

Electronic Supplementary Information belonging to the manuscript:

Rationalizing the influence of α -cationic phospholes on π - catalysis

*Iván Cortés,^{a,b} Jorge Juan Cabrera-Trujillo,^b and Israel Fernández^{*b}*

a. Instituto de Química Rosario (IQUIR, CONICET-UNR), Facultad de Ciencias Bioquímicas y Farmacéuticas and Universidad Nacional de Rosario, Suipacha 531, 2000 Rosario (Argentina).

b. Departamento de Química Orgánica I and Centro de Innovación en Química Avanzada (ORFEO-CINQA), Facultad de Ciencias Químicas, Universidad Complutense de Madrid, 28040 Madrid (Spain).

israel@quim.ucm.es

Contents:

1. Figure S1.....	S2
2. Cartesian coordinates and energies.....	S3

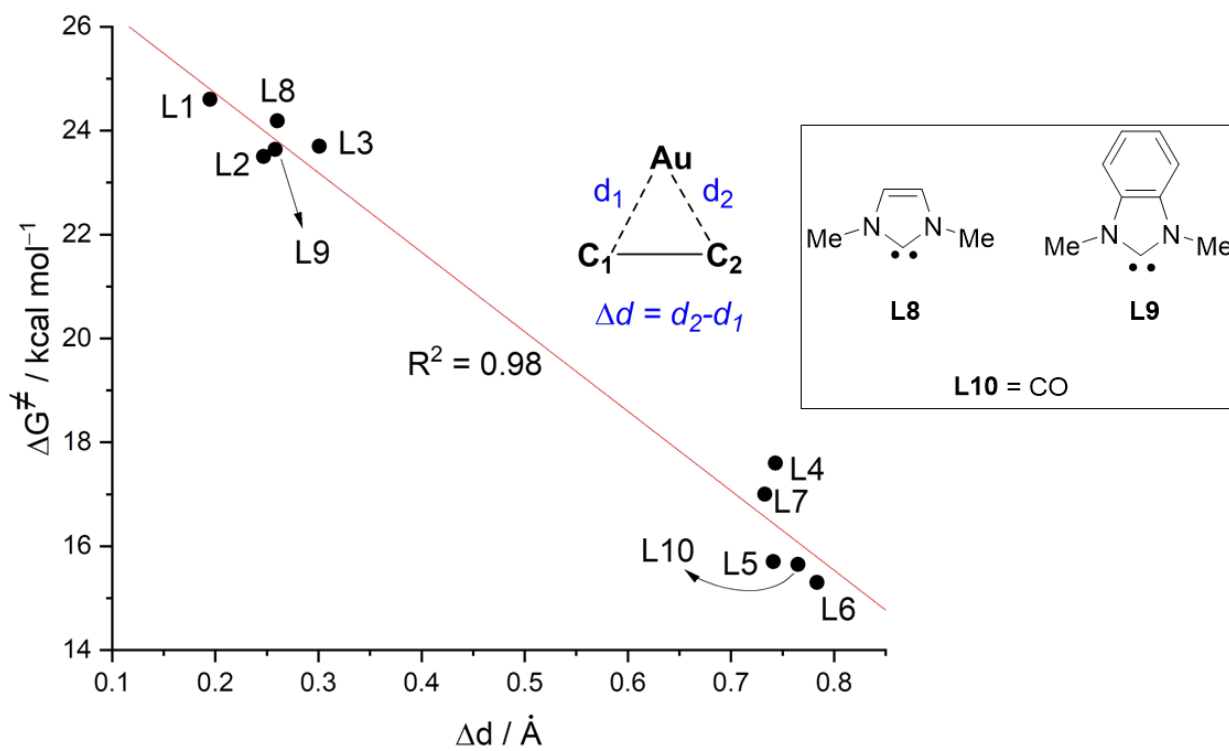


Figure S1. Plot of the geometrical parameter Δd versus the computed free activation barriers. All data have been computed at the PCM(CH₂Cl₂)-B3LYP-D3/def2-TZVPP//B3LYP-D3/def2-SVP level. For the definition of ligands **L1-L7** see main text.

Cartesian coordinates (in Å), electronic and free energies (in a.u.) of all the stationary points discussed in the text. All calculations have been performed at the PCM(dichloromethane)/B3LYP-D3/def2-TZVPP//B3LYP-D3/def2-SVP level.

Mesitylene:

E = -350.350693

G = -350.389305

C	-0.020838000	-1.412170000	0.000193000
C	-1.217317000	-0.672938000	0.001090000
C	1.191589000	-0.717732000	-0.001012000
H	-2.173507000	-1.206205000	0.001957000
H	2.131486000	-1.279185000	-0.001813000
C	-1.212546000	0.724263000	0.000583000
C	1.233506000	0.688124000	-0.001133000
C	0.025809000	1.390966000	-0.000478000
H	0.041860000	2.485687000	-0.000780000
C	-0.064838000	-2.921508000	0.000010000
H	0.944165000	-3.359872000	0.002835000
H	-0.602257000	-3.304157000	0.884086000
H	-0.597081000	-3.304014000	-0.887293000
C	-2.497890000	1.516693000	-0.000303000
H	-3.381713000	0.861717000	0.012950000
H	-2.556381000	2.181716000	0.877797000
H	-2.567847000	2.160486000	-0.893399000
C	2.562649000	1.404510000	0.000723000
H	2.438198000	2.497337000	-0.023117000
H	3.149566000	1.151100000	0.899816000
H	3.172772000	1.114146000	-0.871082000

[L1-Au-phenylacetylene]⁺:

E = -1480.855779

G = -1480.921478

C	-2.235895000	-2.878963000	-0.236867000
C	-2.982049000	-1.890937000	-0.160411000
Au	-0.614324000	-1.346539000	-0.091946000
P	1.169503000	0.148367000	0.021363000
H	-1.980250000	-3.925827000	-0.340518000
C	1.807040000	0.335829000	1.718897000
C	2.171932000	1.594008000	2.225094000
C	1.976971000	-0.815560000	2.507253000
C	2.708352000	1.693784000	3.512054000
C	2.517652000	-0.707950000	3.789361000
C	2.883286000	0.546372000	4.292018000
H	2.036789000	2.493894000	1.621209000
H	1.688014000	-1.796938000	2.120013000
H	2.989832000	2.673095000	3.906060000
H	2.650156000	-1.603976000	4.400026000
H	3.302052000	0.629270000	5.297674000
C	0.618475000	1.797471000	-0.540563000
C	-0.672630000	2.242510000	-0.204448000
C	1.478099000	2.633198000	-1.272175000
C	-1.093496000	3.515545000	-0.590645000
C	1.047838000	3.906341000	-1.657627000
C	-0.234225000	4.348219000	-1.317181000

H	-1.355216000	1.595272000	0.353696000
H	2.479108000	2.292159000	-1.545395000
H	-2.097901000	3.856123000	-0.328884000
H	1.717736000	4.553472000	-2.228402000
H	-0.567579000	5.342797000	-1.622813000
C	2.572278000	-0.339802000	-1.033617000
C	2.307022000	-0.829560000	-2.324685000
C	3.898687000	-0.199800000	-0.594899000
C	3.362773000	-1.166963000	-3.172099000
C	4.950755000	-0.544627000	-1.448739000
C	4.685015000	-1.025308000	-2.734234000
H	1.275146000	-0.947145000	-2.667917000
H	4.113337000	0.173011000	0.408826000
H	3.154495000	-1.546818000	-4.174891000
H	5.982274000	-0.438313000	-1.105335000
H	5.510518000	-1.295524000	-3.396960000
C	-3.818956000	-0.739827000	-0.063885000
C	-4.342433000	-0.352503000	1.190177000
C	-4.092738000	0.032154000	-1.215161000
C	-5.133776000	0.789919000	1.282225000
C	-4.883220000	1.173469000	-1.107207000
C	-5.403253000	1.551807000	0.137558000
H	-4.122886000	-0.952074000	2.075628000
H	-3.678773000	-0.270318000	-2.179042000
H	-5.544741000	1.089235000	2.248779000
H	-5.097951000	1.770614000	-1.995941000
H	-6.026153000	2.446140000	0.216317000

[L2-Au-phenylacetylene]⁺:

E = -1706.679465

G = -1706.746234

C	2.204544000	-2.821803000	-1.145849000
C	2.880848000	-1.804982000	-0.911309000
Au	0.445769000	-1.552660000	-0.739454000
P	-1.400273000	-0.271673000	-0.283253000
H	2.077314000	-3.877219000	-1.359207000
C	3.619288000	-0.617519000	-0.654168000
C	4.248279000	0.065488000	-1.720641000
C	3.700292000	-0.110157000	0.663313000
C	4.962621000	1.232204000	-1.461186000
C	4.407935000	1.063675000	0.902909000
C	5.041125000	1.730940000	-0.153655000
H	4.175364000	-0.330591000	-2.735417000
H	3.194849000	-0.630759000	1.478798000
H	5.460819000	1.757126000	-2.279115000
H	4.467924000	1.461488000	1.917866000
H	5.600899000	2.648614000	0.042616000
O	-1.459195000	0.208584000	1.266022000
O	-1.501626000	1.114076000	-1.119362000
O	-2.788274000	-0.979225000	-0.602106000
C	-4.052795000	-0.368584000	-0.402380000
C	-4.701643000	-0.565035000	0.813703000
C	-4.611027000	0.373731000	-1.439678000
C	-5.966246000	0.004370000	0.991053000
H	-4.224053000	-1.155259000	1.596994000
C	-5.876203000	0.936212000	-1.246130000
H	-4.061152000	0.502327000	-2.372758000
C	-6.552546000	0.752753000	-0.035150000
H	-6.494586000	-0.141477000	1.935864000
H	-6.334209000	1.518621000	-2.048716000
H	-7.541815000	1.192685000	0.108489000

C	-0.597942000	2.155125000	-0.858919000
C	0.692122000	2.101573000	-1.389373000
C	-1.021959000	3.216661000	-0.060431000
C	1.586197000	3.134897000	-1.092229000
H	0.984367000	1.268743000	-2.031802000
C	-0.122044000	4.249862000	0.217830000
H	-2.038913000	3.214622000	0.334810000
C	1.182551000	4.206223000	-0.288864000
H	2.599993000	3.098327000	-1.495830000
H	-0.442652000	5.090911000	0.836795000
H	1.881720000	5.014693000	-0.064318000
C	-0.420522000	-0.021110000	2.178971000
C	-0.313901000	-1.270410000	2.793395000
C	0.477430000	1.011401000	2.449865000
C	0.722788000	-1.487632000	3.706957000
H	-1.042430000	-2.051139000	2.565079000
C	1.500394000	0.783600000	3.375451000
H	0.365702000	1.971254000	1.944534000
C	1.628711000	-0.462143000	4.000361000
H	0.813527000	-2.459053000	4.198099000
H	2.199878000	1.589727000	3.609031000
H	2.428755000	-0.631911000	4.724388000

[L3-Au-phenylacetylene]⁺:

E = -1329.565462

G = -1329.628373

C	-1.519573000	-0.970851000	1.596300000
C	-2.432003000	-1.966927000	1.439747000
C	-3.114373000	-2.003877000	0.101828000
C	-2.726737000	-1.036612000	-0.771941000
C	-0.671440000	-0.607005000	2.775702000
H	-0.805476000	0.454366000	3.046148000
H	0.401545000	-0.751463000	2.561872000
H	-0.920265000	-1.210362000	3.659311000
C	-2.789475000	-2.985658000	2.481274000
H	-2.227642000	-2.848058000	3.413376000
H	-2.591413000	-4.005713000	2.112876000
H	-3.864242000	-2.941662000	2.721696000
C	-4.143807000	-3.059083000	-0.175590000
H	-4.567666000	-2.975742000	-1.183885000
H	-4.972901000	-3.000577000	0.548365000
H	-3.707322000	-4.066303000	-0.073648000
C	-3.196382000	-0.740249000	-2.162754000
H	-4.031141000	-1.389759000	-2.459417000
H	-2.387309000	-0.876410000	-2.900368000
H	-3.538065000	0.305403000	-2.249737000
C	-2.026041000	1.643926000	0.291833000
C	-3.278150000	1.823899000	0.908210000
H	-3.868244000	0.955881000	1.214089000
C	-3.764186000	3.112672000	1.126683000
H	-4.736334000	3.252569000	1.604957000
C	-3.008086000	4.224453000	0.733139000
H	-3.392490000	5.232545000	0.905419000
C	-1.765033000	4.047650000	0.119934000
H	-1.176776000	4.914864000	-0.188481000
C	-1.270615000	2.758619000	-0.102350000
H	-0.298384000	2.624313000	-0.583351000
P	-1.427832000	-0.055545000	0.031499000
C	2.419694000	-0.441169000	-2.302518000
C	3.131975000	-0.286987000	-1.295930000
Au	0.642655000	-0.206155000	-1.019044000

H	2.273982000	-0.615399000	-3.362489000
C	3.939687000	-0.108996000	-0.140515000
C	4.371378000	1.186814000	0.226616000
C	4.317805000	-1.228833000	0.636415000
C	5.173514000	1.351837000	1.352131000
C	5.120200000	-1.047615000	1.759319000
C	5.546812000	0.238459000	2.116675000
H	4.075811000	2.045804000	-0.379040000
H	3.980840000	-2.225771000	0.345465000
H	5.513222000	2.350044000	1.636259000
H	5.419044000	-1.909971000	2.359038000
H	6.177950000	0.374028000	2.998272000

[L4-Au-phenylacetylene]²⁺:

E = -1481.212033

G = -1481.284220

P	1.014605000	0.521943000	0.017529000
N	5.028495000	0.187439000	-0.108245000
N	3.121054000	-2.997952000	0.210952000
C	1.286127000	1.810422000	-1.232797000
C	1.366878000	3.000082000	-0.574133000
C	1.301661000	2.911607000	0.925461000
C	1.166298000	1.654188000	1.430555000
C	2.525474000	-0.474692000	0.027011000
C	3.913005000	-0.486140000	-0.018420000
C	3.178013000	-1.695833000	0.101075000
C	4.998495000	1.651928000	-0.221927000
H	3.960304000	2.004602000	-0.216370000
H	5.545783000	2.098955000	0.622166000
H	5.482934000	1.959262000	-1.161563000
C	6.352940000	-0.441425000	-0.106458000
H	6.949337000	-0.047150000	0.730453000
H	6.260371000	-1.527259000	0.001981000
H	6.873658000	-0.216726000	-1.050010000
C	4.311688000	-3.853076000	0.236323000
H	5.218568000	-3.246390000	0.142709000
H	4.349206000	-4.412222000	1.183888000
H	4.272755000	-4.569918000	-0.598189000
C	1.825621000	-3.678891000	0.312113000
H	1.785267000	-4.262184000	1.244933000
H	1.012345000	-2.942059000	0.310932000
H	1.696651000	-4.363326000	-0.540790000
C	1.301154000	1.507079000	-2.699900000
H	0.314885000	1.155058000	-3.047093000
H	1.566081000	2.392006000	-3.293923000
H	2.027738000	0.713305000	-2.943240000
C	1.504910000	4.340295000	-1.230864000
H	0.647599000	4.984864000	-0.976157000
H	2.405312000	4.864711000	-0.871829000
H	1.561754000	4.271480000	-2.323822000
C	1.377781000	4.164399000	1.744776000
H	0.555798000	4.849680000	1.480791000
H	1.320693000	3.968193000	2.822105000
H	2.314882000	4.709256000	1.544955000
C	1.058709000	1.180092000	2.847543000
H	1.267844000	1.988049000	3.561356000
H	0.048814000	0.793851000	3.067246000
H	1.768680000	0.361889000	3.056505000
C	-2.665536000	-1.958702000	-0.366385000
C	-3.742035000	-1.311261000	-0.225053000
Au	-0.934761000	-0.752022000	-0.161384000

H	-2.509011000	-3.019426000	-0.586087000
C	-4.894981000	-0.548706000	-0.064268000
C	-5.495604000	-0.424090000	1.222804000
C	-5.501402000	0.072239000	-1.195488000
C	-6.669064000	0.302051000	1.363991000
C	-6.674450000	0.794710000	-1.033858000
C	-7.255480000	0.908036000	0.240259000
H	-5.029168000	-0.909232000	2.082560000
H	-5.038760000	-0.034388000	-2.178694000
H	-7.139805000	0.398537000	2.344438000
H	-7.149190000	1.269695000	-1.894790000
H	-8.182369000	1.475237000	0.358857000

[L5-Au-phenylacetylene]²⁺:

E = -1776.253432

G = -1776.326051

P	-0.725247000	1.095258000	0.018487000
N	-2.740228000	-0.846978000	0.023646000
C	-0.605570000	2.410895000	-1.216939000
C	-0.420159000	3.580367000	-0.539148000
C	-0.485325000	3.476758000	0.951717000
C	-0.714496000	2.224113000	1.440982000
C	-2.477144000	0.422773000	-0.062140000
C	-3.742212000	1.261307000	-0.247564000
C	-4.836709000	0.245402000	0.168057000
H	-5.091581000	0.405576000	1.226118000
H	-5.757326000	0.381709000	-0.414348000
C	-4.257153000	-1.166164000	-0.009214000
C	-4.638876000	-2.102709000	1.136724000
H	-5.724833000	-2.270339000	1.082529000
H	-4.421141000	-1.665633000	2.118636000
H	-4.145187000	-3.081024000	1.053464000
C	-4.613059000	-1.821738000	-1.348893000
H	-4.109270000	-2.790870000	-1.465482000
H	-4.378038000	-1.186900000	-2.210871000
H	-5.696754000	-2.007380000	-1.355399000
C	-3.817446000	2.529013000	0.617696000
H	-3.109326000	3.295219000	0.282521000
H	-3.633414000	2.314587000	1.679835000
H	-4.832169000	2.945554000	0.529390000
C	-3.862577000	1.662526000	-1.742122000
H	-4.860326000	2.098213000	-1.900087000
H	-3.758021000	0.808946000	-2.425565000
H	-3.117943000	2.420507000	-2.012810000
C	-1.790028000	-1.947034000	0.070032000
C	-1.404093000	-2.461195000	1.327909000
C	-0.603594000	-3.612496000	1.335520000
H	-0.298272000	-4.034645000	2.296121000
C	-0.198655000	-4.219501000	0.147271000
H	0.401693000	-5.131960000	0.177634000
C	-0.538160000	-3.649271000	-1.079108000
H	-0.180089000	-4.099168000	-2.008403000
C	-1.330490000	-2.494307000	-1.150979000
C	-1.593920000	-1.882644000	-2.506021000
H	-2.264996000	-2.513634000	-3.108492000
H	-2.040310000	-0.882792000	-2.455128000
H	-0.649255000	-1.795251000	-3.063665000
C	-1.764533000	-1.819217000	2.644731000
H	-2.255550000	-0.845316000	2.534860000
H	-2.431497000	-2.468479000	3.232452000
H	-0.855835000	-1.668842000	3.247309000

C	-0.495994000	2.149999000	-2.693015000
H	0.558628000	2.043352000	-2.999364000
H	-1.013777000	1.227061000	-2.990859000
H	-0.926584000	2.974433000	-3.280133000
C	-0.129200000	4.898296000	-1.188694000
H	-0.137195000	4.838849000	-2.283811000
H	-0.863719000	5.659267000	-0.878708000
H	0.859627000	5.273789000	-0.876931000
C	-0.305747000	4.706401000	1.787863000
H	-1.098729000	5.439492000	1.563069000
H	-0.337551000	4.497496000	2.863709000
H	0.651766000	5.201786000	1.560641000
C	-0.831348000	1.756161000	2.859740000
H	-0.491725000	2.527790000	3.563508000
H	-1.873754000	1.511220000	3.127819000
H	-0.227907000	0.852904000	3.038615000
C	2.624963000	-1.830399000	-0.009653000
C	3.760484000	-1.279631000	-0.029473000
Au	1.034225000	-0.440527000	-0.013598000
H	2.314131000	-2.878853000	0.013479000
C	4.990794000	-0.625146000	-0.049492000
C	5.623871000	-0.333235000	-1.292054000
C	5.639170000	-0.290099000	1.174171000
C	6.870937000	0.275303000	-1.300344000
C	6.886141000	0.317985000	1.145882000
C	7.499281000	0.598295000	-0.086340000
H	5.123932000	-0.599907000	-2.225342000
H	5.150640000	-0.523629000	2.122249000
H	7.366373000	0.497531000	-2.247646000
H	7.393116000	0.573072000	2.078684000
H	8.483804000	1.072990000	-0.100766000

[L6-Au-phenylacetylene]²⁺:

E = -1481.293388

G = -1481.361150

C	-2.541763000	-2.068895000	-0.255699000
C	-3.643398000	-1.450941000	-0.167113000
H	-2.382041000	-3.141081000	-0.417337000
C	-4.828596000	-0.733054000	-0.066352000
C	-5.462147000	-0.574300000	1.202285000
C	-5.438428000	-0.195109000	-1.238876000
C	-6.669774000	0.102414000	1.284787000
C	-6.645630000	0.479291000	-1.135210000
C	-7.258263000	0.626084000	0.121027000
H	-4.992904000	-0.996141000	2.093344000
H	-4.950656000	-0.328204000	-2.206604000
H	-7.166261000	0.223620000	2.249672000
H	-7.123513000	0.889783000	-2.027005000
H	-8.212540000	1.154378000	0.193829000
P	1.099938000	0.480336000	0.051110000
N	2.999034000	-1.684196000	0.150864000
C	1.060539000	1.680964000	1.412927000
C	0.884876000	2.910267000	0.849130000
C	0.922306000	2.941660000	-0.652253000
C	1.128019000	1.737780000	-1.256251000
C	2.742157000	-0.353417000	0.065136000
N	3.942846000	0.269153000	-0.050330000
C	4.962091000	-0.666152000	-0.057110000
C	4.364745000	-1.905398000	0.072625000
C	4.988198000	-3.259057000	0.131447000
H	6.075019000	-3.177955000	0.008138000

H	4.612633000	-3.916976000	-0.668095000
H	4.804109000	-3.751508000	1.100151000
C	1.070075000	1.263320000	2.852128000
H	0.160542000	0.695635000	3.113117000
H	1.933040000	0.615939000	3.081925000
H	1.123139000	2.131238000	3.523048000
C	0.658671000	4.180585000	1.611418000
H	0.671397000	4.029961000	2.697489000
H	1.423758000	4.932787000	1.359863000
H	-0.314297000	4.623093000	1.341670000
C	0.742279000	4.245108000	-1.369039000
H	1.517441000	4.968475000	-1.066962000
H	0.782569000	4.137578000	-2.459584000
H	-0.226907000	4.700354000	-1.108131000
C	1.227728000	1.381007000	-2.708251000
H	1.243601000	2.276353000	-3.343928000
H	2.145030000	0.805912000	-2.923501000
H	0.376901000	0.757677000	-3.031379000
Au	-0.808998000	-0.878029000	-0.086466000
C	6.403644000	-0.306674000	-0.182257000
H	6.753352000	0.278767000	0.683868000
H	7.017722000	-1.213877000	-0.234819000
H	6.596789000	0.280306000	-1.093868000
C	2.011498000	-2.756958000	0.308274000
H	1.427561000	-2.878373000	-0.614548000
H	2.535809000	-3.693650000	0.519765000
H	1.343001000	-2.536758000	1.149716000
C	4.155291000	1.715305000	-0.158893000
H	3.493750000	2.237792000	0.541038000
H	5.194136000	1.942799000	0.100087000
H	3.951714000	2.053640000	-1.183835000

[L7-Au-phenylacetylene]²⁺:

E = -1632.501936

G = -1632.574303

C	-2.668126000	-0.640030000	-2.057513000
C	-3.771729000	-0.411758000	-1.487990000
Au	-1.006389000	-0.248725000	-0.796758000
P	0.916016000	0.131760000	0.494665000
H	-2.440450000	-0.990703000	-3.068711000
C	1.121905000	-1.036744000	1.875532000
C	-0.033260000	-1.518082000	2.517136000
C	2.393474000	-1.425738000	2.336975000
C	0.085680000	-2.376593000	3.612280000
C	2.502737000	-2.288751000	3.429234000
C	1.350695000	-2.763020000	4.067242000
H	-1.025609000	-1.224726000	2.164288000
H	3.301114000	-1.057244000	1.852476000
H	-0.812688000	-2.748067000	4.110001000
H	3.490048000	-2.589150000	3.787395000
H	1.440246000	-3.437339000	4.922024000
C	1.112377000	1.840333000	1.094751000
C	1.936503000	2.124110000	2.198249000
C	0.463558000	2.882950000	0.409537000
C	2.121139000	3.449333000	2.598358000
C	0.658803000	4.205835000	0.815103000
C	1.487967000	4.488766000	1.906142000
H	2.422466000	1.319271000	2.754123000
H	-0.193074000	2.667074000	-0.437789000
H	2.755363000	3.671226000	3.459597000
H	0.154139000	5.016494000	0.284759000

H	1.631930000	5.523162000	2.226925000
C	-4.958908000	-0.141618000	-0.810615000
C	-5.620794000	-1.177639000	-0.090115000
C	-5.536198000	1.159600000	-0.875558000
C	-6.825971000	-0.910467000	0.543453000
C	-6.741660000	1.407846000	-0.234881000
C	-7.383566000	0.376750000	0.470603000
H	-5.175963000	-2.174053000	-0.052606000
H	-5.026783000	1.945683000	-1.436493000
H	-7.343560000	-1.699431000	1.092855000
H	-7.194195000	2.400352000	-0.283123000
H	-8.335307000	0.578713000	0.968837000
C	2.397021000	-0.148229000	-0.509535000
C	3.495549000	0.320926000	-1.214424000
C	3.207367000	-1.066695000	-1.156533000
N	3.459876000	-2.320140000	-1.434340000
N	4.234518000	1.325827000	-1.608864000
C	2.574280000	-3.380660000	-0.936026000
H	1.772664000	-2.947407000	-0.325457000
H	2.137361000	-3.929799000	-1.784374000
H	3.151840000	-4.084261000	-0.317173000
C	4.605854000	-2.749550000	-2.240445000
H	4.253309000	-3.288918000	-3.133097000
H	5.196050000	-1.882888000	-2.557094000
H	5.245821000	-3.422966000	-1.649762000
C	5.423349000	1.156454000	-2.449273000
H	5.567881000	0.099862000	-2.698860000
H	5.304580000	1.730555000	-3.381001000
H	6.313334000	1.526114000	-1.916900000
C	3.906087000	2.701696000	-1.213134000
H	4.751947000	3.136075000	-0.658511000
H	3.721428000	3.310788000	-2.111421000
H	3.015044000	2.710502000	-0.575911000

[L8-Au-phenylacetylene]⁺:

E = -749.186825

G = -748.260468

C	-1.201034000	-1.295790000	-1.807012000
C	-2.000795000	-0.747571000	-1.029267000
H	-0.945436000	-1.909452000	-2.663033000
C	-2.952098000	-0.134507000	-0.164361000
C	-3.401334000	-0.817186000	0.988948000
C	-3.461307000	1.147832000	-0.471555000
C	-4.350267000	-0.221905000	1.815728000
C	-4.410498000	1.730089000	0.364295000
C	-4.853748000	1.048063000	1.504942000
H	-3.005807000	-1.808743000	1.217993000
H	-3.112230000	1.667565000	-1.366018000
H	-4.703795000	-0.748529000	2.704705000
H	-4.810874000	2.717983000	0.126828000
H	-5.600030000	1.509394000	2.156176000
N	2.831304000	-0.420997000	1.250022000
C	2.101493000	0.231962000	0.309342000
N	2.779538000	1.380860000	0.056924000
C	3.922436000	1.446470000	0.830533000
C	3.955496000	0.310393000	1.581768000
H	4.676511000	-0.031994000	2.319589000
Au	0.377094000	-0.412923000	-0.583161000
H	4.607763000	2.289001000	0.786773000
C	2.524740000	-1.728220000	1.825135000
H	3.209280000	-2.489370000	1.422947000

H	2.629886000	-1.682692000	2.917815000
H	1.493202000	-2.002402000	1.575107000
C	2.395143000	2.420654000	-0.894055000
H	1.415353000	2.177049000	-1.320841000
H	2.333921000	3.390168000	-0.379852000
H	3.136558000	2.482229000	-1.703761000

[L9-Au-phenylacetylene]⁺:

E = -902.896540

G = -901.768012

C	-2.359202000	-2.103085000	0.210327000
C	-2.951215000	-1.015819000	0.100962000
H	-2.320191000	-3.180618000	0.319960000
C	-3.661846000	0.212067000	-0.022587000
C	-4.013752000	0.943809000	1.134528000
C	-4.029910000	0.689026000	-1.301309000
C	-4.728285000	2.131878000	1.007210000
C	-4.744660000	1.878592000	-1.412825000
C	-5.092896000	2.598571000	-0.262500000
H	-3.728050000	0.567475000	2.118810000
H	-3.756248000	0.117259000	-2.190269000
H	-5.006751000	2.696996000	1.899241000
H	-5.035778000	2.247477000	-2.398616000
H	-5.655370000	3.530601000	-0.356299000
N	2.149247000	0.195443000	1.079003000
C	1.402688000	-0.211996000	0.021087000
N	2.167892000	-0.065060000	-1.090339000
C	3.417539000	0.445204000	-0.747563000
C	3.405813000	0.611874000	0.646602000
Au	-0.504983000	-0.949705000	0.093897000
C	1.744822000	0.212638000	2.477495000
H	2.405770000	-0.440153000	3.066838000
H	1.805929000	1.237906000	2.871579000
H	0.712860000	-0.146601000	2.564509000
C	1.786156000	-0.377116000	-2.460259000
H	0.766791000	-0.779972000	-2.473300000
H	1.824967000	0.533235000	-3.076846000
H	2.475281000	-1.125674000	-2.878505000
C	4.538840000	0.770774000	-1.517462000
H	4.550174000	0.642578000	-2.600679000
C	4.515273000	1.110894000	1.336682000
H	4.509319000	1.239869000	2.419863000
C	5.645768000	1.268700000	-0.831059000
H	6.544474000	1.536177000	-1.390643000
C	5.634222000	1.435524000	0.570589000
H	6.524359000	1.828249000	1.066329000

[L10-Au-phenylacetylene]⁺:

E = -557.552896

G = -557.593409

C	0.119801000	-1.542005000	-0.000957000
C	1.269574000	-1.008163000	-0.000738000
H	-0.135786000	-2.609050000	-0.001624000
C	2.501411000	-0.368074000	-0.000251000
C	3.140659000	-0.051719000	-1.236082000
C	3.140973000	-0.053997000	1.235991000
C	4.384689000	0.560604000	-1.224634000
C	4.385022000	0.558305000	1.225347000
C	5.002791000	0.863027000	0.000558000
H	2.643751000	-0.299292000	-2.176246000

H	2.644305000	-0.303284000	2.175830000
H	4.884247000	0.805538000	-2.164022000
H	4.884840000	0.801471000	2.165056000
H	5.984302000	1.344286000	0.000878000
C	-3.011853000	1.064853000	0.000867000
Au	-1.459295000	-0.175996000	-0.000138000
O	-3.902473000	1.753374000	0.001302000

TS1 :

E = -1831.195685

G = -1831.271532

C	-2.152411000	-0.730418000	0.025504000
C	-2.820780000	0.383915000	0.107499000
Au	-0.064125000	-0.582856000	0.025648000
P	2.261358000	-0.251867000	0.008357000
H	-2.634060000	-1.713818000	-0.029731000
C	3.020442000	-0.406509000	1.664866000
C	4.027941000	0.465803000	2.105981000
C	2.595959000	-1.458969000	2.494490000
C	4.608618000	0.279239000	3.364185000
C	3.183889000	-1.643238000	3.746925000
C	4.190523000	-0.774033000	4.182990000
H	4.359447000	1.291247000	1.472386000
H	1.803689000	-2.134556000	2.159530000
H	5.391259000	0.961226000	3.704873000
H	2.852416000	-2.464067000	4.387268000
H	4.646578000	-0.916077000	5.165704000
C	2.662873000	1.435864000	-0.580649000
C	1.816563000	2.496070000	-0.211011000
C	3.801357000	1.695754000	-1.360486000
C	2.115521000	3.801251000	-0.605484000
C	4.092725000	3.004787000	-1.756030000
C	3.254074000	4.057765000	-1.377571000
H	0.916587000	2.303752000	0.379388000
H	4.459851000	0.878951000	-1.664162000
H	1.451638000	4.618024000	-0.312938000
H	4.978999000	3.201037000	-2.364049000
H	3.485497000	5.079202000	-1.689135000
C	3.179030000	-1.400059000	-1.078653000
C	2.610171000	-1.746809000	-2.316375000
C	4.438362000	-1.908788000	-0.723049000
C	3.301126000	-2.584405000	-3.193496000
C	5.122610000	-2.752043000	-1.603686000
C	4.557583000	-3.088119000	-2.837522000
H	1.624270000	-1.361771000	-2.592132000
H	4.884753000	-1.651800000	0.239907000
H	2.856010000	-2.850541000	-4.155100000
H	6.101104000	-3.148417000	-1.322470000
H	5.094861000	-3.748494000	-3.522433000
C	-2.571562000	1.820695000	0.047659000
C	-2.894960000	2.681958000	1.114891000
C	-1.919539000	2.349302000	-1.086247000
C	-2.562822000	4.034250000	1.053833000
C	-1.586336000	3.703684000	-1.140646000
C	-1.908978000	4.548375000	-0.073879000
H	-3.394981000	2.281564000	1.999106000
H	-1.658232000	1.680231000	-1.908306000
H	-2.809122000	4.691735000	1.890658000
H	-1.069997000	4.098524000	-2.018371000
H	-1.653180000	5.609730000	-0.119048000
C	-4.853841000	0.196019000	0.242549000

C	-4.997936000	-0.735116000	1.330151000
C	-5.047389000	-0.233565000	-1.113596000
C	-5.144609000	-1.599876000	-1.366271000
C	-5.164267000	-2.532048000	-0.315344000
C	-5.114036000	-2.078245000	1.027927000
H	-5.046981000	1.247744000	0.459394000
H	-5.231891000	-1.953126000	-2.396422000
H	-5.178065000	-2.813224000	1.834771000
C	-5.282127000	-4.003432000	-0.589035000
H	-6.206268000	-4.401644000	-0.136871000
H	-5.296481000	-4.228953000	-1.663885000
H	-4.445630000	-4.553072000	-0.126650000
C	-5.137527000	0.785235000	-2.208788000
H	-6.112054000	1.301043000	-2.159142000
H	-4.364904000	1.562352000	-2.097629000
H	-5.044783000	0.329298000	-3.204096000
C	-4.916057000	-0.240236000	2.744260000
H	-5.268185000	-0.994259000	3.461789000
H	-3.867433000	-0.002505000	2.995688000
H	-5.504321000	0.679928000	2.885208000

TS2:

E = -2057.018161

G = -2057.098105

C	2.259302000	0.569547000	0.048985000
C	2.780238000	-0.498926000	0.577466000
Au	0.181318000	0.630226000	-0.133795000
P	-2.096125000	0.521373000	-0.443830000
H	2.862528000	1.404620000	-0.326674000
C	2.396104000	-1.826242000	1.033236000
C	2.658961000	-2.273753000	2.344052000
C	1.679458000	-2.664580000	0.151713000
C	2.212210000	-3.524671000	2.763302000
C	1.227788000	-3.912915000	0.581750000
C	1.496497000	-4.347447000	1.883146000
H	3.205332000	-1.629667000	3.035703000
H	1.456906000	-2.320392000	-0.860107000
H	2.415487000	-3.859651000	3.782926000
H	0.660810000	-4.541031000	-0.107629000
H	1.147950000	-5.328070000	2.215737000
C	4.853784000	-0.460712000	0.747746000
C	5.064060000	0.781934000	1.437908000
C	5.106634000	-0.566689000	-0.660216000
C	5.353009000	0.601813000	-1.376807000
C	5.451269000	1.844509000	-0.727264000
C	5.323258000	1.911424000	0.683281000
H	4.923759000	-1.377933000	1.333510000
H	5.495748000	0.551319000	-2.458815000
H	5.444904000	2.878630000	1.178264000
C	5.733940000	3.100550000	-1.499878000
H	6.702442000	3.527279000	-1.187974000
H	5.766101000	2.926232000	-2.583850000
H	4.971337000	3.868226000	-1.289512000
C	5.095281000	-1.914813000	-1.315223000
H	5.986447000	-2.489186000	-1.009223000
H	4.218887000	-2.503537000	-0.999640000
H	5.098173000	-1.839712000	-2.411314000
C	4.906834000	0.840082000	2.929309000
H	5.335605000	1.760653000	3.348958000
H	3.835039000	0.820140000	3.193823000
H	5.382584000	-0.023294000	3.419893000

O	-2.905400000	1.854234000	-0.883128000
O	-2.814502000	-0.052851000	0.889975000
O	-2.606528000	-0.422413000	-1.662308000
C	-4.104100000	-0.589441000	1.013406000
C	-5.206939000	-0.032397000	0.363391000
C	-4.225569000	-1.710237000	1.835680000
C	-6.459897000	-0.626421000	0.546780000
C	-5.485334000	-2.288371000	2.011806000
C	-6.603917000	-1.749779000	1.366475000
H	-5.091449000	0.844363000	-0.273771000
H	-3.335098000	-2.110123000	2.323956000
H	-7.330277000	-0.200832000	0.042099000
H	-5.591457000	-3.163751000	2.656831000
H	-7.587383000	-2.204155000	1.504330000
C	-2.614937000	3.109089000	-0.332967000
C	-2.611581000	3.303973000	1.050363000
C	-2.358092000	4.152769000	-1.221746000
C	-2.335764000	4.582095000	1.547895000
C	-2.093095000	5.425338000	-0.709306000
C	-2.077797000	5.641672000	0.673412000
H	-2.835577000	2.475035000	1.724116000
H	-2.377619000	3.956623000	-2.295148000
H	-2.332971000	4.747426000	2.627772000
H	-1.897818000	6.252080000	-1.396261000
H	-1.870835000	6.638635000	1.068525000
C	-1.979753000	-1.641786000	-1.935527000
C	-2.479620000	-2.811306000	-1.361330000
C	-0.885748000	-1.660986000	-2.803406000
C	-1.867667000	-4.029193000	-1.673164000
C	-0.281271000	-2.885262000	-3.104260000
C	-0.771448000	-4.069608000	-2.542089000
H	-3.340009000	-2.758349000	-0.692134000
H	-0.532188000	-0.725739000	-3.241271000
H	-2.257473000	-4.952432000	-1.238045000
H	0.567538000	-2.913383000	-3.791647000
H	-0.304840000	-5.025791000	-2.789984000

TS3:

E = -1679.904893

G = -1679.979956

C	-1.944514000	-0.580139000	-0.311039000
C	-2.608518000	0.459221000	0.106132000
H	-2.433658000	-1.490593000	-0.677076000
C	-2.353307000	1.727775000	0.779418000
C	-1.676475000	1.712688000	2.017407000
C	-2.699365000	2.966026000	0.203725000
C	-1.341159000	2.909912000	2.652194000
C	-2.365415000	4.158187000	0.843848000
C	-1.686490000	4.133502000	2.069063000
H	-1.402878000	0.752909000	2.460200000
H	-3.218971000	2.988765000	-0.756329000
H	-0.812010000	2.886890000	3.607746000
H	-2.629914000	5.113241000	0.384334000
H	-1.428544000	5.070075000	2.568960000
C	-4.643435000	0.340409000	-0.065042000
C	-4.820999000	-0.636858000	0.971813000
C	-4.806761000	-0.024860000	-1.447368000
C	-4.922619000	-1.366054000	-1.758253000
C	-4.956033000	-2.359141000	-0.745646000
C	-4.919679000	-1.977159000	0.606173000

H	-4.837131000	1.380801000	0.200004000
H	-4.999885000	-1.676828000	-2.803572000
H	-4.995189000	-2.743706000	1.380955000
C	-5.076760000	-3.803172000	-1.138092000
H	-6.022972000	-3.970813000	-1.680329000
H	-4.265953000	-4.088280000	-1.828418000
H	-5.051097000	-4.476204000	-0.270486000
C	-4.744344000	1.036806000	-2.505710000
H	-5.330615000	1.924864000	-2.222299000
H	-3.698692000	1.363336000	-2.644417000
H	-5.110491000	0.669949000	-3.474581000
C	-4.893817000	-0.195097000	2.401863000
H	-4.802860000	-1.039086000	3.099323000
H	-4.111980000	0.545812000	2.632574000
H	-5.861698000	0.300756000	2.590227000
Au	0.145398000	-0.461573000	-0.295062000
C	2.980009000	1.505750000	0.088992000
C	3.685047000	1.946759000	-0.986703000
C	3.900052000	0.926626000	-2.064992000
C	3.353962000	-0.294385000	-1.820009000
C	2.570928000	2.223414000	1.338414000
H	2.886282000	1.664209000	2.236153000
H	1.473902000	2.332538000	1.397050000
H	3.012140000	3.228042000	1.398467000
C	4.236150000	3.332548000	-1.157366000
H	4.028547000	3.975389000	-0.292663000
H	3.807700000	3.816838000	-2.050627000
H	5.327826000	3.307115000	-1.307785000
C	4.674465000	1.299789000	-3.295809000
H	4.751886000	0.469172000	-4.008356000
H	5.696773000	1.621460000	-3.036962000
H	4.200137000	2.148600000	-3.815495000
C	3.383158000	-1.547967000	-2.638591000
H	4.005368000	-1.438088000	-3.537491000
H	2.369730000	-1.839323000	-2.963211000
H	3.786599000	-2.391891000	-2.052758000
C	3.351589000	-1.293546000	0.949663000
C	4.742000000	-1.150015000	1.106580000
H	5.281092000	-0.397337000	0.525035000
C	5.429410000	-1.968056000	2.003066000
H	6.509395000	-1.855098000	2.123824000
C	4.736626000	-2.932619000	2.746258000
H	5.277949000	-3.572265000	3.447511000
C	3.355772000	-3.078683000	2.591466000
H	2.815622000	-3.832035000	3.169667000
C	2.660493000	-2.260992000	1.694358000
H	1.580441000	-2.377204000	1.572894000
P	2.474459000	-0.211449000	-0.231807000

TS4:

E = -1831.559829

G = -1831.645458

C	2.254471000	-0.470028000	0.405311000
C	2.950336000	0.256008000	-0.411062000
H	2.698638000	-1.194528000	1.099825000
C	2.915584000	1.356097000	-1.342120000
C	3.178022000	1.173107000	-2.717399000
C	2.568648000	2.641228000	-0.867295000
C	3.085118000	2.249312000	-3.595711000
C	2.473125000	3.712815000	-1.755734000
C	2.733819000	3.519878000	-3.117333000

H	3.456415000	0.183738000	-3.085487000
H	2.370963000	2.780840000	0.197486000
H	3.288695000	2.103095000	-4.658802000
H	2.205439000	4.704625000	-1.384217000
H	2.670202000	4.362914000	-3.809405000
C	5.105065000	-0.227822000	-0.341838000
C	5.049455000	-1.646816000	-0.512168000
C	5.298749000	0.352217000	0.950642000
C	5.252359000	-0.485596000	2.064250000
C	5.114201000	-1.877037000	1.922161000
C	5.024883000	-2.439605000	0.623748000
H	5.338860000	0.384991000	-1.213653000
H	5.358804000	-0.058060000	3.064286000
H	4.956155000	-3.526219000	0.523940000
C	5.129913000	-2.777498000	3.124018000
H	6.134442000	-3.222514000	3.237997000
H	4.900750000	-2.236022000	4.052370000
H	4.424098000	-3.614772000	3.012775000
C	5.576049000	1.820423000	1.077280000
H	6.644282000	2.012725000	0.875012000
H	5.006527000	2.407913000	0.341063000
H	5.356540000	2.196284000	2.086491000
C	4.949253000	-2.232180000	-1.892496000
H	5.201140000	-3.301846000	-1.900432000
H	3.918166000	-2.130246000	-2.275074000
H	5.614582000	-1.714264000	-2.600259000
P	-2.099293000	0.321614000	0.449214000
N	-5.708924000	-1.064554000	-0.721320000
N	-2.776573000	-3.267025000	-1.409033000
C	-2.907246000	0.677768000	2.038650000
C	-3.397759000	1.946787000	1.972241000
C	-3.222084000	2.633216000	0.648342000
C	-2.603685000	1.892633000	-0.312887000
C	-3.151383000	-0.936786000	-0.323244000
C	-4.430241000	-1.333933000	-0.686207000
C	-3.309178000	-2.165012000	-0.944558000
C	-6.209465000	0.197853000	-0.161792000
H	-5.374400000	0.781718000	0.243232000
H	-6.714832000	0.777559000	-0.949615000
H	-6.931875000	-0.014477000	0.641372000
C	-6.707930000	-1.969950000	-1.294821000
H	-7.245887000	-1.462554000	-2.110357000
H	-6.224939000	-2.869403000	-1.691702000
H	-7.433740000	-2.263370000	-0.520736000
C	-3.562774000	-4.333987000	-2.032916000
H	-4.624984000	-4.066987000	-2.046692000
H	-3.220795000	-4.494697000	-3.067061000
H	-3.436450000	-5.270626000	-1.468174000
C	-1.328825000	-3.485414000	-1.319100000
H	-0.909128000	-3.612859000	-2.329119000
H	-0.845719000	-2.627914000	-0.833035000
H	-1.126551000	-4.395492000	-0.733189000
C	-2.888267000	-0.297104000	3.175872000
H	-1.861704000	-0.462020000	3.544767000
H	-3.494097000	0.054124000	4.021941000
H	-3.281654000	-1.282173000	2.871863000
C	-4.065590000	2.673533000	3.100968000
H	-3.502064000	3.584219000	3.362518000
H	-5.076974000	3.004426000	2.813803000
H	-4.151205000	2.059897000	4.005879000
C	-3.704589000	4.042098000	0.473267000

H	-3.201956000	4.715131000	1.187071000
H	-3.523228000	4.426430000	-0.537720000
H	-4.784428000	4.119181000	0.680394000
C	-2.228520000	2.247265000	-1.719772000
H	-2.710254000	3.179085000	-2.045681000
H	-1.137310000	2.380063000	-1.820178000
H	-2.521634000	1.455738000	-2.429995000
Au	0.190252000	-0.159970000	0.410772000

TS5:

E = -2126.606537

G = -2126.690272

C	2.398231000	-0.590662000	-0.350169000
C	3.029709000	0.229749000	0.419333000
H	2.885412000	-1.278999000	-1.053210000
C	2.961336000	1.141469000	1.530581000
C	3.356643000	2.492508000	1.422076000
C	2.432377000	0.673643000	2.755003000
C	3.209576000	3.355496000	2.504913000
C	2.279186000	1.547201000	3.832368000
C	2.668486000	2.886015000	3.710742000
H	3.780285000	2.853922000	0.483384000
H	2.139484000	-0.374767000	2.840185000
H	3.521146000	4.398633000	2.415777000
H	1.869529000	1.179917000	4.776132000
H	2.562388000	3.564704000	4.560285000
C	5.264437000	0.168869000	0.013529000
C	5.235118000	0.355043000	-1.400088000
C	5.419385000	-1.128376000	0.587744000
C	5.393442000	-2.233044000	-0.262412000
C	5.295293000	-2.076776000	-1.656599000
C	5.223899000	-0.773143000	-2.206723000
H	5.466590000	1.033350000	0.647081000
H	5.478713000	-3.238178000	0.157888000
H	5.176138000	-0.661021000	-3.293271000
C	5.330875000	-3.271011000	-2.567191000
H	4.669119000	-3.139628000	-3.436697000
H	6.353719000	-3.402778000	-2.962807000
H	5.057660000	-4.198944000	-2.045472000
C	5.626684000	-1.268664000	2.067329000
H	6.662746000	-0.992337000	2.328681000
H	4.967878000	-0.590947000	2.633262000
H	5.458933000	-2.298759000	2.411248000
C	5.134452000	1.740639000	-1.974895000
H	5.446706000	1.768732000	-3.028255000
H	4.087556000	2.091276000	-1.929966000
H	5.749919000	2.459719000	-1.412969000
P	-1.968692000	-1.036573000	0.134608000
N	-2.871009000	1.497942000	-0.607563000
C	-2.320131000	-1.785710000	1.744508000
C	-2.763361000	-3.054980000	1.512795000
C	-2.955694000	-3.411623000	0.074035000
C	-2.651042000	-2.425257000	-0.818042000
C	-3.208226000	0.359153000	-0.080940000
C	-4.677899000	0.332974000	0.338064000
C	-5.227653000	1.571851000	-0.415842000
H	-5.678036000	1.245279000	-1.364788000
H	-6.011856000	2.082030000	0.158905000
C	-4.041881000	2.503296000	-0.709458000
C	-4.112906000	3.120401000	-2.105836000

H	-4.973777000	3.805099000	-2.126082000
H	-4.273116000	2.365072000	-2.884684000
H	-3.213386000	3.705245000	-2.343641000
C	-3.847390000	3.611793000	0.332592000
H	-2.940815000	4.196896000	0.126406000
H	-3.802451000	3.228365000	1.358748000
H	-4.706962000	4.294205000	0.266319000
C	-5.436067000	-0.939487000	-0.073284000
H	-5.111490000	-1.812604000	0.504293000
H	-5.319029000	-1.159256000	-1.143944000
H	-6.507287000	-0.781468000	0.123394000
C	-4.774609000	0.503117000	1.876400000
H	-5.829844000	0.672009000	2.137476000
H	-4.195676000	1.358853000	2.250181000
H	-4.439218000	-0.401466000	2.397074000
C	-1.541598000	1.912992000	-1.023391000
C	-1.165132000	1.734783000	-2.371938000
C	0.073559000	2.256780000	-2.770382000
H	0.387349000	2.130697000	-3.809422000
C	0.897364000	2.927816000	-1.869129000
H	1.846966000	3.348257000	-2.207699000
C	0.524206000	3.036755000	-0.531358000
H	1.191446000	3.514805000	0.187152000
C	-0.690428000	2.513981000	-0.068402000
C	-0.970894000	2.555679000	1.414543000
H	-1.154223000	3.583052000	1.764306000
H	-1.833577000	1.947531000	1.710475000
H	-0.093861000	2.177445000	1.962299000
C	-1.992910000	0.985979000	-3.387012000
H	-2.862337000	0.477118000	-2.954657000
H	-2.357660000	1.661696000	-4.176026000
H	-1.373932000	0.222828000	-3.882702000
C	-1.911042000	-1.155045000	3.045951000
H	-0.870446000	-1.418868000	3.301688000
H	-1.965480000	-0.057386000	3.010779000
H	-2.550585000	-1.491201000	3.874938000
C	-3.010493000	-4.078240000	2.578997000
H	-2.866416000	-3.677503000	3.589819000
H	-4.034484000	-4.479477000	2.509242000
H	-2.329504000	-4.936810000	2.455465000
C	-3.449102000	-4.778553000	-0.290448000
H	-4.456865000	-4.944902000	0.126307000
H	-3.504760000	-4.935288000	-1.374204000
H	-2.800174000	-5.559106000	0.137663000
C	-2.713054000	-2.441080000	-2.315389000
H	-2.817385000	-3.464701000	-2.699638000
H	-3.572248000	-1.863587000	-2.698491000
H	-1.804599000	-2.008094000	-2.761197000
Au	0.321048000	-0.655363000	-0.183021000

TS6:

E = -1831.645911

G = -1831.726124

C	-2.250861000	-0.676983000	0.004009000
C	-2.758796000	0.506336000	-0.003157000
H	-2.823106000	-1.613829000	0.010400000
C	-2.558352000	1.925973000	-0.097687000
C	-2.642435000	2.751000000	1.045931000
C	-2.219186000	2.497540000	-1.345140000

C	-2.384053000	4.116268000	0.941304000
C	-1.960286000	3.865561000	-1.439274000
C	-2.045331000	4.675594000	-0.299854000
H	-2.917965000	2.310317000	2.005923000
H	-2.159156000	1.857127000	-2.227269000
H	-2.457363000	4.752730000	1.826194000
H	-1.705610000	4.305148000	-2.406466000
H	-1.860474000	5.749639000	-0.379900000
C	-5.057214000	0.421245000	0.161378000
C	-5.146075000	-0.410700000	1.315519000
C	-5.212799000	-0.113365000	-1.151590000
C	-5.303211000	-1.497385000	-1.293738000
C	-5.322995000	-2.345590000	-0.171723000
C	-5.253201000	-1.781318000	1.125154000
H	-5.141301000	1.501577000	0.292069000
H	-5.392537000	-1.931374000	-2.292868000
H	-5.302525000	-2.444768000	1.992893000
C	-5.486639000	-3.830063000	-0.334338000
H	-6.546729000	-4.102966000	-0.186516000
H	-5.196259000	-4.172069000	-1.337727000
H	-4.907742000	-4.388355000	0.416875000
C	-5.316107000	0.807951000	-2.332377000
H	-6.367194000	1.116062000	-2.471136000
H	-4.734563000	1.730288000	-2.185036000
H	-4.991918000	0.321712000	-3.263829000
C	-5.056469000	0.188927000	2.691886000
H	-5.582095000	-0.427178000	3.435405000
H	-4.001568000	0.254439000	3.013397000
H	-5.479373000	1.204054000	2.723234000
P	2.181722000	-0.777175000	0.067686000
N	2.471542000	2.077771000	0.332929000
C	2.871798000	-1.713120000	-1.324419000
C	3.439799000	-2.837578000	-0.805674000
C	3.481212000	-2.902096000	0.693579000
C	2.937388000	-1.830449000	1.338520000
C	3.032813000	0.860411000	0.113221000
N	4.351138000	1.076505000	-0.124756000
C	4.625332000	2.432386000	-0.081585000
C	3.434797000	3.067371000	0.209919000
C	3.148483000	4.520796000	0.383908000
H	4.047540000	5.110808000	0.167624000
H	2.842221000	4.755542000	1.416507000
H	2.353722000	4.862984000	-0.297307000
C	2.647705000	-1.307528000	-2.749618000
H	2.968212000	-0.267190000	-2.931775000
H	3.202613000	-1.951392000	-3.445236000
H	1.580009000	-1.365600000	-3.021379000
C	4.002755000	-3.968725000	-1.611501000
H	3.920515000	-3.799923000	-2.691967000
H	5.065543000	-4.132700000	-1.369067000
H	3.480295000	-4.910235000	-1.375547000
C	4.079065000	-4.099549000	1.368065000
H	5.123248000	-4.251577000	1.050303000
H	4.062623000	-4.020499000	2.461674000
H	3.530258000	-5.013186000	1.086404000

C	2.777574000	-1.557621000	2.803367000
H	3.366167000	-2.257681000	3.411395000
H	3.105500000	-0.537456000	3.064982000
H	1.723067000	-1.650320000	3.115087000
Au	-0.162174000	-0.710910000	0.042167000
C	5.984308000	3.000237000	-0.313672000
H	6.391919000	2.689494000	-1.288420000
H	5.944878000	4.096280000	-0.303000000
H	6.694436000	2.688040000	0.469636000
C	1.070733000	2.357053000	0.671108000
H	0.727671000	1.674923000	1.457021000
H	0.993962000	3.381379000	1.046937000
H	0.425861000	2.257515000	-0.212766000
C	5.357450000	0.043658000	-0.385592000
H	5.313687000	-0.275259000	-1.435636000
H	6.349904000	0.451894000	-0.169015000
H	5.177556000	-0.816214000	0.268647000

TS7:

E = -1982.851787

G = -1982.936556

C	2.362586000	-0.903318000	-0.072655000
C	3.072614000	0.175322000	-0.098134000
H	2.762975000	-1.923800000	-0.108655000
C	3.072265000	1.610464000	0.037182000
C	3.328104000	2.456365000	-1.063470000
C	2.741388000	2.178917000	1.288143000
C	3.241950000	3.838656000	-0.916267000
C	2.652362000	3.564712000	1.425073000
C	2.904945000	4.394826000	0.326251000
H	3.593252000	2.018728000	-2.027729000
H	2.546160000	1.521810000	2.137956000
H	3.440715000	4.489584000	-1.770548000
H	2.395086000	3.999662000	2.393536000
H	2.849516000	5.480304000	0.439373000
C	5.264912000	-0.251459000	-0.373482000
C	5.191208000	-1.110701000	-1.511187000
C	5.415346000	-0.780368000	0.943885000
C	5.324740000	-2.161544000	1.115032000
C	5.176745000	-3.023006000	0.014422000
C	5.121595000	-2.478132000	-1.292365000
H	5.510799000	0.799428000	-0.534769000
H	5.402661000	-2.585208000	2.119368000
H	5.040087000	-3.158514000	-2.144427000
C	5.144059000	-4.513181000	0.202590000
H	6.134816000	-4.938030000	-0.037510000
H	4.904257000	-4.796358000	1.237009000
H	4.421980000	-4.991692000	-0.476688000
C	5.697375000	0.140927000	2.094000000
H	6.775792000	0.375218000	2.125259000
H	5.169800000	1.100974000	1.986797000
H	5.429006000	-0.311039000	3.059410000
C	5.117141000	-0.524000000	-2.893204000
H	5.406821000	-1.254888000	-3.661226000
H	4.083354000	-0.204385000	-3.115472000
H	5.765383000	0.359774000	-2.993956000
Au	0.311376000	-0.516125000	0.090678000
P	-1.905655000	0.210738000	0.354899000
C	-2.091752000	1.953682000	-0.157010000

C	-0.985722000	2.809896000	-0.002179000
C	-3.301248000	2.462155000	-0.665917000
C	-1.094944000	4.158454000	-0.347822000
C	-3.399793000	3.811249000	-1.013523000
C	-2.298376000	4.660074000	-0.853644000
H	-0.035117000	2.432838000	0.383869000
H	-4.170888000	1.812149000	-0.792203000
H	-0.230463000	4.814478000	-0.225054000
H	-4.340589000	4.203365000	-1.406681000
H	-2.379990000	5.714737000	-1.126473000
C	-2.611408000	-0.010539000	2.021645000
C	-3.697761000	0.765687000	2.462092000
C	-2.074320000	-1.009100000	2.852947000
C	-4.251707000	0.527469000	3.721640000
C	-2.638196000	-1.243043000	4.110335000
C	-3.726455000	-0.477808000	4.543014000
H	-4.104673000	1.561658000	1.834652000
H	-1.217030000	-1.601845000	2.522356000
H	-5.091634000	1.134112000	4.067758000
H	-2.219622000	-2.017056000	4.757527000
H	-4.160479000	-0.656729000	5.529554000
C	-3.081143000	-0.658876000	-0.713520000
C	-4.093436000	-1.587551000	-0.903006000
C	-3.523402000	-0.901287000	-2.002887000
N	-3.426805000	-0.618792000	-3.278199000
N	-4.940574000	-2.448047000	-0.396431000
C	-2.434973000	0.358634000	-3.742397000
H	-1.872844000	0.758721000	-2.889677000
H	-1.739716000	-0.123000000	-4.447347000
H	-2.943711000	1.189117000	-4.255721000
C	-4.267434000	-1.240156000	-4.303666000
H	-3.639775000	-1.795226000	-5.018135000
H	-4.982100000	-1.931251000	-3.843601000
H	-4.824152000	-0.463860000	-4.851047000
C	-5.867551000	-3.227637000	-1.220207000
H	-5.713656000	-3.006953000	-2.282054000
H	-5.700250000	-4.302711000	-1.052231000
H	-6.906714000	-2.985169000	-0.948434000
C	-5.007807000	-2.672381000	1.053235000
H	-6.023160000	-2.446603000	1.413810000
H	-4.779103000	-3.726024000	1.276209000
H	-4.290465000	-2.026079000	1.570853000

TS8:

E = -1099.524150

G = -1098.056338

C	-0.920449000	-0.642588000	0.022255000
C	-1.561177000	0.489077000	0.100301000
H	-1.441764000	-1.606568000	-0.026653000
C	-1.282801000	1.919247000	0.026094000
C	-1.599252000	2.801953000	1.077474000
C	-0.616374000	2.421288000	-1.112187000
C	-1.247862000	4.148500000	0.997862000
C	-0.263615000	3.770310000	-1.185108000
C	-0.579681000	4.636130000	-0.132777000
H	-2.111612000	2.422803000	1.963986000
H	-0.368354000	1.735771000	-1.925081000
H	-1.490941000	4.822405000	1.822526000
H	0.253016000	4.148505000	-2.070552000
H	-0.309715000	5.693095000	-0.193519000

C	-3.602557000	0.352235000	0.238012000
C	-3.768798000	-0.565990000	1.332944000
C	-3.803995000	-0.083400000	-1.114380000
C	-3.937467000	-1.449013000	-1.356084000
C	-3.984219000	-2.371192000	-0.297667000
C	-3.920784000	-1.907999000	1.041854000
H	-3.769607000	1.410043000	0.445858000
H	-4.032822000	-1.808163000	-2.383484000
H	-4.003824000	-2.634291000	1.854809000
C	-4.146573000	-3.840678000	-0.559190000
H	-3.342103000	-4.414843000	-0.070900000
H	-5.095367000	-4.200369000	-0.125868000
H	-4.144400000	-4.077226000	-1.631794000
C	-3.869486000	0.927556000	-2.218722000
H	-4.839751000	1.452766000	-2.185527000
H	-3.090793000	1.697953000	-2.104780000
H	-3.769539000	0.462401000	-3.209104000
C	-3.673399000	-0.062146000	2.743069000
H	-4.043604000	-0.801433000	3.466819000
H	-2.618910000	0.151294000	2.991606000
H	-4.238590000	0.873379000	2.877210000
N	3.970643000	0.648537000	0.040189000
C	3.222517000	-0.486742000	0.015237000
N	4.123856000	-1.502492000	-0.009877000
C	5.417847000	-1.011447000	0.001350000
C	5.321010000	0.345788000	0.034745000
H	6.090861000	1.112623000	0.053582000
Au	1.160831000	-0.593318000	0.022898000
H	6.288376000	-1.661741000	-0.018651000
C	3.449678000	2.009457000	0.109519000
H	3.602556000	2.426412000	1.116223000
H	3.966110000	2.640946000	-0.627138000
H	2.375969000	2.000576000	-0.114661000
C	3.803146000	-2.924182000	-0.053593000
H	4.190449000	-3.371118000	-0.980985000
H	4.248881000	-3.436815000	0.811198000
H	2.714081000	-3.045546000	-0.022303000

TS9:

E = -902.896540

G = -902.949339

C	-1.590561000	-0.644599000	0.017422000
C	-2.254408000	0.473164000	0.101619000
H	-2.091986000	-1.618936000	-0.034310000
C	-2.007411000	1.909060000	0.032228000
C	-2.343437000	2.781366000	1.086302000
C	-1.351401000	2.428873000	-1.104128000
C	-2.021634000	4.135451000	1.010830000
C	-1.028289000	3.785464000	-1.172783000
C	-1.363935000	4.640965000	-0.118157000
H	-2.847568000	2.388464000	1.971539000
H	-1.087492000	1.751349000	-1.918683000
H	-2.279539000	4.801379000	1.837456000
H	-0.519125000	4.177359000	-2.056565000
H	-1.117138000	5.703759000	-0.175564000
C	-4.292979000	0.291005000	0.244256000
C	-4.435375000	-0.633840000	1.336951000
C	-4.487961000	-0.145096000	-1.108947000
C	-4.590715000	-1.512669000	-1.354354000
C	-4.613111000	-2.438787000	-0.298472000
C	-4.557088000	-1.978194000	1.042244000

H	-4.482822000	1.344253000	0.455680000
H	-4.680203000	-1.871005000	-2.382560000
H	-4.621121000	-2.708621000	1.853211000
C	-4.741580000	-3.910906000	-0.563902000
H	-5.681210000	-4.293769000	-0.130437000
H	-4.735318000	-4.144398000	-1.637156000
H	-3.923384000	-4.467570000	-0.078164000
C	-4.577358000	0.867719000	-2.209924000
H	-5.554555000	1.379132000	-2.167503000
H	-3.808648000	1.648699000	-2.099606000
H	-4.478267000	0.406856000	-3.202369000
C	-4.347840000	-0.131928000	2.748289000
H	-4.699330000	-0.881415000	3.470870000
H	-3.297843000	0.104690000	2.994905000
H	-4.933752000	0.790176000	2.886451000
N	3.268627000	0.732817000	0.025330000
C	2.548804000	-0.421256000	0.009900000
N	3.447072000	-1.440447000	-0.005244000
C	4.748561000	-0.943906000	0.001915000
C	4.633631000	0.455549000	0.022780000
Au	0.489715000	-0.556417000	0.015917000
C	2.730048000	2.083825000	0.050133000
H	3.029065000	2.593606000	0.978666000
H	3.111505000	2.654517000	-0.810024000
H	1.635334000	2.042946000	-0.002502000
C	3.135456000	-2.860512000	-0.025400000
H	3.556490000	-3.326380000	-0.929231000
H	3.560247000	-3.352278000	0.862790000
H	2.046967000	-2.990803000	-0.024857000
C	5.759644000	1.283324000	0.036939000
H	5.672700000	2.370693000	0.055102000
C	5.994132000	-1.577655000	-0.007455000
H	6.085056000	-2.664727000	-0.023937000
C	7.004770000	0.652391000	0.027810000
H	7.911561000	1.260797000	0.038458000
C	7.119936000	-0.752641000	0.005737000
H	8.113643000	-1.205392000	-0.000675000

TS10:

E = -907.903441

G = -907.957771

C	-0.128888000	-0.623482000	-0.008569000
C	-0.674912000	0.551116000	0.078963000
H	-0.724736000	-1.544045000	-0.070559000
C	-0.443487000	1.970966000	0.042695000
C	-0.632621000	2.780167000	1.185221000
C	0.024699000	2.557292000	-1.155376000
C	-0.348672000	4.141097000	1.129713000
C	0.310148000	3.921791000	-1.199414000
C	0.121105000	4.713782000	-0.061476000
H	-0.997916000	2.329309000	2.109828000
H	0.172308000	1.929018000	-2.036109000
H	-0.488108000	4.762468000	2.016985000
H	0.679988000	4.369878000	-2.124316000
H	0.341131000	5.783238000	-0.100078000
C	-2.857005000	0.429686000	0.262359000
C	-2.970320000	-0.498089000	1.346983000
C	-3.055600000	0.008941000	-1.089967000
C	-3.179410000	-1.356266000	-1.345823000
C	-3.205488000	-2.292486000	-0.298121000
C	-3.113562000	-1.841643000	1.043101000

H	-2.964272000	1.492188000	0.484460000
H	-3.287920000	-1.703495000	-2.376180000
H	-3.170272000	-2.576425000	1.850762000
C	-3.382255000	-3.757827000	-0.575132000
H	-2.655097000	-4.360701000	-0.008282000
H	-4.384600000	-4.082431000	-0.245434000
H	-3.283143000	-3.995298000	-1.643097000
C	-3.152473000	1.030259000	-2.183685000
H	-4.166135000	1.467580000	-2.193075000
H	-2.452230000	1.864465000	-2.023829000
H	-2.968506000	0.591726000	-3.174497000
C	-2.850461000	-0.014510000	2.764234000
H	-3.268452000	-0.738959000	3.477136000
H	-1.787224000	0.128929000	3.026365000
H	-3.359231000	0.950742000	2.908712000
C	3.905676000	-0.989109000	0.012811000
Au	1.928534000	-0.786505000	0.003830000
O	5.026425000	-1.115547000	0.015945000

INT1 :

E = -1831.202160

G = -1831.278010

C	-2.160156000	-0.615856000	-0.004316000
C	-2.980678000	0.440681000	0.108194000
C	-4.591953000	0.217666000	0.259776000
C	-4.866840000	-0.744023000	1.355023000
C	-4.989626000	-0.176842000	-1.107186000
C	-5.305114000	-1.502396000	-1.360785000
C	-5.423120000	-2.432412000	-0.311176000
C	-5.238010000	-2.024511000	1.044188000
Au	-0.095441000	-0.521018000	-0.016392000
P	2.255347000	-0.283359000	0.003580000
H	-4.982614000	1.212541000	0.511565000
H	-5.505300000	-1.826698000	-2.384351000
H	-5.392505000	-2.759561000	1.837980000
H	-2.634920000	-1.607468000	-0.030485000
C	2.994471000	-0.520876000	1.661662000
C	4.030486000	0.294697000	2.143037000
C	2.517227000	-1.579902000	2.453362000
C	4.586591000	0.046151000	3.401729000
C	3.081010000	-1.827475000	3.706137000
C	4.115978000	-1.014189000	4.181855000
H	4.403381000	1.125149000	1.539808000
H	1.701852000	-2.210295000	2.087302000
H	5.391573000	0.684873000	3.773030000
H	2.708358000	-2.653827000	4.316156000
H	4.553076000	-1.205336000	5.164911000
C	2.752670000	1.399957000	-0.525468000
C	1.959639000	2.487571000	-0.119693000
C	3.904696000	1.630683000	-1.294454000
C	2.323600000	3.789477000	-0.468405000
C	4.261114000	2.936491000	-1.645053000
C	3.474534000	4.016108000	-1.231264000
H	1.049287000	2.319320000	0.461619000
H	4.523106000	0.793241000	-1.625005000
H	1.700191000	4.627409000	-0.147641000
H	5.157438000	3.109537000	-2.245447000
H	3.756585000	5.035021000	-1.507563000
C	3.145434000	-1.435504000	-1.105537000
C	2.574887000	-1.725306000	-2.357015000
C	4.379352000	-2.006135000	-0.755069000

C	3.238357000	-2.566790000	-3.251732000
C	5.035910000	-2.853722000	-1.652580000
C	4.469136000	-3.132575000	-2.899859000
H	1.607935000	-1.292346000	-2.628837000
H	4.827840000	-1.793584000	0.217769000
H	2.791372000	-2.787588000	-4.223979000
H	5.994533000	-3.298052000	-1.374327000
H	4.984893000	-3.796141000	-3.598171000
C	-2.583968000	1.873247000	0.044923000
C	-3.005438000	2.799914000	1.017279000
C	-1.740629000	2.327141000	-0.988108000
C	-2.575915000	4.127168000	0.976606000
C	-1.316175000	3.657352000	-1.033607000
C	-1.729685000	4.561102000	-0.050830000
H	-3.654253000	2.475345000	1.835364000
H	-1.415612000	1.622251000	-1.755820000
H	-2.899182000	4.825917000	1.751838000
H	-0.658967000	3.986205000	-1.841738000
H	-1.401268000	5.602615000	-0.086953000
C	-5.775238000	-3.857269000	-0.589459000
H	-6.671952000	-4.146961000	-0.015494000
H	-5.951417000	-4.052366000	-1.655164000
H	-4.961474000	-4.515693000	-0.238189000
C	-5.028107000	0.861789000	-2.176854000
H	-5.910177000	1.507819000	-2.016752000
H	-4.150012000	1.524757000	-2.129463000
H	-5.102712000	0.421193000	-3.180009000
C	-4.621611000	-0.291758000	2.755455000
H	-4.883068000	-1.061248000	3.493896000
H	-3.552760000	-0.039173000	2.871571000
H	-5.190530000	0.626030000	2.979220000

INT2 :

E = -2057.024912

G = -2057.104728

C	-2.242401000	-0.411837000	-0.422398000
C	-3.114026000	0.470283000	0.094865000
C	-4.707875000	0.251926000	-0.122742000
C	-5.090847000	-1.126160000	0.277236000
C	-4.907557000	0.627884000	-1.540001000
C	-5.157710000	-0.364703000	-2.472949000
C	-5.389487000	-1.694907000	-2.072914000
C	-5.386964000	-2.048463000	-0.690426000
Au	-0.200917000	-0.411095000	-0.127039000
P	2.076392000	-0.385158000	0.264056000
H	-5.182313000	0.985715000	0.543177000
H	-5.214031000	-0.110950000	-3.533747000
H	-5.622003000	-3.079076000	-0.413197000
H	-2.669191000	-1.236286000	-1.011392000
C	-2.769446000	1.717718000	0.826171000
C	-3.397132000	2.060336000	2.038758000
C	-1.768322000	2.575032000	0.327777000
C	-3.015380000	3.201103000	2.746273000
C	-1.387047000	3.717621000	1.034211000
C	-2.006799000	4.032943000	2.246434000
H	-4.173121000	1.412606000	2.456173000
H	-1.284107000	2.338003000	-0.621608000
H	-3.502142000	3.438658000	3.695183000
H	-0.599434000	4.357377000	0.632589000
H	-1.709395000	4.927071000	2.799300000

C	-5.667284000	-2.757876000	-3.084482000
H	-6.611250000	-3.276118000	-2.844853000
H	-5.718819000	-2.368406000	-4.109386000
H	-4.876107000	-3.526965000	-3.037252000
C	-4.817402000	2.066274000	-1.923036000
H	-5.708505000	2.596998000	-1.542319000
H	-3.948285000	2.554301000	-1.453791000
H	-4.773003000	2.203014000	-3.011673000
C	-5.039758000	-1.466883000	1.728480000
H	-5.360183000	-2.498315000	1.926184000
H	-4.005395000	-1.339944000	2.093484000
H	-5.669326000	-0.778169000	2.316369000
O	2.664754000	-1.423111000	1.369917000
O	2.733202000	0.945753000	0.923073000
O	2.912894000	-0.645796000	-1.103411000
C	2.450885000	2.247751000	0.526607000
C	2.494626000	3.224657000	1.523589000
C	2.168033000	2.580283000	-0.802086000
C	2.262046000	4.557933000	1.181530000
H	2.720505000	2.924335000	2.547994000
C	1.923165000	3.919146000	-1.127204000
H	2.166169000	1.813067000	-1.577651000
C	1.973643000	4.910126000	-0.142703000
H	2.306667000	5.326701000	1.956549000
H	1.708940000	4.186162000	-2.164789000
H	1.796713000	5.955061000	-0.406821000
C	4.275957000	-0.415364000	-1.337356000
C	4.604741000	0.099081000	-2.591942000
C	5.254996000	-0.700196000	-0.382941000
C	5.946933000	0.334419000	-2.899297000
H	3.808626000	0.300786000	-3.310970000
C	6.593460000	-0.453624000	-0.704763000
H	4.979575000	-1.105725000	0.590344000
C	6.943503000	0.061274000	-1.956461000
H	6.213021000	0.734436000	-3.880492000
H	7.367750000	-0.670786000	0.034754000
H	7.992121000	0.247925000	-2.197955000
C	2.155880000	-2.718476000	1.493519000
C	1.695623000	-3.112832000	2.749936000
C	2.138163000	-3.588581000	0.400423000
C	1.209505000	-4.412259000	2.914566000
H	1.731264000	-2.401716000	3.577031000
C	1.641209000	-4.883836000	0.578770000
H	2.520845000	-3.259617000	-0.567486000
C	1.178507000	-5.298064000	1.831285000
H	0.854179000	-4.733619000	3.896517000
H	1.627060000	-5.573877000	-0.268177000
H	0.800307000	-6.313876000	1.966133000

INT3:

E = -1679.911591

G = -1679.985061

C	1.954894000	-0.503034000	0.264186000
C	2.758389000	0.501703000	-0.120247000
H	2.447082000	-1.398253000	0.671385000
C	2.333156000	1.751895000	-0.805063000
C	1.459320000	1.689389000	-1.908666000
C	2.756618000	3.018670000	-0.361477000
C	1.006322000	2.855957000	-2.529821000
C	2.298362000	4.184578000	-0.976885000

C	1.420409000	4.107383000	-2.064081000
H	1.137595000	0.712518000	-2.275261000
H	3.429253000	3.099666000	0.496837000
H	0.332638000	2.785125000	-3.387229000
H	2.624110000	5.158584000	-0.604111000
H	1.068136000	5.019985000	-2.550446000
C	4.373142000	0.385529000	0.084426000
C	4.766179000	-0.562557000	-0.978873000
C	4.678842000	0.004787000	1.485324000
C	5.076788000	-1.275933000	1.759887000
C	5.261647000	-2.232700000	0.716829000
C	5.111801000	-1.858940000	-0.631894000
H	4.749279000	1.394629000	-0.130659000
H	5.255271000	-1.586143000	2.792470000
H	5.310760000	-2.595340000	-1.413587000
C	5.646539000	-3.628499000	1.084095000
H	6.547699000	-3.620343000	1.720534000
H	4.846446000	-4.085016000	1.693042000
H	5.829114000	-4.264745000	0.208479000
C	4.436602000	1.021194000	2.550163000
H	4.993237000	1.950189000	2.342045000
H	3.365001000	1.288036000	2.557895000
H	4.715580000	0.655272000	3.547172000
C	4.766000000	-0.098468000	-2.396260000
H	4.856147000	-0.931973000	-3.105526000
H	3.862850000	0.487433000	-2.628421000
H	5.621955000	0.582719000	-2.551542000
Au	-0.112114000	-0.449436000	0.258021000
C	-3.026774000	1.460050000	0.037314000
C	-3.730420000	1.817472000	1.144369000
C	-3.904669000	0.729861000	2.160739000
C	-3.327798000	-0.457914000	1.835540000
C	-2.655855000	2.263090000	-1.171190000
H	-2.956260000	1.743102000	-2.097308000
H	-1.564582000	2.416888000	-1.229559000
H	-3.136089000	3.251631000	-1.172734000
C	-4.315130000	3.176170000	1.402448000
H	-4.122280000	3.877212000	0.580555000
H	-3.898529000	3.613834000	2.324890000
H	-5.406231000	3.116550000	1.548542000
C	-4.674445000	1.008500000	3.419407000
H	-4.733804000	0.132025000	4.076962000
H	-5.703457000	1.330565000	3.189373000
H	-4.209176000	1.829076000	3.990394000
C	-3.311047000	-1.757557000	2.579207000
H	-3.919890000	-1.718493000	3.493289000
H	-2.284528000	-2.039861000	2.869086000
H	-3.701935000	-2.576523000	1.950789000
C	-3.341285000	-1.281000000	-0.984598000
C	-4.734466000	-1.149236000	-1.124236000
H	-5.278292000	-0.436781000	-0.498133000
C	-5.418203000	-1.926163000	-2.059396000
H	-6.500555000	-1.821522000	-2.166263000
C	-4.718564000	-2.839035000	-2.859323000
H	-5.256698000	-3.446757000	-3.590853000
C	-3.334703000	-2.973586000	-2.722523000
H	-2.788914000	-3.686380000	-3.345299000
C	-2.643581000	-2.196141000	-1.786932000
H	-1.560938000	-2.301943000	-1.679694000
P	-2.461426000	-0.256156000	0.248959000

INT4:

E = -1831.568322

G = -1831.651459

P	-2.056526000	-0.269365000	-0.509947000
N	-5.681703000	1.175428000	0.568766000
N	-2.741145000	3.397317000	1.169998000
C	-2.877260000	-0.711099000	-2.072574000
C	-3.375122000	-1.971615000	-1.935832000
C	-3.204538000	-2.581881000	-0.576023000
C	-2.582351000	-1.789714000	0.340568000
C	-3.122641000	1.023092000	0.189615000
C	-4.401340000	1.440637000	0.527610000
C	-3.279641000	2.278097000	0.753061000
C	-6.180768000	-0.111151000	0.067008000
H	-5.342870000	-0.717685000	-0.296696000
H	-6.698732000	-0.648906000	0.876170000
H	-6.891782000	0.062393000	-0.755584000
C	-6.680724000	2.108068000	1.094509000
H	-7.218134000	1.644523000	1.936259000
H	-6.198291000	3.027832000	1.442876000
H	-7.407740000	2.360335000	0.307030000
C	-3.522428000	4.495419000	1.741394000
H	-4.586226000	4.234841000	1.764293000
H	-3.183428000	4.701992000	2.768489000
H	-3.390213000	5.405193000	1.135308000
C	-1.291697000	3.599135000	1.075378000
H	-0.875277000	3.773655000	2.079821000
H	-0.812946000	2.714285000	0.635383000
H	-1.079393000	4.477149000	0.445457000
C	-2.854784000	0.196676000	-3.264143000
H	-1.826244000	0.345526000	-3.634226000
H	-3.453701000	-0.204079000	-4.093066000
H	-3.253848000	1.195989000	-3.019175000
C	-4.046844000	-2.757895000	-3.022325000
H	-3.494306000	-3.689794000	-3.225743000
H	-5.063843000	-3.058159000	-2.721213000
H	-4.121249000	-2.199186000	-3.963178000
C	-3.694599000	-3.976574000	-0.321914000
H	-3.191108000	-4.692604000	-0.991992000
H	-3.520598000	-4.302249000	0.710938000
H	-4.773594000	-4.061680000	-0.530432000
C	-2.209595000	-2.064655000	1.765665000
H	-2.701989000	-2.969339000	2.147879000
H	-1.119612000	-2.202374000	1.873124000
H	-2.491979000	-1.227917000	2.426782000
C	2.301208000	0.414931000	-0.377144000
C	3.123299000	-0.229443000	0.473125000
C	4.694517000	0.075304000	0.456235000
C	4.949652000	1.542387000	0.535110000
C	5.230589000	-0.635916000	-0.738063000
C	5.701276000	0.096449000	-1.810311000
C	5.826502000	1.500857000	-1.738506000
C	5.468502000	2.200301000	-0.547598000
Au	0.255355000	0.173422000	-0.458787000
H	5.091761000	-0.402823000	1.365688000
H	6.026737000	-0.417618000	-2.717454000
H	5.626524000	3.280970000	-0.509287000
H	2.768754000	1.127793000	-1.071067000
C	2.707635000	-1.289027000	1.433900000
C	3.059806000	-1.221521000	2.794798000

C	1.933984000	-2.382879000	0.998406000
C	2.626896000	-2.194908000	3.697143000
C	1.508183000	-3.362962000	1.899718000
C	1.848355000	-3.269941000	3.252641000
H	3.659797000	-0.384722000	3.163188000
H	1.682535000	-2.469158000	-0.061132000
H	2.899752000	-2.116338000	4.752096000
H	0.923930000	-4.213022000	1.538662000
H	1.523507000	-4.039225000	3.956943000
C	6.391942000	2.269686000	-2.883937000
H	7.402319000	2.627238000	-2.609979000
H	6.476073000	1.671570000	-3.800442000
H	5.794686000	3.174161000	-3.083674000
C	5.248826000	-2.125903000	-0.738220000
H	6.014023000	-2.474582000	-0.021068000
H	4.293568000	-2.544839000	-0.386139000
H	5.491337000	-2.538082000	-1.726478000
C	4.576348000	2.244445000	1.797689000
H	4.774647000	3.323239000	1.749032000
H	3.506537000	2.082848000	2.012347000
H	5.136288000	1.823369000	2.650387000

INT5:

E = -2126.615067

G = -2126.698534

P	1.911051000	1.067069000	0.009244000
N	2.932442000	-1.447317000	-0.608524000
C	2.270162000	1.889624000	1.587928000
C	2.654340000	3.168063000	1.303434000
C	2.789517000	3.484910000	-0.152166000
C	2.511442000	2.454177000	-1.000090000
C	3.234812000	-0.254030000	-0.191657000
C	4.728221000	-0.118205000	0.107600000
C	5.295348000	-1.372355000	-0.606176000
H	5.654970000	-1.085407000	-1.605363000
H	6.148792000	-1.797516000	-0.061777000
C	4.149217000	-2.385964000	-0.748732000
C	4.148125000	-3.080423000	-2.110569000
H	5.047427000	-3.711590000	-2.166449000
H	4.194168000	-2.364190000	-2.940115000
H	3.271746000	-3.730857000	-2.239699000
C	4.110459000	-3.439475000	0.365602000
H	3.227879000	-4.086766000	0.271199000
H	4.124035000	-2.996930000	1.368495000
H	5.003137000	-4.073488000	0.265539000
C	5.386550000	1.160787000	-0.433360000
H	5.061549000	2.051223000	0.116381000
H	5.178984000	1.310226000	-1.502148000
H	6.476253000	1.064933000	-0.312552000
C	4.944433000	-0.180100000	1.641938000
H	6.024095000	-0.267603000	1.834288000
H	4.449927000	-1.042559000	2.109652000
H	4.587669000	0.736422000	2.127179000
C	1.600372000	-1.968412000	-0.864995000
C	1.096497000	-1.925123000	-2.181818000
C	-0.128951000	-2.560792000	-2.423011000
H	-0.535836000	-2.550987000	-3.437152000
C	-0.828056000	-3.190372000	-1.394822000
H	-1.767911000	-3.703629000	-1.609390000
C	-0.345742000	-3.143588000	-0.088806000

H	-0.928598000	-3.573802000	0.727733000
C	0.873957000	-2.522744000	0.212113000
C	1.297794000	-2.430577000	1.657046000
H	1.600419000	-3.412063000	2.053100000
H	2.129158000	-1.735860000	1.824008000
H	0.448706000	-2.082943000	2.262871000
C	1.769021000	-1.186823000	-3.312618000
H	2.646331000	-0.611198000	-2.995063000
H	2.089390000	-1.877668000	-4.107664000
H	1.057688000	-0.479772000	-3.766575000
C	1.915832000	1.268115000	2.907178000
H	0.848052000	0.993463000	2.933946000
H	2.484731000	0.345702000	3.102995000
H	2.108489000	1.954674000	3.742219000
C	2.899258000	4.242055000	2.320427000
H	2.790551000	3.882854000	3.350755000
H	3.914449000	4.656736000	2.210655000
H	2.200779000	5.082754000	2.176757000
C	3.198985000	4.863293000	-0.575567000
H	4.199244000	5.106250000	-0.179654000
H	3.232106000	4.979416000	-1.665452000
H	2.509200000	5.621225000	-0.171107000
C	2.516874000	2.416578000	-2.498300000
H	2.668418000	3.416413000	-2.926427000
H	3.320726000	1.771182000	-2.892235000
H	1.565606000	2.023081000	-2.890648000
C	-2.440869000	0.470868000	-0.364114000
C	-3.250695000	-0.231859000	0.450280000
C	-4.820185000	-0.271652000	0.159681000
C	-5.085610000	-0.666232000	-1.254484000
C	-5.355291000	1.047953000	0.599807000
C	-5.851229000	1.928889000	-0.340459000
C	-5.997038000	1.550595000	-1.693626000
C	-5.629985000	0.240720000	-2.123283000
Au	-0.393935000	0.612975000	-0.238528000
H	-5.224433000	-1.053558000	0.822714000
H	-6.179506000	2.923997000	-0.032219000
H	-5.796735000	-0.032137000	-3.168265000
H	-2.926108000	1.004738000	-1.193617000
C	-2.820664000	-0.958724000	1.676225000
C	-3.214050000	-2.288221000	1.918282000
C	-1.998090000	-0.326166000	2.629130000
C	-2.777557000	-2.973271000	3.054562000
C	-1.570462000	-1.006005000	3.773025000
C	-1.952884000	-2.333932000	3.987780000
H	-3.851850000	-2.808529000	1.198417000
H	-1.713048000	0.716770000	2.473520000
H	-3.087501000	-4.008347000	3.216874000
H	-0.949694000	-0.490000000	4.509895000
H	-1.626957000	-2.863515000	4.885863000
C	-6.586575000	2.494469000	-2.685150000
H	-7.583788000	2.122048000	-2.985638000
H	-6.701644000	3.512636000	-2.291940000
H	-5.983483000	2.518759000	-3.607731000
C	-5.344056000	1.376862000	2.053654000
H	-6.096818000	0.753040000	2.568990000
H	-4.377068000	1.130103000	2.518376000
H	-5.585891000	2.431053000	2.242149000
C	-4.681010000	-2.038252000	-1.677462000
H	-4.918881000	-2.237191000	-2.730649000
H	-3.595356000	-2.159585000	-1.523410000

H -5.178871000 -2.799778000 -1.053461000

INT6:

E = -1831.653792

G = -1831.732775

C	2.294302000	-0.560931000	-0.088438000
C	2.980207000	0.590306000	0.038381000
H	2.880915000	-1.473540000	-0.263603000
C	2.363938000	1.911391000	0.350610000
C	2.588571000	3.037299000	-0.463105000
C	1.519403000	2.053882000	1.469750000
C	1.970397000	4.259114000	-0.184536000
C	0.910454000	3.279776000	1.757336000
C	1.130577000	4.385494000	0.928871000
H	3.239975000	2.955940000	-1.337255000
H	1.354936000	1.193602000	2.122262000
H	2.152565000	5.118937000	-0.833666000
H	0.277082000	3.375564000	2.642834000
H	0.669183000	5.348488000	1.160949000
C	4.569979000	0.598386000	-0.101959000
C	4.984437000	-0.079372000	-1.366567000
C	5.099131000	0.025907000	1.169175000
C	5.713819000	-1.209169000	1.154696000
C	5.987262000	-1.876833000	-0.060734000
C	5.638964000	-1.280618000	-1.308858000
H	4.855896000	1.661320000	-0.158975000
H	6.035551000	-1.666924000	2.092817000
H	5.910934000	-1.801234000	-2.230333000
C	6.697636000	-3.186633000	-0.060405000
H	7.727400000	-3.033004000	-0.435152000
H	6.759742000	-3.639712000	0.937384000
H	6.223270000	-3.891925000	-0.761960000
C	4.951442000	0.814247000	2.425554000
H	5.673626000	1.651135000	2.406065000
H	3.954992000	1.273856000	2.506598000
H	5.154998000	0.211559000	3.320549000
C	4.611356000	0.566683000	-2.658608000
H	4.955648000	-0.010061000	-3.526983000
H	3.515266000	0.677766000	-2.716622000
H	5.038380000	1.582337000	-2.719512000
P	-2.118232000	-0.875822000	-0.115949000
N	-2.501467000	1.914703000	-0.683584000
C	-2.732009000	-1.686579000	1.387748000
C	-3.300569000	-2.864794000	1.007270000
C	-3.420550000	-3.066077000	-0.473787000
C	-2.924066000	-2.052586000	-1.239676000
C	-3.021085000	0.727839000	-0.280406000
N	-4.313158000	0.964065000	0.059865000
C	-4.605815000	2.309009000	-0.093935000
C	-3.457315000	2.911223000	-0.564923000
C	-3.196604000	4.338096000	-0.911512000
H	-4.057749000	4.958780000	-0.634644000
H	-3.028794000	4.471424000	-1.993062000
H	-2.315079000	4.727095000	-0.378405000
C	-2.441154000	-1.148005000	2.755571000

H	-2.831579000	-0.122694000	2.880531000
H	-2.889420000	-1.770492000	3.541652000
H	-1.355234000	-1.099588000	2.943471000
C	-3.791576000	-3.928673000	1.942121000
H	-3.644798000	-3.665082000	2.996573000
H	-4.864719000	-4.125782000	1.784400000
H	-3.268721000	-4.880807000	1.755394000
C	-4.036691000	-4.325655000	-1.005164000
H	-5.054718000	-4.466668000	-0.607752000
H	-4.092678000	-4.337901000	-2.100388000
H	-3.452105000	-5.204814000	-0.687407000
C	-2.846661000	-1.915979000	-2.730151000
H	-3.486345000	-2.650158000	-3.238477000
H	-3.165647000	-0.913928000	-3.063280000
H	-1.814818000	-2.065043000	-3.092137000
Au	0.242388000	-0.711454000	-0.110128000
C	-5.943163000	2.895114000	0.207857000
H	-6.261854000	2.670745000	1.237818000
H	-5.912696000	3.986066000	0.097522000
H	-6.717591000	2.515790000	-0.479128000
C	-1.150518000	2.158370000	-1.203394000
H	-0.834303000	1.319775000	-1.832730000
H	-1.168467000	3.065107000	-1.816062000
H	-0.437668000	2.293067000	-0.379354000
C	-5.280041000	-0.041823000	0.506108000
H	-5.153903000	-0.247032000	1.577661000
H	-6.292365000	0.333640000	0.323641000
H	-5.136214000	-0.965263000	-0.065218000

INT7:

E = -1982.859093

G = -1982.943162

P	-1.898585000	0.201257000	0.302284000
C	-2.222704000	1.839323000	-0.441737000
C	-1.163831000	2.764538000	-0.474753000
C	-3.481659000	2.203910000	-0.954729000
C	-1.367380000	4.039219000	-1.008598000
C	-3.675370000	3.478578000	-1.491184000
C	-2.619429000	4.397565000	-1.517129000
H	-0.178083000	2.498574000	-0.086898000
H	-4.315850000	1.497798000	-0.939251000
H	-0.537517000	4.749170000	-1.027899000
H	-4.654599000	3.758468000	-1.886543000
H	-2.775423000	5.394191000	-1.936545000
C	-2.582058000	0.171344000	1.997637000
C	-3.726656000	0.909039000	2.345939000
C	-1.955968000	-0.648303000	2.952954000
C	-4.248381000	0.810124000	3.637532000
C	-2.487666000	-0.745349000	4.242349000
C	-3.633432000	-0.019339000	4.583599000
H	-4.204697000	1.569613000	1.619461000
H	-1.054363000	-1.208878000	2.691305000
H	-5.134238000	1.388389000	3.910103000
H	-1.999986000	-1.381518000	4.984464000
H	-4.043133000	-0.089947000	5.593969000
C	-3.050264000	-0.866093000	-0.604226000
C	-4.000520000	-1.874531000	-0.642159000
C	-3.537345000	-1.272091000	-1.834700000

N	-3.528130000	-1.115510000	-3.136457000
N	-4.759605000	-2.728851000	0.000274000
C	-2.634254000	-0.129418000	-3.754810000
H	-2.058475000	0.395157000	-2.982786000
H	-1.944314000	-0.635937000	-4.447606000
H	-3.226737000	0.607959000	-4.318094000
C	-4.375517000	-1.892052000	-4.042096000
H	-3.750734000	-2.481639000	-4.731279000
H	-5.019262000	-2.572259000	-3.473577000
H	-5.009854000	-1.214037000	-4.633927000
C	-5.674823000	-3.645300000	-0.681731000
H	-5.588973000	-3.533586000	-1.768159000
H	-5.432321000	-4.684674000	-0.411275000
H	-6.712910000	-3.435482000	-0.379494000
C	-4.739900000	-2.794573000	1.466348000
H	-5.743479000	-2.571013000	1.860329000
H	-4.450605000	-3.806980000	1.788211000
H	-4.027072000	-2.066522000	1.869034000
C	2.405212000	-0.758321000	-0.044989000
C	3.323307000	0.223277000	-0.122582000
C	4.869878000	-0.130899000	-0.341366000
C	5.036046000	-1.064308000	-1.492538000
C	5.365582000	-0.601543000	0.981647000
C	5.708487000	-1.929551000	1.145289000
C	5.748209000	-2.814905000	0.046500000
C	5.433491000	-2.354910000	-1.266588000
Au	0.376329000	-0.429539000	0.111129000
H	5.352920000	0.828112000	-0.586732000
H	6.000620000	-2.296945000	2.131572000
H	5.523948000	-3.055042000	-2.100817000
H	2.774224000	-1.791414000	-0.114432000
C	3.034779000	1.677802000	0.026149000
C	3.434140000	2.605661000	-0.953265000
C	2.331220000	2.153337000	1.150399000
C	3.115917000	3.959672000	-0.829774000
C	2.023498000	3.510851000	1.281369000
C	2.410154000	4.417510000	0.289534000
H	3.979762000	2.264881000	-1.837402000
H	2.034752000	1.447734000	1.929852000
H	3.423050000	4.662025000	-1.608234000
H	1.488552000	3.862293000	2.166966000
H	2.178746000	5.480088000	0.395204000
C	6.174983000	-4.231804000	0.229909000
H	7.159464000	-4.376619000	-0.252661000
H	6.261481000	-4.519617000	1.285501000
H	5.482531000	-4.917560000	-0.285512000
C	5.483485000	0.381230000	2.095762000
H	6.329795000	1.060065000	1.884902000
H	4.592518000	1.023346000	2.168893000
H	5.668192000	-0.106567000	3.061892000
C	4.703128000	-0.554477000	-2.854496000
H	4.844605000	-1.317665000	-3.630993000
H	3.655302000	-0.209842000	-2.875968000
H	5.328928000	0.319844000	-3.102550000