Supporting Information
A fragment energy assembler for Hartree-Fock calculations of large molecules

Wei Li, Tao Fang, and Shuhua Li*
Department of Chemistry, Institute of Theoretical and Computational Chemistry,
Key Laboratory of Mesoscopic Chemistry of MOE,
Nanjing University, Nanjing, 210093, People's Republic of China
(Dated: Submitted to J. Chem. Phys. on December 17, 2005)

Cartesian coordinates of all compounds

(1). Dotriacontane

C 19.80586600 0.37882300 0.00017800
C 18.53160000 -0.46501800 -0.00011500
C 17.25509000 0.37808100 0.00016400
C 15.97500600 -0.45943400 -0.00012700
C 14.69899600 0.38454900 0.00015300
C 13.41887800 -0.45317600 -0.00013700
C 12.14286100 0.39079000 0.00014300
C 10.86272100 -0.44691200 -0.00014600
C 9.58669200 0.39704000 0.00013500
C 8.30654600 -0.44065400 -0.00015300
C 7.03051200 0.40329200 0.00012900
C 5.75036300 -0.43439800 -0.00015600
C 4.47432900 0.40954600 0.00012600
C 3.19418000 -0.42814300 -0.00015600
C 1.91814500 0.41580000 0.00012400
C 0.63800000 -0.42189500 -0.00014900
C -0.63803800 0.42203700 0.00011000
C -1.91817800 -0.41565800 -0.00006500
C -3.19421800 0.42826100 -0.00005900
C -4.47435300 -0.40944400 -0.00006300
C -5.75039300 0.43447700 -0.00004400
C -7.03052500 -0.40323000 0.00003000
C -8.30656200 0.44069200 -0.00019000
C -9.58668900 -0.39702200 0.00005300
C -10.86272300 0.44690500 -0.00015400
C -12.14284400 -0.39081400 0.00016800
C -13.41886700 0.45312400 -0.00028000
C -14.69896800 -0.38462100 0.00021100
C -15.97498600 0.45933400 -0.00022400
C -17.25505300 -0.37819800 0.00034900
C -18.53157200 0.46487100 -0.00034700
C -19.80582200 -0.37898600 0.00041900
H -19.85239900 -1.01792500 0.87788100
H -14.70057400 -1.03792600 0.87119700
H -4.47593600 -1.06326600 0.87054800
H 0.63640300 -1.07597300 0.87026800
H 20.69309000 -0.24698600 -0.00003000
H 19.85249000 1.01879300 -0.87652800
H 19.85248100 1.01819700 0.87731800
H 18.53164300 -1.11765200 -0.87065100
H 18.53163400 -1.11824300 0.86997700
H 17.25772600 1.03171700 0.87105100
H 17.25773500 1.03230800 -0.87027900
H 15.97347900 -1.11291600 -0.87100400
H 15.97347000 -1.11350700 0.87030700
H 14.70064100 1.03862000 -0.87025400
H 14.70063200 1.03803000 0.87100400
H 13.41729500 -1.10667000 -0.87098800
H 13.41728700 -1.10726000 0.87027000
H 12.14446500 1.04428900 0.87099000
H 12.14447200 1.04487800 -0.87026200
H 10.86112900 -1.10041400 -0.87099200
H 10.86112200 -1.10100300 0.87025800
H 9.58829800 1.05113200 -0.87026900
H 9.58829200 1.05054400 0.87098000
H 8.30495100 -1.09416000 -0.87099800
H 8.30494500 -1.09474800 0.87025000
H 7.03211200 1.05679900 0.87097300
H 7.03211600 1.05738600 -0.87027400
H 5.74876600 -1.08790600 -0.87100100
H 5.74876200 -1.08849300 0.87024600
H 4.47593000 1.06364000 -0.87027800
H 4.47592900 1.06305600 0.87096800
H 3.19258100 -1.08165400 -0.87099700
H 3.19257900 -1.08223500 0.87025000
H 1.91974400 1.06931600 0.87096200
H 1.91974200 1.06988700 -0.87028600
H 0.63641000 -1.07542200 -0.87097900
H -0.63646500 1.07607600 -0.87033800
H -0.63641700 1.07561500 0.87090400
H -1.91971300 -1.06937400 -0.87075500
H -1.91982100 -1.06955800 0.87048700
H -3.19263400 1.08207200 0.87056000
H -3.19263400 1.08206900 -0.87068100
H -4.47594800 -1.06323800 -0.87069600
H -5.74883300 1.08826300 -0.87068200
H -5.74877600 1.08830600 0.87056200
H -7.03206600 -1.05719000 -0.87047600
H -7.03215800 -1.05688300 0.87076800
H -8.30497300 1.09474700 0.87024600
H -8.30498800 1.09425200 -0.87099700
H -9.58829300 -1.05105900 -0.87039600
H -9.58826600 -1.05059600 0.87085000
H -10.86117400 1.10044200 -0.87097800
H -10.86110200 1.10097700 0.87026800
H -12.14439800 -1.04501500 -0.87015600
H -12.14447500 -1.04421500 0.87109200
H -13.41728200 1.10741500 0.86997600
H -13.41731200 1.10642900 -0.87127600

*Electronic mail: shuhua@nju.edu.cn

H -14.70061600 -1.03888100 -0.87005700
H -15.97351100 1.11260400 -0.87126400
H -15.97342100 1.11363500 0.87004200
H -17.25764200 -1.03279500 -0.86981900
H -17.25771600 -1.03147700 0.87150700
H -18.53160100 1.11857200 0.86939100
H -18.53164600 1.11704600 -0.87123100
H -20.69305600 0.24681000 -0.00006500
H -19.85248100 -1.01939700 -0.87596500

(2). $(gly)_{12}$

O -21.48423200 -0.39590700 -0.02070500
O -20.27593600 1.49755200 -0.02613300
C -20.33052200 0.28679300 -0.02129900
C -19.14602500 -0.62518900 -0.01532200
N -17.94085400 0.17048000 -0.01628400
C -16.72651600 -0.40166000 -0.01162200
O -16.57287500 -1.62359600 -0.00630200
C -15.54510100 0.54042600 -0.01323600
N -14.33374600 -0.24312300 -0.00778200
C -13.12379000 0.33133000 -0.00789100
O -12.97013900 1.55498700 -0.01259800
C -11.93924500 -0.60769900 -0.00187100
N -10.73050200 0.18054100 -0.00299000
C -9.51767900 -0.38626600 0.00143200
O -9.35451500 -1.60891000 0.00673200
C -8.33903100 0.56070600 -0.00042900
N -7.12535900 -0.22005400 0.00465200
C -5.91583800 0.35308400 0.00417000
O -5.75845800 1.57663600 -0.00057000
C -4.73219400 -0.58781200 0.00981100
N -3.52268400 0.19947000 0.00817500
C -2.30997700 -0.36665800 0.01207600
O -2.14525200 -1.58927000 0.01734100
C -1.13181100 0.58118400 0.00966200
N 0.08227200 -0.19900500 0.01408300
C 1.29172000 0.37403300 0.01296300
O 1.44948000 1.59759900 0.00819700
C 2.47520000 -0.56714800 0.01791700
N 3.68494200 0.21969900 0.01549400
C 4.89758000 -0.34680500 0.01867300
O 5.06175500 -1.56948400 0.02395600
C 6.07580000 0.60089300 0.01543400
N 7.29006900 -0.17875800 0.01886700
C 8.49941400 0.39524700 0.01700800
O 8.65543300 1.61900700 0.01247600
C 9.68317400 -0.54532600 0.02081700
N 10.89312300 0.24061500 0.01759900
C 12.10571700 -0.32794000 0.02035700
C 13.28432500 0.61869700 0.01591100
O 12.26612800 -1.55092300 0.02620400
N 14.49942300 -0.15826100 0.01881200
C 15.70838800 0.42063800 0.01766500
C 16.89378000 -0.51660800 0.01733200
O 15.85467400 1.64567000 0.01593600
N 18.10439500 0.26433700 0.02550600
C 19.31861100 -0.31388300 0.02791100
C 20.50543600 0.62104000 0.10454700
O 19.45922200 -1.53758500 0.01129400
N 21.67122000 -0.03320400 -0.42967400
H 22.54867100 0.40091900 -0.26884700
H 3.55861800 1.20817700 0.01117600
H -0.03871600 -1.18817700 0.01791200
H -18.05082000 1.15965700 -0.02056600
H -19.19328000 -1.27304400 -0.88124000
H -19.19657900 -1.26594600 0.85567700
H -15.58844400 1.18699900 0.85541000
H -15.58517200 1.17991700 -0.88726400
H -14.45361600 -1.23225300 -0.00397700
H -11.97747800 -1.25435400 -0.87054200
H -11.98060200 -1.24710800 0.87200700
H -10.85651000 1.16899300 -0.00729000
H -8.38429100 1.20684500 0.86825700
H -8.38144300 1.19990400 -0.87437400
H -7.24628600 -1.20921100 0.00847000
H -4.77140600 -1.23436100 -0.85884500
H -4.77387400 -1.22698500 0.88379900
H -3.64932200 1.18792500 0.00388800
H -1.17701300 1.22721200 0.87841500
H -1.17504300 1.22036600 -0.86423700
H -22.27005700 0.14640500 -0.02442300
H 2.43522400 -1.21375500 -0.85066500
H 2.43383100 -1.20628800 0.89194700
H 6.03104200 1.24692900 0.88423200
H 6.03169100 1.24024200 -0.85832600
H 7.16993900 -1.16798000 0.02254600
H 9.64216800 -1.19199100 -0.84774400
H 9.64219900 -1.18487100 0.89463300
H 13.23914700 1.26551500 0.88425100
H 13.23846100 1.25823600 -0.85779200
H 14.38399400 -1.14774400 0.02038000
H 10.76857200 1.22916500 0.01284600
H 16.85398900 -1.15647600 -0.85681000
H 16.84780600 -1.16589800 0.88410800
H 17.98876700 1.25234000 0.00676800
H 20.60584200 0.90876400 1.15335200
H 20.28838600 1.52603700 -0.45063200
H 21.66473400 -1.02594800 -0.37041700

(3). 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

(4). 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

(5). β-strand acetyl(ala)$_{18}$NH$_2$

Structure from:
R. Wieczorek, J. J. Dannenberg,
J. Am. Chem. Soc. **126**, 14198 (2004).
C -29.093450 -0.473930 0.203276
O -29.282421 -1.483994 0.888797

N -27.871738 -0.075276 -0.221177
H -27.736574 0.754966 -0.793940
C -26.632130 -0.766803 0.135358
C -25.478366 0.181336 -0.288044
O -25.694628 1.183273 -0.977838
N -24.251696 -0.178841 0.150540
H -24.095515 -1.006859 0.722114
C -23.027025 0.546425 -0.193102
C -21.855454 -0.371093 0.250473
O -22.060120 -1.380740 0.933129
N -20.631318 0.022223 -0.163216
H -20.484977 0.856729 -0.728371
C -19.394351 -0.673328 0.198688
C -18.239759 0.273815 -0.227833
O -18.461934 1.282166 -0.906982
N -17.011602 -0.093231 0.196651
H -16.851356 -0.929262 0.756002
C -15.786063 0.629964 -0.150182
C -14.616891 -0.297976 0.279539
O -14.826598 -1.316794 0.947162
N -13.392053 0.096180 -0.129121
H -13.241686 0.940197 -0.679247
C -12.156960 -0.609310 0.220740
C -11.000362 0.341504 -0.192903
O -11.222745 1.363968 -0.850751
N -9.771962 -0.038191 0.218378
H -9.611520 -0.887501 0.757520
C -8.544852 0.686792 -0.119622
C -7.378221 -0.256036 0.284446
O -7.591107 -1.290474 0.926669
N -6.152817 0.143028 -0.117015
H -5.999464 1.001497 -0.643558
C -4.919812 -0.576050 0.212298
C -3.760541 0.382229 -0.176205
O -3.981057 1.424855 -0.802346
N -2.532570 -0.013982 0.220124
H -2.373286 -0.881093 0.730568
C -1.303652 0.716315 -0.099624
C -0.139654 -0.244216 0.268991
O -0.355184 -1.299459 0.875524
N 1.086365 0.163625 -0.121447
H 1.242431 1.040431 -0.616017
C 2.317205 -0.571043 0.180580
C 3.479313 0.397402 -0.172693
O 3.261583 1.463892 -0.758316
N 4.706440 -0.017454 0.206790
H 4.863901 -0.904664 0.682014
C 5.937176 0.720698 -0.087001
C 7.098658 -0.257551 0.240577
O 6.880875 -1.335488 0.804899
N 8.325367 0.161464 -0.135748
H 8.483717 1.057308 -0.594085
C 9.554150 -0.588503 0.135485
C 10.718979 0.390160 -0.178204
O 10.504533 1.479969 -0.720425
N 11.945018 -0.042929 0.184377
H 12.100060 -0.948759 0.623803
C 13.177430 0.703536 -0.079853
C 14.336780 -0.289452 0.207989
O 14.117384 -1.387946 0.730346
N 15.564302 0.140986 -0.153084
H 15.724130 1.053096 -0.577387
C 16.791145 -0.622015 0.088716
C 17.958629 0.364625 -0.186923
O 17.748350 1.473683 -0.690044
N 19.183310 -0.084151 0.162023
H 19.334934 -1.004415 0.571288
C 20.417036 0.669709 -0.073045
C 21.575052 -0.333355 0.181559
O 21.355815 -1.447814 0.668480
N 22.803464 0.107234 -0.165942
H 22.963269 1.031064 -0.563533
C 24.028039 -0.666322 0.051518
C 25.198838 0.324630 -0.189336
O 24.996008 1.447638 -0.662472
N 26.421654 -0.137162 0.153242
H 26.566705 -1.066408 0.542898
C 27.655456 0.624482 -0.053250
C 28.814467 -0.382127 0.173271
O 28.603103 -1.508089 0.634654
N 30.043492 0.068205 -0.168149
H 30.200016 1.001323 -0.543206
C 31.263444 -0.713164 0.037054
C 32.441574 0.273366 -0.168566
O 32.262127 1.404823 -0.611872
N 33.668684 -0.199113 0.190028
H -26.604212 -0.906611 1.226538
H -22.988107 0.681679 -1.284432
H -19.367908 -0.807641 1.290481
H -15.753340 0.772253 -1.240774
H -12.129501 -0.759930 1.310346
H -8.516875 0.851567 -1.207162
H -4.891944 -0.756333 1.297363
H -1.279370 0.915718 -1.181432
H 2.344742 -0.791368 1.258230
H 5.959550 0.962574 -1.160153
H 9.581161 -0.853050 1.203158
H 13.200099 0.988405 -1.142403
H 16.817254 -0.928087 1.145266
H 20.441874 0.992419 -1.124686
H 24.051461 -1.008111 1.097151
H 27.682931 0.980842 -1.093920
H 31.278795 -1.082527 1.073749
N -31.490995 -0.300802 0.053060
H -30.206248 0.629828 -1.311353
H 33.806712 -1.145614 0.514392
H 34.475823 0.385482 0.017855
C -30.266659 0.444872 -0.228205
C -32.721169 0.111340 -0.384518
O -32.895040 1.135655 -1.049796
H -31.373533 -1.130109 0.628356
C 31.410568 -1.901223 -0.882596
H 30.507593 -2.558762 -0.802732
H 32.305222 -2.502212 -0.589658
H 31.525140 -1.585676 -1.947751
C 27.813779 1.821350 0.851875

H 26.922241 2.492012 0.754734
H 28.721180 2.403832 0.559363
H 27.913652 1.518193 1.922042
C 24.171350 -1.877469 -0.836790
H 23.271230 -2.535237 -0.731338
H 25.071054 -2.467325 -0.535495
H 24.275987 -1.590223 -1.910897
C 20.578856 1.894291 0.793197
H 19.686235 2.560971 0.680165
H 21.484129 2.468052 0.477728
H 20.684953 1.624654 1.871709
C 16.935981 -1.861906 -0.758545
H 16.036644 -2.516899 -0.631416
H 17.836238 -2.440505 -0.437595
H 17.040598 -1.610556 -1.841612
C 13.339215 1.958307 0.741935
H 12.445029 2.618957 0.607920
H 14.242482 2.522263 0.403806
H 13.448854 1.727235 1.829012
C 9.701937 -1.860002 -0.662952
H 8.803682 -2.511252 -0.511296
H 10.602898 -2.424200 -0.319123
H 9.807089 -1.650605 -1.754853
C 6.095735 2.007839 0.683724
H 5.199816 2.660251 0.523513
H 6.997476 2.560171 0.323071
H 6.206109 1.820849 1.779171
C 2.468863 -1.873822 -0.564942
H 1.572206 -2.520686 -0.387256
H 3.371037 -2.421110 -0.197744
H 2.574259 -1.709090 -1.664444
C -1.151290 2.033400 0.620071
H -2.048886 2.675992 0.431979
H -0.250353 2.574016 0.240173
H -1.043200 1.890150 1.722318
C -4.763539 -1.905009 -0.484503
H -5.658095 -2.547866 -0.283216
H -3.859632 -2.435261 -0.097133
H -4.658319 -1.780675 -1.589320
C -8.400862 2.026959 0.558007
H -9.299949 2.659653 0.345105
H -7.500065 2.558454 0.165142
H -8.297551 1.919657 1.664790
C -11.995182 -1.956293 -0.439322
H -12.887341 -2.596847 -0.220774
H -11.089328 -2.472080 -0.037274
H -11.889990 -1.861860 -1.547097
C -15.651307 1.984777 0.499824
H -16.551521 2.609208 0.268104
H -14.750079 2.511262 0.101287
H -15.554436 1.901275 1.609235
C -19.226741 -2.029765 -0.440522
H -20.116436 -2.670390 -0.212342
H -18.318863 -2.535447 -0.030363
H -19.121660 -1.951943 -1.549592
C -22.901769 1.906761 0.447772
H -23.802286 2.526162 0.204012
H -21.999041 2.433102 0.052582
H -22.813743 1.831887 1.558516
C -26.460080 -2.120840 -0.508947
H -27.346348 -2.765727 -0.279604
H -25.548332 -2.623435 -0.103883
H -26.359707 -2.038745 -1.618117
C -30.163485 1.779332 0.471311
H -29.249070 2.320827 0.127272
H -30.111263 1.659556 1.580263
H -31.057329 2.406572 0.223162
C -33.882719 -0.778055 -0.013333
H -33.989501 -0.843553 1.096235
H -33.741020 -1.806057 -0.425677
H -34.818634 -0.343043 -0.441285

(6). α-strand acetyl(ala)$_{18}$NH$_2$

Structure from:
R. Wieczorek, J. J. Dannenberg,
J. Am. Chem. Soc. **126**, 14198 (2004).

C 12.986775 -0.513145 -1.817050
C 11.872019 -1.022137 -0.870323
N 12.245863 -1.382904 0.382467
C 11.246616 -1.866703 1.356357
C 10.191960 -0.785888 1.729086
N 10.624771 0.498574 1.759735
C 9.679294 1.611215 1.986399
C 8.653226 1.748495 0.829014
N 9.157175 1.642868 -0.424112
C 8.267558 1.632587 -1.602117
C 7.230619 0.475296 -1.536779
N 7.714313 -0.735602 -1.176509
C 6.816341 -1.896974 -1.022723
C 5.717655 -1.650734 0.048563
N 6.129811 -1.102658 1.212211
C 5.165228 -0.766350 2.276497
C 4.091300 0.247631 1.793725
N 4.544321 1.299206 1.078053
C 3.611198 2.291338 0.513194
C 2.597140 1.649095 -0.473703
N 3.107379 0.770816 -1.363053
C 2.230596 0.043535 -2.298910
C 1.172216 -0.820527 -1.558588
N 1.624842 -1.547275 -0.514915
C 0.700943 -2.347374 0.308903
C -0.397216 -1.473046 0.976544
N 0.024196 -0.322359 1.542011
C -0.932569 0.627586 2.138150
C -1.979323 1.133105 1.106668
N -1.496255 1.494215 -0.100889
C -2.400888 1.922844 -1.182370
C -3.421602 0.816295 -1.570919
N -2.922622 -0.432786 -1.684053
C -3.798469 -1.581720 -1.974594
C -4.886393 -1.787028 -0.883631
N -4.470480 -1.686514 0.396772
C -5.429724 -1.783173 1.511409
C -6.504214 -0.659593 1.465191
N -6.050917 0.577792 1.169222
C -6.984059 1.709158 1.032360

C -8.021924 1.484861 -0.101713
N -7.539318 0.991607 -1.263838
C -8.450839 0.725883 -2.389807
C -9.455588 -0.425253 -2.098394
N -8.956096 -1.494101 -1.435722
C -9.807413 -2.658919 -1.147287
C -10.879182 -2.405225 -0.048354
N -10.547955 -1.492328 0.907607
C -11.463559 -1.210279 2.020968
C -12.377581 0.032648 1.813946
N -11.948153 0.957776 0.905991
C -12.659790 2.229517 0.723569
C -13.170244 2.481625 -0.721035
N -12.856237 1.548522 -1.656884
O 10.709249 -1.096369 -1.274163
O 9.039728 -1.129909 2.005178
O 7.456816 1.935957 1.066344
O 6.043114 0.687001 -1.801708
O 4.542140 -1.953201 -0.186550
O 2.899190 0.071275 2.072997
O 1.398293 1.950841 -0.418981
O -0.006643 -0.821039 -1.935198
O -1.578094 -1.843868 0.969634
O -3.177380 1.190847 1.411929
O -4.610361 1.103859 -1.760675
O -6.055088 -2.032414 -1.207435
O -7.691624 -0.916707 1.695681
O -9.213470 1.764759 0.074536
O -10.627202 -0.347473 -2.485118
O -11.939157 -3.029889 -0.073596
O -13.420644 0.130058 2.462590
O -13.842501 3.486371 -0.968426
N 14.022998 0.272309 -1.107729
H 12.462408 0.136484 -2.530529
H 13.218640 -1.298313 0.650260
H 10.662636 -2.668969 0.889069
H 11.523417 0.729057 1.347185
H 9.075713 1.378631 2.870332
H 10.153206 1.496189 -0.552973
H 7.659720 2.545612 -1.603669
H 8.717410 -0.866471 -1.062591
H 6.257267 -2.053975 -1.954028
H 7.121667 -0.948641 1.385945
H 4.591541 -1.661618 2.548543
H 5.544934 1.427418 0.933500
H 2.985312 2.703783 1.314911
H 4.113510 0.611477 -1.405565
H 1.637169 0.761264 -2.879827
H 2.620030 -1.557958 -0.292134
H 0.141612 -3.039280 -0.333915
H 1.020280 -0.104197 1.577850
H -1.531003 0.116516 2.903403
H -0.489966 1.496018 -0.270505
H -3.024963 2.755306 -0.832194
H -1.919569 -0.592561 -1.587720
H -4.368663 -1.387048 -2.892107
H -3.479667 -1.560737 0.605390
H -6.005859 -2.712897 1.419564
H -5.050360 0.749756 1.071324
H -7.591553 1.796560 1.942194
H -6.535480 0.861461 -1.389663
H -9.086382 1.605198 -2.553746
H -7.960251 -1.549003 -1.224367
H -10.398438 -2.896867 -2.040642
H -9.584064 -1.171187 0.977839
H -12.163686 -2.051090 2.091711
H -10.983488 0.920131 0.582042
H -13.560595 2.170053 1.346986
H -12.209738 0.783464 -1.499228
H -13.137865 1.740141 -2.608242
C 13.677408 1.443812 -0.476770
O 12.497855 1.748776 -0.258950
H 14.992833 0.151840 -1.379682
C 14.803231 2.330938 -0.024511
H 14.382493 3.177892 0.572337
H 15.532489 1.771091 0.610099
H 15.341228 2.751243 -0.909725
C 13.572173 -1.684662 -2.560403
H 12.744812 -2.246242 -3.063214
H 14.107890 -2.386416 -1.875232
H 14.289029 -1.340379 -3.346253
C 11.877963 -2.388960 2.618854
H 11.068407 -2.730784 3.312266
H 12.545325 -3.258757 2.400861
H 12.477215 -1.602958 3.140442
C 10.387798 2.924287 2.184927
H 9.627845 3.739316 2.279460
H 11.001394 2.903908 3.118817
H 11.061846 3.162307 1.323042
C 9.039000 1.538111 -2.891730
H 8.319234 1.478825 -3.745553
H 9.682022 2.441048 -3.034884
H 9.692572 0.628992 -2.912843
C 7.574489 -3.151106 -0.674201
H 6.849252 -3.990449 -0.533625
H 8.281486 -3.427235 -1.494784
H 8.161661 -3.025341 0.270924
C 5.851142 -0.215845 3.499395
H 5.080569 0.047582 4.265139
H 6.545644 -0.974194 3.938141
H 6.443400 0.702762 3.255808
C 4.338568 3.410425 -0.185415
H 3.591389 4.114608 -0.627322
H 4.978613 3.976039 0.535658
H 4.993645 3.020590 -1.005852
C 3.017486 -0.836009 -3.235336
H 2.309909 -1.395857 -3.895051
H 3.694404 -0.221512 -3.878446
H 3.643076 -1.574103 -2.671189
C 1.429644 -3.123814 1.374609
H 0.686416 -3.680880 1.996311
H 2.133605 -3.860180 0.914629
H 2.018898 -2.444103 2.041975
C -0.233905 1.812915 2.752189
H -0.998219 2.521803 3.155181
H 0.429961 1.488492 3.590950

H 0.393401 2.351626 1.996526
C -1.641009 2.344057 -2.413390
H -2.367264 2.622943 -3.215800
H -0.993482 3.228382 -2.194150
H -0.988115 1.515965 -2.790971
C -3.012143 -2.857782 -2.129786
H -3.718331 -3.704595 -2.311779
H -2.309275 -2.785362 -2.995884
H -2.413068 -3.079872 -1.209656
C -4.739050 -1.745129 2.849936
H -5.507607 -1.782679 3.660499
H -4.053740 -2.620377 2.965952
H -4.136242 -0.808785 2.969184
C -6.258024 3.005786 0.781570
H -7.005680 3.825600 0.648105
H -5.596878 3.261188 1.645862
H -5.623073 2.944059 -0.139128
C -7.702508 0.399875 -3.656817
H -8.437679 0.182575 -4.470232
H -7.064346 1.261503 -3.972048
H -7.042998 -0.494007 -3.521342
C -8.998589 -3.866795 -0.747318
H -9.693745 -4.714102 -0.527537
H -8.308095 -4.171196 -1.571661
H -8.382622 -3.661540 0.163457
C -10.748644 -1.047168 3.339449
H -11.485034 -0.733498 4.119868
H -10.283399 -2.013348 3.653230
H -9.938650 -0.278585 3.276034
C -11.855710 3.436675 1.143184
H -12.424651 4.364177 0.885984
H -11.673566 3.421609 2.245101
H -10.864857 3.465027 0.624227

(7). 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

(8). 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

(9). PPV-helix (n=6)

C -18.07740500 0.12464300 0.13203700
C -16.70811100 0.05414800 -0.06364800
C -15.90056100 1.18011100 0.11495700
C -16.51624300 2.38102300 0.47173200
C -17.88669100 2.45334800 0.66657300
C -18.67342700 1.32344600 0.50063800
C -14.43773800 1.15233400 -0.06511500
C -13.65851900 0.07245300 -0.01841200
C -12.19858100 0.04213900 -0.20683000
C -11.47362700 -1.05675700 0.25901000
C -11.48912900 1.05822800 -0.84896200
C -10.10031300 -1.12921100 0.11764300
C -10.11552100 0.98685000 -0.98839100
C -9.38724100 -0.09892100 -0.49754400
C -7.92472200 -0.11670500 -0.66312000
C -7.06101800 -0.86213800 0.02622100
C -5.59931600 -0.88625200 -0.14541700
C -4.80086400 -1.39566200 0.88092400
C -4.95680600 -0.43655000 -1.30014200
C -3.42292400 -1.43065200 0.77523200
C -3.57874300 -0.46951400 -1.40495100
C -2.77880200 -0.95299000 -0.36730300
C -1.31573800 -0.95324100 -0.52855900
C -0.41359500 -1.03774800 0.44913100
C 1.04936300 -1.04675600 0.28713900
C 1.68428200 -1.36161500 -0.91543600
C 1.85843900 -0.74345300 1.38431400
C 3.06283800 -1.34269600 -1.01712500
C 3.23706300 -0.72666300 1.28319000
C 3.87102200 -1.01202400 0.07277300
C 5.33315800 -0.99585100 -0.09592200
C 6.21266400 -0.38297300 0.69636900
C 7.67542800 -0.37406100 0.53256600
C 8.42777800 0.60812900 1.18035900
C 8.36558200 -1.31571800 -0.23255100
C 9.80281200 0.66821300 1.05067300
C 9.74038900 -1.25432200 -0.36398600
C 10.48981800 -0.25537300 0.26113200
C 11.94999300 -0.23094500 0.07652300
C 12.75551300 0.80931500 0.29003900
C 14.21706500 0.83023100 0.11378400
C 15.00051400 -0.32392100 0.08812900
C 14.86942100 2.05801500 -0.02219000
C 16.36974800 -0.24851200 -0.09348500
C 16.23777600 2.13241400 -0.20272100
C 17.01761500 0.97666100 -0.25352200
C 18.47941100 0.99741400 -0.45271200
C 19.21961400 2.02223500 -0.85633800
H 18.80595100 2.98256500 -1.09798000
H -18.68007300 -0.75160000 -0.01245600
H -16.27045800 -0.87402100 -0.37522100
H -15.91502900 3.26113500 0.60446100
H -18.33680100 3.38669600 0.94576500
H -19.73484900 1.37636200 0.64800900
H -13.98685800 2.11700300 -0.21673500
H -14.10098400 -0.88186300 0.20611900
H -11.99490900 -1.86545600 0.73642200
H -12.01079600 1.90034600 -1.25960300
H -9.58629200 -2.00129000 0.47145800
H -9.59715500 1.78413300 -1.48769800
H -7.54957800 0.57177400 -1.39941300
H -7.42966000 -1.49746200 0.81191200
H -5.26791700 -1.77090200 1.77238700
H -5.53305500 -0.07653900 -2.12973800
H -2.85010800 -1.84967400 1.57910500
H -3.11301600 -0.11690200 -2.30629500
H -0.97766200 -0.84367000 -1.54372000
H -0.75080300 -1.07467300 1.46980400
H 1.10335800 -1.64162100 -1.77218900
H 1.39939900 -0.51996100 2.32929300
H 3.52265400 -1.59006800 -1.95575700
H 3.82000900 -0.50891100 2.15649500
H 5.68838600 -1.51368500 -0.96913900
H 5.85229800 0.19500900 1.52878800
H 7.92709600 1.33258900 1.79528000
H 7.83221000 -2.11229100 -0.71306100
H 10.34282300 1.42663800 1.58272900

H 10.24361600 -1.99340600 -0.95910700
H 12.36938100 -1.14889000 -0.29545700
H 12.32771400 1.74867300 0.59242000
H 14.54628800 -1.28488900 0.23008000
H 14.29458100 2.96464600 0.01270800
H 16.94736400 -1.15399900 -0.10653700
H 16.69932800 3.09618000 -0.29171000
H 18.97149000 0.06091700 -0.25347600
H 20.28202700 1.92636200 -0.96818000

(10). *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

(11) β**-carotene**

C -10.40616800 0.63310800 -0.42626900
C -9.13845800 0.24841300 -0.27887400
C -7.94048500 1.06346100 -0.53415500
C -6.73625500 0.50891900 -0.31794700
C -5.42394300 1.10983200 -0.49690500
C -4.28587000 0.45073200 -0.24606000
C -2.92390800 0.96928300 -0.39577000
C -1.89484500 0.15716000 -0.09434600
C -0.47401300 0.44497800 -0.16339200
C 0.47400100 -0.44502700 0.16314500
C 1.89483300 -0.15720300 0.09411700
C 2.92389500 -0.96930000 0.39561600
C 4.28585600 -0.45075700 0.24588300
C 5.42392800 -1.10984200 0.49677000
C 6.73624100 -0.50893300 0.31780300
C 7.94047000 -1.06345900 0.53405400
C 9.13844200 -0.24841100 0.27876600
C 10.40614900 -0.63302800 0.42639000
C -11.60235600 -0.20110700 -0.13715100
C -11.82653800 -1.38274500 -0.72742800
C -12.58637400 0.43050900 0.87337100
C -13.04206800 -2.23925800 -0.42332000
C -13.58658900 -0.62318200 1.39489500
C -14.16704000 -1.48737300 0.28179600
C 11.60233800 0.20116600 0.13723100
C 12.58647600 -0.43063500 -0.87305600
C 11.82643800 1.38292500 0.72730100
C 13.58674500 0.62296400 -1.39467100
C 13.04199300 2.23939300 0.42316100
C 14.16705600 1.48738600 -0.28167800
C -10.91991300 -2.01466400 -1.75962100
C -11.82433700 0.98831000 2.09485900
C -13.35272100 1.59350700 0.20046000
C 11.82457900 -0.98867800 -2.09452200
C 13.35274100 -1.59350100 -0.19982600
C 10.91970100 2.01503200 1.75928200
C -8.14611400 2.47513700 -1.02391800
C -2.76524000 2.38885600 -0.88118700
C 2.76522500 -2.38884600 0.88111400
C 8.14609800 -2.47510400 1.02390500
H 8.70380200 -2.48017600 1.95484900
H -10.61202800 1.64271600 -0.73517100
H -8.94432800 -0.75123600 0.06903600
H -6.71902100 -0.50937900 0.03302200
H -5.37951400 2.12288800 -0.84435300
H -4.35292900 -0.56616400 0.10267300
H -2.13538100 -0.83719500 0.24300500
H -0.16657100 1.42018500 -0.49270200
H 0.16656000 -1.42022900 0.49246900
H 2.13537100 0.83712800 -0.24330300
H 4.35291700 0.56612200 -0.10289900
H 5.37949900 -2.12287800 0.84427800
H 6.71900700 0.50935200 -0.03320800
H 8.94431500 0.75116500 -0.06935400

H 10.61201200 -1.64257700 0.73548300
H -12.72456100 -3.08333600 0.18916800
H -13.07584800 -1.26820000 2.10603500
H -14.88863500 -2.19022300 0.68672900
H 13.07608200 1.26783500 -2.10600100
H 12.72454100 3.08334200 -0.18953200
H 14.88868500 2.19016600 -0.68666900
H -10.14705800 -1.34960100 -2.10834600
H -10.44019200 -2.90468700 -1.35826200
H -11.50370200 -2.33456500 -2.61770900
H -11.21110000 0.22012100 2.55221200
H -11.17739000 1.81420500 1.82835600
H -12.53097600 1.34485300 2.83788300
H -13.40926800 -2.67007000 -1.35046900
H -14.70273500 -0.87172700 -0.43326900
H -14.37617500 -0.11745400 1.94311800
H 14.37640100 0.11713600 -1.94270000
H 14.70268000 0.87189100 0.43357000
H 13.40908500 2.67039900 1.35026300
H -14.03964300 2.04799000 0.90765800
H -12.67707800 2.36962500 -0.13970700
H -13.92186000 1.25377900 -0.65554400
H 11.17755700 -1.81448300 -1.82792200
H 11.21143900 -0.22056500 -2.55213400
H 12.53130200 -1.34542200 -2.83737000
H 14.03971300 -2.04815100 -0.90687000
H 13.92181600 -1.25360000 0.65615200
H 12.67705300 -2.36953100 0.14045300
H 10.43997400 2.90494800 1.35769100
H 10.14684800 1.35001600 2.10809400
H 11.50340900 2.33514400 2.61734600
H -8.71651800 3.05202500 -0.30268000
H -7.21702000 2.99552700 -1.19618400
H -8.70380900 2.48026500 -1.95486700
H -3.22076300 2.51242400 -1.85849900
H -3.25533500 3.08177300 -0.20474200
H -1.73205100 2.68754400 -0.96242200
H 1.73203600 -2.68753500 0.96234600
H 3.25533600 -3.08180000 0.20471900
H 3.22073000 -2.51235300 1.85844200
H 7.21700400 -2.99548200 1.19621000
H 8.71649400 -3.05204100 0.30269800

(12) 1,3,5-tris((*E*)-3,5-bis((*E*)-3,5-divinylstyryl)styryl)benzene

C 1.12192900 0.13538000 0.00000000
C 0.93177900 -1.24663400 0.00000000
C -0.33722200 -1.81661800 0.00000000
C -1.43803200 -0.96229600 0.00000000
C -1.28781400 0.42217300 0.00000000
C 0.00000000 0.95777500 0.00000000
C -0.44595600 -3.28742400 0.00000000
C -1.56482100 -4.00898500 0.00000000
C 2.50665200 0.64441000 0.00000000
C 2.89788200 1.91698600 0.00000000
C -2.50942300 1.25028800 0.00000000
C -2.58241400 2.57955100 0.00000000
C -1.67546600 -5.48031900 0.00000000
C -2.95163600 -6.04374800 0.00000000
C -0.57583700 -6.33218500 0.00000000
C -3.14942600 -7.42096000 0.00000000
C -0.73533700 -7.71763900 0.00000000
C -2.02468000 -8.24362700 0.00000000
C -3.80755700 3.40297300 0.00000000
C -3.66630000 4.78839900 0.00000000
C -5.09187700 2.85914900 0.00000000
C -4.77341300 5.63493600 0.00000000
C -6.21951800 3.67341100 0.00000000
C -6.03867300 5.05650000 0.00000000
C 4.28563500 2.41698400 0.00000000
C 4.49540100 3.79242700 0.00000000
C 5.40289400 1.58399200 0.00000000
C 5.77669700 4.34444900 0.00000000
C 6.69677800 2.09845700 0.00000000
C 6.86823600 3.48238000 0.00000000
C -4.53270300 -7.93232200 0.00000000
C -4.91524800 -9.20768600 0.00000000
C 0.39837500 -8.66230100 0.00000000
C 1.69559700 -8.36267800 0.00000000
C 7.82320700 1.14500200 0.00000000
C 9.12238500 1.43616600 0.00000000
C 5.90277000 5.81458300 0.00000000
C 7.03051700 6.52236700 0.00000000
C -7.60016700 3.15339900 0.00000000
C -7.97880700 1.87699500 0.00000000
C -4.67681600 7.10635800 0.00000000
C -3.56507300 7.83897300 0.00000000
C -6.29743800 -9.72133600 0.00000000
C -7.42459600 -8.90110400 0.00000000
C -6.49233900 -11.09939600 0.00000000
C -8.71091400 -9.43142200 0.00000000
C -7.76665000 -11.66428100 0.00000000
C -8.86805100 -10.81626400 0.00000000
C 2.82542300 -9.31050300 0.00000000
C 2.66910100 -10.69575300 0.00000000
C 4.11991300 -8.79940500 0.00000000
C 3.76543400 -11.55243400 0.00000000
C 5.24040900 -9.62854400 0.00000000
C 5.04717400 -11.00505600 0.00000000
C 10.24696800 0.48224300 0.00000000
C 10.08358900 -0.90215300 0.00000000
C 11.54401500 0.98687700 0.00000000
C 11.17573500 -1.76417000 0.00000000
C 12.66044800 0.15228200 0.00000000
C 12.46021000 -1.22324700 0.00000000
C 7.15957200 7.99124500 0.00000000
C 8.43695400 8.54383500 0.00000000
C 6.07035800 8.86118900 0.00000000
C 8.64472000 9.92212900 0.00000000
C 6.24164600 10.24196100 0.00000000
C 7.53554400 10.75989500 0.00000000
C -3.47334900 9.31082200 0.00000000
C -2.21129200 9.89742900 0.00000000
C -4.58540500 10.15154500 0.00000000
C -2.04103100 11.28091200 0.00000000
C -4.45168400 11.53641500 0.00000000

C -3.17212600 12.08880000 0.00000000
C -9.36030600 1.36107100 0.00000000
C -9.55378800 -0.01713500 0.00000000
C -10.48848100 2.17998200 0.00000000
C -10.82756600 -0.58320600 0.00000000
C -11.77430600 1.64848800 0.00000000
C -11.92993900 0.26346900 0.00000000
C -9.85617600 -8.49635300 0.00000000
C -11.14799700 -8.79708300 0.00000000
C -7.88395200 -13.13787900 0.00000000
C -8.99551900 -13.86155200 0.00000000
C 6.57970700 -9.00293000 0.00000000
C 7.75795700 -9.61202000 0.00000000
C 3.51773100 -13.01009200 0.00000000
C 4.41722200 -13.98485700 0.00000000
C 10.92100300 -3.22057100 0.00000000
C 11.81566300 -4.19976700 0.00000000
C 14.00280300 0.77141000 0.00000000
C 15.17800700 0.15645400 0.00000000
C 5.03720300 11.09936600 0.00000000
C 4.98609700 12.42470000 0.00000000
C 10.03477900 10.42507700 0.00000000
C 10.43858600 11.68848500 0.00000000
C -0.66531300 11.82160600 0.00000000
C -0.29611600 13.09551600 0.00000000
C -5.67922800 12.36058500 0.00000000
C -5.76655900 13.68407100 0.00000000
C -12.92039500 2.58262500 0.00000000
C -14.21190000 2.28053900 0.00000000
C -10.94353000 -2.05683200 0.00000000
C -12.05424300 -2.78177700 0.00000000
H -13.03734900 -2.35230400 0.00000000
H 1.79226800 -1.88975200 0.00000000
H -2.43054800 -1.36773100 0.00000000
H 0.12666200 2.02034400 0.00000000
H 0.50297100 -3.79162900 0.00000000
H -2.51306500 -3.50343900 0.00000000
H 3.25118100 -0.13032400 0.00000000
H 2.15606200 2.69454400 0.00000000
H -3.41830300 0.67730100 0.00000000
H -1.67441200 3.15417200 0.00000000
H -3.80719700 -5.39403100 0.00000000
H 0.41064900 -5.91777600 0.00000000
H -2.14064100 -9.30944400 0.00000000
H -2.67663300 5.20096300 0.00000000
H -5.21166300 1.79592800 0.00000000
H -6.90333400 5.69396900 0.00000000
H 3.64575500 4.44988300 0.00000000
H 5.27758400 0.51925600 0.00000000
H 7.85830400 3.88788000 0.00000000
H -5.28063700 -7.16071700 0.00000000
H -4.16679200 -9.97879500 0.00000000
H 0.10101700 -9.69486100 0.00000000
H 1.99599800 -7.33092000 0.00000000
H 7.51857400 0.11452100 0.00000000
H 9.42907200 2.46601900 0.00000000
H 4.96043800 6.33110400 0.00000000
H 7.97283700 6.00589900 0.00000000
H -8.35170400 3.92138800 0.00000000
H -7.22874000 1.10737300 0.00000000
H -5.63005600 7.60228700 0.00000000
H -2.61097700 7.34430600 0.00000000
H -7.31200900 -7.83472500 0.00000000
H -5.63582100 -11.74804300 0.00000000
H -9.85396600 -11.23329300 0.00000000
H 1.68643900 -11.12482900 0.00000000
H 4.26093100 -7.73425900 0.00000000
H 5.89671400 -11.65637500 0.00000000
H 9.09868200 -1.32614500 0.00000000
H 11.69037800 2.05127900 0.00000000
H 13.30650100 -1.87878500 0.00000000
H 9.28908700 7.88944800 0.00000000
H 5.07178000 8.47041100 0.00000000
H 7.67688800 11.82099800 0.00000000
H -1.34189500 9.26609900 0.00000000
H -5.57324200 9.73457200 0.00000000
H -3.05934200 13.15331600 0.00000000
H -8.69656400 -0.66489400 0.00000000
H -10.37733500 3.24645500 0.00000000
H -12.91542200 -0.15456900 0.00000000
H -9.57862700 -7.45648900 0.00000000
H -11.89292100 -8.02543600 0.00000000
H -11.51827600 -9.80394000 0.00000000
H -6.94144300 -13.65744600 0.00000000
H -8.95463500 -14.93328300 0.00000000
H -9.97816400 -13.43086900 0.00000000
H 6.56591800 -7.92675200 0.00000000
H 8.66977200 -9.04730700 0.00000000
H 7.86880000 -10.67912100 0.00000000
H 2.47654200 -13.28247700 0.00000000
H 4.11379400 -15.01355400 0.00000000
H 5.47563200 -13.80955900 0.00000000
H 9.87843000 -3.48772700 0.00000000
H 11.50731400 -5.22701300 0.00000000
H 12.87489500 -4.02973100 0.00000000
H 13.99445000 1.84761200 0.00000000
H 16.09251100 0.71677400 0.00000000
H 15.28352500 -0.91122500 0.00000000
H 4.10762000 10.55693900 0.00000000
H 4.04513200 12.93941600 0.00000000
H 5.85925100 13.04792200 0.00000000
H 10.78518100 9.65360800 0.00000000
H 11.48293800 11.93260800 0.00000000
H 9.76328700 12.52217900 0.00000000
H 0.10571300 11.07067700 0.00000000
H 0.74111000 13.36847100 0.00000000
H -0.99369300 13.91056000 0.00000000
H -6.59373400 11.79319600 0.00000000
H -6.72141000 14.17247400 0.00000000
H -4.91057700 14.33080300 0.00000000
H -12.64408800 3.62277100 0.00000000
H -14.95732500 3.05165500 0.00000000
H -14.58116400 1.27326000 0.00000000
H -10.00033300 -2.57524200 0.00000000
H -12.01236000 -3.85349700 0.00000000