

Supporting Information

Zinc 2-N-Methyl N-confused porphyrin: An Efficient Catalyst for the Conversion of CO₂ into Cyclic Carbonates

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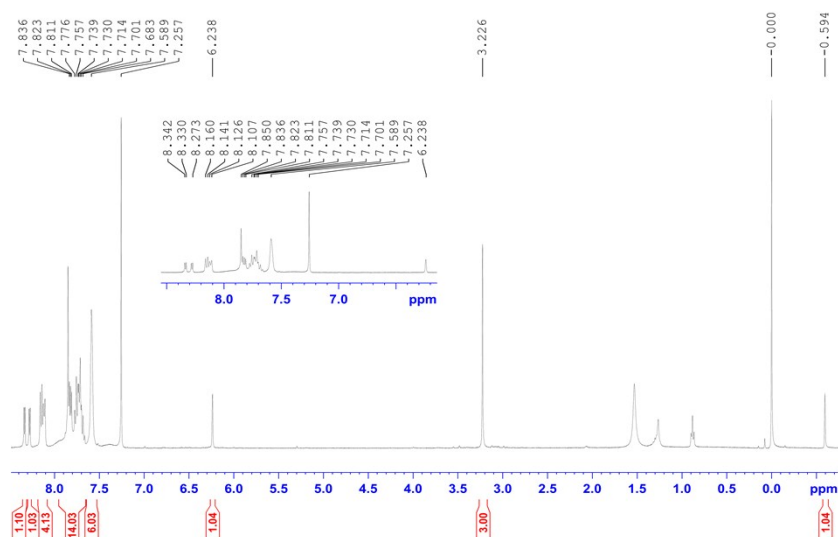
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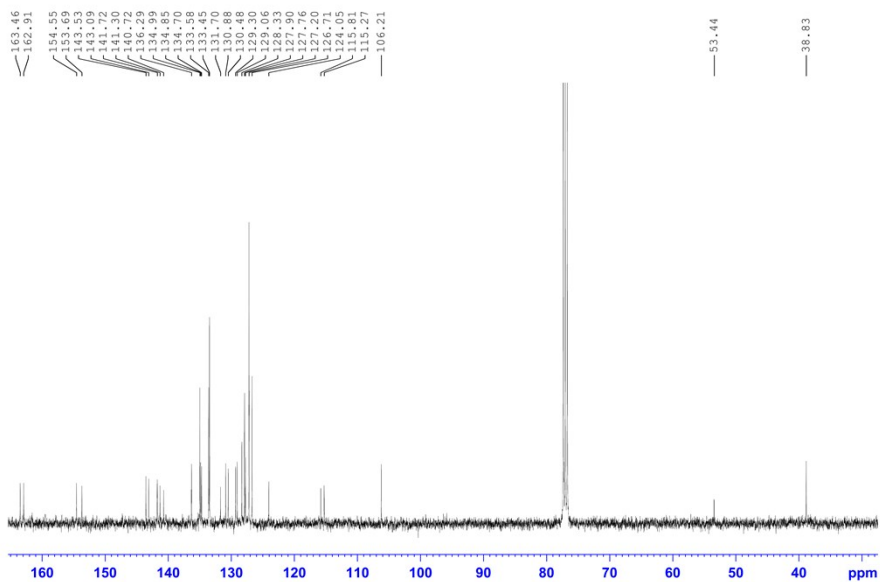
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^1H NMR, ^{13}C NMR, FT-IR and HRMS Spectra of $\text{Zn}(\text{NCP})\text{Cl}$

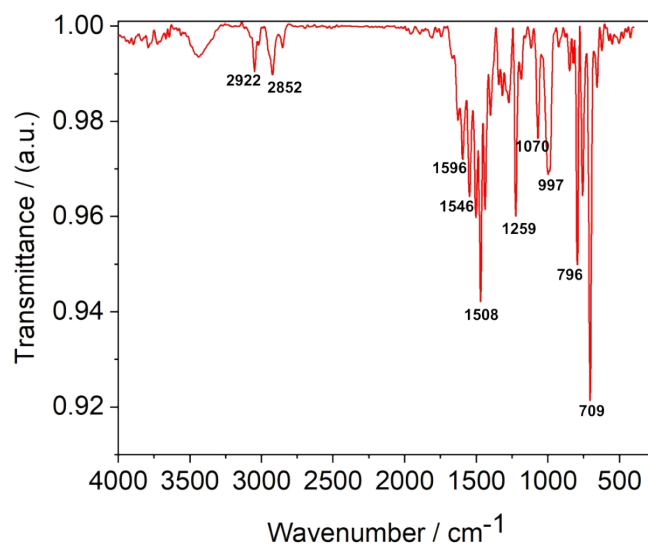
^1H NMR of $\text{Zn}(\text{NCP})\text{Cl}$ (CDCl_3):



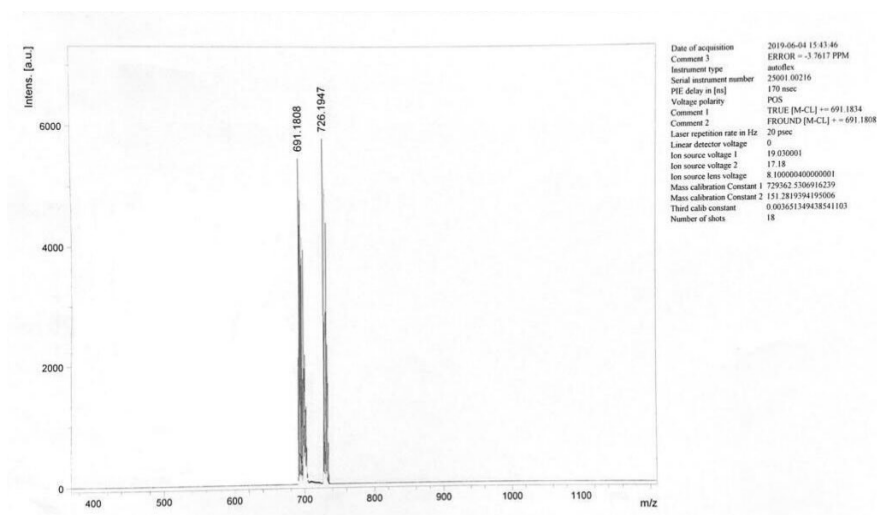
^{13}C NMR of $\text{Zn}(\text{NCP})\text{Cl}$ (CDCl_3):



FT-IR of Zn(NCP)Cl:



HRMS of Zn(NCP)Cl :



Typical procedure for the Cycloaddition of CO₂ with epichlorohydrin in Table 1

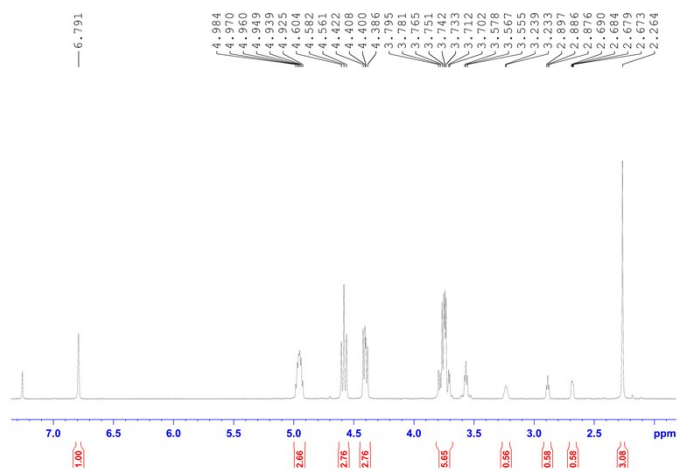
1.00 mg/mL epichlorohydrin solution of Zn(NCP)Cl was prepared in a 25 mL volumetric flask and 1.05 mg/mL epichlorohydrin solution of TBAB was prepared in 50 mL volumetric flask. 0.025 mg/mL Zn(NCP)Cl epichlorohydrin solution was obtained by diluting 0.25 mL of Zn(NCP)Cl epichlorohydrin solution (1.00 mg/mL) to 10 mL in a 10 mL volumetric flask. To get the reactive mixture containing epichlorohydrin (40 mmol), Zn(NCP)Cl (0.004 mol %) and TBAB (0.016 mol %), 1.17 mL Zn(NCP)Cl epichlorohydrin solution (1.00 mg/mL) and 1.96 mL TBAB epichlorohydrin solution (1.05 mg/mL) were added into a 100 mL stainless steel autoclave equipped with a magnetic stir bar. To get the reactive mixture containing epichlorohydrin (40 mmol), Zn(NCP)Cl (0.0001 mol %) and TBAB (0.016 mol %), 1.17 mL Zn(NCP)Cl epichlorohydrin solution (0.025 mg/mL) and 1.96 mL TBAB epichlorohydrin solution (1.05 mg/mL) were added into a 100 mL stainless steel autoclave equipped with a magnetic stir bar. The autoclave was subjected to three cycles of pressurization and depressurization with carbon dioxide, and then pressurized carbon dioxide initial pressure to 1.7 MPa. The reaction mixture was heated to 120 °C with stirring. At the end of the reaction, the reactor was cooled down to room temperature with an ice bath before the excess CO₂ was released. The yield of cyclic carbonate was determined by means of ¹H NMR using mesitylene as an internal standard.

Typical Procedure for the Cycloaddition of CO₂ with Various Epoxides in Table 2

The respective epoxide (40.0 mmol), Zn(NCP)Cl (5.83 mg, 0.008 mmol) and TBAB (10.32 mg, 0.032 mmol) were charged into a 100 mL stainless steel autoclave equipped with a magnetic stir bar. The autoclave was subjected to three cycles of pressurization and depressurization with carbon dioxide, and then pressurized carbon dioxide initial pressure to 1.7 MPa. The reaction mixture was heated to 120 °C with stirring. At the end of the reaction, the reactor was cooled down to room temperature with an ice bath before the excess CO₂ was released. The yield of cyclic carbonate was determined by means of ¹H NMR using mesitylene as an internal standard. The products were purified using column chromatography with ethyl acetate/n-hexane (v/v, 1:4) as the eluent.

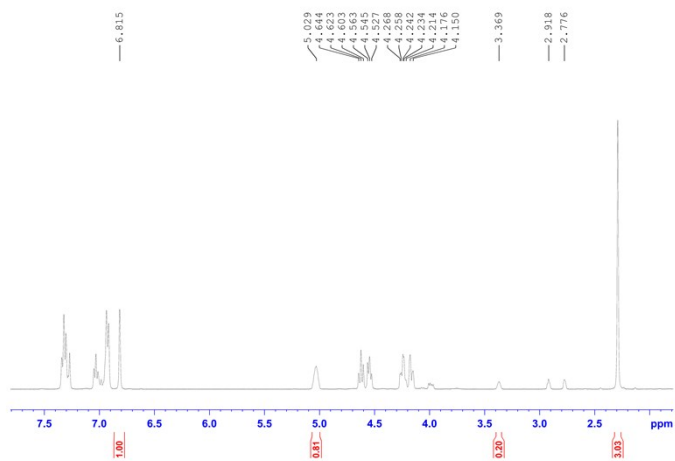
¹H NMR of crude product of chloropropene carbonate (Table 1, Entry 1)

(containing 10 mol % mesitylene)

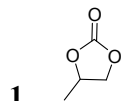


¹H NMR of crude product of phenoxypropylene carbonate (Table 1, Entry 17)

(containing 33.33 mol % mesitylene)

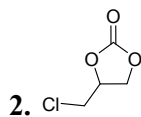
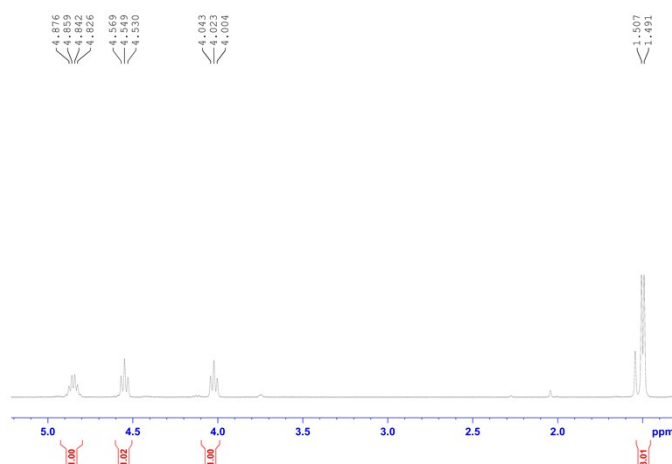


NMR data for the Cyclic Carbonates



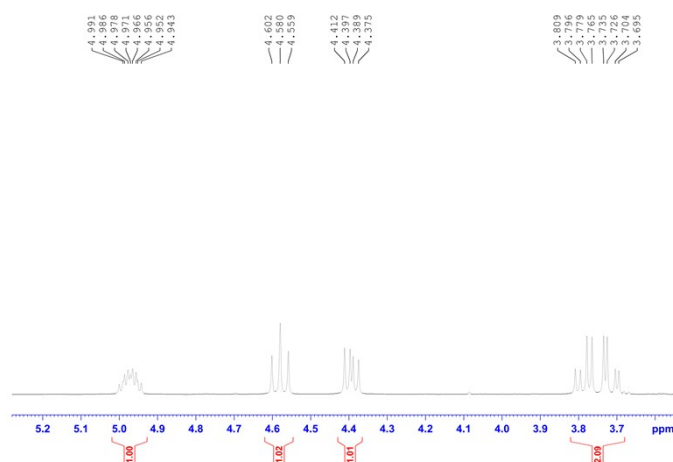
^1H NMR (400 MHz, CDCl_3): δ = 1.49-1.51 (d, 2H, $J=8\text{Hz}$), 4.00-4.04 (t, 1H, $J=16\text{ Hz}$), 4.53-4.57 (t, 1H, $J=16\text{ Hz}$), 4.83-4.88 (m, 1H)

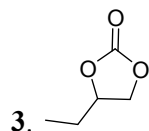
^1H NMR of isolate product :



^1H NMR (400 MHz, CDCl_3): δ = 3.70-3.81 (m, 2H), 4.38-4.41 (dd, 1H, $J=4\text{ Hz}$, $J=8\text{ Hz}$), 4.56-4.60 (t, 1H, $J=8\text{ Hz}$), 4.94-5.00 (m, 1H)

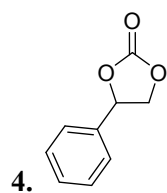
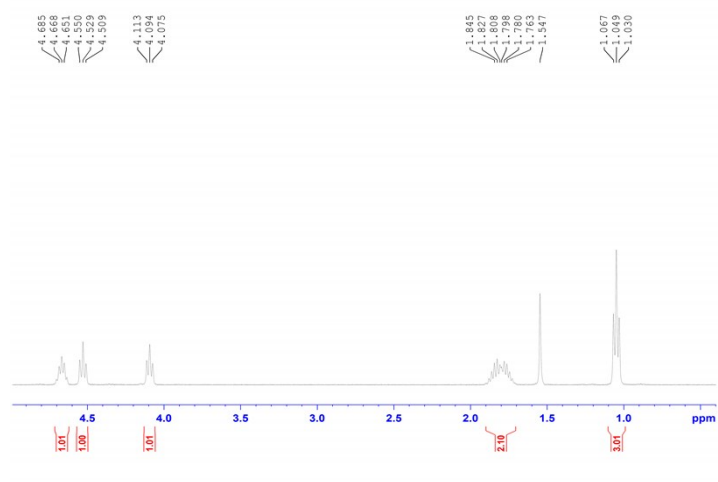
^1H NMR of isolate product :





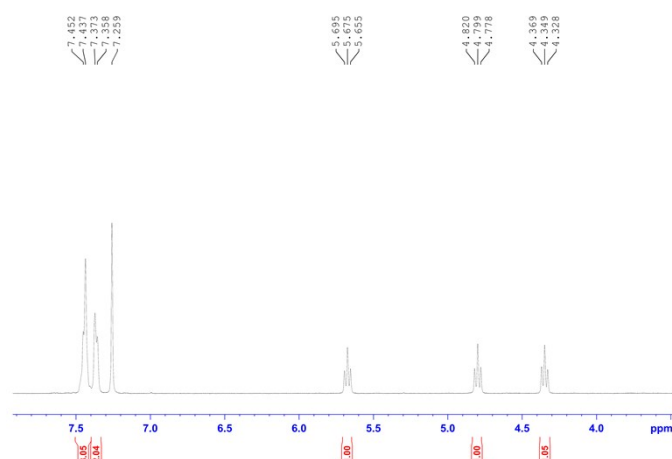
^1H NMR (400 MHz, CDCl_3): δ = 1.03-1.07 (t, 1H, $J=16$ Hz), 1.76-1.85 (m, 2H), 4.08-4.11 (t, 1H, $J=8$ Hz), 4.51-4.55 (t, 1H, $J=8$ Hz), 4.65-4.69 (m, 1H)

^1H NMR of isolate product :

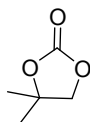


^1H NMR (400 MHz, CDCl_3): δ = 4.33-4.37 (t, 1H, $J=8$ Hz), 4.78-4.82 (t, 1H, $J=8$ Hz), 5.66-5.70 (t, 1H, $J=8$ Hz), 7.36-7.37 (m, 2H), 7.44-7.45(m, 3H)

^1H NMR of isolate product :

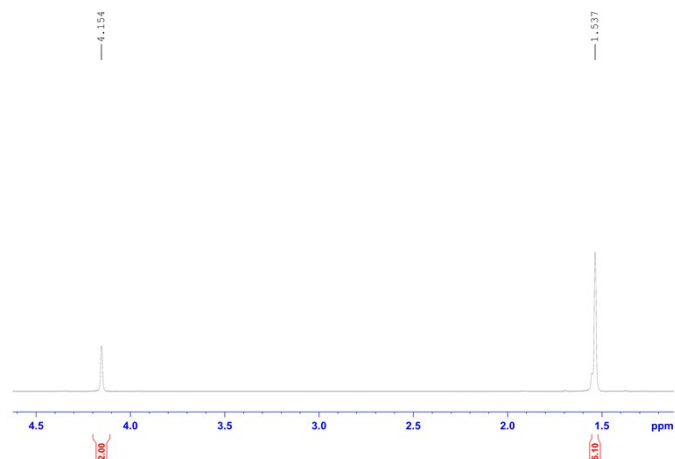


5.

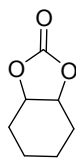


^1H NMR (400 MHz, CDCl_3): δ = 1.54 (s, 6H), 4.15 (s, 2H)

^1H NMR of isolate product :

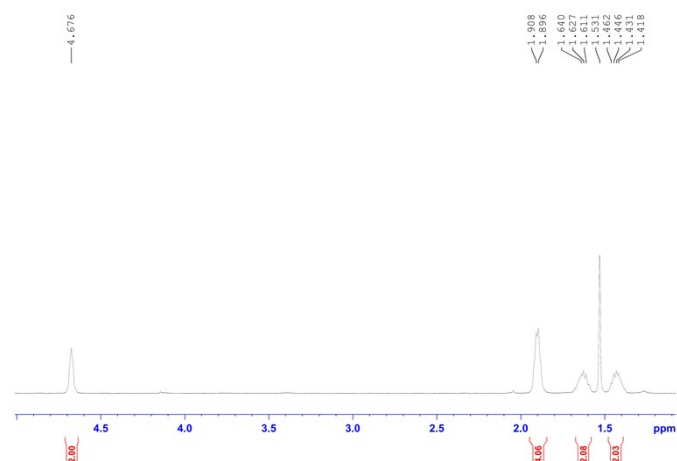


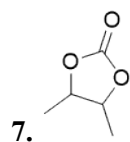
6.



^1H NMR (400 MHz, CDCl_3): δ = 1.42-1.46(m, 2H), 1.61-1.64(m, 2H), 1.90-1.91(m, 4H), 4.68(s, 2H)

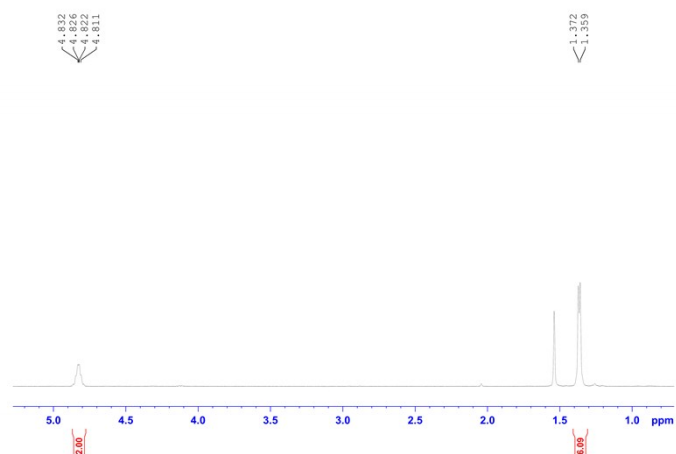
^1H NMR of isolate product :





^1H NMR (400 MHz, CDCl_3): δ = 1.36-1.37 (d, 6H, $J=4$ Hz), 4.81-4.83 (m, 2H)

^1H NMR of isolate product :



X-ray Crystallograph

Table S1. Crystal Data for Zn(NCP)Cl

Empirical formula	C ₄₅ H ₃₃ ClN ₄ Zn
Formula weight	728.58
Space group	I 2/a
Cryst. system	monoclinic
a/Å	18.7682(11)
b/Å	13.7292(6)
c/Å	31.4518(16)
$\alpha/^\circ$	90
$\beta/^\circ$	106.951(6)
$\gamma/^\circ$	90
V/Å ³	7752.2 (7)
Z	8
F(000)	3008.0
D _{c/g} cm ⁻³	1.248
μ/mm^{-1}	0.738
S	1.054
Cryst. size/mm ³	0.29 × 0.28 × 0.27
$\theta/^\circ$	3.262 to 28.431
T/K	291
No. of reflections measured	9751
No. of reflections observed	8465
R ₁ ^a	0.0811(4923)
wR ₂ ^b	0.1958(8465)

Computational Methods

Table S2. Cartesian Coordinates (Å) of the Optimized Structures of all Intermediates and Transition States at B3LYP/6-31 G(d) Level of Theory.

R1			
Zn	0.23497700	0.08170400	-1.23230400
N	0.65379000	-1.89160600	-0.60966200
N	-1.71806500	-0.32351500	-1.14294800
N	-0.15978900	2.05514300	-0.53223100
N	4.12237600	0.21155800	-1.09408000
C	1.84681700	-2.48892700	-0.21840300
C	1.60417600	-3.88617600	0.10245800
H	2.33647400	-4.56342700	0.51603800
C	0.29465400	-4.12802200	-0.14458800
H	-0.24999600	-5.04897400	-0.00127700
C	-0.28921100	-2.88040700	-0.62059200
C	-1.64257500	-2.77005200	-1.01143600
C	-2.28305600	-1.55810100	-1.29015800
C	-3.68141300	-1.41257200	-1.66797400
H	-4.35879300	-2.22867500	-1.86575400
C	-3.96023400	-0.08955300	-1.63765600
H	-4.91060900	0.39216600	-1.80659900
C	-2.73465300	0.59167800	-1.24430200
C	-2.62581700	1.94050700	-0.92162100
C	-1.41982200	2.58132200	-0.52546100
C	-1.38649400	3.95799700	-0.06424200
H	-2.25596000	4.57467600	0.10278000
C	-0.08441500	4.27607400	0.14326200
H	0.31906000	5.19941400	0.53250100
C	0.69511500	3.09613500	-0.16676500
C	2.08342600	3.04062800	-0.15077300
C	2.76011100	1.78234900	-0.24863300
C	2.33612600	0.52021900	0.24834200
H	1.60291300	0.33977300	1.02554900
C	3.17376500	-0.44497100	-0.29090100
C	3.86517800	1.53897400	-1.07289100
H	4.39843500	2.22251100	-1.71673800
C	3.09059800	-1.87125500	-0.17354900
C	-2.48471400	-4.00060500	-0.98175800
C	-2.20731400	-5.09362400	-1.81561000
H	-1.37286300	-5.03075500	-2.50886900
C	-2.99506000	-6.24349200	-1.76514200
H	-2.77120600	-7.08123400	-2.42130000

C	-4.07277700	-6.31266700	-0.88002000
H	-4.68864200	-7.20807700	-0.84037300
C	-4.35578200	-5.22689000	-0.04856300
H	-5.19093900	-5.27238500	0.64556200
C	-3.57012000	-4.07513900	-0.09182700
H	-3.78827600	-3.22722600	0.56034500
C	-3.88429100	2.74117300	-0.88623100
C	-4.05395300	3.86474100	-1.70864100
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H	-5.35271000	5.47353800	-2.30747500
C	-6.25690800	4.23608200	-0.78677100
H	-7.17653600	4.81523000	-0.74756100
C	-6.09464500	3.11733900	0.03256300
H	-6.88558900	2.82069900	0.71652600
C	-4.91782400	2.36933600	-0.01045400
H	-4.79006300	1.49305700	0.62787400
C	2.90500400	4.26338700	-0.12955400
C	2.56678800	5.40231400	-0.88559800
H	1.67798000	5.37509000	-1.50622500
C	3.37752100	6.53418600	-0.87166500
H	3.10144900	7.39890700	-1.46942700
C	4.54964300	6.55362600	-0.11248400
H	5.18204100	7.43745500	-0.10489000
C	4.90837100	5.42548400	0.62829900
H	5.81807900	5.43049800	1.22311200
C	4.10003500	4.29201500	0.61508800
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H	5.93783100	-5.47082100	-1.04112000
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C	-1.08066200	0.14822800	2.31653500
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H	-1.18703800	0.53969300	1.31191600
C	-1.72342900	0.95590400	3.39345600
H	-1.52810800	0.53478800	4.38042300
H	-2.79557900	1.00537800	3.19576700
Cl	-1.06473500	2.66651700	3.42391000
H	-1.26141700	-1.75826600	3.40242700
H	-0.96609700	-1.91685500	1.59462700
Br	-4.24427200	-0.84982100	1.80408900
Cl	1.35694700	0.28508600	-3.23250400
O	3.18489600	-0.91923300	3.13552800
C	2.47803400	-1.85107400	3.15199700
O	1.82560400	-2.81969600	3.19639400
TS1			
Zn	0.35966900	0.09657100	-1.24169400
N	0.75337100	-1.87364100	-0.59850900
N	-1.59794500	-0.32185700	-1.25007000
N	-0.06974600	2.08357200	-0.62164600
N	4.24530300	0.21881700	-0.92249000
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C	1.66729600	-3.85512000	0.19474100
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H	-0.16586900	-5.03378800	-0.03782400
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C	2.16104000	3.07809600	-0.19141200
C	2.83774200	1.81734200	-0.21824300
C	2.37769500	0.57490700	0.29892700

H	1.58848500	0.42563700	1.03809700
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C	-4.05418500	3.81499700	-1.73137400
H	-3.30114800	4.12038900	-2.45278600
C	-5.25055600	4.52315100	-1.62026600
H	-5.42996500	5.38476200	-2.25892200
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C	3.45094900	6.56355500	-0.95259100
H	3.18282800	7.41411200	-1.57386900
C	4.60571900	6.60654900	-0.16803300
H	5.23224700	7.49458200	-0.16448700
C	4.95465300	5.49606500	0.60349300
H	5.85072000	5.51934500	1.21833000
C	4.15377100	4.35723800	0.59583900
H	4.41645800	3.49906400	1.20572000
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C	5.29946500	-2.07602900	1.23173700
H	5.05436800	-1.15333400	1.74692800
C	6.48213100	-2.75348400	1.51530800
H	7.17210400	-2.34580600	2.24958400
C	6.77826900	-3.95620600	0.86901800

H	7.70309100	-4.48283800	1.08907300
C	5.88026400	-4.47382200	-0.06684600
H	6.10883800	-5.40069600	-0.58658300
C	4.69699600	-3.79716200	-0.35465300
H	4.01762200	-4.17958400	-1.10916000
C	5.07376100	-0.44903900	-1.91967300
H	5.60810800	-1.28713400	-1.47441400
H	5.79541400	0.27441400	-2.30555600
H	4.43403800	-0.79655600	-2.73685200
O	0.16374400	-0.06145100	2.36476100
C	-1.09554800	0.54113100	2.30109200
C	-1.48499100	-0.84721800	2.10037500
H	-1.25933100	1.20297100	1.44764700
H	-1.36849000	-1.27416600	1.12286000
C	-1.44408100	1.23718200	3.60497800
H	-0.62435800	1.90586300	3.87509000
H	-1.61847100	0.52315000	4.41165100
Cl	-2.93567000	2.28015900	3.48095000
H	-1.54814300	-1.50280900	2.95390100
Br	-4.00597700	-1.04755700	1.73729900
Cl	1.56916200	0.25588400	-3.20381600
O	2.70342400	-1.08528300	3.22461700
C	1.82595100	-1.86015100	3.23780700
O	1.03253000	-2.71675900	3.29725700
Int1			
Zn	0.32726900	0.06834100	-0.73234600
N	0.73530900	-1.95952600	-0.52756500
N	-1.60508300	-0.25945100	-1.11232800
N	0.02941300	2.12374300	-0.45376100
N	4.24186300	0.09839900	-0.94824300
C	1.90658900	-2.58003600	-0.14197800
C	1.63003800	-3.99264300	0.10579400
H	2.33904800	-4.71165600	0.49002500
C	0.31845300	-4.19279200	-0.17591600
H	-0.24292500	-5.11082300	-0.08317400
C	-0.23046800	-2.90488800	-0.60269900
C	-1.57590200	-2.71526300	-1.02753900
C	-2.17707200	-1.47629000	-1.31572800
C	-3.54095300	-1.27770300	-1.80428900
H	-4.22458300	-2.06562300	-2.08370100
C	-3.76626700	0.06018100	-1.81888200
H	-4.67101700	0.57555100	-2.10593800
C	-2.54708200	0.70157200	-1.33457900

C	-2.39166000	2.06102200	-1.03998100
C	-1.19900700	2.68670200	-0.56461200
C	-1.14113400	4.08004100	-0.13570600
H	-1.98852900	4.74532500	-0.06085100
C	0.15647800	4.34751200	0.16574200
H	0.56889000	5.27017700	0.54863100
C	0.90847300	3.12393800	-0.06647900
C	2.29791000	3.00085000	-0.00491500
C	2.94811800	1.71998800	-0.07942700
C	2.50945800	0.47520100	0.44417300
H	1.76751700	0.34830600	1.22297700
C	3.28395600	-0.52842800	-0.11993900
C	4.02211400	1.43121900	-0.93298000
H	4.55223700	2.08885200	-1.60623000
C	3.15184200	-1.96042200	-0.04258400
C	-2.44758700	-3.92131800	-1.10949700
C	-2.12850500	-4.99520200	-1.95516100
H	-1.23495100	-4.93135600	-2.56906500
C	-2.94687900	-6.12222600	-2.01979800
H	-2.68467800	-6.94128200	-2.68513100
C	-4.10384500	-6.19441900	-1.24173100
H	-4.74309400	-7.07237400	-1.29202800
C	-4.43379900	-5.13084800	-0.39952700
H	-5.32951800	-5.17862400	0.21460700
C	-3.61457700	-4.00480300	-0.33044200
H	-3.86759600	-3.18075400	0.33115300
C	-3.60863400	2.91671100	-1.14400800
C	-3.66832000	3.99666900	-2.03681600
H	-2.81076400	4.20214800	-2.67088700
C	-4.81207900	4.79032600	-2.11796800
H	-4.84443900	5.62003000	-2.81993600
C	-5.91433600	4.51638500	-1.30568400
H	-6.80594000	5.13544000	-1.36795400
C	-5.86360000	3.44501500	-0.41183800
H	-6.71320100	3.22998800	0.23124300
C	-4.72040300	2.65097900	-0.32874600
H	-4.66494500	1.82405900	0.37299900
C	3.16439100	4.19365000	0.01095600
C	2.88563900	5.33435000	-0.76723400
H	2.00943400	5.33160700	-1.40581300
C	3.74007100	6.43375700	-0.75511900
H	3.50899400	7.29903200	-1.37117700
C	4.89959000	6.41906500	0.02337500
H	5.56652200	7.27730300	0.02879600

C	5.20203300	5.28746800	0.78388000
H	6.10332100	5.26376200	1.39122600
C	4.34969000	4.18671400	0.77224100
H	4.57880100	3.30974100	1.36882800
C	4.38084100	-2.75680300	0.13777500
C	5.37316200	-2.29838300	1.02517100
H	5.18687600	-1.38672600	1.58398900
C	6.55698600	-3.00873800	1.20296800
H	7.30469300	-2.64191300	1.90160700
C	6.78181000	-4.19180200	0.49472800
H	7.70755400	-4.74468100	0.63102000
C	5.81136200	-4.65347600	-0.39739200
H	5.98460700	-5.56259000	-0.96773200
C	4.62724400	-3.94282400	-0.57926300
H	3.89306600	-4.27977500	-1.30326500
C	4.91981600	-0.55164700	-2.06457500
H	5.43894800	-1.44791000	-1.72751100
H	5.64735700	0.15000500	-2.47961300
H	4.17127100	-0.79871000	-2.82471900
O	-0.04434500	-0.08817100	1.46631800
C	-1.27719400	0.30037100	1.92385100
C	-2.14886700	-0.95003400	2.15415200
H	-1.81490800	0.96037100	1.22840600
H	-1.84795700	-1.72374500	1.45645300
C	-1.01859500	1.10003000	3.20358300
H	-0.43024800	1.98441900	2.96122100
H	-0.48637900	0.49261200	3.93848000
Cl	-2.53539500	1.71459100	4.05944500
H	-2.12874000	-1.32902700	3.17567200
Br	-4.09088000	-0.66774200	1.74885400
Cl	1.49795100	0.25162300	-2.89518700
O	2.09569900	-1.26477800	3.08709500
C	1.12615900	-1.90187100	2.91837900
O	0.24130500	-2.66821900	2.87738200
TS2			
Zn	0.18536600	0.07415700	-0.23507600
N	0.71487000	-1.89731200	-0.54642700
N	-1.59485900	-0.16701100	-1.08791200
N	0.05963400	2.13684000	-0.32590300
N	4.30716600	0.04557500	-0.79918300
C	1.85959100	-2.56631600	-0.14885200
C	1.55428700	-3.98047000	-0.00293700
H	2.23979800	-4.73346500	0.35721300

C	0.25509400	-4.14729800	-0.36218200
H	-0.31504900	-5.06438200	-0.36664600
C	-0.26048900	-2.83605600	-0.72702200
C	-1.57823700	-2.61682000	-1.20464000
C	-2.15810200	-1.35689100	-1.43581600
C	-3.47415100	-1.10706900	-2.00773500
H	-4.13315800	-1.86354500	-2.40755200
C	-3.69281600	0.23200600	-1.93074900
H	-4.56558100	0.78070500	-2.25304500
C	-2.51304800	0.82040200	-1.31532300
C	-2.35007700	2.16231700	-0.95848800
C	-1.15173600	2.74808000	-0.46069300
C	-1.03955500	4.14589600	-0.08172700
H	-1.85682700	4.85066300	-0.04606800
C	0.27059000	4.37297000	0.20910900
H	0.72498600	5.29609600	0.53953600
C	0.96974800	3.11728100	0.02759500
C	2.35956400	2.95497100	0.07316500
C	2.96872500	1.67045500	0.01278000
C	2.50172600	0.42618600	0.51013500
H	1.83089900	0.30196200	1.35058700
C	3.30013800	-0.57915800	-0.02508700
C	4.05921900	1.36835500	-0.82990000
H	4.61130800	2.02670600	-1.48118200
C	3.12673100	-1.99726000	0.01455000
C	-2.44767300	-3.80727100	-1.42188800
C	-2.08809000	-4.81948600	-2.32512000
H	-1.16137500	-4.72017900	-2.88239400
C	-2.90902200	-5.93004600	-2.51729500
H	-2.61548000	-6.70110400	-3.22537500
C	-4.10818900	-6.04630100	-1.81189600
H	-4.74927400	-6.91139500	-1.96187600
C	-4.47865400	-5.04331400	-0.91397900
H	-5.40806400	-5.12621800	-0.35626600
C	-3.65748300	-3.93387200	-0.71805000
H	-3.94038900	-3.15617700	-0.01404700
C	-3.55274600	3.03599500	-1.07245400
C	-3.57909300	4.14362200	-1.93249000
H	-2.70225100	4.36303600	-2.53434800
C	-4.71657500	4.94499600	-2.02441600
H	-4.72305100	5.79621500	-2.70071600
C	-5.84595000	4.65062900	-1.25780100
H	-6.73246200	5.27589200	-1.32907200
C	-5.83028300	3.54873700	-0.40065100

H	-6.70294700	3.31464000	0.20367500
C	-4.69374300	2.74645100	-0.30723500
H	-4.66887000	1.89051000	0.36055500
C	3.25283900	4.12734000	0.00304200
C	3.00140100	5.20387900	-0.86834000
H	2.13049600	5.16288500	-1.51262300
C	3.88131800	6.28073200	-0.94147300
H	3.67491100	7.09592200	-1.63012700
C	5.03580100	6.30441700	-0.15562600
H	5.72191100	7.14527800	-0.21654600
C	5.30984100	5.23391000	0.69798200
H	6.20795000	5.24058200	1.31042900
C	4.43205800	4.15519100	0.77111100
H	4.63759600	3.32451000	1.43887800
C	4.32178300	-2.84584100	0.19578800
C	5.28628700	-2.46953100	1.14902900
H	5.10396200	-1.58292100	1.74805100
C	6.43876600	-3.22721300	1.33838800
H	7.16574200	-2.92305600	2.08714300
C	6.65802000	-4.37720100	0.57653400
H	7.55891000	-4.96748100	0.72203200
C	5.71511300	-4.75730100	-0.38116400
H	5.88588600	-5.63918300	-0.99335800
C	4.56281300	-3.99885000	-0.57424400
H	3.85299300	-4.27108900	-1.34801100
C	5.02364800	-0.58597100	-1.90443000
H	5.39048100	-1.56651700	-1.60993700
H	5.87212800	0.05082200	-2.16780200
H	4.32935100	-0.64248500	-2.75200200
O	-0.13044300	-0.08264400	1.73689900
C	-1.42178300	0.22355800	2.12292800
C	-2.28002400	-1.05657900	2.09006900
H	-1.89875600	0.97534000	1.47533500
H	-1.90146100	-1.72666300	1.32540700
C	-1.29899900	0.82363800	3.52444700
H	-0.70218000	1.73385200	3.47761100
H	-0.82705600	0.10932500	4.20219600
Cl	-2.89606700	1.28843900	4.30179400
H	-2.33605900	-1.57214400	3.04819100
Br	-4.17349300	-0.73163300	1.55521600
Cl	2.20719400	0.84601800	-3.09105000
O	2.04911900	-1.48570900	3.11273600
C	1.05496300	-2.08478200	2.95780900
O	0.12809600	-2.79709500	2.89619200

Int2			
Zn	-0.08976400	0.04024000	-0.19063300
N	0.24678700	-1.93484800	-0.70046300
N	-1.78424500	0.11075400	-1.19794200
N	0.22946700	2.09401200	-0.43775300
N	4.21666300	-0.63264900	-0.73125600
C	1.26796200	-2.78213100	-0.28211600
C	0.75264800	-4.13774900	-0.20802000
H	1.30767800	-4.99579500	0.14052800
C	-0.53711000	-4.10318200	-0.63212600
H	-1.22867200	-4.92915900	-0.70532900
C	-0.84735800	-2.72118800	-0.95588200
C	-2.11015000	-2.30292500	-1.44937200
C	-2.50811100	-0.96430300	-1.61550200
C	-3.76501500	-0.49325900	-2.17801700
H	-4.52157700	-1.12223100	-2.62356700
C	-3.79267700	0.85737900	-2.01825900
H	-4.57493600	1.54289200	-2.30983700
C	-2.54913700	1.23578300	-1.36840400
C	-2.18242100	2.51283500	-0.94116100
C	-0.89005500	2.88339700	-0.45855800
C	-0.56067000	4.21168100	0.00590500
H	-1.26386700	5.01939100	0.14298700
C	0.78671200	4.23339700	0.22457400
H	1.38449900	5.05688900	0.58677800
C	1.28960100	2.91602700	-0.07608600
C	2.65679000	2.56422900	-0.11191900
C	3.06608800	1.20419500	-0.14068300
C	2.34577200	0.06689100	0.31343200
H	1.61798600	0.07876200	1.11524300
C	3.03342800	-1.07351400	-0.08481700
C	4.23315100	0.70689700	-0.77857100
H	5.07773800	1.21915300	-1.23560400
C	2.60246400	-2.43521000	-0.04902200
C	-3.12615300	-3.35129300	-1.74894100
C	-2.88468000	-4.34849600	-2.70640800
H	-1.93928200	-4.34581700	-3.24101200
C	-3.84220000	-5.32479500	-2.97850700
H	-3.63792800	-6.08664900	-3.72658400
C	-5.06219400	-5.31825300	-2.29988700
H	-5.80969000	-6.07836900	-2.51184400
C	-5.31512000	-4.32927400	-1.34741700
H	-6.25924900	-4.31909400	-0.80895600

C	-4.35708900	-3.35479400	-1.07142500
H	-4.54743800	-2.59092000	-0.32277400
C	-3.24390100	3.55782600	-0.96781000
C	-3.10730400	4.73024700	-1.72620300
H	-2.20435100	4.87788100	-2.31100900
C	-4.11859200	5.68962400	-1.74049200
H	-3.99945800	6.58954100	-2.33845000
C	-5.28304800	5.49230000	-0.99544700
H	-6.07054400	6.24144300	-1.00498400
C	-5.42948600	4.32855500	-0.23866000
H	-6.32942000	4.16916100	0.34940600
C	-4.41976700	3.36726200	-0.22390700
H	-4.52260500	2.46261400	0.36775200
C	3.69097500	3.60779400	-0.24220900
C	3.47101800	4.76841600	-1.01600400
H	2.51939000	4.89821100	-1.51890600
C	4.47820900	5.71066500	-1.18515800
H	4.29182600	6.59220700	-1.79340900
C	5.73855300	5.50409800	-0.61518500
H	6.53312000	6.22854600	-0.77364000
C	5.98364400	4.34675200	0.12105400
H	6.97117500	4.13127100	0.51280000
C	4.96714000	3.41686900	0.31873000
H	5.18132500	2.52062700	0.88766100
C	3.60527200	-3.48774000	0.23332000
C	4.45044000	-3.33422300	1.34612000
H	4.32380000	-2.46350900	1.98157600
C	5.42828100	-4.28342500	1.63143800
H	6.07367100	-4.14785500	2.49472900
C	5.58232200	-5.40214000	0.80928700
H	6.35156000	-6.13799400	1.02701300
C	4.75039000	-5.56424300	-0.30009700
H	4.87494600	-6.42365700	-0.95361700
C	3.77179500	-4.61487100	-0.58745300
H	3.14780600	-4.72186500	-1.46896400
C	5.23441300	-1.43567400	-1.41264900
H	5.58804400	-2.22661400	-0.75449700
H	6.06936300	-0.76273000	-1.63892900
H	4.81300200	-1.88075800	-2.31957600
O	-0.39546100	-0.05816400	1.73399900
C	-1.66618600	0.34521400	2.11582200
C	-2.64833500	-0.83432600	1.95930500
H	-2.04328900	1.19119400	1.51928500
H	-2.30857900	-1.49344800	1.16649000

C	-1.53253400	0.81493100	3.56478200
H	-0.83855300	1.65327800	3.61354700
H	-1.16805500	0.00054300	4.19413200
Cl	-3.10130500	1.38640900	4.31465800
H	-2.79937500	-1.40142700	2.87702100
Br	-4.46609100	-0.26938200	1.37822700
Cl	7.42862800	1.21678000	-0.91954500
O	1.65597000	-1.72966200	3.00213500
C	0.60663200	-2.22608900	2.85500900
O	-0.39370700	-2.82975400	2.78163300
TS3			
Zn	0.00134700	-0.08989100	-0.13335800
N	0.36775500	-2.06563500	-0.51913300
N	-1.70802000	-0.11644200	-1.13794600
N	0.21060800	1.95895500	-0.41242700
N	4.28668600	-0.58342800	-0.73547400
C	1.43919200	-2.85741400	-0.11989500
C	0.97863500	-4.22090300	0.04440000
H	1.58380300	-5.04008500	0.40260800
C	-0.33473600	-4.24999300	-0.30601100
H	-0.99819900	-5.10190500	-0.30552400
C	-0.70679600	-2.90029200	-0.68934700
C	-1.98314700	-2.55075400	-1.20172500
C	-2.40058300	-1.23960500	-1.48393500
C	-3.63858800	-0.84446200	-2.13790100
H	-4.36684200	-1.52614400	-2.55207500
C	-3.68994300	0.51447000	-2.11020700
H	-4.46783800	1.15649200	-2.49694200
C	-2.48532900	0.97355900	-1.44019100
C	-2.17611400	2.28538500	-1.07683100
C	-0.93089100	2.70980500	-0.52272200
C	-0.67399500	4.05733200	-0.07059200
H	-1.41164900	4.84227200	0.00297700
C	0.65721100	4.13141700	0.22567000
H	1.20412100	4.98453800	0.59920500
C	1.22570000	2.83168600	-0.02714400
C	2.60508700	2.54040000	-0.04899400
C	3.06590300	1.19732800	-0.11035300
C	2.39359900	0.02607500	0.32471200
H	1.71357600	-0.03419400	1.16593700
C	3.13474400	-1.08070700	-0.08066900
C	4.24594400	0.75791500	-0.76453100
H	5.06451300	1.31139000	-1.22157600

C	2.77154300	-2.45549600	0.00693800
C	-2.96971300	-3.64240300	-1.43707600
C	-2.68663100	-4.70650900	-2.30781600
H	-1.73010000	-4.72537000	-2.82159900
C	-3.61815000	-5.72111000	-2.52292700
H	-3.38143200	-6.53448700	-3.20414200
C	-4.85392800	-5.68749700	-1.87417800
H	-5.58094300	-6.47790300	-2.04169400
C	-5.14935200	-4.63146700	-1.01034700
H	-6.10680800	-4.59773300	-0.49704300
C	-4.21721100	-3.61810400	-0.79145800
H	-4.44389500	-2.79872700	-0.11558600
C	-3.24356200	3.31028900	-1.24873100
C	-3.05156600	4.43569700	-2.06455700
H	-2.10521900	4.55532400	-2.58351500
C	-4.06132100	5.38445100	-2.21708100
H	-3.89803500	6.24732600	-2.85763100
C	-5.27994800	5.22378900	-1.55446300
H	-6.06646700	5.96486200	-1.67111900
C	-5.48113500	4.10790500	-0.74051000
H	-6.42283600	3.97876600	-0.21367700
C	-4.47279100	3.15731900	-0.58756200
H	-4.61935900	2.29324100	0.05247900
C	3.60293800	3.62221300	-0.14787300
C	3.35860700	4.78641400	-0.90856000
H	2.41327700	4.89266200	-1.42840900
C	4.33767700	5.76275200	-1.04670900
H	4.13339100	6.64650300	-1.64585700
C	5.59421700	5.58829800	-0.45819400
H	6.36748800	6.34003200	-0.59251100
C	5.86473400	4.42784100	0.26391100
H	6.85251500	4.23933400	0.66858400
C	4.87594400	3.46264300	0.42974500
H	5.10843900	2.56369300	0.98721400
C	3.82892100	-3.46425700	0.24232800
C	4.73771600	-3.26249100	1.29520800
H	4.62290000	-2.38537300	1.92425600
C	5.76369900	-4.17341500	1.53104800
H	6.45763700	-4.00179100	2.34892100
C	5.90268800	-5.30044400	0.71740300
H	6.70892500	-6.00651600	0.89641900
C	5.00684600	-5.51048300	-0.33233700
H	5.11751200	-6.37762700	-0.97806900
C	3.97924200	-4.59959300	-0.56962200

H	3.30069400	-4.74447000	-1.40424700
C	5.32402800	-1.33069800	-1.45161000
H	5.71098400	-2.12955900	-0.82319900
H	6.13276500	-0.62226900	-1.66540300
H	4.90672400	-1.75993600	-2.36805600
O	-0.57400600	-0.07056800	1.82112600
C	-1.87539500	0.44345900	2.03083800
C	-2.89019200	-0.69778700	2.20927400
H	-2.15737200	1.00648700	1.14107700
H	-2.51175700	-1.60421900	1.74335200
C	-1.80258300	1.42644700	3.19667200
H	-1.06846400	2.19838600	2.96534400
H	-1.54568100	0.91891700	4.12411200
Cl	-3.38866100	2.28246600	3.47529600
H	-3.17283600	-0.88778900	3.23961200
Br	-4.59154800	-0.32130100	1.24910300
Cl	7.40702500	1.39842700	-0.92795600
O	1.16369000	-1.47684300	2.68008900
C	0.05608900	-1.19125400	3.04925500
O	-0.78405800	-1.34479900	3.89997300
Int3			
Zn	0.02597000	0.06917800	-0.10643100
N	1.76197400	0.01857800	-1.08242900
N	-0.21912400	2.06574200	-0.49925000
C	2.50707800	1.10448700	-1.44619200
C	2.49880300	-1.10949800	-1.34850500
C	0.89043400	2.85032800	-0.67816500
C	-1.25175600	2.90896800	-0.09936900
C	2.14851900	2.43825600	-1.19160000
C	3.73896800	0.64275100	-2.06538300
C	2.12533700	-2.40410500	-0.98086300
C	3.73465500	-0.71596800	-2.00156700
C	0.58360900	4.21644300	-0.29697800
C	-2.60251800	2.57225800	0.01515800
C	-0.72783500	4.24885700	0.06118200
C	3.17773900	3.48362800	-1.45273500
H	4.50078500	1.28213300	-2.48621400
C	0.84703700	-2.77330200	-0.46783100
C	3.15605600	-3.47052300	-1.12252400
H	4.49214300	-1.39750700	-2.35977500
H	1.28571200	5.03674700	-0.30196700
C	-3.03009900	1.21862800	-0.09089700
C	-3.61202500	3.62911300	0.25042400

H	-1.29264800	5.09555000	0.42121000
C	2.92147100	4.55177800	-2.32733800
C	4.43704600	3.41572100	-0.83289900
C	0.50359200	-4.11600400	-0.06265700
N	-0.25411400	-1.96339900	-0.36899000
C	2.94191300	-4.59591000	-1.93289600
C	4.37992300	-3.35358700	-0.44394800
C	-2.34341100	0.07455500	0.31064700
N	-4.19937200	0.78507600	-0.75736700
C	-3.70872200	4.77121300	-0.55974500
C	-4.52911200	3.46695600	1.30269000
C	3.88795500	5.52647000	-2.56990100
H	1.95654400	4.60508400	-2.82242000
C	5.40446400	4.38887200	-1.07909500
H	4.65059100	2.59527500	-0.15441600
C	-0.83580200	-4.12457500	0.19507400
H	1.19572200	-4.94029800	0.01702200
C	-1.32512200	-2.78876800	-0.03345700
C	3.92093900	-5.58014400	-2.05849700
H	2.00258800	-4.68753200	-2.46964900
C	5.35852700	-4.33833800	-0.57069600
H	4.54942600	-2.48419900	0.18364300
C	-3.07261600	-1.05793300	-0.13666500
H	-1.69163800	0.11346300	1.18042600
C	-5.19281000	1.59054300	-1.47344900
C	-4.22354100	-0.55661200	-0.79849500
C	-4.69423000	5.72746700	-0.32220000
H	-3.02297100	4.88647600	-1.39313500
C	-5.51230300	4.42381100	1.53927900
H	-4.45250800	2.58565900	1.93169200
C	5.13432900	5.44910300	-1.94580700
H	3.66974100	6.34295400	-3.25350200
H	6.36981200	4.32053800	-0.58441900
H	-1.43820800	-4.95412000	0.53407600
C	-2.68449700	-2.42354300	-0.08064500
C	5.13285300	-5.45550000	-1.37640400
H	3.73930300	-6.44246800	-2.69476000
H	6.29692200	-4.23435200	-0.03230000
H	-4.73798900	2.03286700	-2.36536100
H	-6.02073000	0.91898500	-1.72964300
H	-5.56568700	2.38345500	-0.82862600
H	-5.06408200	-1.06425600	-1.27170100
C	-5.59940900	5.55674500	0.72662400
H	-4.76476000	6.59979700	-0.96656300

H	-6.21313800	4.28376000	2.35728100
H	5.88869200	6.20845000	-2.13435700
C	-3.73722600	-3.44883200	-0.21496800
H	5.89556800	-6.22374800	-1.47297800
H	-6.37267700	6.29866600	0.90617800
C	-5.00533300	-3.23640200	0.35538400
C	-3.54694400	-4.60382300	-1.00376600
C	-6.04256300	-4.14217700	0.15457200
H	-5.19202100	-2.34183700	0.93682400
C	-4.57567100	-5.52168600	-1.17809000
H	-2.60225700	-4.74746900	-1.51581700
C	-5.82719100	-5.29528000	-0.59714800
H	-7.02329100	-3.91390300	0.55582400
H	-4.41268200	-6.39893500	-1.79904800
H	-6.63860300	-5.99964400	-0.75986100
C	2.01097500	-0.36273900	2.06031300
C	2.19365200	-1.17796400	3.33301400
C	2.99382200	0.81230200	2.01495000
H	2.22478700	-1.01040400	1.21133100
O	0.68085800	0.09588100	1.87573500
H	3.25200400	-1.40870400	3.46902300
H	1.80244800	-0.64185800	4.19428200
Cl	1.31843800	-2.76375800	3.22763100
H	2.67847300	1.54204500	1.27327300
H	3.15943900	1.28741100	2.97522400
Br	4.77452000	0.17072100	1.39835100
C	0.10432900	1.15758300	2.94296500
O	-1.05484900	1.39160200	2.65656400
O	0.94058000	1.47375500	3.77341500
Cl	-7.40491500	-1.06284600	-1.14027800
TS4			
Zn	0.17246300	-0.08714500	-0.44692600
N	0.53665800	-2.08952700	-0.58863100
N	-1.64767300	-0.27535000	-1.20885900
N	0.12012100	1.95983600	-0.58856700
N	4.19018400	-0.31266900	-1.20293000
C	1.67257800	-2.78544700	-0.18186400
C	1.28636900	-4.12570100	0.19780700
H	1.94993300	-4.86376100	0.62278000
C	-0.05083100	-4.24193400	-0.03040900
H	-0.67718200	-5.10352500	0.14653400
C	-0.51020900	-2.96993300	-0.55634700
C	-1.83160900	-2.71843000	-1.01052800

C	-2.31336400	-1.45749800	-1.39487600
C	-3.61657900	-1.17537900	-1.97373800
H	-4.34491600	-1.92119600	-2.25375900
C	-3.73904000	0.17465000	-2.05081500
H	-4.58711900	0.74248600	-2.40238700
C	-2.51718400	0.74696200	-1.51296200
C	-2.29656600	2.09068100	-1.20265400
C	-1.07725900	2.61730600	-0.68260700
C	-0.92169700	3.97326700	-0.20744700
H	-1.71941000	4.69530200	-0.11913700
C	0.39822900	4.14195500	0.10345400
H	0.87224700	5.02460600	0.50685500
C	1.06841500	2.89719100	-0.17569800
C	2.45828400	2.69054100	-0.19266900
C	2.98354200	1.37673000	-0.34597700
C	2.39460000	0.15049700	0.07579200
H	1.86187300	0.01114000	1.01531300
C	3.17271200	-0.89000700	-0.43950800
C	4.12105400	1.02822600	-1.10211300
H	4.81024800	1.66232700	-1.63529900
C	2.97754100	-2.28715700	-0.22863700
C	-2.79126500	-3.85745600	-1.04203700
C	-2.50932200	-5.02498400	-1.76936600
H	-1.57968000	-5.08728900	-2.32754800
C	-3.41015100	-6.08857300	-1.78904500
H	-3.17627200	-6.98278300	-2.36139500
C	-4.61217300	-6.00086200	-1.08409200
H	-5.31529400	-6.82979600	-1.09852500
C	-4.90513400	-4.84196500	-0.36311100
H	-5.83644900	-4.76290500	0.19131500
C	-4.00548100	-3.77691800	-0.33868100
H	-4.23999100	-2.87657400	0.22587800
C	-3.44122900	3.03274900	-1.35748800
C	-3.34159900	4.15932200	-2.18843400
H	-2.41799800	4.33378700	-2.73298400
C	-4.41250300	5.04140500	-2.32326100
H	-4.32067700	5.90632000	-2.97544400
C	-5.60044600	4.80983300	-1.62684500
H	-6.43559500	5.49824000	-1.72908100
C	-5.70845700	3.69166800	-0.79835200
H	-6.62573500	3.50660200	-0.24593800
C	-4.63973400	2.80649400	-0.66056500
H	-4.72394800	1.94179900	-0.00675000
C	3.41517500	3.81179200	-0.16812200

C	3.15646400	5.03767900	-0.81555500
H	2.23010500	5.16561700	-1.36465200
C	4.09910400	6.06058200	-0.79995100
H	3.88547400	6.99576500	-1.31141200
C	5.32742000	5.87577200	-0.15782900
H	6.06598300	6.67356600	-0.15701500
C	5.60939400	4.65540500	0.45636900
H	6.57044600	4.47565200	0.92820900
C	4.66567900	3.63119800	0.45623600
H	4.92551100	2.68108000	0.91542700
C	4.16236600	-3.14047800	-0.02720800
C	5.26070700	-2.61720600	0.68441200
H	5.23558900	-1.60026900	1.06768000
C	6.41138000	-3.37871700	0.86417300
H	7.24928900	-2.94057000	1.39764200
C	6.48891900	-4.67385900	0.34826700
H	7.38947500	-5.26610300	0.48877500
C	5.41154700	-5.19889900	-0.37031900
H	5.47475800	-6.19616800	-0.79834600
C	4.26215100	-4.43756600	-0.56544800
H	3.44776900	-4.82775800	-1.16712700
C	5.25092000	-0.97290300	-1.95585400
H	4.97169700	-2.00379400	-2.16151600
H	6.16619800	-0.91359100	-1.35680400
H	5.39119900	-0.43778400	-2.89863700
O	-0.50305900	-0.07045600	1.63010500
C	-1.84173600	0.38952100	1.91216100
C	-2.57296100	-0.75600200	2.57076200
H	-2.29092100	0.62316500	0.95595400
C	-1.68265600	1.64498400	2.76386200
H	-1.01673700	2.33757000	2.24934800
H	-1.27749400	1.39241800	3.74430900
Cl	-3.24407100	2.51546700	3.02930200
H	-3.11345500	-0.63447900	3.49274400
H	-2.57377000	-1.71743400	2.08820000
Cl	6.69671700	0.78626500	0.56042000
C	-0.01566100	-0.94790900	2.67050700
O	-0.93317300	-1.22336400	3.50554900
O	1.15365100	-1.26913800	2.59199800
Br	-4.75333200	-0.44893900	1.40201800
Int4			
Zn	-0.17770300	0.34642000	-0.48845500
N	-0.92134100	2.25790800	-0.44757900

N	1.48982500	0.88344000	-1.34461900
N	0.07292200	-1.64155400	-0.94064100
N	-4.34615800	0.04482600	-1.07361700
C	-2.12385400	2.73820500	0.06821200
C	-1.92193500	4.09263100	0.53920500
H	-2.66472600	4.68945800	1.04695200
C	-0.63551600	4.43199400	0.25656200
H	-0.13650000	5.36554300	0.46939900
C	-0.01897600	3.28675400	-0.38604500
C	1.30568600	3.28589300	-0.89002700
C	1.96725900	2.16168100	-1.40052400
C	3.29516200	2.14129000	-1.99387500
H	3.89787700	3.01460700	-2.19259800
C	3.62085100	0.84036900	-2.19653400
H	4.54256000	0.44276100	-2.59369500
C	2.50044800	0.04104500	-1.72463800
C	2.47164000	-1.34729900	-1.58836800
C	1.34217600	-2.10537500	-1.16594400
C	1.38541400	-3.52952900	-0.91960100
H	2.26886400	-4.14660900	-0.98924200
C	0.11797200	-3.92413000	-0.60100900
H	-0.21698000	-4.91754500	-0.34119800
C	-0.72268700	-2.75465500	-0.65290100
C	-2.12385800	-2.75666000	-0.57757400
C	-2.84653900	-1.53105600	-0.51669300
C	-2.42501600	-0.29518400	0.04093400
H	-1.79150000	-0.20811700	0.91447700
C	-3.37006600	0.67458100	-0.29155500
C	-4.07107100	-1.26823900	-1.16110200
H	-4.69777400	-1.93183100	-1.73437600
C	-3.34716900	2.06023100	0.05080600
C	2.09796600	4.54412400	-0.78403300
C	1.69741800	5.72005700	-1.43541900
H	0.79364100	5.70877900	-2.03851500
C	2.45126100	6.88783200	-1.32173700
H	2.13079800	7.79026900	-1.83667300
C	3.61833200	6.89349000	-0.55527500
H	4.20735500	7.80311300	-0.46621600
C	4.02406400	5.72631500	0.09528000
H	4.92833100	5.72351600	0.69832300
C	3.27291400	4.55619200	-0.01320400
H	3.57723500	3.64512800	0.50160700
C	3.75892500	-2.07229100	-1.78789200
C	3.88910900	-3.09966600	-2.73451100

H	3.03515400	-3.35959100	-3.35381500
C	5.09853200	-3.77655400	-2.88802300
H	5.18423100	-4.56739800	-3.62919900
C	6.19738400	-3.43358600	-2.09748300
H	7.14010100	-3.96215500	-2.21546700
C	6.07866500	-2.40711900	-1.15854800
H	6.92826800	-2.13272600	-0.53863200
C	4.87134800	-1.72663500	-1.00040400
H	4.77365300	-0.92345100	-0.26887600
C	-2.91294000	-4.00101400	-0.66529000
C	-2.54714500	-5.06921300	-1.50962000
H	-1.66256900	-4.97854900	-2.13053700
C	-3.33660600	-6.21218700	-1.59177000
H	-3.04196700	-7.02196100	-2.25467700
C	-4.51856500	-6.30566400	-0.85104100
H	-5.13841400	-7.19579700	-0.92536600
C	-4.91035600	-5.24050500	-0.03950400
H	-5.84239400	-5.27580300	0.51643900
C	-4.11955800	-4.09788600	0.05706700
H	-4.46762000	-3.27027500	0.67100200
C	-4.62178100	2.71514500	0.40535300
C	-5.57722600	1.98280600	1.13815800
H	-5.38476500	0.94949300	1.41859000
C	-6.80608400	2.55109600	1.46091600
H	-7.52999100	1.95315500	2.00627900
C	-7.10602600	3.85701400	1.06846800
H	-8.06716300	4.29800200	1.32026200
C	-6.17340900	4.58755700	0.32731300
H	-6.41012900	5.59433100	-0.00777300
C	-4.94710100	4.02047800	-0.01027300
H	-4.24699500	4.57123100	-0.62987400
C	-5.55832200	0.61416600	-1.64999200
H	-5.72924000	0.14673000	-2.62313600
H	-5.44004500	1.68772800	-1.77962700
H	-6.38885700	0.37966400	-0.97563500
O	0.20078400	0.39744100	1.62822900
C	2.72906600	-1.78890700	2.47222500
C	2.64270500	-0.85765700	3.69759600
H	3.67790700	-1.65563000	1.95219600
H	3.50038600	-0.18574100	3.73037800
C	2.38984100	-3.24937800	2.71785500
H	2.32487400	-3.78952900	1.77329500
H	1.45135200	-3.35769300	3.26531900
Cl	3.69030700	-4.02393300	3.71584900

H	2.47243800	-1.38250500	4.64000100
Br	3.99431200	1.07209200	1.38113300
O	1.69425500	-1.28295100	1.60409100
C	1.09335700	-0.23700100	2.17225600
O	1.47568800	-0.04367900	3.42674700
Cl	-6.42759900	-1.54880800	0.86300600
TS5			
Zn	-0.47969500	0.21506100	-0.43633100
N	-1.40422700	2.01901700	-0.23560700
N	1.12978500	0.97435600	-1.25553200
N	0.13717300	-1.70284600	-0.63823100
N	-4.53010500	-0.72880800	-0.38275200
C	-2.63229900	2.35341700	0.31202100
C	-2.61970900	3.75381000	0.68029200
H	-3.42426000	4.27041100	1.18268200
C	-1.40731600	4.25409800	0.32136200
H	-1.04221100	5.26146900	0.45318600
C	-0.65705200	3.17135200	-0.28368200
C	0.62172000	3.33810700	-0.86066300
C	1.41394200	2.30235400	-1.37669400
C	2.69321200	2.45456500	-2.04788900
H	3.15404900	3.39775500	-2.29892800
C	3.18787300	1.20654100	-2.24500600
H	4.13267100	0.93188000	-2.68855600
C	2.22221500	0.27424500	-1.68785200
C	2.39825600	-1.10166100	-1.52513900
C	1.42632300	-1.99493100	-1.00216700
C	1.67764500	-3.40427100	-0.78486800
H	2.62012900	-3.90140000	-0.95859600
C	0.51073700	-3.96023000	-0.35127700
H	0.32471800	-4.99228400	-0.09067500
C	-0.46795800	-2.90182700	-0.28712700
C	-1.83067400	-3.09295900	-0.03607800
C	-2.72572300	-2.00203700	0.09484400
C	-2.48082200	-0.68938000	0.57457500
H	-1.77222300	-0.42948500	1.35021800
C	-3.58604600	0.10377100	0.25825200
C	-3.98875500	-1.95521000	-0.53986700
H	-4.49854300	-2.72929100	-1.08764400
C	-3.74002700	1.50360700	0.44469900
C	1.22702900	4.70108700	-0.84849900
C	0.63123500	5.77493400	-1.52605700
H	-0.28735400	5.60534000	-2.08091400

C	1.21331500	7.04214000	-1.50053500
H	0.74277900	7.86366400	-2.03541200
C	2.40186100	7.25043500	-0.79811800
H	2.85746100	8.23765400	-0.77843700
C	3.00286200	6.18478400	-0.12472400
H	3.92749500	6.33792100	0.42577000
C	2.42455600	4.91578000	-0.14530200
H	2.88870400	4.08182300	0.38141200
C	3.75669900	-1.64296300	-1.81756900
C	3.96180900	-2.65320800	-2.76890300
H	3.11121900	-3.03506400	-3.32626600
C	5.24086300	-3.15575100	-3.00650100
H	5.38424800	-3.93542300	-3.75063500
C	6.33368800	-2.65221300	-2.29792600
H	7.33077400	-3.04487400	-2.48207700
C	6.13921100	-1.63818700	-1.35799600
H	6.98389600	-1.23599600	-0.80461800
C	4.86251200	-1.13121200	-1.11592900
H	4.70903500	-0.33015200	-0.39149300
C	-2.42043000	-4.44512800	-0.10937800
C	-2.11865300	-5.32068700	-1.16776200
H	-1.44814200	-4.98247200	-1.94958300
C	-2.71719900	-6.57617100	-1.24119600
H	-2.48257000	-7.23416600	-2.07366500
C	-3.63413200	-6.97930700	-0.26779600
H	-4.10100100	-7.95895200	-0.32910800
C	-3.96047300	-6.11039600	0.77534200
H	-4.67857600	-6.41299000	1.53327200
C	-3.36501000	-4.85317000	0.84878000
H	-3.61277800	-4.17452900	1.65953100
C	-5.07334500	2.05004000	0.77205300
C	-5.88737700	1.38173300	1.70569100
H	-5.50274000	0.48813400	2.18756700
C	-7.15857200	1.85539400	2.01756800
H	-7.76631800	1.32572200	2.74668500
C	-7.64960200	3.00968900	1.40327800
H	-8.64258800	3.37906200	1.64496400
C	-6.85746300	3.67986800	0.46881300
H	-7.23659200	4.56865200	-0.02887300
C	-5.58713300	3.20397700	0.15190000
H	-4.98966400	3.70413600	-0.60276900
C	-5.57376100	-0.28466800	-1.30567900
H	-5.12259500	-0.23327000	-2.30410800
H	-5.97427600	0.67507300	-0.99251100

H	-6.37668100	-1.02693500	-1.30356100
O	0.14219800	0.48391300	1.75343500
C	3.02472200	-1.26695000	2.46753700
C	2.87308600	-0.32857500	3.67948900
H	3.92383300	-1.02339300	1.90115900
H	3.62106400	0.46406000	3.64376900
C	2.88987000	-2.75405200	2.75219600
H	2.85371700	-3.31904900	1.82059000
H	1.99755000	-2.96979000	3.34357600
Cl	4.31931000	-3.33969800	3.70444200
H	2.84668300	-0.84984300	4.63927600
O	1.89440900	-0.92451000	1.64457400
C	1.15389700	0.01391500	2.24132500
O	1.58097500	0.28846400	3.47295600
Br	3.89797200	1.68717100	1.26016800
Cl	-3.00494200	-1.50137200	-3.12827000
P1			
Zn	0.66103900	0.04676300	-1.16387900
N	0.48864300	-1.96967600	-0.58450200
N	-1.32489700	0.15663500	-1.31499900
N	0.71383400	2.01970200	-0.41693800
N	4.40898300	-0.83926000	-0.74223500
C	1.44247200	-2.86410400	-0.11349700
C	0.80695600	-4.14073500	0.16723900
H	1.29652400	-4.99177600	0.61808600
C	-0.49674600	-4.02081400	-0.18564100
H	-1.27861900	-4.76088100	-0.10414500
C	-0.67902200	-2.66909100	-0.69943300
C	-1.89836000	-2.22003500	-1.26220400
C	-2.15820700	-0.88777000	-1.60444300
C	-3.39946700	-0.37528700	-2.16423100
H	-4.23362600	-0.97924700	-2.48514300
C	-3.32777500	0.97604800	-2.11107100
H	-4.09143500	1.68818500	-2.38150500
C	-2.04019100	1.30912300	-1.51924700
C	-1.63362900	2.56868200	-1.08568200
C	-0.37071100	2.84513900	-0.48809100
C	-0.05377200	4.13587000	0.09996700
H	-0.75802900	4.94239100	0.23577200
C	1.25688300	4.10195800	0.45044700
H	1.83033900	4.86659700	0.95381500
C	1.75498900	2.78788300	0.10334900
C	3.08262100	2.38987200	0.21332600

C	3.43535500	1.00672000	0.08785500
C	2.67492100	-0.11779400	0.50280700
H	1.85907500	-0.10538200	1.20918700
C	3.26941700	-1.25221900	-0.02821800
C	4.49631400	0.50943000	-0.67865400
H	5.22937300	1.04939500	-1.25952200
C	2.80300500	-2.60670800	0.02204100
C	-3.01119600	-3.20218300	-1.40380200
C	-2.86477700	-4.35125000	-2.19648900
H	-1.93057700	-4.51037200	-2.72806100
C	-3.90456200	-5.27294100	-2.31248400
H	-3.77704700	-6.15553100	-2.93480600
C	-5.10823400	-5.05592300	-1.63847700
H	-5.92051000	-5.77332700	-1.72869900
C	-5.26311200	-3.91266600	-0.85223300
H	-6.19467800	-3.73182600	-0.32265900
C	-4.22561400	-2.98849400	-0.72948500
H	-4.35931400	-2.09674200	-0.11509400
C	-2.62090200	3.68285600	-1.17398100
C	-2.33310600	4.84738200	-1.90267500
H	-1.37961100	4.92690600	-2.41744200
C	-3.25966200	5.88636700	-1.97613300
H	-3.02493200	6.77976300	-2.54988600
C	-4.48828400	5.77401700	-1.32132300
H	-5.21217300	6.58357400	-1.37848300
C	-4.78180000	4.61735000	-0.59703900
H	-5.73452800	4.51736600	-0.08378000
C	-3.85827500	3.57477700	-0.51795900
H	-4.09745200	2.67150600	0.04564800
C	4.17062900	3.36845400	0.37137600
C	4.17362500	4.59847700	-0.31500100
H	3.35252200	4.82720600	-0.98529900
C	5.23037500	5.49336600	-0.17096800
H	5.21539900	6.43306600	-0.71690400
C	6.31466200	5.17909200	0.65135500
H	7.13982400	5.87799600	0.75994600
C	6.33539900	3.95574100	1.32464800
H	7.17381200	3.70207000	1.96824500
C	5.28021300	3.05903100	1.18200200
H	5.28737600	2.11499100	1.71673100
C	3.77795300	-3.69096100	0.23696100
C	4.84957500	-3.49792700	1.13068600
H	4.91307900	-2.56005900	1.67394200
C	5.80397400	-4.49111500	1.33011000

H	6.61673900	-4.32279300	2.03195500
C	5.71504000	-5.70231600	0.63943400
H	6.46127900	-6.47704000	0.79346400
C	4.66477600	-5.90484400	-0.25845100
H	4.59691600	-6.83551100	-0.81580700
C	3.71167200	-4.91023300	-0.46391500
H	2.92191800	-5.05352000	-1.19349700
C	5.05584900	-1.61222200	-1.79727500
H	5.33449600	-2.59941500	-1.43163600
H	5.95503400	-1.07729500	-2.11107700
H	4.36684800	-1.69711100	-2.64324500
O	0.91550700	1.62483900	2.91591000
C	-2.23994600	0.26269300	3.17228700
C	-1.67189400	-0.42714500	1.93850300
H	-3.22656900	0.67682000	2.95480400
H	-2.11055100	-0.01923000	1.03022700
C	-2.21783200	-0.56899600	4.44916200
H	-2.49014400	0.04579000	5.30797900
H	-1.22864900	-1.00444800	4.61389300
Cl	-3.39453400	-1.94018400	4.36980300
H	-1.76140600	-1.51239100	1.94475000
Br	-4.85655000	0.30368900	0.98071000
O	-1.28504900	1.33894200	3.38790100
C	-0.11552400	1.02052700	2.77741700
O	-0.26111500	-0.08340100	2.01192000
Cl	1.97937100	-0.02035000	-3.05760200