Supporting Information
A localized molecular orbital assembler approach for Hartree-Fock calculations of large molecules

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Cartesian coordinates of all compounds

(1). dodecane

C -7.04109400 -0.30852400 -0.00019100
C -5.75291800 0.51918000 -0.00030500
C -4.48672300 -0.34521800 -0.00001100
C -3.19258500 0.47612800 -0.00012300
C -1.92699500 -0.38890800 0.00017200
C -0.63273300 0.43258400 0.00006000
C 0.63279900 -0.43250900 0.00035000
C 1.92704800 0.38898700 0.00026600
C 3.19259800 -0.47610000 0.00042000
C 4.48671700 0.34522500 0.00074900
C 5.75286300 -0.51925300 -0.00070000
C 7.04102700 0.30842800 -0.00060400
H -7.91879200 0.32854200 -0.00040500
H -7.09471700 -0.94653600 -0.87653100
H -7.09483500 -0.94611100 0.87645100
H -5.74203900 1.17103000 0.86981400
H -5.74192200 1.17060800 -0.87073900
H -4.49891600 -0.99724800 0.87112800
H -4.49879900 -0.99767000 -0.87083500
H -3.18142700 1.12804700 -0.87129900
H -3.18154400 1.12846900 0.87073800
H -1.93806400 -1.04122400 -0.87067100
H -1.93818100 -1.04080100 0.87133000
H -0.62156800 1.08448700 -0.87110200
H -0.62168200 1.08490500 0.87091000
H 0.62161900 -1.08442600 0.87150100
H 0.62175200 -1.08481700 -0.87051100
H 1.93824500 1.04095000 -0.87083800
H 1.93818000 1.04121600 0.87117600
H 3.18162900 -1.12816200 -0.87065000
H 3.18131600 -1.12829800 0.87138800
H 4.49853700 0.99844700 -0.86949800
H 4.49925700 0.99646400 0.87246800
H 5.74233600 -1.17169700 0.86897800
H 5.74142500 -1.17007900 -0.87156900
H 7.91869400 -0.32867100 -0.00147800
H 7.09435900 0.94691300 -0.87662000
H 7.09511500 0.94553900 0.87636600

(2). pentadecane

C -8.95505600 -0.39284100 -0.00000300
C -7.68106400 0.45671600 -0.00000500
C -6.40024900 -0.38585700 0.00000000
C -5.12025200 0.45735600 -0.00000100
C -3.84009700 -0.38595600 0.00000200
C -2.56004600 0.45744700 0.00000200
C -1.28001500 -0.38595800 0.00000400
C 0.00000000 0.45745800 0.00000200
C 1.28001500 -0.38595800 0.00000300
C 2.56004600 0.45744700 0.00000400
C 3.84009700 -0.38595600 0.00000300
C 5.12025200 0.45735700 0.00000200
C 6.40025000 -0.38585700 -0.00000100
C 7.68106400 0.45671500 -0.00000300
C 8.95505600 -0.39284100 -0.00000700
H -9.84352600 0.22911500 -0.00000600
H -8.99796700 -1.03149700 -0.87646700
H -8.99796900 -1.03149200 0.87646400
H -7.68113200 1.10849800 -0.87024200
H -7.68113400 1.10850400 0.87022800
H -6.40124900 -1.03822500 0.87096500
H -6.40124600 -1.03823000 -0.87096100
H -5.12026900 1.10959400 -0.87100700
H -5.12027100 1.10959900 0.87100100
H -3.84010300 -1.03817100 -0.87099000
H -3.84010400 -1.03816600 0.87099800
H -2.56004200 1.10966000 -0.87100700
H -2.56004300 1.10966300 0.87100700
H -1.28001300 -1.03817000 0.87101300
H -1.28001200 -1.03817300 -0.87100400
H 0.00000000 1.10967100 -0.87100900
H 0.00000000 1.10967300 0.87101200
H 1.28001300 -1.03817300 -0.87100500
H 1.28001200 -1.03817100 0.87101200
H 2.56004300 1.10966200 -0.87100300
H 2.56004300 1.10966200 0.87101100
H 3.84010400 -1.03816900 0.87099700
H 3.84010300 -1.03816800 -0.87099100
H 5.12026900 1.10959700 -0.87100100
H 5.12027100 1.10959500 0.87100700
H 6.40124600 -1.03822700 -0.87096500
H 6.40124900 -1.03822900 0.87096100
H 7.68113000 1.10850200 -0.87023700
H 7.68113400 1.10850000 0.87023300
H 8.99797000 -1.03149600 0.87645800
H 8.99796700 -1.03149300 -0.87647300
H 9.84352600 0.22911500 -0.00000800

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(3). tetracosane

C -14.76457400 0.36506200 -0.00111200
C -13.47976600 -0.48613800 -0.00043200
C -12.19932400 0.37845000 -0.00055300
C -10.91183400 -0.47541700 -0.00009500
C -9.63151700 0.38927600 -0.00023900
C -8.34396300 -0.46466500 0.00021000
C -7.06361400 0.40003800 0.00015000
C -5.77604500 -0.45388800 0.00038000
C -4.49569100 0.41080500 0.00029600
C -3.20811700 -0.44311700 0.00051700
C -1.92775600 0.42157600 0.00051400
C -0.64017900 -0.43234300 0.00051900
C 0.64018000 0.43234600 0.00049100
C 1.92775600 -0.42157400 0.00048700
C 3.20811700 0.44311800 0.00054100
C 4.49569100 -0.41080300 0.00032100
C 5.77604600 0.45388900 0.00034900
C 7.06361400 -0.40003800 0.00012100
C 8.34396300 0.46466500 0.00023000
C 9.63151700 -0.38927700 -0.00021400
C 10.91183500 0.47541600 -0.00013000
C 12.19932300 -0.37845300 -0.00058600
C 13.47976600 0.48613500 -0.00041000
C 14.76457400 -0.36506600 -0.00109200
H 14.80465500 -1.00039400 -0.88095700
H -15.64470600 -0.27121100 -0.00087800
H -14.80498200 1.00130900 0.87807400
H -14.80471900 1.00029600 -0.88104100
H -13.47710500 -1.13221700 0.87559500
H -13.47672200 -1.13304000 -0.87585200
H -12.20252100 1.02465600 -0.87641300
H -12.20275600 1.02523300 0.87488100
H -10.90930100 -1.12161000 0.87576500
H -10.90908600 -1.12222300 -0.87550100
H -9.63437700 1.03608000 0.87516700
H -9.63416600 1.03547200 -0.87609100
H -8.34139400 -1.11090600 0.87602700
H -8.34112900 -1.11143000 -0.87522200
H -7.06628500 1.04640500 -0.87557400
H -7.06640500 1.04668500 0.87566900
H -5.77338100 -1.10023500 0.87612200
H -5.77328200 -1.10055400 -0.87512600
H -4.49846400 1.05747000 0.87580300
H -4.49836800 1.05715500 -0.87544200
H -3.20547400 -1.08950700 0.87622300
H -3.20532700 -1.08974200 -0.87501700
H -1.93047500 1.06808900 -0.87510100
H -1.93047900 1.06808200 0.87613600
H -0.63745100 -1.07883400 0.87615400
H -0.63746800 -1.07886800 -0.87509000
H 0.63747000 1.07886900 0.87610300
H 0.63745000 1.07884000 -0.87514000
H 1.93046100 -1.06810800 0.87608700
H 1.93049200 -1.06805700 -0.87515200
H 3.20534400 1.08977300 -0.87496900
H 3.20545600 1.08948200 0.87626800
H 4.49848300 -1.05743600 0.87585100
H 4.49834900 -1.05718500 -0.87539500
H 5.77340000 1.10026800 0.87606800
H 5.77326400 1.10052500 -0.87517800
H 7.06638700 -1.04671200 0.87561700
H 7.06630200 -1.04637500 -0.87562700
H 8.34114800 1.11145800 -0.87517800
H 8.34137700 1.11088000 0.87606800
H 9.63439600 -1.03604500 0.87521600
H 9.63414600 -1.03550700 -0.87604300
H 10.90932100 1.12164400 0.87570500
H 10.90906800 1.12218900 -0.87556000
H 12.20273500 -1.02526300 0.87482700
H 12.20253900 -1.02462900 -0.87646900
H 13.47674000 1.13307100 -0.87580300
H 13.47708700 1.13218300 0.87564100
H 15.64470700 0.27120600 -0.00098800
H 14.80504400 -1.00121900 0.87815900

(4). $(gly)_8$

O 14.27581900 -0.42129100 -0.02447300
O 13.07422100 1.47636400 -0.03184000
C 13.12439500 0.26542800 -0.02485400
C 11.93679000 -0.64243200 -0.01571400
N 10.73428600 0.15716400 -0.01657000
C 9.51806700 -0.41121800 -0.00932700
O 9.36090600 -1.63265900 -0.00150200
C 8.33972600 0.53461000 -0.01129000
N 7.12571300 -0.24463700 -0.00301300
C 5.91778700 0.33448800 -0.00257600
O 5.76929200 1.55873600 -0.00919500
C 4.72985200 -0.60006200 0.00657700
N 3.52377600 0.19202200 0.00553700
C 2.30911300 -0.37155400 0.01244800
O 2.14339700 -1.59375800 0.02022900
C 1.13336500 0.57876600 0.01023000
N -0.08301700 -0.19731400 0.01771600
C -1.29044200 0.38146400 0.01719400
O -1.44086000 1.60579600 0.01064100
C -2.47777800 -0.55430600 0.02520600
N -3.68479000 0.23600100 0.02251400
C -4.89929500 -0.32889400 0.02790300
O -5.06291500 -1.55136600 0.03594200
C -6.07499100 0.62120700 0.02361800
N -7.29249500 -0.15186700 0.02891400
C -8.49954800 0.43128300 0.02775700
O -8.64125800 1.65680800 0.02410600
C -9.68814200 -0.50178800 0.02993400
N -10.89613400 0.28317100 0.03704500
C -12.11216000 -0.29139800 0.04005000
O -12.25624300 -1.51469400 0.02510000
C -13.29625600 0.64702300 0.11524500
N -14.46327200 -0.00385600 -0.42037300
H -10.77748700 1.27076900 0.01677700
H -7.18055500 -1.14172500 0.03194700
H 10.84730100 1.14597000 -0.02281500
H 11.98633700 -1.28182900 0.85635000
H 11.98078000 -1.29204100 -0.88050200

H 8.38098400 1.17244300 -0.88649000
H 8.38630200 1.18266100 0.85610600
H 7.24175500 -1.23418500 0.00238400
H 4.77013900 -1.23816500 0.88148600
H 4.76485300 -1.24848700 -0.86094000
H 3.65239500 1.18006700 -0.00080700
H 1.17722300 1.21660000 -0.86469000
H 1.18181700 1.22628700 0.87776400
H 0.03321700 -1.18693400 0.02289200
H -2.43756100 -1.19218600 0.90029800
H -2.44084200 -1.20306400 -0.84199800
H -3.55726100 1.22412100 0.01583600
H -6.02818800 1.25953200 -0.85093500
H -6.02676000 1.26902700 0.89106400
H 15.06340000 0.11843500 -0.03022300
H -9.64391700 -1.14946800 0.89801600
H -9.65098900 -1.14363000 -0.84288200
H -13.07601500 1.55132100 -0.43979300
H -13.39699700 0.93514500 1.16391800
H -15.33944800 0.43386500 -0.26232800
H -14.46072600 -0.99650600 -0.35929500

(5). adenine-thymine (A-T)

H -8.63758500 2.07849200 -0.03908600
O -8.12638700 1.25168800 0.14528300
C -8.64645600 0.30028700 -0.79536600
H -8.49454700 0.63446600 -1.82872000
H -9.72203500 0.14360000 -0.64845100
C -7.91908500 -1.06322600 -0.60865700
H -8.43269200 -1.80547600 -1.23123700
O -6.55271100 -0.96981400 -1.06283400
C -5.65816900 -1.08980500 0.05694100
H -5.04705800 -1.99802700 -0.05207900
N -4.69941300 0.03447700 0.02620900
C -5.00539000 1.40459800 -0.01348500
H -6.04417900 1.72086300 0.03642400
N -3.95639900 2.18271900 -0.11298900
C -2.86948500 1.26528900 -0.15237400
C -1.46772600 1.46790100 -0.25147900
N -0.89879900 2.71390000 -0.39796500
H 0.12268200 2.82485800 -0.21784900
H -1.50957800 3.49935100 -0.17948300
N -0.65062100 0.38063900 -0.24847800
C -1.24007300 -0.85238300 -0.16375700
H -0.53437300 -1.68597700 -0.16720500
N -2.53300100 -1.17707800 -0.07529600
C -3.31349500 -0.04313100 -0.07439500
C -7.91171300 -1.55213100 0.87166400
H -8.69164000 -1.04576200 1.45184200
C -6.50257700 -1.13448400 1.36251100
H -6.54086000 -0.14901600 1.81723800
H -6.08654500 -1.83854100 2.07763700
O -8.11454600 -2.97179700 0.86249100
H -8.10606800 -3.22462400 1.82042300
H 9.26488700 -0.52918100 1.10532000
C 8.20361800 -0.26131800 1.17558900
O 7.87201500 0.80222000 0.27007800
H 7.99641500 0.02036100 2.21485500
C 7.34418500 -1.50847700 0.82131400
H 8.43288300 1.56076100 0.56841800
H 7.67236700 -2.33951900 1.45754600
O 5.95778500 -1.22972200 1.10287300
C 7.47556800 -1.93117500 -0.67497600
C 5.18950600 -1.30370300 -0.11347400
H 8.36604700 -1.48101200 -1.12875200
C 6.18334200 -1.35861300 -1.30749700
O 7.54622400 -3.36323300 -0.71679800
H 4.54950800 -2.19767000 -0.10167100
N 4.26112100 -0.15934900 -0.16398200
H 6.36597800 -0.36005800 -1.69325400
H 5.80265000 -1.98275700 -2.11095600
H 7.61999500 -3.57453700 -1.68195000
C 4.75136500 1.14454200 0.04815800
C 2.85255800 -0.43144000 -0.21704500
H 5.83585400 1.19654900 0.13966100
C 3.97259700 2.21377600 0.12831200
N 2.03594500 0.72241800 -0.17134400
O 2.40906500 -1.56553100 -0.31755800
C 4.49901800 3.62167500 0.34523400
C 2.48841800 2.04573600 0.00680800
H 0.99726800 0.56003900 -0.22401700
H 4.20489000 4.27484200 -0.47367900
H 4.09842200 4.04791100 1.26265900
H 5.58253100 3.61841800 0.41138300
O 1.69191900 2.98919600 0.06118200

(6). guanine-cytosine (G-C)

H -8.48319000 1.87861700 0.11599400
O -7.89363600 1.09396900 0.23851700
C -8.41123700 0.11258500 -0.67293900
H -8.37934700 0.47493700 -1.70739200
H -9.45166200 -0.14142300 -0.43737400
C -7.54288800 -1.17407700 -0.57284600
H -7.98737800 -1.93548400 -1.22518100
O -6.20885300 -0.88848800 -1.04177000
C -5.26657600 -1.06907000 0.03005500
H -4.63048300 -1.94442200 -0.16441300
N -4.34186000 0.08624200 0.04256900
C -4.85029600 1.38439500 0.02917600
H -5.94011800 1.45012600 0.07429700
C -4.04191000 2.44139400 -0.02783000
H -4.41633300 3.45085000 -0.03038900
C -2.59568600 2.20249700 -0.09719000
N -1.73290600 3.24601700 -0.14686600
H -0.66805600 3.10695700 -0.10225000
H -2.12953800 4.18063800 -0.08283300
N -2.07143400 0.97085500 -0.12520600
C -2.92556000 -0.15040400 -0.05622000
O -2.49363200 -1.30676200 -0.05658400
C -7.45090000 -1.73926200 0.87861800
H -8.24789300 -1.32593800 1.50748900
C -6.06170500 -1.24511800 1.35415000
H -6.15778800 -0.29240500 1.86673000
H -5.57401200 -1.95421100 2.01701700
O -7.54998100 -3.16727400 0.79371400
H -7.49204300 -3.47181000 1.73469200

H 8.54345400 1.92842600 0.72887800
O 8.03093500 1.15692800 0.38036000
C 8.32794700 0.09503000 1.29882600
H 8.04203700 0.35862400 2.32409800
H 9.39925000 -0.14125800 1.30003600
C 7.53984800 -1.18152500 0.88343700
H 7.90827500 -2.01659800 1.49125900
O 6.13394400 -1.01397200 1.15908200
C 7.70678300 -1.53257200 -0.62626200
C 5.39720000 -0.97150100 -0.07693700
H 8.59445200 -1.04303900 -1.04307400
C 6.41336600 -0.95622100 -1.25415700
O 7.80736100 -2.95946300 -0.73445700
H 4.73115800 -1.84453200 -0.14084100
N 4.50422600 0.20295700 -0.06639500
H 6.58225400 0.06299000 -1.58879900
H 6.05722100 -1.54982500 -2.09138600
H 7.90292400 -3.12231800 -1.70710700
C 4.86630900 1.54776300 0.12290800
C 3.11916800 0.19277800 -0.16290100
H 5.91053800 1.81545900 0.24087100
N 3.84027700 2.36077800 0.13974000
C 2.72611600 1.50312000 -0.04553200
N 2.34095300 -0.95190200 -0.35800900
C 1.30142000 1.82088500 -0.10549100
C 1.05342900 -0.62385000 -0.42104100
O 0.76333600 2.94128000 -0.00898800
N 0.51833100 0.65448000 -0.29421100
N 0.12173800 -1.63000100 -0.70365800
H -0.54692100 0.76228900 -0.26392700
H -0.86293700 -1.48983300 -0.40527500
H 0.49608600 -2.56364700 -0.53281200

(7). water cluster (n=14)

O -3.99084000 -1.10337000 -0.00207000
O -5.04579000 -0.93241000 -2.72838000
O -4.47422000 1.67410000 -2.95274000
O -3.66482000 1.53600000 -0.22441000
O -1.85230000 2.18872000 -3.99400000
O -1.07247000 2.33477000 -1.15061000
O -0.74127000 -0.33237000 -4.12222000
O 0.02277000 -0.14191000 -1.41179000
O 1.35005000 -2.13477000 -4.62105000
O 2.03253000 -1.97022000 -2.04632000
O -0.68600000 -4.17731000 -4.17308000
O 0.24092000 -4.24798000 -1.63395000
O -2.65042000 -2.23013000 -3.52838000
O -1.64919000 -2.27041000 -0.94651000
H -2.05469000 -1.51648000 -3.85101000
H -5.23305000 2.14647000 -3.30841000
H -4.72063000 0.71116000 -2.95870000
H 1.87145000 -2.02160000 -3.02885000
H 2.98702000 -1.97439000 -1.92854000
H -0.57980000 -0.86319000 -1.11786000
H 0.89395000 -0.57534000 -1.48099000
H -1.48693000 2.44771000 -3.13315000
H -2.79492000 2.04719000 -3.79664000
H -3.83867000 -0.11972000 -0.00402000
H -4.51480000 -1.29135000 0.78206000
H -0.45536000 -3.75476000 -1.16500000
H 0.98361000 -3.62038000 -1.65192000
H -0.35394000 -4.31120000 -3.24720000
H -0.71661000 -5.04926000 -4.57781000
H -2.05065000 -2.30806000 -1.84323000
H -2.39836000 -2.00387000 -0.38176000
H -1.11956000 0.55524000 -4.31076000
H -0.43534000 -0.23356000 -3.19947000
H -0.51946000 2.98218000 -0.70380000
H -0.55921000 1.49664000 -1.16483000
H -4.36550000 -1.46690000 -3.17590000
H -4.87978000 -1.09973000 -1.78482000
H -2.74807000 1.83728000 -0.35272000
H -4.07862000 1.72875000 -1.08581000
H 0.73511000 -1.38316000 -4.70971000
H 0.76017000 -2.90762000 -4.66317000
H -2.25881000 -3.03891000 -3.90176000

(8). water cluster (n=18)

O 2.82511000 -1.48286000 -4.54411000
O 2.52806000 1.00585000 -3.68371000
O 1.17426000 -2.56506000 -2.59562000
O 0.99138000 0.05148000 -1.55823000
O -1.34247000 -3.09696000 -1.74673000
O -1.63649000 -0.27719000 -0.80703000
O -0.50211000 -3.79371000 0.82982000
O -0.91234000 -1.23510000 1.76939000
O -1.34634000 -4.81943000 3.31204000
O -1.57683000 -2.34042000 4.26476000
O 1.49811000 -5.00530000 3.84583000
O 1.20233000 -2.61867000 5.06171000
O 2.21868000 -3.84032000 1.36480000
O 1.78388000 -1.33636000 2.59743000
O 3.40315000 -2.77042000 -0.95133000
O 3.01364000 -0.27798000 0.28774000
O 5.17440000 -1.54870000 -2.81267000
O 4.66850000 0.87158000 -1.71745000
H -1.58583000 -3.28885000 3.96129000
H 1.59891000 -2.33095000 -3.44405000
H 1.92617000 -2.79861000 -2.00924000
H 2.32916000 -0.70769000 2.09550000
H 2.01264000 -2.19545000 2.18575000
H 1.81757000 0.88264000 -3.02520000
H 3.30610000 1.18021000 -3.12598000
H 4.96476000 0.01072000 -2.11104000
H 5.44779000 1.43389000 -1.67858000
H -1.54312000 -0.45924000 0.14418000
H -1.76174000 -1.15585000 -1.19767000
H -1.88595000 -3.58458000 -2.37247000
H -0.46426000 -2.97772000 -2.17336000
H 3.32168000 -1.91728000 -0.47252000
H 3.27011000 -3.42400000 -0.24404000
H -0.84669000 -3.80351000 -0.08135000
H -0.68224000 -2.87362000 1.12623000
H 1.57256000 -2.01074000 4.39784000
H 0.24536000 -2.45045000 5.00879000
H 0.05287000 0.13635000 -1.27703000

H 1.02057000 -0.85367000 -1.92348000
H 4.53848000 -1.60416000 -3.54648000
H 4.80507000 -2.15934000 -2.15142000
H 2.81330000 -1.54094000 -5.50403000
H 2.70248000 -0.51734000 -4.31822000
H 0.02053000 -1.09073000 2.02896000
H -1.35631000 -1.43049000 2.61575000
H -0.45367000 -5.09834000 3.58061000
H -1.23971000 -4.64101000 2.35969000
H 1.45136000 -4.16044000 4.36802000
H 1.93329000 -5.64881000 4.41289000
H 1.29146000 -3.90577000 1.05238000
H 2.23146000 -4.41873000 2.14784000
H 3.70740000 0.26252000 -0.12883000
H 2.22014000 -0.07334000 -0.25418000
H -2.34204000 -2.22987000 4.83679000

(9). erucic acid

C -1.91258000 3.13970300 0.40975500
C -0.51891700 3.13282500 0.98271300
C 0.49828700 2.66915000 -0.03809500
C 1.89167400 2.62246900 0.55131900
C 2.91289000 2.21615800 -0.48951200
C 4.27996800 2.01185400 0.12759400
C 5.32583700 1.73476400 -0.93235300
C 6.59891200 1.15949100 -0.33970200
C 6.40721500 -0.19954800 0.22710300
C 5.91783000 -1.22976200 -0.46932600
C 5.67700200 -2.57808900 0.10085200
C 4.31410100 -2.67788900 0.76284400
C 3.19317100 -2.25670700 -0.16299300
C 1.84248700 -2.39369100 0.50682100
C 0.75330700 -1.74774500 -0.32278400
C -0.60495100 -1.91741500 0.32326800
C -1.67218500 -1.16111600 -0.43846400
C -3.03679500 -1.35792600 0.18619300
C -4.09219500 -0.55297200 -0.54177100
C -5.45747800 -0.75902500 0.07796700
C -6.50305300 0.06801800 -0.63996000
C -7.87313500 -0.22413100 -0.12068900
O -8.34941800 -1.28023300 0.30443500
O -8.71090500 0.85285700 -0.14707900
H -9.58600400 0.59490400 0.18566200
H -1.97312100 3.82227400 -0.47219200
H 1.91303900 1.89385100 1.40436900
H 4.23774800 1.14898400 0.84504800
H 6.69438700 -0.31862900 1.28461500
H 6.97718700 1.85087400 0.45978000
H 5.74953400 -3.34483500 -0.71641100
H 5.63727200 -1.11376800 -1.52970600
H 3.21726800 -2.87925000 -1.09545100
H 0.74157500 -2.20075600 -1.34887800
H -1.69233300 -1.50901900 -1.50478100
H -1.41880500 -0.06683800 -0.45171500
H -0.25102000 4.16374100 1.33567500
H -0.48321500 2.45808600 1.87867200
H -2.20771000 2.11334900 0.07881500
H -2.64623400 3.48758600 1.17633300
H 7.38607400 1.11800600 -1.14126600
H 4.57191000 2.91989700 0.71723300
H 2.15979600 3.62838000 0.96914900
H 6.46559200 -2.82667200 0.86109400
H 3.35107600 -1.18806700 -0.47342400
H 0.97688400 -0.65371500 -0.44665500
H 4.91161100 1.01672500 -1.68921900
H 5.56939300 2.68591400 -1.47472300
H 2.58343600 1.26300900 -0.98425300
H 2.97031300 3.00209300 -1.28762300
H 0.21545400 1.64830900 -0.41164900
H 0.48544800 3.36018400 -0.92168600
H 4.14850000 -3.73518100 1.09890600
H 4.30122000 -2.02910000 1.67846100
H 1.60674900 -3.47891500 0.66382400
H 1.87339700 -1.91255600 1.52022600
H -0.86934300 -3.00687800 0.36335700
H -0.56740700 -1.54744200 1.38195600
H -3.30926600 -2.44596900 0.16215400
H -3.00561400 -1.04851100 1.26427900
H -4.11779800 -0.85592400 -1.62179400
H -3.82225800 0.53632200 -0.50885500
H -5.74218600 -1.84394700 0.03138300
H -5.42963200 -0.47128200 1.16186300
H -6.28636200 1.16335000 -0.52789600
H -6.50231000 -0.17007400 -1.73819900

(10). 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

(11). polyacetylene (n=12)

C -14.19245200 -0.26950400 0.00000000
C -13.04531800 0.37245400 0.00000000
C -11.71907000 -0.29298600 0.00000000
C -10.56608700 0.35744000 0.00000000
C -9.24316200 -0.30298100 0.00000000
C -8.08944800 0.34911300 0.00000000
C -6.76713300 -0.31021900 0.00000000
C -5.61324100 0.34224700 0.00000000
C -4.29106800 -0.31677800 0.00000000
C -3.13713600 0.33579900 0.00000000
C -1.81499600 -0.32313300 0.00000000
C -0.66105700 0.32947600 0.00000000
C 0.66107600 -0.32943600 0.00000000
C 1.81501400 0.32317100 -0.00000100
C 3.13715000 -0.33576700 0.00000000
C 4.29108100 0.31680500 -0.00000100
C 5.61324700 -0.34223000 -0.00000100
C 6.76713900 0.31022900 -0.00000100
C 8.08944400 -0.34911500 -0.00000100
C 9.24315800 0.30297000 0.00000000
C 10.56607400 -0.35746400 0.00000000
C 11.71905700 0.29295400 0.00000100
C 13.04529800 -0.37249600 0.00000100
C 14.19243100 0.26945600 0.00000100
H 14.24464900 1.34983200 0.00000200
H 9.25064700 1.38704500 0.00000000
H 4.29767600 1.40089800 -0.00000100
H -8.08248800 1.43321700 0.00000000
H -15.14028800 0.25072600 0.00000000
H -14.24466500 -1.34987900 0.00000000
H -13.02862100 1.45677800 0.00000000
H -11.72981000 -1.37702900 0.00000000
H -10.55788500 1.44158900 0.00000000
H -9.25064200 -1.38705400 0.00000000
H -6.77392400 -1.39430600 0.00000000
H -5.60660400 1.42634500 0.00000000
H -4.29765700 -1.40087000 0.00000000
H -3.13059500 1.41989500 0.00000000
H -1.82152300 -1.40722700 0.00000000
H -0.65454100 1.41357100 -0.00000100
H 0.65455900 -1.41353100 0.00000000
H 1.82154300 1.40726600 -0.00000100
H 3.13060600 -1.41986300 0.00000000
H 5.60660400 -1.42632900 0.00000000
H 6.77393600 1.39431800 -0.00000100
H 8.08247500 -1.43322100 -0.00000100
H 10.55786300 -1.44161400 0.00000000
H 11.72980500 1.37699800 0.00000100
H 13.02859600 -1.45682000 0.00000100
H 15.14026400 -0.25077900 0.00000200

(12). trans-retinal

C 2.02085300 -0.51398100 -0.49779800
C 0.83496400 -0.01742900 -0.19858600
C -0.48762900 -0.64962800 -0.49146600
C -1.59251000 -0.01872500 -0.10245400
C -2.99601000 -0.45043000 -0.28029500
C -4.02256800 0.26617900 0.15237700
C -5.46660900 -0.08959700 0.01778200
C -6.37457800 0.74597000 0.51039300
C -7.86927500 0.59133000 0.48750100
O -8.62740900 1.42103000 0.97069200
C 3.33866500 0.13441400 -0.16126500
C 3.65873500 1.35400500 -0.56313200
C 4.29845400 -0.76832100 0.66164300
C 4.98445000 2.03745200 -0.20893700
C 5.43602700 0.07640100 1.30011800
C 6.05948300 1.06064000 0.29848600
C 2.74902300 2.24334100 -1.41057200
C 3.52495900 -1.46877300 1.81332400
C 4.90586400 -1.86279100 -0.26250800
C -0.47222100 -1.98884200 -1.22307600
C -5.79413300 -1.40536700 -0.68575500
H 2.08988200 -1.48005300 -0.98298500
H 0.77353400 0.93454300 0.31427800
H -1.48113600 0.92903500 0.41011300
H -3.16724000 -1.39031000 -0.78523000
H -3.83313300 1.20607800 0.65684500
H -6.04163300 1.65652200 0.99291300
H -8.26179500 -0.31851900 0.00791600
H 4.79001700 2.79139100 0.55508400
H 5.03001200 0.64025300 2.13709100
H 6.86603300 1.61515600 0.77324900
H 1.91980700 1.69120900 -1.83500800
H 2.34602000 3.05874200 -0.81302000
H 3.31783900 2.68704800 -2.22349300
H 3.03333400 -0.73668100 2.44644800
H 2.77105300 -2.14645900 1.42747500
H 4.21309600 -2.04238500 2.42695100
H 5.35507800 2.57081000 -1.08232100
H 6.48906400 0.51791100 -0.53928200
H 6.19747200 -0.59061100 1.69772500
H 5.59757200 -2.48446200 0.29790500
H 4.12907700 -2.50450100 -0.66433200
H 5.44183800 -1.42129100 -1.09588900
H 0.06263300 -2.73421300 -0.63950500
H -1.47209300 -2.36017700 -1.40745000
H 0.03436100 -1.89232200 -2.18015500
H -5.40018400 -1.39783200 -1.69885600
H -5.33684400 -2.23791600 -0.15719500
H -6.86004600 -1.58430200 -0.73947000

(13). PPV-planar (n=4)

C 1.27668700 -11.44064000 0.00000000
C 1.09080000 -10.06958300 0.00000000
C -0.19467800 -9.52193200 0.00000000
C -1.28252000 -10.39759600 0.00000000
C -1.09682500 -11.76975800 0.00000000
C 0.18481800 -12.29691400 0.00000000
C -0.45675500 -8.05175600 0.00000000

C 0.45209300 -7.09126100 0.00000000
C 0.18835100 -5.62302000 0.00000000
C 1.27268200 -4.74138800 0.00000000
C -1.09476600 -5.07167300 0.00000000
C 1.08982100 -3.37243700 0.00000000
C -1.27767400 -3.70272400 0.00000000
C -0.19332900 -2.82105800 0.00000000
C -0.45692500 -1.35313500 0.00000000
C 0.45204600 -0.39213200 0.00000000
C 0.18840900 1.07577100 0.00000000
C 1.27277200 1.95747600 0.00000000
C -1.09476600 1.62712800 0.00000000
C 1.08985900 3.32638500 0.00000000
C -1.27767400 2.99605900 0.00000000
C -0.19333000 3.87773100 0.00000000
C -0.45695500 5.34570300 0.00000000
C 0.45198000 6.30661900 0.00000000
C 0.18839300 7.77490400 0.00000000
C 1.27322900 8.65598700 0.00000000
C -1.09472600 8.32571100 0.00000000
C 1.08956800 10.02507100 0.00000000
C -1.27789300 9.69523600 0.00000000
C -0.19336100 10.57428600 0.00000000
C -0.44884500 12.04808400 0.00000000
C 0.45218300 13.00395000 0.00000000
H 1.51558500 12.81282900 0.00000000
H 1.50362900 6.05011600 0.00000000
H 1.50369100 -0.64864300 0.00000000
H 2.28073900 -11.84558100 0.00000000
H 1.95597600 -9.42133600 0.00000000
H -2.28678600 -9.99355200 0.00000000
H -1.95532900 -12.42929300 0.00000000
H 0.33396400 -13.36903200 0.00000000
H -1.50827300 -7.79468900 0.00000000
H 1.50380600 -7.34728000 0.00000000
H 2.27835000 -5.14203500 0.00000000
H -1.96289500 -5.71601800 0.00000000
H 1.95795200 -2.72808400 0.00000000
H -2.28335100 -3.30208300 0.00000000
H -1.50857100 -1.09659800 0.00000000
H 2.27844300 1.55682700 0.00000000
H -1.96287700 0.98275400 0.00000000
H 1.95795700 3.97077900 0.00000000
H -2.28335000 3.39669800 0.00000000
H -1.50861000 5.60217300 0.00000000
H 2.27876900 8.25503300 0.00000000
H -1.96264300 7.68109500 0.00000000
H 1.95592000 10.67212500 0.00000000
H -2.28343100 10.09636600 0.00000000
H -1.49947000 12.31664000 0.00000000
H 0.16479000 14.04624000 0.00000000

(14) PPP-titled (n=6)

C -12.20669400 -0.00016600 0.00006600
C -11.50891300 1.12952600 0.39858200
C -10.12397100 1.13004700 0.39662600
C -9.40890100 -0.00011300 0.00001300
C -10.12394600 -1.13030100 -0.39656300
C -11.50889000 -1.12983100 -0.39846900
C -7.90245400 -0.00007100 -0.00002600
C -7.18310700 1.13271700 -0.37938300
C -7.18300600 -1.13279400 0.37932700
C -5.80011700 1.13279400 -0.37944600
C -5.80001300 -1.13275900 0.37935700
C -5.08041600 0.00004000 -0.00006300
C -3.57505300 0.00011000 -0.00004900
C -2.85536900 1.13314200 0.37859000
C -2.85526200 -1.13288400 -0.37867700
C -1.47243900 1.13319200 0.37861400
C -1.47235200 -1.13283800 -0.37866600
C -0.75266100 0.00022100 -0.00005100
C 0.75266900 0.00021700 0.00000400
C 1.47235400 -1.13281400 0.37870500
C 1.47245300 1.13316100 -0.37873000
C 2.85526500 -1.13286600 0.37872100
C 2.85538200 1.13310700 -0.37869700
C 3.57506600 0.00009700 0.00001200
C 5.08043400 0.00003800 0.00003700
C 5.80005600 -1.13270300 -0.37954700
C 5.80011900 1.13274400 0.37958900
C 7.18304700 -1.13272700 -0.37947600
C 7.18311300 1.13269200 0.37951200
C 7.90246200 -0.00004000 0.00002900
C 9.40888700 -0.00009000 0.00001200
C 10.12388700 -1.13027300 0.39666800
C 10.12396800 1.13003400 -0.39664800
C 11.50882800 -1.12982200 0.39862100
C 11.50891400 1.12947600 -0.39861500
C 12.20666300 -0.00019800 0.00000000
H 13.28908500 -0.00024200 -0.00000500
H -13.28911500 -0.00018400 0.00008300
H -12.04606700 2.01456300 0.71529900
H -9.59139700 2.01478600 0.71918400
H -9.59135600 -2.01502700 -0.71913100
H -12.04602100 -2.01489000 -0.71516700
H -7.71166100 2.02269400 -0.69422800
H -7.71147600 -2.02281300 0.69419400
H -5.27190000 2.02283400 -0.69457500
H -5.27171700 -2.02274700 0.69450600
H -3.38362700 2.02334500 0.69318400
H -3.38345600 -2.02313100 -0.69325400
H -0.94426300 2.02343000 0.69324100
H -0.94407900 -2.02305200 -0.69321400
H 0.94407700 -2.02300300 0.69331700
H 0.94428200 2.02338200 -0.69341400
H 3.38344100 -2.02308900 0.69338600
H 3.38363900 2.02329100 -0.69334800
H 5.27178200 -2.02263500 -0.69487900
H 5.27189400 2.02271900 0.69488500
H 7.71155300 -2.02267500 -0.69449400
H 7.71166400 2.02262200 0.69450400
H 9.59125200 -2.01494200 0.71932600
H 9.59140400 2.01475100 -0.71929200
H 12.04594200 -2.01485200 0.71543100
H 12.04609100 2.01446700 -0.71542600