.40102000 -15.45045200 0.00000000
H 1.40326200 -16.62459100 0.00000000
H -1.40287100 -17.91697300 0.00000000
H 1.40035200 -19.09345200 0.00000000
H -1.40806500 -20.38230100 0.00000000
H 1.39172700 -21.56730000 0.00000000
H -1.42435600 -22.84212300 0.00000000
H -0.24577700 -24.95609000 0.00000000

C. Glycine peptides

1. *zwitterionic* $(gly)_8$

O 14.39810200 -0.13245100 0.00482900
O 12.88368600 1.56595200 0.00331400
C 13.24934500 0.35424800 0.00373900
C 12.09810800 -0.67858200 0.00275700
N 10.84101300 0.05002000 0.00158600
C 9.63421100 -0.47410500 0.00061500
O 9.37399600 -1.69220800 0.00055700
C 8.48365400 0.52424800 -0.00049700
N 7.25020300 -0.23333200 -0.00115900
C 6.04361600 0.31774000 -0.00189200
O 5.83602300 1.53879400 -0.00208200
C 4.87312200 -0.64856800 -0.00247800
N 3.65691800 0.13341300 -0.00276500
C 2.44273500 -0.41024400 -0.00279900
O 2.23644400 -1.62945800 -0.00263600
C 1.27936300 0.56142300 -0.00310600
N 0.05733800 -0.21094000 -0.00263400
C -1.14977100 0.35037200 -0.00225500
O -1.33501900 1.57236000 -0.00233000
C -2.32944500 -0.60099700 -0.00167600
N -3.53638900 0.19575900 -0.00122100
C -4.75383700 -0.33968700 -0.00062400
O -4.96884300 -1.55676200 -0.00044600
C -5.91448800 0.63581400 -0.00011800
N -7.13535300 -0.14335500 0.00027200
C -8.34126500 0.40604200 0.00041700
O -8.55101800 1.62552300 0.00030200
C -9.52216000 -0.54927900 0.00071700
N -10.71939200 0.27683200 0.00115700
C -11.93884100 -0.20962200 0.00184000
O -12.24576400 -1.40953900 0.00220000
C -13.08788300 0.79849300 0.00220700
N -14.35272200 -0.02170100 0.00324300
H -10.51971000 1.25960300 0.00090500
H -6.99287400 -1.13250200 0.00036800
H 11.01473100 1.03981700 0.00165500
H 12.18264600 -1.31039800 0.87707700
H 12.18422400 -1.31048900 -0.87134500
H 8.54542100 1.16141400 -0.87344800
H 8.54414600 1.16194400 0.87215200
H 7.39226300 -1.22285100 -0.00094700
H 4.91983500 -1.28839600 0.86993000
H 4.92050100 -1.28804900 -0.87511400
H 3.80219200 1.12114700 -0.00284300
H 1.33044600 1.20075300 -0.87578200
H 1.33058000 1.20155500 0.86896700
H 0.18849400 -1.20029000 -0.00253400
H -2.29037600 -1.24107400 0.87101100
H -2.29112500 -1.24121900 -0.87429000
H -3.38445400 1.18240000 -0.00138500
H -5.86658000 1.27401100 -0.87338600
H -5.86589100 1.27383100 0.87324800
H -9.49642600 -1.18486100 0.87597600
H -9.49694100 -1.18468000 -0.87469400
H -13.06503000 1.42259900 -0.87733800
H -13.06396800 1.42323300 0.88127100
H -14.03310400 -1.00242000 0.00300800
H -14.92067000 0.13829800 -0.81258700
H -14.91929900 0.13828700 0.82003100

2. *zwitterionic* $(gly)_{10}$

O -17.99819600 -0.11092100 0.00171400
O -16.48306100 1.58667100 0.00135300
C -16.84886700 0.37514900 0.00145100
C -15.69859200 -0.65845300 0.00121300
N -14.44018400 0.06766700 0.00092400
C -13.23455600 -0.46039500 0.00067500

O -12.97957700 -1.67942300 0.00061700
C -12.08077000 0.53397200 0.00035700
N -10.84916500 -0.22624000 0.00012400
C -9.64119000 0.32363100 -0.00014200
O -9.43381300 1.54447600 -0.00025500
C -8.47241500 -0.64425700 -0.00039700
N -7.25372800 0.13318200 -0.00062500
C -6.04154700 -0.41777200 -0.00080200
O -5.84530800 -1.63834200 -0.00079800
C -4.87319300 0.54712000 -0.00103200
N -3.65383000 -0.22813200 -0.00109900
C -2.44483300 0.33388100 -0.00118900
O -2.26441800 1.55604900 -0.00120800
C -1.26699800 -0.61822300 -0.00122300
N -0.05595900 0.16968000 -0.00118500
C 1.15846100 -0.38153200 -0.00109000
O 1.34920800 -1.60181300 -0.00102500
C 2.32748400 0.58097400 -0.00104700
N 3.54567400 -0.19636500 -0.00083500
C 4.75399100 0.36663300 -0.00066000
O 4.93345300 1.58874200 -0.00067100
C 5.93451900 -0.58238900 -0.00043500
N 7.14153800 0.21373800 -0.00023100
C 8.35800300 -0.32663100 -0.00000500
O 8.56543700 -1.54458200 0.00004700
C 9.52271300 0.64337400 0.00020800
N 10.74077300 -0.13988200 0.00040100
C 11.94832200 0.40762600 0.00049000
O 12.15861400 1.62670300 0.00043000
C 13.12748000 -0.54939000 0.00068300
N 14.32682400 0.27353100 0.00073900
C 15.54464100 -0.21823600 0.00093900
C 16.69840800 0.78426600 0.00100400
O 15.84510500 -1.41956000 0.00108800
N 17.95964700 -0.04140300 0.00114600
H 18.52772900 0.11626500 -0.81512400
H 6.99356000 1.20070900 -0.00027800
H 3.41616600 -1.18550500 -0.00082100
H -14.61056100 1.05781100 0.00094200
H -15.78506700 -1.29039400 -0.87286700
H -15.78468000 -1.29036700 0.87535000
H -12.14009800 1.17183600 0.87302500
H -12.14049400 1.17173600 -0.87235800
H -10.99194300 -1.21545800 0.00019100
H -8.52155200 -1.28413700 -0.87273400
H -8.52119500 -1.28417300 0.87193100
H -7.39301500 1.12150900 -0.00062300
H -4.92217300 1.18772800 0.87098600
H -4.92238700 1.18755400 -0.87316700
H -3.78403400 -1.21718400 -0.00105600
H -1.30931500 -1.25929200 -0.87333100
H -1.30931000 -1.25937200 0.87082400
H -0.19450800 1.15749900 -0.00122000
H 2.27970600 1.22165800 0.87102200
H 2.27989500 1.22148900 -0.87325200
H 5.89627700 -1.22295200 -0.87291500
H 5.89596500 -1.22292700 0.87204900
H 9.47676500 1.28186600 0.87343800
H 9.47707100 1.28190300 -0.87301000
H 10.59694000 -1.12865400 0.00042300
H 13.10074600 -1.18506600 -0.87452000
H 13.10057000 -1.18492400 0.87598400
H 16.67786400 1.40888900 0.88025800
H 16.67802000 1.40884200 -0.87828600
H 17.63688600 -1.02085700 0.00125900
H 14.13141700 1.25697800 0.00064500
H 18.52770000 0.11649000 0.81739000

3. zwitterionic $(gly)_{12}$

O 21.59929900 -0.09637000 0.00629900
O 20.08407900 1.60105800 0.00513100
C 20.44975900 0.38956800 0.00543500
C 19.29980700 -0.64423300 0.00461300
N 18.04084500 0.08084000 0.00366500
C 16.83575100 -0.44903900 0.00280200
O 16.58322900 -1.66848800 0.00266200
C 15.68043700 0.54344000 0.00191200
N 14.44971800 -0.21805900 0.00111600
C 13.24107400 0.33117600 0.00030500
O 13.03368100 1.55190400 0.00013500
C 12.07312700 -0.63750500 -0.00043900
N 10.85326100 0.13784600 -0.00113400
C 9.64207300 -0.41644600 -0.00172400
O 9.45031600 -1.63760100 -0.00174100
C 8.47130100 0.54522500 -0.00239000
N 7.25335900 -0.23183700 -0.00277100
C 6.04337000 0.32975500 -0.00315400
O 5.86397300 1.55187200 -0.00323700
C 4.86663800 -0.62319700 -0.00350600
N 3.65375600 0.16113800 -0.00367900
C 2.44087700 -0.39616900 -0.00373400
O 2.25885200 -1.61751000 -0.00367600
C 1.26806900 0.56088600 -0.00389400
N 0.05171200 -0.21795000 -0.00373200
C -1.15778300 0.34715400 -0.00356100
O -1.33096500 1.56966200 -0.00356400
C -2.33757000 -0.60122100 -0.00336200
N -3.54758700 0.18766200 -0.00306900
C -4.76176300 -0.36661300 -0.00263600
O -4.94691400 -1.58734800 -0.00247000
C -5.93312200 0.59235200 -0.00235100
N -7.14979200 -0.18701400 -0.00167500
C -8.35875300 0.37617800 -0.00130400
O -8.53658200 1.59827100 -0.00148900
C -9.53920600 -0.57249300 -0.00061800
N -10.74672100 0.22269500 -0.00025300
C -11.96248600 -0.32036000 0.00041900
C -13.12941600 0.64673100 0.00074700
O -12.16612500 -1.53878200 0.00077500
N -14.34591800 -0.13882500 0.00150200
C -15.55445300 0.40729900 0.00188600
C -16.73237600 -0.55103900 0.00264700
O -15.76555100 1.62609900 0.00165500

N -17.93310500 0.26980600 0.00299800
C -19.14990700 -0.22507300 0.00374500
C -20.30640400 0.77418300 0.00402600
O -19.44669600 -1.42720100 0.00424100
N -21.56553800 -0.05468200 0.00490900
H -21.24084900 -1.03337900 0.00502800
H -3.41148900 1.17558400 -0.00314500
H 0.17922400 -1.20695300 -0.00370100
H 18.20970000 1.07113100 0.00376000
H 19.38581100 -1.27618400 0.87875000
H 19.38710200 -1.27623100 -0.86936200
H 15.73980000 1.18135200 -0.87074700
H 15.73857100 1.18150300 0.87454200
H 14.59289200 -1.20713300 0.00125500
H 12.12242400 -1.27753800 0.87181200
H 12.12348600 -1.27745300 -0.87269300
H 10.98985200 1.12644200 -0.00109500
H 8.51959400 1.18590500 -0.87445700
H 8.51882800 1.18621800 0.86948500
H 7.38379000 -1.22071400 -0.00267800
H 4.91022100 -1.26467800 0.86832700
H 4.91061700 -1.26448400 -0.87546700
H 3.78730900 1.14941500 -0.00369700
H 1.31441700 1.20204700 -0.87585700
H 1.31441900 1.20237400 0.86782400
H -2.29617000 -1.24281400 0.86851700
H -2.29651800 -1.24273100 -0.87532000
H -5.88718100 1.23308300 -0.87455700
H -5.88646100 1.23346600 0.86953300
H -7.02050300 -1.17604100 -0.00158900
H -9.50021500 -1.21302100 0.87189700
H -9.50096200 -1.21336200 -0.87291800
H -13.08538500 1.28523600 -0.87260200
H -13.08455500 1.28563700 0.87375900
H -14.20103900 -1.12736600 0.00168600
H -10.60085800 1.20987400 -0.00052100
H -16.70423300 -1.18648300 0.87799200
H -16.70502000 -1.18689000 -0.87242800
H -17.74019000 1.25365900 0.00262700
H -20.28807500 1.39860300 -0.87543100
H -20.28719600 1.39914000 0.88308100
H -22.13365000 0.10202500 0.82137900
H -22.13447600 0.10154100 -0.81108100

D. Water clusters

1. $(H_2O)_{12}$ [1]

O 1.794470 0.923410 2.768350
H 2.338250 1.359750 3.430940
H 0.879480 1.303000 2.865760
O -1.794470 -0.923410 2.768350
H -2.338250 -1.359750 3.430940
H -0.879480 -1.303000 2.865760
O 0.923410 -1.794470 -2.768350
H 1.359750 -2.338250 -3.430940
H 1.303000 -0.879480 -2.865760
O -1.752130 -0.741530 -2.896280
H -2.036450 -0.920500 -1.984040
H -0.921210 -1.242140 -2.984230
O -0.885520 1.737840 0.052730
H -1.032320 2.090180 -0.841890
H -1.284090 0.839590 0.017130
O 0.885520 -1.737840 0.052730
H 1.284090 -0.839590 0.017130
H 1.032320 -2.090180 -0.841890
O 1.737840 0.885520 -0.052730
H 2.090180 1.032320 0.841890
H 0.839590 1.284090 -0.017130
O -1.737840 -0.885520 -0.052730
H -2.090180 -1.032320 0.841890
H -0.839590 -1.284090 -0.017130
O 1.752130 0.741530 -2.896280
H 2.036450 0.920500 -1.984040
H 0.921210 1.242140 -2.984230
O 0.741530 -1.752130 2.896280
H 0.920500 -2.036450 1.984040
H 1.242140 -0.921210 2.984230
O -0.923410 1.794470 -2.768350
H -1.359750 2.338250 -3.430940
H -1.303000 0.879480 -2.865760
O -0.741530 1.752130 2.896280
H -0.920500 2.036450 1.984040
H -1.242140 0.921210 2.984230

2. $(H_2O)_{16}$ [2]

O -0.56428200 -0.57338900 -2.52729000
O -3.55903200 -1.84346700 -2.14561800
O -0.78063400 0.54962200 1.55967800
O -2.35205400 -2.18756600 0.72179100
O -2.78794500 1.06514800 -0.80100600
O -0.74385200 3.06647000 3.69618800
O -2.29861000 3.52773600 1.00714000
O 1.90007200 -0.30397000 -0.16400600
O 2.28779600 -2.17860900 -2.79388000
O 0.01715400 -3.56494600 -1.13063900
O 0.67263600 -2.50062900 1.90954000
O 3.70876400 2.34433800 -0.26312700
O 2.31905700 0.88615300 -3.21671700
O 0.33891000 2.59353700 -0.75370300
O 2.57209400 3.99531400 -2.72826800
O 1.88785500 2.39051900 2.22421900
H 1.53406100 3.00110000 2.87973500
H -0.08085800 -1.33585700 -2.19211100
H 0.11906200 -0.06349600 -2.97304900
H -3.97686700 -2.37744500 -2.82376600
H -2.66179800 -1.71876100 -2.47403900
H -1.53851600 -0.01436100 1.37054600
H -0.95128200 1.32283100 1.01030100
H -3.19669300 -2.02667100 0.29159800
H -1.88970200 -2.74345400 0.08577200

H -3.36307900 0.37230000 -1.13843500
H -1.99543200 0.97319700 -1.34128700
H -1.14279300 2.22045400 3.47901900
H -1.26791000 3.69248700 3.18671500
H -3.01299800 2.98891100 0.65372200
H -1.68621300 3.58787500 0.26818700
H 1.03415000 0.11848100 -0.14863100
H 1.85527800 -0.91235000 0.58130600
H 2.60437000 -1.65084200 -2.05460500
H 2.44432200 -1.60560600 -3.55001100
H 0.54816900 -3.51718700 -0.32971900
H 0.67023200 -3.70952500 -1.82308600
H -0.17206900 -2.03811800 1.86062500
H 0.64313000 -2.92886400 2.76701400
H 3.61230100 1.40626000 -0.07095100
H 3.61979000 2.74725900 0.60691000
H 2.54962200 1.07662800 -2.30144100
H 2.41755000 1.73966000 -3.64925100
H 0.66737100 2.95725700 -1.58170300
H 1.07707800 2.72184000 -0.14815400
H 3.26041500 3.80767500 -2.08021500
H 2.75650400 4.89554900 -3.00365600
H 1.31613500 1.62222600 2.32172200

3. $(H_2O)_{32}$ [2]

O -5.297633 -3.258368 -2.917500
H -4.555640 -3.526640 -3.471568
H -6.055243 -3.669168 -3.337921
O -3.588127 -2.893849 -0.229710
H -4.452484 -2.978549 -0.643675
H -2.996644 -2.777467 -0.980941
O -3.554748 -0.454520 -2.421492
H -2.754291 -0.738168 -2.877459
H -4.211370 -1.089780 -2.722408
O -3.024122 1.063887 4.026190
H -2.822590 1.697258 4.723008
H -3.385422 1.620990 3.330426
O -3.238103 4.544063 -3.257114
H -2.759243 4.402619 -2.435988
H -4.116349 4.210806 -3.056105
O -2.675500 2.985631 1.319092
H -3.356776 3.394501 0.775814
H -2.457465 2.192649 0.816724
O -4.109121 2.322147 -1.327362
H -3.281001 2.011155 -1.711593
H -4.668281 1.541861 -1.380198
O -0.781796 -1.971094 -1.598127
H -0.172816 -2.130956 -0.870159
H -0.426945 -1.176684 -2.009621
O -2.352805 -3.016056 -4.129675
H -1.902521 -2.362473 -4.672843
H -1.638454 -3.366377 -3.585369
O 0.834124 -3.761010 -3.760759
H 1.005170 -2.866589 -3.447948
H 1.477278 -3.879841 -4.461444
O 1.020191 -4.406299 -0.533764
H 0.349125 -4.873497 -0.024875
H 0.755876 -4.557847 -1.447470
O -1.350176 -4.339044 1.659902
H -2.152735 -4.143643 1.166077
H -1.568078 -4.045035 2.550107
O 0.697262 -1.977076 1.667690
H -0.221438 -1.832216 1.916250
H 0.721298 -2.920518 1.476300
O -1.909568 -1.906240 3.666101
H -2.595426 -1.253128 3.842346
H -1.238959 -1.699346 4.325595
O -0.842879 -0.165719 -4.379869
H -1.258131 0.636468 -4.713693
H 0.095368 0.022073 -4.479475
O 0.919325 0.311615 -0.422476
H 0.214093 0.409977 0.227969
H 1.577420 -0.204264 0.058915
O -2.198138 -0.223738 0.725036
H -2.411490 -0.431272 -0.191527
H -2.632323 -0.935160 1.208287
O 1.054676 -1.039049 4.747887
H 1.674686 -1.024208 5.483345
H 1.571709 -1.417272 4.028162
O -0.051243 1.290185 2.607374
H -1.000641 1.161940 2.498164
H 0.199062 0.549528 3.168569
O -0.918578 2.713964 -1.703671
H -0.229069 2.044037 -1.768975
H -0.500164 3.391373 -1.162345
O -1.225036 3.042061 -5.005655
H -1.891383 3.658458 -5.324070
H -1.268909 3.164251 -4.051712
O 0.413567 4.146167 0.934236
H 0.687219 4.736721 1.642533
H -0.229077 3.573610 1.367561
O -2.264274 4.037848 4.411603
H -2.303950 4.095271 3.453016
H -1.446255 4.492034 4.630767
O 0.899772 4.118701 4.006384
H 0.694817 3.179281 3.943300
H 1.723096 4.120213 4.503020
O 3.279768 -2.000381 -0.352667
H 2.782826 -2.822022 -0.283881
H 3.430354 -1.910810 -1.297361
O 2.272756 -0.845359 -3.206127
H 2.001410 -0.186264 -2.557468
H 2.621860 -0.306284 -3.923821
O 3.564222 -0.769200 2.600096
H 3.172042 -1.416973 2.002870
H 3.854944 -0.079062 1.994083
O 4.099726 -0.805882 5.754151
H 4.350227 -0.971897 4.838300
H 4.792437 -1.233490 6.261513
O 2.227638 3.059248 -1.531546
H 2.537039 2.331914 -0.981469
H 2.064947 3.756121 -0.888618
O 1.703820 1.869214 -4.507871

H 1.118729 2.410711 -5.047858
H 1.995957 2.478613 -3.820612
O 2.939002 2.142339 1.444049
H 3.207154 2.631047 2.226794
H 1.978369 2.125582 1.513459
O 2.867207 1.866062 4.610181
H 2.701152 1.056959 4.114986
H 3.310663 1.544391 5.400608

4. $(H_2O)_{40}$

O -4.45183800 -1.89774700 -1.07247800
O -4.53101300 0.19580200 -4.32052800
O -4.55650900 1.58831900 -1.34644400
O -5.00972500 2.66106600 2.91209800
O -0.86516300 -4.62923600 -3.16570000
O -2.57074100 -4.21079400 -0.01441600
O -1.33869000 -4.57643800 2.98757700
O -1.87182400 -1.59995600 -3.51198600
O -1.46702200 -1.52781700 1.98478300
O -3.03884900 -1.05242000 4.57128400
O -1.82244100 1.63275500 -3.52009400
O -1.92333000 -0.05407400 -0.70645000
O -1.98701600 3.08331000 0.07603000
O -1.85704700 1.61335600 3.16156400
O -4.31715200 0.04611100 1.53570900
O -0.95533500 0.52471200 6.39530500
O -3.48045500 4.36725200 -2.74712500
O -2.64653400 6.21470100 -0.05839500
O -1.84199000 4.89361400 2.96292700
O 0.08982400 -5.79774800 -0.41423100
O 3.07973500 -4.44773900 0.28886200
O 2.09611700 -3.35987300 -2.86452400
O 0.99807500 -1.08061100 -4.94954300
O 0.09126700 -2.57082800 -0.63272300
O 1.78820700 -1.85973000 1.90371700
O 0.20519900 -2.15282800 4.79556200
O 1.12257100 2.92441000 -3.81130800
O 0.91971600 0.16893400 -2.09085200
O 0.51368600 0.97623100 0.97212200
O 1.03836500 3.16232200 3.11107900
O 2.04810700 1.62569500 5.73385400
O 2.63404900 4.81220900 -1.63991400
O 0.41516200 5.19022800 0.66429000
O 4.05806700 -3.74429400 3.15702300
O 3.58077600 -1.33658300 -0.81375200
O 3.39283000 -1.25770100 5.01883900
O 3.58554100 0.86704700 -3.71601000
O 3.38945500 1.77221800 -0.43075500
O 3.36098100 0.97159400 2.73134100
O 3.61347800 4.29909800 1.46421600
H -3.49088200 -1.84177500 -1.03134300
H -4.63945500 -2.72122300 -0.61056500
H -3.72005100 0.60317600 -4.63923600
H -4.81964500 0.80069600 -3.62975900
H -4.09903000 1.92064100 -0.56760500
H -4.60841700 0.64135200 -1.17298700
H -5.58676700 1.99736400 2.52303600
H -4.13520500 2.35056300 2.65614000
H -1.64381500 -5.17777000 -3.30029000
H -1.07905900 -3.82304800 -3.64574700
H -2.40929200 -4.65530400 -0.85369500
H -1.91274200 -4.61282700 0.56718800
H -1.09763500 -3.69327000 3.28534900
H -1.90401400 -4.89864000 3.69718800
H -1.59575400 -0.80378000 -3.04180600
H -2.82091400 -1.47254300 -3.60271800
H -0.59197500 -1.12605600 1.93595900
H -1.47441000 -2.11325600 1.21899500
H -3.56150200 -1.26872800 3.79001500
H -2.17508500 -1.42349200 4.35459300
H -2.29314200 2.25756600 -2.95870000
H -1.22376000 2.19615200 -4.02034100
H -1.84794400 0.88620100 -0.89620500
H -1.01507000 -0.30002800 -0.49968400
H -1.59824100 3.87088400 -0.31930500
H -2.09991400 3.33711800 0.99751500
H -2.09875200 0.73513900 2.84942100
H -1.83690500 1.50366000 4.11930800
H -3.49644800 -0.22784900 1.11096800
H -4.85828600 -0.74820700 1.48312600
H -0.67290400 -0.35774700 6.13480000
H -1.90687500 0.42925000 6.50564600
H -3.32210300 5.03987800 -2.07668100
H -4.18342800 3.83288900 -2.36336700
H -2.07420900 6.11928900 0.71152400
H -3.50227700 6.42124500 0.33382500
H -1.23136300 5.34294600 3.55593600
H -1.99640700 4.05933500 3.42065200
H 0.19476100 -6.03446900 -1.34232400
H 0.69204400 -5.05292400 -0.31439700
H 3.11503500 -4.84441600 1.16812200
H 3.51860900 -3.60037000 0.42402000
H 1.58765800 -4.14521800 -3.10107000
H 2.60522900 -3.65964900 -2.10424400
H 1.06172300 -1.45901600 -4.06544500
H 0.04944700 -1.02500200 -5.09270200
H 0.68689800 -2.07429300 -1.20461600
H -0.50430200 -2.99259900 -1.26055900
H 1.99820500 -1.19280100 1.24024900
H 1.44259700 -2.58551500 1.37427000
H 0.88109200 -1.82724200 4.18834400
H 0.62455500 -2.92701200 5.18565800
H 0.94992300 3.32747000 -4.66837200
H 1.15936100 3.68511000 -3.22179500
H 1.26775700 0.69988300 -1.36501200
H 0.61466200 0.83383800 -2.71768700
H 1.29718200 1.43450200 1.29271800
H -0.20314300 1.53536200 1.28962300
H 0.30670300 2.86093700 3.66039500
H 1.58957900 3.64862000 3.73360100
H 1.14539800 1.56628200 6.06367100
H 2.33858500 2.49208900 6.03646800
H 3.44505100 5.32478600 -1.56775100

H 2.93431900 3.91378300 -1.46095000
H 1.30866400 4.91720600 0.43057900
H 0.23628200 4.68276600 1.46261300
H 4.58794900 -3.72808900 3.95892200
H 3.56341900 -2.91831000 3.20727100
H 3.04930500 -1.13609900 -1.59235700
H 4.46141000 -1.46262300 -1.18098300
H 3.02981100 -0.50701700 5.49945400
H 3.85978200 -1.75389900 5.69836900
H 3.45313000 1.80917800 -3.86976300
H 2.75723700 0.48269700 -4.02310100
H 3.57345800 1.09664800 0.23157000
H 3.93315000 1.49389000 -1.17582900
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H 2.65287000 1.16301000 3.35665500
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H 3.28787900 3.39160000 1.50448800

5. $(H_2O)_{48}$

O -4.45183800 -1.89774700 -1.07247800
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O -4.00001800 -5.11993600 -2.80813700
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O -2.57074100 -4.21079400 -0.01441600
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O -1.87182400 -1.59995600 -3.51198600
O -1.46702200 -1.52781700 1.98478300
O -3.03884900 -1.05242000 4.57128400
O -1.82244100 1.63275500 -3.52009400
O -1.92333000 -0.05407400 -0.70645000
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O -1.85704700 1.61335600 3.16156400
O -4.31715200 0.04611100 1.53570900
O -0.95533500 0.52471200 6.39530500
O -3.48045500 4.36725200 -2.74712500
O -2.64653400 6.21470100 -0.05839500
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O 0.08982400 -5.79774800 -0.41423100
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O 2.09611700 -3.35987300 -2.86452400
O 0.99807500 -1.08061100 -4.94954300
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O 1.78820700 -1.85973000 1.90371700
O 0.20519900 -2.15282800 4.79556200
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O 0.91971600 0.16893400 -2.09085200
O 0.51368600 0.97623100 0.97212200
O 1.03836500 3.16232200 3.11107900
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O 3.58554100 0.86704700 -3.71601000
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O 3.36098100 0.97159400 2.73134100
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O 3.61347800 4.29909800 1.46421600
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H 0.19476100 -6.03446900 -1.34232400
H 0.69204400 -5.05292400 -0.31439700
H 3.11503500 -4.84441600 1.16812200

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H 2.60522900 -3.65964900 -2.10424400
H 1.06172300 -1.45901600 -4.06544500
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H 2.33858500 2.49208900 6.03646800
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H 4.25668800 4.26612300 0.74766000
H 3.28787900 3.39160000 1.50448800
H 4.28200700 2.78452700 4.27400400

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