

Supporting Information

Insights into quaternary ammonium salts-catalyzed fixation carbon dioxide with epoxides

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Supporting information

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| 1. <i>Supporting Figure</i> | <i>S2</i> |
| 2. <i>Cartesian coordinates for the optimized geometries</i> | <i>S2-S24</i> |

1. Supporting Figure

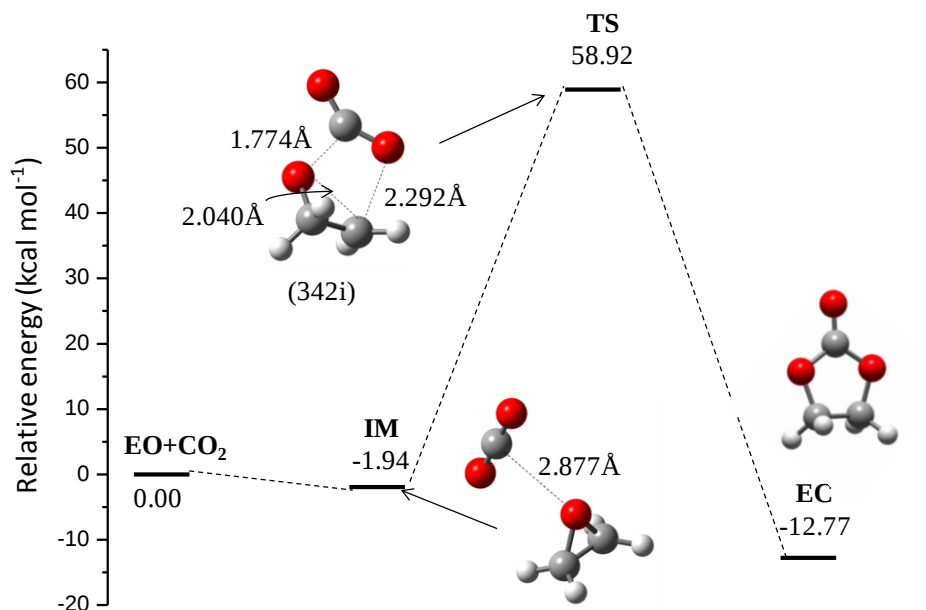


Fig. S1 Potential energy surface profiles for the cycloaddition reaction without catalyst.

2. Cartesian coordinates for the optimized geometries of all species involved in the uncatalyzed and catalytic cycle (values in Angstrom).

CO₂

C	0.00000000	0.00000000	-0.00000300
O	0.00000000	0.00000000	-1.16079800
O	0.00000000	0.00000000	1.16080100

EO

C	-0.66576500	-0.48434900	0.00000000
C	0.00000000	0.82328800	0.00000000
O	0.76245100	-0.38815800	0.00000000
H	-1.10259200	-0.86414600	0.91977500
H	-1.10259200	-0.86414600	-0.91977500
H	0.05008100	1.39996300	0.91977300
H	0.05008100	1.39996300	-0.91977300

IM

C	1.87874100	0.43118000	-0.60581100
C	1.97492800	-0.19200400	0.71813500
O	0.99101900	-0.63098500	-0.22830300

H	1.40849300	1.40566300	-0.70321900
H	2.60020100	0.17139600	-1.37541800
H	1.57919000	0.33178700	1.58410300
H	2.76662600	-0.90809500	0.91999200
C	-1.77631400	0.11262000	0.03044300
O	-2.18045900	-0.96347600	-0.12099000
O	-1.41289000	1.20552100	0.18903500

TS

C	1.57818300	0.64277200	-0.34432300
C	1.47394400	-0.59109200	0.42283700
O	0.29759900	-0.94315500	-0.27365100
H	1.55490900	1.64111500	0.06503500
H	1.71401900	0.53230900	-1.41324900
H	1.33890600	-0.44994200	1.49832200
H	2.26966500	-1.31824900	0.22953700
C	-1.07628100	0.13846300	0.02677400
O	-2.07393400	-0.48069000	-0.06672000
O	-0.56523600	1.23058400	0.21394900

EC

C	1.30070600	-0.75534900	0.12228700
C	1.30069200	0.75536800	-0.12231700
O	-0.07231700	1.11055200	0.10956900
H	1.92786400	-1.31444500	-0.57014700
H	1.56056900	-1.01459000	1.15169600
H	1.56040500	1.01483000	-1.15167800
H	1.92769300	1.31443900	0.57026100
C	-0.85173900	0.00009100	-0.00000900
O	-2.03981200	-0.00009800	0.00000200
O	-0.07218200	-1.11056500	-0.10955900

Et₄NBr

C	3.47163400	-0.61073500	-1.35374500
C	2.98666700	-0.20572600	0.03214800
H	3.45469400	0.21153900	-2.06934800
H	2.90501700	-1.44671200	-1.76538800
H	3.11830100	-1.03180200	0.72910200
H	3.56708400	0.63879400	0.40947000
C	1.31758000	0.63883500	1.60765600
C	-0.09704300	0.57238400	2.17025400
H	1.97533200	-0.00005100	2.19808000
H	1.71940100	1.65269100	1.66170500

H	-0.85601100	1.04020400	1.54721900
H	-0.42676100	-0.45171400	2.33882500
C	1.30410000	1.39999800	-0.79992300
C	0.00892200	2.18261000	-0.65220800
H	2.16961400	2.04956500	-0.64410300
H	1.36994400	0.98547600	-1.80472200
H	-0.88705000	1.55403700	-0.71921500
H	-0.02518900	2.75848200	0.27395000
C	0.58983900	-0.93321000	-0.26321500
C	0.81620200	-2.24729000	0.46798000
H	0.73432500	-1.06270700	-1.33562900
H	-0.44610400	-0.58696000	-0.13210300
H	1.74330700	-2.75352800	0.18682100
H	0.79159300	-2.14050900	1.55400500
N	1.52288100	0.20994500	0.14429100
H	-0.07757300	1.08030400	3.13911100
H	-0.02177000	2.89714500	-1.47975900
H	-0.01688500	-2.90005600	0.19745300
H	4.51045000	-0.93631500	-1.25740100
Br	-2.80998000	-0.22310500	-0.32262200
A			
C	2.49512500	-1.84662200	-1.46931300
C	1.50324600	-0.71259900	-1.25715500
H	2.38120500	-2.64488300	-0.73604900
H	3.53872300	-1.52186700	-1.48835500
H	1.55448400	-0.00021100	-2.07930900
H	0.48009500	-1.10080700	-1.19334100
C	0.52117700	1.13388300	0.00317100
C	0.64695300	2.37357000	0.87762800
H	0.42508000	1.44288800	-1.03675900
H	-0.37056300	0.54767800	0.23592500
H	0.73977400	2.15876300	1.94016100
H	1.46884400	3.02958000	0.58198000
C	1.54280500	-0.86215200	1.20188200
C	1.43176300	-0.27327600	2.59998800
H	0.64121700	-1.44411400	0.97961500
H	2.41810400	-1.50802800	1.13881900
H	2.23952800	0.41280300	2.86520700
H	0.47074000	0.21286000	2.76194800
C	3.03596000	0.78503700	0.07732000
C	3.38647600	1.65389200	-1.12516300
H	3.76999700	-0.01266500	0.19406700
H	3.05389000	1.37645000	0.99049100

H	3.52291500	1.06992800	-2.03614400
H	2.64041400	2.42606600	-1.31698500
N	1.68056100	0.11539000	0.02618400
H	-0.28496900	2.92394100	0.73138800
H	1.47991900	-1.11542600	3.29524500
H	4.33333700	2.15734400	-0.91494300
H	2.27399000	-2.28371300	-2.44628900
C	-3.58458300	1.60383400	0.28198300
C	-3.37934100	1.50672200	-1.16399100
H	-3.33439800	0.73857900	0.88890000
H	-4.33316300	2.28718800	0.67477200
H	-3.97696600	2.11813800	-1.83538200
H	-2.98725900	0.57378000	-1.55824900
Br	-1.71021000	-1.79499300	0.05040000
O	-2.45612400	2.24987900	-0.34276200

TS1

C	0.76078300	-2.61730600	-0.73138900
C	0.88878600	-1.12625500	-1.00279400
H	0.12668600	-2.82866900	0.12914600
H	1.72166500	-3.12510900	-0.61948300
H	1.41715900	-0.94385800	-1.93719200
H	-0.10572900	-0.68423000	-1.07668700
C	1.58985700	1.16275000	-0.42246500
C	2.63665800	2.11956900	0.13504400
H	1.69733600	1.10522900	-1.50501300
H	0.59175900	1.56641000	-0.22953600
H	2.61811000	2.20754800	1.21952100
H	3.65524900	1.88734900	-0.18119200
C	0.84775100	-0.49492800	1.37761200
C	1.12672900	0.48375400	2.50766000
H	-0.20936200	-0.47858400	1.10457300
H	1.07666500	-1.50979500	1.70117800
H	2.17158500	0.49830900	2.82494700
H	0.80549900	1.49805700	2.27180600
C	3.04625700	-0.79812200	0.25747300
C	3.89777700	-0.85846200	-1.00511300
H	2.96976600	-1.78887300	0.70443200
H	3.50202600	-0.14287700	0.99741600
H	3.55312600	-1.62207000	-1.70348100
H	3.94638200	0.09598600	-1.53046500
N	1.62499900	-0.30337400	0.06701100
H	2.37987400	3.10250700	-0.26742500
H	0.53334300	0.14918900	3.36243200

H	4.91660800	-1.12238100	-0.71117900
H	0.25837900	-3.05354500	-1.59792000
C	-2.08494000	1.48145000	0.09082200
C	-1.65484400	1.92093900	-1.24802300
H	-1.32172100	1.21522500	0.79697800
H	-2.96745900	1.94106600	0.51367500
H	-2.49430300	2.19562400	-1.90448500
H	-1.01999900	1.20125300	-1.79898700
Br	-2.84200700	-0.87565400	0.12237400
O	-1.00703500	2.97092400	-0.63352300
B			
C	-1.90412100	2.61431000	0.47645100
C	-1.81800300	1.39893200	-0.43540100
H	-1.35946200	2.47773700	1.41076900
H	-2.92667300	2.92955800	0.70239100
H	-2.25542000	1.62455100	-1.40745300
H	-0.77709900	1.06817500	-0.57108000
C	-2.24914100	-0.92109200	-1.03133700
C	-3.12686600	-2.16644400	-1.06044400
H	-2.36211600	-0.38881100	-1.97638200
H	-1.17578700	-1.13088900	-0.90391500
H	-3.06470700	-2.77295200	-0.15973300
H	-4.17977900	-1.95501500	-1.26373900
C	-1.86999100	-0.25396200	1.39062300
C	-2.26896500	-1.57983400	2.02367400
H	-0.79387500	-0.25765500	1.15468000
H	-2.11335700	0.56266900	2.06986500
H	-3.34557600	-1.72043400	2.15024500
H	-1.85274400	-2.43113500	1.48647400
C	-4.01411800	0.36212700	0.26997500
C	-4.77468900	0.91484900	-0.92996600
H	-4.10090200	1.04203000	1.11803900
H	-4.43929400	-0.59092500	0.57870800
H	-4.46865000	1.92965700	-1.18698500
H	-4.67124700	0.28791500	-1.81679000
N	-2.53698900	0.12901000	0.05849300
H	-2.76169600	-2.78289100	-1.88659000
H	-1.82552300	-1.59191700	3.02302100
H	-5.83654400	0.94825100	-0.67373600
H	-1.42215700	3.44197700	-0.05054000
C	2.72396500	0.40389100	0.13056700
C	1.84614300	-0.72478500	-0.41626200
H	2.55587700	1.33661400	-0.40408000

H	2.57369800	0.54520300	1.19894800
H	2.13440100	-1.66159700	0.10279600
H	2.11175800	-0.87627000	-1.48246600
Br	4.70248500	0.04983900	-0.06696600
O	0.53294300	-0.37115400	-0.22317100
C			
C	-4.14669300	2.18750800	-0.59914500
C	-3.23690900	1.03110000	-0.98808800
H	-3.80998600	2.69635800	0.30373900
H	-5.19562700	1.90274800	-0.48248300
H	-3.53174800	0.62078800	-1.95306200
H	-2.19648700	1.36653700	-1.03489300
C	-2.18272500	-1.14542700	-0.60688600
C	-2.29065700	-2.60614700	-0.18392000
H	-2.30021700	-1.07320000	-1.68824100
H	-1.20166700	-0.73655600	-0.33658200
H	-2.20137900	-2.75436700	0.89011100
H	-3.20019900	-3.09964800	-0.53291200
C	-2.72662800	0.39035800	1.33756600
C	-2.30711400	-0.62315800	2.39105200
H	-1.88497000	1.03890900	1.08384100
H	-3.55161200	0.99950200	1.70721700
H	-3.07833200	-1.35815900	2.63469800
H	-1.37847800	-1.12187600	2.11695400
C	-4.58142200	-0.77743600	0.14950300
C	-5.27634600	-1.19013700	-1.14322500
H	-5.18800400	-0.04674500	0.68492300
H	-4.45626100	-1.63529200	0.80720900
H	-5.56758500	-0.33265300	-1.75113800
H	-4.66641700	-1.85570800	-1.75536600
N	-3.21030300	-0.15902200	-0.01526100
H	-1.44487600	-3.12208000	-0.64590500
H	-2.10409400	-0.05587300	3.30342600
H	-6.18952900	-1.73013700	-0.88118700
H	-4.09714100	2.91885200	-1.40959900
C	3.47174400	0.31181100	-0.65336900
C	2.92804400	1.06183200	0.55305100
H	2.78032500	-0.45553200	-0.98831200
H	3.73221200	0.98595900	-1.46578000
H	3.66226700	1.78394400	0.91498800
H	2.67351500	0.36182400	1.34951300
Br	5.15267000	-0.64013200	-0.18589100
O	1.78674300	1.82451800	0.16609300

C	0.54803200	1.16294800	0.13954300
O	-0.40308600	1.90517000	-0.17653000
O	0.53246600	-0.05460400	0.43110700
TS2			
C	-4.34889000	2.05693800	-0.06943600
C	-3.37538800	1.08635600	-0.72245000
H	-3.96872400	2.46738100	0.86588500
H	-5.34163700	1.63355600	0.10131100
H	-3.73477700	0.79010900	-1.70680100
H	-2.39027200	1.54584400	-0.82388500
C	-2.06648600	-0.98288800	-0.79992000
C	-1.98072700	-2.49421000	-0.61981800
H	-2.30344900	-0.75700000	-1.83946800
H	-1.11213000	-0.50949600	-0.56107800
H	-1.76456000	-2.80083600	0.40129100
H	-2.87053600	-3.02348400	-0.96506700
C	-2.54456600	0.16169900	1.41036800
C	-1.94221900	-0.95294000	2.25192400
H	-1.79007700	0.91897300	1.19128200
H	-3.37265200	0.62856100	1.94308700
H	-2.62614600	-1.78293500	2.44258600
H	-1.01113700	-1.32550500	1.82734500
C	-4.39396600	-1.01981600	0.22215700
C	-5.17988600	-1.30394200	-1.05309500
H	-5.00754000	-0.45712200	0.92571000
H	-4.11159200	-1.94925400	0.71253300
H	-5.61482700	-0.40172800	-1.48488100
H	-4.57893000	-1.79809300	-1.81772300
N	-3.11697900	-0.22499300	0.03733700
H	-1.14458400	-2.83216800	-1.23743800
H	-1.69366000	-0.51241400	3.22096900
H	-6.00427400	-1.97505300	-0.80055300
H	-4.46939600	2.89809800	-0.75640800
C	2.60655600	-0.05829400	0.02358500
C	2.93836900	1.40963800	-0.17159200
H	2.63561400	-0.50418700	1.00002200
H	2.49905800	-0.71258600	-0.82180400
H	3.47618000	1.56425000	-1.10340900
H	3.54096400	1.78195600	0.65392100
Br	5.05488400	-0.71202400	-0.07732200
O	1.73353600	2.22383400	-0.23348700
C	0.58630500	1.53477600	-0.05301900
O	-0.49024600	2.13317600	-0.07960200

O	0.73951100	0.26611700	0.13374800
D			
C	0.99555200	-0.55522900	1.24636600
H	0.65418300	-1.55832700	1.00147600
H	0.15599700	0.13254500	1.10865800
C	1.21418700	-0.31353000	-1.17680300
H	0.60709800	-1.20905900	-1.05513300
H	0.53175800	0.54080300	-1.19047000
C	2.38109500	1.29843900	0.40061900
H	1.42922600	1.82017600	0.53959300
H	2.92496800	1.28908300	1.34450300
C	3.23010100	-1.03775900	0.17880100
H	3.76601600	-0.77782900	1.09233800
H	3.85324400	-0.73086300	-0.65887700
N	1.99690200	-0.16268300	0.14331800
C	-3.64732100	-0.30226100	-0.78112800
C	-3.59533300	-0.44213800	0.74772300
H	-3.22705900	0.64927700	-1.10641000
H	-4.63599100	-0.47235800	-1.20554300
H	-4.50025900	-0.87204800	1.18052400
H	-3.32859000	0.49696600	1.22978700
Br	-1.14637400	2.22797700	0.07974800
O	-2.51344400	-1.37919100	0.96229000
C	-2.07947800	-1.86720900	-0.21341700
O	-1.17647100	-2.65369300	-0.32233600
O	-2.77453800	-1.36162500	-1.24528300
C	1.51514900	-0.49335300	2.67504000
H	1.75680700	0.51938400	2.99940000
H	2.37602700	-1.14198600	2.85575200
C	3.20312400	2.01259900	-0.66272400
H	2.62080600	2.22105400	-1.55924700
H	4.12485700	1.49462300	-0.93706500
C	2.02050800	-0.43171100	-2.46482600
H	2.61996900	-1.34312100	-2.51327200
H	2.66510300	0.42047600	-2.66929000
C	2.96571600	-2.53829800	0.12599100
H	2.36214800	-2.83010000	-0.73399800
H	2.47094600	-2.90537900	1.02543800
H	0.70506500	-0.84715200	3.31751600
H	3.92855600	-3.04904600	0.04613800
H	1.29142000	-0.48822000	-3.27740700
H	3.48832200	2.97946400	-0.24006000

E			
C	-1.62128400	1.10147000	-0.52052700
H	-2.23115900	0.70276600	-1.33102300
H	-0.76052900	1.62398800	-0.95443400
C	-0.18505300	-0.83416600	-0.89808000
H	-0.76868800	-0.74124000	-1.81482200
H	0.70231000	-0.20714300	-1.02150700
C	-0.10771700	0.41945500	1.30713000
H	0.49682200	1.19577900	0.82555500
H	-0.78777900	0.88498300	2.02121700
C	-2.08067500	-1.01274700	0.78495800
H	-2.51615600	-0.45812500	1.61728700
H	-1.56485300	-1.87392700	1.20582400
N	-1.01310000	-0.12061700	0.18875800
C	4.48491600	0.09360600	0.23025100
C	4.32235900	-0.46019500	-1.11405500
H	3.95466100	1.01232500	0.46316100
H	5.38955400	-0.11826900	0.79464400
H	5.10691300	-1.08072900	-1.53977900
H	3.68118500	0.07833800	-1.80590500
Br	1.70956200	2.35948400	-1.15803200
O	3.63635900	-1.05221800	0.00898300
C	0.17042100	-2.30392000	-0.68327400
C	1.02999700	-2.80101200	-1.85766400
H	-0.73042700	-2.92442100	-0.62221600
H	0.72848100	-2.45196800	0.24067700
C	1.41709600	-4.27508400	-1.71501100
H	0.48657100	-2.65228900	-2.79853700
H	1.93333900	-2.18828900	-1.91654600
H	2.02054000	-4.60575500	-2.56416100
H	2.00447100	-4.44033700	-0.80719300
H	0.53298500	-4.91935400	-1.66559300
C	-3.17973400	-1.47285600	-0.17103600
C	-4.08813700	-2.51580100	0.49786000
H	-2.74607300	-1.90435000	-1.07800600
H	-3.79005500	-0.62223400	-0.48731400
C	-5.22478700	-2.98115000	-0.41591400
H	-3.48633700	-3.37973700	0.80303800
H	-4.50871900	-2.09481600	1.41879700
H	-5.85413300	-3.72062200	0.08508800
H	-5.86530700	-2.14444400	-0.71028400
H	-4.83626200	-3.44022300	-1.32988400
C	-2.44292600	2.05940300	0.33535500
C	-3.03481400	3.16542900	-0.55448400

H	-1.81359600	2.52964700	1.09459100
H	-3.25807700	1.54455200	0.85768200
C	-3.83372100	4.19887400	0.24345900
H	-2.21861800	3.66193600	-1.08886000
H	-3.67850400	2.71394400	-1.31912900
H	-4.24241200	4.97051900	-0.41370700
H	-4.67221300	3.73549800	0.77358600
H	-3.20284700	4.69690000	0.98541100
C	0.80359900	-0.56640500	2.03024900
C	1.46894700	0.14232000	3.22241000
H	1.58798100	-0.91767400	1.35686200
H	0.25462000	-1.43878000	2.40244100
C	2.44204100	-0.76871400	3.97543600
H	2.00007200	1.02778200	2.85795300
H	0.69737100	0.50585400	3.91248100
H	2.91132900	-0.23960100	4.80896300
H	1.93012700	-1.64570400	4.38493300
H	3.23639900	-1.12570000	3.31427700

TS3

C	-0.11720800	1.45652900	-0.53967900
H	-0.77721900	1.74395300	-1.35757100
H	0.76712400	0.97690700	-0.96270600
C	-1.10520400	-0.77695500	-0.80158100
H	-1.32841100	-0.26100400	-1.73571700
H	-0.16189200	-1.30857400	-0.94610000
C	0.08502000	-0.10092400	1.35854400
H	1.08966600	-0.09519300	0.93105400
H	0.04878700	0.70059100	2.09655800
C	-2.14569700	0.86050400	0.83425300
H	-1.85984800	1.57535300	1.60592600
H	-2.60904000	0.01092400	1.33440300
N	-0.85301100	0.34658900	0.22813600
C	2.55286500	-1.72072500	-0.98626500
C	1.92151700	-1.61026200	-2.31324700
H	1.91297000	-1.65111000	-0.12723900
H	3.39881300	-2.38622700	-0.88419600
H	2.63759300	-1.70691400	-3.14355200
H	1.33783100	-0.68502000	-2.47850900
Br	3.65766700	0.37044100	-0.27337200
O	1.20347100	-2.74681000	-2.00748400
C	-2.21150200	-1.79425300	-0.52278500
C	-2.27807700	-2.78381500	-1.70212500
H	-3.18730800	-1.31248700	-0.40340100

H	-2.01703000	-2.35434700	0.39285000
C	-3.29208000	-3.90486500	-1.46493000
H	-2.54602000	-2.23629900	-2.61408200
H	-1.27861700	-3.19507300	-1.87560300
H	-3.32935100	-4.58162700	-2.32201900
H	-3.02497200	-4.50165400	-0.58723100
H	-4.30253300	-3.51231300	-1.30712800
C	-3.13170400	1.51096400	-0.13510500
C	-4.46204100	1.81733000	0.57035700
H	-3.32158900	0.85989000	-0.99300100
H	-2.71749500	2.44299300	-0.53038700
C	-5.47023200	2.51440100	-0.34669500
H	-4.89483100	0.88419700	0.94921200
H	-4.27165700	2.44573000	1.44842500
H	-6.40427900	2.71955700	0.18165300
H	-5.07986500	3.46823900	-0.71363200
H	-5.70972800	1.89569500	-1.21660500
C	0.30855600	2.68324800	0.26029200
C	0.99963800	3.69297600	-0.67159100
H	1.01869100	2.40173100	1.04092900
H	-0.54914100	3.16618700	0.74256400
C	1.48478500	4.93760000	0.07555500
H	1.85059700	3.19922900	-1.15071900
H	0.30886500	3.98867900	-1.47085200
H	1.97125700	5.63773800	-0.60786400
H	0.65612800	5.46560900	0.55905400
H	2.21177700	4.67115300	0.84782300
C	-0.20048500	-1.43663900	2.03605000
C	0.76850000	-1.63754800	3.21392900
H	-0.06720700	-2.25827000	1.32814800
H	-1.22898800	-1.48650700	2.40878800
C	0.58402100	-2.99509300	3.89678200
H	1.79841700	-1.54353200	2.85418600
H	0.62390700	-0.83417200	3.94613200
H	1.27883700	-3.10917400	4.73230100
H	-0.43104600	-3.11034500	4.29014500
H	0.76774200	-3.81642300	3.19834500
F			
C	-1.16581800	1.51896200	-0.38582100
H	-1.57436100	1.55930200	-1.39597600
H	-0.06606800	1.48237300	-0.43448800
C	-0.88636200	-0.85822500	-0.82360000
H	-1.04807900	-0.42525100	-1.81209800

H	0.18708100	-0.77052300	-0.60755300
C	-0.89655600	0.02821800	1.55485400
H	0.14800900	0.33359900	1.37936100
H	-1.41911800	0.76916000	2.16102300
C	-3.03634000	-0.05692900	0.26980700
H	-3.37313900	0.60809100	1.06651000
H	-3.20130300	-1.07754900	0.61238300
N	-1.54064900	0.12830400	0.16192400
C	3.69137400	-0.10274800	-0.72394700
C	2.90594800	0.82260500	0.20890700
H	3.57678300	-1.14701600	-0.44023700
H	3.40936400	0.04342300	-1.76459600
H	3.13788300	1.86937500	-0.07788400
H	3.31313400	0.69539700	1.23364700
Br	5.68613400	0.22070900	-0.68384000
O	1.57525700	0.50425700	0.09912300
C	-1.39014700	-2.30032000	-0.83773300
C	-0.56046300	-3.12234200	-1.83887600
H	-2.44408600	-2.35339900	-1.13369100
H	-1.31600700	-2.76822200	0.14450400
C	-1.02123400	-4.57915400	-1.93248500
H	-0.61832500	-2.65574100	-2.82929300
H	0.49383300	-3.08471900	-1.54666200
H	-0.41467300	-5.13772700	-2.64970500
H	-0.93861600	-5.08446200	-0.96529000
H	-2.06489100	-4.64830000	-2.25568000
C	-3.84159000	0.20306200	-1.00246000
C	-5.31659300	-0.17696100	-0.80438900
H	-3.43249400	-0.36831600	-1.84097500
H	-3.78184000	1.25877100	-1.28178500
C	-6.17287200	0.11056700	-2.04063900
H	-5.38723300	-1.24089700	-0.54980000
H	-5.72103700	0.37094800	0.05497100
H	-7.21487400	-0.17216800	-1.87239900
H	-6.15442800	1.17400300	-2.29734900
H	-5.81348700	-0.44744300	-2.91048800
C	-1.64265500	2.72445000	0.41755400
C	-1.28228500	4.01998200	-0.32879900
H	-1.16109200	2.74721200	1.39824700
H	-2.72606000	2.70436000	0.58768700
C	-1.67997300	5.27901000	0.44593500
H	-0.20456200	4.03086900	-0.52111400
H	-1.77105700	4.02379900	-1.31046900
H	-1.41315700	6.18243500	-0.10823100

H	-2.75836800	5.30978900	0.63220900
H	-1.17301700	5.32299100	1.41438400
C	-0.92868200	-1.31920600	2.26944200
C	-0.43413600	-1.13944300	3.71419100
H	-0.26448600	-2.02523800	1.76630800
H	-1.93085300	-1.76202900	2.29205400
C	-0.36431500	-2.46054800	4.48469000
H	0.55587100	-0.67200100	3.69534400
H	-1.09631500	-0.44226300	4.24181400
H	-0.01051500	-2.30173400	5.50655300
H	-1.34639500	-2.94066000	4.54422300
H	0.32194400	-3.16312900	4.00272300
G			
C	-2.26790000	1.27836900	-0.77358600
H	-2.60070100	0.93020800	-1.75153100
H	-1.23649300	1.63566600	-0.84697300
C	-1.16311900	-0.89456300	-0.60725200
H	-1.34550400	-0.75344300	-1.67329800
H	-0.17701400	-0.48035700	-0.36786800
C	-1.62011600	0.48721300	1.46866000
H	-0.81246600	1.17768800	1.21392900
H	-2.43578400	1.04218800	1.93387400
C	-3.52216000	-0.63080600	0.30347900
H	-4.11170700	0.05297500	0.91566900
H	-3.34909800	-1.52738000	0.89711600
N	-2.17199300	0.02404700	0.10960300
C	4.42611000	0.63947200	-1.00268600
C	4.01127400	1.28767400	0.30923800
H	3.69659600	-0.09562600	-1.32889300
H	4.61164700	1.37781100	-1.77902900
H	4.77853500	1.98605900	0.64867400
H	3.84204600	0.52520000	1.07028400
Br	6.13466400	-0.35410400	-0.78826200
O	2.83500700	2.06618800	0.10128300
C	1.60037200	1.39265000	0.14347900
O	0.62198600	2.14312200	-0.03892100
O	1.62007500	0.15895500	0.35568000
C	-3.17634300	2.39947000	-0.27818200
C	-3.16717000	3.55810400	-1.28922200
H	-2.82711100	2.78020400	0.68446700
H	-4.20787300	2.05465700	-0.13963100
C	-4.03938400	4.73502400	-0.84483700
H	-2.13563800	3.89583100	-1.42987700

H	-3.51207700	3.19482300	-2.26490300
H	-4.01295000	5.54223100	-1.58099900
H	-5.08453100	4.43423800	-0.71878900
H	-3.69241200	5.14531100	0.10808600
C	-1.10320800	-0.57742500	2.42968100
C	-0.72739400	0.08250100	3.76668700
H	-0.20810800	-1.04172700	2.01215400
H	-1.84738300	-1.35944400	2.61851700
C	-0.13418700	-0.91488000	4.76532100
H	-0.00493600	0.88277500	3.57661700
H	-1.61338900	0.55864300	4.20484800
H	0.12415500	-0.42235400	5.70622000
H	-0.84109600	-1.71901100	4.99431100
H	0.77654700	-1.37181100	4.36825200
C	-1.20376300	-2.38980700	-0.29108800
C	-0.03885600	-3.08986700	-1.01230700
H	-2.14578200	-2.84532900	-0.61525000
H	-1.11199700	-2.57570000	0.77959600
C	-0.00947200	-4.59862500	-0.75574800
H	-0.11456700	-2.90410500	-2.09041300
H	0.90187400	-2.63577900	-0.68732800
H	0.82693600	-5.06838600	-1.27916100
H	0.10450100	-4.81686600	0.31053300
H	-0.92983500	-5.08258500	-1.09877800
C	-4.28860500	-0.97976400	-0.97197700
C	-5.54372900	-1.80278600	-0.64546300
H	-3.65589000	-1.54698500	-1.66079400
H	-4.58791400	-0.06803500	-1.49704100
C	-6.36947300	-2.14141200	-1.88943900
H	-5.24805700	-2.72874100	-0.13864700
H	-6.16670600	-1.24924600	0.06700400
H	-7.25049900	-2.73244400	-1.62791400
H	-6.71572900	-1.23504100	-2.39494300
H	-5.78268300	-2.72015400	-2.60904400
TS4			
C	-2.45198000	1.20624300	-0.74527400
H	-2.87065700	0.80310100	-1.66732300
H	-1.48541200	1.66447200	-0.96543100
C	-1.12360600	-0.84953700	-0.70183900
H	-1.45819100	-0.75282200	-1.73528900
H	-0.16409600	-0.33684400	-0.60831200
C	-1.43650100	0.53432800	1.39995300
H	-0.72570600	1.27848600	1.03652000

H	-2.22908700	1.04148800	1.95102300
C	-3.35532600	-0.78910800	0.51319800
H	-3.91908600	-0.15204800	1.19542300
H	-3.01512900	-1.65147000	1.08404700
N	-2.11272700	-0.01108500	0.13143800
C	3.60186600	0.23875200	-0.29945800
C	3.89954300	1.69077700	-0.62368100
H	3.68608500	-0.13283800	0.70402700
H	3.44339700	-0.47475400	-1.08719200
H	4.41799500	1.77545200	-1.57499300
H	4.51129800	2.14060200	0.15619700
Br	6.03573800	-0.41356600	-0.48099400
O	2.68004700	2.47431900	-0.73460600
C	1.55135100	1.80082300	-0.41284100
O	0.46862600	2.38587300	-0.45058600
O	1.73351000	0.56429700	-0.09041100
C	-3.39992800	2.23937100	-0.14517200
C	-3.66839500	3.35711300	-1.16741600
H	-2.96401100	2.68929800	0.74991600
H	-4.35450100	1.78782800	0.14738900
C	-4.59240900	4.44663200	-0.61784600
H	-2.71357800	3.80034900	-1.46769100
H	-4.10960000	2.92509900	-2.07362000
H	-4.76484400	5.22594400	-1.36398600
H	-5.56720700	4.03858400	-0.33231900
H	-4.15809900	4.92470000	0.26502900
C	-0.72619400	-0.45635900	2.31666600
C	-0.25468900	0.27057500	3.58751100
H	0.14907200	-0.86813700	1.81096300
H	-1.37722800	-1.28842400	2.60682900
C	0.52934700	-0.64553000	4.53053800
H	0.37175800	1.12157900	3.30020400
H	-1.12174700	0.68625100	4.11524800
H	0.84731800	-0.10564700	5.42568100
H	-0.07637300	-1.49794000	4.85424700
H	1.42690300	-1.03762500	4.04428100
C	-0.97703500	-2.33366800	-0.36667800
C	0.09904600	-2.95932700	-1.27119900
H	-1.91884400	-2.87003800	-0.51948200
H	-0.69012100	-2.48308500	0.67477300
C	0.29044300	-4.45488400	-1.00694800
H	-0.17388600	-2.80522800	-2.32195200
H	1.04601700	-2.43267700	-1.11918100
H	1.05924300	-4.87118700	-1.66181100

H	0.60273400	-4.63808100	0.02541700
H	-0.63452300	-5.01384600	-1.18134800
C	-4.24984800	-1.23834100	-0.64103700
C	-5.36619500	-2.16454800	-0.13371300
H	-3.66668200	-1.76257500	-1.40379700
H	-4.70438700	-0.37276600	-1.13124400
C	-6.31567300	-2.61270700	-1.24788000
H	-4.91912800	-3.04471500	0.34280900
H	-5.93732600	-1.65010500	0.64806400
H	-7.09495500	-3.27127800	-0.85730500
H	-6.80931200	-1.75695700	-1.71782700
H	-5.78020500	-3.15927400	-2.02974400
H			
C	0.08707200	0.96711900	-1.03502600
H	-0.12425900	1.77466100	-0.33664300
H	-0.77851600	0.29798400	-1.05335500
C	0.64522800	-0.29738200	0.98083000
H	0.08727300	0.56288200	1.34727600
H	-0.08333500	-1.07986600	0.75006000
C	1.41574200	-1.08912000	-1.30248700
H	0.41075100	-1.48310800	-1.48286600
H	1.81350500	-0.68517900	-2.23378700
C	2.49284000	0.91111200	-0.26925100
H	2.86894200	1.04737900	-1.28415400
H	3.19982100	0.26865200	0.25328000
N	1.20528000	0.12579500	-0.39168900
C	-4.11231300	-0.25309300	1.60591600
C	-4.41016500	0.55029300	0.33024500
H	-3.70069700	-1.23371400	1.36759300
H	-4.95880900	-0.32557800	2.28790200
H	-5.36951600	1.06982900	0.35175000
H	-4.30730600	-0.06278200	-0.56385800
Br	-2.08536000	-2.06868100	-0.82873300
O	-3.36506200	1.55099700	0.30989200
C	-2.62782100	1.48052100	1.43189800
O	-1.68016400	2.18389800	1.66119900
O	-3.07826000	0.52286400	2.25991600
C	0.36279400	1.52200200	-2.42936300
C	-0.81162400	2.41040700	-2.87416700
H	0.48024800	0.71369100	-3.15608600
H	1.28341100	2.11664600	-2.45312000
C	-0.61806200	2.97817900	-4.28228700
H	-1.73541100	1.82512200	-2.83434100

H	-0.93837200	3.23016500	-2.15854300
H	-1.46349500	3.60818200	-4.57010000
H	0.28778400	3.58993300	-4.34611300
H	-0.53359600	2.17866500	-5.02458100
C	2.31724200	-2.21683200	-0.81052100
C	2.50289200	-3.24756000	-1.93651000
H	1.85763300	-2.71956200	0.04286400
H	3.30054600	-1.85211500	-0.49370700
C	3.34304200	-4.45065500	-1.50060200
H	1.51773400	-3.58880000	-2.27051800
H	2.97535100	-2.76356200	-2.79992100
H	3.46055500	-5.16448800	-2.31972800
H	4.34413500	-4.14445900	-1.18002300
H	2.87157200	-4.97882200	-0.66671800
C	1.63544700	-0.73369400	2.05968300
C	0.85747400	-1.21972700	3.29512400
H	2.27955400	0.09977800	2.35921200
H	2.29262800	-1.53509800	1.71908600
C	1.77995600	-1.62970200	4.44573900
H	0.17827200	-0.42849500	3.62996100
H	0.22261000	-2.06458200	3.00881100
H	1.20221700	-1.97379800	5.30722500
H	2.44932300	-2.44360600	4.14959900
H	2.40099700	-0.79137200	4.77706600
C	2.38273700	2.26122500	0.43797200
C	3.77358600	2.86830700	0.67572100
H	1.86459400	2.15815100	1.39539600
H	1.78840700	2.95623700	-0.16102200
C	3.70866500	4.24558000	1.34112900
H	4.36588500	2.18777200	1.29890600
H	4.30573300	2.94939200	-0.27990000
H	4.71012100	4.65125000	1.50469500
H	3.15702000	4.95898300	0.72187900
H	3.20681700	4.19296800	2.31170700
I			
C	-2.82513400	2.03164400	0.37816500
C	-1.88341700	1.22338000	-0.50199600
H	-2.33837800	2.40699600	1.27826500
H	-3.73579900	1.49616300	0.65944200
H	-2.36337800	0.97808500	-1.44867100
H	-0.96426700	1.78489000	-0.70937000
C	-0.43887500	-0.68300100	-0.99184300
C	-0.12127300	-2.17106800	-0.93618500

H	-0.91206100	-0.45081000	-1.94614400
H	0.45710500	-0.06068600	-0.91824900
H	0.38738000	-2.47516000	-0.02569300
H	-0.99557200	-2.80740900	-1.09219800
C	-0.63257300	0.22349400	1.37514700
C	0.14962000	-0.89856000	2.04154100
H	0.04703600	1.03494300	1.09246000
H	-1.39503800	0.60428300	2.05431400
H	-0.44767800	-1.78557200	2.26777400
H	1.03081800	-1.17897200	1.46548700
C	-2.53690000	-1.04724500	0.39164700
C	-3.48601900	-1.33495200	-0.76547500
H	-3.07983100	-0.59908600	1.22402000
H	-2.09248400	-1.97088600	0.75679800
H	-4.05863600	-0.45611100	-1.06403900
H	-2.97043600	-1.72632600	-1.64343600
N	-1.38969300	-0.11278000	0.07919100
H	0.57103600	-2.36735600	-1.75880400
H	0.50385300	-0.50037300	2.99655900
H	-4.19967700	-2.09506800	-0.43822700
H	-3.12942500	2.90608800	-0.20254000
C	3.89323200	-0.16832100	0.61460300
C	3.80707200	-0.48890000	-0.81058900
H	3.38249600	0.72665700	0.95733900
H	4.74361600	-0.51670500	1.19530300
H	4.59346900	-1.07390400	-1.28099500
H	3.24114700	0.18923000	-1.44242600
O	3.01771600	-1.21836100	0.15197300
Cl	1.39743600	2.25615300	-0.50101000
TS5			
C	0.90272600	-2.63077800	-0.67942100
C	0.68681600	-1.15513700	-0.97896700
H	0.32564100	-2.96511300	0.18219700
H	1.95322400	-2.90366300	-0.55322600
H	1.15141100	-0.87680600	-1.92360300
H	-0.38305300	-0.95349300	-1.04315800
C	0.84520700	1.24354800	-0.44195200
C	1.64584100	2.42802300	0.08603300
H	0.94873300	1.19583700	-1.52536700
H	-0.21592800	1.40105400	-0.23640900
H	1.62551300	2.52383300	1.16977200
H	2.68501300	2.43678700	-0.24786600
C	0.53960900	-0.51264900	1.39353700

C	0.60533600	0.51897000	2.50905600
H	-0.49662400	-0.74762400	1.14013500
H	1.00514500	-1.44121600	1.72231600
H	1.62413400	0.77883900	2.80470800
H	0.05392700	1.42902400	2.27331100
C	2.72952900	-0.30985800	0.23254000
C	3.54921500	-0.19480800	-1.04719300
H	2.89534200	-1.28187300	0.69612100
H	3.03167100	0.44858400	0.95214500
H	3.38179300	-1.03323300	-1.72417500
H	3.36101700	0.73218800	-1.59000200
N	1.22864800	-0.16500200	0.06530300
H	1.15890200	3.31754100	-0.32104300
H	0.12101900	0.06712100	3.37850000
H	4.60667500	-0.20419000	-0.77204500
H	0.52165800	-3.18596400	-1.53979800
C	-2.75207200	0.69054700	0.13498800
C	-2.49472200	1.18838300	-1.22610000
H	-1.93435500	0.69513700	0.83005800
H	-3.72564500	0.88124100	0.56416200
H	-3.39029200	1.18356500	-1.86626200
H	-1.68768200	0.66916900	-1.77757400
O	-2.17328400	2.40101000	-0.65523400
Cl	-2.78684700	-1.63631000	0.25274900
J			
C	-1.52872900	2.64642200	0.45542600
C	-1.31902400	1.45335400	-0.46532700
H	-0.91758100	2.59460800	1.35689700
H	-2.57144300	2.81098400	0.74134700
H	-1.84996100	1.60372800	-1.40497600
H	-0.24940900	1.27963200	-0.66945500
C	-1.43118900	-0.91211500	-1.03889800
C	-2.11985400	-2.27147200	-1.01342700
H	-1.68429500	-0.40741400	-1.97193500
H	-0.33177500	-0.95977300	-0.98691800
H	-1.91718600	-2.85393400	-0.11762800
H	-3.20245700	-2.21558700	-1.15221600
C	-0.98379800	-0.17553200	1.35062100
C	-1.11030000	-1.55085300	1.99010800
H	0.05744600	0.00195600	1.04413000
H	-1.31236000	0.58821700	2.05521600
H	-2.13718800	-1.86758100	2.18960800
H	-0.59866800	-2.31841500	1.41061600

C	-3.27314000	0.09305100	0.39347000
C	-4.19455800	0.51211300	-0.74627900
H	-3.40289600	0.75812300	1.24791400
H	-3.52097900	-0.91207100	0.72967800
H	-4.07417800	1.56243300	-1.01444500
H	-4.05141700	-0.09165800	-1.64348000
N	-1.79703900	0.09066900	0.07262600
H	-1.71948200	-2.83695100	-1.85942300
H	-0.59973300	-1.49293600	2.95525800
H	-5.22777200	0.37376400	-0.41823700
H	-1.20313700	3.53318900	-0.09480100
C	3.48988100	-0.00466600	0.36815200
C	2.57902700	0.08303700	-0.86123200
H	3.33042500	0.84387700	1.03202700
H	3.32655500	-0.93630900	0.90809300
H	2.84648100	-0.75724200	-1.53536800
H	2.85198800	1.00667100	-1.41343600
O	1.26976900	0.05826900	-0.44714700
Cl	5.29001500	0.02069500	-0.05384400

K

C	-3.34612600	2.30066400	-0.54734600
C	-2.49249900	1.10903400	-0.95752500
H	-2.99145900	2.77094900	0.36953700
H	-4.40905000	2.06711400	-0.44435600
H	-2.80320700	0.73335400	-1.93162200
H	-1.43650700	1.39358000	-0.99522500
C	-1.55654000	-1.12897800	-0.62484800
C	-1.73898200	-2.58909900	-0.22623000
H	-1.67727300	-1.03173000	-1.70388800
H	-0.55351000	-0.77734000	-0.35425600
H	-1.64173000	-2.76162100	0.84336500
H	-2.67994700	-3.02444200	-0.56904200
C	-2.01009400	0.39419800	1.35253800
C	-1.63673300	-0.66053700	2.38256800
H	-1.13702400	1.00380100	1.10813800
H	-2.80141100	1.03640800	1.73942100
H	-2.44039400	-1.36429700	2.61419800
H	-0.73245500	-1.19553100	2.09528100
C	-3.92884200	-0.64706300	0.14821300
C	-4.64625800	-0.99921300	-1.15016400
H	-4.49424600	0.10639600	0.69674800
H	-3.84897700	-1.52143100	0.79108000
H	-4.88206800	-0.11688300	-1.74619400

H	-4.07798700	-1.69325400	-1.77079700
N	-2.52709300	-0.10053000	-0.00913400
H	-0.93037300	-3.14238400	-0.71095300
H	-1.40550700	-0.12256300	3.30600500
H	-5.59166300	-1.48456300	-0.89573200
H	-3.25336600	3.04719800	-1.33999400
C	4.14337600	-0.02190300	-0.73039800
C	3.67608500	0.74333000	0.50004400
H	3.38431400	-0.72569600	-1.06085400
H	4.41856200	0.65444100	-1.53732800
H	4.46696000	1.40811100	0.85310900
H	3.39876600	0.04531200	1.29095600
O	2.57827200	1.58469400	0.15711800
C	1.30004800	1.00366100	0.14738300
O	0.39142300	1.80863900	-0.13907000
O	1.21300600	-0.21503100	0.42190200
Cl	5.63335200	-1.00307100	-0.34521700
TS6			
C	-3.53555300	2.20810200	-0.03811900
C	-2.62650500	1.18392800	-0.70233100
H	-3.13622500	2.57459200	0.90744000
H	-4.55702400	1.85266400	0.11714600
H	-3.00206900	0.92609200	-1.69149400
H	-1.61273600	1.57791300	-0.79680300
C	-1.46407400	-0.97013500	-0.80996800
C	-1.47723600	-2.48514100	-0.64099900
H	-1.69363300	-0.72108800	-1.84589400
H	-0.47837600	-0.56366500	-0.57562200
H	-1.26923100	-2.81252500	0.37531500
H	-2.40454800	-2.95207500	-0.97777200
C	-1.85337200	0.18132200	1.41581000
C	-1.31927900	-0.97716200	2.24418800
H	-1.05253600	0.89093200	1.20167800
H	-2.64720100	0.69435300	1.95806600
H	-2.05435800	-1.76184800	2.43757700
H	-0.41865900	-1.40788900	1.80902500
C	-3.78249400	-0.85931300	0.22349800
C	-4.59001200	-1.07838200	-1.05082000
H	-4.35406000	-0.26246100	0.93408500
H	-3.56045900	-1.80932400	0.70500000
H	-4.97070700	-0.14560900	-1.46852000
H	-4.02389400	-1.59797800	-1.82491400
N	-2.45577100	-0.15118300	0.04103000

H	-0.67306000	-2.87343300	-1.27129100
H	-1.03332300	-0.55982900	3.21323400
H	-5.45290000	-1.70095000	-0.80261900
H	-3.59120900	3.06779200	-0.71039200
C	3.24267000	-0.39229400	-0.01120500
C	3.69317200	1.04350000	-0.20812900
H	3.25494700	-0.84105600	0.96450000
H	3.09453000	-1.03920700	-0.85598300
H	4.21801000	1.15701700	-1.15320400
H	4.34590500	1.35733400	0.60275700
O	2.55631900	1.95272300	-0.23146400
C	1.36551600	1.34471900	-0.05733500
O	0.33164100	2.01400600	-0.06114000
O	1.43196400	0.06300200	0.10129400
Cl	5.51687200	-1.14259800	-0.12915300
L			
C	0.87137700	-0.46249800	1.25472000
H	0.47988800	-1.43622700	0.96932000
H	0.05797900	0.26552400	1.18597300
C	1.01094300	-0.09755000	-1.15910300
H	0.36910900	-0.97160100	-1.06039700
H	0.36557800	0.78305300	-1.10128800
C	2.29670200	1.38231900	0.45698200
H	1.37047200	1.92974400	0.65818000
H	2.87584200	1.29908800	1.37612600
C	3.04607200	-0.96660700	0.08054100
H	3.61824900	-0.77979400	0.98972900
H	3.65518000	-0.63360300	-0.75782800
N	1.84586500	-0.04769500	0.13641700
C	-3.70822900	0.48583600	-0.81560600
C	-3.76590200	0.27716500	0.70767500
H	-3.24510900	1.43843500	-1.06736300
H	-4.67012500	0.35821800	-1.31363000
H	-4.76695600	0.06847600	1.08574700
H	-3.29694400	1.10539700	1.23683900
O	-2.95695600	-0.90394900	0.92177300
C	-2.39138900	-1.29697400	-0.23193600
O	-1.59035900	-2.18946100	-0.32243800
O	-2.83081500	-0.57011900	-1.27229500
C	1.44499100	-0.49925600	2.66369800
H	1.73546000	0.48524200	3.03205900
H	2.28774700	-1.18592200	2.77754300
C	3.10670200	2.12073100	-0.59882100

H	2.50110700	2.39509200	-1.46154900
H	3.99924200	1.58650200	-0.93271200
C	1.76595400	-0.18033900	-2.48042400
H	2.32632500	-1.11017400	-2.59786000
H	2.43661700	0.65589400	-2.66631200
C	2.72496900	-2.45134600	-0.05017900
H	2.09444200	-2.67115200	-0.91230800
H	2.23461800	-2.85062600	0.83800500
H	0.64657100	-0.85925400	3.31733900
H	3.66591700	-2.99187800	-0.17996600
H	1.00635800	-0.16667000	-3.26651600
H	3.44134700	3.05428900	-0.13897200
Cl	-1.02929800	2.35324500	0.32078300