

Supplementary information

Chiral Differentiation of L- and D-Alanine by Permethylated β -cyclodextrin: IRMPD Spectroscopy and DFT Methods

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Normal mode

Normal mode – (D-2)

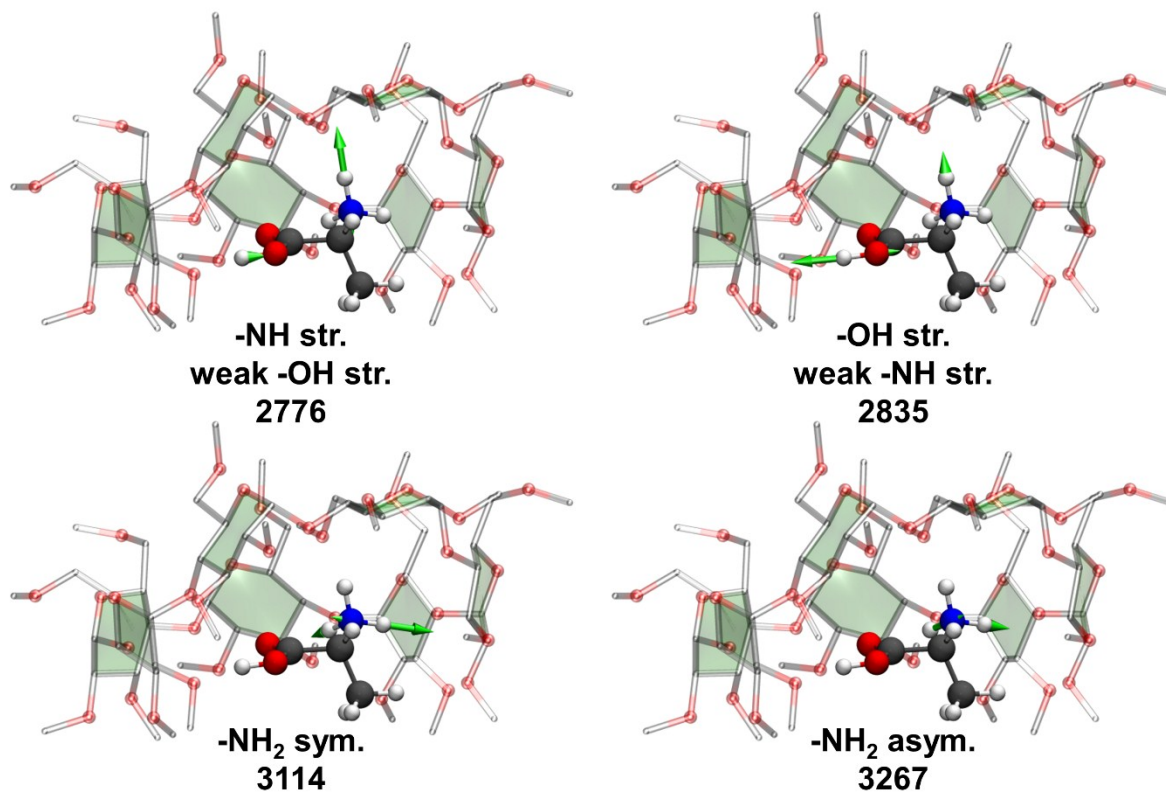


Figure 1S. Normal modes of the absorption bands of (D-2).

Normal mode – (D-3)

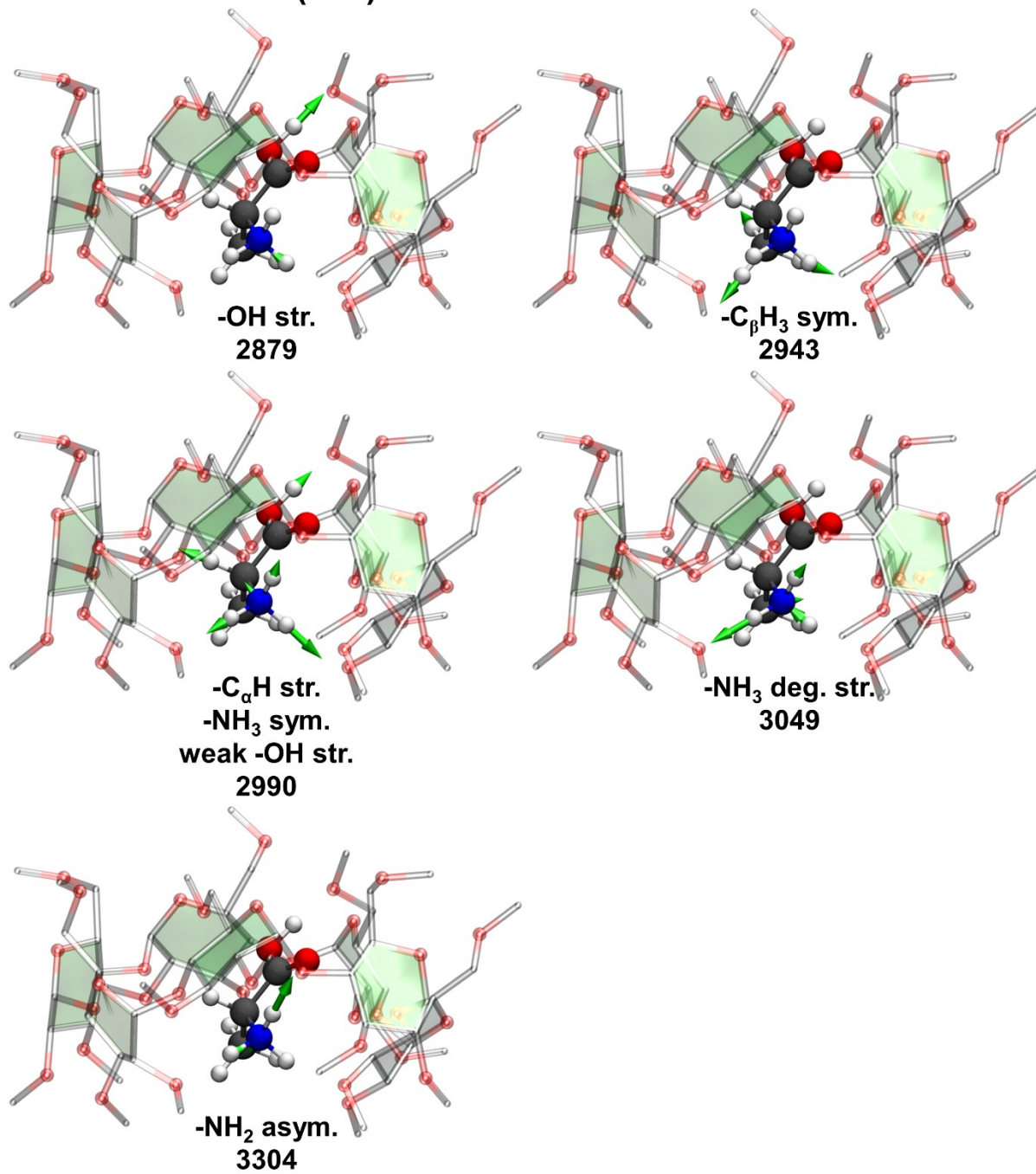
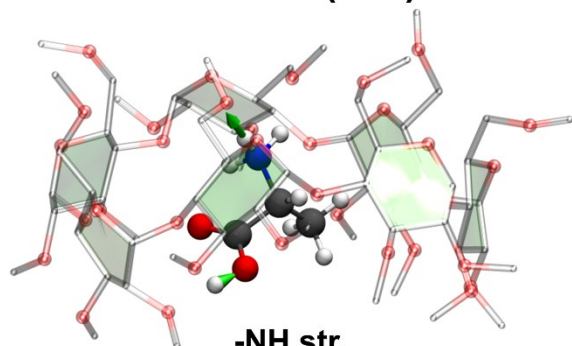
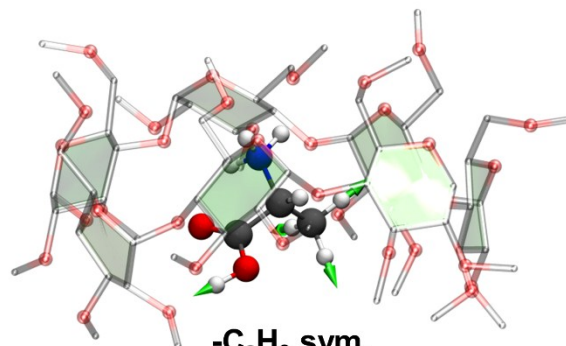


Figure 2S. Normal modes of the absorption bands of (D-3).

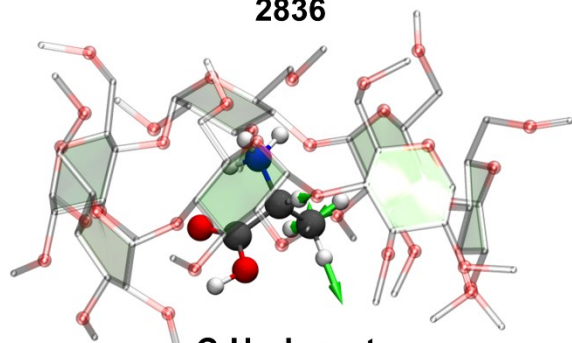
Normal mode – (D-4)



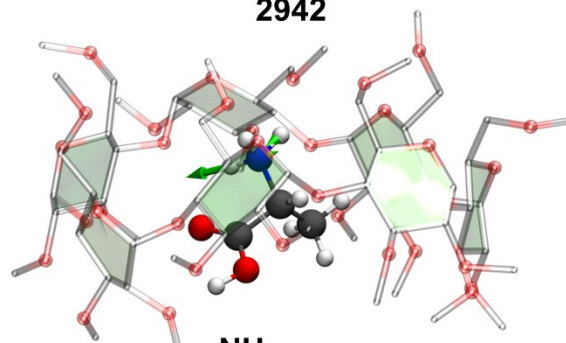
-NH str.
weak -OH str.
2836



-C_βH₃ sym.
weak - OH str.
2942



-C_βH₃ deg. str.
weak -C_αH str.
3018



-NH₂ asym.
3246

Figure 3S. Normal modes of the absorption bands of (D-4).

Normal mode – (L-2)

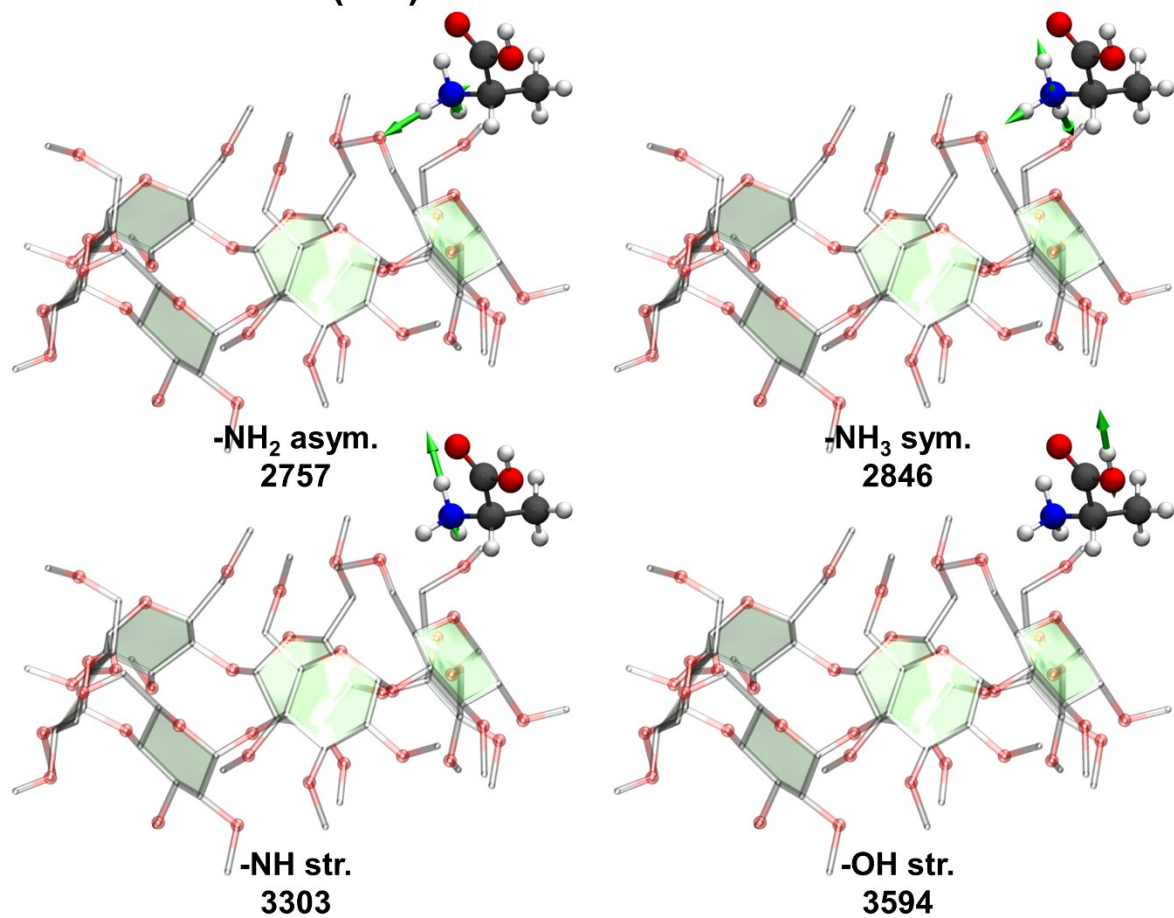


Figure 4S. Normal modes of the absorption bands of (L-2).

Normal mode – (L-3)

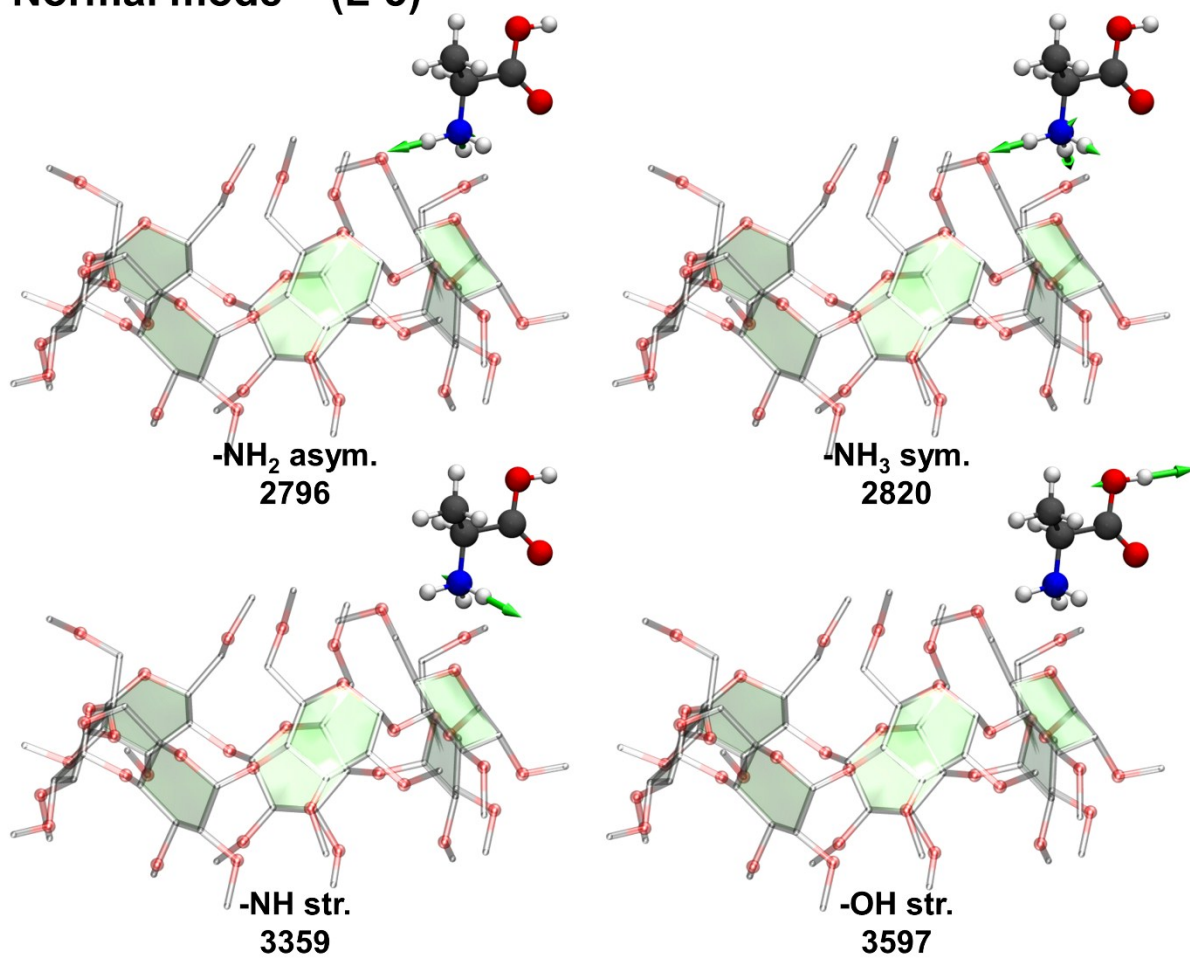
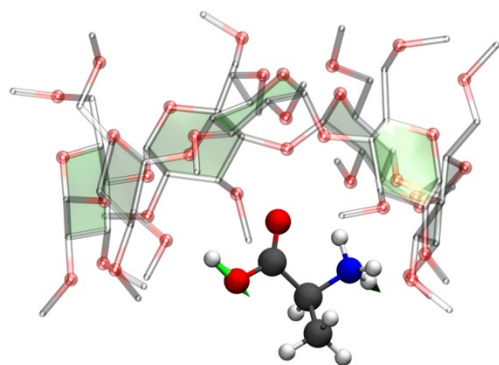
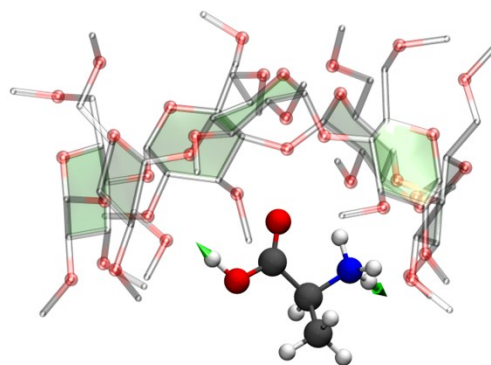


Figure 5S. Normal modes of the absorption bands of (L-3).

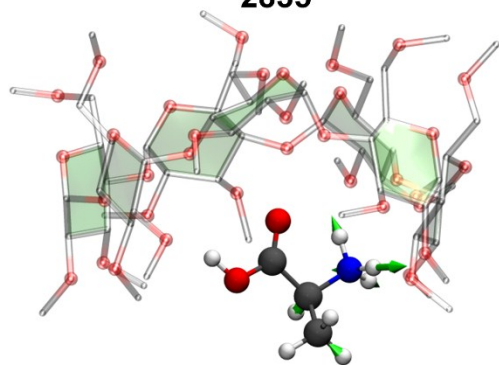
Normal mode – (L-4)



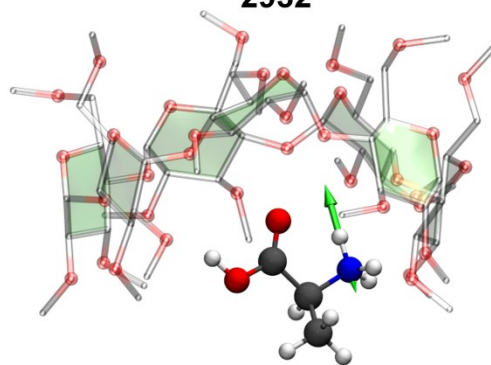
-NH str.
-OH str.
2835



-NH str.
-OH str.
2932



-NH₃ sym.
-C_{α,β} H str.
3005



-NH str.
3236

Figure 6S. Normal modes of the absorption bands of (L-4).

Table 1S. Relative electronic energies (ΔE_0) and Gibbs free energies (ΔG) in kcal/mol of the three lowest energy conformers (D2-4 and L2-4) and conformers D1 and L1. Calculations were carried out at the levels of B3LYP/G-31G** and M06-2X/6-311G**.

Name	ΔE_0		ΔG	
	B3LYP	M06-2X	B3LYP	M06-2X
D1	22.26	29.81	21.09	26.39
D2	1.20	1.54	2.78	3.80
D3	2.16	0.44	2.64	1.83
D4	0.00	0.00	0.00	0.00
L1	19.32	19.09	17.07	17.71
L2	6.00	4.98	3.35	2.81
L3	5.25	7.69	2.27	4.08
L4	0.00	0.00	0.00	0.00

Cartesian Coordinates

(D-1)

H	-1.54536800	6.35476700	1.44254200
C	5.66816600	-2.69942100	-0.18448400
C	6.63452100	-1.91983600	0.73124600
C	6.22956100	-0.45159300	0.88744000
C	5.88770400	0.19872600	-0.45449100
C	4.97382500	-0.68694600	-1.31930800
C	4.79841700	-0.16590200	-2.74852900
O	6.72439700	-2.46993800	2.03201800
O	7.31091500	0.26788700	1.46314700
O	5.26425700	1.45279000	-0.14763500
O	5.53654400	-2.01133100	-1.41405800
O	6.01052900	0.22375900	-3.37549100
H	6.08297100	-3.67468400	-0.45415400
H	7.62040100	-1.93949500	0.24055900
H	5.34013000	-0.39713200	1.52840000
H	6.81952400	0.37027700	-1.00495600
H	3.98227400	-0.74719800	-0.84961000
H	4.28435100	-0.94031300	-3.33711700
H	4.16901300	0.72627900	-2.72496000
C	1.49498800	-5.86034400	0.65190200
C	2.30210400	-5.59068700	1.92935200
C	3.05905400	-4.25916500	1.84411200
C	3.89635600	-4.19745700	0.55950100
C	3.05561800	-4.57820600	-0.67750400
C	3.87557300	-4.73276600	-1.96005900
O	1.44097300	-5.62973400	3.05158500
O	3.89234900	-4.16736400	2.99043700
O	4.41279600	-2.86702300	0.45023100
O	2.37640800	-5.83543900	-0.45696900
O	5.03425900	-5.53912500	-1.81557200
H	1.08392900	-6.87533600	0.67638500
H	3.04447500	-6.39895600	1.99292200
H	2.32496600	-3.44239800	1.83276900
H	4.72154700	-4.91279600	0.65556800
H	2.30926500	-3.78867100	-0.84511300
H	3.22077100	-5.12056000	-2.75368100
H	4.23036500	-3.74412500	-2.25957900
C	-3.34597500	-4.35120500	-1.09896600
C	-3.28896600	-5.06603400	0.25640500
C	-1.91331700	-4.90915200	0.91294600
C	-0.79284900	-5.34196800	-0.04557000
C	-0.97319200	-4.69889500	-1.44021300
C	-0.07900300	-5.30724000	-2.51529800
O	-4.32926900	-4.59678800	1.10256000
O	-1.88015400	-5.70986700	2.08362600
O	0.44916700	-4.91890400	0.53003100
O	-2.32598000	-4.84739400	-1.93046200
O	0.06987500	-4.44793700	-3.63804500
H	-4.28217200	-4.60087300	-1.60902600
H	-3.44150000	-6.13192000	0.03679200
H	-1.76159400	-3.85056700	1.15920000
H	-0.81527500	-6.43776500	-0.12747600
H	-0.73536800	-3.63348000	-1.34071300
H	0.91335600	-5.48059800	-2.09824400
H	-0.49682200	-6.28023100	-2.81108200
C	-4.84067200	0.64421700	-2.18831100
C	-5.87327500	-0.47977100	-2.00949700
C	-5.19893900	-1.56201400	-1.16471300
C	-3.94513500	-2.12630400	-1.85446300
C	-3.01632700	-0.94186900	-2.22759600
C	-1.88906500	-1.31706800	-3.19164600
O	-7.05505500	-0.05507100	-1.33943900
O	-6.11847500	-2.54160000	-0.66289000
O	-3.25378600	-2.94865100	-0.91541600
O	-3.74187200	0.11465700	-2.88516500
O	-0.85066500	-0.35652300	-3.17231200

H	-5.22438700	1.45702500	-2.80803800
H	-6.12933400	-0.85995900	-3.00955500
H	-4.81822700	-1.08789400	-0.25749300
H	-4.19987100	-2.69824800	-2.75730900
H	-2.58925800	-0.56196400	-1.29179500
H	-1.50802900	-2.31960300	-2.96880500
H	-2.30455100	-1.32585100	-4.20562700
C	-3.47217800	4.86873100	0.63445300
C	-4.55180500	4.07341900	1.41472800
C	-4.68746800	2.62314900	0.91855400
C	-4.64900700	2.51265000	-0.61456300
C	-3.52674400	3.37887500	-1.21468500
C	-3.47512300	3.40620000	-2.74150800
O	-4.29679500	4.00540500	2.80089800
O	-5.93420700	1.99430100	1.32638900
O	-4.47605000	1.12046100	-0.90164100
O	-3.73075200	4.72604300	-0.75336500
O	-4.74094500	3.59561100	-3.36240900
H	-3.58499400	5.94024900	0.83697100
H	-5.50230100	4.60013500	1.21868000
H	-3.84872500	2.05335200	1.33944400
H	-5.60817400	2.86493500	-1.01122200
H	-2.55607300	3.01311400	-0.85907200
H	-2.76206500	4.18701800	-3.03731200
H	-3.08997900	2.44604000	-3.09550500
C	1.79459500	5.66017100	1.05515700
C	1.07789900	5.53505600	2.41769600
C	-0.27870800	4.83566900	2.29127200
C	-1.12853100	5.38299800	1.14151100
C	-0.29963500	5.53856500	-0.15001300
C	-0.99074700	6.32208400	-1.26215400
O	1.81270800	4.82321400	3.38891800
O	-1.02490900	5.00919100	3.48979500
O	-2.19982600	4.42746400	0.98997700
O	0.90685500	6.26419200	0.12364600
O	-0.49607300	5.85880900	-2.51313400
H	2.63018700	6.35790100	1.13227800
H	0.88646700	6.56480100	2.75939900
H	-0.09975600	3.77015600	2.09584500
H	-0.06436900	4.53259400	-0.51802100
H	-2.07841500	6.19727500	-1.22840200
H	-0.75180700	7.38630100	-1.11983300
C	5.58752500	2.56605300	-0.94329500
C	5.91211800	3.78800200	-0.05580000
C	4.66480900	4.23306400	0.71612800
C	3.43180900	4.39504400	-0.19215000
C	3.28632400	3.22516000	-1.18297300
C	2.31291700	3.53834900	-2.30744700
O	6.92886200	3.57771500	0.89903000
O	4.86582800	5.41105000	1.50424900
O	2.24460200	4.40252600	0.62207200
O	4.53586500	2.92860300	-1.81787900
O	1.82485000	2.32360700	-2.85577300
H	6.42470300	2.32955800	-1.60625100
H	6.21717300	4.57593400	-0.76475100
H	4.42837100	3.45273200	1.44509100
H	3.50158300	5.33631700	-0.75477100
H	2.93019000	2.35044900	-0.62519900
H	1.48364900	4.15533400	-1.94252600
H	2.84982800	4.12027200	-3.07316600
C	4.83277700	-6.93536900	-1.98746800
H	4.35114400	-7.14976000	-2.95279800
H	5.82296600	-7.39750900	-1.97989100
H	4.22047500	-7.36953200	-1.18958600
C	-0.76705900	-4.75892500	-4.74226000
H	-0.51376800	-4.05384900	-5.53760300
H	-0.58474000	-5.78006200	-5.10755300
H	-1.83095200	-4.66064500	-4.49373000
C	0.16459100	-0.64080200	-2.21614800
H	0.68002100	-1.58010600	-2.46176600
H	0.87090300	0.19073100	-2.24502100
H	-0.24073900	-0.72122900	-1.19557800
C	-5.13034500	4.95253600	-3.54468000

H	-5.29734100	5.46646100	-2.59175000
H	-4.37084800	5.50597900	-4.11426600
H	-6.05849200	4.93846400	-4.12100900
C	-0.75222800	6.75973900	-3.57478700
H	-0.33479000	6.31697300	-4.48155100
H	-1.83068600	6.92512900	-3.72384500
H	-0.27476400	7.73487600	-3.39956200
C	1.01135200	2.54121200	-3.99771500
H	0.57543100	1.58029800	-4.27696600
H	0.20009400	3.25092000	-3.77769200
H	1.60027300	2.93713700	-4.83876000
C	6.73284600	-0.82506800	-4.00568800
H	7.55794900	-0.35560400	-4.54745700
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H	6.10021500	-1.36478100	-4.72598700
C	1.96198200	-6.33086200	4.17537000
H	1.20527700	-6.26761300	4.96107000
H	2.13519500	-7.39125400	3.94007900
H	2.89640100	-5.88439100	4.52798400
C	3.86411400	-2.91092500	3.65492100
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H	4.52916200	-2.99996500	4.51695800
H	4.22866900	-2.10712600	3.01069900
C	7.53937000	-3.62444300	2.14025800
H	8.55463500	-3.43624300	1.76242100
H	7.59567500	-3.87236500	3.20205000
H	7.11950100	-4.48804600	1.60665900
C	7.10064600	0.69885200	2.79978200
H	6.88636700	-0.14782200	3.46302800
H	8.02854500	1.17684800	3.12335100
H	6.29059800	1.43650800	2.85768500
C	8.21830300	3.32334300	0.35936900
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H	8.92999300	3.44896500	1.17840900
H	8.30758000	2.29928100	-0.01929300
C	5.62227900	6.46554000	0.92722900
H	6.68020700	6.19658700	0.83327000
H	5.24072700	6.77996800	-0.05510800
H	5.53623300	7.31112900	1.61374100
C	2.79552900	5.58424300	4.08442700
H	2.35901300	6.49965300	4.51042300
H	3.15257400	4.95343500	4.90174600
H	3.64299900	5.83848500	3.43988900
C	-1.03146500	3.88107200	4.35436200
H	-0.01455800	3.57989900	4.62410400
H	-1.56890600	4.18301300	5.25722200
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H	-3.43085100	5.83238000	3.32856000
H	-5.22715700	5.83897400	3.19985700
C	-6.46465300	2.29894300	2.61930000
H	-6.73301000	3.35279700	2.72024100
H	-7.38630500	1.71361200	2.70818700
H	-5.77226200	2.04128900	3.42710600
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H	-8.21571000	0.19169700	-3.06053100
H	-8.83087800	0.91271600	-1.55081000
C	-6.96038100	-3.19935300	-1.61427300
H	-7.68898100	-2.50882300	-2.05119600
H	-6.37409500	-3.66550600	-2.41298500
H	-7.48584200	-3.98208000	-1.06499500
C	-5.00502100	-5.62908600	1.81994500
H	-5.69950100	-5.13642000	2.50372900
H	-5.57284700	-6.27990200	1.13852700
H	-4.30290400	-6.24018100	2.39364800
C	-1.63709200	-4.99693100	3.29215000
H	-1.67044100	-5.73575300	4.09656300
H	-0.64860600	-4.53026800	3.28507100
H	-2.41684700	-4.24364500	3.47336400
C	-6.49353800	-1.29040300	2.68835200
C	-7.40058900	-2.45489900	3.08929700

O	-7.08811200	-3.31931900	3.86608300
O	-8.61793400	-2.35875000	2.50331900
H	-9.16381900	-3.09520200	2.83109700
H	-6.42098000	0.13995900	1.11217000
H	-6.73784700	-1.45192000	0.58745600
H	-7.91673700	-0.55952300	1.32855200
N	-6.91310400	-0.75041100	1.34846400
C	-5.01639400	-1.66935500	2.69495600
H	-4.40110800	-0.79199500	2.47753700
H	-4.75792600	-2.03303600	3.69083600
H	-4.79385300	-2.46487700	1.97705400
H	-6.68219900	-0.49196800	3.41481300

(D-2)

H	2.20004300	-5.60790500	0.40746000
C	-5.84377400	2.43513800	0.18269700
C	-6.79240400	1.49515300	0.94598500
C	-6.32419900	0.04100900	0.86414600
C	-5.96884900	-0.37487500	-0.56689500
C	-5.15828400	0.69244900	-1.32934800
C	-5.06818600	0.43077600	-2.83626900
O	-6.90825300	1.84208500	2.31540500
O	-7.36916800	-0.80516700	1.32515300
O	-5.23403500	-1.60363300	-0.44045000
O	-5.76660800	1.99094000	-1.16165800
O	-6.29344000	0.04373100	-3.43873700
H	-6.24290100	3.45233200	0.13509100
H	-7.77334600	1.55912100	0.45327100
H	-5.42677200	-0.07370200	1.48381800
H	-6.90152000	-0.55654500	-1.11268400
H	-4.13946200	0.71879800	-0.92177300
H	-4.66539800	1.33588000	-3.31543200
H	-4.37148100	-0.39143700	-3.00829200
C	-1.33136700	5.09827200	0.93314500
C	-1.84840100	4.52608100	2.25692000
C	-2.81471700	3.35167300	2.07803500
C	-3.90677600	3.67786100	1.04312000
C	-3.28514100	4.27758900	-0.23968000
C	-4.29990300	4.81660400	-1.25409400
O	-0.71965800	4.15327900	3.06256700
O	-3.33892000	3.10063100	3.37289600
O	-4.56748600	2.43189400	0.79375500
O	-2.41947400	5.38545600	0.08565000
O	-5.35044100	5.58044000	-0.68479300
H	-0.83301500	6.05261000	1.10802200
H	-2.38582600	5.33509800	2.76592800
H	-2.25637900	2.47828600	1.71406500
H	-4.61193400	4.39757400	1.47584600
H	-2.69929300	3.48781300	-0.72929500
H	-3.74738400	5.40491000	-2.00109400
H	-4.77404700	3.97178700	-1.75690300
C	3.30238700	4.33700400	-1.50065300
C	3.04107600	5.45340800	-0.47635000
C	1.85396200	5.09111300	0.42348600
C	0.62416600	4.76973600	-0.44235700
C	0.95756900	3.77677500	-1.57416000
C	-0.16482700	3.69350800	-2.60737200
O	4.17333900	5.74525700	0.32052100
O	1.50509400	6.18691900	1.25959900
O	-0.41510500	4.18121900	0.35713300
O	2.13801500	4.17433100	-2.29313500
O	0.09882200	2.73676200	-3.62405600
H	4.09119400	4.62856500	-2.19979800
H	2.75356700	6.34277000	-1.05644700
H	2.10478900	4.20935300	1.02679100
H	0.26292600	5.70928000	-0.88249400
H	1.11681700	2.78661800	-1.13072200
H	-1.07953400	3.38405700	-2.09546700
H	-0.33373100	4.68731100	-3.04488300
C	6.20486100	-0.13919800	-1.23984500
C	6.89680000	1.23586300	-1.15306500
C	5.93373200	2.35057400	-0.71350100
C	4.60275400	2.28758000	-1.47973600
C	4.04967900	0.85382600	-1.48475600
C	2.75718600	0.64829000	-2.27416600
O	7.99589700	1.22082100	-0.26082000
O	6.50548300	3.62412900	-0.95701800
O	3.66017900	3.14532800	-0.83340200
O	5.03584900	-0.02965200	-2.04563900
O	1.71650100	0.21761400	-1.37958000
H	6.85022200	-0.85958000	-1.74585700
H	7.23659500	1.48161200	-2.17099900
H	5.70804700	2.22563500	0.35474100
H	4.77040100	2.61221600	-2.51509800

H	3.86124300	0.56714700	-0.44317900
H	2.42623000	1.56443400	-2.77270000
H	2.93319800	-0.12567100	-3.03161900
C	3.97808500	-4.13413200	1.13337200
C	4.70500600	-3.35754000	2.24028400
C	5.24777400	-1.99193700	1.80142100
C	5.84823500	-1.97620600	0.37997600
C	5.03635400	-2.85107900	-0.60547000
C	5.72780300	-3.12862500	-1.95400600
O	3.86444500	-3.22712700	3.37382800
O	6.19269000	-1.63479400	2.79393700
O	5.86940400	-0.57545200	0.05307900
O	4.78567900	-4.14658200	-0.02016500
O	7.13712600	-3.23665200	-1.88870400
H	3.88211800	-5.17543900	1.44611300
H	5.57812700	-3.97742200	2.48435000
H	4.41630400	-1.26864000	1.79902600
H	6.87403700	-2.35790700	0.42541400
H	4.07647700	-2.36074500	-0.81170500
H	5.28476800	-4.04510500	-2.36829500
H	5.50870300	-2.30665200	-2.63763600
C	-1.07734100	-5.36792000	-0.15728900
C	-0.52067700	-5.65103700	1.25870600
C	0.66656300	-4.75133300	1.63558100
C	1.68683700	-4.64427500	0.50006200
C	0.99595800	-4.34013100	-0.84134300
C	1.93368800	-4.38254100	-2.03767200
O	-1.49119800	-5.52083300	2.27426500
O	1.35554800	-5.29044300	2.75109000
O	2.66976200	-3.63015600	0.85241600
O	0.00714000	-5.34662200	-1.08076000
O	1.33778300	-3.67011700	-3.10830100
H	-1.69562300	-6.20886600	-0.47987100
H	-0.12784900	-6.67844800	1.22789300
H	0.27604600	-3.74747300	1.86461000
H	0.51995400	-3.35044600	-0.79947100
H	2.90540300	-3.94843400	-1.77781500
H	2.09600400	-5.43658500	-2.30975800
C	-5.42871700	-2.59691300	-1.41097500
C	-5.54886700	-3.98591200	-0.74748000
C	-4.22117600	-4.39850200	-0.09869400
C	-3.00348200	-4.18462000	-1.01731900
C	-3.06643300	-2.85338200	-1.78491200
C	-2.10904700	-2.80552600	-2.96537200
O	-6.53489700	-4.08415700	0.25606900
O	-4.21586900	-5.73567700	0.40712700
O	-1.81407700	-4.17672400	-0.19992000
O	-4.36746200	-2.66026000	-2.34894500
O	-1.96104900	-1.44751400	-3.36554000
H	-6.31222200	-2.37242400	-2.01580900
H	-5.78769400	-4.66832300	-1.57981200
H	-4.07452400	-3.76811100	0.78306000
H	-2.94443200	-5.00777500	-1.74250000
H	-2.83392400	-2.03871800	-1.08766700
H	-1.13641800	-3.24450100	-2.71255700
H	-2.55109700	-3.39930500	-3.77941200
C	-5.05371300	6.95245100	-0.45617200
H	-4.70986700	7.44106300	-1.37906700
H	-5.98498700	7.42406400	-0.13396200
H	-4.28750600	7.09009600	0.31455700
C	0.58978000	3.28528300	-4.84299600
H	0.72736600	2.44765300	-5.53097800
H	-0.13603800	3.98368600	-5.28286600
H	1.54425000	3.80250700	-4.70119200
C	0.52352300	-0.19160400	-2.08203200
H	0.69684300	-1.13991600	-2.60140400
H	-0.26204900	-0.31558700	-1.33510700
H	0.21632600	0.58599900	-2.78477600
C	7.62365100	-4.51659700	-1.49600400
H	7.33770400	-4.77289800	-0.46907900
H	7.25008400	-5.30170400	-2.16761200
H	8.71207300	-4.47369300	-1.56977900
C	2.01858300	-3.85988000	-4.33686700

H	1.48756600	-3.28046900	-5.09474500
H	3.06012700	-3.50773700	-4.28485500
H	2.02339900	-4.91791800	-4.63503300
C	-1.56205100	-1.30054800	-4.71596600
H	-1.48467700	-0.22852000	-4.91163200
H	-0.58499600	-1.76898600	-4.90935700
H	-2.30008300	-1.73858200	-5.40294100
C	-7.15959400	1.11303800	-3.79362400
H	-7.99029700	0.67228900	-4.35035800
H	-7.54795800	1.64551000	-2.91845600
H	-6.64697900	1.84020000	-4.44077300
C	-0.83851700	4.42832000	4.46653600
H	0.07820200	4.05977500	4.93152200
H	-0.91388100	5.50918000	4.63238600
H	-1.71018300	3.92490900	4.88686300
C	-3.76545000	1.76596500	3.64821100
H	-3.06875900	1.03349700	3.21871400
H	-3.76242600	1.66060600	4.73722800
H	-4.77216500	1.58428900	3.26778900
C	-7.93970100	2.77347600	2.60633800
H	-8.92442800	2.37807700	2.32184000
H	-7.92084700	2.93874600	3.68548500
H	-7.78847400	3.73796100	2.10176800
C	-7.09544000	-1.49461400	2.53702500
H	-6.85264800	-0.79735000	3.34848200
H	-8.00810200	-2.03532500	2.79995300
H	-6.28389800	-2.22075800	2.40751800
C	-7.87104300	-3.89585700	-0.19284000
H	-8.07560200	-4.47398800	-1.10625100
H	-8.52236400	-4.25959900	0.60482800
H	-8.09656700	-2.83791300	-0.36838000
C	-4.86250600	-6.73238500	-0.37015900
H	-5.95092600	-6.60593600	-0.36684400
H	-4.50762900	-6.76552800	-1.41097800
H	-4.62251900	-7.68853500	0.10142200
C	-2.16575900	-6.72753700	2.61792500
H	-1.45525400	-7.49221500	2.96186800
H	-2.84830700	-6.47900300	3.43254300
H	-2.75595100	-7.11304300	1.78193600
C	0.97518100	-4.76917900	4.01878700
H	-0.09368400	-4.90349800	4.20531100
H	1.54967500	-5.32287500	4.76484000
H	1.23362700	-3.70443200	4.09806800
C	4.48981400	-3.53614800	4.62148300
H	3.72704800	-3.40559400	5.39170000
H	4.83455600	-4.57844300	4.64014900
H	5.33435700	-2.86973200	4.81680500
C	6.50406800	-0.24861400	2.92632800
H	5.58942200	0.35236400	3.04101700
H	7.09836500	-0.15966600	3.83832500
H	7.07090300	0.13416900	2.07371700
C	9.18459700	0.64599500	-0.79202300
H	9.07429700	-0.42709800	-0.99780100
H	9.49360400	1.15346700	-1.71611100
H	9.96112200	0.77854300	-0.03655700
C	7.18530900	4.19205000	0.16109300
H	6.48031200	4.40179700	0.97566200
H	7.98484900	3.53747400	0.51862300
H	7.61729400	5.13290400	-0.18657400
C	4.99332000	6.78057600	-0.20777300
H	5.77484000	6.97267600	0.52946200
H	5.46768300	6.48786500	-1.15359700
H	4.41754300	7.70281000	-0.36442800
C	2.10110300	6.17809400	2.55303500
H	1.70680500	7.05033000	3.08015900
H	1.82477400	5.27141900	3.10731700
H	3.19064500	6.24752400	2.49438500
C	1.78419200	0.09110300	2.13326300
H	2.73431100	0.56218600	1.87297200
C	1.83976600	-0.52998700	3.53090600
C	0.65090600	1.12002100	2.05020200
H	0.86670800	-0.95214700	3.80276000
H	2.59600900	-1.31787500	3.58102000

H	2.08569500	0.25017700	4.25433300
O	-0.42100700	0.82192700	1.54824700
O	0.98357200	2.25134800	2.62571300
H	0.23073800	2.93040000	2.65212100
H	1.96520500	-1.84801400	1.21919400
H	0.46103400	-1.07955600	1.09769600
H	1.70917700	-0.56159300	0.12441900
N	1.48102100	-0.94086500	1.08409900

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H	3.82000100	4.31107100	-1.89630500
C	-6.14543300	-0.65321800	1.08628300
C	-6.99739200	0.41511500	0.37451200
C	-6.13470800	1.60026300	-0.06967600
C	-5.24739700	2.12111100	1.06426200
C	-4.56189400	0.99694200	1.86602200
C	-3.97773600	1.49027500	3.19336000
O	-7.65857700	-0.08293900	-0.77232400
O	-6.95986600	2.67552700	-0.49363000
O	-4.25321500	2.96074200	0.45070200
O	-5.49288200	-0.05120800	2.19075200
O	-4.86941400	2.27849000	3.96135400
H	-6.76721500	-1.43788200	1.52675100
H	-7.73271800	0.78295400	1.10734300
H	-5.47957400	1.26937200	-0.88596800
H	-5.86416000	2.71199400	1.75021500
H	-3.74550000	0.58207800	1.25824900
H	-3.63329400	0.61505500	3.76487300
H	-3.11654500	2.12717000	2.98368000
C	-3.35010400	-4.83439800	-0.59511000
C	-4.45388100	-4.43657100	-1.58152100
C	-4.84286600	-2.96482100	-1.40327000
C	-5.15340800	-2.64374100	0.06495500
C	-4.08654400	-3.21329000	1.02626800
C	-4.50786200	-3.15382600	2.49716500
O	-4.00464900	-4.69563200	-2.89892000
O	-5.98114600	-2.71125200	-2.21499600
O	-5.22231800	-1.21571300	0.17431500
O	-3.79936400	-4.59505600	0.72405900
O	-5.82584000	-3.61032000	2.74763700
H	-3.16065900	-5.91113700	-0.65699500
H	-5.32969300	-5.05665800	-1.34369000
H	-3.99417400	-2.34620200	-1.72251900
H	-6.12433200	-3.08572600	0.31495900
H	-3.16686000	-2.62325800	0.90828100
H	-3.77530200	-3.71926500	3.09194800
H	-4.48858100	-2.10859500	2.81505100
C	2.01340300	-4.63373100	-0.83083000
C	1.33395400	-4.32309500	-2.18442100
C	-0.17372700	-4.04496500	-2.13192700
C	-0.93084100	-4.81433600	-1.03681200
C	-0.11320400	-4.86351400	0.26863100
C	-0.73300900	-5.73060600	1.35997700
O	1.94076100	-3.20979400	-2.85762500
O	-0.70181700	-4.37967800	-3.40450700
O	-2.16748700	-4.11041300	-0.87616400
O	1.17838600	-5.43058000	-0.02809400
O	-0.04153900	-5.59689000	2.59590600
H	2.90475300	-5.23798300	-0.99292400
H	1.44964800	-5.22031100	-2.80506100
H	-0.32745600	-2.98052200	-1.91700100
H	-1.11780400	-5.83432200	-1.39689600
H	0.01833400	-3.85059200	0.66568200
H	-1.76352700	-5.40663000	1.52815600
H	-0.74710500	-6.77964100	1.03064600
C	5.60186200	-1.80295300	1.65641500
C	5.93993700	-3.17987000	1.05712100
C	4.80997300	-3.55186400	0.08893900
C	3.42661900	-3.50444500	0.78032200
C	3.24607000	-2.26466300	1.68949200
C	2.12648200	-2.39788200	2.72515400
O	7.15194400	-3.21104200	0.33603300
O	5.02136700	-4.77464600	-0.61312100
O	2.38437100	-3.41076100	-0.21144800
O	4.42709800	-1.96444700	2.44227600
O	0.88343800	-2.06633000	2.12684800
H	6.36801700	-1.45246500	2.35324900
H	5.98171700	-3.88392300	1.90304100
H	4.80171700	-2.79370800	-0.69775800
H	3.27897800	-4.41202100	1.37856500

H	3.00559400	-1.40446800	1.05821500
H	2.09263200	-3.41470100	3.14228300
H	2.35108700	-1.70198400	3.54703500
C	5.40043000	3.09277100	-0.16123500
C	6.44695100	2.33929600	-0.97914900
C	6.24687400	0.82918100	-0.82415200
C	6.06234300	0.40771500	0.65073800
C	5.21596700	1.39302600	1.49262800
C	5.38119700	1.19199800	3.00267700
O	6.32697700	2.74367300	-2.33608100
O	7.37714900	0.20151000	-1.41030100
O	5.41774700	-0.88205500	0.60472400
O	5.56465600	2.76542700	1.19936900
O	6.71197300	0.96893200	3.43746800
H	5.55960000	4.17151500	-0.25281200
H	7.43464100	2.61306300	-0.58463400
H	5.33234300	0.56792400	-1.37230800
H	7.05567000	0.30647400	1.10020300
H	4.16011700	1.24241100	1.24659600
H	4.94054400	2.06232200	3.51095700
H	4.81693900	0.30204600	3.29318500
C	0.55757700	4.75490800	-1.62576200
C	1.18867500	3.79087700	-2.66314400
C	2.16818300	2.85878600	-1.93627000
C	3.25080800	3.67892400	-1.20177800
C	2.47728400	4.55542500	-0.18645200
C	3.30161200	5.45077600	0.72302500
O	0.25900000	2.98025700	-3.34568200
O	2.66357900	1.79132900	-2.74297700
O	4.09997100	2.72551700	-0.58396900
O	1.57867900	5.41393100	-0.90184400
O	2.42162800	5.97564800	1.70132000
H	0.00467800	5.55259800	-2.12237700
H	1.73148600	4.42958500	-3.37962500
H	1.61086000	2.33979600	-1.15588600
H	1.91548000	3.86896400	0.45747200
H	4.09326200	4.86278300	1.20799700
H	3.76649900	6.26051500	0.13713500
C	-4.01887500	4.23887100	0.97264100
C	-3.82549400	5.25112500	-0.18079100
C	-2.58183000	4.86941200	-0.99682200
C	-1.33607600	4.72129900	-0.10008400
C	-1.65983600	3.85727600	1.13354900
C	-0.56201700	3.87867200	2.18940500
O	-4.90828300	5.33195700	-1.07738000
O	-2.32475300	5.72812300	-2.10782600
O	-0.30385300	4.00157600	-0.80005900
O	-2.85523200	4.28756500	1.78927900
O	-0.47442700	2.57693000	2.79870600
H	-4.83372300	4.54455500	1.63553800
H	-3.66856700	6.22489600	0.31297100
H	-2.77437300	3.89174100	-1.44887700
H	-0.95795300	5.70369400	0.21173000
H	-1.78986200	2.83324900	0.76535100
H	0.40720100	4.15496300	1.76575700
H	-0.82577100	4.61510000	2.95771500
C	-5.96287100	-5.01509000	2.92277200
H	-5.28418700	-5.38395000	3.70535800
H	-6.99349900	-5.19101200	3.23962600
H	-5.76396700	-5.57167600	2.00041800
C	0.87078000	-6.64664900	2.88388500
H	1.30164000	-6.42983400	3.86465900
H	0.35924300	-7.61864100	2.93627300
H	1.67216000	-6.71110200	2.13848500
C	-0.19218700	-2.16129000	3.05474300
H	-0.01807200	-1.51527500	3.92842400
H	-1.08910200	-1.81638400	2.53656100
H	-0.33080500	-3.19626800	3.39024800
C	7.49374200	2.14531500	3.60908600
H	7.67301300	2.66722100	2.66242500
H	7.00640100	2.84437700	4.30378000
H	8.44715100	1.82878800	4.03792400
C	3.06252700	6.87441800	2.58747000

H	2.30986500	7.21586400	3.30120900
H	3.88383200	6.39049300	3.13818300
H	3.46904400	7.74737500	2.05568300
C	0.45915100	2.53096200	3.87841300
H	0.45651100	1.50906800	4.26133300
H	1.46843600	2.79281400	3.53846800
H	0.15231700	3.21734800	4.67579100
C	-5.74388200	1.55306700	4.81670400
H	-6.27275700	2.29359800	5.42157600
H	-6.46806700	0.94985400	4.25955000
H	-5.17999400	0.88760400	5.48716700
C	-4.96738400	-5.31637000	-3.74450700
H	-4.49082300	-5.44343500	-4.71911600
H	-5.25638700	-6.30697000	-3.36403400
H	-5.86563000	-4.69995800	-3.85109800
C	-5.86725300	-1.58993400	-3.08035100
H	-5.02770200	-1.70978600	-3.78023300
H	-6.79677400	-1.54255600	-3.65239700
H	-5.75502100	-0.65838500	-2.51912300
C	-8.80864500	-0.87118800	-0.50826900
H	-9.52237700	-0.33608900	0.13408400
H	-9.28036700	-1.07275200	-1.47189000
H	-8.56023900	-1.83218700	-0.03865400
C	-7.08630700	2.81022900	-1.90455800
H	-7.47470100	1.89379300	-2.36048900
H	-7.79720300	3.62217500	-2.07621600
H	-6.12564100	3.08277200	-2.36043100
C	-6.08991200	5.90896500	-0.53233300
H	-5.86686800	6.83478200	0.01833700
H	-6.73634600	6.15215500	-1.37816000
H	-6.62067400	5.20828500	0.12144800
C	-2.45665100	7.12953300	-1.89796800
H	-3.50316200	7.41233200	-1.74406000
H	-1.85261400	7.49203500	-1.05453700
H	-2.09424600	7.60731300	-2.81062300
C	-0.57115000	3.67924200	-4.27326200
H	0.03765200	4.24453300	-4.99405800
H	-1.13831700	2.91889800	-4.81379900
H	-1.26644200	4.36247700	-3.77395700
C	3.38242300	2.13607700	-3.93104000
H	4.31157600	2.65879700	-3.68807700
H	3.63080500	1.19132100	-4.41926300
H	2.76267400	2.72671200	-4.61344100
C	7.56626600	2.91857800	-3.01911500
H	7.32158700	3.21698600	-4.04106500
H	8.16889000	3.71244100	-2.55539800
H	8.14732500	1.99199600	-3.03442200
C	7.12800300	-0.96582500	-2.18564000
H	6.29431700	-0.80590300	-2.88570200
H	8.03465800	-1.14928600	-2.76831400
H	6.92619800	-1.83848500	-1.55935400
C	8.32682800	-3.18146500	1.13774100
H	8.46576000	-2.21758000	1.64395300
H	8.31349300	-3.97873500	1.89455200
H	9.16876100	-3.34547100	0.46324800
C	5.46572400	-5.89535300	0.14402700
H	6.49059000	-5.75286700	0.50260700
H	4.80910700	-6.11973300	0.99607900
H	5.44804100	-6.74756700	-0.53803000
C	3.14046800	-3.54412600	-3.56424900
H	3.49485100	-2.62640200	-4.03913800
H	3.91760500	-3.93114600	-2.89526400
H	2.92870800	-4.28614900	-4.34318300
C	-1.30117200	-3.32174200	-4.13439900
H	-1.62215500	-3.74819600	-5.08742200
H	-2.18228500	-2.92432100	-3.62050100
H	-0.58092600	-2.51619000	-4.33866300
C	0.49771300	-0.50414200	-0.77589700
C	0.64342700	0.41416700	0.43949800
O	1.72380600	0.86093600	0.79062300
O	-0.51365900	0.64386300	1.02511900
H	-0.41355200	1.33517300	1.75517900
H	1.94114400	-1.51597100	-1.93462800

H	2.02428200	0.19711400	-2.10015300
H	2.57263800	-0.52581600	-0.72749900
N	1.84524400	-0.59966900	-1.44815300
C	-0.57968700	-0.05613000	-1.76275500
H	-0.62536000	-0.73767000	-2.61623700
H	-1.54782600	-0.07482700	-1.26007400
H	-0.39817700	0.95799900	-2.13188800
H	0.29244900	-1.50056900	-0.37648400

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H	5.45816000	-4.17628600	1.44489600
C	-5.94494600	-0.72621600	-0.50812500
C	-6.30652300	-2.00456900	0.27485900
C	-5.10297500	-2.93978500	0.44429100
C	-4.33846000	-3.13474800	-0.86744800
C	-4.11192600	-1.81284900	-1.62067100
C	-3.55003300	-2.01430600	-3.03182500
O	-6.80765800	-1.72940100	1.56769500
O	-5.55268500	-4.21360400	0.87715000
O	-3.08153800	-3.74582000	-0.53343400
O	-5.34800400	-1.09487100	-1.74281300
O	-4.20785700	-3.01491300	-3.78458900
H	-6.84046700	-0.16589000	-0.78908300
H	-7.06040400	-2.54208200	-0.32164900
H	-4.41479600	-2.49898600	1.17771600
H	-4.91922500	-3.80366500	-1.51114000
H	-3.39636000	-1.19920800	-1.05210000
H	-3.57834400	-1.04503500	-3.55403600
H	-2.50907600	-2.33819500	-2.94755700
C	-4.49083900	4.16528400	0.92721700
C	-5.06282700	3.35712700	2.10002300
C	-4.92668400	1.84857900	1.86524400
C	-5.47383300	1.44963200	0.48942400
C	-4.95921800	2.38113900	-0.62839500
C	-5.65807000	2.16615700	-1.97427500
O	-4.42510100	3.73997500	3.30235900
O	-5.64747400	1.18499900	2.89363700
O	-5.07660400	0.09063800	0.25325300
O	-5.15086700	3.76184400	-0.26486800
O	-7.07101300	2.09267300	-1.89302700
H	-4.73538700	5.22493600	1.05144300
H	-6.13441700	3.59739200	2.13983600
H	-3.86024000	1.59158900	1.91408400
H	-6.56661500	1.51852900	0.52535500
H	-3.88538100	2.19151400	-0.77265100
H	-5.34221800	2.96254000	-2.66377700
H	-5.32959700	1.20614500	-2.38008400
C	0.43708000	5.88974100	-0.28591200
C	-0.08313700	6.22972100	1.11510700
C	-1.17439300	5.24662700	1.55521600
C	-2.28485400	5.13622300	0.50326300
C	-1.70960500	4.96325800	-0.92071400
C	-2.75156500	5.17673800	-2.01456700
O	0.98445300	6.24150100	2.04773800
O	-1.73668100	5.69528800	2.77792600
O	-3.09372700	3.99677500	0.84334200
O	-0.65394500	5.89997700	-1.19397600
O	-2.31172100	4.69642000	-3.28120100
H	1.12418500	6.66329800	-0.63516500
H	-0.53327500	7.22913200	1.03800400
H	-0.71518100	4.25741200	1.67735000
H	-2.89248800	6.05010800	0.55392500
H	-1.32208000	3.93809900	-0.99399800
H	-3.66260000	4.63467800	-1.75494700
H	-2.99469800	6.24706500	-2.06661900
C	4.45456300	2.68682100	-1.65481100
C	4.69468100	4.14333300	-1.20642100
C	3.50519800	4.69814600	-0.41664000
C	2.18933100	4.46442200	-1.16315700
C	2.06465500	3.04031300	-1.73627800
C	0.93715700	2.98054300	-2.76223400
O	5.85109100	4.25621400	-0.40042000
O	3.62353000	6.10111500	-0.23713600
O	1.08658300	4.63558700	-0.26530600
O	3.25324900	2.60899600	-2.40413500
O	0.27928800	1.70347900	-2.73258400
H	5.23237400	2.36523900	-2.35153900
H	4.80140600	4.75027700	-2.11934200
H	3.44324400	4.18608400	0.55203500
H	2.12913700	5.19209300	-1.98399100

H	1.84742500	2.37591000	-0.88890500
H	0.19963800	3.76467300	-2.57172300
H	1.37308900	3.14063400	-3.75699100
C	6.21990100	-1.78859400	0.55433100
C	6.74035000	-0.53784000	1.27432900
C	5.78195200	0.64836400	1.07154200
C	5.48301800	0.85977900	-0.42059100
C	5.10749700	-0.46661600	-1.11289500
C	4.98075600	-0.36157000	-2.63338500
O	6.91672500	-0.82523000	2.64805800
O	6.40378800	1.80138000	1.61926300
O	4.40528400	1.80628700	-0.54193800
O	6.09381900	-1.47585900	-0.83064100
O	6.04875200	0.31211800	-3.27654700
H	6.95063700	-2.60376200	0.60996500
H	7.70356700	-0.28584100	0.80949800
H	4.84475600	0.42248300	1.59543900
H	6.38628900	1.26341700	-0.88955600
H	4.13611300	-0.79437300	-0.71592600
H	4.85560900	-1.37841200	-3.03436200
H	4.08124200	0.21833400	-2.86187600
C	2.09920800	-5.17858200	1.04292000
C	2.54496100	-4.63763700	2.42411000
C	3.62951800	-3.54926600	2.42404100
C	4.59185300	-3.54082500	1.21677300
C	3.89297400	-4.02212300	-0.07109000
C	4.81960100	-4.32199500	-1.24164500
O	1.45414700	-4.10973600	3.19521100
O	4.34656500	-3.71292700	3.63934000
O	4.99804400	-2.16283800	1.12670200
O	3.20614800	-5.26192600	0.18108000
O	4.05992500	-4.22854100	-2.44462500
H	1.74838700	-6.20561800	1.15165800
H	2.97150700	-5.49178600	2.96296300
H	3.12238200	-2.58244500	2.39830900
H	3.17529100	-3.24966300	-0.37044600
H	5.65567400	-3.61764200	-1.28209900
H	5.21299000	-5.34136800	-1.11301200
C	-2.62564600	-4.81630800	-1.32397600
C	-2.22797700	-6.01892300	-0.43657300
C	-1.03797700	-5.64039200	0.45561900
C	0.13116700	-5.05984200	-0.36363800
C	-0.37302300	-3.99179900	-1.35090800
C	0.68370300	-3.57468200	-2.36148400
O	-3.24976700	-6.48111900	0.41400100
O	-0.59243000	-6.68992900	1.31335200
O	1.05433000	-4.38576200	0.50780900
O	-1.49706300	-4.44900600	-2.10429000
O	0.53046100	-2.17234900	-2.65540900
H	-3.38340000	-5.10082700	-2.05862400
H	-1.93181400	-6.81245300	-1.14343800
H	-1.37630800	-4.85393700	1.13747000
H	0.65098300	-5.85477200	-0.91485500
H	-0.66789900	-3.12354600	-0.74825700
H	1.69751200	-3.76736800	-2.00012200
H	0.52741600	-4.15131300	-3.28130700
C	-7.74947400	3.34384100	-1.91483000
H	-7.46593100	3.93045100	-2.80036700
H	-8.81701300	3.11877900	-1.96919200
H	-7.54493100	3.94189300	-1.02053300
C	-1.78320300	5.69723200	-4.14554200
H	-1.51969800	5.19841800	-5.08146700
H	-2.53400700	6.47000500	-4.36130500
H	-0.89376000	6.17528900	-3.72093700
C	-0.75669700	1.61160000	-3.72025300
H	-0.32556800	1.64986200	-4.72859200
H	-1.24787500	0.64530100	-3.58242800
H	-1.48026900	2.42634200	-3.60483900
C	7.19875000	-0.48225500	-3.54505300
H	7.70632600	-0.79978300	-2.62850300
H	6.93153600	-1.37783200	-4.12488400
H	7.87198800	0.13580800	-4.14322800
C	4.73983000	-4.77799600	-3.56050500

H	4.08698700	-4.66212900	-4.42862500
H	5.68918100	-4.25814700	-3.75747600
H	4.95333600	-5.84678500	-3.41527500
C	1.35567900	-1.75523400	-3.74865800
H	1.29518200	-0.66592800	-3.80033700
H	2.39629100	-2.06118300	-3.58951900
H	0.99157800	-2.18793000	-4.68806800
C	-5.38806500	-2.59096200	-4.45977100
H	-5.71098000	-3.43137900	-5.07822000
H	-6.18828800	-2.31597100	-3.76506900
H	-5.18105100	-1.73006300	-5.11185600
C	-5.30757600	3.98036500	4.39344600
H	-4.68112600	4.24228000	5.24897400
H	-5.98459200	4.82107100	4.18451100
H	-5.90123500	3.09204400	4.63221800
C	-4.93620900	0.15382700	3.56194600
H	-4.03107000	0.54564100	4.04847100
H	-5.60526800	-0.23914000	4.33072100
H	-4.67106500	-0.66019400	2.88088200
C	-8.16637700	-1.32099400	1.61022700
H	-8.82272100	-2.06357300	1.13500300
H	-8.43460800	-1.23065400	2.66429800
H	-8.32681000	-0.34735100	1.12819000
C	-5.30840900	-4.50659200	2.24666800
H	-5.76356400	-3.75649500	2.90272100
H	-5.76697000	-5.47843200	2.44325500
H	-4.23257900	-4.58240400	2.44956500
C	-4.35477700	-7.08907200	-0.24389500
H	-4.02222700	-7.81475300	-1.00062700
H	-4.92240800	-7.61719900	0.52470100
H	-5.01344300	-6.34690100	-0.70746600
C	-0.52066300	-8.00285900	0.76804600
H	-1.51866500	-8.40407700	0.56453900
H	0.08627800	-8.05104800	-0.14696600
H	-0.04195900	-8.62041700	1.53075100
C	0.71966300	-5.07706700	3.96138100
H	1.39485900	-5.58739700	4.65734900
H	-0.02322400	-4.51799300	4.53395100
H	0.21652900	-5.80394400	3.31658900
C	4.52821700	-2.52618800	4.40760100
H	3.56131900	-2.06741900	4.65944200
H	5.01753800	-2.83580800	5.33462500
H	5.16011700	-1.79828300	3.89033000
C	8.12845500	-0.33443200	3.21321700
H	8.11649600	-0.61747500	4.26791200
H	9.00673100	-0.79266200	2.73595000
H	8.19948000	0.75407600	3.12459500
C	5.59474600	2.55099600	2.51144600
H	5.33250800	1.96390300	3.40299300
H	6.18436200	3.41788300	2.81710000
H	4.67679800	2.90248000	2.02857500
C	7.07066700	4.38542900	-1.11657300
H	7.28401000	3.50941200	-1.74428000
H	7.06773900	5.28078200	-1.75381100
H	7.86221800	4.47735600	-0.37100800
C	4.19472400	6.50851600	1.00398400
H	3.58453200	6.15613900	1.84422200
H	5.22164900	6.14685300	1.10988500
H	4.19281700	7.60117800	0.99751700
C	0.99525400	7.38121300	2.90309700
H	1.83438000	7.25035100	3.59003700
H	1.14761600	8.30952600	2.33413600
H	0.06489900	7.46165600	3.47493800
C	-1.48780400	4.85164200	3.89610300
H	-1.91672400	5.35611300	4.76541700
H	-1.98172500	3.88154600	3.77693000
H	-0.41130900	4.71431900	4.06103500
C	-0.35237200	-0.48627300	0.47760000
H	-1.23457700	-1.04642000	0.16035900
C	-0.75107000	0.78059800	1.23753200
C	0.56541100	-1.38102100	1.32406900
H	0.13386300	1.34628000	1.54486900
H	-1.39198900	1.42693300	0.63197200

H	-1.30699900	0.49999500	2.13495500
O	1.77659800	-1.27043500	1.20631300
O	-0.07934600	-2.19202200	2.12704600
H	0.54960800	-2.86985000	2.53593400
H	0.17516300	0.67019000	-1.29160700
H	1.43208200	-0.02327800	-0.40809500
H	0.49679900	-0.97792100	-1.40641000
N	0.46605900	-0.16451900	-0.73807100

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H	-1.10919400	-6.10073400	1.19834300
C	4.96442500	2.92024400	-0.35995800
C	5.93463900	2.33654100	0.66848500
C	5.84151600	0.80722100	0.74350800
C	5.87610000	0.15827400	-0.65561600
C	4.95260500	0.89032400	-1.66063200
C	5.14626000	0.48376400	-3.12605200
O	5.67640800	2.95595300	1.92570500
O	6.92323200	0.38727900	1.55831800
O	5.48385900	-1.20429200	-0.43928400
O	5.19694900	2.31790000	-1.60601000
O	6.50155000	0.31767500	-3.51502000
H	5.15316500	3.98840700	-0.49548700
H	6.94501900	2.59803700	0.32561900
H	4.88479100	0.53236700	1.21089300
H	6.90539200	0.19362500	-1.03293000
H	3.90678800	0.69694800	-1.39088300
H	4.64998400	1.24031800	-3.75121400
H	4.65407400	-0.47517700	-3.28682700
C	0.03079700	4.87295000	-0.38230100
C	0.53202000	4.57807800	1.04477100
C	1.59727800	3.47466900	1.04508300
C	2.73941800	3.83932700	0.08613700
C	2.15770100	4.17232400	-1.31141600
C	3.19237000	4.71069400	-2.30187100
O	-0.51156900	4.39858200	1.99753400
O	2.02901700	3.32253100	2.41215600
O	3.61620300	2.71709000	0.06764300
O	1.14052600	5.18482900	-1.19992100
O	4.01017700	5.73682200	-1.75913300
H	-0.59026200	5.76904500	-0.37696200
H	1.02013400	5.51137700	1.35702700
H	1.16491800	2.52066500	0.72166400
H	3.26493800	4.72596200	0.46410400
H	1.72699500	3.25149800	-1.72776900
H	2.65584800	5.06186900	-3.19337200
H	3.85783800	3.89559400	-2.59399400
C	-4.32497400	3.01749000	-2.65856800
C	-4.24636600	4.42695200	-2.03814700
C	-3.03693100	4.50694600	-1.09925000
C	-1.75036700	4.07061700	-1.81884600
C	-1.92786800	2.79489100	-2.67067400
C	-0.78330000	2.63923300	-3.67373200
O	-5.39287700	4.79452300	-1.30282600
O	-2.82683300	5.84174900	-0.64323400
O	-0.71085900	3.77150600	-0.85768300
O	-3.14265700	2.82570100	-3.42795300
O	-0.79163900	1.39769600	-4.35224100
H	-5.14425500	2.94719700	-3.38116500
H	-4.09041500	5.13199300	-2.87020700
H	-3.21575900	3.83315000	-0.25220200
H	-1.42250500	4.89933400	-2.46033600
H	-1.93843600	1.93083500	-1.99555300
H	0.15912500	2.69596900	-3.12131000
H	-0.81599200	3.47672800	-4.38653700
C	-6.30585100	-1.48741500	-0.51503200
C	-7.17205900	-0.22080000	-0.37031300
C	-6.35540000	1.06472400	-0.57310800
C	-5.42347700	0.99432300	-1.79441000
C	-4.69743000	-0.35975200	-1.86759200
C	-3.92224100	-0.60725100	-3.15832400
O	-7.81300100	-0.12864300	0.89167100
O	-7.22023300	2.17630300	-0.76462600
O	-4.46691200	2.05942600	-1.64646500
O	-5.66029600	-1.41715000	-1.77647300
O	-3.06067700	-1.72967600	-3.04995400
H	-6.92417000	-2.38791200	-0.55016800
H	-7.92477700	-0.26498600	-1.17239700
H	-5.72116700	1.21730700	0.31072200
H	-6.02152900	1.15109800	-2.70245400

H	-4.01086800	-0.41530300	-1.01539900
H	-3.36089300	0.29191200	-3.43983000
H	-4.63848900	-0.83761100	-3.95474900
C	-2.94092200	-4.67308000	1.97162900
C	-3.57579600	-3.72626000	3.00167000
C	-4.20735200	-2.48270700	2.36479300
C	-5.08529700	-2.83117400	1.14979700
C	-4.36180700	-3.82679100	0.21266700
C	-5.21474400	-4.39236500	-0.92997500
O	-2.62058200	-3.36203200	3.98119600
O	-4.94997900	-1.86226700	3.40541800
O	-5.37175100	-1.56135300	0.53549600
O	-3.90435000	-4.96476600	0.97156800
O	-6.55121100	-4.71452100	-0.57096800
H	-2.72222300	-5.62878900	2.45495000
H	-4.39078500	-4.30275400	3.46220000
H	-3.39967400	-1.81740700	2.02352100
H	-6.01858200	-3.28628300	1.50256000
H	-3.49911900	-3.31510400	-0.23371700
H	-4.69542700	-5.27821800	-1.32236700
H	-5.27580000	-3.64724300	-1.72403300
C	2.06136600	-5.51716100	0.31055200
C	1.65224800	-5.71405800	1.78564300
C	0.40026000	-4.91219900	2.16510900
C	-0.71711400	-5.07750100	1.12792000
C	-0.17230300	-4.86035600	-0.29561100
C	-1.18346200	-5.17439700	-1.38396900
O	2.68691800	-5.37497300	2.69061200
O	-0.10562300	-5.37876700	3.40759800
O	-1.76127400	-4.13434800	1.42011500
O	0.93914100	-5.74160300	-0.52182300
O	-0.67931100	-4.70345800	-2.62232900
H	2.78585900	-6.28176600	0.01794500
H	1.38716800	-6.77680800	1.89123000
H	0.65744200	-3.84575200	2.22363300
H	0.15189300	-3.81691500	-0.39847600
H	-2.14025800	-4.69519100	-1.14791600
H	-1.34499600	-6.26361100	-1.42133200
C	5.78913600	-2.16568700	-1.42808000
C	6.19530400	-3.49815700	-0.76819800
C	5.01566400	-4.10180900	0.00612300
C	3.69878100	-4.11658600	-0.80162400
C	3.48503600	-2.82100000	-1.60216600
C	2.43740300	-2.94438500	-2.69481000
O	7.28535700	-3.39893100	0.12839000
O	5.28579300	-5.39758800	0.54154300
O	2.60790500	-4.23301600	0.12001200
O	4.69312400	-2.43345800	-2.27609200
O	2.05984500	-1.62984800	-3.08222000
H	6.57620600	-1.79120800	-2.08957500
H	6.46577100	-4.15318200	-1.61116000
H	4.83481800	-3.47728300	0.88538200
H	3.70000500	-4.96928400	-1.49461100
H	3.18224200	-2.03407200	-0.90213500
H	1.56909300	-3.51968000	-2.35154900
H	2.88786700	-3.48552400	-3.54204700
C	3.53944400	7.06408800	-1.96421800
H	3.39458500	7.27121500	-3.03363700
H	4.31361900	7.73298900	-1.58088800
H	2.59620800	7.25454400	-1.44026400
C	-1.43863200	1.41115500	-5.62201800
H	-1.33077000	0.40636000	-6.03532600
H	-0.95597300	2.12813800	-6.30157400
H	-2.50076200	1.65938300	-5.53596900
C	-1.81815700	-1.43384800	-2.42202500
H	-1.28967100	-0.62953200	-2.94899400
H	-1.22325200	-2.34791400	-2.45419100
H	-1.94434200	-1.13972300	-1.36822700
C	-6.71693200	-5.97442500	0.06739000
H	-6.22611500	-6.01306500	1.04618000
H	-6.31362100	-6.78708700	-0.55365700
H	-7.79221400	-6.12494700	0.19067500
C	-1.56327600	-4.95751500	-3.70289400

H	-1.06049900	-4.62441300	-4.61366300
H	-2.50420900	-4.40040700	-3.59329400
H	-1.78591200	-6.03083700	-3.79414900
C	1.39159400	-1.59418500	-4.33105500
H	1.06077700	-0.56514200	-4.49028600
H	0.51086700	-2.25174200	-4.34098600
H	2.05903400	-1.89705600	-5.15260200
C	7.17674800	1.51077500	-3.88825900
H	8.15691500	1.21223400	-4.26786900
H	7.30662200	2.19995400	-3.04569300
H	6.63479000	2.03930000	-4.68604400
C	-1.11539600	3.10039600	2.10031500
H	-2.00024500	3.23409900	2.72550200
H	-0.44072700	2.38676700	2.58691300
H	-1.41543700	2.71892300	1.12409500
C	2.63637200	2.06749800	2.79332100
H	2.18604800	1.24936200	2.22556600
H	2.41255400	1.92319900	3.85493100
H	3.71223800	2.09987800	2.62348300
C	6.84342200	3.24371700	2.69365300
H	7.40318800	2.33453200	2.92566300
H	6.50249100	3.71442300	3.62010900
H	7.50176200	3.94748100	2.16495300
C	6.72100800	-0.79457600	2.33402800
H	5.75018600	-0.76595700	2.84993400
H	7.51521600	-0.80566600	3.08533700
H	6.78012000	-1.69958400	1.72592500
C	8.54258800	-3.15891100	-0.48625800
H	8.74697000	-3.89003700	-1.28189000
H	9.29917600	-3.26475300	0.29373400
H	8.61716400	-2.14879400	-0.91074900
C	5.94774600	-6.32737900	-0.30078000
H	7.00058400	-6.06125000	-0.45512000
H	5.46223700	-6.44447900	-1.28060300
H	5.90752800	-7.28902300	0.21622500
C	3.53312400	-6.45711500	3.05334000
H	2.96020000	-7.27169000	3.51924800
H	4.24869000	-6.06502600	3.77943900
H	4.09397200	-6.84374300	2.19597000
C	0.28127200	-4.61133600	4.53910500
H	1.36926500	-4.59695700	4.66081500
H	-0.17509100	-5.09173300	5.40860800
H	-0.10035700	-3.58532100	4.46430000
C	-3.09379200	-3.42517900	5.31984100
H	-2.25187900	-3.15410200	5.96198900
H	-3.41898300	-4.44213500	5.58499300
H	-3.92324400	-2.73090500	5.48757900
C	-5.17074600	-0.46253700	3.29816000
H	-4.25211000	0.06294900	2.99554800
H	-5.45623100	-0.11815700	4.29684100
H	-5.96754700	-0.22584100	2.58812900
C	-8.94994200	-0.96818600	1.04079500
H	-8.68991700	-2.03444600	1.01380800
H	-9.69793300	-0.76852300	0.26062600
H	-9.38331900	-0.74037400	2.01658100
C	-7.51317900	2.91720000	0.41428400
H	-6.61128700	3.40899500	0.80262100
H	-7.95456600	2.28286600	1.18814900
H	-8.23319000	3.68691500	0.12569300
C	-6.52829000	5.11801400	-2.09707600
H	-7.24112800	5.61628300	-1.43709900
H	-7.00495600	4.22091700	-2.50770100
H	-6.26188800	5.80529700	-2.91237900
C	-3.45087700	6.17035500	0.59490500
H	-3.25760600	7.23312900	0.76235000
H	-3.00999100	5.59578900	1.42216100
H	-4.52901100	5.99866500	0.55814900
C	0.81311400	5.64737200	4.61563100
H	0.13381400	5.28801900	3.82877700
C	0.49586000	4.96873300	5.94620600
C	0.73296400	7.17311700	4.63662900
H	1.17583100	5.29523500	6.74024200
H	0.55815500	3.88194800	5.84639300

H	-0.52102400	5.22322300	6.24849700
O	1.60516800	7.87622800	4.16644900
O	-0.39666400	7.61074000	5.18481200
H	-0.40758800	8.58356500	5.13555300
H	2.81755100	5.06038100	4.91554000
H	2.59127100	6.18884800	3.72661400
H	2.19728900	4.52840900	3.41028500
N	2.20758500	5.32177700	4.13762000

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H	-1.08957000	-6.29188400	-1.69698200
C	5.74410200	2.79037400	0.50674700
C	6.87289200	1.95367000	-0.12529800
C	6.50842100	0.46992300	-0.21263100
C	5.93804600	-0.05668000	1.10645100
C	4.89617200	0.89292600	1.72639300
C	4.50081100	0.50908600	3.15502400
O	7.21191500	2.39193100	-1.42895800
O	7.67568700	-0.28239600	-0.51229000
O	5.36251200	-1.33616200	0.80992600
O	5.42311900	2.23464500	1.77242900
O	5.59599700	0.19580600	4.00194300
H	6.08379500	3.80759000	0.71808400
H	7.74454200	2.04138700	0.54131300
H	5.74657300	0.33616000	-0.99079900
H	6.76471800	-0.17523300	1.81584800
H	3.99102100	0.88154300	1.10425100
H	3.90307400	1.33104400	3.57765800
H	3.88078600	-0.38946800	3.12029400
C	1.55709700	5.59628900	-1.07315100
C	2.36436600	5.10816400	-2.28202400
C	3.21688500	3.87376500	-1.95582600
C	4.03956600	4.09047100	-0.67275400
C	3.15088100	4.64130300	0.46616900
C	3.90966900	5.06186500	1.72877200
O	1.48091800	4.86307100	-3.36157600
O	4.04016700	3.65955200	-3.08877300
O	4.61030300	2.81724800	-0.33938600
O	2.42191400	5.80342000	0.02700300
O	5.07922500	5.82889300	1.48981300
H	1.11770200	6.57041000	-1.29557800
H	3.05353900	5.92779500	-2.53356300
H	2.54602400	3.01580400	-1.80078200
H	4.83640500	4.81275100	-0.88609900
H	2.44333100	3.84805700	0.74693300
H	3.20921600	5.61202500	2.37456100
H	4.23886900	4.16361800	2.25500500
C	-3.50847600	4.63695900	0.15861100
C	-3.10024200	5.67138500	-0.90773600
C	-1.68147600	5.40886800	-1.42880100
C	-0.68782600	5.23168800	-0.26893900
C	-1.22758700	4.30108500	0.83195800
C	-0.38726600	4.36765500	2.10353800
O	-3.98146700	5.71061200	-2.01076100
O	-1.22497700	6.51405500	-2.19130100
O	0.53213500	4.66997700	-0.75743500
O	-2.56567200	4.67153300	1.21416100
O	-0.89765200	3.51081400	3.12177500
H	-4.46317100	4.91281500	0.62038800
H	-3.09090100	6.64847500	-0.39884700
H	-1.67795400	4.49014400	-2.02953900
H	-0.50141900	6.22302300	0.16747400
H	-1.23236000	3.27238500	0.45043800
H	0.62997600	4.04664700	1.86741300
H	-0.34464800	5.40487500	2.46007900
C	-5.69301700	-0.24104600	-0.27599500
C	-6.31245100	0.86464800	-1.15621500
C	-5.33808200	2.02677700	-1.38494800
C	-4.70609000	2.51504800	-0.07514700
C	-4.23176400	1.34424900	0.81246800
C	-3.89756000	1.80914000	2.22545200
O	-6.71878600	0.40553400	-2.42344000
O	-6.03329300	3.11952700	-1.95504000
O	-3.60500100	3.35236600	-0.41974200
O	-5.27075400	0.35124000	0.95642700
O	-3.50234600	0.73571700	3.09281700
H	-6.45085400	-0.97556300	0.01607700
H	-7.17793500	1.26035700	-0.59814100
H	-4.52997000	1.68243300	-2.04272300
H	-5.46810900	3.09438100	0.46707800

H	-3.35872000	0.88104600	0.33808100
H	-3.12075200	2.57738700	2.20555600
H	-4.79621600	2.24200500	2.68088600
C	-3.12698000	-4.75754200	-1.60409500
C	-3.98598200	-4.13273800	-2.73001900
C	-4.28626200	-2.63703100	-2.51783700
C	-4.65697200	-2.30499200	-1.06621300
C	-3.67027900	-2.98747800	-0.10746200
C	-3.88857900	-2.73910100	1.37452100
O	-3.41520100	-4.24413100	-4.01271000
O	-5.37626200	-2.25912600	-3.33812200
O	-4.62547100	-0.87717200	-0.92497700
O	-3.72259600	-4.39962400	-0.34909000
O	-5.22792700	-2.97248700	1.85294600
H	-3.18912500	-5.85109800	-1.63628800
H	-4.95412400	-4.66018000	-2.69475000
H	-3.38358000	-2.06522800	-2.77245800
H	-5.66833400	-2.67835600	-0.86619700
H	-2.65722400	-2.62055000	-0.32245900
H	-3.17204800	-3.34948400	1.94007300
H	-3.70070300	-1.68136400	1.56795700
C	2.06978100	-5.58363800	-0.64231800
C	1.69052300	-5.60851900	-2.14008100
C	0.36912000	-4.88685000	-2.42232600
C	-0.74113900	-5.28047600	-1.44507200
C	-0.23592300	-5.24763900	0.01187200
C	-1.20173400	-5.83890200	1.03556100
O	2.66286400	-5.02547500	-2.97888400
O	-0.07254700	-5.21153900	-3.73188500
O	-1.80252200	-4.33405300	-1.67991200
O	0.95958700	-6.03288200	0.12734500
O	-1.04430600	-5.14957200	2.27648700
H	2.85544100	-6.31539400	-0.44452600
H	1.54112200	-6.66806200	-2.40053600
H	0.53673300	-3.80638700	-2.32189200
H	-0.03225500	-4.20212800	0.27640500
H	-2.24221000	-5.75420500	0.70667400
H	-0.95112600	-6.90230200	1.15221300
C	5.53353100	-2.37743500	1.73605900
C	5.98789000	-3.66585800	1.01661500
C	4.88815100	-4.16366300	0.07161000
C	3.50938500	-4.24024200	0.75459600
C	3.21711200	-3.00199300	1.62165300
C	2.06440300	-3.23657500	2.58199700
O	7.16073900	-3.53220600	0.24514100
O	5.19502600	-5.40612900	-0.56773300
O	2.48722600	-4.30076800	-0.25521800
O	4.34185200	-2.67113700	2.44326900
O	1.60224400	-1.98099100	3.05953000
H	6.24755800	-2.08644000	2.51195500
H	6.14933300	-4.39783900	1.82572700
H	4.80258600	-3.44563300	-0.74874100
H	3.45980000	-5.13759800	1.38770300
H	2.97695600	-2.16422800	0.95608500
H	1.25262000	-3.78785600	2.09207500
H	2.43574800	-3.85192400	3.41713100
C	4.86683600	7.22023000	1.28700600
H	4.30285200	7.65916800	2.12287300
H	5.85513400	7.68455300	1.24728200
H	4.32570300	7.42797000	0.35785900
C	-1.53503100	4.19589300	4.19272600
H	-1.88572000	3.43328000	4.89300500
H	-0.83210900	4.85599600	4.71935200
H	-2.38908400	4.78821100	3.84356800
C	-2.11345400	0.37240700	3.00411100
H	-1.48486800	1.25777800	3.13510900
H	-1.92467400	-0.34356400	3.80595500
H	-1.88109100	-0.10103800	2.04281600
C	-5.56257400	-4.35162800	2.07729700
H	-5.55568100	-4.90827200	1.13906800
H	-4.85264700	-4.81418500	2.77453000
H	-6.56372900	-4.36527100	2.51348200
C	-1.48929600	-5.90896800	3.38433500

H	-1.31873700	-5.30773500	4.28069700
H	-2.56220100	-6.15188400	3.31719100
H	-0.93210100	-6.85195300	3.47812300
C	0.70701300	-2.11667000	4.13953200
H	0.42403900	-1.10901200	4.45674800
H	-0.19774700	-2.67755600	3.85153900
H	1.17058900	-2.63266700	4.99468800
C	6.24268300	1.31255200	4.59618000
H	6.96899400	0.91182800	5.30791300
H	6.75836200	1.93844400	3.85992600
H	5.52443400	1.94258300	5.14222300
C	1.96698700	5.28428600	-4.63187100
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H	2.14712500	6.36967800	-4.65155300
H	2.89008000	4.76466100	-4.90168600
C	4.40116300	2.31303000	-3.37856900
H	3.54986100	1.63318000	-3.23406000
H	4.68948400	2.28947100	-4.43354600
H	5.24377600	1.98586300	-2.76639300
C	8.10901100	3.49032500	-1.47438500
H	9.05160400	3.25764600	-0.95905800
H	8.31782000	3.68339100	-2.52850800
H	7.68216300	4.40058500	-1.03104800
C	7.72853900	-0.81314700	-1.82877700
H	7.67220100	-0.01937000	-2.58305400
H	8.69069200	-1.32295700	-1.92031200
H	6.92961200	-1.54630500	-1.99604100
C	8.33924400	-3.24974700	0.98653600
H	8.43241500	-3.90881600	1.86289600
H	9.18179900	-3.43570100	0.31688100
H	8.38011000	-2.20292900	1.30760100
C	5.82182300	-6.41079300	0.21517400
H	6.85135200	-6.13780800	0.47232500
H	5.26972900	-6.64452400	1.13746300
H	5.84374000	-7.30930300	-0.40613500
C	3.68031700	-5.91018700	-3.43491500
H	3.24640000	-6.79810100	-3.91709300
H	4.26121900	-5.35651600	-4.17592000
H	4.34856100	-6.21146700	-2.62223200
C	0.07701800	-4.16817000	-4.68727800
H	1.11698200	-3.83035500	-4.74637200
H	-0.21972600	-4.58577000	-5.65258600
H	-0.58078600	-3.32100800	-4.45329300
C	-3.35159000	-5.56463900	-4.53816700
H	-3.15649100	-5.46582100	-5.60790800
H	-2.53175500	-6.13749000	-4.09062800
H	-4.30405600	-6.09666500	-4.40113500
C	-5.02347600	-1.55542500	-4.52411600
H	-4.35543500	-2.14957700	-5.15563400
H	-5.95567100	-1.36565200	-5.06051100
H	-4.55375200	-0.59209700	-4.28761200
C	-7.92205600	-0.34568700	-2.44343000
H	-7.79028900	-1.35254300	-2.02780300
H	-8.72662100	0.17351100	-1.90254600
H	-8.21075400	-0.44876900	-3.49079600
C	-5.81780300	3.30262800	-3.35296100
H	-4.78318200	3.60580300	-3.55042800
H	-6.06574900	2.39650000	-3.91453700
H	-6.48597600	4.10901100	-3.66349500
C	-5.20482100	6.39240900	-1.77255600
H	-5.67521400	6.54525700	-2.74599500
H	-5.88886500	5.80394000	-1.14828500
H	-5.03259700	7.37273800	-1.30626600
C	-1.41709100	6.40457100	-3.59928000
H	-0.94501400	7.28499500	-4.04190600
H	-0.92573000	5.50542600	-3.98745200
H	-2.48001800	6.39139700	-3.85851900
C	-6.86095200	-0.27508400	3.65744100
H	-6.80189700	0.41855200	2.81711600
C	-8.01207400	-1.26641600	3.44908400
C	-7.01884400	0.48152700	4.97280900
H	-8.07722200	-1.97927300	4.27709900
H	-8.95691000	-0.72276200	3.38975500

H	-7.86918500	-1.81637500	2.51556400
O	-6.36733200	0.22511200	5.96242500
O	-7.97583800	1.40975000	4.89725800
H	-8.06777300	1.82374900	5.77401700
H	-5.49832200	-1.79748400	3.07277500
H	-4.74712700	-0.32886900	3.48198700
H	-5.39953600	-1.28059100	4.70460000
N	-5.54238300	-0.98027100	3.73344500

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H	-1.54261900	-6.05027800	-1.99864400
C	5.91959600	2.37314500	0.66162300
C	6.99131100	1.47873900	0.01118400
C	6.51771500	0.03125600	-0.13848500
C	5.88815900	-0.50039300	1.15142400
C	4.91156100	0.50221500	1.79464000
C	4.46389400	0.09500200	3.20135100
O	7.37878300	1.94228600	-1.27016000
O	7.63055300	-0.79424800	-0.45237700
O	5.22418600	-1.72134800	0.79707700
O	5.53968100	1.79677000	1.90147500
O	5.51476900	-0.34976500	4.04569700
H	6.33135900	3.35396100	0.91306800
H	7.85748800	1.47383800	0.69031100
H	5.76075300	-0.01544800	-0.93131400
H	6.69179100	-0.70766500	1.86705600
H	4.01886600	0.58632400	1.16045300
H	3.93536700	0.94856900	3.65267200
H	3.76822600	-0.74310000	3.12178600
C	1.98506300	5.54175000	-0.87908500
C	2.76432800	5.02333600	-2.09376600
C	3.51475200	3.71825000	-1.79400000
C	4.33799000	3.83625800	-0.49892000
C	3.48523700	4.42648900	0.64769400
C	4.26476200	4.75675000	1.92462200
O	1.87627700	4.87637200	-3.18698300
O	4.33255600	3.47163000	-2.92442400
O	4.80244600	2.51344400	-0.19550600
O	2.85124200	5.65228400	0.23382200
O	5.49286200	5.43471400	1.71183100
H	1.62532300	6.55234300	-1.08066600
H	3.51814600	5.79281200	-2.31710000
H	2.77752800	2.91136500	-1.66915600
H	5.19151500	4.49780300	-0.68822700
H	2.71611700	3.68397600	0.90478100
H	3.60467900	5.34551700	2.57888600
H	4.51767800	3.82346200	2.43212400
C	-3.15480500	4.96272200	0.27127000
C	-2.64915400	5.99278200	-0.75635000
C	-1.25008600	5.62868400	-1.27012700
C	-0.28971300	5.33789100	-0.10531600
C	-0.91727200	4.42508400	0.96297400
C	-0.09035700	4.39379700	2.24509400
O	-3.50839500	6.13612000	-1.86785700
O	-0.69303600	6.71264500	-1.99526800
O	0.88706300	4.69165300	-0.59545300
O	-2.22729000	4.88880900	1.33974900
O	-0.68289700	3.56174500	3.23933500
H	-4.09110200	5.29976900	0.73038400
H	-2.56688600	6.94993700	-0.21699200
H	-1.31627700	4.73005300	-1.89694900
H	-0.02903600	6.29841000	0.36102400
H	-0.99632400	3.41011500	0.55394000
H	0.89931800	3.99362100	2.01261000
H	0.03457400	5.41591500	2.62503300
C	-5.68231900	0.27610900	-0.34409400
C	-6.21286000	1.44935900	-1.19427300
C	-5.15225800	2.54129200	-1.37507600
C	-4.51077800	2.94928500	-0.04261400
C	-4.14027500	1.72605000	0.82432100
C	-3.81065100	2.13234300	2.25647100
O	-6.63744000	1.06103200	-2.47863000
O	-5.75151500	3.69860800	-1.92653800
O	-3.34420500	3.70932700	-0.34955400
O	-5.24923900	0.80463000	0.91491300
O	-3.48906100	1.01508100	3.10408900
H	-6.48722400	-0.41978800	-0.08695000
H	-7.05326500	1.88804400	-0.63028800
H	-4.35942800	2.15467900	-2.02786800
H	-5.23683300	3.57222200	0.50035900

H	-3.28927600	1.21722800	0.35699600
H	-2.99470400	2.85911600	2.27186500
H	-4.69614000	2.59622700	2.70674800
C	-3.44907900	-4.35699800	-1.86258700
C	-4.22165600	-3.59756800	-2.96762100
C	-4.39392600	-2.09494200	-2.67549100
C	-4.77541900	-1.81551200	-1.21556000
C	-3.87057200	-2.63113800	-0.27892800
C	-4.10170500	-2.44831000	1.21182800
O	-3.62964600	-3.68918400	-4.24248900
O	-5.42265100	-1.57606600	-3.49666300
O	-4.63872100	-0.40446000	-0.98897100
O	-4.04182000	-4.01845800	-0.60110800
O	-5.47248200	-2.51868900	1.63592700
H	-3.60199800	-5.43775800	-1.95885500
H	-5.23309800	-4.03737100	-2.98346900
H	-3.43763700	-1.59274800	-2.87576300
H	-5.81741700	-2.11858400	-1.06041600
H	-2.82462400	-2.34641300	-0.45703200
H	-3.49176600	-3.18388700	1.75318900
H	-3.77436700	-1.44208500	1.48139600
C	1.64564300	-5.64725700	-0.86373900
C	1.29342800	-5.57424500	-2.36633400
C	0.03879700	-4.73627300	-2.63293400
C	-1.11693300	-5.08480300	-1.69121000
C	-0.63654700	-5.16350900	-0.22760200
C	-1.66579200	-5.72230800	0.75026400
O	2.32520600	-5.03361400	-3.16192700
O	-0.40570400	-4.96168400	-3.96215200
O	-2.09212000	-4.04325100	-1.88988700
O	0.49137200	-6.04490700	-0.13253200
O	-1.45090300	-5.13507300	2.03436300
H	2.37199800	-6.44321500	-0.68855500
H	1.06546500	-6.60527700	-2.67899100
H	0.28956600	-3.67859800	-2.47763700
H	-0.35694700	-4.15117600	0.09059400
H	-2.68903500	-5.51063000	0.42368000
H	-1.52444400	-6.81114300	0.79713500
C	5.29973600	-2.80504200	1.68654500
C	5.66714500	-4.10039800	0.93052700
C	4.54816500	-4.48870800	-0.04291700
C	3.15503300	-4.47566500	0.61417500
C	2.94480300	-3.24862500	1.51993000
C	1.76229700	-3.42874700	2.45529200
O	6.85728300	-4.03273800	0.17690800
O	4.77032400	-5.73593600	-0.70851800
O	2.15033800	-4.41704500	-0.41299600
O	4.07797000	-3.03103900	2.36718500
O	1.38442800	-2.15943600	2.96970900
H	6.02113300	-2.59715200	2.48202100
H	5.76311700	-4.86531300	1.71938200
H	4.53269400	-3.74746600	-0.84682900
H	3.02120400	-5.38768100	1.21297100
H	2.77866400	-2.37324900	0.88060300
H	0.92098500	-3.90167700	1.93456200
H	2.07283600	-4.09760400	3.27399400
C	5.39071100	6.84102100	1.52770400
H	4.84452700	7.30916400	2.35950500
H	6.41201500	7.22912100	1.51412100
H	4.88568400	7.10281900	0.59192000
C	-1.27526600	4.27564600	4.31670300
H	-1.70128300	3.53089600	4.99428000
H	-0.52659600	4.86059700	4.86860500
H	-2.06969500	4.94708800	3.97012500
C	-2.13052000	0.55277900	2.99324500
H	-1.43790100	1.38348300	3.15516500
H	-1.99485800	-0.20697600	3.76488500
H	-1.93798000	0.10147500	2.01302800
C	-6.03059000	-3.83732000	1.73823700
H	-6.06269100	-4.32012400	0.76005500
H	-5.43664400	-4.45623900	2.42309400
H	-7.04052000	-3.71244500	2.13287400
C	-1.99509700	-5.90816700	3.08670200

H	-1.76954900	-5.38963300	4.02181700
H	-3.08774600	-6.02088500	2.99665300
H	-1.55058000	-6.91308200	3.12220500
C	0.45070700	-2.26678000	4.01960600
H	0.23296400	-1.25261900	4.36663800
H	-0.48352400	-2.74919200	3.68709900
H	0.85041500	-2.84524900	4.86714100
C	6.25521700	0.67974000	4.68635800
H	6.93215300	0.18784400	5.38951600
H	6.83599800	1.28066400	3.97825200
H	5.59170200	1.35449900	5.24796400
C	2.40567800	5.29569800	-4.44043300
H	1.61928000	5.13199700	-5.18144700
H	2.65950300	6.36640400	-4.42979500
H	3.29439000	4.72100900	-4.71412100
C	4.58546700	2.10968400	-3.25296600
H	3.67904100	1.49850100	-3.14105700
H	4.88681700	2.09510000	-4.30442000
H	5.38908900	1.69470500	-2.64160600
C	8.37515300	2.95247800	-1.26262600
H	9.29153600	2.60574100	-0.76444400
H	8.60161600	3.17971800	-2.30626300
H	8.03593600	3.87453900	-0.77047700
C	7.65968500	-1.28331300	-1.78568800
H	7.66822400	-0.46268500	-2.51283300
H	8.58402900	-1.85726400	-1.88661400
H	6.81222300	-1.95115400	-1.98428900
C	8.04324900	-3.85458800	0.93835400
H	8.07725100	-4.53859900	1.79987100
H	8.87852800	-4.08669200	0.27395000
H	8.15593100	-2.82103400	1.28415000
C	5.29933900	-6.80575400	0.06011700
H	6.34299400	-6.62379100	0.33998800
H	4.71418300	-7.01431300	0.96808100
H	5.25886000	-7.68883700	-0.58195000
C	3.28488800	-5.97399900	-3.63227800
H	2.79751200	-6.81081700	-4.15333400
H	3.91849100	-5.43891500	-4.34317500
H	3.91329700	-6.35150500	-2.81959800
C	-0.13456500	-3.90043800	-4.86999000
H	0.93488000	-3.66758400	-4.90041400
H	-0.45508100	-4.24574700	-5.85603700
H	-0.70751200	-3.00099400	-4.60911300
C	-3.67335400	-4.97867900	-4.84116200
H	-3.43317800	-4.84072600	-5.89732900
H	-2.92740200	-5.65208900	-4.40447100
H	-4.67603700	-5.42321200	-4.76274600
C	-4.97779600	-0.84342000	-4.63238600
H	-4.36596300	-1.46561500	-5.29338800
H	-5.87527000	-0.52079100	-5.16428600
H	-4.41046800	0.04740200	-4.33280800
C	-7.88865000	0.39324200	-2.52834700
H	-7.83340400	-0.62497700	-2.12318600
H	-8.66463300	0.95851100	-1.99218800
H	-8.16561500	0.32298100	-3.58146700
C	-5.49792900	3.89946500	-3.31534100
H	-4.43846600	4.12079000	-3.48929500
H	-5.80977800	3.03179100	-3.90517000
H	-6.09192300	4.76619400	-3.61384400
C	-4.67696300	6.90694600	-1.62574700
H	-5.11919000	7.12254200	-2.60048700
H	-5.41567100	6.35953700	-1.02688500
H	-4.43389800	7.85755100	-1.13040400
C	-0.88281600	6.66427200	-3.40707700
H	-0.32735500	7.50990400	-3.81973500
H	-0.47433700	5.73532300	-3.82050900
H	-1.94010000	6.75775200	-3.67230700
C	-6.20964600	-0.66322400	4.77331400
H	-5.51280800	-1.39115700	5.20148800
C	-6.15714300	0.63863400	5.57962100
C	-7.60073000	-1.29127100	4.74709100
H	-6.87228700	1.37124200	5.19200300
H	-6.40612200	0.43699800	6.62245700

H	-5.15322200	1.06836200	5.53238500
O	-8.23787200	-1.45895300	3.73089500
O	-8.00996200	-1.61676700	5.97784800
H	-8.90347900	-1.99765000	5.90958000
H	-4.85808300	0.04313200	3.29253100
H	-5.75513400	-1.31907900	2.78759400
H	-6.45490600	0.16896000	2.86358400
N	-5.79583600	-0.43477000	3.36158000

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H	-3.09378700	5.31025000	1.52356900
C	6.00966900	-1.42848500	-0.63440700
C	6.89257700	-0.42570700	0.13586300
C	6.17378700	0.90598500	0.37251700
C	5.51524500	1.43567800	-0.90318300
C	4.73140100	0.34753500	-1.65883900
C	4.28330600	0.78620100	-3.05625400
O	7.30775400	-0.91277900	1.39814600
O	7.11231600	1.87853600	0.81128400
O	4.65264600	2.51060800	-0.49986100
O	5.55915800	-0.81963000	-1.83005100
O	5.29846600	1.42966800	-3.80963700
H	6.58963900	-2.29387100	-0.96743600
H	7.76926500	-0.22067700	-0.49850300
H	5.38854100	0.75672000	1.12516100
H	6.29859100	1.81809000	-1.56694100
H	3.83987600	0.07727100	-1.07575700
H	3.89948800	-0.09725500	-3.58737400
H	3.47045600	1.50833300	-2.95992500
C	2.74027800	-5.36918700	0.75740600
C	3.68631000	-4.95393600	1.89128600
C	4.15159000	-3.50031900	1.72900900
C	4.71963600	-3.26313600	0.32188800
C	3.77188200	-3.80708500	-0.76811100
C	4.37424100	-3.80017100	-2.17435300
O	3.04996200	-5.16334500	3.13799200
O	5.14064000	-3.26044700	2.72022500
O	4.93013000	-1.85326800	0.17775000
O	3.41322800	-5.17490600	-0.47206700
O	5.67986500	-4.35244700	-2.24466800
H	2.53520600	-6.44402700	0.81459800
H	4.56814600	-5.60362600	1.80143600
H	3.28741500	-2.83892500	1.87827000
H	5.67596800	-3.79349200	0.24681300
H	2.86228500	-3.19034400	-0.78339000
H	3.68456200	-4.32087500	-2.85395300
H	4.46649300	-2.76221500	-2.50138300
C	-2.50886800	-4.99191300	-0.31762200
C	-2.15965800	-5.24346500	1.15270800
C	-0.75268400	-4.76262500	1.52199200
C	0.29704100	-5.31083100	0.53374700
C	-0.16157100	-5.04985000	-0.92219400
C	0.69147800	-5.71494300	-2.00028700
O	-3.14980400	-4.63046000	2.00219400
O	-0.51088800	-5.20442000	2.84829300
O	1.52955400	-4.64169300	0.83454600
O	-1.49680500	-5.55321300	-1.12304800
O	0.50490700	-5.11576500	-3.27409700
H	-3.42345600	-5.51863500	-0.59256600
H	-2.19727300	-6.32753000	1.30788900
H	-0.72376100	-3.66517000	1.46243800
H	0.40742000	-6.39044600	0.70857700
H	-0.14314300	-3.96544200	-1.08450900
H	1.74598400	-5.59971000	-1.75053300
H	0.45463600	-6.78910100	-2.02535400
C	-5.30242300	-0.97716400	-2.23669000
C	-5.89198800	-2.38693000	-2.06148300
C	-5.00596000	-3.21201300	-1.11781300
C	-3.53735700	-3.19953100	-1.58344200
C	-3.05712000	-1.79116800	-1.98359900
C	-1.76559200	-1.80212100	-2.80177800
O	-7.21578900	-2.36329600	-1.55001200
O	-5.43482600	-4.57045000	-1.07983200
O	-2.66861800	-3.60418300	-0.51081100
O	-4.02087200	-1.11240100	-2.80816100
O	-1.10927700	-0.54535400	-2.77518300
H	-5.87963800	-0.37047300	-2.94033100
H	-5.88248400	-2.86754800	-3.05036700

H	-5.04031900	-2.77138400	-0.11393300
H	-3.43630100	-3.89167700	-2.43082600
H	-2.90666900	-1.22986000	-1.05601700
H	-1.09702400	-2.60015400	-2.45685800
H	-2.02576600	-2.00247600	-3.84618400
C	-4.64065500	3.54304500	0.46962600
C	-5.67094000	2.65895200	1.19406800
C	-5.75508600	1.20483100	0.70475000
C	-5.57051400	1.03222000	-0.81812500
C	-4.46563300	1.97378500	-1.34423000
C	-4.31303900	2.01480200	-2.86815500
O	-5.43024800	2.70392500	2.60830600
O	-7.01534900	0.75739000	1.18194900
O	-5.25059700	-0.35306500	-0.96521800
O	-4.77427600	3.32179300	-0.91045500
O	-5.54023500	2.00745400	-3.57961300
H	-4.90497600	4.59441000	0.62954800
H	-6.64605900	3.11240500	0.98093400
H	-4.95118500	0.61051400	1.16246000
H	-6.51121500	1.26638700	-1.33024800
H	-3.49813100	1.67601500	-0.92079100
H	-3.71231000	2.90072300	-3.11978300
H	-3.76678800	1.12294400	-3.18015500
C	0.26808700	5.56460200	1.00531400
C	-0.34230900	5.16159500	2.36724800
C	-1.41254700	4.08337900	2.16065900
C	-2.47932900	4.48957400	1.12638100
C	-1.76782500	4.95987400	-0.16908600
C	-2.65695800	5.62100400	-1.21807500
O	0.56262900	4.64780600	3.31077100
O	-2.00244200	3.66227000	3.40273600
O	-3.31903600	3.32548100	0.93955600
O	-0.79336500	5.96271500	0.15158600
O	-1.98805400	5.52055600	-2.46500100
H	0.88371400	6.45878600	1.11792200
H	-0.81909600	6.08048200	2.74851200
H	-0.90273600	3.18842300	1.78804500
H	-1.28479800	4.08426900	-0.61925700
H	-3.63669500	5.13975400	-1.28545900
H	-2.79395200	6.67518900	-0.93033000
C	4.64791800	3.68367200	-1.27055500
C	4.68336700	4.92838300	-0.35576600
C	3.40090900	5.00506800	0.48071900
C	2.12877400	4.86107500	-0.37342200
C	2.24869400	3.73366000	-1.41319000
C	1.17934200	3.80966000	-2.49333100
O	5.76473100	4.97408600	0.54717300
O	3.31519200	6.17145900	1.30786800
O	1.02126700	4.50656800	0.48570700
O	3.50384000	3.78999100	-2.09833300
O	0.91657100	2.49634800	-2.95808000
H	5.49026800	3.68756100	-1.96826200
H	4.73247700	5.78408700	-1.04989700
H	3.41784800	4.16854700	1.18541100
H	1.90761900	5.80774300	-0.88419400
H	2.15370300	2.77946000	-0.88091900
H	0.26211300	4.27502800	-2.11275100
H	1.56086300	4.44429400	-3.30798500
C	5.73678200	-5.75840000	-2.44697900
H	5.16670300	-6.05285500	-3.33999800
H	6.78861600	-6.00955100	-2.60397900
H	5.35175400	-6.31842500	-1.58773200
C	-0.48022900	-5.72990900	-4.09204300
H	-0.45657900	-5.21095200	-5.05352200
H	-0.25337600	-6.79288700	-4.26202500
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H	0.54471000	-1.14516400	-1.65418100
H	0.20853200	0.60615800	-1.75789000
H	-0.78810700	-0.44440600	-0.70216000
C	-6.16245700	3.27515000	-3.73693600
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H	-7.01087600	3.12804900	-4.40921800
C	-2.56740800	6.33567500	-3.46773900
H	-1.99286200	6.17733500	-4.38238500
H	-3.61838100	6.06834800	-3.65633600
H	-2.52354400	7.40089500	-3.19691200
C	0.03587200	2.47303800	-4.07188300
H	-0.21249800	1.42756700	-4.26103400
H	-0.88840600	3.02942600	-3.85737600
H	0.50851800	2.91225800	-4.96262500
C	6.16022700	0.55997400	-4.53196600
H	6.80232600	1.19564300	-5.14693400
H	6.77933000	-0.05733000	-3.87211400
H	5.58714400	-0.10654900	-5.19322800
C	3.87012300	-5.76557600	4.13371800
H	3.25490700	-5.85543700	5.03210100
H	4.19444800	-6.77129800	3.82928300
H	4.75194000	-5.15506300	4.34994500
C	4.99780700	-2.03919700	3.43309500
H	4.02093000	-1.98492500	3.93579400
H	5.78358400	-2.02888500	4.19229700
H	5.13018800	-1.17469400	2.77848000
C	8.37406300	-1.84730100	1.35719300
H	9.24928300	-1.43375200	0.83606900
H	8.64539200	-2.06165900	2.39271700
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C	7.04708600	2.19485500	2.19441300
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C	7.04545300	5.09121800	-0.06101000
H	7.05332800	5.87319700	-0.83497900
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H	7.37949300	4.14061200	-0.49034700
C	3.75394400	7.40459300	0.75250000
H	4.84038200	7.41663600	0.61628200
H	3.26546700	7.63999300	-0.20373200
H	3.48197400	8.17664600	1.47592300
C	1.41409800	5.61693400	3.92426400
H	0.82671100	6.44969300	4.34081900
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H	2.16136400	6.00393400	3.22545100
C	-2.43762200	4.66606000	4.31905100
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H	-8.10431100	-0.76985000	1.93893600
H	-7.24616200	-1.18829100	0.42694700
C	-8.22392600	-2.18997500	-2.53907800
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H	-9.18382200	-2.21896700	-2.01999200
C	-6.33900400	-4.89259300	-0.02905500
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H	-7.27830900	-4.33998400	-0.11979000
H	-6.53842800	-5.96401600	-0.10962800
C	-3.62231900	-5.47967000	3.06221700
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H	-4.16652300	-6.33474300	2.64629900
H	-2.78994700	-5.82758100	3.67777400
C	0.07495900	-4.24693400	3.72632000
H	0.12632500	-4.72657500	4.70700800
H	1.08528600	-3.97817400	3.41491700
H	-0.55692700	-3.35070000	3.80925400
C	-2.92752300	-0.04297400	3.80114000
H	-1.93495300	-0.04151200	4.26527500
C	-4.00165300	-0.20294600	4.87454300
C	-2.91596700	-1.15791700	2.73472100

H	-5.00309400	-0.20944000	4.43350600
H	-3.85376800	-1.14840600	5.39734700
H	-3.94360400	0.60824000	5.60568900
O	-2.78778900	-0.88563900	1.55298200
O	-3.02478000	-2.35490900	3.26401400
H	-3.00394500	-3.11317300	2.59022600
H	-2.78352800	1.07054100	2.07797200
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N	-3.07123300	1.24366000	3.05275200