

Conformational preferences of the phenylalanine cyclohexane analogue 1- amino-2-phenylcyclohexanecarboxylic acid

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Table S1	S2-S30	Coordinates and energies of Ac- <i>c</i> -L-c ₆ Phe-NHMe and Ac- <i>t</i> -L-c ₆ Phe-NHMe

Table S1. Atomic Coordinates (in Å), energies (in atomic units) and free energies (in atomic units) of the minimum energy conformations calculated for Ac-*c*-L-c₆Phe-NHMe and Ac-*t*-L-c₆Phe-NHMe.

Ac-*c*-L-c₆Phe-NHMe

1

E= -880.353232 a.u.

C	0.38552300	0.69692700	-0.09480000
C	0.92000400	0.97450300	1.30008400
N	1.01239400	-0.10488500	2.12121500
C	1.39503100	-0.17797800	3.54746000
C	2.91367600	0.09239600	3.80642200
N	3.51334900	1.00577200	3.00824800
C	4.87994000	1.43541300	3.27274500
H	1.08886700	1.10166700	-0.82715100
H	0.21674100	-0.36323900	-0.30160000
H	-0.55934500	1.23563400	-0.21551600
O	1.24537700	2.12207400	1.63196300
H	0.88480200	-1.00375200	1.67518700
C	1.02252400	-1.62513900	4.05014600
C	-0.50594900	-1.80277000	4.20059700
O	3.49814700	-0.45299000	4.74575300
H	2.92039500	1.59070500	2.42278300
H	5.20962200	2.07242000	2.44962800
H	4.95602500	1.99248000	4.21440900
H	5.53835900	0.56654000	3.34270600
C	-1.15263700	-0.73166600	5.08471500
C	-0.85895900	0.66348700	4.52719600
H	1.46729200	-1.67899100	5.04805400
H	-0.99689800	-1.77149800	3.21935500
H	-0.69381600	-2.80349300	4.60653200
H	-2.23366200	-0.90581800	5.14741200
H	-0.76013400	-0.80830900	6.10875800
H	-1.33941000	0.78022500	3.54634800
H	-1.28325500	1.43976500	5.17503200
C	0.64982500	0.89085800	4.40455600
H	0.85801000	1.88032800	3.99215600
H	1.10029500	0.85065200	5.40389500
C	1.65395500	-2.75162400	3.22398400
C	2.94243300	-3.22106900	3.53796900
C	0.97859900	-3.37177600	2.15658300
C	3.53474400	-4.25090100	2.80531200
H	3.48184400	-2.75980100	4.35777100
C	1.57275400	-4.40022200	1.41653500
H	-0.03850400	-3.08272400	1.90696900
C	2.85635200	-4.84298900	1.73601700
H	4.53024800	-4.59314400	3.07437700
H	1.02274300	-4.86012100	0.60002300
H	3.31799300	-5.64512500	1.16742900

2

E= -880.3476484 a.u.

C	-0.05130400	-0.57878600	0.09436200
C	-0.12521900	-0.16558800	1.55443100
N	1.06745300	-0.06724400	2.19945600
C	1.32168200	0.18315600	3.64173700
C	1.00744000	1.69891900	3.94573100
N	-0.29318900	2.05803200	3.84288800
C	-0.69455000	3.44707400	4.01487000

H	-0.53043400	0.19504500	-0.51182800
H	0.96648300	-0.74259500	-0.26931700
H	-0.62822800	-1.49927300	-0.03324800
O	-1.22106800	0.06662800	2.08272000
H	1.88659400	-0.30473700	1.65625000
C	2.85906100	-0.03918700	3.89444100
C	3.18761700	-0.06081200	5.41507800
O	1.88946800	2.49861100	4.26415800
H	-0.92869700	1.41047200	3.37701700
H	-1.78430400	3.50075100	3.97553600
H	-0.34933200	3.82303000	4.98138600
H	-0.27265900	4.09158000	3.23437500
C	2.27880100	-0.94905500	6.27612800
C	0.80001300	-0.63859300	6.01350500
H	3.33677200	0.86737900	3.51256900
H	4.23609300	-0.35674900	5.53422500
H	3.10585900	0.97116200	5.76986500
H	2.47189900	-2.01171200	6.08117900
H	2.51869900	-0.78690400	7.33407300
H	0.15584400	-1.31897600	6.58299700
H	0.56740300	0.37558800	6.36519800
C	0.45800600	-0.75566200	4.52184500
H	0.62907500	-1.78314000	4.18008100
H	-0.60071600	-0.55346600	4.35586100
C	3.48633700	-1.19740400	3.11891400
C	4.43084300	-0.89150200	2.12163800
C	3.20853100	-2.55797800	3.34667700
C	5.06967000	-1.89096000	1.38077700
H	4.67939500	0.15022900	1.93189600
C	3.84404500	-3.56051700	2.61039900
H	2.49298500	-2.84986600	4.10528500
C	4.77680200	-3.23386400	1.62220500
H	5.79689900	-1.61670100	0.62165200
H	3.60837100	-4.60182900	2.81202100
H	5.26962500	-4.01615900	1.05240600

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E= -880.3468163 a.u.

C	-0.21522800	-1.17125400	0.19013700
C	-0.22016500	-0.64833900	1.61627400
N	1.00166800	-0.42946400	2.16781200
C	1.33545300	-0.03265800	3.55331600
C	0.99209700	1.47485200	3.83321700
N	-0.22456000	1.89161300	3.42002100
C	-0.68929800	3.24260900	3.69838900
H	-0.68229100	-2.16084800	0.18429800
H	-0.83362900	-0.51391600	-0.42681200
H	0.78285000	-1.24760100	-0.24920500
O	-1.28901100	-0.44232100	2.20741900
H	1.79563500	-0.50215400	1.54399900
C	2.88862600	-0.24647200	3.76529300
C	3.16793000	-1.65456400	4.32562100
O	1.77141800	2.21612100	4.43930200
H	-0.86642400	1.20559800	3.02394200
H	-0.78253700	3.42040200	4.77573000
H	0.01076400	3.98105400	3.29705800
H	-1.66421100	3.37744300	3.22599400
C	2.59658500	-1.80429600	5.75194800
C	1.27035500	-1.02607800	5.91474300
H	3.15016900	0.47732600	4.54176400
H	2.73257800	-2.41794400	3.66805200

H	4.24780900	-1.83583000	4.33292300
H	2.43991600	-2.86819500	5.96714200
H	3.32941500	-1.44373400	6.48348500
H	0.62131400	-1.52341300	6.64365900
H	1.46230900	-0.02187100	6.31043400
C	0.53884500	-0.91219600	4.57270600
H	0.41419700	-1.90945600	4.13537200
H	-0.46706300	-0.51004100	4.70371100
C	3.73861400	0.11585100	2.54941600
C	4.19200500	-0.85326700	1.63695000
C	4.09952900	1.45594500	2.31990000
C	4.97176600	-0.49754700	0.53024700
H	3.95479000	-1.90147200	1.79531100
C	4.87846100	1.81201500	1.21744000
H	3.76057500	2.21545800	3.01758400
C	5.31621400	0.83767300	0.31485200
H	5.31438300	-1.26775900	-0.15535400
H	5.14832500	2.85359000	1.06630200
H	5.92508800	1.11567400	-0.54062600

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E= -880.3488609 a.u.

C	0.45602100	-0.27479300	-0.11543300
C	0.28112500	0.07368800	1.35159900
N	1.36155100	-0.14825300	2.14626500
C	1.54162400	0.19041400	3.58089600
C	0.64329200	-0.78376700	4.43514100
N	-0.69667200	-0.61859300	4.32227500
C	-1.61077300	-1.53604000	4.98850100
H	0.41064900	0.65144200	-0.69631700
H	1.39643500	-0.78564600	-0.33918300
H	-0.38102200	-0.90381400	-0.42847700
O	-0.79036000	0.53568700	1.76514800
H	2.17223100	-0.55282100	1.69888200
C	1.18338200	1.69435500	3.87753700
C	1.62520800	2.06252600	5.32049700
O	1.14276500	-1.64449100	5.16102300
H	-1.03494000	-0.06976600	3.53233500
H	-2.63134500	-1.17635200	4.84303700
H	-1.52623800	-2.55505400	4.59173500
H	-1.39079600	-1.57483700	6.05816900
C	3.10094600	1.77735000	5.63033500
C	3.46294800	0.31861000	5.31344600
H	0.09441500	1.75965300	3.87419100
H	1.39246400	3.11930600	5.49253900
H	1.00087700	1.48878500	6.01887900
H	3.74222000	2.46614500	5.06841100
H	3.29434600	1.98187700	6.69034400
H	4.54549600	0.16759300	5.40531000
H	2.98661900	-0.34464100	6.04063700
C	3.02276400	-0.11528500	3.90497400
H	3.63973300	0.38608200	3.15025700
H	3.18153300	-1.19345100	3.79860700
C	1.63398600	2.70391900	2.81819300
C	0.63786600	3.45155400	2.16520100
C	2.97000700	2.97548300	2.47163400
C	0.95254800	4.42591900	1.21542300
H	-0.40462600	3.25252200	2.39504800
C	3.29149500	3.94659800	1.51853300
H	3.78259600	2.43800800	2.94300000
C	2.28554900	4.67880200	0.88505900

H	0.15386500	4.98293600	0.73332500
H	4.33467600	4.13120400	1.27649200
H	2.53730100	5.43496500	0.14697400

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E= -880.346982 a.u.

C	0.49303500	-0.13370700	-0.26015700
C	0.18834800	-0.43565500	1.20039700
N	1.19267700	-0.13287800	2.07285400
C	1.32582100	-0.09143700	3.55488000
C	0.77888200	-1.31254500	4.36171800
N	-0.02336500	-2.20809700	3.75629500
C	-0.58111000	-3.31715200	4.51776000
H	-0.26441900	0.56339400	-0.62989500
H	1.48441600	0.29267600	-0.43631300
H	0.39296200	-1.05857200	-0.83465500
O	-0.89585700	-0.94121700	1.50411600
H	2.01257200	0.23724200	1.61488300
C	0.70545500	1.22550400	4.17134100
C	1.43246800	2.48272200	3.65098700
O	1.12495900	-1.41657000	5.54376700
H	-0.49285700	-1.91593200	2.89471700
H	-1.09134500	-3.98977300	3.82530400
H	0.21717100	-3.85957000	5.02969500
H	-1.29421800	-2.97176900	5.27610000
C	2.93745200	2.44667200	3.94780000
C	3.58507300	1.19000300	3.35457200
H	0.94136700	1.13533000	5.23834600
H	1.28070600	2.59374300	2.56906400
H	0.97530800	3.36371800	4.11525500
H	3.42185500	3.34911600	3.55592000
H	3.09228900	2.45214000	5.03557400
H	3.59618500	1.27048800	2.25554300
H	4.63922900	1.12176800	3.64792800
C	2.86297300	-0.08149100	3.82312200
H	3.30121900	-0.97333600	3.35815300
H	2.98992700	-0.19385700	4.90170400
C	-0.81223700	1.32458000	4.07147500
C	-1.60676800	0.77854200	5.09321000
C	-1.46041300	1.97274300	3.00979400
C	-2.99980500	0.86216800	5.04777000
H	-1.12504400	0.28328100	5.93219500
C	-2.85364800	2.06008000	2.96047900
H	-0.88045800	2.41816100	2.20740300
C	-3.63035000	1.50277600	3.97813100
H	-3.59090400	0.43235400	5.85181700
H	-3.33134700	2.56373900	2.12462800
H	-4.71378400	1.57132700	3.94085500

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E= -880.3476922 a.u.

C	-0.44198100	0.07329900	0.32314900
C	-0.11681000	-0.36986000	1.73978800
N	1.19351100	-0.17169800	2.11919200
C	1.63375600	-0.14410700	3.51687200
C	0.93798200	1.08142200	4.19598900
N	0.89142400	1.09717700	5.55952600
C	0.21679700	2.17938800	6.26717000
H	-0.83585400	1.09494700	0.36529100
H	0.42764900	0.06496300	-0.34085300

H	-1.21972500	-0.57670800	-0.08111900
O	-0.96720100	-0.87228700	2.46808500
H	1.68387700	0.49523700	1.53558200
C	3.20494900	0.05930000	3.53757100
C	3.92456700	-1.16316600	2.91952800
O	0.51343400	2.01889000	3.52810500
H	1.06461100	0.24105700	6.06222300
H	0.42792300	2.08713900	7.33477100
H	0.58811000	3.14081000	5.90660300
H	-0.86725700	2.15344600	6.10705300
C	3.54353200	-2.48410200	3.59966600
C	2.02372200	-2.68567800	3.60341100
H	3.46478300	0.08369400	4.60366200
H	3.68409400	-1.23713800	1.85302300
H	5.00584000	-0.99539800	2.98670900
H	4.04374900	-3.31841300	3.09328100
H	3.91278000	-2.48145200	4.63603400
H	1.65940100	-2.82504700	2.57884000
H	1.75815000	-3.59282300	4.15907300
C	1.31773400	-1.48271800	4.23923600
H	0.23763900	-1.63118200	4.26206400
H	1.67684000	-1.40638500	5.27525400
C	3.68537600	1.38111300	2.94603300
C	3.87029600	2.49153800	3.78532200
C	3.97695900	1.53885300	1.58068900
C	4.31211500	3.71614200	3.28372000
H	3.66090800	2.39389100	4.84744000
C	4.41567700	2.76515300	1.07161500
H	3.88700700	0.69707100	0.90004400
C	4.58272400	3.86024100	1.92046900
H	4.44440700	4.55784300	3.95764000
H	4.63365300	2.85855000	0.01137300
H	4.92595900	4.81231500	1.52650200

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E= -880.34425 a.u.

C	0.48357900	0.42430000	-0.20762400
C	0.17655400	0.11718200	1.25335900
N	1.27042700	0.08679700	2.06005800
C	1.43106600	-0.11569300	3.50656400
C	2.98667000	0.03567800	3.68399200
N	3.49187400	-0.09309100	4.93453300
C	4.91811500	0.06896000	5.19141300
H	-0.05283000	1.33561300	-0.48810000
H	1.54736300	0.55464000	-0.42241000
H	0.08956400	-0.38866800	-0.82385200
O	-0.98555900	-0.08417900	1.61302700
H	2.17499300	0.23885000	1.61996800
C	0.98539200	-1.54286700	4.03099000
C	-0.53815000	-1.66060100	4.26794400
O	3.72640600	0.27693700	2.72721900
H	2.87369800	-0.24720900	5.71456200
H	5.10776900	-0.13701600	6.24638000
H	5.49734500	-0.62490100	4.57629300
H	5.24648900	1.08654900	4.95680500
C	-1.06916300	-0.54159400	5.17343200
C	-0.76047900	0.83986500	4.58372700
H	1.43874200	-1.62879500	5.02797200
H	-1.07273200	-1.62788000	3.31747500
H	-0.72658200	-2.64001400	4.72462800
H	-2.15057300	-0.65998500	5.30906300

H	-0.61891800	-0.62817400	6.17561700
H	-1.30522700	0.96069500	3.64514600
H	-1.09323500	1.63030800	5.26854100
C	0.74669600	1.01204800	4.34535500
H	0.96060800	1.96879400	3.85575100
H	1.23526600	1.05408400	5.32742000
C	1.55080300	-2.69351300	3.20904600
C	2.69379600	-3.37864600	3.64917900
C	0.94687600	-3.11892400	2.01439400
C	3.22777900	-4.44498900	2.92073500
H	3.17285400	-3.07567300	4.57699500
C	1.47673100	-4.18458800	1.28336700
H	0.05160400	-2.62206700	1.65579700
C	2.62092200	-4.85091500	1.73071200
H	4.11311200	-4.95815300	3.28588000
H	0.99040000	-4.49706300	0.36332400
H	3.03010500	-5.68063500	1.16149100

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E= -880.347474 a.u.

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.51924200
N	1.24193900	0.00000000	2.11265000
C	1.46561900	0.29202700	3.54271800
C	0.67184500	-0.74088900	4.40462400
N	0.69038400	-2.02231600	3.94263300
C	-0.08930600	-3.06185400	4.59997000
H	-0.14580700	1.02872200	-0.34697600
H	0.92924000	-0.38247000	-0.43296800
H	-0.84232500	-0.59819900	-0.35239200
O	-1.03841200	-0.01025500	2.17208300
H	2.02707200	0.18887800	1.50287400
C	1.01403600	1.75387500	3.92610100
C	1.59845800	2.21772000	5.29382900
O	0.16003500	-0.43850700	5.47831900
H	0.94563000	-2.15670800	2.97499600
H	0.22893500	-4.03614500	4.22182200
H	0.08528900	-3.01916200	5.67649100
H	-1.16415500	-2.93575400	4.42177500
C	3.08960300	1.92399300	5.51430500
C	3.41688800	0.45370100	5.22040200
H	-0.06640500	1.68710100	4.07122300
H	1.40703500	3.29177600	5.39993100
H	1.02810300	1.70651200	6.07322500
H	3.71516400	2.57169900	4.88656500
H	3.35207500	2.16424500	6.55173200
H	4.49269800	0.26912700	5.32583500
H	2.91203600	-0.18923000	5.95151200
C	2.97986200	0.06291100	3.80276500
H	3.54679200	0.66066500	3.07579900
H	3.21811900	-0.98760100	3.60186900
C	1.22094500	2.77347000	2.80723900
C	0.08477300	3.34469700	2.20787400
C	2.47824600	3.21127400	2.35215100
C	0.19216100	4.30675700	1.19992700
H	-0.90001500	3.02461900	2.53700600
C	2.59237300	4.17038700	1.34114300
H	3.38766300	2.81710800	2.79058000
C	1.44988300	4.72342100	0.75806200
H	-0.70831100	4.73017700	0.76330500
H	3.57882000	4.48952300	1.01539800

H	1.53947600	5.47191300	-0.02398800
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9

E= -880.3439793 a.u.

C	-0.21215500	-0.33286100	0.22437000
C	-0.08053100	0.22569700	1.63342400
N	1.13926200	0.03026600	2.23582900
C	1.40166800	0.27024100	3.67061900
C	1.15976400	1.77784300	3.99431900
N	1.51688700	2.65825500	3.01763900
C	1.25206300	4.08240800	3.16532200
H	-0.58952400	0.45528100	-0.43229300
H	0.72255400	-0.72796700	-0.18351400
H	-0.95889200	-1.13298100	0.23678100
O	-0.99987800	0.83179300	2.17484700
H	1.78283300	-0.59775700	1.77154600
C	2.93823700	-0.00236100	3.92970000
C	3.23687100	-0.06003300	5.45296600
O	0.76876900	2.14889100	5.09741600
H	1.63768200	2.28711300	2.08671000
H	1.79522000	4.62606500	2.38883500
H	0.18136500	4.30560400	3.08381400
H	1.59591500	4.41606800	4.14610700
C	2.35809600	-1.05157000	6.22550600
C	0.87056700	-0.73012000	6.02852400
H	3.46122500	0.88022600	3.54591800
H	4.29906600	-0.29568700	5.58535400
H	3.07694700	0.94262200	5.86634300
H	2.57835900	-2.07903800	5.90993600
H	2.61192100	-1.00124500	7.29131200
H	0.25046400	-1.50465700	6.49731600
H	0.63723300	0.21621700	6.52241200
C	0.47713500	-0.62280300	4.54435700
H	0.47627100	-1.62075200	4.08960400
H	-0.54229000	-0.24031000	4.45603000
C	3.54868300	-1.17917400	3.16487300
C	4.67483000	-0.92716900	2.35988600
C	3.08816600	-2.50772800	3.23105300
C	5.32386600	-1.94868700	1.66197300
H	5.05366700	0.08939600	2.28561500
C	3.73013400	-3.53253400	2.52983600
H	2.22110500	-2.75618100	3.82995200
C	4.85239600	-3.26040200	1.74421000
H	6.19411200	-1.71687500	1.05440200
H	3.34986300	-4.54760000	2.60273700
H	5.35076800	-4.05935800	1.20316700

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E= -880.343258 a.u.

C	0.40640700	0.65155600	-0.18666000
C	0.21705900	-0.02392000	1.16789300
N	1.29470800	0.08462300	2.00952400
C	1.47186800	-0.17964700	3.46506100
C	3.01534800	-0.16786100	3.71890000
N	3.81700800	-0.50680400	2.66577500
C	5.25021600	-0.69204300	2.86158100
H	-0.31787200	1.46782100	-0.26967400
H	1.41018100	1.05110900	-0.35740500
H	0.17152000	-0.07384900	-0.96964600
O	-0.82443400	-0.62355200	1.41726600

H	2.00295200	0.71751500	1.66127300
C	0.97328300	-1.57303000	4.02810100
C	-0.55020300	-1.66204800	4.27983800
O	3.47484300	0.12502800	4.81895500
H	3.38025300	-1.00660700	1.90236200
H	5.73666100	-0.74173300	1.88507400
H	5.64832000	0.15472900	3.42256200
H	5.46850500	-1.60847700	3.42272800
C	-1.07359700	-0.47320600	5.09762200
C	-0.68063400	0.86180100	4.45198800
H	1.43676600	-1.57502600	5.02334400
H	-1.08580000	-1.71179000	3.33185800
H	-0.73583500	-2.59955300	4.81842000
H	-2.16372700	-0.54480900	5.19158200
H	-0.66603400	-0.51400500	6.11874400
H	-1.17326700	0.95615700	3.47783400
H	-1.02946800	1.69939600	5.06863400
C	0.84239600	0.96554200	4.30221700
H	1.12680200	1.92230800	3.84659700
H	1.31216300	0.94040300	5.29006400
C	1.52779800	-2.79289800	3.30221400
C	2.59385800	-3.50990900	3.87103300
C	0.99205400	-3.25790700	2.08946300
C	3.12054600	-4.64464900	3.24823400
H	3.01486500	-3.17566100	4.81645300
C	1.51844100	-4.39152000	1.46299200
H	0.15295100	-2.73778500	1.63979000
C	2.58574700	-5.08850600	2.03627000
H	3.94185800	-5.18307600	3.71332100
H	1.08485700	-4.73516700	0.52759900
H	2.98833600	-5.97244300	1.54972100

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E= -880.3443322 a.u.

C	0.66913500	-0.74798700	-0.15076600
C	0.49152400	-0.71053400	1.35866900
N	1.40168200	0.06150000	2.03750300
C	1.62506600	0.01416300	3.49530100
C	1.38117000	-1.46175000	3.96928700
N	0.46385900	-1.68688700	4.94551100
C	0.15250800	-3.05939400	5.32992100
H	-0.31520000	-0.72167800	-0.62265500
H	1.28240000	0.06992300	-0.54116700
H	1.14310900	-1.69854800	-0.41814400
O	-0.40583300	-1.33032500	1.91854800
H	2.17482900	0.41012900	1.48872100
C	0.85692500	1.15214100	4.27126100
C	1.38020500	2.55138900	3.84664300
O	2.10015200	-2.35211600	3.52225300
H	-0.28730900	-1.01572700	5.03084100
H	-0.51116800	-3.03778400	6.19719100
H	-0.33099400	-3.60503300	4.51105900
H	1.07334300	-3.58298100	5.59296300
C	2.88591400	2.72379600	4.07056800
C	3.66932500	1.62440700	3.34831800
H	1.15019300	1.01267300	5.32044700
H	1.14215100	2.71675700	2.78792600
H	0.82422200	3.30928400	4.40936900
H	3.20607600	3.71646500	3.73151200
H	3.10181800	2.67478300	5.14765600
H	3.60014600	1.78130500	2.26139700

H	4.73779300	1.68429100	3.58723700
C	3.15156500	0.23388600	3.73602200
H	3.68486400	-0.55914000	3.20556800
H	3.34100100	0.07361400	4.80481400
C	-0.66955500	1.17018100	4.25247000
C	-1.37666600	1.04011700	5.46012200
C	-1.40994100	1.42463100	3.08694400
C	-2.77202200	1.12703500	5.50245700
H	-0.82637000	0.88058600	6.38556700
C	-2.80164800	1.51185000	3.12311500
H	-0.89668500	1.55394200	2.14118900
C	-3.49132500	1.35893800	4.32959000
H	-3.29012300	1.01998200	6.45139200
H	-3.35025800	1.69730300	2.20403800
H	-4.57505300	1.42582100	4.35394900

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E= -880.3410094 a.u.

C	-0.50457300	0.77998100	0.19967100
C	-0.28850700	0.90223000	1.70243500
N	0.92079100	0.41399600	2.14730700
C	1.36902400	0.21126300	3.54439500
C	2.91028400	-0.02382700	3.49518100
N	3.58178000	0.61760300	2.49713200
C	5.03777400	0.63108400	2.44884200
H	-1.36120900	0.12282400	0.02414500
H	-0.76098800	1.76740800	-0.19316600
H	0.35870000	0.38884900	-0.34583000
O	-1.13961500	1.42355000	2.41641400
H	1.36530600	-0.21050700	1.48637500
C	0.68049200	-1.02399600	4.24956600
C	-0.52362400	-0.56459700	5.09587700
O	3.49566100	-0.70387000	4.33562200
H	3.06633000	1.27016900	1.92373100
H	5.46461400	1.30215100	3.20399100
H	5.41578600	-0.37512200	2.63847900
H	5.35689600	0.95678200	1.45643400
C	-0.06279600	0.32547700	6.27223800
C	1.14877500	1.21128300	5.89170200
H	1.43986000	-1.39890300	4.94285300
H	-1.23377400	-0.01318400	4.47268900
H	-1.05038100	-1.44551500	5.47926600
H	-0.90234600	0.95374900	6.59237200
H	0.20312000	-0.30109400	7.13218800
H	1.11941400	2.15477600	6.44785300
H	2.08532900	0.71606300	6.17143600
C	1.15740000	1.51242100	4.38820500
H	0.20522100	1.95711200	4.09584200
H	1.94351600	2.23448300	4.13802400
C	0.38060100	-2.16138300	3.28319100
C	-0.86992700	-2.30722600	2.66121600
C	1.37727600	-3.10880600	2.99235300
C	-1.11655800	-3.36261000	1.77794400
H	-1.66285100	-1.59646700	2.87243900
C	1.13553200	-4.16215300	2.10606700
H	2.34679000	-3.02008300	3.47508600
C	-0.11387200	-4.29338500	1.49372600
H	-2.09584100	-3.45928000	1.31672200
H	1.92062400	-4.88561700	1.90327200
H	-0.30675000	-5.11606100	0.81101100

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E= -880.3430331 a.u.

C	-0.00538400	-0.36405900	-0.05732300
C	0.11223600	-0.55500900	1.44464600
N	1.29455100	-0.12558600	2.00575800
C	1.49535400	0.05720700	3.45382500
C	1.16700100	-1.28439000	4.18736000
N	1.64089200	-2.40746000	3.57983300
C	1.31276500	-3.72770400	4.09998400
H	-0.55201600	-1.20953500	-0.47924500
H	-0.58896500	0.54403200	-0.24389000
H	0.96168100	-0.26405900	-0.55929800
O	-0.77899700	-1.07017400	2.11069300
H	1.89437100	0.43029400	1.41002500
C	0.62739300	1.23697100	4.07340900
C	1.44110200	2.08189000	5.09387600
O	0.62734900	-1.31082800	5.28889500
H	1.88094400	-2.32888600	2.60215300
H	1.50909700	-3.75370700	5.17331200
H	0.25660500	-3.97485200	3.93776000
H	1.94004800	-4.47044200	3.60167100
C	2.35516000	1.23280900	5.98288400
C	3.40996400	0.47338200	5.13849800
H	-0.16809800	0.74149100	4.63369200
H	2.04381900	2.83293900	4.56742200
H	0.72891800	2.64658400	5.70608000
H	2.85327000	1.87352300	6.71944000
H	1.74329700	0.51673600	6.53783600
H	4.37824000	0.98600500	5.17914600
H	3.57187300	-0.52517100	5.55854100
C	3.00470100	0.34811900	3.65652700
H	3.23093800	1.28722600	3.13264500
H	3.59537400	-0.43515300	3.16935000
C	-0.03384400	2.13992300	3.03944900
C	0.69453700	3.05971600	2.26444900
C	-1.42328500	2.08623200	2.85342600
C	0.06060300	3.88855000	1.33551900
H	1.77121300	3.14429700	2.38974200
C	-2.06530400	2.91742000	1.93080000
H	-2.00471800	1.37198000	3.42893800
C	-1.32555000	3.82179200	1.16533200
H	0.64821100	4.59203500	0.75166400
H	-3.14331100	2.85492000	1.81076500
H	-1.82147500	4.47046900	0.44885800

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E= -880.3364631 a.u.

C	0.63262700	0.29003300	-0.01731100
C	0.59649100	0.91195100	1.37349600
N	1.22713400	0.17111200	2.33731800
C	1.32580500	0.35550600	3.80434800
C	2.80279700	-0.11839400	4.06085200
N	3.73148400	0.79887900	4.41900000
C	5.13891000	0.44128600	4.54630700
H	0.96542900	1.05098300	-0.72754300
H	1.27881900	-0.58846400	-0.09916000
H	-0.38784300	0.00503600	-0.29141400
O	0.03685500	1.99041000	1.55956900
H	1.59717900	-0.72334200	2.04109000

C	0.39087000	-0.68463600	4.52926400
C	0.36941700	-0.42899800	6.06060900
O	3.10512000	-1.29863500	3.86806700
H	3.46802200	1.76801100	4.49265400
H	5.67715300	1.28592900	4.98043700
H	5.24609100	-0.43023300	5.19649900
H	5.57697400	0.19407200	3.57315700
C	0.02349700	1.01479400	6.44008200
C	1.00528700	1.99133100	5.77908100
H	0.89466500	-1.64449000	4.38612800
H	-0.33263600	-1.13178700	6.52243700
H	1.36262400	-0.67274100	6.46394600
H	-1.00346800	1.24939900	6.13468100
H	0.05649200	1.13013000	7.53021600
H	0.72087200	3.02789700	5.99566400
H	1.99755900	1.84184500	6.22511800
C	1.04903100	1.80926600	4.24921900
H	0.10046300	2.12453700	3.81978600
H	1.77597600	2.48867800	3.78700800
C	-1.00512500	-0.87314800	3.93864600
C	-1.41253900	-2.18915200	3.65417600
C	-1.93418500	0.15430700	3.70431000
C	-2.68987500	-2.47483200	3.16733400
H	-0.71352200	-3.00567600	3.81967400
C	-3.21204100	-0.12448400	3.21091400
H	-1.67091100	1.18871800	3.88290600
C	-3.59925500	-1.43885500	2.94291900
H	-2.96987700	-3.50413500	2.96045200
H	-3.90272500	0.69465500	3.03159400
H	-4.59352500	-1.65175100	2.56081200

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E= -880.3393302 a.u.

C	-0.41798100	-0.76606300	0.31496200
C	-0.25025600	-0.53748400	1.80710100
N	1.04205200	-0.61569800	2.27054900
C	1.41469400	-0.11577200	3.59754500
C	1.11534500	1.41697600	3.61693200
N	0.79291600	1.97968500	4.81702300
C	0.44368700	3.39268300	4.90596700
H	-1.32897000	-1.34386000	0.14612800
H	-0.54102700	0.20832000	-0.17016100
H	0.43291200	-1.27884500	-0.14240300
O	-1.20971300	-0.30456900	2.53793700
H	1.75484800	-0.49917100	1.56037200
C	2.98208200	-0.30987400	3.80238400
C	3.26648900	-1.73956100	4.31410100
O	1.24898600	2.09456500	2.60168700
H	0.49191400	1.37689300	5.56649700
H	1.20086700	3.98870800	4.39323100
H	-0.52605100	3.60105000	4.43880500
H	0.40842500	3.68155900	5.95873900
C	2.72639400	-1.95080100	5.74493700
C	1.44821500	-1.12077200	5.99477200
H	3.25413800	0.38350400	4.60736900
H	2.80658100	-2.46361700	3.63172500
H	4.34455400	-1.92762400	4.28507300
H	2.51761900	-3.01623200	5.89765600
H	3.49414900	-1.67759000	6.47880200
H	0.81212900	-1.61489700	6.73756600
H	1.72187600	-0.15156000	6.43158100

C	0.65308900	-0.92712900	4.69501600
H	0.43637900	-1.91332300	4.27234700
H	-0.32570000	-0.47673300	4.87285900
C	3.84195100	0.07416700	2.60371100
C	4.16421300	-0.84789900	1.59248600
C	4.36687500	1.37174000	2.49926600
C	4.97000800	-0.48086100	0.50997700
H	3.79807800	-1.86873800	1.65233200
C	5.17429100	1.74162400	1.42306900
H	4.13219500	2.10386200	3.26629100
C	5.47737100	0.81666200	0.42035200
H	5.20540500	-1.21353500	-0.25697600
H	5.56375200	2.75405500	1.36677000
H	6.10576800	1.10280700	-0.41802500

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E= -880.3391094 a.u.

C	-0.25675900	1.13615000	0.11541200
C	-0.21918000	0.81616300	1.60330500
N	0.98498400	0.36876600	2.06999900
C	1.40943800	0.17784600	3.47939400
C	2.93505400	-0.12923100	3.40918200
N	3.31559900	-1.04728800	2.46603900
C	4.69887200	-1.50641800	2.39706500
H	-1.10329600	0.60973000	-0.33267000
H	-0.43650000	2.20907700	-0.00386400
H	0.65743700	0.86881300	-0.42217400
O	-1.22210300	0.95038200	2.30308500
H	1.73412600	0.35202900	1.39264000
C	0.72208600	-1.05202400	4.23765400
C	-0.49716700	-0.58242000	5.06509800
O	3.75117800	0.42322800	4.13911600
H	2.60216400	-1.66369100	2.09662400
H	5.36692900	-0.64361300	2.38524500
H	4.96778400	-2.13055300	3.25799800
H	4.83315100	-2.08111100	1.47832600
C	-0.07910500	0.38276200	6.19698500
C	1.13173000	1.25809700	5.79879100
H	1.47961200	-1.37334000	4.96503600
H	-1.21207200	-0.09433400	4.39897000
H	-0.99448100	-1.46331200	5.48582200
H	-0.93668100	1.01733400	6.45015900
H	0.16399500	-0.18437700	7.10432200
H	1.08108200	2.22753400	6.30705300
H	2.06961600	0.79511400	6.12123200
C	1.18362200	1.48712800	4.28322300
H	0.23636500	1.92066000	3.95239600
H	1.98498800	2.18640700	4.02989800
C	0.41744900	-2.27288200	3.38210200
C	-0.70583400	-2.33340200	2.53844500
C	1.23510200	-3.41286800	3.46818300
C	-0.98429900	-3.48366500	1.79661200
H	-1.37245200	-1.48026300	2.47057400
C	0.95966200	-4.56626000	2.72632000
H	2.09222400	-3.40266800	4.13785900
C	-0.15174200	-4.60368400	1.88203200
H	-1.86080000	-3.50661500	1.15475000
H	1.60644700	-5.43439900	2.81910400
H	-0.37418000	-5.49795700	1.30700600

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E= -880.3307251 a.u.

C	0.45435700	0.29575800	-0.25514400
C	0.31912400	0.78689800	1.18233900
N	1.18717700	0.19266200	2.06630000
C	1.38063400	0.41830800	3.52136000
C	2.92887000	0.18703300	3.70060100
N	3.37985600	-1.09509800	3.52982100
C	4.80158400	-1.40553200	3.63733500
H	0.66355100	1.15763100	-0.89478800
H	1.23508500	-0.45588200	-0.40469500
H	-0.50694500	-0.12160800	-0.56755800
O	-0.51047300	1.64172100	1.47183800
H	1.80276200	-0.49791500	1.66124100
C	0.55598900	-0.62563500	4.36767300
C	0.70539900	-0.32622600	5.88556600
O	3.71474000	1.11015500	3.87645500
H	2.72670800	-1.86144400	3.57974900
H	4.96274500	-2.43297800	3.30437000
H	5.37381600	-0.72522400	3.00340500
H	5.16447400	-1.29587400	4.66563000
C	0.37521700	1.12056300	6.27342700
C	1.21030700	2.11003500	5.44937000
H	1.02596800	-1.60427900	4.21325800
H	0.08133100	-1.03316400	6.44375700
H	1.74665500	-0.53311700	6.17281000
H	-0.69504000	1.31231700	6.13225800
H	0.57199800	1.26035800	7.34344800
H	0.90274000	3.13915700	5.66991600
H	2.26415000	2.03080700	5.73778100
C	1.07194100	1.87438600	3.93512200
H	0.06801600	2.12515700	3.59808300
H	1.75657900	2.53237600	3.39462100
C	-0.89044000	-0.86446400	3.93219800
C	-1.25977100	-2.17486400	3.58113000
C	-1.89452300	0.11723400	3.90599700
C	-2.56942100	-2.50047500	3.22105300
H	-0.50729600	-2.96084700	3.59388600
C	-3.20603200	-0.20124000	3.54653300
H	-1.66239500	1.14675400	4.14126800
C	-3.55262800	-1.50960600	3.20363700
H	-2.81720800	-3.52443100	2.95523600
H	-3.95590300	0.58422400	3.52535100
H	-4.57342700	-1.75199400	2.92258600

Ac-t-L-c₆Phe-NHMe

1

E= -880.351682 a.u.

C	-0.41240200	0.50711100	0.68887100
C	-0.15071800	0.15741800	2.14388200
N	1.09283100	0.45383500	2.60497800
C	1.70603100	0.16446200	3.92519600
C	1.11270700	1.09680900	5.03493900
N	-0.23705400	1.11570100	5.11108600
C	-0.92038000	1.91273500	6.11897400
H	-1.29163500	1.15489900	0.63672100
H	0.42903000	0.99875100	0.19361000
H	-0.65234300	-0.41478700	0.15076200

O	-1.03946300	-0.35961500	2.83435900
H	1.68040500	0.99627600	1.98437600
C	3.25646200	0.33193100	3.70562900
C	4.08267100	-0.06192800	4.95181100
O	1.81822000	1.73194700	5.82362600
H	-0.77784800	0.55368200	4.45425200
H	-1.99628800	1.77349900	5.99795200
H	-0.62750100	1.60650400	7.12853700
H	-0.68021300	2.97531200	6.00927300
C	3.75784500	-1.49150900	5.41117500
C	2.24894400	-1.69997400	5.59840500
H	5.14472700	0.01354600	4.69021900
H	3.89206300	0.64770100	5.75948500
H	4.12677700	-2.20735800	4.66145900
H	4.29137000	-1.71290500	6.34329200
H	2.03712300	-2.74783900	5.84218600
H	1.89630500	-1.10535800	6.45093500
C	1.46241900	-1.31662100	4.33557200
H	1.78502300	-1.94420300	3.49395300
H	0.39539700	-1.49801800	4.47221600
C	3.71065000	1.64613500	3.07315400
C	3.76153300	2.86452100	3.77388200
C	4.14406100	1.63892400	1.73491700
C	4.21956200	4.02679200	3.14967700
H	3.42800400	2.89594100	4.80413200
C	4.60028300	2.80299200	1.10730800
H	4.14465000	0.70250900	1.17984300
C	4.63749700	4.00483700	1.81528300
H	4.24978400	4.95619600	3.71179800
H	4.93223600	2.76461500	0.07344400
H	4.99329700	4.91277100	1.33666700
H	3.46982100	-0.43823700	2.95005300

2

E= -880.3484977 a.u.

C	0.27021200	0.20766200	0.04922900
C	0.34513400	-0.01819000	1.55193600
N	1.58600200	0.10354400	2.09211900
C	1.96312300	-0.05128200	3.50186000
C	3.49976800	0.22624300	3.48217200
N	4.16145900	0.25950700	4.66449100
C	5.59102700	0.54265000	4.71878800
H	-0.37930700	1.06737100	-0.14104300
H	1.24276000	0.38399700	-0.41787300
H	-0.19866000	-0.66538400	-0.41296300
O	-0.67013600	-0.28410000	2.20418200
H	2.38275200	0.27474200	1.48583600
C	1.58460000	-1.50553300	3.99773100
C	1.62722100	-1.66635400	5.53423200
O	4.09933900	0.42773100	2.42280800
H	3.65488400	0.14189700	5.52548100
H	5.91671200	0.48813700	5.75920900
H	6.14970400	-0.18638800	4.12504800
H	5.80907400	1.53929000	4.32264100
C	0.75876600	-0.61612400	6.24021600
C	1.18326000	0.81067600	5.86826700
H	1.26694200	-2.67322200	5.77432900
H	2.65658100	-1.62808300	5.91592600
H	-0.28828000	-0.76596500	5.94570700
H	0.80444500	-0.75542100	7.32715700
H	0.48855400	1.53694200	6.30702700

H	2.15801800	1.04292300	6.32170200
C	1.20282300	1.02321500	4.34541000
H	0.16878700	0.99871800	3.99077100
H	1.60634900	2.01156400	4.09602500
C	2.31128800	-2.62048600	3.25752000
C	3.62158100	-3.01297800	3.57521200
C	1.64883400	-3.31180900	2.23074200
C	4.25063300	-4.05198200	2.88505500
H	4.16244600	-2.50591800	4.36822700
C	2.27337100	-4.35148500	1.53724700
H	0.62862700	-3.03396200	1.97911400
C	3.57975800	-4.72491300	1.86094400
H	5.26595500	-4.33530800	3.14865000
H	1.73709600	-4.87096800	0.74783500
H	4.06830300	-5.53351700	1.32483800
H	0.52767900	-1.58103700	3.72317500

3

E= -880.3475663 a.u.

C	0.02044400	-0.55996600	0.16784300
C	0.89411300	-0.81675100	1.38440000
N	1.01325800	0.22084800	2.25555700
C	1.73964100	0.30323000	3.55700100
C	3.28640800	0.31449400	3.30936100
N	3.78994900	-0.74622000	2.64033400
C	5.21675900	-0.85675700	2.37714600
H	-0.77634100	-1.30889200	0.14943600
H	-0.42688200	0.43743800	0.14283200
H	0.62568000	-0.70369800	-0.73167200
O	1.44881300	-1.91352700	1.53389300
H	0.55402100	1.07648200	1.97765000
C	1.31020600	-0.90938100	4.46716900
C	-0.16253900	-0.75442900	4.93712000
O	3.99084800	1.23680700	3.72195700
H	3.14750200	-1.44452000	2.27230900
H	5.40224000	-1.80254700	1.86449100
H	5.57102600	-0.03119500	1.75025100
H	5.78379200	-0.83520600	3.31280600
C	-0.47585900	0.59870700	5.58508100
C	-0.12283400	1.74581200	4.62977300
H	-0.81703000	-0.88636600	4.06485800
H	-0.39230800	-1.57560500	5.62490300
H	-1.53829500	0.64315600	5.85351600
H	0.08457900	0.70691200	6.52185800
H	-0.80697200	1.71527100	3.76893900
H	-0.28787900	2.71675900	5.11164500
C	1.33921800	1.66825000	4.16277500
H	1.55723600	2.45177500	3.42623300
H	2.01432600	1.87786800	4.99239900
H	1.32931400	-1.78245300	3.81311700
C	2.25672300	-1.25893000	5.61677600
C	2.66131500	-2.60078700	5.73518700
C	2.71028100	-0.35938500	6.59552500
C	3.47551000	-3.03230200	6.78366000
H	2.33363400	-3.31916500	4.98759600
C	3.53051800	-0.78427200	7.64485300
H	2.44321700	0.68859100	6.54874300
C	3.91545800	-2.12189500	7.74740400
H	3.76922600	-4.07672700	6.84249300
H	3.87099000	-0.06114100	8.38065700
H	4.55321600	-2.44913700	8.56349700

4

E= -880.3469283 a.u.

C	0.41224600	-0.07495400	-0.03431600
C	0.40334100	0.02249900	1.48554100
N	1.65154200	0.08167600	2.06770900
C	1.95619100	-0.03387900	3.51649300
C	3.45459600	0.33271200	3.69463600
N	3.96000000	1.22489600	2.79287300
C	5.29469000	1.78637400	2.95555300
H	-0.13960300	0.77885100	-0.43753600
H	1.41275400	-0.09388000	-0.47528600
H	-0.12496200	-0.98074300	-0.32903000
O	-0.65388000	0.07074800	2.10611100
H	2.39303400	-0.25766700	1.46774000
C	1.57888700	-1.47587700	4.01919300
C	1.68940900	-1.63811200	5.55408300
O	4.13949800	-0.09822300	4.62020500
H	3.31679100	1.67177700	2.15480200
H	5.58461300	2.28273700	2.02702500
H	5.33568400	2.50818700	3.78003000
H	6.00260700	0.98452800	3.17296100
C	0.90110700	-0.55093300	6.29896100
C	1.31879400	0.85638300	5.84979600
H	1.29855000	-2.62914700	5.81504100
H	2.73754300	-1.60894200	5.86018700
H	-0.17423900	-0.68414200	6.11192100
H	1.04893500	-0.66221300	7.37994700
H	0.70488900	1.61293200	6.35343200
H	2.35852900	1.04136900	6.14402300
C	1.14843600	1.02255500	4.33237700
H	0.09586700	0.90509300	4.06642600
H	1.45114000	2.02740900	4.01262800
C	2.25189000	-2.60334300	3.24395000
C	3.59635200	-2.96530600	3.43978900
C	1.50221000	-3.33903700	2.31061000
C	4.16722500	-4.01670800	2.71731800
H	4.19778000	-2.41844800	4.15715400
C	2.07037800	-4.39162200	1.58700700
H	0.45426300	-3.09085800	2.15826000
C	3.40989100	-4.73314600	1.78623100
H	5.20813500	-4.27852900	2.88759100
H	1.46464200	-4.94609400	0.87529500
H	3.85643700	-5.55187800	1.22901400
H	0.50958000	-1.53634400	3.78155200

5

E= -880.3493295 a.u.

C	0.25431500	0.23729300	0.01218700
C	0.35751300	-0.18790700	1.47060200
N	1.58980600	-0.00728900	2.04315100
C	1.93021600	-0.12296500	3.48453300
C	3.46205600	0.10316200	3.60022000
N	4.21863600	-0.29545600	2.52975800
C	5.67456200	-0.26091300	2.60439900
H	-0.49743600	1.02835700	-0.06624300
H	1.19473500	0.59529200	-0.41654900
H	-0.10404200	-0.61356500	-0.57341600
O	-0.60880500	-0.67406600	2.05508500
H	2.24255700	0.53697400	1.49600300

C	1.54418500	-1.55013400	4.05470000
C	1.69412900	-1.58728900	5.59214300
O	3.96952300	0.62793600	4.58764500
H	3.80460500	-0.97609200	1.90592700
H	6.08331400	-0.38180500	1.59888700
H	5.98946000	0.70081900	3.01158300
H	6.06970100	-1.05282100	3.25247900
C	0.81470800	-0.52979300	6.27092100
C	1.18946600	0.87754400	5.79283500
H	1.41592900	-2.59125300	5.93320700
H	2.73725800	-1.42756500	5.88936600
H	-0.24093900	-0.73601800	6.04284700
H	0.92223200	-0.59927100	7.36018200
H	0.49225400	1.61719900	6.20636900
H	2.18936600	1.13305000	6.15299300
C	1.15243800	0.97961600	4.26026600
H	0.11245800	0.90489800	3.92493100
H	1.53111500	1.95671900	3.93821500
C	2.23080900	-2.71954000	3.35783000
C	3.48223100	-3.21114000	3.76752300
C	1.59096900	-3.36478800	2.28623500
C	4.07725800	-4.29951400	3.12365300
H	4.00025300	-2.74646900	4.60134600
C	2.18406500	-4.45131800	1.63690900
H	0.61124000	-3.01714900	1.97065900
C	3.43219900	-4.92263500	2.05167200
H	5.04231700	-4.66416900	3.46507000
H	1.66450100	-4.93541600	0.81439700
H	3.89187400	-5.77156000	1.55362000
H	0.47657500	-1.63671500	3.83525100

6

E= -880.3451983 a.u.

C	-0.20763400	-0.30873200	0.30267400
C	-0.18754200	-0.44466000	1.81838500
N	1.05721100	-0.48060000	2.37748700
C	1.59192800	-0.38034900	3.77116000
C	0.96191900	-1.36244000	4.80409300
N	-0.20678400	-1.96677700	4.50960600
C	-0.83323500	-2.84677200	5.48550500
H	-0.71200900	0.62934000	0.05207200
H	0.78136100	-0.31415400	-0.16374900
H	-0.80665400	-1.12328500	-0.11243200
O	-1.25141200	-0.53651700	2.43713000
H	1.79945200	-0.42575400	1.69472300
C	1.51646000	1.12127000	4.25779200
C	2.43521100	1.39400500	5.47364500
O	1.56120900	-1.57416400	5.86501600
H	-0.78803800	-1.55505100	3.77427700
H	-1.70455600	-3.31262200	5.02088500
H	-0.13045600	-3.62218300	5.79974000
H	-1.15144300	-2.30020000	6.38182600
C	3.89728200	1.03980700	5.17943300
C	4.03555300	-0.42832800	4.76227900
H	2.34465700	2.45679700	5.72685600
H	2.08777100	0.82316400	6.33986600
H	4.27531500	1.69289500	4.37763300
H	4.51565900	1.24017300	6.06245600
H	5.06516000	-0.63994800	4.44637400
H	3.80792700	-1.07701000	5.61006000
C	3.09897000	-0.76672700	3.59540200

H	3.46102900	-0.21646300	2.71256800
H	3.15732000	-1.83398500	3.35160600
C	0.11527500	1.67074400	4.48185900
C	-0.65866300	1.30369200	5.59478100
C	-0.41192100	2.62125100	3.59632000
C	-1.92486300	1.85511100	5.79895300
H	-0.27201400	0.58572400	6.31190500
C	-1.67743500	3.17779400	3.79736500
H	0.17863300	2.93388200	2.73770200
C	-2.44169600	2.79244100	4.90012800
H	-2.50756900	1.55417100	6.66526700
H	-2.06317200	3.91100500	3.09441400
H	-3.42672900	3.22076000	5.06154300
H	1.94150500	1.68313300	3.41354900

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E= -880.3449982 a.u.

C	-0.00965500	-0.29262700	-0.04097000
C	0.65838100	0.39896300	1.13594300
N	0.67498700	-0.31494300	2.30657300
C	1.50583600	0.05729200	3.47041900
C	2.98484300	0.03865300	2.97781400
N	3.76899800	1.10208100	3.27372300
C	5.14574400	1.17712900	2.80446200
H	0.76966500	-0.61505000	-0.73940400
H	-0.60763300	-1.16265900	0.24519400
H	-0.64415000	0.42965800	-0.55936600
O	1.14130800	1.52471300	1.03125500
H	0.48230600	-1.30285800	2.21195300
C	1.33482300	-1.10377100	4.52200700
C	-0.11823400	-1.13860900	5.07460300
O	3.40823600	-0.94974200	2.37716900
H	3.32955900	1.94890700	3.59861900
H	5.65483900	1.98631600	3.33229800
H	5.65188300	0.23328700	3.01537600
H	5.19445400	1.36003100	1.72458700
C	-0.67607000	0.21211100	5.55527600
C	-0.45087200	1.32662300	4.52328400
H	-0.77465700	-1.51244200	4.27849600
H	-0.16430400	-1.87826700	5.88191400
H	-1.74792300	0.10219500	5.76081400
H	-0.21740100	0.49413800	6.50968500
H	-1.09219200	1.15813100	3.65034700
H	-0.74397000	2.29559700	4.94436700
C	1.01384300	1.39924000	4.06109000
H	1.12404400	2.18442600	3.30907800
H	1.64806500	1.65426200	4.91840900
H	1.47799300	-2.02470600	3.94489500
C	2.42516300	-1.15656800	5.59401600
C	3.40873400	-2.15567100	5.48680600
C	2.50079500	-0.29143300	6.69922000
C	4.42348100	-2.28865100	6.43642100
H	3.38605500	-2.82843100	4.63454900
C	3.51458300	-0.42018300	7.65318200
H	1.76833600	0.49418100	6.83545600
C	4.48172700	-1.41899100	7.52752200
H	5.16768700	-3.07160600	6.32051900
H	3.54316000	0.26358700	8.49716300
H	5.26793100	-1.51891800	8.27033900

8

E= -880.346228 a.u.

C	-0.44789800	-0.01917800	0.29059400
C	-0.25861300	-0.40581300	1.74958300
N	1.04570900	-0.38111300	2.19818500
C	1.48845800	-0.39569800	3.60801100
C	0.75320200	-1.51288200	4.40185100
N	0.63177900	-2.70505500	3.75307900
C	-0.14267500	-3.78932800	4.34246300
H	-0.84410200	1.00113000	0.25563300
H	0.47354700	-0.05698400	-0.29838200
H	-1.19330700	-0.68077800	-0.15530500
O	-1.20074600	-0.74183200	2.45556600
H	1.73117100	-0.01951900	1.54761500
C	1.37916300	1.05060300	4.22113300
C	2.07636900	1.17620600	5.59881700
O	0.43948000	-1.37820400	5.58209900
H	0.69765100	-2.68039900	2.74581700
H	0.05395900	-4.70786500	3.78469300
H	0.16153900	-3.92718300	5.38111400
H	-1.21783300	-3.57345400	4.32142300
C	3.54060400	0.71907900	5.54806100
C	3.67109000	-0.69151200	4.95939600
H	2.02437200	2.22719700	5.90633300
H	1.52784200	0.59094500	6.33979100
H	4.12288300	1.42062800	4.93151300
H	3.97742900	0.75090200	6.55326600
H	4.72698700	-0.97015600	4.85858900
H	3.21542100	-1.42119400	5.63938900
C	3.00053900	-0.77860900	3.58193900
H	3.50719200	-0.07985400	2.89828200
H	3.10938500	-1.78175300	3.15719400
C	0.00451800	1.70809100	4.21133900
C	-1.01309400	1.35855400	5.11403000
C	-0.24234700	2.75714200	3.31228800
C	-2.23610100	2.03055800	5.10297300
H	-0.85110800	0.54327800	5.80919600
C	-1.46709400	3.43175200	3.29750200
H	0.53999400	3.06089300	2.61921100
C	-2.47154900	3.06770100	4.19543700
H	-3.01160100	1.73808600	5.80559000
H	-1.63009100	4.24225700	2.59207600
H	-3.42543000	3.58766700	4.19199200
H	1.98949700	1.64430800	3.52291900

9

E= -880.3417086 a.u.

C	0.32783200	-0.24147000	-0.06526500
C	0.20590600	-0.19728900	1.44949900
N	1.37710500	-0.03165700	2.12994100
C	1.53919200	0.13482200	3.60213200
C	0.94291300	1.54262700	3.93258900
N	-0.38402900	1.58230200	4.22672800
C	-1.06002800	2.86363400	4.38664600
H	-0.24934500	0.58725400	-0.48568500
H	1.35702300	-0.18107500	-0.42967900
H	-0.12409100	-1.17075100	-0.42245700
O	-0.89414700	-0.31549400	1.99693500
H	2.18919200	0.19392800	1.57261700
C	3.08817100	0.15920200	3.85727600
C	3.71645700	-1.23198000	3.55865100
O	1.64482600	2.55116100	3.88651500

H	-0.93972900	0.80008200	3.89983200
H	-2.05708500	2.68548000	4.79502200
H	-0.49251900	3.48908700	5.07792100
H	-1.14966800	3.40306400	3.43531600
C	3.03878000	-2.39263900	4.29820200
C	1.52616600	-2.40076600	4.03949900
H	3.65564500	-1.42652300	2.47916900
H	4.78314800	-1.18790500	3.80429600
H	3.48126200	-3.34155500	3.97143800
H	3.23736400	-2.31814000	5.37374100
H	1.33831500	-2.66372100	2.99050700
H	1.03907800	-3.17614400	4.64263800
C	0.86289100	-1.04634600	4.34280200
H	-0.19030700	-1.10614100	4.06816000
H	0.89572900	-0.83506200	5.41459600
H	3.48621200	0.86185500	3.11640400
C	3.56053200	0.72417800	5.19987500
C	4.48662800	1.78137800	5.16939800
C	3.19702100	0.22538500	6.46145600
C	5.02803800	2.31811000	6.33672100
H	4.76950700	2.20627700	4.21051400
C	3.73009900	0.76498400	7.63739900
H	2.49225200	-0.59059400	6.55373200
C	4.64986400	1.81174900	7.58307400
H	5.73592300	3.13972300	6.27202900
H	3.42224700	0.35796800	8.59668700
H	5.06348900	2.22927100	8.49651700

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E= -880.3421203 a.u.

C	-0.06774000	-0.07359100	0.32247600
C	0.16030300	-0.04751800	1.82477000
N	1.45928600	0.13366200	2.22105400
C	1.94165300	-0.07641200	3.60722700
C	1.59124200	-1.56699200	3.94639600
N	0.83766500	-1.85299300	5.02897200
C	0.42257000	-3.21940100	5.31371500
H	-0.94887100	0.52867700	0.09010400
H	0.78536300	0.29148600	-0.25653100
H	-0.27977500	-1.10543000	0.02347000
O	-0.77086800	-0.17617000	2.61845500
H	2.15644400	0.00715500	1.50042300
C	1.32431100	1.06672900	4.49763700
C	1.90271600	2.44427600	4.05748700
O	2.03433700	-2.44942300	3.20728200
H	0.40722200	-1.10201900	5.54607700
H	-0.03560700	-3.24579400	6.30439300
H	-0.29800200	-3.57979600	4.57064900
H	1.28967700	-3.88362000	5.29683600
C	3.43510100	2.50395800	4.05712000
C	4.02470800	1.39926100	3.16960200
H	1.53743200	2.65828100	3.04606900
H	1.48920700	3.21791200	4.71381900
H	3.76541600	3.48766400	3.70210200
H	3.81559600	2.40436800	5.08122900
H	3.78771000	1.62103900	2.12005200
H	5.11915000	1.38985700	3.23834900
C	3.49027000	0.00733800	3.54482400
H	3.83708600	-0.75363900	2.83785400
H	3.89029000	-0.29444600	4.51728600
H	0.26382700	1.08016300	4.23791900

C	1.36474500	0.92874500	6.02171100
C	0.16340900	1.16273300	6.71849100
C	2.50887900	0.65051500	6.79062300
C	0.10057700	1.11876300	8.11377400
H	-0.73897300	1.38412300	6.15322800
C	2.45094000	0.60209900	8.18599600
H	3.46081600	0.45891800	6.31188900
C	1.24824100	0.83556000	8.85660000
H	-0.84502000	1.30447600	8.61544300
H	3.35305900	0.37933700	8.74903600
H	1.20722500	0.79693700	9.94116400

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E= -880.3425103 a.u.

C	0.31108700	-0.24806400	-0.00682600
C	0.24097400	0.06807500	1.48030300
N	1.44420100	0.06464500	2.14431500
C	1.59570000	0.13545100	3.61928500
C	0.99768700	1.46982600	4.15295600
N	1.19349300	2.56226400	3.36425700
C	0.62242900	3.85353400	3.71902800
H	-0.26242900	0.50522500	-0.55241800
H	1.32951200	-0.28543100	-0.40488300
H	-0.17032800	-1.21571200	-0.18049100
O	-0.82205300	0.32586800	2.03460100
H	2.24524600	-0.26009300	1.62163000
C	3.15516600	0.12500700	3.87301800
C	3.75509900	-1.28851000	3.60852800
O	0.46892500	1.53448000	5.25723800
H	1.44701400	2.39617900	2.40162100
H	1.09592200	4.63005600	3.11362300
H	-0.46206200	3.87682200	3.55640200
H	0.81409700	4.05282800	4.77478500
C	3.01480700	-2.42975100	4.31750400
C	1.51913900	-2.40879300	3.97300600
H	3.74221400	-1.49045000	2.52668200
H	4.81213400	-1.27124400	3.89558700
H	3.46211900	-3.38798100	4.02640200
H	3.14858700	-2.34503900	5.40258700
H	1.38882700	-2.64047000	2.90613200
H	0.99032400	-3.19669200	4.52189200
C	0.87540800	-1.05397700	4.29524600
H	-0.17256200	-1.03602600	3.98614700
H	0.87148800	-0.87494100	5.37214700
H	3.56846100	0.79038000	3.10466800
C	3.64553000	0.71698900	5.19385300
C	4.60729400	1.73956300	5.13342000
C	3.24994100	0.27235800	6.46580600
C	5.15920200	2.29648900	6.28913100
H	4.92856700	2.10948100	4.16245800
C	3.79597100	0.82759500	7.62507600
H	2.49498400	-0.49593100	6.56925900
C	4.75463100	1.83984400	7.54471700
H	5.89923900	3.08753400	6.20554500
H	3.46183700	0.46987300	8.59478800
H	5.17559000	2.27045400	8.44863500

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E= -880.3393909 a.u.

C	-0.03028700	-0.12864900	0.11883600
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C	0.19046900	-0.18531300	1.62081800
N	1.47668100	-0.03223500	2.03587700
C	2.02813500	0.01282600	3.42101500
C	1.98746600	-1.41951700	4.05488000
N	0.79061800	-2.04226100	4.05702500
C	0.62007200	-3.33992700	4.69207800
H	-0.50911900	-1.05933900	-0.19812600
H	-0.72459000	0.68794600	-0.09907400
H	0.88561500	0.01881200	-0.45982700
O	-0.76317500	-0.35554400	2.39091800
H	2.17225200	0.02719700	1.30539400
C	1.22507500	1.09657700	4.27196900
C	2.01766700	2.42841700	4.31834200
O	3.00663100	-1.93369900	4.52230200
H	-0.01914100	-1.54503700	3.69233400
H	1.35136300	-4.05534100	4.30544100
H	0.75505300	-3.27073700	5.77749100
H	-0.38766100	-3.70114100	4.47826400
C	3.41678100	2.31403100	4.94883200
C	4.16275400	1.03967100	4.47612900
H	2.11019700	2.79845300	3.28879800
H	1.41966200	3.17256600	4.85580600
H	3.98939700	3.21145800	4.68612100
H	3.33282100	2.31563400	6.04052400
H	5.20865000	1.27140400	4.24640100
H	4.19016900	0.27958600	5.26073800
C	3.51516900	0.42464000	3.23125900
H	3.55646200	1.16273100	2.41931300
H	4.08313100	-0.45484300	2.91597700
H	0.32053300	1.29810000	3.69799900
C	0.72172200	0.68904800	5.65703100
C	-0.63894300	0.89138200	5.94466000
C	1.53706100	0.18575300	6.68406600
C	-1.16828800	0.61224600	7.20651500
H	-1.29554500	1.26216000	5.16164800
C	1.01079200	-0.10056000	7.94680600
H	2.58603800	-0.01451500	6.50354800
C	-0.34243000	0.11450200	8.21712400
H	-2.22538800	0.77806600	7.39532900
H	1.66486600	-0.49558700	8.71929200
H	-0.74824100	-0.10769000	9.19995400

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E= -880.3393561 a.u.

C	-0.43357900	0.19182500	0.24081200
C	-0.18280400	0.12256800	1.73754700
N	1.12156000	0.05132500	2.11647000
C	1.71300800	0.02635800	3.48572300
C	1.43437800	-1.35938900	4.16117200
N	0.14596200	-1.75676500	4.20966400
C	-0.23645300	-2.98410300	4.89052200
H	-1.07824700	-0.64459700	-0.04323700
H	-0.97906200	1.11458200	0.02310900
H	0.47673100	0.16501100	-0.36421300
O	-1.12932800	0.13809500	2.53468300
H	1.79597800	-0.02065300	1.36751200
C	1.14281800	1.25538300	4.32702400
C	2.15618100	2.42750800	4.30424300
O	2.35789100	-2.03588100	4.62056200
H	-0.57161100	-1.13139500	3.84911400
H	0.35011600	-3.82821200	4.51725100

H	-0.06920800	-2.90659400	5.97091400
H	-1.29610300	-3.16883100	4.70397600
C	3.53477900	2.08690800	4.89885900
C	4.02703300	0.68608000	4.45521000
H	2.27703200	2.74476600	3.26012900
H	1.71639100	3.28100900	4.83192500
H	4.24730100	2.85912600	4.58527500
H	3.49106400	2.13975100	5.99170300
H	5.09020300	0.71932100	4.19249400
H	3.94262700	-0.04208500	5.26574000
C	3.24409100	0.15853900	3.24789900
H	3.39395700	0.85171700	2.40944400
H	3.63652400	-0.81783100	2.95119000
H	0.26625300	1.59594400	3.77602900
C	0.62584900	0.97866300	5.73921600
C	-0.66522900	1.43055300	6.06206400
C	1.37231100	0.36058600	6.75588200
C	-1.19185000	1.28159200	7.34693400
H	-1.27162500	1.89589900	5.28904600
C	0.84769500	0.20440100	8.04195600
H	2.36127000	-0.02997400	6.55034600
C	-0.43448300	0.66652200	8.34649300
H	-2.19487300	1.63956800	7.56225500
H	1.44686600	-0.28402600	8.80552600
H	-0.83930400	0.54380700	9.34702200

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E= -880.335818 a.u.

C	0.09460800	-0.50750000	0.11967200
C	0.04093700	-0.20811300	1.61476300
N	1.26454600	-0.02322100	2.18638100
C	1.71299600	0.21185700	3.57522900
C	3.27925200	0.21477400	3.38941500
N	4.04210600	0.72384800	4.38331200
C	5.49717100	0.65340300	4.31337600
H	-0.46102000	0.27324900	-0.40786900
H	1.10619600	-0.56464700	-0.29098300
H	-0.42191000	-1.45434300	-0.06169900
O	-1.04636300	-0.14170100	2.18918600
H	2.07026100	-0.20559800	1.59205900
C	1.25456100	-0.98881000	4.52776200
C	-0.19548700	-0.80160200	5.06772400
O	3.79408700	-0.19987700	2.34498700
H	3.62680300	0.85772700	5.29280700
H	5.91321200	1.24679200	5.12967500
H	5.85443100	-0.37938600	4.39581200
H	5.83790600	1.05982100	3.35939400
C	-0.56880400	0.61005500	5.55482300
C	-0.21675800	1.68749500	4.52240300
H	-0.88098800	-1.05795700	4.25860400
H	-0.34979400	-1.52812900	5.87419600
H	-1.64552900	0.63065300	5.76104900
H	-0.07748400	0.84539500	6.50817700
H	-0.85652500	1.57441300	3.64565200
H	-0.39887500	2.68482200	4.94256200
C	1.26012500	1.59589400	4.11664200
H	1.50575700	2.35033700	3.36083000
H	1.86307800	1.83945700	5.00001500
H	1.22727100	-1.85099800	3.85451100
C	2.25356000	-1.37467100	5.61897200
C	3.14524000	-2.43338000	5.37500500

C	2.32078400	-0.74768300	6.87597400
C	4.07504900	-2.84247200	6.33360300
H	3.11015900	-2.94489500	4.41644300
C	3.25114200	-1.15176500	7.83918300
H	1.63684000	0.05693800	7.12007100
C	4.13597600	-2.19906700	7.57228700
H	4.74664100	-3.66756400	6.11317400
H	3.27530300	-0.65058000	8.80307300
H	4.85450700	-2.51595400	8.32248800

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E= -880.3347844 a.u.

C	0.18907000	-0.52876900	0.09422300
C	0.11600300	-0.23873500	1.58722000
N	1.32088600	-0.07107200	2.19658300
C	1.61055000	0.22006600	3.60955200
C	3.15030700	0.48745500	3.58002100
N	3.68590800	1.18490300	4.60658600
C	5.12680300	1.37438300	4.72261900
H	-0.33959500	-1.46533600	-0.10451500
H	-0.34068200	0.26551500	-0.43982600
H	1.20868100	-0.60104700	-0.29386900
O	-0.97422700	-0.15992000	2.15953600
H	2.16826700	-0.21298300	1.65402800
C	1.27674900	-1.06854100	4.51813400
C	-0.14509700	-0.96864700	5.12703100
O	3.84430100	0.09228100	2.63747500
H	3.11549700	1.37190400	5.41663300
H	5.63426600	0.43719000	4.97691400
H	5.52657000	1.73679900	3.77368700
H	5.32003600	2.11360200	5.50239400
C	-0.47387600	0.33028000	5.91030200
C	0.46806100	1.49472100	5.56050900
H	-0.84231500	-1.04252100	4.29093300
H	-0.30790700	-1.84633800	5.76237000
H	-1.50079400	0.62404000	5.66424800
H	-0.46243400	0.15850100	6.99293900
H	-0.00319300	2.45104400	5.81408700
H	1.37018200	1.43762500	6.18580200
C	0.82044700	1.48564100	4.06756900
H	-0.11587700	1.50531700	3.50573300
H	1.38551800	2.38074200	3.78753700
H	1.23593800	-1.88014100	3.78575500
C	2.36325200	-1.49551800	5.50891100
C	3.44537400	-2.26107300	5.03835600
C	2.32002400	-1.21250600	6.88363500
C	4.45373000	-2.70437400	5.89571400
H	3.50024900	-2.50981900	3.98210000
C	3.32662200	-1.65537900	7.74826500
H	1.48895800	-0.65557800	7.30047600
C	4.40164000	-2.39944600	7.25872600
H	5.27464100	-3.29515100	5.49880100
H	3.26143100	-1.42420400	8.80808000
H	5.18082500	-2.74737900	7.93072100

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E= -880.3310409 a.u.

C	0.26575800	-0.58676600	0.15023800
C	0.13318400	-0.39856000	1.65240400
N	1.27263000	-0.02617300	2.30228400

C	1.42391000	0.29176900	3.75419200
C	0.64517300	1.63400900	3.96762900
N	-0.68900600	1.51443200	4.20325000
C	-1.53351900	2.70162900	4.24832600
H	-0.04518100	-1.60481500	-0.10011300
H	-0.42369100	0.09957600	-0.34972500
H	1.27690100	-0.41854000	-0.23048400
O	-0.94783900	-0.59248800	2.21852000
H	2.05509700	0.22984400	1.71699200
C	2.94920400	0.54234900	3.95075800
C	3.76957000	-0.74732100	3.58958000
O	1.21717700	2.71921300	3.89189100
H	-1.11849400	0.64430000	3.90176300
H	-1.08539500	3.44145100	4.91398100
H	-1.64983400	3.16200500	3.25897100
H	-2.51658900	2.41867600	4.63065600
C	3.04419300	-2.07874500	3.89380800
C	2.02089600	-1.90304700	5.01815500
H	4.05361200	-0.72161600	2.53051900
H	4.70923800	-0.70778500	4.14728500
H	2.52939300	-2.44198800	2.99583600
H	3.78011500	-2.84525000	4.16129000
H	1.55852500	-2.86392400	5.27180300
H	2.53534100	-1.55601400	5.92173800
C	0.91277900	-0.90884800	4.61605700
H	0.14228700	-1.43310400	4.04875300
H	0.41404300	-0.52891200	5.51109000
H	3.21220800	1.31972900	3.22399700
C	3.38652100	1.13357500	5.29702500
C	4.68115000	1.67913100	5.35716100
C	2.61386900	1.18179500	6.46438700
C	5.19135000	2.23122300	6.53160200
H	5.29937700	1.68133900	4.46218000
C	3.11818000	1.73438300	7.64641700
H	1.59907400	0.80411600	6.47255800
C	4.40984100	2.25813400	7.69005300
H	6.19493600	2.64745600	6.53857300
H	2.48992000	1.75775900	8.53255900
H	4.79931400	2.68871500	8.60791000

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E= -880.4036155 a.u.

C	0.38840600	-0.68556300	-0.03251800
C	0.28254300	-0.59716900	1.48372900
N	1.38368500	-0.08498200	2.11688100
C	1.49302900	0.25829100	3.56201000
C	2.95532300	0.77780900	3.72197000
N	3.92560200	0.00292400	3.14882400
C	5.33711700	0.30195700	3.36400300
H	0.15766100	-1.70941000	-0.33829300
H	-0.37165400	-0.03280200	-0.47244600
H	1.36882600	-0.40495100	-0.42812700
O	-0.72581200	-0.97863900	2.07351700
H	2.10764300	0.28964500	1.51981000
C	1.21277600	-1.04507800	4.44988600
C	-0.11864500	-0.90920400	5.23547500
O	3.21963100	1.83953600	4.27643600
H	3.68370700	-0.95296300	2.92523100
H	5.51224600	1.36273400	3.17809100
H	5.64620300	0.07657000	4.39153800
H	5.93368400	-0.29074000	2.66722700

C	-0.22327200	0.34090200	6.12554500
C	0.30464500	1.61304200	5.41202500
H	-0.91982400	-0.89839800	4.49215900
H	-0.25664000	-1.81459000	5.83759100
H	-1.27613700	0.46915300	6.40300100
H	0.31766600	0.18568700	7.06560900
H	-0.39176300	2.44673900	5.55579900
H	1.25562800	1.93719900	5.84366600
C	0.50196800	1.39982000	3.90296600
H	-0.45584300	1.14890100	3.43853900
H	0.86577400	2.32255500	3.44199500
H	1.04227300	-1.84448100	3.72529500
C	2.34755100	-1.53720900	5.34628200
C	2.78476100	-2.86545100	5.20387100
C	2.94024700	-0.76165400	6.35809500
C	3.77388100	-3.40361500	6.03213500
H	2.33432800	-3.49227500	4.43715400
C	3.93035200	-1.29447800	7.18744500
H	2.64703200	0.27274400	6.49500600
C	4.35253400	-2.61752500	7.03068100
H	4.08739500	-4.43520900	5.89721700
H	4.37179700	-0.67012900	7.95936500
H	5.12094000	-3.02918900	7.67861800

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E= -880.3313571 a.u.

C	1.51095000	-1.54028400	0.45367000
C	0.85887000	-0.82963200	1.63262900
N	1.73473500	-0.18421700	2.47615300
C	1.40972000	0.42474200	3.79129600
C	2.65134300	1.26686500	4.20007000
N	3.34622100	1.83280000	3.16797900
C	4.42464600	2.77986300	3.41937000
H	1.23841200	-2.59899600	0.48917000
H	1.09542100	-1.12794400	-0.47012000
H	2.60062200	-1.45128500	0.42503400
O	-0.35974800	-0.83417400	1.77561800
H	2.69799200	-0.48048600	2.38318000
C	1.00272200	-0.71368100	4.80837700
C	0.04811200	-0.21453200	5.94342300
O	2.97288600	1.46365600	5.36763900
H	2.95257300	1.77606900	2.23968900
H	4.04622200	3.73929200	3.79181500
H	5.10248700	2.36976800	4.17044700
H	4.97288400	2.94506600	2.48945900
C	0.10552800	1.28792800	6.25316400
C	-0.08456800	2.16155500	4.98655000
H	-0.97650000	-0.46998300	5.64592500
H	0.24700900	-0.78626800	6.85542400
H	-0.66886100	1.52790500	6.99128600
H	1.06865500	1.52347100	6.70896900
H	-1.11603900	2.52783000	4.92554900
H	0.55233800	3.04976000	5.06453700
C	0.21173800	1.40780500	3.67132900
H	-0.65405700	0.81842300	3.36653000
H	0.40354800	2.11902500	2.85916200
H	0.38043700	-1.35457300	4.17764800
C	2.15635700	-1.59907500	5.26853100
C	2.44505600	-2.77104400	4.54882100
C	2.93206500	-1.32391400	6.40729400
C	3.48109200	-3.62883800	4.93198300

H	1.83243400	-3.03015200	3.68831000
C	3.96293800	-2.18058000	6.79819900
H	2.74216600	-0.42488200	6.98128000
C	4.24727700	-3.33416700	6.06089500
H	3.67531300	-4.53099400	4.35813500
H	4.54817400	-1.94342400	7.68250400
H	5.04898100	-3.99911900	6.36958300

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E= -880.332319 a.u.

C	0.39320600	0.23141800	-0.09541100
C	0.25216000	0.26050200	1.41964200
N	1.43342600	0.25617600	2.12568400
C	1.52503100	0.04885500	3.59350700
C	0.75798500	1.18995400	4.32006700
N	0.86524100	2.42466000	3.76809700
C	0.16592800	3.56803400	4.33408200
H	-0.01721900	-0.71375800	-0.46436600
H	-0.21113400	1.03762100	-0.51882700
H	1.42410300	0.33053000	-0.44794200
O	-0.84466500	0.31130800	1.96362000
H	2.27343000	0.06946100	1.59489800
C	3.08494400	0.09529900	3.93383100
C	3.63335600	-1.34542700	4.09716400
O	0.15933000	0.98457400	5.37287300
H	1.23615800	2.49015300	2.83227300
H	-0.91567800	3.50218700	4.16652800
H	0.34381800	3.60845200	5.41067100
H	0.54890400	4.48053800	3.87190200
C	2.96551600	-2.14655900	5.22939600
C	1.43003900	-1.93649300	5.26375700
H	3.48468700	-1.87397100	3.14579200
H	4.71657700	-1.29456500	4.25351800
H	3.20530500	-3.20668500	5.08491800
H	3.40688200	-1.86402200	6.19090900
H	0.92124300	-2.89157600	5.43632400
H	1.13975600	-1.28749900	6.09360400
C	0.89346200	-1.32645500	3.96340100
H	1.09854900	-2.01074000	3.13099200
H	-0.18909900	-1.20622900	4.01917900
H	3.56093100	0.50307700	3.03410400
C	3.57336100	1.01959800	5.05038900
C	4.61134000	1.91760100	4.74760600
C	3.11201000	0.98098400	6.37610000
C	5.17350500	2.74433000	5.72254700
H	4.98907200	1.97058000	3.72857300
C	3.66816900	1.80935300	7.35436800
H	2.29265300	0.32957000	6.64979800
C	4.70210100	2.69243200	7.03595900
H	5.97448400	3.42750600	5.45388600
H	3.28435800	1.76347700	8.36965400
H	5.13174700	3.33369400	7.80018500

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E= -880.3319589 a.u.

C	0.29548000	0.21277000	0.06451900
C	0.22622600	-0.05346000	1.55878000
N	1.44083400	-0.05989700	2.20841900
C	1.54017300	0.03370700	3.67835500
C	0.92102300	1.40721800	4.07858800

N	0.31452700	1.49957200	5.28530900
C	-0.24761400	2.75824600	5.75631000
H	-0.46630900	-0.38772200	-0.43624000
H	0.06194800	1.26917200	-0.10811800
H	1.27645900	-0.00396500	-0.36841300
O	-0.83974100	-0.25273700	2.13276800
H	2.17885200	0.41618500	1.70595100
C	3.10541500	0.04179900	4.00408000
C	3.63072400	-1.41277000	4.05281400
O	1.03665600	2.38009500	3.33220000
H	0.20033700	0.67489400	5.85175500
H	0.51745600	3.53945000	5.76026300
H	-1.06847100	3.08586600	5.11031800
H	-0.62223500	2.61527300	6.77162900
C	2.93195300	-2.34488000	5.08008300
C	1.55537300	-1.80918700	5.50746100
H	3.48849000	-1.83010100	3.04994500
H	4.71201500	-1.39192700	4.22571300
H	2.79931000	-3.33152500	4.61988900
H	3.56555400	-2.50955300	5.95851500
H	0.95103000	-2.62040500	5.92930100
H	1.66921600	-1.06625100	6.30724000
C	0.82252200	-1.20405400	4.30581000
H	0.75694000	-1.96864200	3.52618800
H	-0.21402100	-0.95346400	4.54006600
H	3.56204200	0.49831300	3.11784200
C	3.58178500	0.94271000	5.15148800
C	3.76988900	2.31331400	4.89396200
C	3.92898200	0.47336800	6.42815600
C	4.25312000	3.18086500	5.87432300
H	3.51955100	2.70879800	3.91461100
C	4.41757500	1.33766000	7.41335200
H	3.84051700	-0.57803200	6.67012600
C	4.57712100	2.69749400	7.14461100
H	4.38302600	4.23377500	5.64004000
H	4.67973700	0.93964700	8.38984500
H	4.95912900	3.36840100	7.90869100

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E= -880.3319945 a.u.

C	-0.49428800	-0.01220300	0.44952500
C	-0.15615300	0.15427600	1.91984600
N	1.18531400	0.26118900	2.20436900
C	1.73917400	0.06544100	3.55294000
C	1.35773800	-1.39711900	3.98689900
N	1.50732500	-1.74640500	5.28930400
C	1.21844400	-3.10623400	5.72894400
H	-0.63544000	-1.08043400	0.25128400
H	-1.43527700	0.50010300	0.24120600
H	0.28591400	0.36615900	-0.21779200
O	-1.02948800	0.20382800	2.78267400
H	1.79383500	-0.03787100	1.45398400
C	1.27315000	1.31120800	4.44509100
C	2.32653900	2.44291100	4.34364800
O	1.09236700	-2.23090400	3.12212800
H	1.52454900	-1.01842700	5.98891600
H	0.14759500	-3.33232500	5.66740300
H	1.75151200	-3.82008300	5.09744600
H	1.55153000	-3.21604200	6.76308600
C	3.77251000	2.07947900	4.76482800
C	4.05082000	0.57489500	4.59489600

H	2.33960000	2.75494000	3.29286900
H	1.96799700	3.30911400	4.90999800
H	4.46983600	2.64816100	4.13701200
H	3.98005900	2.39153700	5.79404400
H	5.12484400	0.39322700	4.47700100
H	3.74519200	0.01622200	5.48741400
C	3.29771200	0.03990900	3.37585800
H	3.55149400	0.67000600	2.51288100
H	3.61358500	-0.97849300	3.12725200
H	0.39731600	1.68062500	3.91350300
C	0.74577100	1.06039400	5.86044300
C	-0.61657300	0.73497500	6.01206900
C	1.51730900	1.19437800	7.02792300
C	-1.17740700	0.53746300	7.27432500
H	-1.22639900	0.62450100	5.12056900
C	0.95629800	0.99579000	8.29555900
H	2.56489100	1.46297900	6.96548100
C	-0.39283500	0.66401800	8.42519800
H	-2.23135800	0.28716500	7.35815600
H	1.57824900	1.10988000	9.17923200
H	-0.82904100	0.51317100	9.40848700