

Cucurbiturils as Promising Hydrogen Storage Materials: A Case Study of Cucurbit[7]uril

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Supporting Information

Cartesian coordinates of the optimized geometries

	(CH ₃) ₂ C ₄ H ₂ N ₄ O ₂ (CH ₃) ₂		
0 1			
C	-1.46270600	-2.56949800	-0.08840800
C	1.96411000	-2.27579100	0.05232600
N	1.39391100	-0.97623700	0.30552000
C	0.06951100	-0.77249700	0.81637600
C	1.92080200	0.16705400	-0.25495400
C	-0.06962600	0.77251000	0.81635300
N	-1.02073700	-1.19568600	-0.03497300
H	-0.02998200	-1.22483500	1.81199100
N	1.02074300	1.19568500	-0.03484500
O	2.98925500	0.25887300	-0.81321800
N	-1.39395300	0.97624100	0.30530100
H	0.02972300	1.22486400	1.81197500
C	-1.92075500	-0.16705500	-0.25524300
O	-2.98914000	-0.25888800	-0.81363700
C	1.46271200	2.56949800	-0.08824500
C	-1.96411900	2.27579000	0.05201000
H	-1.56332600	-2.99491000	0.91879600
H	-2.43656800	-2.58258200	-0.57738100
H	3.03494500	-2.14954700	-0.10359400
H	1.79950500	-2.92463000	0.91658400
H	1.56323200	2.99491900	0.91896500
H	2.43662300	2.58258200	-0.57712200
H	-3.03493700	2.14954800	-0.10402700
H	-1.79960900	2.92465100	0.91627000

H	1.53726800	-2.75029300	-0.83800600
H	-0.77201200	-3.18777500	-0.66486500
H	0.77207100	3.18776700	-0.66477500
H	-1.53717600	2.75026800	-0.83828600



0 1

C	1.74091800	2.22707500	-0.51196800
C	-1.65738900	2.49768000	-0.12877400
N	-1.24829600	1.17118500	0.26466300
C	0.05073800	0.85305600	0.78155800
C	-1.92748300	0.04565000	-0.14092800
C	-0.03918100	-0.67098000	1.02878500
N	1.15926700	0.95605600	-0.14656300
H	0.25626400	1.43654700	1.68731300
N	-1.18007500	-1.05325500	0.22117100
O	-3.00854300	0.03059400	-0.69364100
N	1.24174800	-1.14273900	0.59085600
H	-0.20750900	-0.94006300	2.07885300
C	1.90077900	-0.20478500	-0.16911400
O	2.96349900	-0.36942700	-0.73297500
C	-1.76460800	-2.37251700	0.29072200
C	1.64625300	-2.52738000	0.62244300
H	1.85502300	2.87071500	0.36789100
H	2.72407000	2.03870400	-0.94122900
H	-2.74210100	2.50361500	-0.23048000
H	-1.36725600	3.21156000	0.64622800
H	-1.85611100	-2.70495200	1.33157100
H	-2.75777200	-2.32548400	-0.15397800
H	2.72960600	-2.57001000	0.51458700
H	1.36423800	-2.96406600	1.58359900
H	-1.21805900	2.80078700	-1.08391300
H	1.12889300	2.74151900	-1.25584800
H	-1.16641900	-3.09670400	-0.26635400
H	1.19514300	-3.10954200	-0.18682500
H	-4.94284100	-1.48200800	-0.72815500
H	-3.49902200	1.52570400	-2.59588900
H	-2.66325100	-1.48781900	-2.61603200
H	3.45147000	-2.38993200	-2.04962900
H	2.54026300	0.46026900	-3.02993300
H	4.94422200	1.04644800	-1.09854500
H	-1.85565200	1.97345900	3.40739000
H	-3.46361300	-0.65959700	2.50228000
H	0.14371200	-1.70104500	-2.08836500
H	-0.24370100	0.84852800	-2.49200700

H	-3.55662600	2.03410700	-3.14033100
H	-2.44643600	-1.98805000	-3.12627100
H	-5.46987200	-2.01037500	-0.69429900
H	-1.97995700	1.64917500	2.74704200
H	-3.77726900	-0.55011500	1.83470200
H	-0.90035100	0.95848800	-2.82851300
H	0.78996800	-1.88234200	-2.41380800
H	5.47663600	1.56950800	-1.13027500
H	2.26344400	0.76742400	-3.65166900
H	3.54558900	-3.04161600	-2.40280800
H	1.94123300	-0.92394000	3.81362000
H	3.47430700	1.30554300	2.08108000
H	3.77220500	0.98939400	1.47494500
H	2.06107900	-0.82151200	3.08434700
H	0.80996200	4.16674100	2.95803300
H	0.49818100	3.85608700	2.35737900

1H₂@CB[7]

0 1

C	-5.55551200	1.81155000	0.17247800
C	-4.87772400	3.21102300	0.05753900
N	-4.12699400	3.10905700	-1.17169400
C	-4.48341700	1.98936700	-1.91126700
N	-5.31612900	1.22240300	-1.11252000
N	-4.87926500	1.21405700	1.29953700
H	-6.63761500	1.86646600	0.36609800
N	-4.12238800	3.31162700	1.27213100
H	-5.59883200	4.04006800	-0.00649100
C	-3.52412800	4.24247500	-1.82451000
O	-4.17872800	1.75764300	-3.05687400
C	-3.46119900	4.49747200	1.74034000
C	-4.12089200	2.13774700	2.00678100
O	-3.60905900	1.97043600	3.08795300
N	-2.18567600	4.77117500	1.13234600
C	-2.03342000	5.42945300	-0.14057800
C	-1.03224800	4.82641800	1.90186800
C	-0.50858500	5.76159700	-0.19356200
N	-2.23963600	4.62700300	-1.31236600
H	-2.67533900	6.32314800	-0.17966200
N	-0.03436700	5.35769900	1.10053200
O	-0.93166300	4.52750500	3.06804400
N	-0.04117400	4.99656000	-1.32064800
H	-0.30148700	6.83101700	-0.35307300
C	-1.07469000	4.39763800	-2.02552900
O	-0.98612000	3.83648900	-3.09175900

C	1.26647100	5.66994700	1.62793400
N	2.34292300	4.84098300	1.15956700
C	3.00982600	4.98741000	-0.10153800
C	2.89251400	3.84285800	1.94792400
C	4.23606700	4.03251200	0.02775200
N	2.32354700	4.47630800	-1.26493700
H	3.28900800	6.04022400	-0.25940500
N	3.93753700	3.28272700	1.22578800
O	2.56333600	3.55853600	3.07490300
N	4.22253500	3.30773100	-1.20912800
H	5.19378700	4.56246300	0.14267000
C	3.09775500	3.56833900	-1.97444800
C	1.25156200	5.17589300	-1.92242000
C	5.26730200	2.43587200	-1.67065400
C	4.89275300	2.42845200	1.88186900
O	2.86747300	3.13402900	-3.07794400
N	5.26379700	1.11238700	-1.10769700
N	5.00246800	1.10845900	1.32675800
C	5.00926600	-0.00074000	-1.89338500
C	5.80628500	0.77688100	0.18139300
C	5.80555300	-0.78569400	0.17875200
N	5.25182800	-1.11655100	-1.10729700
C	4.58694000	-0.00683700	2.03666900
N	5.01124200	-1.12015200	1.32927600
C	5.25739400	-2.43802900	-1.67547800
C	4.89704800	-2.44216600	1.87799100
O	4.01681400	-0.00804800	3.10182300
O	4.69720900	0.00088700	-3.06041900
N	4.21536900	-3.31344600	-1.21501400
N	3.93601200	-3.28954300	1.22082300
C	3.08731600	-3.56950100	-1.97695000
C	4.23033400	-4.03900600	0.02132000
C	3.00203700	-4.99143800	-0.10621000
N	2.31333100	-4.47727100	-1.26688300
O	2.85440600	-3.13223800	-3.07872600
C	1.24003600	-5.17541300	-1.92384700
N	2.33900100	-4.84581600	1.15700600
C	2.89240800	-3.84977200	1.94528700
O	2.56715800	-3.56698800	3.07377300
C	1.26111100	-5.67235900	1.62642400
N	-0.05175400	-4.99581200	-1.32020300
N	-0.03969300	-5.35692500	1.10083700
C	-1.08672400	-4.39878300	-2.02452700
C	-0.51719400	-5.76058600	-0.19206700
C	-2.04158100	-5.42717000	-0.13579300
N	-2.25055900	-4.62861900	-1.30966300

O	-1.00014500	-3.83886400	-3.09156200
C	-3.53586800	-4.24344700	-1.81928600
N	-2.18940500	-4.76457200	1.13553600
C	-1.03475700	-4.82170700	1.90309000
O	-0.93127000	-4.52128500	3.06863000
C	-3.46299600	-4.48715700	1.74595400
N	-4.13510700	-3.10708100	-1.16835100
N	-4.12309800	-3.30147000	1.27593500
C	-4.88219400	-3.20373600	0.06340100
C	-4.12105600	-2.12664400	2.00908300
C	-5.55793200	-1.80293800	0.17585200
N	-4.88123500	-1.20445100	1.30195400
C	-4.48964700	-1.98788000	-1.90943100
N	-5.31748900	-1.21620000	-1.11013800
O	-3.60742400	-1.95753500	3.08911700
O	-4.18726300	-1.75976500	-3.05638100
C	-5.32666700	0.00574100	1.93788300
C	-5.90946200	0.00297600	-1.59014700
H	5.13183200	2.31648700	-2.74859500
H	6.23567000	2.91357100	-1.46448100
H	5.88434500	2.90710200	1.85852200
H	4.55788700	2.31649300	2.91662800
H	5.88650000	-2.92473600	1.84909800
H	4.56596600	-2.33362000	2.91431300
H	5.11954900	-2.31506500	-2.75271900
H	6.22709100	-2.91480900	-1.47304000
H	1.47297700	-6.25211500	-1.95771000
H	1.17794300	-4.77729000	-2.94036500
H	1.49577800	-6.72043400	1.39250700
H	1.20197500	-5.53547700	2.70920300
H	-4.21641500	-5.10568000	-1.74499600
H	-3.39789800	-3.96870300	-2.86838300
H	-4.13570900	-5.34340800	1.59045700
H	-3.27568500	-4.34899000	2.81388200
H	-5.79338900	0.00170900	-2.67685900
H	-6.97562800	0.00400400	-1.32536600
H	-4.91269200	0.00652500	2.94999200
H	-6.42793200	0.00657700	1.98415800
H	-4.20354000	5.10603600	-1.75475700
H	-3.38369600	3.96427900	-2.87237600
H	-3.27676500	4.36191700	2.80909600
H	-4.13206800	5.35438200	1.58076500
H	6.81127200	1.21287600	0.29063600
H	6.81099400	-1.22294100	0.27824500
H	3.27889500	-6.04448900	-0.26657000
H	5.18724100	-4.57091800	0.13381400

H	-0.31132000	-6.83018600	-0.35195100
H	-2.68428200	-6.32050400	-0.17003900
H	-6.64015800	-1.85597600	0.36935000
H	1.50400200	6.71753600	1.39467800
H	1.20537000	5.53286100	2.71058000
H	1.19073700	4.77901900	-2.93949800
H	1.48513700	6.25248300	-1.95466500
H	-5.60455500	-4.03206400	0.00432900
H	-2.80664800	-0.00664900	-0.24551800
H	-2.29196000	-0.00515300	-0.78329200

2H₂@CB[7]

0 1

C	5.83375600	-0.76463500	0.10989100
C	5.80828500	0.79328700	0.19192400
N	4.92861300	1.04850800	1.30578700
C	4.62924100	-0.10476600	2.01751300
N	5.16311900	-1.16943700	1.31038700
N	5.15948900	-1.03660500	-1.13749600
H	6.85078000	-1.18464400	0.08672300
N	5.33738700	1.18587900	-1.10592600
H	6.79750600	1.23735900	0.38137500
C	4.79072900	2.33871800	1.92515200
O	4.06569100	-0.16508200	3.08419000
C	5.32627500	2.53239500	-1.60968700
C	4.98161300	0.10924200	-1.90116400
O	4.64157500	0.15446800	-3.05932900
N	4.25195900	3.36650100	-1.14424600
C	4.21348700	4.03039200	0.12563600
C	3.15563000	3.66113800	-1.93874500
C	2.99490200	4.99267700	-0.00831900
N	3.86345500	3.22319300	1.27124600
H	5.16576800	4.55204300	0.30584500
N	2.34561800	4.52377100	-1.21140100
O	2.97269300	3.28731400	-3.07272800
N	2.29026400	4.80386700	1.22535100
H	3.28118500	6.04938300	-0.12063200
C	2.79493200	3.75654400	1.97929800
O	2.41464100	3.41559500	3.07399100
C	1.29413400	5.25057100	-1.87520700
N	-0.01724900	5.05185500	-1.32523200
C	-0.52807400	5.75417300	-0.18051300
C	-1.00157000	4.37681300	-2.02937600
C	-2.05057900	5.40559100	-0.19065200

N	-0.08838900	5.29217700	1.10971600
H	-0.32788000	6.83202200	-0.28231400
N	-2.18438100	4.52881600	-1.32270900
O	-0.86667800	3.81505400	-3.09039800
N	-2.26802300	4.82382600	1.10623900
H	-2.69842000	6.28642000	-0.31954000
C	-1.13076500	4.83016600	1.89874700
C	1.19231100	5.60823600	1.68408300
C	-3.56583200	4.55687100	1.66554600
C	-3.44481400	4.13717800	-1.88859800
O	-1.07204300	4.54643400	3.07161000
N	-4.19954100	3.35032100	1.21021000
N	-4.09098600	3.03715300	-1.22087100
C	-4.20129700	2.19420200	1.97339700
C	-4.89748800	3.19754500	-0.03264500
C	-5.58126500	1.80515400	0.11141500
N	-4.91848700	1.23981500	1.26402100
C	-4.44403200	1.90273900	-1.93975500
N	-5.32621200	1.18043200	-1.15258100
C	-5.36322600	0.03904500	1.91869600
C	-5.92199300	-0.04570700	-1.60967300
O	-4.09796900	1.62674800	-3.06367300
O	-3.72247400	2.06271900	3.07450700
N	-4.90345900	-1.17805200	1.30721400
N	-5.33911800	-1.25880200	-1.10375600
C	-4.11595700	-2.06786200	2.02538800
C	-5.57572100	-1.81139300	0.19849100
C	-4.89274800	-3.21227200	0.12332300
N	-4.10615000	-3.26026900	1.32183600
O	-3.59034000	-1.86169600	3.09322600
C	-3.42206800	-4.42242000	1.81488000
N	-4.17272500	-3.16001700	-1.12625300
C	-4.52757800	-2.05810500	-1.89200600
O	-4.23713500	-1.86309700	-3.04825800
C	-3.58784400	-4.31849400	-1.75065600
N	-2.16037900	-4.70649600	1.18242500
N	-2.28753200	-4.68243100	-1.26412800
C	-0.99011600	-4.73747600	1.92840100
C	-2.03897200	-5.42456700	-0.06195100
C	-0.51303600	-5.74341900	-0.14445800
N	-0.01357400	-5.30905600	1.12926100
O	-0.86174500	-4.39034000	3.07843300
C	1.30145400	-5.59526700	1.63429600
N	-0.08044000	-4.99563100	-1.29829700
C	-1.14133700	-4.44802400	-2.00504500
O	-1.08608000	-3.92254200	-3.09151600

C	1.19747800	-5.18365000	-1.93090300
N	2.35643200	-4.76599100	1.11883600
N	2.28661200	-4.47936400	-1.31169400
C	2.99559100	-4.95856200	-0.15281900
C	2.99616300	-3.51788300	-2.01381800
C	4.24152800	-4.01879500	-0.07978800
N	4.12810500	-3.22557000	-1.27100600
C	3.01088500	-3.84341700	1.91932000
N	4.06613100	-3.33573700	1.17629100
O	2.71514400	-3.06456400	-3.09786500
O	2.74994600	-3.58002900	3.06906800
C	5.14004600	-2.33387500	-1.76155200
C	5.07630200	-2.51879700	1.79511500
H	-3.42638100	4.45785000	2.74503100
H	-4.23419000	5.40210900	1.44794200
H	-4.11974000	5.00821600	-1.89009200
H	-3.25335400	3.81493900	-2.91566000
H	-6.98943300	-0.03140900	-1.35108800
H	-5.80023700	-0.07153100	-2.69538400
H	-4.95803600	0.06284300	2.93413900
H	-6.46481200	0.03029900	1.95567000
H	-4.08814800	-5.29111400	1.70515300
H	-3.21112800	-4.24650700	2.87285000
H	-4.26309800	-5.17836700	-1.62435100
H	-3.47916300	-4.08368500	-2.81274000
H	1.54000500	-6.64742400	1.42064600
H	1.26729900	-5.43207700	2.71458400
H	1.43167600	-6.26011100	-1.95541200
H	1.10773100	-4.79950900	-2.95071900
H	4.82616200	-2.46232500	2.85760600
H	6.05781300	-2.99808800	1.66613800
H	4.93907400	-2.16874200	-2.82341400
H	6.12245600	-2.81384400	-1.63563500
H	5.78012500	2.82216100	1.97548100
H	4.40925300	2.17048400	2.93604400
H	5.22352900	2.45940700	-2.69524400
H	6.27949500	3.01446200	-1.35359100
H	-5.61313800	4.02288200	-0.16669700
H	-6.66550000	1.86825100	0.28948600
H	-5.61056800	-4.04646400	0.11114200
H	-6.65755900	-1.86460100	0.39400200
H	-2.67158300	-6.32541400	-0.03956600
H	-0.29926700	-6.81378600	-0.28781300
H	5.19881600	-4.56215400	-0.08152400
H	1.52580800	6.32730500	-1.85510000
H	1.26962000	4.89526000	-2.90897200

H	1.09960100	5.44436100	2.76067300
H	1.42746200	6.66355800	1.48390700
H	3.25640700	-6.01988600	-0.28496000
H	-2.74263500	-0.03543000	-0.31517100
H	-2.37957800	-0.09903200	-0.96195300
H	2.51883600	-1.09572100	0.02997900
H	2.00129700	-0.88595000	0.52143300

3H₂@CB[7]

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C	5.72410700	1.23343000	-0.05934100
C	5.17595600	2.69225000	0.01484800
N	4.37869500	2.68378000	1.21704200
C	4.56566500	1.53012400	1.96590400
N	5.33811800	0.67006300	1.20199600
N	5.07916600	0.70071700	-1.23435800
H	6.81758700	1.18257100	-0.17510200
N	4.47243000	2.84548000	-1.22631700
H	5.96795500	3.45276600	0.09334600
C	3.87928200	3.88136900	1.84005200
O	4.18206300	1.33659700	3.09477300
C	3.95360800	4.08551600	-1.73258400
C	4.42796100	1.67949800	-1.97177900
O	3.96503400	1.55445700	-3.08053400
N	2.70268100	4.50995900	-1.16296700
C	2.58482600	5.19853000	0.09475600
C	1.55981900	4.61134900	-1.94161700
C	1.10727400	5.70591300	0.09309300
N	2.65850700	4.39131300	1.28206500
H	3.32567100	6.01114100	0.14774200
N	0.60262500	5.25819000	-1.17612700
O	1.44149900	4.26103200	-3.09167600
N	0.54383800	5.09248200	1.26598500
H	1.02156200	6.80107300	0.16656500
C	1.47490300	4.37500900	2.00106600
O	1.30257000	3.88226400	3.09052100
C	-0.65502100	5.66659100	-1.74131900
N	-1.81475600	4.97880800	-1.24425000
C	-2.48183700	5.27157800	-0.01000800
C	-2.43787800	3.97684300	-1.96989800
C	-3.78410900	4.41789000	-0.09346600
N	-1.85690400	4.79062800	1.19995100
H	-2.67193400	6.35280900	0.06889600
N	-3.54519600	3.57071100	-1.23737200
O	-2.11331000	3.57798500	-3.06288800

N	-3.84129700	3.77382900	1.18680300
H	-4.69215200	5.01943000	-0.25220100
C	-2.71423700	4.00463900	1.95828200
C	-0.73354800	5.44081300	1.82169800
C	-4.96708900	3.03612200	1.69091900
C	-4.57577200	2.78710600	-1.86394100
O	-2.53899100	3.64355900	3.09758500
N	-5.11712800	1.69859800	1.18562200
N	-4.82411200	1.51483100	-1.24049800
C	-4.78617300	0.58870100	1.94603400
C	-5.67899100	1.35467900	-0.08791000
C	-5.85622100	-0.19100600	0.00321900
N	-5.10911100	-0.53153300	1.19159600
C	-4.72025400	0.34536100	-1.98079600
N	-5.33225300	-0.65741600	-1.24636500
C	-5.16140500	-1.82845400	1.81084700
C	-5.44032700	-2.00205200	-1.74336400
O	-4.24153400	0.23259100	-3.08416300
O	-4.35730500	0.59540900	3.07518000
N	-4.27661000	-2.80135800	1.22991100
N	-4.50281800	-2.95056500	-1.20641400
C	-3.27752700	-3.38763100	1.99478500
C	-4.61713500	-3.59153100	0.07154400
C	-3.49080300	-4.67008500	0.03464400
N	-2.80342800	-4.47448200	1.27898000
O	-2.93036600	-3.05141600	3.10182200
C	-1.80693700	-5.35941100	1.81729800
N	-2.76345400	-4.34554100	-1.16806600
C	-3.42309700	-3.40484000	-1.94591200
O	-3.14635100	-3.08768900	-3.07822500
C	-1.78434200	-5.21892800	-1.75791700
N	-0.48904000	-5.22449700	1.25888000
N	-0.46929500	-5.11787600	-1.18723900
C	0.55882100	-4.68700600	1.98941000
C	-0.06685100	-5.80279100	0.01465100
C	1.48251000	-5.61263900	0.03334100
N	1.70489100	-4.82830400	1.22133900
O	0.49502100	-4.23718900	3.10881900
C	3.00514900	-4.60077100	1.79072300
N	1.75482000	-4.97384900	-1.22305400
C	0.61014900	-4.71953600	-1.96130200
O	0.56518800	-4.29032200	-3.08971600
C	3.06766000	-4.79844800	-1.78211100
N	3.74861400	-3.52967200	1.18275800
N	3.82030900	-3.69015900	-1.26242600
C	4.53336800	-3.68996400	-0.01722900

C	4.01025400	-2.53076300	-1.99536900
C	5.36297700	-2.36952300	-0.07653000
N	4.83423800	-1.70509900	-1.24329300
C	4.16111800	-2.44419300	1.94271500
N	5.10078400	-1.75584300	1.19273800
O	3.58936500	-2.30726500	-3.10536900
O	3.81535800	-2.18358700	3.07035700
C	5.44499100	-0.54923800	-1.84216000
C	5.78143600	-0.59983800	1.70997700
H	-4.82996300	2.95190100	2.77174100
H	-5.88509400	3.59804800	1.47080400
H	-5.51174700	3.36982600	-1.88222600
H	-4.24744400	2.58311500	-2.88675100
H	-6.45892200	-2.36461100	-1.54970900
H	-5.25756500	-1.95599800	-2.81983300
H	-4.85694700	-1.69666200	2.85277800
H	-6.19424200	-2.21088300	1.76870200
H	-2.14597200	-6.39574000	1.67785500
H	-1.72299900	-5.13395400	2.88344000
H	-2.13387800	-6.26065100	-1.67401700
H	-1.69827700	-4.93983500	-2.81156400
H	3.59252100	-5.53082200	1.72516000
H	2.85334200	-4.33171500	2.83944700
H	3.64467900	-5.72066900	-1.62481000
H	2.93418000	-4.61864000	-2.85177600
H	5.60494400	-0.58688300	2.78842400
H	6.85594000	-0.70575200	1.50655300
H	5.10788000	-0.51101600	-2.88168200
H	6.54058500	-0.66127700	-1.80758100
H	4.64991500	4.66614700	1.78369600
H	3.67688200	3.63487700	2.88574100
H	3.78171200	3.94591800	-2.80293900
H	4.70667300	4.87119500	-1.57255400
H	-6.62663200	1.89350000	-0.23969700
H	-6.90538000	-0.50472600	0.11342300
H	-3.87605100	-5.69962100	-0.02432600
H	-5.62491500	-4.01816300	0.19036800
H	-0.37583300	-6.85853700	-0.03268600
H	2.03676600	-6.56160800	0.09967300
H	6.44383900	-2.53816500	-0.19779600
H	-0.79195700	6.74391900	-1.57074300
H	-0.59612200	5.46286000	-2.81344900
H	-0.72665200	5.12820200	2.86947400
H	-0.86434700	6.53253200	1.75697000
H	5.15686800	-4.59408900	0.05742200
H	-2.52772200	-0.91840800	-0.25006700

H	-2.16583900	-0.80325200	-0.89026600
H	-0.28337900	2.15532700	-0.65435100
H	-0.31656400	2.69092800	-0.13887900
H	2.24095000	-0.25484100	0.69471200
H	2.76828300	-0.28334600	0.17024300

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C	-1.98592500	-5.47224900	0.14191800
C	-0.45675600	-5.79203500	0.17213900
N	0.00796400	-5.08455500	1.33479200
C	-1.01424900	-4.46644800	2.03596300
N	-2.17718500	-4.65335600	1.30715600
N	-2.16756900	-4.83774000	-1.13727200
H	-2.61941500	-6.37041000	0.20663700
N	0.00895800	-5.31818500	-1.10361100
H	-0.23949800	-6.86637300	0.27548800
C	1.31308900	-5.24584100	1.91101400
O	-0.92118100	-3.92204600	3.11048400
C	1.30744800	-5.60550000	-1.65076700
C	-1.01156700	-4.82707100	-1.90206900
O	-0.92257100	-4.50894100	-3.06415400
N	2.37598000	-4.77510600	-1.16882100
C	3.04951500	-4.95411400	0.08492900
C	2.94850700	-3.78968800	-1.95643900
C	4.26609000	-3.98198100	-0.01692100
N	2.35731200	-4.49508800	1.26428500
H	3.34231200	-6.00813400	0.20744000
N	4.00159500	-3.24986500	-1.23101200
O	2.63137000	-3.50096900	-3.08560100
N	4.20224800	-3.24401000	1.21173200
H	5.23412200	-4.50032300	-0.09394800
C	3.09481800	-3.56321300	1.98046400
O	2.85245400	-3.15268000	3.09031400
C	4.96933800	-2.39978300	-1.87398600
N	5.06335500	-1.06935700	-1.34279000
C	5.79659000	-0.70583200	-0.16398900
C	4.55783400	0.02320600	-2.02774000
C	5.76172100	0.85544500	-0.18574900
N	5.19322600	-1.03248200	1.10390900
H	6.81498000	-1.12074000	-0.21303600
N	4.90132900	1.15376400	-1.30147900
O	3.98277100	-0.00092500	-3.08977800
N	5.26666600	1.19533200	1.11897500

H	6.75147200	1.31170300	-0.34163700
C	4.98007200	0.08619400	1.89705900
C	5.21835300	-2.34786600	1.68706400
C	5.24683700	2.52364500	1.66846000
C	4.77415200	2.46272900	-1.88069800
O	4.66651600	0.08918600	3.06358000
N	4.18045000	3.37228700	1.21214600
N	3.83561600	3.32669400	-1.21472500
C	3.04809100	3.60025600	1.97683200
C	4.16366400	4.08678500	-0.03006900
C	2.93798700	5.03609000	0.11887500
N	2.25044700	4.48909800	1.26701400
C	2.79545000	3.90303400	-1.93126600
N	2.27613800	4.92000400	-1.14622300
C	1.16591200	5.16306600	1.92943300
C	1.20331800	5.76024100	-1.60365300
O	2.44732200	3.61580200	-3.05177600
O	2.82765000	3.15746700	3.07873300
N	-0.11813900	4.97972600	1.30877800
N	-0.10490600	5.44668300	-1.09683000
C	-1.15921200	4.39536700	2.01807700
C	-0.58883500	5.78744100	0.20961400
C	-2.10678700	5.43415700	0.13367500
N	-2.32508500	4.65769700	1.31936300
O	-1.07276400	3.82154500	3.07751900
C	-3.60893900	4.24670800	1.81215700
N	-2.22066300	4.74221700	-1.12721000
C	-1.06843000	4.85103400	-1.89368200
O	-0.94694800	4.54466000	-3.05591800
C	-3.48144200	4.43963600	-1.75311700
N	-4.17270100	3.08928400	1.16629800
N	-4.12934300	3.24970300	-1.27880300
C	-4.51133800	1.96950200	1.91399500
C	-4.90437200	3.15639800	-0.07625700
C	-5.55766200	1.74406800	-0.17961400
N	-5.31333900	1.17285000	1.11286900
O	-4.21752800	1.75876500	3.06647300
C	-5.88347800	-0.05417400	1.59857200
N	-4.86801600	1.14558500	-1.29777400
C	-4.10832200	2.07005300	-2.00292300
O	-3.58146100	1.89766300	-3.07608100
C	-5.30308900	-0.06754400	-1.93534300
N	-5.27380500	-1.26479300	1.11916100
N	-4.85039900	-1.27271000	-1.29495900
C	-5.51948300	-1.86339900	-0.15985700
C	-4.10619300	-2.20415000	-2.00745500

C	-4.83749900	-3.25922500	-0.03962400
N	-4.10262300	-3.37347000	-1.26483100
C	-4.42560500	-2.01950000	1.91330000
N	-4.06552300	-3.13993700	1.17519500
O	-3.60879400	-2.04591000	-3.09657900
O	-4.11082700	-1.77846200	3.05410700
C	-3.44934600	-4.56567400	-1.72960400
C	-3.45629700	-4.26851800	1.83124600
H	5.12595400	2.41098200	2.74874800
H	6.20277600	3.01793700	1.44686100
H	5.76524000	2.94453600	-1.89672900
H	4.41007200	2.32966800	-2.90307600
H	1.44268500	6.80137500	-1.34769000
H	1.15012700	5.64494500	-2.68911100
H	1.09949000	4.74297500	2.93687500
H	1.38638600	6.24164800	1.98872000
H	-4.30639500	5.09261800	1.71669600
H	-3.48156700	3.98743800	2.86637100
H	-4.17014600	5.28698300	-1.61772100
H	-3.27654200	4.29265300	-2.81666500
H	-6.95108800	-0.07398900	1.34008100
H	-5.76142700	-0.04792800	2.68461000
H	-6.40425500	-0.07454000	-1.98622700
H	-4.88508400	-0.06707100	-2.94578600
H	-3.30391300	-3.98285000	2.87552200
H	-4.13768100	-5.13203000	1.77549400
H	-3.27922100	-4.44014000	-2.80189700
H	-4.11880300	-5.41964200	-1.55229400
H	1.57732700	-6.31516100	1.90150900
H	1.25525500	-4.88589600	2.94185200
H	1.23687400	-5.44333500	-2.72940000
H	1.55788100	-6.65639300	-1.44444400
H	5.11676000	4.61865600	-0.17101600
H	3.21437300	6.08484500	0.30560200
H	-2.76126900	6.31929200	0.13853700
H	-0.39837000	6.85179500	0.41569200
H	-5.63960700	3.97456500	-0.03831400
H	-6.63983500	1.77797500	-0.37783800
H	-5.55572600	-4.08874100	0.04724000
H	5.96146700	-2.87243100	-1.81501300
H	4.66179600	-2.30660300	-2.91886100
H	5.05643600	-2.21844000	2.76038900
H	6.20212600	-2.80670400	1.50831500
H	-6.60262900	-1.92218900	-0.34669200
H	0.53202400	2.64766900	-0.30506200
H	0.42005400	2.29498600	-0.95109000

H	1.95172500	-0.75883700	-0.19667600
H	2.55889200	-1.08916900	0.07839200
H	-2.26485000	0.02213000	0.79164000
H	-2.78386400	0.01626500	0.25786900
H	-0.23711300	-2.46800900	-0.13483700
H	-0.96604100	-2.33822400	-0.06320600

5H₂@CB[7]

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C	1.98097900	5.46317900	0.06806700
C	3.36397000	4.75413000	-0.04234300
N	3.21475400	3.93311800	-1.22178900
C	2.09288800	4.28609300	-1.96132500
N	1.36577600	5.18274300	-1.19563200
N	1.39214000	4.84415600	1.23283000
H	2.05968600	6.55095900	0.21663700
N	3.48418500	4.07065300	1.21161300
H	4.20308300	5.45459600	-0.17155900
C	4.32658800	3.28686500	-1.87128100
O	1.83098900	3.92863500	-3.08494000
C	4.67047100	3.41403100	1.68706100
C	2.32298800	4.11814600	1.96533500
O	2.17069900	3.66781700	3.07555500
N	4.91810100	2.10958400	1.13510000
C	5.53648200	1.87344900	-0.14183400
C	4.87002600	0.97514500	1.92970400
C	5.84719400	0.34236900	-0.11639900
N	4.70380000	2.02361400	-1.30458700
H	6.43756100	2.49806600	-0.24171200
N	5.33229000	-0.08020700	1.15956000
O	4.54600400	0.92740000	3.09248600
N	5.17343600	-0.15380500	-1.28438500
H	6.92274100	0.11619900	-0.18059400
C	4.54029100	0.84200300	-2.00928000
O	4.00252500	0.71525600	-3.08366400
C	5.57369000	-1.37244800	1.74267400
N	4.73093400	-2.43316900	1.26430900
C	4.92568400	-3.15446300	0.04166400
C	3.63402700	-2.87780900	1.98354700
C	3.89927500	-4.32157300	0.14791700
N	4.53263600	-2.48799400	-1.17793900
H	5.96930500	-3.49617100	-0.03224500
N	3.06775500	-3.92181800	1.26112700
O	3.27595100	-2.47457400	3.06417900
N	3.28647100	-4.33744500	-1.14761800

H	4.36652800	-5.29625300	0.35551800
C	3.65816500	-3.25800000	-1.93268800
C	5.33675000	-1.47712600	-1.81520900
C	2.39278500	-5.35392300	-1.63202900
C	2.13788900	-4.81201800	1.90440800
O	3.33034300	-3.05975900	-3.07831200
N	1.04051100	-5.29215700	-1.14767500
N	0.85336300	-4.89838600	1.26382100
C	0.00622900	-4.80007100	-1.92717900
C	0.59646500	-5.75931300	0.13233100
C	-0.95511200	-5.71487500	0.01199800
N	-1.16003300	-4.93369000	-1.18581500
C	-0.30247800	-4.62947000	1.98695400
N	-1.36711900	-5.11860100	1.24758800
C	-2.44157400	-4.80553500	-1.82496400
C	-2.71896800	-5.07536600	1.73625500
O	-0.36408700	-4.12053000	3.08056600
O	0.09606300	-4.38963500	-3.05969500
N	-3.30226400	-3.81214700	-1.24132200
N	-3.55778700	-4.04513600	1.18758900
C	-3.74713200	-2.74121600	-2.00605200
C	-4.16324300	-4.07568600	-0.11276900
C	-5.11264300	-2.83731100	-0.09411400
N	-4.79601500	-2.15746800	-1.31666400
O	-3.33760100	-2.41862000	-3.09558000
C	-5.53657700	-1.05135700	-1.85750100
N	-4.75711600	-2.16605300	1.13175000
C	-3.92075000	-2.93323300	1.92965600
O	-3.61540000	-2.70706300	3.07639800
C	-5.54307700	-1.10561200	1.70636000
N	-5.24943200	0.23004100	-1.27228100
N	-5.27244800	0.20139900	1.17694600
C	-4.60483200	1.22195800	-1.99327800
C	-5.82773300	0.71259600	-0.04752400
C	-5.42363000	2.22237200	-0.02424800
N	-4.64602400	2.37443500	-1.22571700
O	-4.14895300	1.11809300	-3.10724600
C	-4.21280100	3.63470100	-1.75958200
N	-4.72719200	2.36078100	1.22622600
C	-4.68755800	1.18437000	1.95754500
O	-4.27823500	1.05469800	3.08682200
C	-4.34451200	3.61539000	1.81383700
N	-3.02388800	4.17279800	-1.15097200
N	-3.13828600	4.19817200	1.29436000
C	-3.04848100	4.93987900	0.07075000
C	-1.95492200	4.19484300	2.01404900

C	-1.62092400	5.56303700	0.13030300
N	-1.02456100	4.90825200	1.26938400
C	-1.90509400	4.45417100	-1.92410400
N	-1.07090700	5.25180400	-1.15704000
O	-1.78307800	3.71590100	3.10930800
O	-1.72091800	4.11991600	-3.06999500
C	0.20511700	5.34433800	1.87273200
C	0.15554500	5.78751400	-1.68206500
H	2.34431700	-5.23540000	-2.71728900
H	2.81040600	-6.33746700	-1.37871200
H	2.58383000	-5.81884400	1.96395200
H	1.96729500	-4.42355100	2.91220800
H	-3.18670800	-6.05139200	1.54773500
H	-2.66283700	-4.89029600	2.81179300
H	-2.25315400	-4.50559700	-2.85932900
H	-2.95592400	-5.78047200	-1.80760500
H	-6.61004900	-1.26082300	-1.74593300
H	-5.27757900	-0.98079900	-2.91697700
H	-6.61148400	-1.33199500	1.56542600
H	-5.30668300	-1.07374500	2.77332000
H	-5.03088100	4.36567200	-1.66053100
H	-3.98538500	3.47376000	-2.81677700
H	-5.16433800	4.33703100	1.68662000
H	-4.17458400	3.42714500	2.87697300
H	0.13215500	5.62427700	-2.76241400
H	0.19261700	6.86398100	-1.46523600
H	0.21203100	4.96647400	2.89884900
H	0.23357600	6.44637900	1.88010100
H	5.19808600	3.96069700	-1.85313700
H	4.02455300	3.09922100	-2.90518000
H	4.55120900	3.28049900	2.76527700
H	5.53358300	4.06286000	1.48060400
H	0.99371400	-6.76783000	0.32351800
H	-1.41524000	-6.70865000	-0.09953700
H	-6.18007100	-3.10641500	-0.07977700
H	-4.69152300	-5.03003800	-0.25968900
H	-6.91705500	0.55409100	-0.06060100
H	-6.28709500	2.90480500	-0.04853300
H	-1.62673900	6.65321000	0.28332600
H	6.62123500	-1.65731900	1.56936000
H	5.38705200	-1.26977900	2.81468000
H	5.03142300	-1.44574700	-2.86461600
H	6.39933600	-1.75721900	-1.74215600
H	-3.85057500	5.69258500	0.02747200
H	-1.41055500	-2.26940500	0.37995600
H	-1.29153400	-1.92508500	1.02922800

H	1.09557800	-2.09712700	-1.05003100
H	1.20523800	-2.43524600	-0.39580600
H	-2.45284600	0.37626200	0.08782500
H	-2.33998000	1.10511500	-0.00996800
H	0.09717000	2.22429200	-0.78340300
H	0.11723300	2.74378900	-0.25032000
H	2.52167600	0.10549400	0.18608600
H	2.40587400	0.83555000	0.10249200

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C	3.49257800	-4.64980100	-0.13069900
C	4.61067300	-3.56396600	-0.10877600
N	4.35930000	-2.85429000	1.12172700
C	3.43133100	-3.50426300	1.92064500
N	2.90752500	-4.54522000	1.17487600
N	2.66865000	-4.25319400	-1.24808300
H	3.87765000	-5.66807900	-0.29132700
N	4.39094200	-2.83866400	-1.32648900
H	5.62700400	-3.98579400	-0.09946800
C	5.29747600	-1.92723000	1.69936000
O	3.17712500	-3.25219100	3.07611500
C	5.28805200	-1.85697200	-1.87043900
C	3.26560500	-3.25988400	-2.01136100
O	2.90857000	-2.88259200	-3.10345100
N	5.19974900	-0.54989600	-1.27773300
C	5.84894500	-0.16761400	-0.05259900
C	4.72827100	0.53389100	-1.99799700
C	5.67858600	1.38543800	-0.02126100
N	5.22579600	-0.59391500	1.17169700
H	6.90105700	-0.49024100	-0.07010300
N	4.94711200	1.66250900	-1.22895600
O	4.27324900	0.50651500	-3.11890500
N	4.99362900	1.62043300	1.22192100
H	6.63538700	1.92895100	-0.02990300
C	4.78652100	0.46206500	1.94979300
O	4.36449000	0.39084900	3.08165700
C	4.72317800	2.97917800	-1.75763500
N	3.62497200	3.68972100	-1.15556800
C	3.75096100	4.43722800	0.07185500
C	2.56389900	4.13082500	-1.93152600
C	2.43124500	5.26591100	0.12171700
N	3.71553400	3.68323500	1.29133700
H	4.65704700	5.06121600	0.04158600
N	1.84917100	5.03797800	-1.16929900

O	2.34305300	3.83317800	-3.08302400
N	1.73525300	4.70705600	1.25563200
H	2.59736000	6.34267100	0.27660500
C	2.54343200	3.86248100	2.00324300
C	4.81254900	2.91781300	1.81543400
C	0.59132800	5.33421200	1.86117000
C	0.71340000	5.74300800	-1.69806800
O	2.29822700	3.42174600	3.10234700
N	-0.66070500	5.02364600	1.22488400
N	-0.56962200	5.31939900	-1.20649600
C	-1.69010400	4.44706100	1.95337400
C	-1.14361300	5.70867600	0.04823200
C	-2.61682000	5.21296700	-0.06298800
N	-2.83992700	4.55615900	1.19208300
C	-1.42277800	4.54116900	-1.96980800
N	-2.58932400	4.37486000	-1.23873700
C	-4.11542000	4.10271900	1.67464500
C	-3.78132700	3.88023100	-1.87699400
O	-1.21398100	4.14115000	-3.09200500
O	-1.61323800	3.99521500	3.07288500
N	-4.56470600	2.84438400	1.14361000
N	-4.32618600	2.68869100	-1.28931800
C	-4.67078000	1.72093100	1.94460900
C	-5.19161800	2.67988400	-0.13981000
C	-5.72163400	1.21123600	-0.09844600
N	-5.27412600	0.73385000	1.18453100
O	-4.35859300	1.63983400	3.11082500
C	-5.68151900	-0.51444900	1.77065600
N	-5.12344400	0.60895900	-1.25818800
C	-4.34511500	1.49273500	-1.98515100
O	-3.83484000	1.27993300	-3.06119700
C	-5.50011400	-0.66831800	-1.79537800
N	-4.99582300	-1.67628600	1.27550600
N	-4.86469600	-1.79630600	-1.16559300
C	-3.98446800	-2.29096700	1.99128900
C	-5.33038700	-2.37765100	0.07125800
C	-4.49722100	-3.68997500	0.17488600
N	-3.60132800	-3.41790200	1.27632300
O	-3.56305800	-1.94841300	3.07178800
C	-2.82003600	-4.44015800	1.92040900
N	-3.90788000	-3.80862000	-1.12679900
C	-4.12336600	-2.69339500	-1.91768100
O	-3.78503700	-2.55788900	-3.07141600
C	-3.18568700	-4.95322100	-1.61093200
N	-1.56822200	-4.72570600	1.27193900
N	-1.83564700	-5.09346700	-1.13640200

C	-1.45645800	-5.61950600	0.14127900
C	-0.74513500	-4.75852800	-1.92023500
C	0.08208200	-5.81200100	0.00752000
N	0.39263100	-5.06219400	-1.18806900
C	-0.38205900	-4.64732000	1.98811000
N	0.58882000	-5.29248700	1.24306800
O	-0.78063900	-4.34279100	-3.05573700
O	-0.23646100	-4.16349500	3.08723500
C	1.67591000	-5.11306800	-1.83484800
C	1.93585400	-5.45281900	1.72094800
H	0.52694000	4.96688100	2.88881300
H	0.73723300	6.42607200	1.86754900
H	0.83318200	6.81444100	-1.48762100
H	0.71358300	5.57242500	-2.77745800
H	-4.55107100	4.66744000	-1.86769700
H	-3.51378700	3.63926900	-2.90915500
H	-4.02072000	3.97123700	2.75545000
H	-4.86585000	4.87452400	1.45383600
H	-6.76005800	-0.65527900	1.61350000
H	-5.46909900	-0.44240000	2.83999300
H	-6.59296300	-0.77607200	-1.72292400
H	-5.19753300	-0.68261800	-2.84556200
H	-3.41676300	-5.36475100	1.98605400
H	-2.58559900	-4.08188300	2.92639100
H	-3.74416500	-5.86084700	-1.34634300
H	-3.12994000	-4.85177900	-2.69740800
H	1.91659500	-5.27716000	2.79905500
H	2.25513900	-6.48319900	1.51561500
H	1.52629300	-4.78007400	-2.86534700
H	2.04874100	-6.14985200	-1.83220500
H	6.31880600	-2.31396900	1.56129600
H	5.06750800	-1.86194100	2.76608200
H	5.03581500	-1.74272000	-2.92772000
H	6.31747000	-2.22903200	-1.76813200
H	-1.05557700	6.79716900	0.18225800
H	-3.34459500	6.02744400	-0.19599900
H	-6.81786800	1.14042100	-0.16407600
H	-5.98866200	3.42851700	-0.26502800
H	-6.41585900	-2.55079500	0.02388600
H	-5.10664200	-4.57891600	0.39669600
H	0.38318400	-6.86323600	-0.11338200
H	5.64449100	3.57050300	-1.64483800
H	4.48774800	2.86375400	-2.81861100
H	4.61164900	2.75620400	2.87726800
H	5.73799800	3.49832200	1.69452600
H	-1.99872800	-6.55579600	0.34094700

H	-2.14440500	0.96823100	0.18863100
H	-2.61997600	0.39649500	0.18454500
H	0.30544100	2.20275400	-0.74840400
H	0.32811800	2.72560400	-0.21859200
H	-1.41335200	-1.91250400	-1.09868000
H	-1.53630800	-2.24148400	-0.44230500
H	0.93844100	-2.11638200	1.05936900
H	1.03110100	-2.46114800	0.40605200
H	2.44327400	0.62616700	-0.04219300
H	2.53511400	-0.10680300	0.04634500
H	-5.19592300	-3.83073500	3.88337500
H	-5.68498700	-4.34918300	3.66805800
H	0.07124800	-7.23427300	3.95714100
H	-0.03069500	-6.50348900	4.05850900
H	6.03785700	-4.79066800	3.20877400
H	5.43351700	-4.47892200	3.51206300
H	6.57260700	1.30851700	3.91304900
H	7.23400000	1.63476200	3.80852500
H	3.03473500	5.88388400	3.76893000
H	3.18329600	6.54446000	3.45948200
H	-1.53060900	6.42412800	3.87283200
H	-1.43797100	7.15118100	3.74072500
H	-7.51884300	1.54137900	3.66816200
H	-6.78891100	1.62990000	3.78757800
H	-6.19059300	1.50442800	-4.04912500
H	-6.92017500	1.59662700	-3.93158500
H	-6.17905100	-3.00650700	-3.76374300
H	-6.90328300	-3.12589700	-3.63705800
H	-0.15943700	-6.68441700	-3.82319500
H	-0.00551300	-7.40305700	-3.70242500
H	7.10521200	1.83634100	-3.85240300
H	6.44489700	1.50864800	-3.95893200
H	4.44687500	-5.73698000	-3.50962200
H	4.12662000	-5.13245200	-3.80319900
H	-3.22037700	6.65442000	-3.57541400
H	-2.73511900	6.13123800	-3.78806300
H	4.76474000	5.95518900	-3.40377400
H	4.24562700	5.47067300	-3.62808300

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C	5.27216400	2.57553000	0.09659600
C	4.38401800	3.85067700	0.19828600

N	3.47907100	3.53107900	1.28033700
C	3.89138000	2.40864000	1.98547600
N	4.94828200	1.85237100	1.29074900
N	4.85042600	1.98545700	-1.15294400
H	6.35010400	2.79317800	0.06835900
N	3.81274600	3.95745700	-1.11214200
H	4.95183900	4.76153000	0.43956200
C	2.65782400	4.51819900	1.93120000
O	3.45090500	2.02849300	3.04657100
C	3.03619400	5.06931500	-1.58653600
C	4.07649300	2.85574100	-1.90563600
O	3.75041500	2.70970800	-3.06160300
N	1.67626600	5.12847700	-1.12335900
C	1.26074800	5.64799900	0.14486200
C	0.61205600	4.71290800	-1.90188800
C	-0.28163400	5.76900800	-0.00617000
N	1.39853800	4.76482300	1.28133600
H	1.75981700	6.60790300	0.34324100
N	-0.54670800	4.97756300	-1.18770800
O	0.68080600	4.25996000	-3.02253200
N	-0.77552200	5.25398100	1.23615800
H	-0.63034700	6.80177500	-0.15292400
C	0.21198600	4.64393800	1.98805100
O	0.07799700	4.15235600	3.08620100
C	-1.82449500	4.96211300	-1.84888000
N	-2.79392400	4.08332500	-1.25047500
C	-3.64037100	4.47145000	-0.14614900
C	-3.33787000	3.04146600	-1.98827600
C	-4.71538200	3.34431000	-0.10952300
N	-3.06112700	4.41425700	1.16542900
H	-4.06266000	5.47042300	-0.32935900
N	-4.45584200	2.59612500	-1.30523400
O	-2.94739900	2.63997500	-3.06030700
N	-4.44969400	2.67375800	1.13915200
H	-5.74686400	3.72677300	-0.12380200
C	-3.54549100	3.36568700	1.92598800
C	-2.13188400	5.37172400	1.69918700
C	-5.33772300	1.69781500	1.71215000
C	-5.34278000	1.61031500	-1.86132600
O	-3.27335400	3.13759500	3.08361700
N	-5.19874200	0.37295600	1.17312000
N	-5.24917300	0.30066400	-1.27725400
C	-4.73189900	-0.66657000	1.95809400
C	-5.84906200	-0.08328200	-0.02801200
C	-5.63503800	-1.62951500	0.01214800
N	-4.95138800	-1.83856500	1.25902700

C	-4.73434300	-0.77175200	-1.98161400
N	-4.88539100	-1.89380400	-1.18733300
C	-4.70381500	-3.12796800	1.84355000
C	-4.65263600	-3.20913600	-1.71560100
O	-4.29347600	-0.74837900	-3.10879800
O	-4.27849700	-0.56842000	3.07626000
N	-3.57385300	-3.83828100	1.30890600
N	-3.52446800	-3.89226800	-1.13968100
C	-2.37622000	-3.92313300	1.99235300
C	-3.58707700	-4.61894600	0.10543500
C	-2.21986000	-5.36782100	0.14663000
N	-1.53173000	-4.73311500	1.24765500
O	-2.13266000	-3.43390100	3.07258100
C	-0.34899900	-5.28112200	1.85772200
N	-1.68373700	-5.14633400	-1.16506800
C	-2.45522700	-4.28695100	-1.92498800
O	-2.26185100	-3.98934400	-3.08299100
C	-0.51254300	-5.78595000	-1.70029700
N	0.87782200	-4.93336100	1.19322100
N	0.74672300	-5.27988100	-1.22740400
C	1.90843300	-4.33131800	1.89927400
C	1.35909900	-5.62765000	0.01989100
C	2.80932200	-5.08440800	-0.12848500
N	3.04828900	-4.43044700	1.12306600
O	1.84213300	-3.86207200	3.01302200
C	4.33662400	-4.00012200	1.59458300
N	2.71316600	-4.23527400	-1.29384900
C	1.54428800	-4.45826300	-2.00323400
O	1.28940400	-4.06346600	-3.11904800
C	3.85894400	-3.64605900	-1.93158900
N	4.78715100	-2.72513600	1.10867500
N	4.35072200	-2.45496900	-1.28958600
C	5.30643700	-2.48024900	-0.20609100
C	4.39291800	-1.25993000	-1.99388900
C	5.79243700	-1.00104400	-0.12643400
N	5.23300900	-0.40635800	-1.30598300
C	4.75941800	-1.59118200	1.89947600
N	5.26426800	-0.54941300	1.13864600
O	3.84735100	-1.03458600	-3.05043000
O	4.42137600	-1.53364200	3.06020100
C	5.55486100	0.90531400	-1.79450600
C	5.64791000	0.69051900	1.76207000
H	-5.10672300	1.63860700	2.77822900
H	-6.37834900	2.02986600	1.57682200
H	-6.37455500	1.97604500	-1.76343300
H	-5.08564600	1.50488300	-2.91784500

H	-5.55873900	-3.81726300	-1.57221300
H	-4.45137300	-3.09576400	-2.78345100
H	-4.51041400	-2.96619500	2.90608700
H	-5.59884200	-3.75292100	1.72145600
H	-0.44221300	-6.37836400	1.90382300
H	-0.29194100	-4.87476500	2.87077100
H	-0.56366700	-6.86085900	-1.48174200
H	-0.53593900	-5.62738500	-2.78083900
H	5.07641100	-4.76402800	1.32244500
H	4.27365000	-3.91898300	2.68159000
H	4.67167800	-4.38788100	-1.98335700
H	3.55441700	-3.36731300	-2.94337500
H	5.43356500	0.58618700	2.82767400
H	6.72512900	0.85423200	1.61665900
H	5.28499600	0.93929600	-2.85270300
H	6.63829200	1.05858600	-1.68301500
H	3.21977200	5.46277700	2.00975900
H	2.43279700	4.14286400	2.93294000
H	3.00454300	4.99255800	-2.67508600
H	3.54040500	6.00066500	-1.29921500
H	-6.90923600	0.21083300	-0.01470300
H	-6.57610700	-2.19994800	-0.00076700
H	-2.31937600	-6.44691700	0.33646700
H	-4.45524200	-5.29466700	0.10518800
H	1.30997800	-6.71575500	0.17464000
H	3.55979600	-5.87220400	-0.29166200
H	6.88761800	-0.89856900	-0.13722200
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H	-1.65262900	4.60842700	-2.86844400
H	-2.11891900	5.22783300	2.78143800
H	-2.49036800	6.38258800	1.46513500
H	6.11191300	-3.19405100	-0.43365400
H	-2.41146900	-0.71597800	-0.11808200
H	-0.99943600	2.04859100	1.09354200
H	1.42851100	1.89514900	-1.03652100
H	2.20811800	-1.70374500	0.30653600
H	-0.34228500	-2.61962000	-0.46185500
H	-0.62040000	-1.52288100	2.27468300
H	1.44293100	6.98882400	3.84011900
H	-1.74489700	5.38183600	5.40585800
H	4.99668000	1.57842900	4.92208100
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H	-4.93613100	2.73325100	4.88657500
H	-4.80115400	-2.52322400	5.54461400
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H	-6.96321600	-1.79309100	-3.34433100
H	-2.78858100	-6.38467900	-3.77737700
H	-3.75642500	4.56342200	-4.39420100
H	2.89572100	-4.57096900	-4.94373400
H	-0.92381800	5.70616000	-5.35133300
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H	1.52256800	7.38016200	-3.39096400
H	-5.84825800	0.09762600	-4.78581000
H	-5.72644200	4.88584800	-2.49545900
H	-3.98873700	-4.15406600	-4.86216600
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H	0.83275700	-5.61887100	5.44976200
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H	1.55389900	2.23093700	-0.38400800
H	1.91124400	-1.39885000	0.91729000
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H	6.61327200	-2.78287800	-3.51856100
H	4.15539600	-3.31636200	4.92757800
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H	5.06436100	-0.21966300	-5.00531400
H	5.58981400	-0.01550800	-5.49262800
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H	4.41743900	-3.89388200	5.31810500
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C	-0.30971300	5.71150100	1.76383300
C	-2.28286900	4.26177200	1.99188800
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O	1.81750600	3.73596300	-2.96623000
C	4.05653400	3.53639200	1.89972600
N	4.47787500	2.30991400	1.27387600
C	5.37591800	2.27717800	0.14115600
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C	5.81034900	0.78351000	0.07551800
N	4.79842200	2.50582100	-1.15202700
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O	4.02455900	0.94485400	3.09544600

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O	4.30362300	1.27654600	-3.05057100
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C	4.24470800	-4.03897500	-0.06371300
N	3.52852300	-3.89719800	-1.30360100
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C	2.69153200	-4.91251200	-1.88207300
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C	-0.50603300	-5.78750700	-0.13714800
N	-0.85608600	-4.93912600	-1.25134800
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H	4.31137400	2.90506700	5.60965200
H	-1.42806500	-4.24658700	5.08943800
H	1.21115400	6.24567500	4.44210500
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H	-4.02913000	-4.90290600	4.30679100
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H	5.69213800	-5.26919600	-2.45081600
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