

Supporting Information

**Computational Insight into Asymmetric Cross-Aldol  
Carboligation in Choline Chloride/Ethylene Glycol Deep  
Eutectic Solvent**

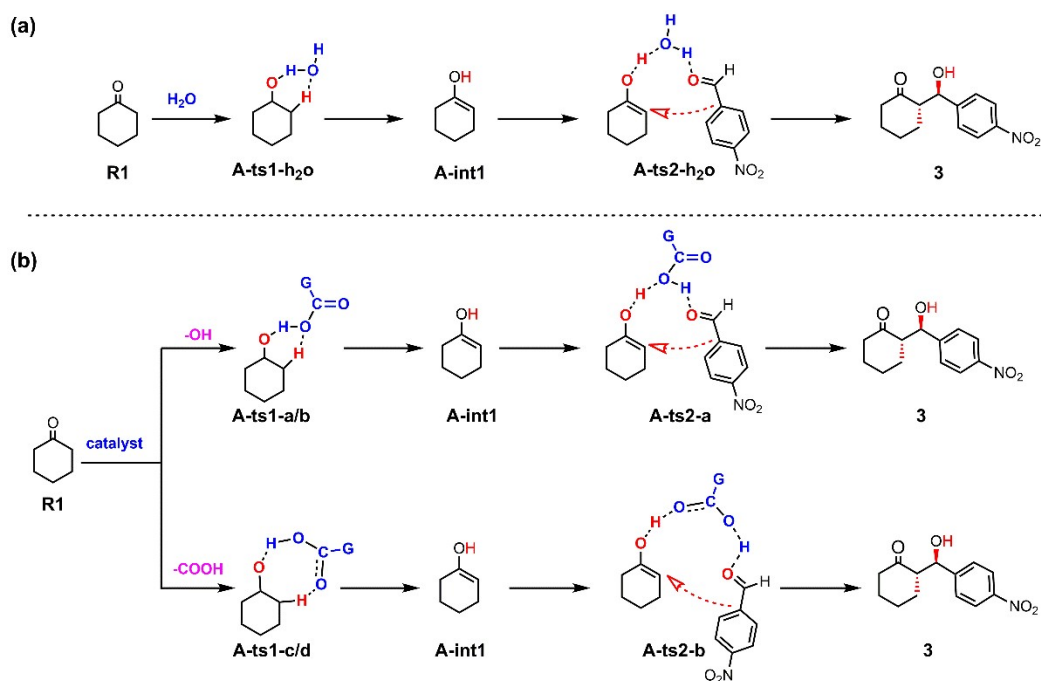
Yan Zhang<sup>1</sup>, Yong Sheng Yang<sup>2</sup>, Shi Jia Zhao<sup>1</sup>, Cui Wei<sup>1</sup>,

Ning Zou<sup>1\*</sup>, Ying Xue<sup>3\*</sup> and Wen Jun Zhou<sup>1\*</sup>

<sup>1\*</sup>College of Chemistry and Chemical Engineering, Neijiang Normal  
University, Neijiang 641112  
People's Republic of China

<sup>2</sup>School of Pharmacy and Institute of Pharmacy,  
North Sichuan Medical College, Nanchong 637100,  
People's Republic of China

<sup>3\*</sup>College of Chemistry,  
Key Lab of Green Chemistry and Technology in Ministry of Education,  
Sichuan University, Chengdu 610064,  
People's Republic of China



Scheme S1. The reaction mechanism involved  $\text{H}_2\text{O}$  and catalyst.

### The interaction energy analysis of A-ts1-b and A-ts1-c

The interaction energy ( $E_{\text{int}}$ ) reported in the paper is valued by following equation, the transition state is divided into two fragments, and the two distorted parts to form the transition state would release energy. Here, the BSSE correction is also adopt to calculate the  $E_{\text{int-BSSE}}$ , and the results is suggested in Figure S1. The  $E_{\text{int-BSSE}}$  for A-ts1-b, A-ts1-b is 109.1 kcal/mol and 66.3 kcal/mol respectively, there is slight difference with the  $E_{\text{int}}$  valued by the equation. This result suggests that both two methods could apply to measure the interaction energy.

$$E_{\text{int}} = E_{A-B}^{\ddagger} - E_{\text{dis-A}}^{\ddagger} - E_{\text{dis-B}}^{\ddagger}$$

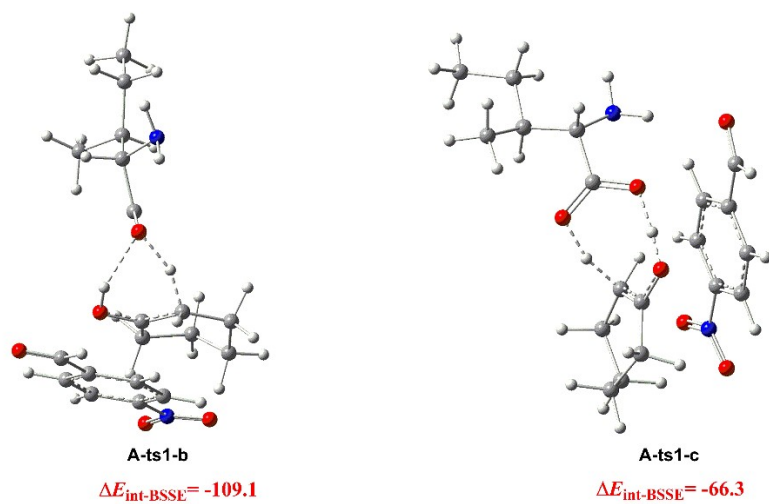


Figure S1. The interaction energy with BSSE correction for A-ts1-b and A-ts1-c.

## Coordinates

R1

0 1

C	-1.00522300	-1.25965000	-0.28935800
C	0.38845500	-1.28181800	0.35850800
C	0.38845500	1.28181800	0.35850800
C	-1.00522300	1.25965000	-0.28935800
C	-1.77899500	0.00000000	0.10476500
H	0.27265000	-1.35936400	1.44860100
H	0.99225300	-2.12585100	0.01912300
H	-0.89423800	-1.28699500	-1.38052600
H	-1.55835500	-2.15970000	-0.00496100
H	0.27265000	1.35936400	1.44860100
H	0.99225300	2.12585100	0.01912300
H	-1.55835500	2.15970000	-0.00496100
H	-0.89423800	1.28699500	-1.38052600
H	-1.94613400	0.00000000	1.19049800
H	-2.76574100	0.00000000	-0.36861400
C	1.15071800	0.00000000	0.07052000
O	2.28226700	0.00000000	-0.35848300

R2

0 1

C	0.47677200	1.27982000	0.00005600
C	1.03738800	0.01059200	-0.00000600
C	0.28222300	-1.15744300	-0.00005500
C	-1.09955100	-1.04194900	-0.00004000
C	-1.69267000	0.22355700	0.00002200
C	-0.90973200	1.37772300	0.00006900
H	1.12103100	2.14968300	0.00009100
H	0.78410000	-2.11673000	-0.00010300
H	-1.74077500	-1.91703200	-0.00007600
H	-1.38610900	2.35427600	0.00011700
N	2.50911400	-0.10435200	-0.00002100
O	2.98230400	-1.22436900	-0.00008300
O	3.15096700	0.92871700	0.00002900
C	-3.17732900	0.33708200	0.00003600
O	-3.91740100	-0.61559900	-0.00000200
H	-3.57160400	1.37397200	0.00008600

## Catalyst

0 1

C	3.30936500	0.04849800	0.34878800
C	1.98039700	0.69329500	-0.03978100
H	4.11341200	0.78853800	0.35568900
H	3.24800100	-0.38952800	1.35040900
H	3.59538400	-0.74458700	-0.34642200
C	0.77413100	-0.24260900	0.11223600
H	1.82031900	1.57456800	0.58955800
H	2.03654800	1.04427800	-1.08172900
C	-0.51341300	0.44941100	-0.35690500
H	0.64667800	-0.47107700	1.17792000
H	-0.54422500	0.40977200	-1.46304600
C	0.97394300	-1.55030000	-0.65736200
H	0.07556100	-2.16894700	-0.62263100
H	1.21816700	-1.34330600	-1.70674000
H	1.79235200	-2.13622400	-0.23345800
C	-1.74366700	-0.31205700	0.11968600
O	-1.76313300	-1.33182700	0.75852900
O	-2.87602400	0.31371100	-0.26834800
H	-3.61451600	-0.20353900	0.08752900
N	-0.63825100	1.81125700	0.16787400
H	0.05634600	2.40524700	-0.27358700
H	-1.54754900	2.18349800	-0.09003400

## [ChCl/2 EG]

0 1

C	2.10120300	-0.21205000	-1.79308700
C	3.17873300	-0.67217500	-0.81833600
H	2.34038000	-0.56331000	-2.80410300
H	1.15530200	-0.66517900	-1.48612300
H	4.15211300	-0.25756100	-1.11530700
H	2.95070500	-0.30066200	0.19054500
O	3.28030900	-2.07050800	-0.85994600
H	2.51952300	-2.40993700	-0.35634300
O	1.90329200	1.20712700	-1.79052000
H	2.73192000	1.62103500	-2.05959600
C	1.65973100	2.36356700	1.15112000
C	1.09223200	1.02725600	1.59345100
H	1.72902100	3.07110900	1.98154300
H	2.67055500	2.20658800	0.75281800
H	0.14842200	1.20969600	2.14008600
H	0.84695300	0.46640500	0.68098500
O	2.00966700	0.30825300	2.36877500

H	1.77572900	-0.62863300	2.25280700
O	0.79669100	2.92342700	0.16887300
H	1.02613200	2.45606800	-0.65153500
N	-2.45180700	0.66678700	-0.39078800
C	-2.25702300	-0.14878400	0.88049600
H	-1.18480300	-0.15077800	1.08062000
H	-2.78468100	0.38589500	1.67606400
C	-2.76283600	-1.58878800	0.79756700
H	-3.85806900	-1.61216000	0.78569500
H	-2.42976400	-2.06582700	1.72807900
O	-2.30891300	-2.27592100	-0.33420800
H	-1.36990100	-2.50684000	-0.14575000
Cl	0.51704300	-2.15586100	0.80201800
C	-2.39419800	2.12109300	-0.04193500
H	-2.51122800	2.69759700	-0.96132300
H	-3.20690600	2.34925800	0.64853000
H	-1.41748500	2.34419400	0.39743800
C	-1.34134900	0.38702200	-1.36434000
H	-1.28713900	-0.68797300	-1.51806000
H	-1.56436600	0.91715000	-2.29219400
H	-0.41625600	0.76966800	-0.93452500
C	-3.76028700	0.34958200	-1.03247900
H	-4.55734700	0.50390000	-0.30326700
H	-3.89749500	1.02143900	-1.88059100
H	-3.73400000	-0.68839300	-1.36383000

#### A-tsl-self

0 1

C	-1.01245900	-1.34873500	-0.20459400
C	0.47045900	-1.21247700	0.09821900
C	0.31711200	1.37255400	0.20013800
C	-1.12501700	1.18459400	-0.30580500
C	-1.76652700	-0.09069100	0.25350000
H	0.85271300	-1.79849300	0.93694800
H	1.86894900	-1.17623600	-0.38776900
H	-1.17449100	-1.48503300	-1.28157500
H	-1.42979500	-2.23369300	0.28338000
H	0.30388900	1.63174400	1.26742600
H	0.84572300	2.16818500	-0.32969800
H	-1.71705500	2.06451000	-0.03907700
H	-1.11496800	1.12946900	-1.40130600
H	-1.76065100	-0.04402000	1.35028000
H	-2.81429700	-0.14019500	-0.06040200
C	1.05442800	0.07903800	0.08239600

O	2.31400100	-0.00274100	-0.13516700
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A-ts1-cata

0 1

C	-3.07157500	-1.43506100	-1.04759500
C	-2.29071100	-0.14267600	-0.86625800
C	-3.75115800	0.50728600	1.12217500
C	-4.64206900	-0.67844100	0.75363800
C	-3.79528900	-1.84146600	0.23663600
H	-1.11274500	-0.32340500	-0.27574700
H	-1.86363500	0.29484800	-1.77116500
H	-3.80950100	-1.31854900	-1.85195300
H	-2.39003500	-2.23053000	-1.36504700
H	-3.19763300	0.30331600	2.04874800
H	-4.31666700	1.42608400	1.30363600
H	-5.23379900	-0.97609000	1.62360100
H	-5.35139300	-0.37591700	-0.02646900
H	-3.05950400	-2.12389300	1.00087500
H	-4.42117000	-2.71932000	0.05228700
C	-2.71345600	0.81567100	0.07865900
O	-2.12792100	1.94881200	0.20917900
C	5.17422800	-1.41082800	0.95246000
C	4.42348000	-0.20744800	0.38586000
H	6.19589100	-1.13832300	1.22916000
H	4.67414700	-1.79030100	1.84980600
H	5.23424500	-2.23045300	0.23190600
C	2.93023600	-0.46892800	0.14755000
H	4.52177100	0.63327000	1.07911200
H	4.89108100	0.09924100	-0.56264700
C	2.25146900	0.77082800	-0.45835100
H	2.45754600	-0.65902300	1.11963900
H	2.44339200	0.75921000	-1.55014700
C	2.71791200	-1.68481500	-0.75791100
H	1.66559400	-1.80055400	-1.02085900
H	3.30036800	-1.57682300	-1.68166100
H	3.04054800	-2.60592100	-0.26680000
C	0.72609200	0.74225900	-0.33412700
O	0.15262800	-0.31036400	0.07165400
O	0.12425700	1.80119800	-0.67136700
H	-1.13867700	1.93797700	-0.27308700
N	2.68799500	2.01404300	0.17603700
H	3.62850700	2.24088000	-0.13040200
H	2.07903800	2.76052200	-0.14718900

A-tsl-h<sub>2</sub>O

0 1

C	-0.95770000	-1.50735300	-0.36146800
C	0.36376000	-0.77685600	-0.52094600
C	-0.72609900	1.43216400	0.17653200
C	-2.06148700	0.70414000	0.03514600
C	-1.93027600	-0.73549700	0.53196600
H	1.54250500	-0.99635100	0.28880500
H	0.99968500	-1.12803800	-1.33734900
H	-1.43126200	-1.65611900	-1.34174200
H	-0.78813300	-2.50928200	0.04823400
H	-0.53338400	1.69038500	1.22601200
H	-0.70189100	2.37865200	-0.37300700
H	-2.83958200	1.24446200	0.58235200
H	-2.36399800	0.68993900	-1.01932200
H	-1.55957000	-0.72836600	1.56591300
H	-2.90517300	-1.23201600	0.54367300
C	0.45494100	0.61715500	-0.29730000
O	1.58081300	1.22149300	-0.33068500
H	2.40423300	0.30930200	0.01023300
O	2.71884300	-0.70744200	0.45924200
H	2.92049600	-0.57749700	1.39415600

## A-tsl-a

0 1

C	-2.72497900	0.95267100	-0.94957200
C	-2.50458900	0.46319600	0.47389600
C	-4.25827800	-1.38201800	0.16222800
C	-4.63673300	-0.67086900	-1.13624100
C	-3.38034000	-0.12437600	-1.81802300
H	-1.40655800	-0.11457200	0.75698900
H	-2.34062900	1.24575100	1.22112900
H	-3.34912800	1.85380900	-0.93762400
H	-1.76440500	1.25080200	-1.38589900
H	-3.73682800	-2.33091900	-0.03110700
H	-5.11525100	-1.62130100	0.80078800
H	-5.16537800	-1.36914800	-1.78989300
H	-5.32580600	0.15518700	-0.92320700
H	-2.67592100	-0.95129300	-1.97761200
H	-3.62393000	0.29034100	-2.79973100
C	-3.27782700	-0.60908300	0.96811800
O	-3.04436300	-1.08502000	2.15667300
C	1.74790300	2.80397200	-0.78970700
C	0.68348800	2.69764000	0.10001600



C	0.73212000	1.92955900	1.25532900
C	1.89301700	1.21801600	1.52283700
C	2.97723900	1.30603400	0.65022700
C	2.90915300	2.10186400	-0.49719800
H	1.64497000	3.41097600	-1.68003900
H	-0.12841100	1.86943600	1.90744200
H	1.95795300	0.56782000	2.38797700
H	3.76064100	2.15341500	-1.17024700
N	-0.56858100	3.40575500	-0.21790200
O	-1.45229600	3.39820100	0.62280700
O	-0.65251000	3.94349200	-1.30485800
C	4.20442700	0.50966600	0.93157600
O	4.30821700	-0.23785200	1.87306300
H	5.03244900	0.64164400	0.20500300
C	3.04965700	-2.21880300	-2.90280900
C	2.77185300	-2.08179200	-1.40796400
H	4.12324900	-2.28124900	-3.09986200
H	2.58529000	-3.12744100	-3.29834700
H	2.65924600	-1.37079400	-3.47347200
C	1.28283500	-2.02759400	-1.05388200
H	3.21523300	-2.92526900	-0.86990600
H	3.25073400	-1.16758800	-1.02587600
C	1.10055900	-2.31179100	0.45518700
H	0.76810900	-2.84703000	-1.57694200
H	1.81493400	-1.70196700	1.02245100
C	0.63596500	-0.70856200	-1.47993800
H	-0.45203400	-0.75309400	-1.36620500
H	1.00728400	0.11915500	-0.86772400
H	0.84823200	-0.48058800	-2.52803400
C	-0.31939500	-1.91038600	0.85413700
O	-1.27031000	-2.59084300	0.47038300
O	-0.44628200	-0.78855300	1.51360700
H	-2.09741600	-0.88382900	2.37856700
N	1.37587600	-3.72571000	0.69690100
H	1.45502100	-3.89182600	1.69635600
H	0.55118500	-4.24020800	0.38933300

A-tsl-b

0 1

C	-0.20181400	-2.50916800	1.57877600
C	-0.33319700	-1.20946300	0.78925100
C	0.24758100	-2.42339300	-1.40608800
C	0.69581100	-3.57555000	-0.50590600
C	-0.26717400	-3.73913500	0.67080500

H	-1.14497900	-0.53721400	1.08648300
H	0.54072900	-0.32957600	0.94143800
H	0.75316300	-2.50672900	2.11572300
H	-0.99447100	-2.55480200	2.32975400
H	-0.63540100	-2.70624900	-1.99509400
H	1.02967800	-2.09756400	-2.09636100
H	0.75726100	-4.49177300	-1.09829800
H	1.70169600	-3.34934700	-0.13503000
H	-1.29180100	-3.85895400	0.29630600
H	-0.02083200	-4.63650200	1.24527100
C	-0.14974700	-1.23095600	-0.61538200
O	-0.23789400	-0.11624200	-1.28602200
C	-4.11812500	0.18207300	1.17427200
C	-3.60398500	-0.34528700	-0.00323100
C	-3.36443900	0.41587500	-1.14354400
C	-3.65552100	1.77110600	-1.09307300
C	-4.17564400	2.32987200	0.07731800
C	-4.40644200	1.54112000	1.20443500
H	-4.27730000	-0.46408200	2.02831000
H	-2.95129200	-0.05353900	-2.02719400
H	-3.48637100	2.41706700	-1.94806100
H	-4.81026100	1.99123200	2.10693800
N	-3.27486400	-1.78068900	-0.03690000
O	-2.88967200	-2.24397800	-1.09670900
O	-3.38852800	-2.41229100	0.99558800
C	-4.48439200	3.78784500	0.11744600
O	-4.31713100	4.52514700	-0.82176500
H	-4.88553600	4.16034000	1.08178400
C	7.44569200	0.94223500	0.00579800
C	6.09791600	1.50327800	0.45494000
H	8.26983700	1.43605800	0.52744900
H	7.50777300	-0.12996900	0.22025700
H	7.60542100	1.07684300	-1.06715900
C	4.89163000	0.73510400	-0.09994600
H	6.04878700	1.48202300	1.54809900
H	6.02351900	2.55876600	0.14976400
C	3.57547900	1.37443200	0.36394900
H	4.91399400	-0.28456100	0.30574700
H	3.37551200	2.24967500	-0.28636000
C	4.92942100	0.65964900	-1.62790700
H	4.01797700	0.20009700	-2.01255100
H	5.02773500	1.66510900	-2.05716200
H	5.77707300	0.06456400	-1.97705000
C	2.37348500	0.43818300	0.17105900

O	2.46559500	-0.64751900	-0.40212900
O	1.25906400	0.89541300	0.67279000
H	-0.02891900	0.62550200	-0.66110400
N	3.59816600	1.73095500	1.78488700
H	4.15769200	2.56771500	1.91781500
H	2.64551500	1.96285000	2.05251300

A-ts1-c

01

C	-1.67914300	1.97536100	-1.08549300
C	-0.92731700	1.30917600	0.06267700
C	-2.34262200	2.55365000	1.78459300
C	-2.80958200	3.42159700	0.61567300
C	-3.01638600	2.56388600	-0.63305400
H	-0.61034500	0.27957400	-0.11399900
H	0.34519400	1.66140000	0.21598000
H	-1.06875900	2.77249500	-1.52657200
H	-1.83791700	1.24236600	-1.88383600
H	-3.18454800	1.97378600	2.18896800
H	-1.94791600	3.13741600	2.62162800
H	-3.72815400	3.94442100	0.89503500
H	-2.05622000	4.18988900	0.40371200
H	-3.72000000	1.75057500	-0.40718800
H	-3.46134400	3.15494000	-1.43815000
C	-1.31714900	1.52830900	1.39714800
O	-0.77825800	0.89488100	2.37944300
C	-3.03874100	-1.32867700	0.41556700
C	-2.70048500	-1.36742100	-0.92972100
C	-1.48221200	-1.85332400	-1.39600100
C	-0.56350700	-2.32434100	-0.46737200
C	-0.87964400	-2.29536500	0.89531000
C	-2.10621000	-1.79776000	1.33436500
H	-4.00182900	-0.93458600	0.71558300
H	-1.27221500	-1.83866600	-2.45818400
H	0.41647700	-2.67785100	-0.77306300
H	-2.32533100	-1.76396100	2.39782400
N	-3.66312800	-0.82499600	-1.90592400
O	-3.32190100	-0.79282700	-3.07314700
O	-4.73555700	-0.43444300	-1.48122800
C	0.10054700	-2.80172500	1.89574900
O	1.10563400	-3.40240800	1.60001400
H	-0.16325900	-2.60585100	2.95415000
C	6.06532100	0.60578300	-2.23800500
C	5.19057400	-0.19119000	-1.27213900

H	6.74379700	-0.05402700	-2.78454400
H	5.44799400	1.13462400	-2.97180200
H	6.67422400	1.34849300	-1.71662800
C	4.08608200	0.64288100	-0.60888200
H	4.72523200	-1.01617700	-1.82129200
H	5.82395600	-0.63911100	-0.49130700
C	3.29857000	-0.19526900	0.40766200
H	3.38056200	0.95840700	-1.38752600
H	3.89601400	-0.26034200	1.33673000
C	4.65958100	1.88598100	0.07605300
H	3.88879100	2.41530400	0.63897000
H	5.46505000	1.60436500	0.76569400
H	5.07414100	2.58547600	-0.65350500
C	1.97260700	0.45527200	0.80772900
O	1.64495100	1.57437700	0.31535500
O	1.24490100	-0.21362700	1.59792600
H	0.11063200	0.35677700	2.04504800
N	2.92986400	-1.51479200	-0.11697200
H	3.77387600	-2.05871200	-0.26971100
H	2.40487200	-2.01109300	0.60021400

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0 1

C	-1.81872900	0.94336200	-2.26284400
C	-0.72077900	1.81709500	-1.67206600
C	-2.34834900	2.84950000	-0.01355400
C	-3.46632900	2.23966500	-0.85943500
C	-3.05847100	0.85734600	-1.36811800
H	0.12035600	1.18864300	-0.85089500
H	0.07665700	2.10673700	-2.36021500
H	-2.11204900	1.34682400	-3.24009900
H	-1.42349600	-0.06210000	-2.45080600
H	-2.22670700	2.30574500	0.93524100
H	-2.53842100	3.89174300	0.25786900
H	-4.38435800	2.18234400	-0.26771500
H	-3.67726600	2.89666800	-1.71230200
H	-2.85259900	0.21102100	-0.50805300
H	-3.87974200	0.39558800	-1.92441100
C	-1.01930100	2.79726700	-0.70724000
O	-0.12936100	3.60825300	-0.25394100
C	-2.88847000	-2.53112700	0.54986400
C	-1.66023700	-2.35657000	-0.07415100
C	-0.73538400	-1.39435100	0.31202500
C	-1.07332400	-0.54402100	1.35683500

C	-2.30878500	-0.68671800	1.99626700
C	-3.20489600	-1.68370400	1.60507200
H	-3.56157700	-3.30505500	0.20345900
H	0.21315000	-1.30006200	-0.20188400
H	-0.38720200	0.23682000	1.67072100
H	-4.15889700	-1.78396400	2.11553900
N	-1.32716400	-3.22458800	-1.22027800
O	-0.32547100	-2.95302200	-1.85524100
O	-2.08051600	-4.14898000	-1.46036500
C	-2.69776200	0.26152700	3.07379100
O	-2.08147400	1.26824600	3.32976100
H	-3.61936600	-0.00464900	3.63115400
C	4.98440000	-2.46282000	1.18781200
C	4.93063400	-0.99585400	0.76639400
H	5.93064000	-2.69258800	1.68398100
H	4.17450000	-2.69283200	1.88818100
H	4.88679900	-3.13569300	0.33204700
C	3.56457500	-0.56709900	0.21627600
H	5.17092600	-0.36675400	1.62898300
H	5.70112200	-0.80731900	0.00301700
C	3.58873400	0.90435700	-0.22626600
H	2.83066400	-0.65128200	1.02868000
H	4.03658500	0.94601300	-1.23876900
C	3.13092800	-1.46081500	-0.95035800
H	2.25389800	-1.05920900	-1.46285200
H	3.94183700	-1.54839800	-1.68401300
H	2.87906500	-2.46937400	-0.61281400
C	2.18781900	1.49539100	-0.39248200
O	1.17792600	0.73768600	-0.23041500
O	2.11399200	2.71354300	-0.68926100
H	0.86127600	3.29667000	-0.52119400
N	4.27571500	1.77084900	0.73108100
H	5.27710500	1.61508100	0.67420300
H	4.10883600	2.73515700	0.45607300

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0 1

C	1.84986200	0.91460300	0.66900400
C	1.84961400	-0.20327100	-0.36096200
C	4.04461800	-1.13166900	0.58826500
C	4.15132400	0.18756100	1.35011600
C	2.77161900	0.61125800	1.85216900
H	0.87896900	-1.22809900	-0.47067900
H	1.52094200	0.09793900	-1.35962500

H	2.16596900	1.85657400	0.20056200
H	0.83257800	1.08888800	1.04232600
H	3.88528000	-1.96921600	1.28014600
H	4.95369300	-1.37383000	0.02850700
H	4.86009900	0.08312500	2.17657000
H	4.54540300	0.96642500	0.68594800
H	2.34508600	-0.20035700	2.45704800
H	2.84623600	1.48916600	2.50032200
C	2.90258500	-1.15055800	-0.39603100
O	2.85216300	-2.15699500	-1.18549900
C	-2.31115000	1.66406500	0.64775700
C	-1.47887500	1.35289700	-0.42057100
C	-1.48922000	0.12027700	-1.06209700
C	-2.36514100	-0.85017200	-0.59692300
C	-3.21702100	-0.56566800	0.47211700
C	-3.19423500	0.68718100	1.08843500
H	-2.24892600	2.64186400	1.10796300
H	-0.81315100	-0.07891700	-1.88308700
H	-2.39191500	-1.83484000	-1.05094600
H	-3.86287100	0.89304800	1.91979700
N	-0.51515000	2.37339300	-0.87273300
O	0.16757000	2.11060200	-1.84561700
O	-0.45249000	3.40792300	-0.23630400
C	-4.14720200	-1.61499800	0.97048800
O	-4.19538300	-2.73315500	0.51927800
H	-4.80769600	-1.30207200	1.80540400
O	0.48212100	-2.20501200	-1.14947400
H	1.66152700	-2.32083200	-1.37330700
H	0.20231400	-2.93855400	-0.58749100

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0 1

C	2.73973900	-0.11414000	1.59300900
C	1.60496100	0.68500000	0.96529400
C	2.92495300	0.95856800	-1.20718600
C	4.13041000	0.45017300	-0.41523700
C	3.70464800	-0.66405800	0.53992600
H	0.59556800	0.38200400	1.25689400
H	1.11509500	1.98107200	1.39705700
H	3.30335800	0.50655500	2.30225400
H	2.32004400	-0.94239300	2.17167800
H	2.64178000	0.22304300	-1.97100900
H	3.12841400	1.89558900	-1.73401200
H	4.90307900	0.10262400	-1.10723100

H	4.56860400	1.27431800	0.16273800
H	3.20419900	-1.45788900	-0.02825700
H	4.57847900	-1.10931000	1.02586900
C	1.68872800	1.15465000	-0.36546100
O	0.74769300	1.85879400	-0.87814300
C	-1.62829000	-1.68951800	0.82647700
C	-0.87739300	-1.26161300	-0.26126700
C	-1.31618300	-0.30061100	-1.16555800
C	-2.56981200	0.25770300	-0.96037100
C	-3.35078700	-0.15622800	0.12086400
C	-2.88386700	-1.12556800	1.00993100
H	-1.22296400	-2.43592300	1.49762900
H	-0.67135900	0.01307100	-1.97574600
H	-2.96042800	1.02151100	-1.62403900
H	-3.50326300	-1.43535700	1.84706500
N	0.46053700	-1.84634600	-0.45254400
O	1.03929400	-1.59989100	-1.49532100
O	0.90775400	-2.53858200	0.44302500
C	-4.69447900	0.44881100	0.33040600
O	-5.17096800	1.28540200	-0.39670600
H	-5.24631100	0.07473100	1.21745900
O	0.26147300	2.84076700	1.23449800
H	0.26220200	2.47197200	0.15491700
H	0.64202600	3.72786600	1.25075700

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0 1

C	-0.82066100	-1.07735900	1.91302600
C	-0.02691900	-1.00535400	0.62379500
C	-1.46126300	-2.82241000	-0.40898900
C	-1.98830800	-3.11238900	0.99721700
C	-2.16034700	-1.80624500	1.76992700
H	1.05396300	0.40589800	-1.65780000
H	0.99318400	-0.63792000	0.71715600
H	-0.20656700	-1.59325300	2.66216600
H	-0.97826600	-0.06704200	2.30816000
H	-2.22851100	-2.29301400	-0.99387700
H	-1.21073300	-3.72913800	-0.96550500
H	-2.93626300	-3.65227700	0.92944400
H	-1.28229100	-3.76591300	1.52334800
H	-2.88179000	-1.17329900	1.23968800
H	-2.57677400	-1.99936000	2.76261400
C	-0.24785800	-1.94534600	-0.37968000
O	0.51820800	-2.06328600	-1.42384000

C	7.60278300	1.22301600	1.29859000
C	6.73925800	0.62978600	0.18714500
H	8.64778600	1.29379700	0.98609500
H	7.26107000	2.23099700	1.55623300
H	7.57005800	0.61691200	2.20760800
C	5.23477200	0.67088400	0.48388800
H	6.92417900	1.18210400	-0.73941600
H	7.04282100	-0.41330700	0.00749600
C	4.43685000	0.01973500	-0.65360000
H	4.92059400	1.72098700	0.53642500
H	4.49067300	-1.08012700	-0.52157200
C	4.90617900	-0.01237000	1.81320600
H	3.82697500	-0.06126300	1.96813700
H	5.31219200	-1.03187400	1.83004900
H	5.33663300	0.53144700	2.65739800
C	2.94627000	0.36498000	-0.58580400
O	2.45070400	1.03782200	0.30846900
O	2.24887100	-0.13714400	-1.58043600
H	1.30299300	-1.42990200	-1.42099200
N	4.89762100	0.44832200	-1.97525700
H	5.78547400	0.00467600	-2.18803300
H	4.22665300	0.11822500	-2.66326600
C	-3.89017600	1.58905700	0.93918600
C	-4.69416400	1.02879700	-0.04361300
C	-4.18039700	0.40942500	-1.17775900
C	-2.80238200	0.32755400	-1.31410200
C	-1.96471100	0.84446700	-0.31835200
C	-2.51159000	1.49641700	0.79032800
H	-4.34760100	2.08331300	1.78687500
H	-4.85927000	0.01398300	-1.92286500
H	-2.35175500	-0.12581000	-2.19122800
H	-1.85627100	1.94178700	1.53240300
N	-6.15696000	1.10950200	0.11341400
O	-6.84199300	0.61412500	-0.76134700
O	-6.58393400	1.66200900	1.10955800
C	-0.49560700	0.71086400	-0.45568500
O	-0.04415300	0.58076200	-1.65911400
H	0.12422500	1.24924600	0.26749800

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0 1

C	0.79563300	1.52299100	1.83655500
C	0.03646900	0.94588900	0.65727400
C	1.32197500	2.43565900	-0.95235500



C	1.75594400	3.24973200	0.26784000
C	2.04810200	2.31284600	1.43752700
H	-1.19436000	-1.69194400	-0.56309100
H	-0.97284700	0.59764300	0.86907200
H	0.11855200	2.18193000	2.39463400
H	1.06560200	0.71864500	2.53306000
H	2.16324800	1.82705500	-1.31316200
H	1.00026700	3.06210200	-1.78812600
H	2.63793400	3.84532800	0.01823300
H	0.95946200	3.95221000	0.54139400
H	2.85169600	1.62707900	1.14609600
H	2.40990100	2.87701900	2.30198800
C	0.19299300	1.50710100	-0.61724400
O	-0.55890600	1.17850800	-1.61106000
C	-7.64041200	0.96330700	0.63137000
C	-6.66821300	-0.21020500	0.73362700
H	-8.47664700	0.83837900	1.32380400
H	-7.13764700	1.90411200	0.87904000
H	-8.05549600	1.06128900	-0.37476900
C	-5.37828300	-0.01336700	-0.07374800
H	-6.40249800	-0.35867000	1.78505800
H	-7.16997800	-1.12928300	0.39379000
C	-4.47671100	-1.25195000	0.02770600
H	-4.82533000	0.82796200	0.36304900
H	-4.85575000	-2.01116300	-0.68367300
C	-5.67875900	0.29642800	-1.54232800
H	-4.76259500	0.32283300	-2.13432300
H	-6.34609700	-0.46572200	-1.96360500
H	-6.17006300	1.26613400	-1.65019300
C	-3.04299700	-0.96570500	-0.41421300
O	-2.71089600	0.13974900	-0.86841500
O	-2.23839600	-1.95841000	-0.25210400
H	-1.37695500	0.61782700	-1.32686100
N	-4.37801500	-1.76222500	1.39800400
H	-5.26284500	-2.18266000	1.66422300
H	-3.68551100	-2.50594900	1.40743700
C	4.28656800	-0.94980700	1.20907900
C	4.86020400	-0.73498800	-0.03652100
C	4.10920900	-0.61484800	-1.20074700
C	2.72721800	-0.69303700	-1.10321700
C	2.11710400	-0.86704700	0.14371200
C	2.90086400	-1.02009400	1.28988800
H	4.92254200	-1.06215100	2.07802800
H	4.61406900	-0.47227200	-2.14808300

H	2.09438900	-0.62871200	-1.98326400
H	2.42614400	-1.20497500	2.24898500
N	6.32658900	-0.64855200	-0.13043700
O	6.80826900	-0.45609600	-1.23120100
O	6.96371500	-0.77064300	0.89938400
C	0.62758400	-0.93694000	0.21814700
O	0.00756800	-1.32523700	-0.83274600
H	0.25301000	-1.25737900	1.20330400

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0 1

C	-1.65225300	1.62186600	1.46965400
C	-2.25630300	0.47683200	0.66850600
C	-1.40911100	1.53592100	-1.49405900
C	-1.14421000	2.81205300	-0.69336700
C	-0.62133700	2.44961200	0.69401900
H	-3.26608900	-2.14059800	0.18144900
H	-3.19047400	0.09298400	1.07710400
H	-2.46107200	2.28590500	1.79966100
H	-1.19950800	1.22406100	2.38718700
H	-0.45980000	1.01355600	-1.68195700
H	-1.86846200	1.72640200	-2.46694600
H	-0.42601100	3.43853900	-1.22873300
H	-2.07217500	3.39025000	-0.60508000
H	0.31144600	1.88578300	0.58319700
H	-0.38250300	3.35257000	1.26354400
C	-2.29502800	0.58238000	-0.74740700
O	-3.00742400	-0.18863300	-1.47464600
O	-4.21693500	-1.88063300	-0.21691000
H	-3.63914700	-0.88674500	-0.92634800
C	2.33640500	-0.18412300	1.30210300
C	2.75119200	-0.42656900	0.00003400
C	1.89966200	-0.92860400	-0.97863300
C	0.57769100	-1.17552500	-0.63639400
C	0.11739600	-0.90141200	0.65559100
C	1.00645200	-0.43145800	1.62412000
H	3.04931200	0.18176600	2.03024400
H	2.28535600	-1.12110200	-1.97212100
H	-0.12444700	-1.59325200	-1.35192800
H	0.65942300	-0.26571400	2.64015400
N	4.15312000	-0.15639900	-0.35394500
O	4.49490700	-0.37097300	-1.50234100
O	4.88324100	0.26996800	0.52220400
C	-1.32972700	-1.16765000	0.97644100

O	-1.88119300	-2.12055900	0.31603400
H	-1.51787000	-1.08600000	2.06506400
H	-4.83555800	-1.65691700	0.48475300

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0 1

C	2.19109600	-0.91066200	-1.82307400
C	1.27273200	-1.64512200	-0.86855800
C	3.18543300	-3.17318200	-0.13938200
C	3.95238100	-2.65427600	-1.35567100
C	3.67831200	-1.16560600	-1.56443100
H	0.31704100	-1.27309200	0.38970000
H	0.25686100	-1.75171500	-1.26903800
H	1.97780700	-1.22525700	-2.85560000
H	1.98834700	0.17175800	-1.81364500
H	3.57588000	-2.71752200	0.78221500
H	3.28478800	-4.25392000	-0.01467300
H	5.02500000	-2.83885500	-1.24072500
H	3.62915500	-3.20365700	-2.24890100
H	4.01473000	-0.62908900	-0.66554300
H	4.27182500	-0.77277600	-2.39647100
C	1.69140100	-2.87138400	-0.22488400
O	0.89434200	-3.63896700	0.32498500
C	1.90905100	2.98317700	-0.49517600
C	0.68585300	3.42088600	-0.00889200
C	-0.02406400	2.75117500	0.98382300
C	0.50295900	1.57844900	1.49544800
C	1.72133400	1.08138300	0.99161500
C	2.43278100	1.80649500	0.02102600
H	2.42326700	3.56042700	-1.25283700
H	-0.96136600	3.15783400	1.34246700
H	-0.03358100	1.05893700	2.28230800
H	3.39362700	1.44292600	-0.32937100
N	0.12170500	4.67022700	-0.55604300
O	-0.94757600	5.03876000	-0.11201800
O	0.76614800	5.24269000	-1.41375900
C	2.33443500	-0.12506700	1.51951200
O	1.81242700	-0.91635800	2.35363000
H	3.39533000	-0.28703400	1.31584800
C	-5.92932600	-1.16895700	-1.30781300
C	-4.47390700	-1.60945900	-1.16529800
H	-6.46419000	-1.81534800	-2.00794600
H	-6.44497700	-1.22061600	-0.34327400
H	-6.01064300	-0.14328700	-1.67650800

C	-3.71084700	-0.86440800	-0.06341800
H	-4.44679900	-2.68004000	-0.94077300
H	-3.95293200	-1.46597000	-2.12437800
C	-2.24575800	-1.32189000	-0.02082000
H	-4.15703300	-1.12649700	0.90416900
H	-1.70934500	-0.79473300	-0.84034800
C	-3.78023000	0.65246700	-0.25483600
H	-3.15064500	1.17263000	0.47042500
H	-3.44969400	0.92725300	-1.26423500
H	-4.79954100	1.02223000	-0.12547000
C	-1.56779500	-0.85433100	1.25856300
O	-2.05906300	-0.24718200	2.17195700
O	-0.26073300	-1.21385800	1.31052000
H	0.73989200	-0.99260100	2.16619200
N	-2.09901400	-2.77212000	-0.06424200
H	-2.32784500	-3.11378100	-0.99144200
H	-1.14320200	-3.07377600	0.14094300

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0 1

C	0.78438300	2.26980700	-0.49701000
C	0.39705300	1.21241800	0.53272900
C	-1.68893200	2.68985500	1.08408000
C	-1.21183700	3.68507800	0.02459400
C	-0.44159700	2.97014100	-1.08350200
H	-0.69089600	0.30076500	0.14897400
H	1.22931600	0.87539700	1.14637200
H	1.42778600	3.02632700	-0.02703300
H	1.37735500	1.82602800	-1.30456800
H	-2.50212500	2.07964600	0.66772000
H	-2.08442000	3.17894400	1.97733200
H	-2.06970400	4.23102900	-0.37959800
H	-0.55262900	4.42980100	0.48765700
H	-1.08840600	2.23100200	-1.57858100
H	-0.13195300	3.68375000	-1.85314800
C	-0.62955100	1.69642900	1.54797900
O	-0.64621400	1.25246700	2.67671100
C	4.09546200	-1.29335300	1.09193600
C	4.99901100	-0.81206200	0.15109200
C	4.61021700	-0.27060300	-1.06552800
C	3.25245800	-0.20652600	-1.35361500
C	2.32075400	-0.67472800	-0.42338900
C	2.74404200	-1.21929800	0.79464200
H	4.46058100	-1.70620800	2.02351200

H	5.36358300	0.08098200	-1.75888400
H	2.90268200	0.18713300	-2.30127500
H	2.00793300	-1.56852200	1.51352900
N	6.43972000	-0.88594700	0.45980300
O	7.21271600	-0.45206700	-0.37269900
O	6.75792500	-1.37585500	1.52629700
C	0.88103900	-0.62681200	-0.73668600
O	0.55729400	-0.29683500	-1.93518000
H	0.22695300	-1.28919200	-0.16653400
C	-6.42832500	-2.36196200	1.45473500
C	-5.84893200	-1.68969700	0.21149100
H	-7.37297300	-2.85833100	1.21914400
H	-5.73973000	-3.12063700	1.84143200
H	-6.62316600	-1.64696700	2.25735000
C	-4.41777100	-1.16163000	0.39781200
H	-5.84697400	-2.40884500	-0.61199900
H	-6.50204500	-0.85560400	-0.08850800
C	-3.92851500	-0.49608200	-0.91170300
H	-3.76650000	-2.02433200	0.59405700
H	-4.29413800	0.55303800	-0.89694300
C	-4.34236300	-0.19723600	1.58494300
H	-3.33401100	0.18460500	1.74500600
H	-5.02145600	0.65068300	1.42653700
H	-4.64934400	-0.69612300	2.50674500
C	-2.41399100	-0.34561300	-0.98372000
O	-1.77165500	-0.24649000	0.11677100
O	-1.87188000	-0.29051300	-2.11167800
H	-0.52006700	-0.30438700	-2.07305100
N	-4.34704100	-1.23078900	-2.09786000
H	-5.33141100	-1.06713100	-2.27746300
H	-3.82413400	-0.89011400	-2.89843700

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0 1

C	-2.99011200	-0.49450000	1.83815900
C	-2.06295200	-0.48761900	0.64000800
C	-3.93943400	-1.16237300	-0.91554500
C	-4.73654900	-1.49679600	0.34380500
C	-4.46650800	-0.46138200	1.43405300
H	-2.83641000	1.26498000	0.00198500
H	-0.99974700	-0.55805700	0.85816100
H	-2.81340800	-1.39647400	2.44469100
H	-2.77096100	0.35210700	2.50228900
H	-4.37844700	-0.28558400	-1.41661800

H	-3.97349000	-1.97032800	-1.65165700
H	-5.80526800	-1.55686600	0.11408900
H	-4.43292100	-2.48524300	0.71146100
H	-4.72938800	0.53740100	1.05671900
H	-5.09831000	-0.64195500	2.30936000
C	-2.45926700	-0.87656600	-0.65051900
O	-1.68226100	-0.91462500	-1.65152900
C	2.58501100	-0.98824700	-0.57047300
C	3.53089900	-0.18318500	0.04955100
C	3.27741600	1.11821000	0.47450700
C	2.01059600	1.63642500	0.26646800
C	1.03636300	0.84618000	-0.36276100
C	1.31503200	-0.46541500	-0.77837000
H	2.85090700	-1.99358400	-0.87088700
H	4.06522200	1.68638500	0.95196900
H	1.76265900	2.64524600	0.57772300
H	0.51333300	-1.04291100	-1.23822000
N	4.88293600	-0.73650100	0.27550800
O	5.69770000	-0.01413700	0.81714400
O	5.08918700	-1.87514400	-0.09575600
C	-0.30067200	1.34688300	-0.60966100
O	-0.61154100	2.53082700	-0.25480500
H	-0.97156000	0.72181300	-1.21970000
O	-3.02371100	2.17812600	-0.36683900
H	-1.64824000	2.61472200	-0.38987900
H	-3.46845300	2.03378800	-1.21109400

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C	1.42468500	-0.78619200	2.16981600
C	2.00822800	-0.93864200	0.77005600
C	-0.00977100	-2.32847500	0.04168000
C	-0.41782100	-2.34615300	1.51617900
C	-0.08676100	-1.00958000	2.17866900
H	2.51295900	-0.05491500	0.37401800
H	3.17967700	-1.59855100	0.66486100
H	1.89503000	-1.49360200	2.86410700
H	1.66247500	0.21303800	2.54972400
H	-0.74603300	-1.75554000	-0.54735800
H	0.03903800	-3.32597000	-0.40791300
H	-1.49138400	-2.55540700	1.59493100
H	0.10284100	-3.15285700	2.04665400
H	-0.57583200	-0.21046200	1.60433300
H	-0.49218900	-0.96239500	3.19269000

C	1.28142000	-1.61957900	-0.22273000
O	1.69251400	-1.68752100	-1.44499700
C	0.14334900	1.62212600	-0.46268700
C	0.79896400	2.21612100	0.60375000
C	2.14786200	2.57153300	0.58042800
C	2.86315500	2.32981100	-0.58207100
C	2.22393700	1.73320200	-1.67881000
C	0.87870400	1.37601900	-1.61849000
H	-0.89772200	1.32907200	-0.39312400
H	2.60657600	3.00810100	1.45907300
H	3.92372700	2.55249700	-0.64822700
H	0.39203600	0.88291500	-2.45622700
N	0.04151500	2.42199600	1.84081200
O	0.64952500	2.69024000	2.85735700
O	-1.17792600	2.29408300	1.78827700
C	2.99284200	1.47298100	-2.92672800
O	4.10976000	1.89058600	-3.12367800
H	2.45900700	0.87308100	-3.69009800
C	9.27322400	-0.51396800	1.71281700
C	8.35099800	-0.17626400	0.54297600
H	10.10492500	0.19282600	1.77164000
H	8.72667900	-0.46853200	2.66077000
H	9.69700700	-1.51708000	1.61997100
C	7.06395900	-1.01131400	0.51139800
H	8.07867500	0.88229800	0.60329100
H	8.89603900	-0.31600600	-0.40317000
C	6.21715000	-0.66976600	-0.72276800
H	6.46777800	-0.75498800	1.39616000
H	6.64902600	-1.20027400	-1.59288000
C	7.36931900	-2.51107800	0.53542400
H	6.45904200	-3.09772100	0.40068800
H	8.07436600	-2.76932700	-0.26472100
H	7.81834300	-2.81047700	1.48546800
C	4.77273500	-1.16566400	-0.60820100
O	4.41588500	-1.83198300	0.41309000
O	3.99784300	-0.83097100	-1.54258700
H	2.67862400	-1.29839500	-1.52421100
N	6.10739700	0.77593200	-0.94533000
H	7.01406500	1.14070600	-1.22170900
H	5.48658400	0.93345700	-1.73729800
C	-4.53964400	2.91338700	-1.49030300
C	-3.11019800	2.98875100	-0.97237700
H	-4.68730500	3.63976800	-2.29765200
H	-4.71485800	1.91091800	-1.89285400

H	-2.92308900	3.97277300	-0.52074100
H	-2.97800800	2.22449800	-0.19222000
O	-2.20478500	2.82519800	-2.03238100
H	-2.20917800	1.87180500	-2.23415400
O	-5.50620200	3.10844700	-0.45400500
H	-5.37210600	3.98584900	-0.07671900
C	-4.30652500	1.36587500	2.22156100
C	-3.30147100	0.26659000	2.52417900
H	-4.90136300	1.57163400	3.12206700
H	-3.76148300	2.28330500	1.95852900
H	-3.84368600	-0.65803900	2.76235100
H	-2.70336400	0.08281600	1.61655300
O	-2.51190600	0.58041700	3.64460000
H	-1.92003100	1.29800700	3.37604900
O	-5.12928400	0.94336500	1.14704000
H	-5.38591100	1.73278200	0.63098100
N	-5.97289000	-2.09639500	-0.27793800
C	-4.55000600	-2.31409200	0.21589900
H	-4.10507700	-1.31711400	0.27594400
H	-4.62938500	-2.74411600	1.21966500
C	-3.71900500	-3.24723600	-0.66807100
H	-4.04315700	-4.28414000	-0.52647100
H	-2.69013900	-3.17493400	-0.28985400
O	-3.79914000	-2.97101300	-2.03720400
H	-3.28700700	-2.14394900	-2.18363500
Cl	-2.56412600	-0.24708600	-1.60559000
C	-6.80984900	-1.64617000	0.87809400
H	-7.81899600	-1.44861100	0.51237100
H	-6.83382800	-2.44449100	1.62113900
H	-6.36352800	-0.73395700	1.28104100
C	-5.98440000	-1.00960100	-1.31769900
H	-5.38599300	-1.34066900	-2.16207600
H	-7.02323600	-0.83325100	-1.60320600
H	-5.53579200	-0.12411500	-0.86731800
C	-6.55225100	-3.34484700	-0.85349600
H	-6.50610900	-4.13327400	-0.10019000
H	-7.59199900	-3.14600200	-1.11694800
H	-5.97596600	-3.61666400	-1.73692900

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C	-1.26694700	-0.49473400	-1.61765500
C	-2.14244400	-0.75702200	-0.39511000
C	-0.49310800	-2.48442800	0.49623700



C	0.07374400	-2.48537600	-0.92208200
C	0.14708500	-1.05295900	-1.45084500
H	-2.69763000	0.10154000	-0.01423500
H	-3.28392000	-1.38403400	-0.63850100
H	-1.72276900	-0.94447400	-2.50771000
H	-1.23658000	0.58288800	-1.81531000
H	0.24993800	-2.05898800	1.18708100
H	-0.73856500	-3.48367300	0.86851300
H	1.06043100	-2.95400200	-0.94510700
H	-0.57121900	-3.08046500	-1.58011400
H	0.70982000	-0.43765100	-0.72993200
H	0.69530800	-1.02698500	-2.39610800
C	-1.71132500	-1.62022800	0.63190900
O	-2.37980500	-1.76623400	1.72129000
C	-0.91625100	1.70837000	1.54530900
C	-1.36679200	2.41309800	0.43671200
C	-2.70751000	2.72117100	0.21788400
C	-3.63717800	2.31013200	1.16311600
C	-3.20789200	1.60551000	2.29329000
C	-1.86019400	1.30094800	2.48091600
H	0.13639200	1.47980300	1.65489900
H	-2.99827600	3.25138600	-0.68046000
H	-4.70001100	2.48051600	1.01929700
H	-1.55049200	0.72997600	3.35141800
N	-0.38726800	2.80296700	-0.58370300
O	-0.78276000	3.36607700	-1.58129400
O	0.78857200	2.52436300	-0.37351300
C	-4.20288200	1.16523100	3.31371500
O	-5.34833100	1.54478000	3.32899000
H	-3.81344300	0.46920700	4.08275100
C	-9.05495500	-0.17929200	-2.88544400
C	-8.44164300	-0.01837800	-1.49576200
H	-9.88481900	0.51732200	-3.02793100
H	-8.31023200	0.02251600	-3.66260100
H	-9.43945000	-1.18949600	-3.04572200
C	-7.15493200	-0.83006500	-1.29258200
H	-8.21833100	1.04073500	-1.33143100
H	-9.18025400	-0.31465000	-0.73536100
C	-6.63110300	-0.68471500	0.14459600
H	-6.38666900	-0.42558500	-1.96367500
H	-7.20990500	-1.37275400	0.78988800
C	-7.37217200	-2.30962500	-1.62052100
H	-6.49286900	-2.90281600	-1.36464300
H	-8.23245200	-2.70033500	-1.06295500

H	-7.57055000	-2.45465200	-2.68489400
C	-5.16969300	-1.11767600	0.28484800
O	-4.56975900	-1.63723300	-0.69997400
O	-4.62816200	-0.88847800	1.40624900
H	-3.38095300	-1.33849200	1.61714200
N	-6.67569800	0.70083500	0.62385900
H	-7.64480300	0.99608900	0.69574200
H	-6.30445100	0.72530900	1.57122600
C	3.69634300	-1.68896100	1.90946500
C	4.79310000	-2.74427800	1.99042700
H	3.17073200	-1.62428200	2.86972200
H	4.16846800	-0.72510200	1.70541900
H	4.35017200	-3.71993400	2.23770200
H	5.29130800	-2.83958300	1.01585800
O	5.68889500	-2.40890200	3.01425000
H	6.27338200	-1.72373100	2.64364000
O	2.76128700	-1.93214000	0.84627300
H	2.46803800	-2.84944200	0.92423500
C	4.19659300	-2.74837300	-1.88286700
C	5.40349800	-1.91620200	-1.49151200
H	4.33407200	-3.24071000	-2.84859100
H	4.03915600	-3.52769500	-1.12423100
H	5.66054800	-1.24914800	-2.33407200
H	5.09663800	-1.28349400	-0.64671000
O	6.48139300	-2.72706800	-1.11742900
H	7.01229500	-2.19283700	-0.50139900
O	3.06492700	-1.89315500	-1.99107600
H	2.82866200	-1.67413300	-1.07361700
N	4.12403100	2.00240100	-1.23709800
C	5.58726200	1.73530500	-1.54374500
H	5.76627200	0.69151400	-1.28265300
H	5.71138600	1.87529000	-2.62200200
C	6.57312700	2.63236100	-0.79270700
H	6.53925600	3.65157400	-1.19258300
H	7.56723400	2.22357200	-1.01709900
O	6.33602000	2.71225400	0.58374900
H	6.62982400	1.85343000	0.96476500
Cl	6.91266500	-0.26256000	0.96165300
C	3.28337000	1.45078900	-2.34722700
H	2.23628300	1.62374900	-2.09126700
H	3.53725700	1.97550300	-3.26929900
H	3.47590000	0.37792900	-2.44054600
C	3.72748300	1.29633500	0.02843200
H	4.41978700	1.58835300	0.81398300

H	2.69976000	1.57376300	0.26009800
H	3.79582400	0.22522400	-0.15954900
C	3.85800000	3.46539700	-1.09306100
H	4.20981200	3.97225700	-1.99349300
H	2.78222300	3.59976900	-0.97874700
H	4.39598800	3.82189600	-0.21486700

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C	2.49355200	-1.55541700	-2.29428500
C	1.97267900	-1.09737000	-0.93607000
C	0.82295800	-3.34365500	-0.55218700
C	1.04469100	-3.58431400	-2.04288500
C	2.42415900	-3.07368700	-2.46423100
H	2.65622900	-0.48688700	-0.34495900
H	1.15768900	-0.03043300	-1.02335200
H	1.90902400	-1.08234200	-3.09290100
H	3.52333600	-1.20276100	-2.42350800
H	1.46346700	-4.01453700	0.04181100
H	-0.20469100	-3.52906700	-0.23087400
H	0.93370100	-4.65004100	-2.26129000
H	0.26716900	-3.05101800	-2.60303800
H	3.19754600	-3.54669600	-1.84258600
H	2.63885400	-3.34667300	-3.50158000
C	1.22459500	-1.96724800	-0.12808300
O	0.85573500	-1.62949900	1.06913100
C	4.59489700	-2.27400800	0.87336700
C	5.20233400	-1.30066400	0.09256200
C	5.09003500	0.06277100	0.34995700
C	4.33080300	0.46929500	1.44065800
C	3.70344700	-0.49398800	2.23865400
C	3.83327600	-1.85400100	1.95754800
H	4.71125000	-3.31918300	0.61550700
H	5.57083400	0.77165400	-0.31255600
H	4.16063600	1.52253600	1.65323200
H	3.31322500	-2.58282600	2.57302800
N	5.95244000	-1.73573700	-1.09948300
O	6.42302000	-0.87058400	-1.81436100
O	6.04490100	-2.93288700	-1.30059300
C	2.86175300	-0.07376100	3.39289200
O	2.83678900	1.04993400	3.83430600
H	2.24979200	-0.88264400	3.84183900
C	3.03432200	5.96612000	-1.50178100
C	2.49787200	5.15602800	-0.32311900

H	3.63120900	6.81240800	-1.15212100
H	3.67469200	5.34577900	-2.13789300
H	2.23110600	6.36519800	-2.12641600
C	1.82586600	3.83569400	-0.72791400
H	3.32283000	4.92881300	0.35742400
H	1.77587400	5.76724400	0.24075200
C	1.29833200	3.08967900	0.51713000
H	2.58995800	3.19689900	-1.19254700
H	0.30185900	3.50404400	0.76824600
C	0.70938300	4.08116700	-1.74379700
H	0.20587700	3.14956300	-1.99935600
H	-0.02552800	4.78705400	-1.33195500
H	1.10281700	4.51491500	-2.66641600
C	1.03971600	1.59961700	0.25951700
O	0.81010200	1.21135800	-0.92898800
O	1.08700800	0.83625200	1.25644700
H	0.95612900	-0.59191800	1.17968200
N	2.24578100	3.16867200	1.62747500
H	2.20711600	4.08767100	2.05552600
H	1.98614200	2.48964100	2.33876100
C	-3.64895200	-1.70854300	2.16048000
C	-3.10375300	-3.00744400	1.57986800
H	-3.29908400	-1.59125500	3.19331700
H	-3.25254500	-0.87865400	1.56702800
H	-3.50679300	-3.86277900	2.13882000
H	-3.41825200	-3.10811200	0.53177200
O	-1.70739300	-3.03224800	1.72872200
H	-1.34498100	-2.36282100	1.12200700
O	-5.07610200	-1.61427300	2.09943100
H	-5.44181400	-2.33790200	2.62166100
C	-6.27711400	-2.13617100	-0.78902900
C	-4.91050400	-1.73130300	-1.30886300
H	-6.96090800	-2.38945400	-1.60338500
H	-6.16335600	-3.02267200	-0.15217400
H	-5.03717300	-0.94125400	-2.07263200
H	-4.36185000	-1.28886800	-0.46450400
O	-4.22018100	-2.83800500	-1.81462600
H	-3.27956000	-2.58869600	-1.79442900
O	-6.84095300	-1.04753900	-0.06678700
H	-6.40503800	-1.07953900	0.79955400
N	-4.67196000	2.23334600	-0.22044500
C	-3.62852900	1.71030200	-1.20066800
H	-3.71113300	0.62172100	-1.19628400
H	-3.91616900	2.09655900	-2.18327900

C	-2.19229200	2.11017800	-0.88895200
H	-2.04888200	3.19137300	-0.99390500
H	-1.57027600	1.61489500	-1.64370100
O	-1.79576200	1.74293200	0.40753300
H	-1.52158600	0.80357000	0.33352200
Cl	-1.70513700	-1.10009100	-0.87095600
C	-6.02466800	2.08139900	-0.84273400
H	-6.76841200	2.47392900	-0.14728700
H	-6.04933100	2.64431600	-1.77624000
H	-6.21698900	1.01764000	-1.00619200
C	-4.66541400	1.43310900	1.05083100
H	-3.67118600	1.49464500	1.48647600
H	-5.42684200	1.84955700	1.71314200
H	-4.92170200	0.40526400	0.79869700
C	-4.41601000	3.66436700	0.10544500
H	-4.35359500	4.23492800	-0.82269800
H	-5.24073300	4.03224000	0.71697700
H	-3.47834800	3.73012500	0.65710000

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C	2.28927700	-1.98045900	-1.60307000
C	1.94298600	-1.07954300	-0.42460600
C	1.19758200	-3.08639600	0.96403300
C	1.33989800	-3.90619900	-0.32056700
C	2.52543400	-3.42318400	-1.15652800
H	2.57063100	-0.19822000	-0.28700600
H	0.89760300	-0.30643600	-0.62618900
H	1.47320600	-1.95696500	-2.33476500
H	3.17116700	-1.58278700	-2.11597800
H	1.89457000	-3.44216700	1.73600800
H	0.19114800	-3.18526400	1.38787300
H	1.43790000	-4.96342700	-0.06197700
H	0.41655700	-3.81234400	-0.90279000
H	3.44870000	-3.47282400	-0.56254700
H	2.67077400	-4.07095900	-2.02534000
C	1.52103700	-1.63356700	0.79469700
O	1.33411600	-0.89190700	1.84112900
C	5.03876400	-0.90715700	0.95787400
C	5.22265600	-0.43303700	-0.33318300
C	4.86603700	0.85206100	-0.73254700
C	4.29607600	1.70041200	0.20888500
C	4.10241100	1.24672500	1.51860000
C	4.46830100	-0.04743600	1.88954600

H	5.32931900	-1.92087900	1.20369000
H	5.01697100	1.15320000	-1.76173900
H	3.95474400	2.69543400	-0.06261000
H	4.29437500	-0.38621700	2.90704900
N	5.76503800	-1.36215600	-1.34282300
O	5.87837700	-0.94908900	-2.48096800
O	6.04890600	-2.48718000	-0.97471900
C	3.49998800	2.14491500	2.54098200
O	3.28202400	3.31891700	2.36447100
H	3.27196600	1.65916000	3.51211100
C	-1.28352600	5.08198700	-3.26315600
C	-0.51158400	4.81126200	-1.97325600
H	-1.12048400	6.10626200	-3.60745000
H	-0.95734600	4.40326700	-4.05789700
H	-2.35841800	4.94229900	-3.12747200
C	-0.56696900	3.34329100	-1.53037100
H	0.53468500	5.09871100	-2.12355600
H	-0.91099000	5.44654900	-1.16814700
C	0.14657300	3.14243700	-0.18502000
H	-0.03304800	2.74156800	-2.27652400
H	-0.54575400	3.45972500	0.61932800
C	-2.01340600	2.84901300	-1.42894900
H	-2.06854600	1.87147600	-0.94717300
H	-2.62296200	3.54651700	-0.84160800
H	-2.47624500	2.72890900	-2.41127800
C	0.45950900	1.67459900	0.09681700
O	0.17114800	0.79371900	-0.75780400
O	1.02296800	1.42675200	1.21221300
H	1.27873900	0.18198700	1.54887300
N	1.44653200	3.81808300	-0.11718900
H	1.30604600	4.81997700	-0.20399500
H	1.84819800	3.66598800	0.80585500
C	-1.89005700	-0.71910900	-2.20285000
C	-3.09072900	-1.10090700	-3.05754100
H	-1.22163400	-0.05580900	-2.76229300
H	-2.25063500	-0.16722600	-1.33411300
H	-2.75889500	-1.63878100	-3.95689800
H	-3.76088100	-1.76978900	-2.49753400
O	-3.74035700	0.07067700	-3.47682500
H	-4.25557500	0.38239900	-2.71061900
O	-1.15975100	-1.84730900	-1.69251900
H	-0.93437000	-2.41554500	-2.43959200
C	-3.15291000	-3.89911100	-0.22118700
C	-4.14866600	-2.77129600	-0.01762200

H	-3.49657600	-4.83745800	0.22132500
H	-3.01395100	-4.06157200	-1.29853100
H	-4.40893200	-2.71529300	1.05628900
H	-3.63978200	-1.83789200	-0.28126500
O	-5.28344100	-2.92904600	-0.82282200
H	-5.65424100	-2.03635000	-0.92373500
O	-1.92678900	-3.54116200	0.40831900
H	-1.53771700	-2.87195400	-0.18374600
N	-2.31374700	-0.21192400	2.65443000
C	-3.81751600	-0.01888800	2.70996200
H	-4.22623900	-0.59135000	1.87358800
H	-4.15634900	-0.44744000	3.65833700
C	-4.27461700	1.44015100	2.61484300
H	-4.05397800	1.96462800	3.55102400
H	-5.36658500	1.39693500	2.50932900
O	-3.67577500	2.16395400	1.57744900
H	-4.07865600	1.83187300	0.74101900
Cl	-4.97337300	0.37908800	-0.53279300
C	-1.96360500	-1.56757400	3.17925700
H	-0.87707700	-1.67108400	3.13110100
H	-2.31158400	-1.65123400	4.20956500
H	-2.42511300	-2.32160700	2.53725800
C	-1.84028900	-0.15406800	1.23407900
H	-2.07907800	0.82749000	0.83549700
H	-0.77199500	-0.34070600	1.24481000
H	-2.35664900	-0.93172300	0.67889300
C	-1.59078500	0.83160200	3.43989400
H	-1.93800100	0.79945800	4.47429100
H	-0.52328300	0.61394600	3.38361300
H	-1.79577600	1.80126200	2.98671000

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C	-5.69323500	1.10222100	0.93127300
C	-4.27840200	0.54544800	1.05443200
C	-4.92108300	-0.77281700	3.14507600
C	-6.18925200	0.08070200	3.16101100
C	-6.70562000	0.28620400	1.73667700
H	-3.76696600	0.34802200	0.11058700
H	-3.31909700	1.40786400	1.38914500
H	-5.72359700	2.14470200	1.27106400
H	-5.98015700	1.12148100	-0.12584500
H	-5.17417400	-1.82750400	2.96735600
H	-4.37504700	-0.74812500	4.09296100

H	-6.94310800	-0.39769700	3.79227600
H	-5.97048800	1.05792700	3.60862600
H	-6.85530900	-0.69098000	1.25676800
H	-7.67667200	0.78915900	1.74588700
C	-3.96763800	-0.41072300	2.04176300
O	-2.82448700	-0.99263800	2.09304000
C	-4.71773300	-2.31678200	-0.74071700
C	-5.17072400	-1.31792500	-1.59114300
C	-4.31696100	-0.49937800	-2.32626300
C	-2.94877200	-0.70049100	-2.20555200
C	-2.46674800	-1.70421900	-1.35859500
C	-3.34378700	-2.50157600	-0.62505000
H	-5.43154800	-2.91582600	-0.18895400
H	-4.73260000	0.27741900	-2.95577000
H	-2.23229000	-0.06886600	-2.72207600
H	-2.94957900	-3.25876900	0.04644400
N	-6.62200600	-1.08477000	-1.68216600
O	-7.00256000	-0.15716800	-2.37254400
O	-7.35470200	-1.82937800	-1.05487700
C	-0.99572900	-1.92475100	-1.24495200
O	-0.20622400	-1.43357300	-2.01835600
H	-0.65746000	-2.58830300	-0.42751200
C	0.23933400	5.91977500	-1.15845300
C	0.35758500	4.39702200	-1.15689600
H	0.72041300	6.34941300	-2.04135600
H	-0.81184100	6.22732000	-1.16812900
H	0.70642500	6.36644100	-0.27639700
C	-0.45634500	3.71758900	-0.04749700
H	0.01262700	4.01321700	-2.12231500
H	1.41326600	4.10244700	-1.06255200
C	-0.22903700	2.19710300	-0.04142600
H	-1.52060800	3.89393100	-0.24914000
H	0.69654900	1.98166700	0.52655200
C	-0.11722900	4.29487500	1.32902900
H	-0.60157000	3.72300900	2.12235400
H	0.96872100	4.26913900	1.49320600
H	-0.44226900	5.33429000	1.42067100
C	-1.32701000	1.44509200	0.70929000
O	-2.20578700	2.09168000	1.35768700
O	-1.30800700	0.18553200	0.61479700
H	-2.11628500	-0.50109100	1.39891600
N	-0.18932700	1.62036800	-1.38633700
H	0.63458000	1.98265100	-1.86056100
H	-0.02497600	0.61917800	-1.28250700



C	3.99969300	-3.02067900	-1.48394400
C	2.94182700	-3.65952200	-0.59205900
H	3.89194700	-3.39044900	-2.51072800
H	3.82472000	-1.94130000	-1.48780000
H	3.06663500	-4.75078200	-0.58489500
H	3.05928300	-3.29940800	0.43925400
O	1.67007600	-3.38669300	-1.11866900
H	1.52299100	-2.42758600	-1.03035700
O	5.33699100	-3.21904800	-1.01536600
H	5.50799600	-4.16811800	-1.00054700
C	5.82747000	-2.67578600	2.03080100
C	4.64480100	-1.72537200	2.01640800
H	6.27104200	-2.76179800	3.02614300
H	5.48452400	-3.67162100	1.72232400
H	4.95162400	-0.77461200	2.49038100
H	4.41729800	-1.51625600	0.96256500
O	3.52588000	-2.28213900	2.64808900
H	2.75472800	-1.83599600	2.25883300
O	6.82490200	-2.17440300	1.14893500
H	6.51646700	-2.42922600	0.26378700
N	5.79782500	1.39208800	-0.38147600
C	4.73781300	1.66241300	0.67731300
H	4.37287100	0.68553400	0.99783100
H	5.24725500	2.16140100	1.50699800
C	3.56274200	2.51723700	0.20471700
H	3.87234000	3.55608000	0.04581400
H	2.84757800	2.51406500	1.03942700
O	2.98189100	2.05942900	-0.98499800
H	2.50542000	1.22358600	-0.74493000
Cl	2.10119200	-0.50215900	0.30326300
C	7.07144000	1.00834500	0.30560700
H	7.81913000	0.78977100	-0.45883100
H	7.40242400	1.84344500	0.92391400
H	6.89739600	0.10900400	0.90429400
C	5.38586000	0.23861900	-1.25295100
H	4.39699900	0.44633700	-1.65474300
H	6.12939900	0.13370000	-2.04530500
H	5.37372200	-0.65846100	-0.63421800
C	6.02078700	2.59686300	-1.23222600
H	6.26854700	3.44252200	-0.58857700
H	6.85036800	2.38932100	-1.90906900
H	5.10659500	2.79190900	-1.79282100

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C	5.66910000	1.24339400	-0.73505700
C	4.40591000	0.43495000	-1.01291700
C	5.66318200	-1.06245400	-2.65451500
C	6.79826200	-0.04132400	-2.55839400
C	6.93454800	0.48065400	-1.12720900
H	3.75286600	0.26997000	-0.15458800
H	3.41273100	1.09217700	-1.59925100
H	5.63990700	2.19192900	-1.28423100
H	5.69580100	1.51509000	0.32567200
H	5.98132600	-2.02770700	-2.23464700
H	5.35886000	-1.26847600	-3.68516000
H	7.72833800	-0.50013100	-2.90380600
H	6.59108200	0.80186000	-3.22800900
H	7.08605100	-0.36142600	-0.43755000
H	7.81115800	1.12749400	-1.03607700
C	4.44571000	-0.68504600	-1.86332700
O	3.41858700	-1.44415800	-2.03930500
C	5.15220200	-1.81578300	1.46246000
C	5.00824700	-0.61856700	2.14927500
C	3.77501300	-0.02747700	2.40689300
C	2.62866700	-0.66293800	1.94468300
C	2.74909600	-1.86844600	1.24271000
C	3.99932600	-2.44148600	1.00462000
H	6.14121100	-2.22338500	1.29447100
H	3.73444800	0.91826900	2.93288000
H	1.64938200	-0.20693800	2.06646800
H	4.06970400	-3.36924600	0.44349100
N	6.23344100	0.08706700	2.57537400
O	6.09630600	1.16026800	3.12932200
O	7.29958900	-0.44522700	2.32866600
C	1.54959400	-2.55511500	0.71231800
O	0.40897400	-2.22389100	0.95273200
H	1.75938500	-3.42852300	0.06310100
C	-0.70280600	5.19208300	0.53943600
C	-0.84414900	3.68113600	0.36101800
H	-1.36647700	5.55869300	1.32712400
H	0.32289600	5.45463000	0.81840800
H	-0.95059800	5.73312900	-0.37659700
C	0.18801400	3.08475700	-0.60617700
H	-0.73295100	3.19621400	1.33780000
H	-1.84782400	3.45181100	-0.02446200
C	0.06936600	1.55120100	-0.69854900
H	1.18765900	3.31265300	-0.21300400

H	-0.72626500	1.32546100	-1.43109300
C	0.03786400	3.69417600	-2.00273200
H	0.71500900	3.21891500	-2.71435300
H	-0.99270100	3.55757300	-2.35016200
H	0.26304300	4.76317600	-1.99695200
C	1.33658500	0.90864200	-1.26132400
O	2.23823400	1.63085100	-1.77414000
O	1.42069700	-0.35399600	-1.15502900
H	2.52346500	-0.97887300	-1.63460900
N	-0.16354100	0.91966200	0.60635700
H	-1.10505700	1.11915500	0.93981800
H	-0.07919700	-0.08911200	0.50919400
C	-4.21494000	1.12244300	2.20604700
C	-5.56088300	1.81983900	2.04996900
H	-3.88662500	1.16609700	3.25068200
H	-4.34658200	0.07510200	1.92571100
H	-5.47999500	2.86852900	2.36732500
H	-5.86507000	1.81018200	0.99425300
O	-6.50329900	1.19307300	2.87840300
H	-6.75344500	0.36929800	2.42374900
O	-3.19898700	1.65956100	1.34336300
H	-3.04769300	2.58230900	1.58521400
C	-4.32987900	2.18233600	-1.63658800
C	-5.21711000	0.96616200	-1.45065100
H	-4.44731500	2.63051400	-2.62599900
H	-4.59262200	2.93894400	-0.88495600
H	-5.06609100	0.28447500	-2.30677400
H	-4.86210500	0.44904500	-0.54652300
O	-6.55884700	1.33490000	-1.30393800
H	-6.97258000	0.62541500	-0.78172100
O	-2.97082700	1.77751700	-1.50461700
H	-2.86102000	1.60696600	-0.55366500
N	-2.72452000	-2.33634600	-0.80287000
C	-4.10057300	-2.47358500	-1.43083500
H	-4.63405700	-1.55243400	-1.19522900
H	-3.94632100	-2.54657500	-2.51184000
C	-4.91157400	-3.67553900	-0.94383200
H	-4.49280200	-4.60475700	-1.34541900
H	-5.91075000	-3.54802300	-1.38073500
O	-4.95957900	-3.80092300	0.44871800
H	-5.58072300	-3.10577900	0.76566500
Cl	-6.52661200	-1.19886100	0.70496000
C	-1.86545500	-1.49156800	-1.69258500
H	-0.89539800	-1.34186000	-1.20965700

H	-1.73229700	-2.01117900	-2.64276000
H	-2.36448100	-0.52950300	-1.84833100
C	-2.82938600	-1.63788000	0.52360700
H	-3.57866600	-2.15133600	1.12132600
H	-1.84511400	-1.66253400	0.99229800
H	-3.13480600	-0.60880200	0.32908500
C	-2.08438300	-3.67109100	-0.60637800
H	-2.04641300	-4.18335000	-1.56954000
H	-1.08198200	-3.49987900	-0.21470600
H	-2.68762900	-4.23195400	0.10713800

H<sub>2</sub>O-A

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C	2.39454000	2.39795200	1.95120000
C	2.48640700	1.03524800	1.27350500
C	0.71626700	0.07066400	2.83368200
C	0.95537400	1.30365200	3.70170600
C	1.13566800	2.52928100	2.80839700
H	2.71286600	1.05022300	0.20465500
H	3.58620900	0.32381800	1.51725500
H	3.28034200	2.57353500	2.57306800
H	2.40159900	3.17647800	1.18026100
H	-0.30345000	0.10224200	2.41989800
H	0.79141000	-0.87119200	3.38652200
H	0.09818900	1.43624500	4.36504200
H	1.84954600	1.16493400	4.32218700
H	0.25859700	2.59660600	2.15336900
H	1.17264600	3.44696400	3.40216400
C	1.61987800	-0.00681000	1.64498000
O	1.61169000	-1.13388600	1.00745700
C	-0.11789200	1.00475300	-0.95245400
C	0.30824400	2.32131800	-1.01317600
C	1.45154300	2.72699400	-1.69780400
C	2.20459500	1.75488300	-2.33883600
C	1.79301500	0.41709300	-2.30058000
C	0.63359500	0.04639800	-1.62297100
H	-1.01989400	0.73907400	-0.41512900
H	1.72576600	3.77430400	-1.71340300
H	3.11312900	2.00645000	-2.87588000
H	0.29961800	-0.98758500	-1.62467300
N	-0.48552800	3.33880400	-0.31446800
O	-0.15802700	4.50048700	-0.42890900
O	-1.42931700	2.95572900	0.36838700
C	2.60126200	-0.62637300	-2.98712000

O	3.61798600	-0.38630700	-3.59758200
H	2.20437500	-1.65628900	-2.91048500
C	9.72703800	-1.29351300	0.51735000
C	8.47739100	-1.23621500	-0.35960800
H	10.63156300	-1.16892500	-0.08337800
H	9.70956300	-0.49574000	1.26727100
H	9.80937200	-2.24686800	1.04536500
C	7.16432800	-1.21347000	0.43389900
H	8.52978300	-0.33350000	-0.97739600
H	8.47166200	-2.09687800	-1.04523000
C	5.95750300	-1.24718800	-0.50959900
H	7.10970700	-0.26861300	0.98761100
H	5.86728900	-2.26337700	-0.93395400
C	7.07941400	-2.37724300	1.42374000
H	6.10918600	-2.39397500	1.92600700
H	7.22030900	-3.33485000	0.90754600
H	7.84581600	-2.29839100	2.19814800
C	4.64413400	-0.97034000	0.21900200
O	4.66515500	-0.39876300	1.34634500
O	3.58234100	-1.28093600	-0.40176100
H	2.46933400	-1.19845300	0.31211800
N	6.03246700	-0.20000600	-1.53363700
H	6.81743500	-0.39315500	-2.14840800
H	5.20549500	-0.25197900	-2.12557200
C	-4.85361600	1.78720500	-2.17544700
C	-3.51894100	2.17636500	-1.55593500
H	-5.03913700	2.36779200	-3.08599300
H	-4.83722700	0.72529400	-2.43565500
H	-3.55963000	3.21691100	-1.20560200
H	-3.34504800	1.53202600	-0.68314500
O	-2.46894700	2.08679400	-2.48253000
H	-2.30626300	1.13505600	-2.60996400
O	-5.92422800	1.96448600	-1.23696700
H	-6.06920400	2.91168100	-1.12717000
C	-4.26807900	1.65264600	1.82229700
C	-2.96176700	0.95156200	2.15596800
H	-4.76290200	1.97482200	2.74792000
H	-4.04464900	2.55211700	1.23094100
H	-3.16046700	0.05866000	2.75974300
H	-2.48609300	0.60478800	1.22813200
O	-2.11254300	1.78621600	2.91527700
H	-1.83830400	2.50920700	2.33461600
O	-5.09520100	0.76090500	1.09401700
H	-5.47222000	1.22435400	0.32125500

N	-5.60775900	-2.67709100	0.57215000
C	-4.10069900	-2.68402100	0.80437300
H	-3.75572700	-1.67960800	0.54759300
H	-3.94167600	-2.84672500	1.87417300
C	-3.36086500	-3.76600100	0.01519800
H	-3.55534300	-4.74792200	0.46038400
H	-2.29812600	-3.54102400	0.15450200
O	-3.72948100	-3.84827100	-1.33689200
H	-3.32191500	-3.07889100	-1.78864000
Cl	-2.65759700	-1.05230800	-1.92350500
C	-6.26766900	-2.02091500	1.74274600
H	-7.34197300	-1.98358200	1.55291900
H	-6.06810700	-2.61916100	2.63271800
H	-5.86634100	-1.00996700	1.83669500
C	-5.92041000	-1.87491800	-0.66042800
H	-5.43766900	-2.35472500	-1.50772100
H	-7.00556300	-1.84639500	-0.77621300
H	-5.51373900	-0.87445600	-0.51488200
C	-6.14843800	-4.05906800	0.41603000
H	-5.88275000	-4.64092700	1.30022400
H	-7.23391800	-3.99017900	0.33153300
H	-5.71775500	-4.49884300	-0.48239800
O	-1.26281800	-1.54473000	0.86657800
H	-0.30512500	-1.67966200	0.82220500
H	-1.55949500	-1.38787100	-0.04991600

## H<sub>2</sub>O-B

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C	1.58340600	-1.22464000	1.86332200
C	2.29760200	-1.23152100	0.51540800
C	0.67284900	-2.98023500	-0.38793100
C	0.20690300	-3.15210200	1.05815100
C	0.16798100	-1.79592200	1.76459800
H	2.67790500	-0.26627300	0.17619900
H	3.55942400	-1.68829700	0.51399700
H	2.15149100	-1.80935900	2.59732000
H	1.56568900	-0.20048500	2.25348700
H	-0.14412200	-2.55232100	-0.98934600
H	0.95361500	-3.92382700	-0.86592200
H	-0.78300600	-3.61386600	1.07353400
H	0.89226700	-3.81807600	1.59743700
H	-0.47260200	-1.11127100	1.18732400
H	-0.27378700	-1.89581900	2.76178000
C	1.79963300	-2.01109400	-0.54436100

O	2.31638300	-1.95466000	-1.72843700
C	0.38188300	1.15232600	-0.81814600
C	0.91013700	1.80827400	0.28461400
C	2.20149800	2.33273600	0.32689300
C	2.99703100	2.19720800	-0.80086000
C	2.48842800	1.54469500	-1.93174500
C	1.19543000	1.02447700	-1.94006500
H	-0.61147700	0.71426400	-0.78545400
H	2.56304500	2.80487800	1.23187800
H	4.02788400	2.53827300	-0.80755100
H	0.82371000	0.48843400	-2.80901100
N	0.08909000	1.87996100	1.49664000
O	0.56966300	2.37069900	2.49778900
O	-1.04758700	1.42117800	1.43674400
C	3.34665400	1.38531800	-3.13895400
O	4.40479900	1.94937500	-3.28458800
H	2.93783600	0.71455700	-3.92057500
C	9.22682800	0.42346900	2.18981500
C	8.42605000	0.56372000	0.89669800
H	9.93036700	1.25194400	2.30546900
H	8.56032400	0.42555400	3.05884800
H	9.80226000	-0.50532500	2.21338400
C	7.29109400	-0.46026200	0.76080900
H	7.99597500	1.56941000	0.85482100
H	9.10507900	0.46691400	0.03561900
C	6.56422200	-0.30317900	-0.58420700
H	6.55788900	-0.26402200	1.55349300
H	7.16219700	-0.82422400	-1.35664100
C	7.81238200	-1.89177300	0.91032200
H	7.02730600	-2.61882700	0.69803900
H	8.64772400	-2.06575500	0.22036000
H	8.17289100	-2.07917100	1.92458200
C	5.19103200	-0.98345100	-0.59921600
O	4.84458600	-1.71235200	0.38066400
O	4.46164500	-0.74291200	-1.59803200
H	3.22285600	-1.40533600	-1.70916600
N	6.31307800	1.10046400	-0.92600800
H	7.19684000	1.55785800	-1.12908100
H	5.77399600	1.12931900	-1.78913600
C	-4.12389100	3.55409100	-0.80167900
C	-3.08552000	2.45033100	-0.90992900
H	-3.98145300	4.29410700	-1.59798400
H	-5.12019900	3.11946700	-0.92624100
H	-2.07212300	2.88491100	-0.83451600

H	-3.19991000	1.76733500	-0.05586700
O	-3.28932900	1.80263600	-2.13916500
H	-2.88900700	0.91668800	-2.06370800
O	-4.12146900	4.17185500	0.48054200
H	-3.23625600	4.50816200	0.66238800
C	-4.00290700	1.62021800	2.62693800
C	-3.58973800	0.18471600	2.35938800
H	-4.29146600	1.73653800	3.67959800
H	-3.15250300	2.28539300	2.42841100
H	-4.44476600	-0.47674100	2.54137100
H	-3.30122600	0.08361200	1.30157200
O	-2.55130800	-0.25651500	3.21065500
H	-1.75982600	0.23786400	2.95157200
O	-5.08818500	1.91994500	1.76199000
H	-4.95709200	2.83125700	1.45086400
N	-6.48118900	-0.85654300	-0.53081300
C	-5.55339300	-1.88303800	0.10527100
H	-4.67229800	-1.33574900	0.43573400
H	-6.06475000	-2.28208600	0.98591800
C	-5.15386900	-3.03867600	-0.81239100
H	-5.99507400	-3.72930500	-0.93602400
H	-4.36430600	-3.57059100	-0.26708500
O	-4.75741100	-2.64206400	-2.09881700
H	-3.86337800	-2.25047500	-2.02033300
Cl	-2.32502900	-1.02044000	-1.14835200
C	-7.22822700	-0.14885500	0.55342200
H	-7.86670800	0.60653200	0.09150100
H	-7.83878600	-0.87553500	1.09067400
H	-6.51157600	0.34331100	1.21470600
C	-5.65884800	0.16551300	-1.26729800
H	-5.04193400	-0.34637300	-1.99957300
H	-6.34070800	0.87093100	-1.74649900
H	-5.03774600	0.67605600	-0.53008900
C	-7.45087700	-1.49673900	-1.46622300
H	-8.00991100	-2.26054500	-0.92283500
H	-8.13296200	-0.72636100	-1.82834300
H	-6.89168300	-1.93776700	-2.29031800
O	-3.00280900	-2.63350200	1.57242000
H	-2.69115700	-2.10283200	2.32229300
H	-2.61058800	-2.18972200	0.80038900
2H <sub>2</sub> O			
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C	2.41134000	1.80600500	2.48508200



C	2.49962100	0.62263600	1.52767900
C	0.70944500	-0.64273300	2.82628000
C	0.95703000	0.36346800	3.94800000
C	1.15180700	1.75468800	3.34952200
H	2.73385800	0.86707300	0.48900500
H	3.59265000	-0.13638500	1.60732700
H	3.29657700	1.83747200	3.13123800
H	2.41935900	2.73397200	1.90334300
H	-0.30542700	-0.50464200	2.42311000
H	0.76717800	-1.68519300	3.15557900
H	0.09855400	0.35524600	4.62307200
H	1.84663200	0.07973300	4.52409000
H	0.27250900	1.97311200	2.73254700
H	1.19526400	2.51864600	4.13066700
C	1.62225600	-0.46606400	1.65426500
O	1.60945700	-1.42365900	0.78175400
C	-0.11320000	1.12790500	-0.70550400
C	0.39484800	2.37800600	-0.39439700
C	1.57000400	2.88604600	-0.94394500
C	2.27672100	2.08462200	-1.82520500
C	1.79832400	0.80530100	-2.14088000
C	0.60650000	0.33550700	-1.59617600
H	-1.03498700	0.77317500	-0.25994400
H	1.89975000	3.87978500	-0.66805800
H	3.20613200	2.41942800	-2.27421600
H	0.22159500	-0.64469300	-1.86641200
N	-0.31613200	3.18901400	0.60127300
O	0.24389200	4.16079400	1.05458000
O	-1.42390700	2.79997700	0.95629200
C	2.57098700	-0.06893600	-3.06175700
O	3.60480900	0.26808000	-3.59306200
H	2.13055100	-1.06816000	-3.24248000
C	9.73105100	-1.38275600	0.21959700
C	8.46959600	-1.16015500	-0.61286800
H	10.62550200	-1.10978200	-0.34613400
H	9.70804500	-0.77047700	1.12719300
H	9.83780800	-2.42709300	0.52361900
C	7.16644800	-1.33995700	0.17685900
H	8.49666300	-0.14288500	-1.01752900
H	8.47129100	-1.84904700	-1.47100000
C	5.94894300	-1.19060600	-0.74121900
H	7.10140100	-0.54143300	0.92554100
H	5.86906800	-2.09304500	-1.37388700
C	7.11566000	-2.69446100	0.88687800

H	6.15150500	-2.84229000	1.37909300
H	7.27003300	-3.51165700	0.17152200
H	7.88893100	-2.77124300	1.65469300
C	4.63940900	-1.09820600	0.03921500
O	4.66526500	-0.80685300	1.26951000
O	3.57600500	-1.25747500	-0.63284700
H	2.46412400	-1.33472300	0.08647000
N	5.99523100	0.05314000	-1.51740500
H	6.77303500	0.00827500	-2.16895400
H	5.15988400	0.11371500	-2.09660200
C	-4.87825900	1.99029100	-1.88802600
C	-3.46582900	2.22391600	-1.37456000
H	-5.08317800	2.64810300	-2.74037500
H	-4.97862700	0.95316200	-2.22074700
H	-3.36921600	3.23018500	-0.94668100
H	-3.24444100	1.49185500	-0.58704700
O	-2.53895900	2.13529100	-2.43536700
H	-2.36943200	1.18485300	-2.58275100
O	-5.85019000	2.18678000	-0.85565400
H	-5.82798300	3.11664400	-0.59911000
C	-4.19782000	1.26503000	1.98018500
C	-2.92955500	0.48903200	2.28966400
H	-4.73234200	1.48566400	2.91422000
H	-3.92225400	2.22232500	1.51406900
H	-3.18618200	-0.47572900	2.74358600
H	-2.40122000	0.26501500	1.35249300
O	-2.11796100	1.17907200	3.21538000
H	-1.84113500	2.00055100	2.78456500
O	-4.99901900	0.49135000	1.10293600
H	-5.43651100	1.09425500	0.47065300
N	-5.53150700	-2.87752400	0.26656600
C	-4.01656100	-2.89747900	0.43664800
H	-3.68707600	-1.86726200	0.28398400
H	-3.81269800	-3.17925800	1.47353200
C	-3.30459300	-3.87541200	-0.49962700
H	-3.47825400	-4.90367500	-0.16413500
H	-2.23857600	-3.65862900	-0.37671400
O	-3.72565700	-3.80431100	-1.83772800
H	-3.32696600	-2.99427800	-2.21721600
Cl	-2.64498100	-0.94698500	-2.12100400
C	-6.14578300	-2.35297200	1.52509500
H	-7.22764400	-2.31066400	1.38580400
H	-5.90227200	-3.03539100	2.34037800
H	-5.74977300	-1.35122100	1.70360100

C	-5.89392800	-1.95046000	-0.85984900
H	-5.44906600	-2.33783800	-1.77263800
H	-6.98297900	-1.91186400	-0.92603100
H	-5.47700400	-0.97144900	-0.62430900
C	-6.07358600	-4.23872100	-0.01439100
H	-5.77007400	-4.90976300	0.79092000
H	-7.16185200	-4.16995400	-0.04773400
H	-5.67894600	-4.57723300	-0.97127500
O	-1.23369700	-1.76093400	0.56970300
H	-0.27742800	-1.89559500	0.49794600
H	-1.53292800	-1.47584700	-0.31411600
O	-1.22796800	4.39250000	-1.60880900
H	-1.50034200	3.59649300	-2.09980200
H	-0.96137000	5.02989900	-2.27683100

H<sub>2</sub>O-A-H

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C	2.00520500	-3.06818400	-0.25452900
C	2.18664700	-1.57391300	-0.49626700
C	0.58801700	-1.64239500	-2.48184100
C	0.72164200	-3.16139100	-2.40492600
C	0.74938300	-3.60435400	-0.94184500
H	2.35900400	-0.96519400	0.39333600
H	3.36619900	-1.23420400	-1.01462400
H	2.87779000	-3.62644400	-0.61568100
H	1.95002800	-3.24049900	0.82455700
H	-0.45099700	-1.34593500	-2.27953200
H	0.83101200	-1.24290500	-3.47190900
H	-0.11406600	-3.61444500	-2.94286600
H	1.64909000	-3.48672300	-2.89252500
H	-0.13371900	-3.19441700	-0.42973200
H	0.70519700	-4.69506900	-0.86092400
C	1.42254400	-0.91603700	-1.47321600
O	1.46366500	0.37000900	-1.60516800
C	0.52797900	-0.72043200	2.53049800
C	1.64038400	-1.41093300	3.00669100
C	2.91067500	-0.82575500	2.97204100
C	3.07311100	0.46416100	2.48197400
C	1.95103400	1.16605600	2.02332100
C	0.68742600	0.57390700	2.03895300
H	-0.45868700	-1.17447600	2.55683600
H	3.77260100	-1.38034200	3.32911700
H	4.05463800	0.92725300	2.42279300
H	-0.18403400	1.12004200	1.68489000
C	2.07591300	2.55678700	1.53312000

O	3.09679700	3.20826200	1.53983400
H	1.12912200	2.99821100	1.15562500
C	9.55568600	-0.08108000	-0.01788200
C	8.31698600	0.80859400	0.06606100
H	10.36414500	0.31537100	0.60182500
H	9.32887800	-1.09304800	0.33421600
H	9.93156600	-0.16054800	-1.04112600
C	7.08448800	0.21763100	-0.63106900
H	8.07244700	0.97790900	1.11917300
H	8.54412900	1.79154400	-0.37460600
C	5.89484700	1.18711100	-0.55220800
H	6.79509700	-0.69644200	-0.09703500
H	6.02392500	1.94985200	-1.34485600
C	7.38414100	-0.13163800	-2.09094600
H	6.47899100	-0.44430600	-2.61391700
H	7.80642200	0.73750300	-2.61095100
H	8.10733900	-0.94746000	-2.16399600
C	4.55828600	0.51049500	-0.86714800
O	4.53685600	-0.69908900	-1.23606800
O	3.53177400	1.23368000	-0.71887200
H	2.38674500	0.79213100	-1.12447000
N	5.74384800	1.78001000	0.77677900
H	6.49829800	2.43934800	0.94034800
H	4.87691200	2.31595800	0.81212900
C	-5.11844000	-1.61107100	2.61930200
C	-3.74751800	-2.23641200	2.39528400
H	-5.42850600	-1.74489200	3.66193900
H	-5.05402600	-0.53988300	2.40967800
H	-3.79614400	-3.31877400	2.57800600
H	-3.46320100	-2.07492800	1.34556100
O	-2.80583400	-1.69755800	3.28293800
H	-2.63706900	-0.79057300	2.96744300
O	-6.10390300	-2.13997300	1.72759300
H	-6.21522800	-3.07917900	1.91394300
C	-4.58145700	-2.38417100	-1.23356300
C	-3.18718100	-1.85257800	-1.52472100
H	-4.98947200	-2.84619000	-2.14176200
H	-4.51781400	-3.17129500	-0.46679700
H	-3.23047500	-1.07528800	-2.29391100
H	-2.76774600	-1.37881400	-0.62635800
O	-2.35681500	-2.88336100	-2.03273400
H	-2.12317000	-3.46793300	-1.30264700
O	-5.41929900	-1.33306300	-0.79132000
H	-5.79054600	-1.59371400	0.07290300

N	-5.61523100	2.19224300	-1.25257700
C	-4.11586200	2.05920400	-1.49232600
H	-3.82773800	1.10645500	-1.04403200
H	-3.96723700	2.00212100	-2.57420900
C	-3.29218700	3.21734300	-0.92909600
H	-3.43577300	4.11372200	-1.54205500
H	-2.25116800	2.89702300	-1.03919100
O	-3.61968100	3.56624900	0.39194700
H	-3.26290000	2.85400200	0.96164300
Cl	-2.76107800	0.76569000	1.35546800
C	-6.32586200	1.30814700	-2.22624500
H	-7.39913600	1.39065100	-2.04528500
H	-6.09151000	1.64321300	-3.23728800
H	-5.99629800	0.28168300	-2.05333500
C	-5.95573800	1.72541400	0.13596900
H	-5.47010500	2.39010600	0.84482500
H	-7.04256600	1.75056100	0.23819300
H	-5.56954000	0.71213300	0.24370800
C	-6.07162500	3.60023500	-1.42827900
H	-5.78715000	3.94039700	-2.42555100
H	-7.15735200	3.62327400	-1.32356500
H	-5.59888400	4.21198900	-0.66074200
O	-1.41857500	0.78809300	-1.57558700
H	-0.46127000	0.91280200	-1.65257400
H	-1.58954000	0.66624200	-0.62478900
H	1.52047000	-2.41451800	3.40464200

## H<sub>2</sub>O-A-Cl

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C	-2.38483700	-2.14360800	2.31217200
C	-2.45214700	-0.87838200	1.46407000
C	-0.69885400	0.26740100	2.91350100
C	-0.98452500	-0.82819400	3.93889900
C	-1.15966700	-2.16860000	3.22704600
H	-2.66297400	-1.02698400	0.40219300
H	-3.55516600	-0.14007600	1.60537500
H	-3.29556500	-2.24161600	2.91534800
H	-2.36303200	-3.01128200	1.64358500
H	0.31953700	0.14665700	2.51371100
H	-0.75978800	1.27779300	3.33020900
H	-0.15675500	-0.87519300	4.65151200
H	-1.89280300	-0.58832200	4.50619600
H	-0.26076900	-2.35549400	2.62891800
H	-1.24647100	-2.98491900	3.95038800

C	-1.58555200	0.19710500	1.71323400
O	-1.55730700	1.23496200	0.93807700
C	0.12031200	-1.26470300	-0.75243000
C	-0.38554600	-2.55663500	-0.71045500
C	-1.55912000	-2.92140100	-1.36988000
C	-2.24025700	-1.95592300	-2.09727700
C	-1.73797100	-0.65260400	-2.17077200
C	-0.56143000	-0.31441400	-1.50611000
H	1.02122500	-0.99271200	-0.21134200
H	-1.91960200	-3.94192800	-1.30925100
H	-3.16245700	-2.19130200	-2.61917700
H	-0.15858000	0.69206700	-1.58215000
C	-2.45504900	0.37759900	-2.95816100
O	-3.47838100	0.16677900	-3.57138300
H	-1.98192900	1.37891800	-2.96201700
C	-9.69745800	1.14802300	0.27552100
C	-8.41831700	1.06149300	-0.55526200
H	-10.57659000	0.93321500	-0.33741400
H	-9.67496000	0.42298600	1.09591500
H	-9.83265500	2.14125300	0.71111500
C	-7.13208600	1.16138600	0.27518100
H	-8.41648900	0.10581400	-1.08990000
H	-8.42142800	1.85691300	-1.31566500
C	-5.89686900	1.15477900	-0.63145800
H	-7.06298200	0.27368600	0.91522900
H	-5.82479300	2.13346600	-1.13945400
C	-7.12127800	2.41282900	1.15554600
H	-6.16874200	2.51288900	1.68123800
H	-7.28007700	3.31300400	0.54901900
H	-7.90894500	2.37539700	1.91164100
C	-4.59855200	0.98552500	0.15514600
O	-4.63846400	0.53870100	1.33790000
O	-3.52952600	1.24817100	-0.47206600
H	-2.41751200	1.22892400	0.24045200
N	-5.90551900	0.02285800	-1.56425600
H	-6.67153900	0.14169000	-2.22055400
H	-5.05876300	0.05261400	-2.12999700
C	4.74881900	-2.16879900	-1.93306700
C	3.35891900	-2.64113100	-1.52212900
H	5.04597700	-2.65797700	-2.86794600
H	4.72630900	-1.08880800	-2.09738100
H	3.37364500	-3.72214900	-1.32636200
H	3.08288600	-2.14261000	-0.57871900
O	2.42038400	-2.41125100	-2.53300000

H	2.29511100	-1.44675100	-2.58127000
O	5.72043300	-2.40587100	-0.90995800
H	5.80404800	-3.35719600	-0.77881400
C	4.39495600	-1.55909300	1.93023500
C	3.13323800	-0.73377200	1.72066300
H	4.56074700	-1.72909500	2.99982200
H	4.25942300	-2.54427500	1.45894300
H	3.17624000	0.19510500	2.29907400
H	3.06199200	-0.44727700	0.66001200
O	1.98543400	-1.43006400	2.16488300
H	1.83819300	-2.18894300	1.58320400
O	5.51857400	-0.89828000	1.37772900
H	5.72986900	-1.35924100	0.54415800
N	5.59163000	2.68755400	0.40504100
C	4.07934500	2.76832100	0.56726800
H	3.71106100	1.74932700	0.44547000
H	3.88099200	3.09343200	1.59231900
C	3.39245300	3.72389800	-0.40946600
H	3.58745000	4.76155600	-0.11757900
H	2.32176900	3.53218000	-0.27771700
O	3.81250100	3.58495400	-1.74171100
H	3.40248900	2.76226700	-2.08226400
Cl	2.73049400	0.72124000	-1.88455100
C	6.17961100	2.17778100	1.68168600
H	7.26114200	2.10262900	1.55531000
H	5.94424300	2.88201800	2.48035900
H	5.76932100	1.18525300	1.87773100
C	5.93240600	1.71029700	-0.68555000
H	5.47873600	2.05787100	-1.60962400
H	7.02043400	1.66094100	-0.76122000
H	5.51970600	0.74272800	-0.39874200
C	6.17798300	4.02073700	0.08331000
H	5.89007800	4.72758300	0.86342000
H	7.26374600	3.91832500	0.05865900
H	5.79768100	4.33761800	-0.88694200
O	1.32078000	1.63278900	0.79904000
H	0.35800500	1.73131600	0.75964100
H	1.59026900	1.29057000	-0.07299100
Cl	0.47831100	-3.78143700	0.19360700

H<sub>2</sub>O-A-Br

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C	-2.70849400	-2.35116900	2.01426500
C	-2.73806700	-1.05616400	1.21048900

C	-0.82682800	-0.08848200	2.59155100
C	-1.07895400	-1.23464200	3.56777800
C	-1.40637300	-2.51434200	2.79930600
H	-3.00634700	-1.15424700	0.15661500
H	-3.78561200	-0.25216400	1.41569300
H	-3.55741800	-2.38600700	2.70775600
H	-2.83718800	-3.19312800	1.32655400
H	0.16518700	-0.19878000	2.12968100
H	-0.81649600	0.89425900	3.07402500
H	-0.18826100	-1.36538100	4.18622900
H	-1.91779200	-0.98762200	4.23039600
H	-0.59364900	-2.73329400	2.09452100
H	-1.47912200	-3.36691400	3.48126500
C	-1.79010800	-0.04741700	1.44864000
O	-1.74686400	1.02309500	0.72292900
C	0.33269000	-1.08677800	-0.98750400
C	0.09169300	-2.43102800	-0.75316200
C	-1.04581900	-3.08616300	-1.22211600
C	-1.97434700	-2.35334400	-1.94711700
C	-1.75584800	-0.99301200	-2.19561800
C	-0.60305300	-0.36738400	-1.72465700
H	1.23786400	-0.60637900	-0.63630100
H	-1.18826700	-4.14214200	-1.02341900
H	-2.88103300	-2.81231500	-2.32910300
H	-0.41241300	0.68261100	-1.93586300
C	-2.76982600	-0.20767400	-2.94050400
O	-3.80633600	-0.67892400	-3.35431900
H	-2.52070900	0.85952600	-3.09340500
C	-9.83441100	1.72386900	0.48654400
C	-8.62196900	1.53013200	-0.42235000
H	-10.76524600	1.63284800	-0.07910300
H	-9.84793500	0.96801800	1.27881500
H	-9.83189200	2.70745900	0.96316300
C	-7.28803300	1.45549300	0.33158500
H	-8.75495600	0.60192100	-0.98771600
H	-8.57881100	2.35104600	-1.15408500
C	-6.11720100	1.33923000	-0.65025300
H	-7.28478200	0.54337000	0.94031300
H	-5.96107200	2.32209200	-1.13142900
C	-7.08309800	2.66626400	1.24430600
H	-6.09757900	2.63955700	1.71538300
H	-7.17052400	3.59919700	0.67381800
H	-7.82643700	2.69270500	2.04445000
C	-4.80208100	1.00157000	0.04902100



O	-4.81906900	0.52148300	1.21891500
O	-3.74792100	1.17582300	-0.63348000
H	-2.62273200	1.08182100	0.04845800
N	-6.31571300	0.25078100	-1.61075400
H	-7.07142600	0.49579500	-2.24290000
H	-5.48567500	0.14787400	-2.19261200
C	5.07104100	-1.23245700	-2.19046800
C	3.75819000	-1.82611500	-1.69946900
H	5.38405000	-1.71754800	-3.12164200
H	4.93665900	-0.16454900	-2.38220900
H	3.90947100	-2.87752800	-1.41851600
H	3.45334900	-1.27551800	-0.79547100
O	2.77118500	-1.79346800	-2.69071900
H	2.50355200	-0.86100900	-2.77676200
O	6.09518300	-1.34876100	-1.19161100
H	6.36482000	-2.27362900	-1.14875200
C	4.17740200	-1.33614100	1.81040400
C	2.84484600	-0.69777400	2.16401700
H	4.68401500	-1.66360100	2.72806300
H	3.99107800	-2.22483900	1.19000800
H	3.02018400	0.22659900	2.72575400
H	2.32011100	-0.40207000	1.24446600
O	2.06449500	-1.54178500	2.98551100
H	1.72302400	-2.24943800	2.42291700
O	4.95457500	-0.38043000	1.11186100
H	5.43046400	-0.80504000	0.37221100
N	5.29065600	3.08860100	0.63278500
C	3.77536600	2.99589600	0.77961000
H	3.51048400	1.97491100	0.49551700
H	3.54607300	3.13426700	1.83996900
C	3.01245600	4.03772700	-0.04093900
H	3.11680700	5.02430700	0.42390800
H	1.96085000	3.74187500	0.03453200
O	3.45201900	4.16065100	-1.36871800
H	3.10777900	3.38078900	-1.85326000
Cl	2.56388200	1.31884700	-2.04259500
C	5.92569100	2.46801600	1.83565800
H	7.00899600	2.49703200	1.70423200
H	5.64220500	3.04791600	2.71493200
H	5.58220200	1.43422600	1.90632600
C	5.72157900	2.31688200	-0.58311000
H	5.24379100	2.76179500	-1.45229000
H	6.81006400	2.37015600	-0.64783000
H	5.38694300	1.28761700	-0.45603900

C	5.74919500	4.50356000	0.51231900
H	5.39623200	5.06112400	1.38149000
H	6.83994200	4.50499900	0.49054400
H	5.34298500	4.92097900	-0.40784800
O	1.06682500	1.67349100	0.71704300
H	0.10041200	1.69845900	0.65651800
H	1.38330900	1.55298800	-0.19781300
Br	1.38866600	-3.43382200	0.20477400