

Theoretical Investigations on Stereoselectivity of Proline-catalyzed Mannich Reaction in DMSO

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Table S1 Total energy and number of imaginary frequency of compounds

compound	total energy	#imaginary fregeuncy
iminium1	-634.6426817	0
iminium1+h2o	-711.1022423	0
s-cis enamine1	-634.6553017	0
s-trans enamine1+h2o	-711.1027338	0
TS1	-634.6264577	1, 1139.31i
TS1a	-711.0737491	1, 1475.20i
imine2	-325.7086803	0
cpx12	-960.3719927	0
int3	-960.3821723	0
TS12	-960.3584494	1, 1009i
cpx12a	-960.3711158	0
int3a	-960.3713881	0
TS12a	-960.3513143	1, 94i

Cartesian coordinate of iminium1

C	3.08330400	0.97644900	-0.42874600
C	3.62839500	-0.28801100	0.24813500
C	2.60056500	-0.87172800	1.22458700
C	1.24854900	-1.16476700	0.52904400
C	0.73358200	0.06668400	-0.16432400
C	1.71497200	0.71705200	-1.09912200
H	2.97029300	-1.80383400	1.66537600
H	3.86970200	-1.03706400	-0.51855500
H	4.56376400	-0.05939700	0.77174000
H	2.97520700	1.77534600	0.31735100
H	3.78224900	1.34652600	-1.18673000
H	1.37939800	-1.93430600	-0.23920800
H	0.52754600	-1.56414000	1.24144800
H	1.84502100	-0.00499500	-1.91816600
H	1.32103800	1.62885700	-1.54892400
H	2.44381800	-0.17202500	2.05723400
N	-0.42961100	0.59505600	0.10554700
C	-1.56066200	-0.19518700	0.62410200
C	-2.73644800	0.79341600	0.75642000
C	-2.14526400	2.17614700	0.42150600
C	-0.95140300	1.85786100	-0.47860600
H	-1.29869500	-0.66283200	1.57380000
H	-3.51843700	0.50048800	0.05152700
H	-3.18281100	0.76766400	1.75291400
H	-2.85906300	2.83964100	-0.07428800
H	-1.79349200	2.68168700	1.32807300
H	-1.25983300	1.65975300	-1.51210000
H	-0.18259400	2.63059200	-0.47261900
C	-1.85542500	-1.41271100	-0.40821500
O	-0.95527600	-1.61697000	-1.25477100
O	-2.93682800	-1.96910300	-0.16727600

Cartesian coordinate of iminium1_h2o

C	3.34386500	-0.89247300	-0.11498200
C	3.63641300	0.60004800	0.08125500
C	2.77461800	1.42901900	-0.87448800
C	1.27569300	1.21559500	-0.61237900
C	0.90569800	-0.24578300	-0.41426200
C	1.86066800	-1.18755600	-0.17165000
H	3.00584600	2.49678900	-0.78877300
H	3.41281100	0.89034500	1.11796100
H	4.70087300	0.80471300	-0.08186700
H	3.83173200	-1.23796400	-1.04080100
H	3.80663200	-1.47607900	0.69232700
H	0.96340200	1.78896200	0.27216100
H	0.70874500	1.63271600	-1.45100600
H	0.91697200	-0.87038500	1.90859500
H	1.57567300	-2.23219500	-0.08715900
H	3.00656900	1.13692500	-1.90756800
N	-0.45271300	-0.55299300	-0.42229000
C	-1.52192000	0.36864300	-0.81073100
C	-2.67182000	-0.56963500	-1.25231700
C	-2.44664700	-1.83139900	-0.40822400
C	-0.91906100	-1.94493000	-0.35100200
H	-1.23132500	1.01564400	-1.64252200
H	-3.65099600	-0.10643700	-1.11514000
H	-2.55091500	-0.79814100	-2.31695400
H	-2.85333900	-1.69681100	0.60015100
H	-2.91118700	-2.72199100	-0.84014500
H	-0.57431500	-2.42434000	0.57188000
H	-0.51988400	-2.52336300	-1.19951300
C	-2.00248200	1.33261300	0.29821900
O	-1.63300000	1.09316500	1.56326300
O	-2.72206000	2.26901800	0.01979700
O	0.17811300	-0.77674000	2.54156200
H	-1.01729200	0.33126500	1.67630700
H	0.55442300	-0.46709400	3.37447600

Cartesian coordinate of s-cis enamine1

C	-3.27296300	0.90980100	0.30600600
C	-3.56586300	-0.58170400	0.11788800
C	-2.66179800	-1.16790300	-0.97484500
C	-1.22668800	-0.71079500	-0.84989800
C	-0.82875700	0.31796100	-0.07469900
C	-1.81695400	1.13174900	0.74085900
H	-2.69654700	-2.26477800	-0.94429900
H	-3.38290400	-1.10801100	1.06479600
H	-4.62025500	-0.74147400	-0.13567300
H	-3.45517000	1.43627000	-0.64093700
H	-3.94714300	1.35193000	1.04868700
H	0.90225200	-0.66955000	1.70132900
H	-0.49779400	-1.28686900	-1.41185000
H	-1.69641900	0.86166500	1.80155300
H	-1.57703200	2.19929800	0.67999800
H	-3.05038700	-0.88833900	-1.96676800
N	0.53888600	0.64391600	0.15422900
C	1.58665000	-0.18874400	-0.45072600
C	2.86331400	0.66558600	-0.30565700
C	2.33711300	2.08622300	-0.54052100
C	0.94791400	2.07946600	0.12124200
H	1.40532500	-0.40381000	-1.51268400
H	3.27116200	0.56543600	0.70703400
H	3.63576100	0.35557900	-1.01252000
H	2.99142400	2.85906400	-0.12692600
H	2.23933000	2.27345700	-1.61570700
H	0.98342500	2.48559200	1.13906100
H	0.23257000	2.67745500	-0.45274300
C	1.74810000	-1.53346100	0.26844700
O	1.33945700	-1.53428400	1.55320000
O	2.26426800	-2.49814100	-0.24701600

Cartesian coordinate of s-trans enamine1_h2o

C	3.34386500	-0.89247300	-0.11498200
C	3.63641300	0.60004800	0.08125500
C	2.77461800	1.42901900	-0.87448800
C	1.27569300	1.21559500	-0.61237900
C	0.90569800	-0.24578300	-0.41426200
C	1.86066800	-1.18755600	-0.17165000
H	3.00584600	2.49678900	-0.78877300
H	3.41281100	0.89034500	1.11796100
H	4.70087300	0.80471300	-0.08186700
H	3.83173200	-1.23796400	-1.04080100
H	3.80663200	-1.47607900	0.69232700
H	0.96340200	1.78896200	0.27216100
H	0.70874500	1.63271600	-1.45100600
H	0.91697200	-0.87038500	1.90859500
H	1.57567300	-2.23219500	-0.08715900
H	3.00656900	1.13692500	-1.90756800
N	-0.45271300	-0.55299300	-0.42229000
C	-1.52192000	0.36864300	-0.81073100
C	-2.67182000	-0.56963500	-1.25231700
C	-2.44664700	-1.83139900	-0.40822400
C	-0.91906100	-1.94493000	-0.35100200
H	-1.23132500	1.01564400	-1.64252200
H	-3.65099600	-0.10643700	-1.11514000
H	-2.55091500	-0.79814100	-2.31695400
H	-2.85333900	-1.69681100	0.60015100
H	-2.91118700	-2.72199100	-0.84014500
H	-0.57431500	-2.42434000	0.57188000
H	-0.51988400	-2.52336300	-1.19951300
C	-2.00248200	1.33261300	0.29821900
O	-1.63300000	1.09316500	1.56326300
O	-2.72206000	2.26901800	0.01979700
O	0.17811300	-0.77674000	2.54156200
H	-1.01729200	0.33126500	1.67630700
H	0.55442300	-0.46709400	3.37447600

Cartesian coordinate of TS1

C	3.22383400	1.04381500	-0.27151400
C	3.51184100	-0.46006700	-0.28279700
C	2.70713700	-1.14230300	0.82815800
C	1.21653000	-0.82443000	0.73848200
C	0.78121300	0.42193800	0.18189300
C	1.74146400	1.33628300	-0.55060700
H	2.83813100	-2.22943300	0.78077500
H	3.23783200	-0.88357300	-1.25886100
H	4.58308900	-0.64360300	-0.14405100
H	3.49915000	1.45409800	0.70935100
H	3.83118700	1.57235100	-1.01455500
H	0.51296200	-1.54026400	-0.07309900
H	0.65794800	-1.12548500	1.63067700
H	1.53302500	1.22992500	-1.62578000
H	1.51556600	2.37990600	-0.30569900
H	3.11136400	-0.82673000	1.80173900
N	-0.51991200	0.69287400	0.11260300
C	-1.60023700	-0.24863200	0.55220700
C	-2.89429400	0.59149700	0.48669400
C	-2.43366200	2.04510100	0.29123500
C	-1.12527600	1.89796900	-0.48720200
H	-1.38132700	-0.55678900	1.58189600
H	-3.49249100	0.24162300	-0.35771300
H	-3.50251200	0.45988400	1.38404700
H	-3.16517700	2.65311900	-0.24787600
H	-2.23257200	2.53181500	1.25259600
H	-1.31244000	1.72230700	-1.55549500
H	-0.46453700	2.75974100	-0.39058200
C	-1.68027600	-1.56143000	-0.31934500
O	-0.55414200	-2.05903300	-0.71737300
O	-2.79829100	-2.02190000	-0.52748000

Cartesian coordinate of TS1a

C	-3.22913700	0.92773600	0.07911800
C	-3.57309500	-0.56501400	0.02772500
C	-2.77754200	-1.24331200	-1.09110200
C	-1.26328600	-1.11636400	-0.86367100
C	-0.81906200	0.28605100	-0.50333400
C	-1.72352600	1.17174200	0.15190700
H	-3.03289600	-2.30564700	-1.16952500
H	-3.33023100	-1.03796600	0.98925000
H	-4.64880400	-0.70098500	-0.13122200
H	-3.65333500	1.42430500	-0.80655800
H	-3.70654800	1.39843800	0.94700400
H	-0.94735500	-1.78138800	-0.04752000
H	-0.72225000	-1.45373000	-1.75284300
H	-1.18916400	0.82736900	1.34430900
H	-1.44950700	2.22687600	0.12921300
H	-3.04337700	-0.78376500	-2.05276700
N	0.47782300	0.57836000	-0.59403000
C	1.55697300	-0.40631600	-0.81333800
C	2.75404400	0.47970900	-1.19437400
C	2.56229700	1.72019500	-0.30851600
C	1.03741400	1.91169200	-0.24961600
H	1.29694400	-1.09012000	-1.62241000
H	3.69703400	-0.04220600	-1.02586600
H	2.69113100	0.74746600	-2.25568700
H	2.95049600	1.52840000	0.69650900
H	3.06730600	2.60750100	-0.69900900
H	0.70066300	2.21674700	0.74394100
H	0.67763100	2.64217100	-0.98413900
C	1.87869500	-1.30105700	0.43213200
O	1.28037600	-1.07215200	1.56154100
O	2.70747800	-2.18309000	0.23902900
O	-0.34526300	0.55270200	2.30762600
H	0.48419300	-0.24717500	1.87574100
H	-0.75007500	0.20513400	3.11263400

Cartesian coordinate of imine2

C	1.34453500	1.31171700	-0.03581200
C	-0.03053700	1.10374500	-0.16368400
C	-0.55048100	-0.20181100	-0.14727600
C	0.32848400	-1.29076500	-0.03306100
C	1.69780000	-1.07469200	0.11585000
C	2.21233100	0.22670400	0.11444600
H	1.73813400	2.32396300	-0.06240100
H	-0.69842600	1.94744900	-0.31008400
H	-0.08220600	-2.29530600	-0.05328100
H	2.36716600	-1.92381800	0.22000000
H	3.28104200	0.39194400	0.21286900
N	-1.92823400	-0.48036500	-0.30055000
C	-2.79032100	0.23272900	0.30753700
H	-3.84897400	0.02855200	0.14785500
H	-2.52995800	1.04400700	1.00089100

Cartesian coordinate of cpx12

N	-1.41070600	0.61454900	0.84609700
C	-1.21944800	1.97083700	0.32399500
H	-2.14700300	2.55976900	0.33088800
C	-0.67966600	2.06776600	-1.11038500
O	-1.00397300	2.98224800	-1.83943500
C	-0.20011200	2.59338300	1.30611600
H	-0.27428400	3.68311200	1.31770300
H	0.81946000	2.32621500	1.00577900
C	-0.55311800	1.92941200	2.64145800
C	-0.95595600	0.50240100	2.24083600
H	-0.11416500	-0.20015900	2.32016000
H	-1.76564100	0.11929600	2.87409400
O	0.20941300	1.14692200	-1.50715500
H	0.43230300	0.45055200	-0.83439700
H	-1.40462000	2.44256700	3.10284100
H	0.27399400	1.94660100	3.35707800
C	-4.28326800	-0.74818700	-1.26534600
C	-3.03807100	0.09871100	-0.96459800
C	-2.36688500	-0.28259600	0.34529400
C	-2.65755600	-1.45406300	0.96631800
C	-3.64455000	-2.47300300	0.44095900
C	-4.00948400	-2.23563000	-1.02971000
H	-2.31736800	-0.00505100	-1.78749400
H	-3.32156500	1.15654400	-0.94845100
H	-5.10943000	-0.42682500	-0.61646000
H	-4.60166000	-0.56479300	-2.29792600
H	-2.17006700	-1.70526300	1.90365900
H	-3.23180100	-3.48398000	0.56539700
H	-4.56285700	-2.45716500	1.05045300
H	-3.17811500	-2.55584000	-1.67337000
H	-4.88007900	-2.84066200	-1.30947200
C	5.09986400	-1.23980900	0.70452700
C	3.72003300	-1.44967600	0.73654000
C	2.89359300	-0.82694000	-0.21302900
C	3.45802600	0.03033900	-1.17041500
C	4.83950800	0.22030800	-1.20545800
C	5.66496700	-0.41281800	-0.27046600
H	5.73200700	-1.71600500	1.44848200
H	3.28143000	-2.06880700	1.51356500
H	2.80649800	0.52899000	-1.88101000
H	5.27054000	0.87290300	-1.95886900
H	6.73846200	-0.25107600	-0.29196700
N	1.48245800	-0.98568200	-0.21749700
C	0.95784800	-2.12546400	0.01554000
H	-0.12809900	-2.20468100	0.04509700
H	1.55192900	-3.03148200	0.18367200

Cartesian coordinate of int3

N	1.75898700	-0.45002500	0.72122400
C	2.38042400	-1.61015900	0.02294800
H	3.41094400	-1.36162100	-0.23934900
C	1.60590700	-1.97221800	-1.32790200
O	2.16389300	-2.88813100	-1.94657900
C	2.31716600	-2.76542900	1.04524100
H	3.23356600	-3.35742900	1.03264500
H	1.49446400	-3.43736500	0.78268600
C	2.05116700	-2.08794500	2.39729100
C	1.17791000	-0.89178900	2.02254600
H	0.13399200	-1.17197000	1.85252000
H	1.21401500	-0.07846500	2.74756800
O	0.56210500	-1.31010000	-1.56813300
H	-0.77327900	-0.34481200	-0.61681900
H	2.98544500	-1.74015400	2.85380200
H	1.54848500	-2.74166100	3.11516100
C	2.89803200	2.50874000	-1.00573000
C	2.27609500	1.09860700	-1.10871600
C	1.57229400	0.71145100	0.16380100
C	0.60945000	1.72108600	0.74295500
C	1.20537400	3.15091500	0.74694500
C	1.86110400	3.55270100	-0.58112200
H	1.52773200	1.07530500	-1.91061600
H	3.03102500	0.36394600	-1.38634500
H	3.72595300	2.49405600	-0.28359700
H	3.33430300	2.76402100	-1.97707100
H	0.35611200	1.44813400	1.76866000
H	0.41133100	3.85652300	1.01808400
H	1.95722200	3.21014700	1.54525700
H	1.10169500	3.65760200	-1.36598400
H	2.33423500	4.53534100	-0.47298300
C	-4.98070900	0.64502100	0.53665500
C	-3.61743300	0.95078000	0.55084300
C	-2.68567600	0.09133300	-0.06257700
C	-3.16749800	-1.07903300	-0.68569500
C	-4.52809900	-1.37671700	-0.68576900
C	-5.45055900	-0.51758700	-0.07744100
H	-5.67842900	1.32585400	1.01727800
H	-3.28906400	1.85385800	1.05593000
H	-2.46000700	-1.74351900	-1.17490300
H	-4.87054100	-2.28380200	-1.17644000
H	-6.51117100	-0.74865100	-0.08535700
N	-1.30046400	0.30960400	-0.02834900
C	-0.73282900	1.64390700	-0.05577800
H	-0.57599700	1.99970400	-1.08581700
H	-1.41239500	2.35176200	0.42228600

Cartesian coordinate of TS12

N	-0.84913500	0.68921300	0.90547700
C	-0.94207300	2.08918900	0.43124900
H	-1.88062400	2.54062200	0.77194700
C	-0.87915500	2.31402100	-1.11172700
O	-1.46161700	3.31752600	-1.52434900
C	0.25045000	2.77515300	1.13053100
H	0.05442600	3.83684500	1.29264100
H	1.14451600	2.68871800	0.50281700
C	0.43492000	1.97165900	2.42392700
C	0.15248500	0.53163200	1.97902500
H	1.06261700	0.04390000	1.61017400
H	-0.26225200	-0.09019800	2.77964100
O	-0.18820100	1.48678700	-1.82446000
H	0.37762100	0.34381900	-1.46320500
H	-0.29873700	2.28370900	3.17646800
H	1.43255000	2.07932300	2.85945000
C	-4.06624300	-0.96612800	-0.10953700
C	-2.94662900	0.07904200	-0.23571800
C	-1.70752300	-0.30189900	0.55289700
C	-1.42512400	-1.63555900	0.80966600
C	-2.42958900	-2.74857700	0.60167200
C	-3.54437700	-2.37872100	-0.38900700
H	-2.67713400	0.21509600	-1.29253300
H	-3.31025500	1.05491400	0.09870900
H	-4.48927800	-0.92847500	0.90355200
H	-4.87713600	-0.70810700	-0.79957100
H	-0.58028800	-1.87143400	1.45031700
H	-1.91324100	-3.65775700	0.26234500
H	-2.88170900	-3.01832500	1.56947300
H	-3.16487200	-2.42469100	-1.41882100
H	-4.35716300	-3.11121800	-0.32643900
C	3.92197400	-1.89430300	0.49572600
C	2.59667300	-1.88047100	0.05656400
C	2.12287200	-0.80118400	-0.70749800
C	2.98648800	0.26683700	-1.00555300
C	4.30677100	0.24422800	-0.55891800
C	4.78290700	-0.83636200	0.19118000
H	4.27925100	-2.73477600	1.08371500
H	1.94166800	-2.70542600	0.31651000
H	2.61089800	1.09657600	-1.59671200
H	4.96654100	1.07175800	-0.80224700
H	5.81215000	-0.85294200	0.53606400
N	0.80465100	-0.71413200	-1.20427600
C	-0.06801600	-1.68984900	-1.20377500
H	-0.97656000	-1.53372200	-1.76914600
H	0.21607500	-2.71052300	-0.96732200

Cartesian coordinate of cpx12a

N	-1.30977300	-0.47259800	-0.76699800
C	-2.30124100	-1.44107600	-0.30447500
H	-3.32472900	-1.15087400	-0.58505000
C	-2.31520800	-1.64357500	1.21607500
O	-3.30513100	-2.03291900	1.79841300
C	-1.91070200	-2.75183700	-1.02269100
H	-2.76167800	-3.43135800	-1.10469300
H	-1.11936200	-3.26735000	-0.46559300
C	-1.38112600	-2.24762300	-2.37040600
C	-0.64179600	-0.95104900	-2.00394500
H	0.42320900	-1.13711600	-1.81537100
H	-0.71133500	-0.21163100	-2.80702000
O	-1.15630200	-1.44500200	1.86329700
H	-0.45424400	-1.08147000	1.27619300
H	-2.21944700	-2.02582900	-3.04075500
H	-0.73246500	-2.97035100	-2.87466200
C	-0.48279200	3.21696600	-0.47957900
C	-0.46296500	1.82428900	-1.12561800
C	-1.53711000	0.90610300	-0.56622200
C	-2.58877800	1.39093700	0.13117400
C	-2.80226700	2.85803300	0.42421700
C	-1.90987700	3.77128000	-0.42655300
H	-0.59551600	1.93215400	-2.21214800
H	0.51941100	1.35891900	-0.98364800
H	-0.08304900	3.15026800	0.54160900
H	0.17970600	3.88956800	-1.03742600
H	-3.32646700	0.71537100	0.55310000
H	-3.85847900	3.11196200	0.26332200
H	-2.61483700	3.05311700	1.49277500
H	-2.31042100	3.82833500	-1.44830900
H	-1.91629400	4.79146500	-0.02455800
C	4.50120500	1.04537900	-0.11831700
C	3.39955600	0.92468100	0.73200800
C	2.66715900	-0.27296500	0.76775300
C	3.03717700	-1.33387900	-0.07348200
C	4.15087700	-1.21348500	-0.90421100
C	4.88569600	-0.02301800	-0.93250500
H	5.05546200	1.97911200	-0.14713000
H	3.08753800	1.76465900	1.34555300
H	2.45591900	-2.25036200	-0.04793800
H	4.44139600	-2.04718200	-1.53687900
H	5.74352300	0.07379500	-1.59100900
N	1.52453100	-0.43943000	1.58909700
C	1.55813600	-0.06586200	2.80783400
H	0.65859600	-0.17531200	3.41178100
H	2.45606400	0.34787600	3.28315200

Cartesian coordinate of int3a

N	-1.46211500	-0.26662500	-0.60275900
C	-2.29455800	-1.08272900	0.34537300
H	-2.87574000	-0.39830400	0.96189900
C	-1.29525800	-1.91345000	1.27122900
O	-1.06578500	-1.37785400	2.38512000
C	-3.16788500	-1.96763100	-0.56796500
H	-4.23131500	-1.82436600	-0.35912600
H	-2.90465800	-3.00918200	-0.37309700
C	-2.80811900	-1.58803600	-2.01988300
C	-1.40432100	-1.00341400	-1.89290900
H	-0.65471900	-1.79102700	-1.75579000
H	-1.10355200	-0.35473900	-2.71245800
O	-0.82196900	-2.93795400	0.74465000
H	0.69198300	-0.56817500	2.08863800
H	-3.49261400	-0.82947200	-2.41723900
H	-2.82462000	-2.44498500	-2.69795900
C	-0.07545100	3.15293900	-1.13544100
C	-0.17704300	1.64352300	-1.44735200
C	-0.87572400	0.87082300	-0.34930200
C	-0.87247500	1.46720100	1.02732400
C	-1.41542900	2.93050300	1.00772000
C	-1.31792500	3.61956700	-0.36892600
H	-0.73031300	1.51678700	-2.38313800
H	0.81749200	1.20711200	-1.60800000
H	0.82779700	3.37083900	-0.55639700
H	0.02860000	3.69572500	-2.08053500
H	-1.46663100	0.84580400	1.69677800
H	-2.45520600	2.93590900	1.35057000
H	-0.84701200	3.50700700	1.74803400
H	-2.20921800	3.38560200	-0.96841700
H	-1.31048900	4.70709500	-0.24169700
C	3.99493100	0.23775900	-0.85308400
C	3.06547800	0.68531800	0.08959500
C	2.18215800	-0.22031400	0.71508300
C	2.27839800	-1.58784200	0.37382700
C	3.21948900	-2.02029200	-0.55844800
C	4.08316400	-1.11560400	-1.18812600
H	4.66761200	0.95717200	-1.31338000
H	3.05766500	1.73667500	0.36088500
H	1.59249200	-2.29854400	0.82811200
H	3.26859800	-3.07843500	-0.80138700
H	4.81277000	-1.45912200	-1.91495600
N	1.25946000	0.17877600	1.68416000
C	0.58472400	1.44820100	1.66415900
H	0.42684000	1.79899400	2.69117800
H	1.20992500	2.19391200	1.17227600

Cartesian coordinate of TS12a

N	-1.60407200	-0.20674000	-0.78968100
C	-2.54736500	-0.92701200	0.10353400
H	-3.37012000	-0.24972200	0.35889200
C	-1.85387800	-1.37562400	1.42742900
O	-2.28125500	-0.90567000	2.49529000
C	-3.02264700	-2.13254600	-0.73775100
H	-4.09031500	-2.32039100	-0.59740700
H	-2.47094300	-3.02184200	-0.42060800
C	-2.65990600	-1.77736500	-2.18807500
C	-1.37459400	-0.95981600	-2.03181900
H	-0.49912700	-1.61762200	-1.92492200
H	-1.19997800	-0.29227200	-2.87703200
O	-0.84445700	-2.15276700	1.26884800
H	0.38805600	-1.31617200	1.57012600
H	-3.43839600	-1.15511600	-2.64546000
H	-2.51562400	-2.65851300	-2.82052900
C	0.39604000	2.99709000	-1.17282100
C	-0.26051700	1.67981900	-1.60932100
C	-1.10785600	1.03495900	-0.52383900
C	-1.34039300	1.69754500	0.66904500
C	-1.06759900	3.17667500	0.86205600
C	-0.60564700	3.87849400	-0.42310500
H	-0.90118800	1.87218700	-2.48232400
H	0.50810100	0.97495100	-1.94678500
H	1.25789200	2.78658200	-0.52511500
H	0.79034000	3.51086300	-2.05707400
H	-2.00024800	1.23370400	1.39438600
H	-1.97877800	3.65834400	1.24059700
H	-0.31600100	3.33908700	1.65372300
H	-1.47257900	4.06472800	-1.07203300
H	-0.16893000	4.85628500	-0.18894900
C	4.31308100	0.16296000	-0.19369100
C	3.20107600	0.37994100	0.61984900
C	2.21171000	-0.60971700	0.72009200
C	2.35274700	-1.81780700	0.01884800
C	3.47064500	-2.02298500	-0.78904500
C	4.45301400	-1.03464900	-0.90272900
H	5.07867900	0.92986600	-0.26439700
H	3.12273600	1.30381600	1.18328800
H	1.58062900	-2.57550000	0.11296100
H	3.57365700	-2.95920900	-1.32934000
H	5.32414200	-1.19816500	-1.52951900
N	1.06343900	-0.46980300	1.53157800
C	0.56701100	0.63751700	2.02044300
H	-0.27078100	0.54000900	2.69736100
H	1.10936000	1.57251700	1.94917200