

Geometry of the stationary structures based on the structure of Ramakrishnan

Reactant

C	-1.54661000	-4.48701900	-0.49233900
O	-2.99835300	-4.35706100	-0.80009500
C	-3.45033600	-3.03304200	-0.40461000
N	-4.83088300	-3.14244500	0.03251400
C	-5.88228800	-2.29267500	-0.27058900
N	-5.91196100	-1.16566900	-1.02781600
C	-7.14866300	-0.61702500	-1.11932100
N	-8.28229200	-1.05407700	-0.54317600
C	-8.23751600	-2.18129700	0.22281100
N	-9.37645800	-2.61791400	0.80019500
C	-7.00342500	-2.84366400	0.37284700
N	-6.66053900	-4.01122700	1.05504100
C	-5.36353600	-4.15932300	0.82934000
C	-2.44672800	-2.59452000	0.69289300
O	-2.47267500	-1.20761300	0.98667300
C	-1.12539500	-3.15966900	0.13404600
O	-0.73132800	-2.19472400	-0.91189200
N	1.21973600	0.29783500	-1.05262600
C	0.88035100	-0.77313400	-1.98706200
C	0.61182800	-2.07744300	-1.24917800
O	1.44902100	-2.90855200	-0.87191000
C	4.44688400	-2.53432600	2.33538900
O	5.70584700	-1.74617100	2.42069800
C	5.73768200	-0.78256900	1.33981000
N	7.08617500	-0.79732500	0.76337100
C	7.46210800	-0.26344400	-0.45705200
N	6.68693100	0.29998800	-1.41806000
C	7.39923100	0.71258000	-2.49243700
N	8.73184900	0.61087800	-2.67219900
C	9.49235700	0.03574600	-1.69773500
N	10.82547500	-0.06438500	-1.89304500
C	8.85339900	-0.42878100	-0.52958300
N	9.33584600	-1.05300400	0.62281500
C	8.25770700	-1.25340200	1.37170500
C	4.64346600	-1.23442500	0.34298000
O	4.14314600	-0.19557800	-0.49066700
C	3.59235100	-1.83000500	1.28444000
O	2.88131800	-0.69114600	1.90369100
N	-0.23293500	0.61627000	1.84057600
C	0.90472300	0.40221900	2.72920800
C	1.58313200	-0.88755100	2.31491000
O	1.04066400	-1.99994000	2.31213700
H	-1.01150600	-4.69965600	-1.41836600
H	-1.42750000	-5.32395300	0.20165800
H	-0.32429500	-3.23241400	0.86927900
H	-2.48484800	-0.03238200	-1.86467400
H	-0.00381100	-0.50668900	-2.56983100
H	-2.69179100	-3.12098700	1.62159600
H	-3.42846400	-2.33614800	-1.24784800
H	-7.23167100	0.27358000	-1.72973400
H	-10.22958100	-2.10419200	0.64982400

H	-4.75678900	-4.97942000	1.17063900
H	3.98534500	-2.53980500	3.32250500
H	4.69476900	-3.55733100	2.03554800
H	6.83835000	1.17234300	-3.29559800
H	11.22088900	0.28834600	-2.74944600
H	2.19056700	0.27796700	-0.74456000
H	0.54875500	0.45210000	-0.29888000
H	1.61391400	1.22472400	2.62455200
H	-0.57817000	1.57078900	1.76493200
H	-0.96846900	-0.08323700	1.90302800
H	2.87241200	-2.47470300	0.78061000
H	5.05230500	-2.06609500	-0.25270300
H	5.50912800	0.21856300	1.72035000
H	8.23319100	-1.72063100	2.34000900
H	4.90781400	0.14696300	-1.04189500
C	-3.75090700	2.72853700	-2.87867800
O	-2.28797200	2.94963200	-2.89777400
C	-1.79615200	2.76930800	-1.55276900
N	-1.90323900	4.06893600	-0.84412500
C	-1.76445700	4.33469000	0.51239300
N	-1.56740700	3.47978500	1.54659000
C	-1.49912300	4.11103600	2.74109000
N	-1.59623400	5.43688100	2.98040300
C	-1.78108400	6.27973300	1.92780900
N	-1.87093800	7.60823000	2.16604300
C	-1.87072700	5.73117900	0.63226900
N	-2.04965100	6.32606300	-0.61683000
C	-2.05256100	5.31010100	-1.46993500
C	-2.68842900	1.68173700	-0.92413400
O	-2.04384900	0.39822200	-1.08228900
C	-4.00992000	1.67588600	-1.79531200
O	-4.16250500	0.37718500	-2.41596200
H	-4.03092900	2.36172100	-3.86440600
H	-4.25896000	3.67516200	-2.66053200
H	-4.88408500	1.91622700	-1.18309300
H	-2.17755300	-0.65532500	0.19945800
H	-2.86094800	1.84551200	0.13848100
H	-0.75397800	2.44720600	-1.60783600
H	-1.34576000	3.48009500	3.60764000
H	-1.79397700	7.94014000	3.11350200
H	-2.15018400	5.38167900	-2.53860000
H	-4.77688500	-0.23826500	-1.88917300
H	-2.00002000	8.25516700	1.40544500
H	1.72260000	-0.93443900	-2.66428400
H	0.64483500	0.31020000	3.80058500
H	-9.37426800	-3.45067800	1.36676000
H	11.41457700	-0.48456400	-1.19275800

TS

C	-3.77434800	-4.18808500	-0.82277100
O	-5.09523000	-3.53708400	-0.63581100
C	-4.84547800	-2.12194600	-0.44518300
N	-6.03984400	-1.53997400	0.13801800
C	-6.57094200	-0.29469000	-0.14444800
N	-6.13309600	0.66184100	-1.00090400
C	-6.93768000	1.75104100	-1.03440400

N	-8.05967200	1.96072800	-0.31962800
C	-8.48116400	0.99344700	0.54388900
N	-9.60742800	1.20873500	1.25774300
C	-7.72504700	-0.19093400	0.64946800
N	-7.91006800	-1.34913300	1.40625900
C	-6.88999100	-2.13039900	1.07456100
C	-3.56615300	-2.05079300	0.41070800
O	-2.78530300	-0.88964000	0.07564900
C	-2.72770400	-3.28769000	-0.13673000
O	-1.79744700	-2.68567000	-1.04373700
N	0.79663400	-3.35695300	-2.33026300
C	0.78977500	-2.22690000	-1.42292300
C	0.15243800	-2.53767900	-0.08213100
O	0.22351900	-3.55830900	0.60015500
C	4.36750700	-1.29058500	3.13535500
O	4.85117700	-0.07573100	2.43144100
C	4.84605400	-0.31645100	1.00027200
N	6.15672800	0.05425700	0.45966000
C	6.66178400	-0.31250000	-0.77703100
N	6.12673300	-1.14795600	-1.70305000
C	6.90470700	-1.27775900	-2.80392200
N	8.09253600	-0.68316800	-3.03318200
C	8.61499900	0.14950100	-2.08814800
N	9.80695600	0.73540600	-2.33177400
C	7.88569700	0.36108200	-0.89940700
N	8.13823100	1.13438200	0.23629900
C	7.08667800	0.93384400	1.02079700
C	4.53243300	-1.82377900	0.82270100
O	3.91529800	-2.15722600	-0.41084800
C	3.67378600	-2.11787500	2.05477700
O	2.31984900	-1.58230700	1.79395100
N	-0.17709200	-1.20275800	0.76644100
C	-0.03301400	-1.43709000	2.23224800
C	1.31467600	-1.97773400	2.64903000
O	1.50998500	-2.62832200	3.67490600
H	-3.54873800	-4.26346700	-1.89073400
H	-3.86473500	-5.18241700	-0.38289400
H	-2.18983200	-3.81793300	0.66118400
H	-2.25596600	-0.10750200	-2.62532900
H	1.82423400	-1.92707400	-1.20232100
H	-3.79377600	-2.09885200	1.47799900
H	-4.66020600	-1.60871200	-1.39617700
H	-6.64557600	2.54073800	-1.71510200
H	-10.10949800	2.07230500	1.13011600
H	-6.71686300	-3.12984100	1.43264600
H	3.70302800	-0.96996300	3.93515100
H	5.22051400	-1.83104700	3.55948400
H	6.53290000	-1.92983200	-3.58329300
H	10.27421300	0.54594700	-3.20370200
H	-0.14874500	-3.65179200	-2.55454900
H	1.37186500	-4.12938000	-2.01133000
H	-0.21608600	-0.48731300	2.74575500
H	0.39429300	-0.39371100	0.45961600
H	-1.20048400	-0.96307700	0.58708800
H	3.58589400	-3.17725300	2.29551100
H	5.47584400	-2.37696600	0.96068100

H	4.06678300	0.29325800	0.53213500
H	6.92573500	1.36605600	1.99257600
H	4.58081800	-1.95289700	-1.13458900
C	-2.57870000	2.89591100	-3.25951200
O	-1.27681400	3.41313600	-2.79424100
C	-0.72684900	2.51878000	-1.78847100
N	-0.40485800	3.34394800	-0.61331000
C	0.35695000	2.96698800	0.48192100
N	0.91283200	1.76151600	0.78428200
C	1.64408100	1.80700900	1.92788000
N	1.82331500	2.85750700	2.75594300
C	1.23243700	4.04476400	2.44927000
N	1.40356800	5.09324300	3.28470800
C	0.47459200	4.12968100	1.26535600
N	-0.19606300	5.19939900	0.67519900
C	-0.70161700	4.69684500	-0.44470400
C	-1.78985900	1.45029100	-1.50929600
O	-1.41836100	0.27654200	-2.26832600
C	-3.10157300	2.03051900	-2.10780400
O	-3.94377500	0.98594700	-2.61683900
H	-2.43866100	2.27618700	-4.14945000
H	-3.19810300	3.76154500	-3.49630100
H	-3.61899100	2.63672800	-1.35496700
H	-2.20186400	-1.44272300	-0.76482400
H	-1.89073200	1.20671700	-0.45046100
H	0.19278500	2.05459600	-2.15270800
H	2.15666200	0.89584400	2.20483700
H	1.97123000	4.97511900	4.10795300
H	-1.25989300	5.23724600	-1.18675400
H	-4.71580700	0.78318600	-1.99795600
H	0.98713100	5.98550500	3.07354700
H	0.26308500	-1.38417000	-1.87743800
H	-0.78299800	-2.15997200	2.54959400
H	-9.94853900	0.50805600	1.89559400
H	10.21913700	1.35814100	-1.65616500

Product

C	-0.87847600	-4.92222400	1.87374500
O	-1.01607800	-5.23476200	0.42798100
C	-0.44304700	-4.16457100	-0.33711800
N	-1.54444300	-3.27015200	-0.77939400
C	-1.50859500	-2.29465500	-1.76190900
N	-0.47388900	-1.85489500	-2.52299600
C	-0.83607000	-0.90176400	-3.41467400
N	-2.05693500	-0.36314600	-3.58801600
C	-3.08634000	-0.81035800	-2.81563400
N	-4.30868000	-0.25993800	-2.99506000
C	-2.82917000	-1.82285500	-1.87263900
N	-3.66713400	-2.49201800	-0.98273900
C	-2.87116500	-3.35167800	-0.35920400
C	0.60358500	-3.45613000	0.56292000
O	1.91920000	-3.85460800	0.13013600
C	0.36874700	-4.05340600	2.00932800
O	1.51602200	-4.85126100	2.39451600
N	3.35820900	-3.08251700	4.01149300

C	3.41387100	-1.91049300	3.16646900
C	2.13058000	-1.06110800	3.12952400
O	1.08628600	-1.39210500	3.74485700
C	-1.46840200	4.00942800	-0.32229000
O	-2.72690400	4.14691100	0.45330200
C	-3.18982800	2.82900500	0.84526600
N	-4.64818500	2.81591300	0.73507200
C	-5.45374900	1.69597500	0.60883100
N	-5.09115400	0.39727300	0.47081700
C	-6.14878100	-0.44018100	0.34320900
N	-7.45458900	-0.09667200	0.35156400
C	-7.79930600	1.21459600	0.50165900
N	-9.11048300	1.53928600	0.51404600
C	-6.77212200	2.17320400	0.63105600
N	-6.79009000	3.56335900	0.77081100
C	-5.51080200	3.91120600	0.83472900
C	-2.48995100	1.84379000	-0.12085400
O	-2.35854100	0.51929100	0.37671600
C	-1.12674000	2.52286800	-0.30995700
O	-0.31511600	2.27354000	0.89260200
N	2.19820500	0.08777000	2.38350500
C	1.06386600	0.98504700	2.30520700
C	0.55860200	1.20706600	0.89908500
O	0.87453300	0.57803500	-0.11462600
H	-0.76720900	-5.87140600	2.39491900
H	-1.78152600	-4.40257800	2.21793800
H	0.24833300	-3.26424000	2.75357300
H	3.29610300	-2.60830900	-1.82302300
H	4.24211300	-1.25615100	3.47447000
H	0.48469600	-2.36945700	0.54201700
H	0.03979500	-4.58065800	-1.22203300
H	-0.05163800	-0.53747400	-4.06567100
H	-4.43158500	0.42546500	-3.72271500
H	-3.18344500	-4.07387800	0.37233200
H	-0.69669100	4.60923200	0.16113400
H	-1.65209000	4.37779300	-1.33574800
H	-5.90851900	-1.48580200	0.19967100
H	-9.79492300	0.80567400	0.42523500
H	2.75328500	-3.81817500	3.64590000
H	3.14988100	-2.87476200	4.98175000
H	0.25394400	0.53267600	2.89198300
H	3.05428900	0.33179900	1.87793700
H	2.53507000	-3.09841400	-0.08319400
H	-0.58782100	2.16395600	-1.18694100
H	-3.02265400	1.87286500	-1.08368700
H	-2.89113100	2.61533200	1.87731100
H	-5.12895600	4.91195000	0.93421400
H	-3.28545100	0.14126800	0.45067900
C	3.71500500	-0.03528600	-3.59338100
O	5.05674200	-0.39434600	-3.07539300
C	4.99871200	-0.29830800	-1.63667600
N	5.30633500	1.10917800	-1.26772300
C	5.16844200	1.77829400	-0.05467100
N	4.55725100	1.40086000	1.09842900
C	4.66466900	2.32938400	2.08040100
N	5.27141100	3.53162800	2.02033700

C	5.86440200	3.90342500	0.85315600
N	6.46960100	5.10958400	0.78484700
C	5.82658100	3.00932700	-0.23493800
N	6.36391600	3.10866100	-1.51671300
C	6.04759400	1.96096300	-2.09697300
C	3.58459500	-0.75884300	-1.24670600
O	3.62433300	-2.18509800	-0.97660600
C	2.71421300	-0.53863700	-2.54884600
O	2.19162900	-1.81910700	-2.98178700
H	3.59495200	-0.55122800	-4.54393900
H	3.66010400	1.05077200	-3.73216700
H	1.90393700	0.16346700	-2.34696000
H	2.10816500	-4.88001700	1.59781200
H	3.17801300	-0.25000000	-0.37884700
H	5.75975300	-0.96237800	-1.22642200
H	4.20340800	2.07703300	3.02742800
H	6.47954000	5.69833700	1.60180600
H	6.31319200	1.66074000	-3.09477300
H	1.22841800	-1.95899000	-2.69760200
H	6.92784000	5.40257100	-0.06273600
H	3.64656700	-2.22212100	2.13904200
H	1.27728600	1.96553600	2.74818700
H	-5.09256200	-0.55701000	-2.43726900
H	-9.40027800	2.49696100	0.62815600

Geometry of the stationary structures based on the structure of Steitz

Reactant

N	-1.98171400	3.01193300	-2.31924700
H	-1.07852500	2.54595700	-2.25070800
C	-2.92620500	2.28735800	-1.50430700
C	-2.94438300	0.78824400	-1.73658100
H	-2.70051000	2.43584800	-0.44075400
H	-3.94260900	2.66579400	-1.66270200
O	-2.29895600	0.18392900	-2.55377700
H	-2.26219900	2.98700800	-3.29423600
N	0.91615500	-0.88649900	-0.23447000
C	1.51725300	-1.07274400	-1.56240200
C	2.81696400	-0.29351500	-1.51314400
H	1.71992900	-2.11818100	-1.81810700
H	0.86090000	-0.62201400	-2.31192300
O	2.89285900	0.91061000	-1.56859800
O	3.86867600	-1.10318200	-1.30224000
O	-3.82317600	0.17130900	-0.89896100
C	-3.90722700	-1.24421100	-1.03661400
C	-5.05116500	-1.78339500	-0.16229800
H	-4.05772100	-1.48114900	-2.09405200
C	-2.65156300	-1.98553300	-0.52167900
H	-5.38581300	-1.03249700	0.56150700
O	-4.52745800	-2.90255600	0.55230500
C	-3.28750300	-3.28568300	-0.04159200
H	-1.93904400	-2.14254300	-1.33585800
O	-1.98342800	-1.27692900	0.49425000
H	-2.68717200	-3.79513400	0.71570700
H	-2.47472300	-1.35421000	1.35659000
H	-5.90798000	-2.10231600	-0.76488500

H	-3.46815900	-3.96775800	-0.88507800
H	1.57161800	-1.18257800	0.48752800
H	0.04167300	-1.39647400	-0.12089800
C	5.03637400	-0.46061800	-0.78851400
C	6.19836400	-1.46412100	-0.82496800
C	4.83473000	-0.17949500	0.73943300
H	5.22407500	0.44942700	-1.35949000
O	6.74850600	-1.48110300	0.48265200
H	6.99391200	-1.19078400	-1.51961100
H	5.80272900	-2.45413900	-1.09272600
C	5.66208700	-1.29961700	1.36934400
H	5.27504700	0.79505100	0.98022400
H	5.03829900	-2.20554900	1.43119600
H	6.05796600	-1.05937200	2.35688400
O	-3.47050300	-1.43419200	2.71205400
H	-3.93001900	-0.57387600	2.63687000
H	-4.10733300	-2.10854100	2.43411000
O	3.50240900	-0.25841500	1.16475700
H	3.07648600	0.62217300	1.18786700
O	-0.24369400	1.53480500	-0.57832700
C	-0.01819000	2.59294000	0.31904800
C	1.45308700	2.89184700	0.54443100
C	-0.47096100	2.17562200	1.73297400
H	-0.56704800	3.46198300	-0.06050400
O	1.88932700	1.91725200	1.50623100
H	1.59354700	3.89891200	0.95961000
H	2.04629100	2.76440900	-0.36269800
C	0.77668100	1.45857300	2.28368100
H	-0.71245900	3.05783400	2.33317500
H	0.67035700	0.37481100	2.15206700
H	0.96264300	1.67453000	3.33949800
O	-1.61999000	1.36280700	1.72260400
O	-4.36190100	1.07211000	1.88317800
H	-3.48125000	1.45196200	2.04846000
H	-4.37352300	0.94833200	0.92311900
H	-1.53506200	0.70961200	0.99985400
H	0.32317200	0.73996300	-0.36391900

TS1

N	-1.72916100	2.90556400	-2.91891400
H	-0.90951300	3.32161800	-2.47921800
C	-2.55014100	2.23135900	-1.91740100
C	-1.92850400	0.93911600	-1.35948600
H	-2.84341200	2.93279200	-1.13049200
H	-3.48142800	1.91178800	-2.40006700
O	-1.43206200	0.11845000	-2.13107500
H	-1.36214800	2.18165900	-3.53816400
N	0.55659400	-1.31023800	-0.21665200
C	1.21905200	-1.65936900	-1.49101000
C	2.49556600	-0.84012700	-1.60818400
H	1.44725700	-2.72826900	-1.51242900
H	0.53839200	-1.39380500	-2.30059900
O	2.55616100	0.30182800	-2.01778900
O	3.54955700	-1.51116500	-1.08277200
O	-3.06944900	0.34356800	-0.42655400
C	-3.61379000	-0.87954700	-0.89105100

C	-5.01889600	-1.11903500	-0.28126300
H	-3.66485700	-0.83019000	-1.98181000
C	-2.80979400	-2.17135100	-0.48842100
H	-5.35901800	-0.28781000	0.34099200
O	-4.92629100	-2.29443400	0.54075200
C	-3.94092000	-3.12555100	-0.09967500
H	-2.23479900	-2.53742200	-1.34368200
O	-1.95007900	-1.97529100	0.61902400
H	-3.62609300	-3.89357900	0.60943200
H	-2.72829600	-1.81859100	2.21659100
H	-5.76485700	-1.29265500	-1.06954300
H	-4.38579500	-3.60443400	-0.98575100
H	1.25024300	-1.33996600	0.53431300
H	-1.00592500	-1.83378500	0.28664700
C	4.69518200	-0.71608700	-0.72224300
C	5.91218800	-1.64960500	-0.58782500
C	4.49486300	-0.16366000	0.72900800
H	4.81799800	0.07413000	-1.46303600
O	6.34585300	-1.58651800	0.77278100
H	6.75560800	-1.34845100	-1.21588700
H	5.61456300	-2.67180300	-0.86208200
C	5.21995200	-1.22622000	1.55988700
H	5.03260700	0.79109100	0.80849400
H	4.54150800	-2.07866300	1.72814800
H	5.58271600	-0.86325100	2.52452000
O	-3.47660700	-1.50829500	2.78817700
H	-3.40015300	-0.07232900	2.44684600
H	-4.24343600	-1.84549700	2.27138700
O	3.15675800	-0.03520000	1.14463300
H	2.79768200	0.83174600	0.85718600
O	-0.89173000	1.29379400	-0.13088900
C	-0.41404700	2.57601200	0.18334500
C	1.02161800	2.81970500	-0.32439600
C	-0.24263300	2.64086100	1.76144200
H	-1.09663100	3.36314100	-0.15381900
O	1.88794500	2.40327200	0.74193000
H	1.19203400	3.88957000	-0.52749500
H	1.26302700	2.22395700	-1.20559000
C	1.26719400	2.84328000	1.95366400
H	-0.81915500	3.45121600	2.21476100
H	1.66463200	2.25019200	2.77963100
H	1.49617400	3.90772200	2.11929200
O	-0.70192300	1.41301200	2.33692300
O	-3.26531400	0.88343000	2.01334100
H	-2.35999300	1.21954300	2.30729600
H	-3.16381700	0.68593300	0.96670800
H	-0.69155600	0.80162400	1.55761600
H	0.25052200	-0.33478400	-0.29744300

Intermediate

N	-3.69375800	2.65251200	-2.15001000
H	-3.35324600	2.49785500	-3.09444700
C	-2.58280800	2.78830600	-1.24118500
C	-1.51788400	1.70768200	-1.39359600
H	-2.09454400	3.76092100	-1.39440900
H	-2.95065900	2.76286900	-0.21086900

O	-1.50487200	0.90355900	-2.29134100
H	-4.21623300	1.82313800	-1.87752000
N	0.92890300	-0.97424200	-0.24041600
C	1.41176100	-0.66750100	-1.59907600
C	2.75361500	0.01881600	-1.45132000
H	1.50612000	-1.59161300	-2.17236400
H	0.70310800	0.00848200	-2.08012800
O	2.90154000	1.21180500	-1.29826000
O	3.75940200	-0.86411400	-1.36268800
O	-3.91524800	0.21659100	-0.42877000
C	-3.76772600	-1.02537700	-1.06129500
C	-4.70269800	-2.13534700	-0.51457000
H	-3.95885800	-0.85916400	-2.12735000
C	-2.34881700	-1.64705300	-0.92635800
H	-5.30011500	-1.78178900	0.33086500
O	-3.86753400	-3.20048300	-0.06124200
C	-2.66995200	-3.13346100	-0.82549800
H	-1.73078100	-1.40784400	-1.79677200
O	-1.70936100	-1.16677000	0.24707600
H	-1.89555200	-3.70418300	-0.30683000
H	-2.36260800	-1.96371800	1.83554100
H	-5.37497100	-2.51143300	-1.29647800
H	-2.83579100	-3.56511400	-1.82541200
H	1.56910900	-1.63343700	0.20171300
H	-0.72161400	-1.17769500	0.05978300
C	4.98243000	-0.34254900	-0.85004300
C	6.04513300	-1.44110600	-0.89328400
C	4.87210500	0.00792800	0.67542100
H	5.26860600	0.53689000	-1.43045500
O	6.85083900	-1.19894500	0.24335500
H	6.68158300	-1.41439900	-1.77836400
H	5.55073200	-2.42209100	-0.82369000
C	5.94844500	-0.89850000	1.29238700
H	5.11204000	1.06592100	0.81945500
H	5.45327100	-1.81040600	1.65894300
H	6.50949400	-0.43542800	2.10494400
O	-2.97136800	-2.34640200	2.49353200
H	-4.08167500	-0.89997900	2.50622100
H	-3.45032400	-3.00305500	1.96587800
O	3.62092800	-0.30306900	1.23758100
H	3.06291500	0.48636700	1.32053900
O	-0.49110700	1.66816700	-0.50140400
C	-0.36867100	2.60080900	0.57188300
C	1.10695100	2.69489500	0.90270400
C	-0.94106900	1.97250600	1.86037900
H	-0.81402400	3.56552500	0.32366800
O	1.38551800	1.47157700	1.59145100
H	1.29944600	3.55272400	1.56200900
H	1.74311800	2.73377100	0.01759700
C	0.23921000	1.11273900	2.37547400
H	-1.15513700	2.77893100	2.56923000
H	0.03088600	0.04670200	2.22792100
H	0.44978200	1.28842600	3.43471200
O	-2.13772200	1.27610500	1.68500300
O	-4.53158600	-0.08105700	2.21060200
H	-3.95357200	0.63682600	2.50468400

H	-4.19687700	0.09092200	0.50757700
H	-2.03138600	0.53434200	1.04798200
H	1.01616700	-0.10958600	0.29750000

TS2

N	-1.37376069	2.03078227	-3.04642514
H	-0.55411269	2.44683627	-2.60672914
C	-2.19474069	1.35657727	-2.04491214
C	-1.57310369	0.06433427	-1.48699714
H	-2.48801169	2.05801027	-1.25800314
H	-3.12602769	1.03700627	-2.52757814
O	-1.07666169	-0.75633173	-2.25858614
H	-1.00674769	1.30687727	-3.66567514
N	0.55659400	-1.31023800	-0.21665200
C	1.21905200	-1.65936900	-1.49101000
C	2.49556600	-0.84012700	-1.60818400
H	1.44725700	-2.72826900	-1.51242900
H	0.53839200	-1.39380500	-2.30059900
O	2.55616100	0.30182800	-2.01778900
O	3.54955700	-1.51116500	-1.08277200
O	-3.06944900	0.34356800	-0.42655400
C	-3.61379000	-0.87954700	-0.89105100
C	-5.01889600	-1.11903500	-0.28126300
H	-3.66485700	-0.83019000	-1.98181000
C	-2.80979400	-2.17135100	-0.48842100
H	-5.35901800	-0.28781000	0.34099200
O	-4.92629100	-2.29443400	0.54075200
C	-3.94092000	-3.12555100	-0.09967500
H	-2.23479900	-2.53742200	-1.34368200
O	-1.95007900	-1.97529100	0.61902400
H	-3.62609300	-3.89357900	0.60943200
H	-2.72829600	-1.81859100	2.21659100
H	-5.76485700	-1.29265500	-1.06954300
H	-4.38579500	-3.60443400	-0.98575100
H	1.25024300	-1.33996600	0.53431300
H	-1.00592500	-1.83378500	0.28664700
C	4.69518200	-0.71608700	-0.72224300
C	5.91218800	-1.64960500	-0.58782500
C	4.49486300	-0.16366000	0.72900800
H	4.81799800	0.07413000	-1.46303600
O	6.34585300	-1.58651800	0.77278100
H	6.75560800	-1.34845100	-1.21588700
H	5.61456300	-2.67180300	-0.86208200
C	5.21995200	-1.22622000	1.55988700
H	5.03260700	0.79109100	0.80849400
H	4.54150800	-2.07866300	1.72814800
H	5.58271600	-0.86325100	2.52452000
O	-3.47660700	-1.50829500	2.78817700
H	-3.40015300	-0.07232900	2.44684600
H	-4.24343600	-1.84549700	2.27138700
O	3.15675800	-0.03520000	1.14463300
H	2.79768200	0.83174600	0.85718600
O	-0.89173000	1.29379400	-0.13088900
C	-0.41404700	2.57601200	0.18334500
C	1.02161800	2.81970500	-0.32439600
C	-0.24263300	2.64086100	1.76144200

H	-1.09663100	3.36314100	-0.15381900
O	1.88794500	2.40327200	0.74193000
H	1.19203400	3.88957000	-0.52749500
H	1.26302700	2.22395700	-1.20559000
C	1.26719400	2.84328000	1.95366400
H	-0.81915500	3.45121600	2.21476100
H	1.66463200	2.25019200	2.77963100
H	1.49617400	3.90772200	2.11929200
O	-0.70192300	1.41301200	2.33692300
O	-3.26531400	0.88343000	2.01334100
H	-2.35999300	1.21954300	2.30729600
H	-3.16381700	0.68593300	0.96670800
H	-0.69155600	0.80162400	1.55761600
H	0.12109605	-0.15025357	-0.27857115

Product

N	-4.95698200	-2.59687500	-0.01896000
H	-4.96841200	-1.61073800	0.23142800
C	-3.57544700	-3.00445400	-0.16502500
C	-2.83152600	-2.28208100	-1.28681300
H	-3.05176300	-2.85671000	0.78512800
H	-3.53315400	-4.07697000	-0.39301200
O	-3.39994000	-1.89712800	-2.29786900
H	-5.41651300	-2.67071700	-0.92304000
N	-1.48714200	-2.12802700	-1.09962200
C	-0.67870200	-1.43151300	-2.06020400
C	-0.51536500	0.03423800	-1.71522400
H	0.30675500	-1.88860300	-2.16207700
H	-1.19039200	-1.47325300	-3.02873000
O	-1.36522700	0.71367200	-1.17323100
O	0.65054000	0.52491900	-2.12480400
O	0.76529600	-1.61091500	0.51753400
C	1.88532200	-2.32600500	0.05262500
C	2.73497900	-2.99965200	1.16087700
H	1.51141200	-3.08899000	-0.64195000
C	2.91290400	-1.43289000	-0.69268600
H	2.39333300	-2.71540100	2.16011300
O	4.07499600	-2.54291700	0.99173100
C	4.21564500	-2.14391900	-0.36703300
H	2.71238200	-1.38460400	-1.77182000
O	2.96741400	-0.13607900	-0.14579900
H	5.08552500	-1.48879700	-0.44611600
H	3.72901700	0.07343600	1.54726300
H	2.70700000	-4.09281000	1.06971800
H	4.35439200	-3.02400400	-1.01368500
H	-1.05666400	-2.29870200	-0.19712600
H	2.06645400	0.23299800	-0.02567600
C	0.81529200	1.94802500	-2.04635300
C	2.19429600	2.30022600	-2.60145500
C	0.84677100	2.52487900	-0.59417100
H	0.00823000	2.41487900	-2.61756700
O	2.52105600	3.50783400	-1.94562200
H	2.21411700	2.47383000	-3.67814400
H	2.90061900	1.49879200	-2.33379500
C	2.17143600	3.30928100	-0.58472800
H	-0.02401900	3.16482900	-0.43454300

H	2.93160100	2.69933900	-0.07465600
H	2.10186000	4.28705300	-0.10676200
O	3.90915200	-0.06619400	2.49607700
H	2.18844000	-0.26511300	2.92693900
H	4.32833600	-0.93812900	2.49892900
O	0.89668600	1.53626100	0.41061000
H	-0.00270900	1.27601700	0.68011700
O	-3.30322600	-0.04276200	0.64072500
C	-3.40962200	1.16717500	1.36025100
C	-3.25210500	2.44593800	0.50712000
C	-2.26260200	1.30950800	2.41005600
H	-4.37936500	1.14630700	1.86467600
O	-1.99885600	3.01485400	0.86306900
H	-4.05508400	3.16014900	0.73830500
H	-3.24784200	2.23767100	-0.56433600
C	-1.84781700	2.76398400	2.24949800
H	-2.58574500	1.05896900	3.42626100
H	-0.80582700	2.94221900	2.52669300
H	-2.50592100	3.42204100	2.83813100
O	-1.16114900	0.49691100	2.03709200
O	1.27030700	-0.61416300	2.89508400
H	0.64601600	0.12215500	2.95200000
H	0.96878300	-1.22070100	1.41408000
H	-1.51975700	-0.31972900	1.65014900
H	-2.73938800	0.10681700	-0.14401500

Geometry of the stationary structures based on the structure of Polacek

Reactant

C	-1.29315200	5.66063700	0.33778400
O	-0.73062500	4.90317900	-0.75393500
C	-0.87674400	3.51444000	-0.50907600
N	0.30242900	2.82230400	-0.98492700
C	0.33113800	1.61864600	-1.66081900
N	-0.69604500	0.83868700	-2.03109200
C	-0.27916200	-0.25595600	-2.68467400
N	0.97392700	-0.63185600	-2.96319800
C	1.98589300	0.16323400	-2.56702600
N	3.25689800	-0.21231100	-2.85535800
C	1.68491100	1.36498600	-1.89433800
N	2.47877800	2.37617400	-1.38059000
C	1.62267100	3.21515500	-0.85133900
C	-1.12328000	3.39456500	1.01295700
O	-1.62402600	2.16920700	1.45239300
C	-1.96659200	4.65635200	1.27367000
O	-3.32406200	4.37131300	0.85367400
N	-5.66202400	4.46795500	-0.83377500
C	-5.62274300	4.94119400	0.54515800
C	-4.25415000	5.34028000	1.10111400
O	-3.99834900	6.36915400	1.68248700
C	3.45720800	-3.62990800	1.47834600
O	4.65306900	-2.99573400	1.97932300
C	4.66855100	-1.63581800	1.60845500
N	5.96453700	-1.32838200	0.98453500
C	6.26393600	-0.23359600	0.20042400
N	5.43004200	0.70185800	-0.29287000

C	6.08142400	1.63504500	-1.00363100
N	7.39145700	1.71019000	-1.26539900
C	8.20209000	0.74983900	-0.77602600
N	9.52142100	0.80578200	-1.06336200
C	7.64613100	-0.28663600	0.00511400
N	8.20097700	-1.37616200	0.65042000
C	7.17459000	-1.95784900	1.22563600
C	3.47682000	-1.40399800	0.64504800
O	2.90991500	-0.13254600	0.72401800
C	2.50506700	-2.50830800	1.08537900
O	1.78451500	-2.08044600	2.25238700
N	-1.29611000	-0.35600200	3.31591000
C	-0.02894500	-1.04682300	3.38411300
C	0.54258700	-1.55844300	2.06230200
O	-0.02778800	-1.54938800	0.99268300
H	-1.99188900	6.39808700	-0.06222000
H	-0.48923800	6.19514200	0.85977900
H	-1.97928800	4.97902700	2.31580400
H	-2.34347600	1.86413100	0.85888700
H	-6.27136000	5.81384500	0.65423300
H	-0.16411200	3.54451100	1.52436500
H	-1.72456100	3.09368300	-1.06412200
H	-1.06686800	-0.92406600	-3.02349100
H	3.38799800	-1.13918900	-3.23452700
H	1.87771500	4.15293400	-0.37830500
H	3.04795100	-4.26357200	2.26848900
H	3.70683500	-4.25333100	0.60961200
H	5.45670000	2.42304100	-1.41775200
H	9.88091800	1.62690900	-1.52684800
H	-5.03182200	3.67950700	-0.97000900
H	-5.35846400	5.20222100	-1.46979600
H	0.73004700	-0.39729000	3.83650400
H	-1.99280700	-0.92129500	2.83270100
H	-1.20504000	0.49541700	2.76258000
H	1.79769400	-2.77944900	0.30095600
H	3.81022400	-1.64693500	-0.37607000
H	4.55182500	-1.00320500	2.49741700
H	7.21411000	-2.85438000	1.82727000
H	3.56411100	0.48185300	0.31952700
C	-4.89993200	-0.22882500	1.12404300
O	-3.67123300	-0.96796300	1.20995900
C	-3.20272000	-1.26174500	-0.10058800
N	-3.21981400	-2.69813300	-0.34458600
C	-4.31589300	-3.54062200	-0.40203600
N	-5.61838000	-3.23120700	-0.30023300
C	-6.39141000	-4.31568300	-0.42103000
N	-6.02589700	-5.59160000	-0.61609400
C	-4.71244300	-5.86993000	-0.70463400
N	-4.32723500	-7.16354900	-0.86352800
C	-3.78087700	-4.81731700	-0.60025900
N	-2.39767200	-4.78295000	-0.65925300
C	-2.11083600	-3.51441200	-0.49506500
C	-4.10401400	-0.46492200	-1.09562700
O	-3.44688200	0.04305400	-2.21884700
C	-4.79479000	0.56160400	-0.17418300
O	-3.92774400	1.70636400	-0.05911200

H	-4.97263100	0.39599700	2.02021000
H	-5.75457200	-0.91601800	1.08224000
H	-5.76642100	0.88152000	-0.56644900
H	-2.65650400	0.56274000	-1.95240000
H	-4.88634800	-1.13169700	-1.46661100
H	-2.15699500	-0.95493200	-0.16689800
H	-7.46396700	-4.14401100	-0.35485200
H	-5.03906800	-7.83211700	-1.11996700
H	-1.11695800	-3.08955600	-0.45684700
H	-4.29055900	2.32655300	0.59427800
H	-3.37235800	-7.35070300	-1.13183500
H	-6.03435700	4.15889800	1.19922300
H	-0.10642800	-1.91697200	4.05145600
H	4.02360800	0.21902300	-2.35596300
H	10.15898700	0.16742000	-0.61215300

TS1

C	-1.42508831	5.65385055	-1.70796733
O	-0.42173431	4.69380455	-2.06964933
C	-0.57408031	3.60322855	-1.17228733
N	0.53763069	2.70224255	-1.33319033
C	0.45910969	1.46339455	-1.94418033
N	-0.63702231	0.79327455	-2.32671933
C	-0.32836031	-0.37415845	-2.90905033
N	0.88211469	-0.90439045	-3.11555833
C	1.96324869	-0.21838145	-2.69950333
N	3.18713869	-0.77925345	-2.87232133
C	1.77994869	1.03923555	-2.08867033
N	2.66345169	1.98855855	-1.59833233
C	1.89030369	2.95637755	-1.17367433
C	-0.73509931	4.30776655	0.18396267
O	-1.31860626	3.45790119	1.14441733
C	-1.67336631	5.50227055	-0.18130933
O	-3.01998731	5.27692555	0.16660867
N	-3.01749279	4.13841314	4.28287924
C	-2.75164279	3.55358514	2.98007324
C	-1.75946579	4.32010314	2.11485824
O	-1.16380479	5.31791214	2.44219824
C	2.96690700	-4.05620800	1.55256500
O	4.20496800	-3.50040000	2.04308200
C	4.33963900	-2.16491000	1.61068200
N	5.68170900	-1.98526900	1.04150600
C	6.10476300	-0.91907700	0.27704100
N	5.37712400	0.10107200	-0.21226500
C	6.12666200	0.96296600	-0.91327100
N	7.44087700	0.90357100	-1.16340200
C	8.14441200	-0.13541400	-0.66995000
N	9.46639400	-0.21480600	-0.94681600
C	7.47657500	-1.11404000	0.09779400
N	7.90487700	-2.26261700	0.73738300
C	6.81470200	-2.74141200	1.29059100
C	3.21338500	-1.89717900	0.57874900
O	2.74315900	-0.58259600	0.56907800
C	2.13600300	-2.88568300	1.04809900
O	1.43607800	-2.29402800	2.15868300
N	-1.43552600	-0.16833000	2.98347900

C	-0.07694200	-0.68365200	3.01014500
C	0.28008100	-1.64133300	1.88032200
O	-0.35254000	-1.77637100	0.85495700
H	-2.36259131	5.45720855	-2.24606233
H	-1.04935131	6.63792555	-1.99801933
H	-1.37790131	6.39640755	0.36881367
H	-2.57072024	2.35991919	0.36904306
H	-2.40853079	2.51440614	3.08982224
H	0.22750269	4.66921355	0.55228067
H	-1.46991431	3.01905255	-1.40833133
H	-1.17506231	-0.95983245	-3.25915733
H	3.25169069	-1.56435645	-3.50457933
H	2.23895469	3.88487955	-0.74274133
H	2.47813900	-4.58874600	2.37205200
H	3.17859600	-4.76299100	0.73970100
H	5.59088200	1.81200300	-1.33143200
H	9.91373100	0.57970800	-1.37965300
H	-3.24061479	5.12599814	4.16740124
H	-2.16654579	4.11821914	4.84239024
H	0.64202600	0.14287100	2.91597200
H	-2.08428300	-0.88148200	3.31220000
H	-1.72298100	-0.01381800	2.01758200
H	1.42157600	-3.14776300	0.26702500
H	3.56377400	-2.21752300	-0.41409400
H	4.22779900	-1.47921600	2.46037200
H	6.75163300	-3.64323300	1.88183700
H	3.47580700	-0.03458600	0.20144300
C	-4.57980100	0.79711000	0.95809800
O	-3.65569900	-0.31182600	0.91558500
C	-3.46781900	-0.76145400	-0.41929600
N	-3.91070500	-2.13938400	-0.55511300
C	-5.19860800	-2.63505300	-0.46035700
N	-6.34639000	-1.95774500	-0.30202100
C	-7.39953000	-2.78134800	-0.26813700
N	-7.42447100	-4.11932900	-0.36524200
C	-6.25508000	-4.76882800	-0.51058500
N	-6.26385500	-6.12636900	-0.56893000
C	-5.06039600	-4.02252800	-0.56595900
N	-3.73201800	-4.38994900	-0.70611600
C	-3.09004400	-3.24792400	-0.68204100
C	-4.21657500	0.24014400	-1.34927300
O	-3.55074700	0.52193000	-2.54611800
C	-4.48925400	1.45249800	-0.41714200
O	-3.43165200	2.42243100	-0.47888900
H	-4.18024000	1.44462400	1.74168500
H	-5.59000400	0.44632400	1.19291800
H	-5.40202200	1.97889000	-0.70428700
H	-2.66621600	0.89792600	-2.34703900
H	-5.18428600	-0.18909400	-1.61915100
H	-2.39588200	-0.76951500	-0.63053400
H	-8.37070800	-2.30572400	-0.14668500
H	-7.15459500	-6.57995100	-0.71140800
H	-2.01578700	-3.12614200	-0.73529500
H	-3.37441370	4.24717585	-0.22841363
H	-5.42744300	-6.60032200	-0.87636000
H	-3.68751779	3.51545414	2.40822524

H	0.13610200	-1.15939900	3.97255700
H	4.01247969	-0.21986345	-2.71160233
H	10.03174900	-0.90229700	-0.47168000

Intermediate

C	-1.43685300	5.73881100	-1.18051000
O	-0.47240900	4.77922900	-1.61779200
C	-0.75259000	3.57754700	-0.94407200
N	0.36334300	2.68461900	-1.09104300
C	0.30861000	1.43341800	-1.66022800
N	-0.77100200	0.74900400	-2.05013900
C	-0.44443800	-0.43286700	-2.57608600
N	0.77212600	-0.95738100	-2.74210600
C	1.83255300	-0.24772200	-2.33437500
N	3.06722300	-0.76774600	-2.49405600
C	1.62775000	1.02002300	-1.75694700
N	2.49053800	1.98187800	-1.26733800
C	1.70196700	2.95146100	-0.89039600
C	-1.05814000	4.04318300	0.47719100
O	-1.75509600	3.03203500	1.17942400
C	-1.93948400	5.28729200	0.21343600
O	-3.31125400	4.98197600	0.24116700
N	-4.48359900	3.28133200	2.70381800
C	-3.24632600	2.54682200	2.97645600
C	-2.05846300	3.34270900	2.48365700
O	-1.51664600	4.24947400	3.05567700
C	3.16371400	-3.78124800	1.43165200
O	4.28119500	-3.15564600	2.07541800
C	4.39974900	-1.82605700	1.65171700
N	5.74643600	-1.60685900	1.12005500
C	6.12728100	-0.60236700	0.26476000
N	5.36012800	0.31430500	-0.35313100
C	6.08388200	1.14958600	-1.09835600
N	7.40555400	1.15374700	-1.29385400
C	8.14508400	0.21878800	-0.67777700
N	9.47425000	0.19820000	-0.87970600
C	7.50831300	-0.72223000	0.15784500
N	7.98210900	-1.76598500	0.92236000
C	6.90662400	-2.25547600	1.48196300
C	3.33799300	-1.58391300	0.56200500
O	2.77935400	-0.31175500	0.60395200
C	2.30140800	-2.65963200	0.88250400
O	1.46516800	-2.15722800	1.92362800
N	-1.19818400	0.31399500	2.32200600
C	-0.05987900	-0.50953700	2.65703600
C	0.44556200	-1.37109100	1.51807600
O	0.01043100	-1.35068300	0.39207000
H	-2.28895800	5.76892000	-1.87071600
H	-0.94457600	6.71311200	-1.17386800
H	-1.78705100	6.04915500	0.97806600
H	-3.12821600	1.99036300	0.13035300
H	-3.13986700	2.38679100	4.05026300
H	-0.13609800	4.31221400	1.00123900
H	-1.62416500	3.05431300	-1.36666100
H	-1.28249900	-1.03698400	-2.91916000
H	3.16664100	-1.58574600	-3.07657700

H	2.02514000	3.89754600	-0.47675100
H	2.63456600	-4.38489900	2.17130000
H	3.51763900	-4.42623500	0.61849700
H	5.51852600	1.92584700	-1.61010800
H	9.89739300	0.93679200	-1.42024000
H	-4.47454600	3.59823600	1.73394200
H	-4.49726400	4.13189400	3.26408500
H	0.78824400	0.11808000	2.95509000
H	-2.01356200	-0.26498600	2.12153200
H	-1.00054300	0.81462500	1.45607700
H	1.69689900	-2.93976900	0.01788700
H	3.78015400	-1.81289100	-0.41567600
H	4.23683700	-1.14617400	2.49640700
H	6.87127100	-3.09894200	2.15753500
H	3.42773000	0.30005600	0.19453500
C	-5.07019600	0.61336100	0.63351600
O	-3.87485100	-0.16163800	0.87166800
C	-3.40968000	-0.67004900	-0.36837100
N	-3.54650200	-2.11083000	-0.42747300
C	-4.71005700	-2.84307500	-0.37480600
N	-5.97174700	-2.40321200	-0.27078800
C	-6.83850500	-3.41180900	-0.26443900
N	-6.59800000	-4.72740300	-0.34204100
C	-5.32633600	-5.13298800	-0.43951900
N	-5.05836600	-6.45755600	-0.48886100
C	-4.30021600	-4.16983100	-0.46381000
N	-2.92831200	-4.27109200	-0.57201900
C	-2.52331400	-3.03015000	-0.54153400
C	-4.21509000	0.06767300	-1.47605500
O	-3.48493600	0.35044900	-2.62384900
C	-4.76429600	1.27252800	-0.69932600
O	-3.75975700	2.27638900	-0.55519300
H	-5.19203500	1.31492500	1.46275500
H	-5.93484100	-0.05441300	0.55838500
H	-5.62172700	1.73987700	-1.18519500
H	-2.68508600	0.85299300	-2.36778200
H	-5.06138100	-0.56022600	-1.77286100
H	-2.33492100	-0.46670200	-0.45150700
H	-7.88790400	-3.13652500	-0.18820200
H	-5.83148100	-7.08763200	-0.63956500
H	-1.49378800	-2.69471200	-0.59249000
H	-3.49645100	4.18531000	-0.29509400
H	-4.12724500	-6.75318300	-0.74011700
H	-3.27427100	1.57266900	2.48749000
H	-0.28724300	-1.15082100	3.51448900
H	3.88267700	-0.21790000	-2.25485000
H	10.05065400	-0.44786300	-0.36290300

TS2

C	-1.14038600	5.80855800	-0.61268500
O	-0.18622100	4.98920100	-1.30735000
C	-0.54165600	3.65077800	-1.02214300
N	0.55615000	2.78937800	-1.41225500
C	0.45292500	1.57722600	-2.05966800
N	-0.64951300	0.94868200	-2.49438200
C	-0.36045600	-0.21287700	-3.09403900

N	0.84109100	-0.77929500	-3.27508800
C	1.92620100	-0.13479900	-2.81256300
N	3.14391900	-0.74158000	-2.94128600
C	1.76738500	1.11358300	-2.18264500
N	2.66538500	2.01148200	-1.63149500
C	1.90399100	2.98486700	-1.18561900
C	-0.88239900	3.63835200	0.49223600
O	-1.64602100	2.55745700	0.87610000
C	-1.57087100	5.03995100	0.66439700
O	-2.97712200	4.98164300	0.83435800
N	-3.04058600	3.72056200	3.66999500
C	-2.77308300	2.31595500	3.47609900
C	-1.37602500	1.96516100	2.98477100
O	-0.33037900	2.41904400	3.36533800
C	2.75316900	-3.83502300	1.46899300
O	3.96762600	-3.32923100	2.05529300
C	4.20358800	-2.00671800	1.62384100
N	5.57105200	-1.90236100	1.10380300
C	6.06438000	-0.86605100	0.33806000
N	5.39663900	0.17816900	-0.18326300
C	6.20255300	0.99200200	-0.87834100
N	7.51895400	0.86864000	-1.09135200
C	8.16174400	-0.19184600	-0.56248000
N	9.48585000	-0.33347300	-0.80046800
C	7.42959900	-1.12699900	0.20140000
N	7.78606300	-2.28483100	0.86912100
C	6.66057700	-2.70566700	1.39705200
C	3.14415200	-1.66870200	0.54134400
O	2.71393800	-0.34114900	0.56686200
C	2.00850200	-2.63793900	0.90076100
O	1.21362400	-2.02835400	1.94950700
N	-1.29553100	0.58454000	2.22015300
C	-0.21958300	-0.31439200	2.67005700
C	0.21861100	-1.22628700	1.53896200
O	-0.27765400	-1.21737900	0.43438900
H	-2.02649700	5.97957100	-1.24014300
H	-0.65580700	6.76861300	-0.41720900
H	-1.19634300	5.53557700	1.56416800
H	-2.93744200	2.39366200	-0.13176900
H	-2.87640300	1.78414700	4.43777800
H	0.07809700	3.66789700	1.03895200
H	-1.41421300	3.32544100	-1.60317800
H	-1.21439400	-0.76448100	-3.47925800
H	3.20033500	-1.47552300	-3.63474300
H	2.25749900	3.88681000	-0.70661600
H	2.18325900	-4.35259500	2.24475800
H	2.99545900	-4.54666000	0.66904100
H	5.71818100	1.85698900	-1.32529000
H	9.97875100	0.43077500	-1.23823900
H	-3.07745000	4.18959200	2.76035800
H	-2.29286400	4.14718100	4.21333200
H	0.62593300	0.31232200	2.96727500
H	-2.22118500	0.14430800	2.11389000
H	-1.12189100	1.03070400	1.27030400
H	1.36172600	-2.87405400	0.05592400
H	3.53464500	-1.95552700	-0.44505500

H	4.09792800	-1.31537400	2.46952600
H	6.54014000	-3.59565100	1.99761700
H	3.44855200	0.19132900	0.18031400
C	-4.96845200	1.03879900	0.56785300
O	-3.87841000	0.09686300	0.78630600
C	-3.51686800	-0.47232400	-0.47722900
N	-3.82117400	-1.89655800	-0.50198400
C	-5.05691200	-2.51205300	-0.40223700
N	-6.26776300	-1.94756000	-0.27770800
C	-7.23577300	-2.86805400	-0.22257900
N	-7.12901900	-4.20482500	-0.27175000
C	-5.90093800	-4.74055600	-0.38850300
N	-5.77598200	-6.09444900	-0.40106600
C	-4.78449100	-3.88280500	-0.46332700
N	-3.42757200	-4.12408600	-0.59833200
C	-2.89938800	-2.92460800	-0.61296000
C	-4.25306800	0.35567600	-1.57584000
O	-3.50596600	0.54704000	-2.74037100
C	-4.68022200	1.63237600	-0.80542900
O	-3.66377400	2.61935300	-0.79007700
H	-4.94088500	1.77802000	1.37025600
H	-5.91842500	0.49369300	0.58373700
H	-5.56627800	2.08754000	-1.25735300
H	-2.69129900	1.05098000	-2.52663300
H	-5.15944200	-0.18138700	-1.86910800
H	-2.43478300	-0.39422500	-0.60056100
H	-8.24996500	-2.48545900	-0.12769900
H	-6.61798200	-6.63326800	-0.54517500
H	-1.84423100	-2.70223100	-0.70032900
H	-3.35026000	4.30843900	0.22783600
H	-4.89851700	-6.49037400	-0.70528300
H	-3.51278300	1.89114900	2.79803200
H	-0.53887400	-0.89732900	3.53885600
H	3.96624400	-0.16785400	-2.81178800
H	10.00776500	-1.03921100	-0.30309900

Product

C	-0.77475100	5.89548900	0.05193000
O	0.18899300	5.25328200	-0.80171500
C	-0.08311500	3.86880500	-0.74297700
N	1.05241700	3.13860700	-1.26545800
C	1.00019700	1.91766600	-1.90377900
N	-0.07682300	1.21281400	-2.27975200
C	0.26108600	0.07016300	-2.88920300
N	1.48804200	-0.41043400	-3.13538900
C	2.55073000	0.31778500	-2.74623200
N	3.79476700	-0.18957700	-2.96638800
C	2.33636600	1.55016500	-2.09728600
N	3.19572300	2.51260700	-1.59453200
C	2.39420500	3.42860600	-1.10427900
C	-0.37648800	3.60339400	0.74253300
O	-1.06570500	2.38552200	0.88621400
C	-1.16468400	4.88467000	1.16867600
O	-2.55652600	4.69393700	1.30579500
N	-3.62018500	2.50740700	3.63351200
C	-3.33339000	1.08698300	3.66860000

C	-1.85002500	0.69847500	3.66958800
O	-0.94602900	1.51626300	3.45899800
C	2.35479000	-3.97054000	0.98441100
O	3.66216700	-3.72764800	1.54202300
C	3.98624700	-2.35769800	1.42514200
N	5.31342000	-2.23764800	0.81180800
C	5.87186900	-1.08554200	0.30171900
N	5.31038900	0.12865300	0.17218000
C	6.14442200	1.00902300	-0.39721800
N	7.40195500	0.80631100	-0.81431100
C	7.94164800	-0.42005200	-0.66740100
N	9.20202100	-0.63368500	-1.11504000
C	7.16678900	-1.44406600	-0.08317100
N	7.41793700	-2.77666300	0.18823000
C	6.29890500	-3.20643400	0.72303600
C	2.86926800	-1.69405900	0.57378300
O	2.60997900	-0.35954800	0.88319000
C	1.68113500	-2.60988000	0.89006200
O	1.16525700	-2.26456300	2.19543900
N	-1.57501200	-0.61368500	3.91195200
C	-0.25158800	-1.15188300	3.69973100
C	-0.01737300	-1.62275600	2.26531200
O	-0.78307600	-1.45642900	1.34329900
H	-1.67456200	6.16022700	-0.52017900
H	-0.31087300	6.81239500	0.42369000
H	-0.82715900	5.23138200	2.14871400
H	-2.56465700	2.36635700	-0.13827800
H	-3.81509900	0.63812400	4.54817900
H	0.58172900	3.56885100	1.27738200
H	-0.95123500	3.58907900	-1.35350400
H	-0.57116400	-0.54151400	-3.22826000
H	3.86526500	-0.94216300	-3.63704200
H	2.70624900	4.35309300	-0.63972900
H	1.82339400	-4.65912900	1.64549300
H	2.44852900	-4.42585300	-0.01034500
H	5.73801500	2.00379100	-0.55809400
H	9.75349400	0.16784800	-1.38401800
H	-3.20149200	2.94947400	2.81483600
H	-3.19943600	2.96968500	4.43736300
H	0.47437700	-0.36156000	3.90896500
H	-2.35336000	-1.26057400	3.92331500
H	-1.01295100	2.09665500	1.82635800
H	0.87903000	-2.54895000	0.15470100
H	3.12109600	-1.83339800	-0.48952800
H	4.01709000	-1.89305800	2.41874100
H	6.10946800	-4.21317800	1.06530300
H	3.42027100	0.13635100	0.61553800
C	-5.00757600	1.52283400	0.12991100
O	-4.17153700	0.42601200	0.57011400
C	-3.55816100	-0.18169000	-0.56242700
N	-4.00751300	-1.55933200	-0.71359800
C	-5.27643500	-2.02201800	-1.01437900
N	-6.38195300	-1.31693700	-1.30007100
C	-7.42310000	-2.11601500	-1.55312100
N	-7.47537600	-3.45721900	-1.54778700
C	-6.35331300	-4.13492200	-1.24732800

N	-6.40305300	-5.49366900	-1.19730500
C	-5.17451500	-3.41650400	-0.96305400
N	-3.89061500	-3.81874300	-0.63404200
C	-3.24084800	-2.68928300	-0.48839500
C	-3.88370800	0.72869200	-1.78933000
O	-2.87651000	0.79796400	-2.75431400
C	-4.28836000	2.05414800	-1.10247700
O	-3.14843100	2.84701800	-0.77107600
H	-5.06639500	2.23888800	0.95330300
H	-6.00851900	1.15132200	-0.12189500
H	-4.91965000	2.67484600	-1.74216300
H	-2.07880900	1.24178400	-2.39178700
H	-4.77037900	0.32892500	-2.28834300
H	-2.47926800	-0.23720000	-0.38987300
H	-8.35717300	-1.61518000	-1.79961500
H	-7.21243600	-5.93927200	-1.60512400
H	-2.20144600	-2.59065600	-0.20460900
H	-2.90735900	4.25245600	0.50285200
H	-5.53105600	-6.00237500	-1.19236500
H	-3.78187700	0.61151400	2.78678400
H	-0.05406400	-1.97920100	4.38836500
H	4.58859600	0.42696700	-2.86671600
H	9.67081200	-1.49421800	-0.87445900