

Supporting Information

Influence of Odd-Even Effect and Intermolecular Interactions in 2D

Molecular Layers of Bisamide Organogelators

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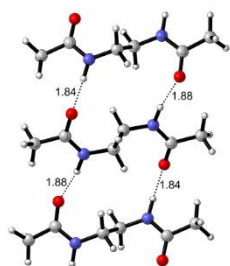
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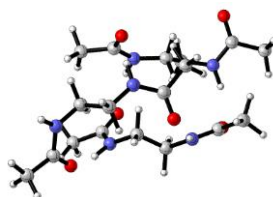
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I. Structures of Trimers (B3LYP-D3/6-311+G**)



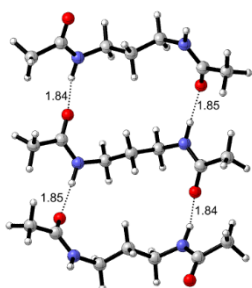
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2-anti-t-D



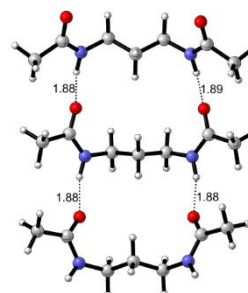
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2-para-t-D



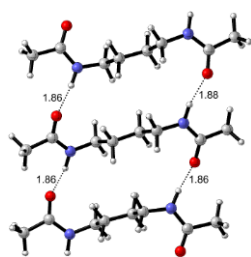
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3-anti-t-D



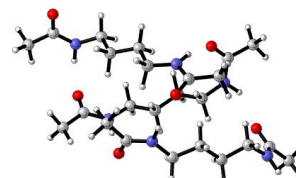
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3-para-t-D



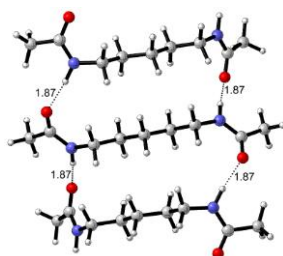
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4-anti-t-D



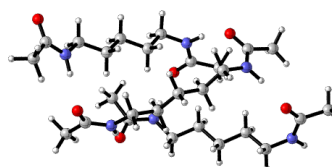
(-1723.484601)

4-para-t-D



(-1841.385854)

5-anti-t-D



(-1841.391285)

5-para-t-D

Figure S1. Structures of 2-anti-t-D, 2-para-t-D, 3-anti-t-D, 3-para-t-D, 4-anti-t-D, 4-para-t-D, 5-anti-t-D and 5-para-t-D. (B3LYP/6-311+G** (Solvent=Benzene)). (Gibbs free energies (a.u) are given in parentheses).

II. Energetics of Trimers

Table S1. Gibbs Free Energies (G_{rel} , kcal/mol) of trimers calculated at B3LYP/6-311+G** // B3LYP-D3/6-311+G** relative to B3LYP/6-311+G** level of theory (Solvent=(Benzene)).

B3LYP/6-311+G**		B3LYP/6-311+G**//B3LYP-D3/6-311+G**		
n-anti/para	G	n-anti/para	G	G_{rel}
2-anti-t	-1487.616597	2-anti-t-D	-1487.602614	8.8
2-para-t	-1487.608113	2-para-t-D	-1487.583163	15.7
3-anti-t	-1605.508474	3-anti-t-D	-1605.496861	7.3
3-para-t	-1605.500493	3-para-t-D	-1605.493455	4.4
4-anti-t	-1723.403896	4-anti-t-D	-1723.387242	10.5
4-para-t	-1723.401284	4-para-t-D	-1723.369198	20.1
5-anti-t	-1841.295834	5-anti-t-D	-1841.275734	12.6
5-para-t	-1841.294974	5-para-t-D	-1841.263008	20.1

Table S2. Relative Gibbs Free Energies (G_{rel} , kcal/mol) between antiparallel (anti) and parallel (para) arrangements of optimized trimer structures and the total stabilization energies (kcal/mol).*

n-anti/para	G_{rel}	Total Stabilization Energy
2-anti-t	0.0	44.0 (0.0)
2-para-t	6.6	36.1 (7.9)
3-anti-t	0.0	45.9 (0.0)
3-para-t	5.7	42.1 (3.8)
4-anti-t	0.0	48.6 (0.0)
4-para-t	2.2	35.7 (13.0)
5-anti-t	0.0	44.3 (0.0)
5-para-t	1.0	41.7 (2.6)
6-anti-t	0.0	56.2 (0.0)
6-para-t	0.8	39.2 (17.1)
7-anti-t	0.0	42.8 (0.0)
7-para-t	0.1	41.1 (1.7)
8-anti-t	0.0	48.7 (0.0)
8-para-t	0.3	40.1 (8.6)
9-anti-t	0.0	42.6 (0.0)
9-para-t	1.3	40.9 (1.7)

*The relative total stabilization energies (kcal/mol) between antiparallel (anti) and parallel (para) arrangements are indicated in parentheses. (B3LYP-D3/6-311+G**//B3LYP/6-311+G**, Solvent = Benzene)

III. Coordinates and Gibbs Free Energies (a.u) of Dimer and Trimers (B3LYP/6-311+G** (Solvent=Benzene))

2-anti-d

Gibbs Free Energy= -991.744573

C	-1.42331000	-2.17375100	-0.61485400
C	-1.94588400	-1.45422100	0.64213100
N	-2.78154200	-0.31342600	0.31096500
N	-0.62178200	-3.34818700	-0.28770200
C	-4.10949800	-0.44450900	0.06210800
C	0.71648400	-3.30811700	-0.08648900
O	-4.68649200	-1.53165100	0.08898500
O	1.36680200	-2.26489000	-0.18253700
C	1.38541000	-4.62288000	0.25537000
C	-4.85049700	0.84251000	-0.24609000
H	-5.63981000	0.97710800	0.49704800
H	-4.20080200	1.71844000	-0.24578800
H	-2.34898900	0.60381800	0.26136700
H	-1.10348300	-1.10322800	1.24092800
H	-2.53042800	-2.15348800	1.24344700
H	-1.09693600	-4.22998000	-0.17178800
H	0.69221400	-5.46389900	0.30330100
H	-0.80642800	-1.49443400	-1.20390400
H	-2.26673500	-2.49551700	-1.22724700
H	1.88947600	-4.52069200	1.21861300
H	-5.33187900	0.74644200	-1.22175700
H	2.14915800	-4.83258200	-0.49638500
C	1.94585300	1.45413300	-0.64213700
C	1.42328900	2.17371200	0.61482500
N	0.62177000	3.34814200	0.28763200
N	2.78157200	0.31339200	-0.31093600
C	-0.71651400	3.30811200	0.08652900
C	4.10952900	0.44454800	-0.06212200
O	-1.36687900	2.26492600	0.18271000
O	4.68647000	1.53171600	-0.08905100
C	4.85059200	-0.84242100	0.24612900
C	-1.38539800	4.62286800	-0.25543900
H	-2.14912300	4.83266400	0.49631200
H	-0.69217200	5.46385700	-0.30346200
H	1.09694800	4.22990600	0.17159300
H	2.26672200	2.49549600	1.22719800
H	0.80640500	1.49442600	1.20390700
H	2.34906900	-0.60387300	-0.26131700
H	4.20095100	-1.71839100	0.24582300
H	2.53034700	2.15339200	-1.24351200
H	1.10344900	1.10307000	-1.24088900
H	5.33192900	-0.74630700	1.22181400
H	-1.88948700	4.52061200	-1.21866300
H	5.63994400	-0.97698800	-0.49697400

2-para-d

Gibbs Free Energy= -991.738179

H	2.60798900	-0.89446600	-1.26126700
C	1.67509800	-0.84712800	-0.69962700
H	0.96381900	-0.23325100	-1.26051100
C	1.91909000	-0.20855600	0.67993000
H	1.03054800	-0.34758200	1.30425200
N	1.14299800	-2.19592700	-0.58869900
H	0.17328000	-2.28953000	-0.30808700
C	1.86432400	-3.31345800	-0.86144200
O	3.03647100	-3.29165100	-1.23006600
H	2.76440500	-0.68704900	1.17386700
N	2.20622800	1.21298500	0.57034200
H	1.44478800	1.81681300	0.28109700
C	3.41160700	1.76365800	0.86655800
O	4.37898800	1.11377500	1.25672500
C	3.49849400	3.26981000	0.68525900
H	4.28766400	3.48951700	-0.03718700
H	3.78913400	3.72111200	1.63646800
C	1.12025900	-4.62627700	-0.68322200
H	0.07733400	-4.49502600	-0.39032100
H	1.63489600	-5.21914600	0.07640600
H	2.56397700	3.71834500	0.34434500
H	1.16500700	-5.18423500	-1.62092900
H	-2.50216200	0.03209300	-1.04286100
C	-3.33985800	0.32414100	-0.41060700
H	-4.18746900	0.57019300	-1.05679700
C	-2.94939100	1.54603700	0.44064300
H	-3.76785200	1.81129800	1.11610800
N	-3.69392700	-0.82363800	0.41240200
H	-4.60369400	-0.83988600	0.84709700
C	-2.86201800	-1.87866300	0.62645300
O	-1.73996500	-1.94064400	0.12857300
H	-2.07256800	1.31031400	1.04287500
N	-2.62383900	2.70374000	-0.38018400
H	-3.38046500	3.23592200	-0.78159800
C	-1.34983900	3.10750100	-0.63527400
O	-0.37210200	2.51803800	-0.18037200
C	-1.20228900	4.33340900	-1.51120000
H	-0.63239200	4.06068900	-2.40193500
H	-0.62511000	5.08430000	-0.96814600
C	-3.40045100	-2.98383900	1.51011100
H	-4.40573900	-2.79067900	1.88763000
H	-2.72160100	-3.11824500	2.35459100
H	-2.15511000	4.76795200	-1.81710900
H	-3.40618400	-3.91553300	0.94061000

3-anti-d

Gibbs Free Energy= -1070.338129

C	0.17685300	-3.05139800	-0.85511800
C	1.20413700	-2.18125700	-0.12255600
C	2.19059300	-1.52499600	-1.09804800
N	3.20324800	-0.72049600	-0.43068900
N	-0.77812300	-3.69082400	0.04693100
C	-1.98027000	-3.15658300	0.36514800
C	4.36045500	-1.25524800	0.02945600
O	4.63788200	-2.44971800	-0.08614900
O	-2.37987600	-2.09440800	-0.11793600
C	5.31496300	-0.28193700	0.69667700
C	-2.82623700	-3.94380700	1.34438200
H	6.25970000	-0.28759200	0.14819300
H	4.92811000	0.73716400	0.73582700
H	3.01135700	0.26569500	-0.28326500
H	1.65584800	-0.87478700	-1.79595000
H	0.68078200	-1.40872700	0.44913400
H	2.70130300	-2.29494300	-1.68154100
H	0.68108300	-3.83970300	-1.42076900
H	-0.39944900	-2.45114600	-1.56109500
H	1.76644400	-2.79328800	0.58894200
H	-0.49830400	-4.54336800	0.50702400
H	-3.78097200	-4.18125800	0.87062400
H	-2.35527400	-4.86901900	1.67992800
H	5.52258600	-0.63152000	1.71044200
H	-3.03547500	-3.31544200	2.21273800
C	-2.19067900	1.52487400	-1.09807400
C	-1.20401400	2.18096100	-0.12267100
C	-0.17674700	3.05112200	-0.85522400
N	0.77818400	3.69052600	0.04691000
N	-3.20344300	0.72057500	-0.43065500
C	-4.36059600	1.25549700	0.02944500
C	1.98043000	3.15652100	0.36509900
O	2.38042100	2.09455700	-0.11815400
O	-4.63797300	2.44995400	-0.08635700
C	2.82608300	3.94372700	1.34461800
C	-5.31518400	0.28235700	0.69682200
H	3.78115100	4.18079100	0.87134400
H	2.35520200	4.86913300	1.67974100
H	0.49828300	4.54308300	0.50693100
H	-0.68099200	3.83948400	-1.42077600
H	-1.76616900	2.79294500	0.58899500
H	0.39958000	2.45096800	-1.56125600
H	-1.65614800	0.87454300	-1.79602300
H	-2.70129200	2.29490800	-1.68153800
H	-0.68064600	1.40832700	0.44886000
H	-3.01163000	-0.26562400	-0.28317900
H	-6.25986300	0.28791600	0.14824500
H	-4.92837300	-0.73674600	0.73627100
H	3.03465700	3.31547900	2.21322000
H	-5.52291100	0.63218300	1.71048800

3-para-d

Gibbs Free Energy= -1.070.334846

C	1.26944000	-3.35624300	-0.85688500
C	0.00166300	-3.31621100	0.00587400
C	-1.26682300	-3.35735500	-0.85579000
N	-2.49454900	-3.31380700	-0.06837900
N	2.49784400	-3.31206700	-0.07054700
C	-3.16141500	-2.16433300	0.20679200
C	3.16336700	-2.16204100	0.20550700
C	-4.40667400	-2.30182200	1.05743100
C	4.40961800	-2.29887900	1.05480300
O	2.78295800	-1.06874000	-0.21291200
O	-2.78305200	-1.07106600	-0.21355700
H	-5.25025900	-1.86855600	0.51664500
H	-4.64292100	-3.33455000	1.31832900
H	2.84733400	-4.17218000	0.32251100
H	0.00233800	-4.16338900	0.70116000
H	-1.28793600	-2.50264800	-1.53340000
H	-2.84241500	-4.17385900	0.32625500
H	-1.28820800	-4.26657600	-1.46371500
H	1.29097900	-4.26527900	-1.46506700
H	1.28930400	-2.50133000	-1.53428700
H	5.25181800	-1.86246600	0.51440500
H	4.64828700	-3.33172000	1.31303500
H	0.00152900	-2.40148700	0.60437500
H	-4.27131900	-1.72590500	1.97550200
H	4.27374900	-1.72548400	1.97438800
C	1.27040200	2.24782300	-1.06811500
C	-0.00083100	1.97089200	-0.25561100
C	-1.27200300	2.24674200	-1.06856500
N	-2.48961000	1.90148100	-0.34684500
N	2.48804600	1.90350300	-0.34603300
C	-3.32338700	2.82681200	0.18902900
C	3.32070000	2.82944500	0.19053200
C	-4.53794100	2.26907900	0.91197600
C	4.53546700	2.27261800	0.91382600
O	3.13427000	4.04266500	0.10714000
O	-3.13803900	4.04018900	0.10541300
H	-5.43931100	2.65384000	0.42948500
H	-4.57150200	1.17865200	0.91879100
H	2.70298700	0.91822700	-0.22899700
H	-0.00042400	0.92509000	0.07076400
H	-1.33654300	3.30401100	-1.32940400
H	-2.70385900	0.91605500	-0.22980200
H	-1.25006700	1.67163300	-2.00090200
H	1.24928800	1.67273700	-2.00048400
H	1.33415600	3.30515700	-1.32889600
H	5.43670400	2.65723800	0.43095800
H	4.56934100	1.18220500	0.92146100
H	-0.00125900	2.59339700	0.64421900
H	-4.53341600	2.63776200	1.94012200
H	4.53092400	2.64211700	1.94167100

2-anti-t

Gibbs Free Energy= -1487.616597

C	4.89830600	0.86110300	-0.60616300
C	4.89706000	-0.03426900	0.64673000
N	4.71421800	-1.43585400	0.31581100
N	5.15897500	2.26034700	-0.28498000
C	5.76078900	-2.23717600	-0.00628000
C	4.19132900	3.16534600	-0.01108500
O	6.92244500	-1.83014300	-0.04671600
O	2.99063000	2.88211300	-0.03295400
C	4.65868900	4.56825300	0.31551700
C	5.41342500	-3.68281000	-0.30610700
H	5.93416000	-4.32219400	0.41063200
H	4.34240100	-3.88177300	-0.25571900
H	3.77002800	-1.81294600	0.31298900
H	4.09185600	0.27214500	1.31716300
H	5.84739100	0.07905200	1.17228100
H	6.12023000	2.55862200	-0.22266400
H	5.74463300	4.67228800	0.32663100
H	3.93398800	0.80147300	-1.11127900
H	5.67138400	0.51957800	-1.29607400
H	4.26223800	4.85262600	1.29218300
H	5.78583800	-3.93523700	-1.30123800
H	4.24301300	5.25690600	-0.42329300
C	0.07895800	0.42025900	-0.63958400
C	-0.07748600	-0.42235600	0.63991200
N	-0.26716800	-1.83589300	0.34905800
N	0.26830600	1.83384500	-0.34874000
C	0.76389500	-2.69346700	0.20141300
C	-0.76309600	2.69081900	-0.19988800
O	1.94565600	-2.34007200	0.30219200
O	-1.94470600	2.33673900	-0.29993800
C	-0.39772600	4.13137600	0.09014700
C	0.39799700	-4.13398800	-0.08814100
H	0.81160600	-4.76459600	0.70233100
H	-0.67865500	-4.29132400	-0.15322100
H	-1.21647100	-2.18411300	0.24225500
H	-0.94245500	-0.07002500	1.20454000
H	0.81025900	-0.30994100	1.26424000
H	1.21748300	2.18249300	-0.24224000
H	0.67891500	4.28926800	0.15409000
H	-0.80870200	0.30762100	-1.26399800
H	0.94404800	0.06810400	-1.20414200
H	-0.86696000	4.43043600	1.03017100
H	0.86817400	-4.43397100	-1.02739200
H	-0.81266800	4.76226800	-0.69939600
C	-4.89728500	0.03536700	-0.64721800
C	-4.89896300	-0.85978700	0.60582900
N	-5.15930400	-2.25912000	0.28471300
N	-4.71480300	1.43705400	-0.31651700
C	-4.19142600	-3.16392500	0.01100400
C	-5.76159000	2.23829500	0.00503000
O	-2.99080500	-2.88038000	0.03292400
O	-6.92324000	1.83118300	0.04489600
C	-5.41456300	3.68404100	0.30474200
C	-4.65844900	-4.56691800	-0.31572200
H	-4.24123700	-5.25578800	0.42200300
H	-5.74434800	-4.67157800	-0.32531800
H	-6.12047900	-2.55768400	0.22260600
H	-5.67240700	-0.51829900	1.29534300
H	-3.93486200	-0.79993000	1.11133300
H	-3.77055200	1.81397100	-0.31264300
H	-4.34347100	3.88300000	0.25577200
H	-5.84733500	-0.07819700	-1.17322000
H	-4.09168700	-0.27103700	-1.31717600
H	-5.78840500	3.93694000	1.29920800
H	-4.26331400	-4.85044300	-1.29318100
H	-5.93421400	4.32313200	-0.41305300

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Gibbs Free Energy= -1487.608113

H	5.48054700	0.13127400	-1.01279600
C	4.49398900	-0.17563400	-0.66577300
H	3.74050300	0.27527600	-1.31861500
C	4.26528200	0.30627200	0.77931800
H	3.37821600	-0.18913900	1.18629600
N	4.40019700	-1.62289800	-0.77556800
H	3.47056700	-2.02764800	-0.71743700
C	5.46492700	-2.43356500	-0.99444400
O	6.61966200	-2.02727000	-1.11383300
H	5.12082800	0.04803300	1.40331200
N	4.07202400	1.74590000	0.84598600
H	3.18944600	2.11336800	0.50438500
C	4.98437800	2.60552000	1.36506400
O	6.06421700	2.25140800	1.83572800
C	4.58252300	4.07061800	1.33313900
H	5.33208300	4.62530100	0.76412800
H	4.59202600	4.45893500	2.35409300
C	5.14184000	-3.91568900	-1.09142400
H	4.08105200	-4.13493100	-0.96023900
H	5.71808400	-4.44950700	-0.33253000
H	3.59872000	4.23579700	0.89158700
H	5.46672100	-4.28160100	-2.06809400
H	0.17573300	-0.34597700	-1.48897000
C	-0.67111600	-0.46698100	-0.81337400
H	-1.59250200	-0.29847400	-1.37579700
C	-0.58020700	0.55669800	0.33398300
H	-1.33843500	0.32444000	1.08650600
N	-0.68267800	-1.83790000	-0.32417700
H	-1.57362100	-2.20660600	-0.00597000
C	0.41787300	-2.61913500	-0.27269400
O	1.53073400	-2.23448400	-0.64427500
H	0.40111900	0.50648600	0.80481600
N	-0.79766100	1.91688200	-0.13500900
H	-1.75716300	2.18760400	-0.32726900
C	0.19145500	2.82110600	-0.30847900
O	1.38051200	2.57618200	-0.08635800
C	-0.24365100	4.19006200	-0.79394200
H	0.29975900	4.42635500	-1.71114100
H	0.03740700	4.93341200	-0.04440300
C	0.21277700	-4.02103500	0.26617000
H	-0.82228000	-4.22749600	0.54130300
H	0.85238900	-4.15852400	1.14084600
H	-1.31607000	4.25786400	-0.98122400
H	0.53378600	-4.73857500	-0.49204100
H	-4.99011500	-0.89967700	-0.89370000
C	-5.81156300	-0.85815900	-0.17899200
H	-6.75196200	-0.92415000	-0.73268900
C	-5.75017800	0.46571500	0.60508800
H	-6.53059000	0.48580900	1.37054500
N	-5.70553200	-2.01941700	0.69411700
H	-6.53815000	-2.34873400	1.15793300
C	-4.54232900	-2.68677500	0.91363800
O	-3.48509700	-2.34717400	0.38415800
H	-4.78327000	0.55590100	1.09896400
N	-5.91816900	1.62368000	-0.26223900
H	-6.85252000	1.88290300	-0.53918400
C	-4.88292800	2.37848100	-0.71593200
O	-3.71448500	2.13039800	-0.42198300
C	-5.24940000	3.55289800	-1.59763800
H	-4.70822000	3.46611800	-2.54173100
H	-4.91862200	4.47282000	-1.11059900
C	-4.62027600	-3.88093500	1.83998700
H	-5.61852800	-4.05451300	2.24400800
H	-3.92187900	-3.73127100	2.66577300
H	-6.31813700	3.62563100	-1.80400700
H	-4.29890200	-4.76951300	1.29252000

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Gibbs Free Energy= -1605.50847

C	0.09757900	-1.26578500	1.55069000	H	-4.00438100	-5.09682600	-2.52385700
C	-0.00001800	0.00031000	0.68985200	H	-6.24251000	3.53737400	-1.63726700
C	-0.09861700	1.26620000	1.55087600	H	-2.32815400	-4.51448100	-2.62359800
N	-0.21698200	2.48621000	0.76112300				
N	0.21694700	-2.48560900	0.76080100				
C	1.40622800	-3.01142800	0.40846600				
C	-1.40580400	3.01224800	0.40756600				
O	-2.48692400	2.50612100	0.73651400				
O	2.48691000	-2.50512800	0.73859500				
C	-1.35306400	4.28304900	-0.41602200				
C	1.35459900	-4.28225400	-0.41514900				
H	-1.88502000	5.07156200	0.12112000				
H	-0.33412900	4.61221900	-0.62125900				
H	0.63795900	2.93213500	0.43797400				
H	0.78996300	1.36386000	2.18050400				
H	0.88029500	0.06352300	0.04306900				
H	-0.96949300	1.20835400	2.20699900				
H	-0.79175200	-1.36362900	2.17922800				
H	0.96765800	-1.20803700	2.20787500				
H	-0.87954800	-0.06275200	0.04198700				
H	-0.63760200	-2.93170500	0.43686600				
H	1.88449400	-5.07116200	0.12346600				
H	0.33595700	-4.61067300	-0.62303400				
H	-1.87744700	4.11515700	-1.35955400				
H	1.88161300	-4.11486900	-1.35729400				
C	5.22414000	-0.03330000	0.89695300				
C	4.84151400	0.98360400	-0.18727600				
C	4.91944000	2.42347400	0.33161300				
N	4.55239700	3.41447700	-0.67796800				
N	5.17422800	-1.40961000	0.42818900				
C	6.24519900	-2.01940900	-0.13377400				
C	3.30101600	3.90571000	-0.82419500				
O	2.37214000	3.57983000	-0.07964600				
O	7.33410400	-1.46231000	-0.28301500				
C	3.09670800	4.89820200	-1.94993300				
C	6.02814800	-3.45747500	-0.56859400				
H	2.73196900	5.83708500	-1.52805400				
H	4.00261500	5.09509700	-2.52504700				
H	5.25503000	3.69418400	-1.34504100				
H	5.93344800	2.65223900	0.67065800				
H	5.51494600	0.86141600	-1.04104100				
H	4.24578700	2.56182600	1.17872700				
H	4.54631600	0.05416800	1.75064000				
H	6.23872500	0.16473500	1.25024200				
H	3.82500000	0.78110000	-0.53812000				
H	4.28832700	-1.90509000	0.49600100				
H	6.74218900	-4.09371900	-0.04082400				
H	5.01596800	-3.81442100	-0.37380700				
H	2.32536400	4.51510800	-2.62139800				
H	6.24320500	-3.53918000	-1.63645300				
C	-4.91894300	-2.42381600	0.33227700				
C	-4.84168800	-0.98409000	-0.18711200				
C	-5.22349300	0.03308900	0.89714700				
N	-5.17401700	1.40926800	0.42796700				
N	-4.55265000	-3.41508300	-0.67731900				
C	-3.30122600	-3.90583000	-0.82477200				
C	-6.24545300	2.01886700	-0.13333700				
O	-7.33448400	1.46171700	-0.28146900				
O	-2.37166300	-3.57934100	-0.08134700				
C	-6.02865800	3.45669400	-0.56907400				
C	-3.09767000	-4.89845100	-1.95052400				
H	-6.74364200	4.09300500	-0.04269100				
H	-5.01684900	3.81426400	-0.37351700				
H	-4.28812800	1.90485600	0.49496300				
H	-4.54498500	-0.05412500	1.75032000				
H	-3.82551300	-0.78154600	-0.53890900				
H	-6.23778600	-0.16488300	1.25130900				
H	-5.93260800	-2.65264600	0.67229800				
H	-4.24451400	-2.56180000	1.17883400				
H	-5.51588700	-0.86224700	-1.04032200				
H	-5.25584700	-3.69516900	-1.34364100				
H	-2.73077100	-5.83664500	-1.52900800				

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Gibbs Free Energy= -1605.500493

C	-0.44230500	1.44760100	1.36444700	H	-4.87949700	0.02450900	-0.84528300
C	-0.62224800	0.15387300	0.56077900	H	-4.39894800	-4.37919100	-2.30583800
C	-0.56176400	-1.09099000	1.45524000	H	-4.30729400	4.39532000	-2.05407200
N	-0.76838700	-2.32675400	0.71108900				
N	-0.61510200	2.64079700	0.54665400				
C	0.24765200	-3.11623100	0.30095100				
C	0.41249600	3.39406400	0.10230000				
C	-0.14713900	-4.34438700	-0.49380200				
C	0.03481900	4.59303600	-0.74535900				
O	1.59496800	3.15131500	0.36708100				
O	1.43114300	-2.87180900	0.56061400				
H	0.18503000	-5.23338500	0.04757800				
H	-1.22157300	-4.40749100	-0.66804300				
H	-1.56277800	2.88118700	0.27197100				
H	-1.58693800	0.18205800	0.04312100				
H	0.40946000	-1.16105100	1.94662700				
H	-1.71527600	-2.55716700	0.42725300				
H	-1.32835600	-1.03116700	2.23467000				
H	-1.17150600	1.48722500	2.18039600				
H	0.55481300	1.49061900	1.80441900				
H	0.36243400	5.50106000	-0.23362300				
H	-1.03637000	4.65913900	-0.94006300				
H	0.15565300	0.08916100	-0.20544800				
H	0.37695300	-4.32634000	-1.45172800				
H	0.57182100	4.53741400	-1.69434500				
C	4.86551500	1.16483400	0.87220100				
C	4.44279400	-0.10394600	0.11939900				
C	4.81488000	-1.37507000	0.89456600				
N	4.34677600	-2.59234400	0.24681800				
N	4.46527900	2.39099300	0.19629300				
C	5.16915200	-3.44857500	-0.40589200				
C	5.33450300	3.17823800	-0.48413100				
C	4.48947500	-4.66248600	-1.01732100				
C	4.72817400	4.41802600	-1.11883100				
O	6.53620700	2.93204500	-0.59059900				
O	6.38517100	-3.28362700	-0.50853900				
H	4.93533600	-5.56435900	-0.59150100				
H	3.41172800	-4.67992300	-0.84896000				
H	3.48683100	2.66229600	0.23436000				
H	3.36010900	-0.08504200	-0.04633500				
H	5.89829500	-1.45485300	0.99540000				
H	3.35112900	-2.79445800	0.28341800				
H	4.38520300	-1.33412700	1.90176400				
H	4.42395800	1.16528500	1.87506900				
H	5.95042300	1.19381400	0.98443900				
H	5.24161700	5.29771100	-0.72397100				
H	3.65731600	4.51035000	-0.93422300				
H	4.92304000	-0.12198400	-0.86311700				
H	4.68934300	-4.67249500	-2.09107400				
H	4.91242600	4.38604500	-2.19510500				
C	-5.71134900	1.23420800	0.73913400				
C	-5.73371900	-0.00637100	-0.16367000				
C	-5.68605800	-1.30222700	0.65632000				
N	-5.76466100	-2.50167400	-0.16977400				
N	-5.74237100	2.48520900	-0.01085900				
C	-4.69114800	-3.25461100	-0.51774000				
C	-4.63118600	3.19953400	-0.31819100				
C	-4.97766100	-4.46325100	-1.38381800				
C	-4.84945900	4.47167300	-1.10912800				
O	-3.50476100	2.84090900	0.02798100				
O	-3.54554700	-2.98609100	-0.15398500				
H	-4.63551600	-5.35788400	-0.85960000				
H	-6.03305700	-4.57987400	-1.63497900				
H	-6.63286100	2.82214200	-0.34266600				
H	-6.64164400	0.00530600	-0.77745000				
H	-4.75458000	-1.36046200	1.22047000				
H	-6.66922700	-2.77651900	-0.52054700				
H	-6.51181700	-1.32927700	1.37393400				
H	-6.56766200	1.22592900	1.41984300				
H	-4.80466700	1.24531100	1.34539100				
H	-4.42433000	5.30793600	-0.55067000				
H	-5.89972900	4.68007100	-1.31818100				

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Gibbs Free Energy= -1723.403896

C	-0.00330600	0.72186200	0.25465300	H	-3.87227600	-2.55668800	1.34076400
C	-0.16779300	1.74011700	-0.88127500	H	-4.03618600	-0.05201000	0.77211500
C	0.00347900	-0.72241800	-0.25472400	H	-6.11461100	0.64885000	-1.36382100
C	0.16819900	-1.74058000	0.88124900	H	-4.22427000	2.62878300	-0.28039500
N	0.16420300	-3.12346900	0.41964300	H	-5.78255900	-0.12188700	0.97895400
N	-0.16392000	3.12296300	-0.41947800	H	-5.62349400	-2.64208600	1.53416700
C	1.28998800	-3.79616300	0.10809100	H	-6.61505800	4.93049700	-0.11454300
C	-1.28976800	3.79550700	-0.10792000	H	-4.98540100	4.55218600	0.49819000
O	2.41879600	-3.29728500	0.19960100	H	-4.17469600	-1.80240500	-1.03049500
O	-2.41854600	3.29654400	-0.19951800	H	-4.36439900	0.69893600	-1.60635500
C	1.10247100	-5.22500200	-0.36020300	H	-6.42116100	4.32929400	1.52980700
C	-1.10240000	5.22431000	0.36053200	H	-3.35395800	-6.23161800	-1.51204900
H	-0.73410900	-3.58424400	0.30495900				
H	0.05506000	-5.52625500	-0.39185600				
H	1.65042500	-5.88906600	0.31217400				
H	-0.92948000	-0.93268800	-0.79042600				
H	1.10896400	-1.56590600	1.40663100				
H	0.92957400	0.93208700	0.79052000				
H	-1.10842300	1.56549000	-1.40690400				
H	0.73434300	3.58386400	-0.30486800				
H	-0.81819400	0.86291300	0.97323100				
H	-0.64415400	-1.62962300	1.60508200				
H	-0.05498700	5.52551800	0.39261600				
H	-1.54083600	5.32932200	1.35551500				
H	0.81825400	-0.86346500	-0.97343600				
H	0.64474200	1.62926500	-1.60491700				
H	-1.65006100	5.88845000	-0.31201400				
H	1.54051200	-5.33009100	-1.35535700				
C	4.98178200	1.67673600	0.30066300				
C	4.80948000	2.72145000	-0.80809300				
C	4.97780600	0.24610400	-0.24616800				
C	5.15752500	-0.80268100	0.86034400				
N	5.12745800	-2.17085700	0.36540800				
N	4.78724400	4.09492800	-0.30848800				
C	6.24734900	-2.83063000	-0.01655600				
C	3.65101200	4.76551600	-0.00835500				
O	7.37304000	-2.33206700	0.03418600				
O	2.53075500	4.27332900	-0.16528400				
C	6.03372700	-4.24980300	-0.51147800				
C	3.82196100	6.17205600	0.52682300				
H	4.22435800	-2.62884100	0.28044000				
H	4.98571300	-4.55166000	-0.49926000				
H	6.61444000	-4.93010200	0.11571800				
H	4.03585500	0.05214300	-0.77217500				
H	6.11413700	-0.64851800	1.36396400				
H	5.92136300	1.86710200	0.83284900				
H	3.87189500	2.55694400	-1.34079000				
H	5.66916100	4.54811800	-0.12500400				
H	4.17417700	1.80257000	1.03041500				
H	4.36389700	-0.69894300	1.60619400				
H	3.29456400	6.86452100	-0.13251800				
H	4.86455800	6.48290900	0.60868300				
H	5.78223600	0.12211400	-0.97893100				
H	5.62312900	2.64212700	-1.53419200				
H	3.35400500	6.23238700	1.51164300				
H	6.42288800	-4.32950300	-1.52912900				
C	-4.97817200	-0.24591900	0.24615000				
C	-5.15788500	0.80285200	-0.86037400				
C	-4.98223500	-1.67655500	-0.30067100				
C	-4.80984000	-2.72128200	0.80805800				
N	-4.78742600	-4.09472600	0.30839500				
N	-5.12750900	2.17105100	-0.36549700				
C	-3.65108800	-4.76519300	0.00832200				
C	-6.24725600	2.83106000	0.01642100				
O	-2.53089400	-4.27298300	0.16559700				
O	-7.37308300	2.33279600	-0.03447300				
C	-3.82186200	-6.17162500	-0.52718100				
C	-6.03333400	4.25010300	0.51159400				
H	-5.66927500	-4.54790700	0.12453100				
H	-4.86441400	-6.48263200	-0.60907500				
H	-3.29432200	-6.86418400	0.13194400				
H	-5.92186700	-1.86689900	-0.83277700				

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Gibbs Free Energy= -1723.401284

C	4.57506600	1.57503500	-1.13310600	H	-6.70514600	-0.51815200	-1.00652900
C	4.55069000	0.74059500	0.15473700	H	-6.66657200	-3.35300200	-0.80562300
C	4.53306600	-0.76549100	-0.12276400	H	-4.88284400	-1.89860600	1.03676900
C	4.48603900	-1.59922500	1.16469500	H	-4.85430800	0.67841000	1.13325700
N	4.32416200	-3.02510400	0.91555400	H	-6.61127700	0.66807900	1.22595900
N	4.43620500	3.00468200	-0.89009300	H	-6.64678700	-1.90390600	1.08672400
C	5.34107100	-3.91589600	1.00716200	H	-5.67306900	5.26366000	2.06660500
C	5.48500200	3.86132300	-0.88005300	H	-4.96930800	2.03844200	-0.97082900
O	6.49026300	-3.60629700	1.32371600	H	-4.94664800	-0.53097100	-1.06050500
O	6.64768600	3.51567300	-1.09344800	H	-4.27819900	-4.79376600	-2.56666000
C	4.97377100	-5.35664000	0.69451000	H	-4.30370400	5.93791800	1.15707700
C	5.13979900	5.31252400	-0.58974700	H	-4.00102700	4.92476400	2.56725600
H	5.21801500	-5.97611000	1.56045300	H	-4.47048000	-5.81640600	-1.14418000
H	3.50309100	3.35544300	-0.69654500				
H	3.75698900	1.26389500	-1.79081000				
H	3.65968300	-1.01455700	-0.73771600				
H	3.40253800	-3.35401900	0.64454900				
H	5.40670800	-1.46712800	1.73469500				
H	5.42236200	1.00379700	0.76382300				
H	3.66276700	1.01679300	0.73624700				
H	3.65210400	-1.26513400	1.79168600				
H	4.07253900	5.47803600	-0.43515100				
H	5.51381900	1.41875600	-1.66666600				
H	5.41799800	-1.05549800	-0.69977400				
H	3.92000400	-5.48431600	0.44294500				
H	5.48357300	5.92811300	-1.42398100				
H	5.68694600	5.63117900	0.30051100				
H	5.58944000	-5.70127200	-0.13959000				
C	-0.56701500	1.77229800	-0.84504400				
C	-0.48210600	0.67706700	0.22612300				
C	-0.53089200	-0.72979600	-0.37687200				
C	-0.47514000	-1.82859600	0.69205300				
N	-0.65151500	-3.16574200	0.13862000				
N	-0.64419900	3.11634900	-0.28511500				
C	0.36576700	-4.02704600	-0.06950400				
C	0.43191100	3.91323300	-0.12391200				
O	1.54174700	-3.76633700	0.20702200				
O	1.57438000	3.57514400	-0.45299500				
C	-0.01275600	-5.36887500	-0.66583300				
C	0.16667200	5.27557200	0.48637100				
H	0.54592600	-5.51134500	-1.59336900				
H	-1.55839500	3.43929100	0.01786600				
H	-1.45707400	1.61969200	-1.46224100				
H	-1.45405100	-0.84904500	-0.95620300				
H	-1.59513600	-3.43559600	-0.12329000				
H	0.48389400	-1.80858400	1.21116400				
H	0.44081200	0.81251200	0.80024900				
H	-1.31360500	0.80521100	0.92923300				
H	-1.26220800	-1.66478000	1.43482000				
H	-0.88667000	5.44596700	0.71269200				
H	0.30603300	1.73081300	-1.49823000				
H	0.30045800	-0.87152900	-1.07627900				
H	0.29036300	-6.15855500	0.02530800				
H	0.51513400	6.04471500	-0.20633000				
H	0.75188100	5.36964900	1.40388500				
H	-1.08023600	-5.46089200	-0.87010400				
C	-5.80685000	1.99925000	-0.27336000				
C	-5.76615800	0.69133800	0.52727000				
C	-5.80480500	-0.54287100	-0.38049800				
C	-5.78110400	-1.85107400	0.42016200				
N	-5.78659800	-3.04277300	-0.42352800				
N	-5.72356300	3.19215700	0.56476600				
C	-4.66634300	-3.72829700	-0.75968600				
C	-4.56454600	3.85016100	0.81274600				
O	-3.54891600	-3.39911100	-0.35795300				
O	-3.48943100	3.48931500	0.33054800				
C	-4.86202300	-4.93404100	-1.65455600				
C	-4.66140700	5.06630000	1.70928100				
H	-5.90439100	-5.11245900	-1.92302500				
H	-6.56522400	3.52585000	1.00869700				
H	-6.73024700	2.05947900	-0.85640800				

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Gibbs Free Energy= -1841.295834

C	5.56377400	-0.22328400	-0.96232100	O	-1.24917100	-5.15231400	0.18937600
C	5.01153100	0.81853700	0.02023000	C	-7.03854800	3.31317400	0.80800700
C	4.75054000	2.17376600	-0.64505600	C	-1.79340900	-6.85348300	1.79276700
C	4.21108500	3.22607200	0.32970600	H	-2.67130800	-7.33533300	2.22589700
C	3.92435000	4.56726400	-0.35567100	H	-1.20068100	-6.40806100	2.59463400
N	3.42465600	5.58946000	0.56231700	H	-3.20931900	-4.40618700	-1.14031000
N	5.78942100	-1.52674500	-0.35358100	H	-4.11639500	-6.08222000	1.10266800
C	2.11030200	5.81744400	0.78779600	H	-4.86428500	-4.92761300	-0.82062600
C	6.96942100	-1.87026800	0.21452300	H	-4.96301600	-3.35134100	1.14317500
O	1.22160000	5.19559600	0.20008300	H	-5.71870200	-2.51158300	-1.09237100
O	7.94465800	-1.11777800	0.25296200	H	-4.07795300	-2.01347000	-1.46954500
C	1.77987800	6.89496200	1.79976800	H	-4.90665800	0.38578000	-1.79400900
C	7.02938400	-3.26719700	0.80693800	H	-6.55470200	-0.08940900	-1.36477300
H	6.09598000	-3.81991000	0.69237000	H	-5.75918500	-0.90774500	0.84609200
H	7.27712600	-3.18859600	1.86797500	H	-5.02940900	2.20541600	-0.32930500
H	6.51315900	0.12453200	-1.37534300	H	-7.84355300	3.87143100	0.32486500
H	5.01453100	-2.18461500	-0.33579000	H	-6.10150400	3.85962900	0.69238100
H	4.86556600	-0.36116300	-1.79312800	H	-4.11675600	-0.40683400	0.45979800
H	4.08264100	0.43715800	0.46010400	H	-3.31962600	-2.83121800	0.79339300
H	4.03764500	2.04386700	-1.46966300	H	-7.28426400	3.23629300	1.86963300
H	5.68012300	2.54049900	-1.09852900	H	-1.17561000	-7.61106000	1.30618500
H	4.83213100	4.95620900	-0.82529000				
H	3.17417600	4.44009500	-1.13753700				
H	3.28806800	2.86441900	0.79542300				
H	4.09675100	6.11398600	1.10067300				
H	1.16469800	7.165548700	1.31446700				
H	2.66144300	7.37230800	2.23044700				
H	4.93360900	3.381115500	1.13967000				
H	5.72580000	0.93892800	0.84131300				
H	1.18673900	6.45294900	2.60319300				
H	7.83781400	-3.81862900	0.32160200				
C	0.80893000	-2.46212800	-1.31849200				
C	0.42017600	-1.24837800	-0.46422800				
C	0.03802900	-0.03087700	-1.31273600				
C	-0.35242200	1.18867200	-0.47096700				
C	-0.73909800	2.39826600	-1.33204000				
N	-1.10982900	3.56968300	-0.54587900				
N	1.15939800	-3.63505000	-0.52536400				
C	-2.37872000	3.82815600	-0.17366400				
C	2.42254800	-3.91332800	-0.14841900				
O	-3.33001700	3.09908800	-0.48323000				
O	3.38849200	-3.20429500	-0.45902200				
C	-2.58933000	5.08409100	0.64800000				
C	2.60982000	-5.16813900	0.68075000				
H	1.67635100	-5.70224400	0.86103700				
H	3.06075800	-4.89521000	1.63762900				
H	1.66533700	-2.21745200	-1.94962700				
H	0.40386300	-4.24184600	-0.21835500				
H	-0.02128700	-2.74153600	-1.97320000				
H	-0.41795000	-1.52302700	0.18651700				
H	-0.79589500	-0.29591200	-1.97536400				
H	0.87745900	0.23229500	-1.96918800				
H	0.09697400	2.68365000	-1.97664500				
H	-1.58508100	2.14482800	-1.97378300				
H	-1.19629900	0.93603200	0.17979200				
H	-0.36725900	4.19308200	-0.24122300				
H	-3.29692200	5.73086200	0.12443400				
H	-1.66458800	5.63295100	0.82861900				
H	0.48017000	1.46759200	0.18512400				
H	1.25986900	-0.99587100	0.19212000				
H	-3.03974700	4.80920100	1.60458200				
H	3.30950300	-5.82841600	0.16352600				
C	-3.95570800	-4.53548200	-0.35521200				
C	-4.24342900	-3.19484900	0.33085300				
C	-4.78784000	-2.14369000	-0.64243600				
C	-5.04703700	-0.78812600	0.02296700				
C	-5.60065200	0.25367600	-0.95880000				
N	-5.81493000	1.56000700	-0.35178400				
N	-3.44854000	-5.55567400	0.56102300				
C	-6.99163700	1.91588700	0.21483100				
C	-2.13235300	-5.77811200	0.78130200				
O	-7.97544600	1.17449700	0.25192700				

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Gibbs Free Energy= -1841.29497

C	-5.90724100	-2.40155800	-0.58290000	O	6.47079900	-4.50910700	0.67871800
C	-5.81192600	-1.15752300	0.30944200	C	4.59821300	-5.89687100	1.24883500
C	-5.85465900	0.14309100	-0.50041100	C	4.87606400	5.69432100	1.15132200
C	-5.72364200	1.39812000	0.36976000	H	5.40895100	6.56505600	0.76255900
C	-5.75204900	2.68705200	-0.46108800	H	3.63476900	3.94205500	-0.21656500
N	-5.84018500	-3.65556300	0.16373400	H	4.53527500	2.40169900	-1.80808100
N	-5.60185700	3.89655600	0.34400200	H	6.08748300	2.46324200	-0.96479700
C	-4.41695000	4.52557000	0.53431400	H	3.54216100	1.19878800	0.17631600
C	-4.68854500	-4.33747600	0.37401300	H	4.48594900	-0.12054800	-1.74967700
O	-3.37078700	4.12572200	0.01933400	H	6.05199900	-0.15071500	-0.95679200
O	-3.60655500	-3.95173000	-0.07336700	H	3.48333900	-1.35012100	0.21263300
C	-4.80113100	-5.61161600	1.18443200	H	4.38501000	-2.63920500	-1.75905600
C	-4.44586200	5.76085100	1.40977100	H	5.94361100	-2.76790500	-0.93569100
H	-4.08535200	6.61155900	0.82758000	H	3.42607900	-4.08932900	-0.10653100
H	-6.41581700	4.26219400	0.81350500	H	5.07165500	-1.42220000	0.96564300
H	-6.69339300	2.76392600	-1.01285100	H	5.12459500	1.19846400	0.94522400
H	-4.93905900	2.68369300	-1.18819500	H	5.05866100	-6.80703300	0.85773900
H	-6.53431300	1.42427000	1.10776400	H	3.52073100	-5.93722000	1.08337500
H	-6.79213000	0.18872300	-1.06959200	H	3.81013900	5.80259800	0.94636700
H	-5.04600000	0.13301400	-1.24147300	H	5.03762000	5.66615300	2.23135900
H	-6.63259500	-1.16885600	1.03663800	H	4.79983500	-5.86219100	2.32190100
H	-6.84469200	-2.39631200	-1.14627700				
H	-5.08690000	-2.41128300	-1.30195400				
H	-6.68706400	-4.01177300	0.57905200				
H	-4.88034000	-1.20718800	0.88251000				
H	-4.78488700	1.36335200	0.93238900				
H	-4.42360300	-6.44280000	0.58534500				
H	-5.82051300	-5.83636700	1.50164800				
H	-5.43728200	5.99381800	1.80106700				
H	-3.75787600	5.61632600	2.24531400				
H	-4.16505700	-5.52465400	2.06782700				
C	-0.50075000	-2.53887800	-1.33625500				
C	-0.52677700	-1.25668200	-0.49463800				
C	-0.39420800	0.01166700	-1.34388300				
C	-0.45532300	1.29615900	-0.51079600				
C	-0.38510500	2.56392600	-1.37149000				
N	-0.70882800	-3.74464500	-0.54243200				
N	-0.50908700	3.78925200	-0.59031600				
C	0.55229300	4.51476200	-0.18403800				
C	0.30274700	-4.50372900	-0.07527700				
O	1.71935600	4.21651400	-0.46383100				
O	1.49245900	-4.25575200	-0.30358000				
C	-0.09820900	-5.71140800	0.74952900				
C	0.23807800	5.74871100	0.63920100				
H	0.63192100	6.62610500	0.12125400				
H	-1.44322400	4.06563100	-0.30032900				
H	-1.19000900	2.55703600	-2.11263000				
H	0.56435600	2.60694600	-1.90711400				
H	-1.38507200	1.31336100	0.06968600				
H	-1.19493100	0.02890400	-2.09518300				
H	0.54912700	-0.01774500	-1.90323000				
H	-1.46576800	-1.22333900	0.07010600				
H	-1.28576600	-2.50219000	-2.09743000				
H	0.45824500	-2.63751400	-1.84723700				
H	-1.66592700	-3.97962300	-0.29366700				
H	0.28276600	-1.29985200	0.24181500				
H	0.36770500	1.31198600	0.21171700				
H	0.26619300	-6.61319000	0.25206900				
H	-1.17648000	-5.79251700	0.89227900				
H	-0.82984100	5.88470200	0.81412600				
H	0.75386200	5.67357800	1.59903800				
H	0.39138200	-5.65173300	1.72389900				
C	4.86837000	-2.67277500	-0.77682000				
C	4.55831600	-1.38555500	-0.00130300				
C	4.97215100	-0.12281400	-0.76483100				
C	4.61957200	1.17298600	-0.02635400				
C	5.00653700	2.42809200	-0.81992400				
N	4.41967800	-3.87727500	-0.09091000				
N	4.61189700	3.66783900	-0.16405500				
C	5.47610400	4.44181700	0.53480800				
C	5.25653500	-4.69640000	0.58968100				
O	6.67141700	4.17686000	0.67070900				

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Gibbs Free Energy= -1959.188800

H	-0.28245000	-5.46353800	-1.43784500	H	4.98292000	3.14116100	1.02235200
C	-0.79881400	-6.19242300	-0.81141500	H	3.82812100	1.91015600	0.52554800
H	-1.42141000	-6.81039600	-1.46434900	C	3.55690200	3.81894200	-0.45911200
C	-1.66388600	-5.47602300	0.23224700	H	3.03223000	3.40811200	-1.33150200
H	-1.00724900	-4.91057300	0.90227700	H	4.18457400	4.63595500	-0.83654600
H	-2.17861800	-6.22152600	0.85029800	C	2.52857300	4.38736900	0.52541700
C	-2.69075800	-4.53383000	-0.40546800	H	3.05455100	4.81834400	1.38658600
H	-3.33697800	-5.10077000	-1.08734900	H	1.91541600	3.56749800	0.92051100
H	-2.16605400	-3.79549700	-1.02492500	C	1.61429200	5.44775900	-0.09844900
C	-3.56141900	-3.80162200	0.62215700	H	1.06754500	5.01771800	-0.94476800
H	-2.91170200	-3.26644200	1.32697600	H	2.22206800	6.26745100	-0.50044400
H	-4.11631900	-4.53803900	1.21692900	C	0.60335600	6.01409700	0.90533100
C	-4.54432400	-2.81239200	-0.01296400	H	1.12406900	6.47306400	1.75092900
H	-5.20770600	-3.33805100	-0.70805700	H	-0.02878200	5.21724400	1.29882500
H	-3.99217400	-2.07057700	-0.60165800	N	-0.28491500	7.01760800	0.32267700
C	-5.40276500	-2.08199800	1.02863000	H	0.08097700	7.94598400	0.17703500
H	-4.75836900	-1.57064000	1.75036300	N	6.31204600	1.12800700	-0.27525000
H	-6.01542900	-2.80100000	1.57617900	H	5.95371100	0.17722200	-0.28424000
N	-6.29434400	-1.08857900	0.44623300	C	7.50868800	1.37909400	0.30727700
H	-5.91962900	-0.16144800	0.26662600	C	-1.54147700	6.75686100	-0.10819900
N	0.22425700	-7.05384100	-0.22076000	O	-2.06153500	5.64334900	-0.00852800
H	-0.04484500	-7.97913700	0.07603600	O	7.99611000	2.50789000	0.39038800
C	1.49246500	-6.64862600	0.02263000	C	-2.29384900	7.92136000	-0.71841700
C	-7.57198700	-1.36813300	0.09563100	H	-1.71556600	8.84622700	-0.74550600
O	-8.09033500	-2.47463100	0.25594500	H	-3.20705200	8.08922200	-0.14363300
O	1.89125700	-5.51899600	-0.27135100	H	-2.58819100	7.65502300	-1.73564900
C	-8.35100600	-0.21407500	-0.51097400	C	8.23648400	0.16452000	0.85617600
H	-7.76462600	0.70230300	-0.59072400	H	9.21234400	0.09246100	0.37052600
H	-9.23447600	-0.02644200	0.10363000	H	7.68706400	-0.76562500	0.70544500
H	-8.69898400	-0.50881200	-1.50364600	H	8.41219800	0.31384700	1.92406800
C	2.41062000	-7.66451100	0.66998400				
H	3.26747400	-7.83098400	0.01379100				
H	1.92719800	-8.62132700	0.87264300				
H	2.78745300	-7.25068100	1.60768900				
H	2.98733700	-1.23036400	-1.65719200				
C	2.39693100	-1.98808300	-1.13888800				
H	1.77705200	-2.49688200	-1.88266000				
C	1.50812800	-1.33076400	-0.07535100				
H	2.14844400	-0.82486400	0.65548700				
H	0.96596800	-2.11296100	0.46864000				
C	0.51192500	-0.33351800	-0.67561300				
H	-0.11628700	-0.84578900	-1.41548100				
H	1.05892500	0.44264400	-1.22589600				
C	-0.38660900	0.32988400	0.37411700				
H	0.24157200	0.84247800	1.11405700				
H	-0.93236500	-0.44692400	0.92464700				
C	-1.38565600	1.32519500	-0.22432500				
H	-2.02421500	0.81872500	-0.95602500				
H	-0.84686700	2.11088200	-0.76685400				
C	-2.27714000	1.97495300	0.84137700				
H	-1.65965000	2.48783700	1.58474300				
H	-2.85802400	1.21075300	1.36099400				
N	-3.21184800	2.94979300	0.29248200				
H	-2.87690000	3.89754500	0.14773600				
N	3.32056400	-2.97131000	-0.58495000				
H	2.96429000	-3.90881800	-0.41990800				
C	4.58764800	-2.67567400	-0.23497300				
C	-4.47362000	2.63794700	-0.06505300				
O	-4.94571500	1.50090500	0.05849100				
O	5.08180100	-1.54986900	-0.37578100				
C	-5.30369900	3.77347600	-0.62957100				
H	-4.75771800	4.71637700	-0.67420000				
H	-6.19399500	3.89924300	-0.00921000				
H	-5.63788900	3.50025000	-1.63305900				
C	5.40102200	-3.81682100	0.34347200				
H	6.29284400	-3.95915300	-0.27081600				
H	4.84480200	-4.75352800	0.39394800				
H	5.73287200	-3.54042800	1.34691700				
H	6.13429600	2.98294700	-1.17799900				
C	5.47689900	2.18016700	-0.83802400				
H	4.96597400	1.77006300	-1.71452500				
C	4.44861900	2.73546200	0.15666700				

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Gibbs Free Energy= -1959.188062

C	2.52429600	1.83030400	1.13301600	H	-3.60999500	5.37089300	-1.36948500
C	1.54223800	1.21544700	0.12738200	H	-1.28263700	6.47807700	-1.57726900
C	0.31105800	0.60244500	0.80225900	H	3.74428200	5.96478800	-2.71410300
C	-0.69175800	0.01090500	-0.19570300	C	-5.46520900	3.53726100	-0.43471400
C	-1.95999600	-0.53701200	0.46628100	H	-5.91147500	4.22348200	-1.16064200
N	3.65136400	2.49885700	0.49286600	H	-5.08522100	2.67450400	-0.98300500
C	4.85721700	1.91957900	0.32453400	N	-1.82521500	-5.72076200	-1.06196300
O	5.11716700	0.77670300	0.71871400	C	-2.14612000	-7.03019800	-1.19688000
C	5.90606700	2.75978500	-0.37743400	C	-3.53428400	-7.41293100	-0.71326100
H	5.53969900	3.74506000	-0.66831700	H	-2.50009100	-5.08821000	-0.64270000
H	6.76456500	2.87733700	0.28757300	H	-4.08854600	-6.57048100	-0.29740400
H	2.00831500	2.56825500	1.75474200	H	-3.43767000	-8.19376000	0.04450900
H	3.48988600	3.43195900	0.12420600	H	-4.09252000	-7.83676500	-1.55136200
H	2.92577900	1.05890300	1.79191100	O	-1.38545300	-7.86921400	-1.68154900
H	2.06673400	0.45332600	-0.45923500	N	-4.21509400	-1.52560400	0.04877000
H	0.62716400	-0.17773400	1.50572100	C	-4.49892300	-2.81437200	0.32705600
H	-0.19191000	1.37031100	1.40458300	O	-3.72506300	-3.74762800	0.08413000
H	-2.44632100	0.25805200	1.04358900	C	-5.85054000	-3.07420400	0.96297400
H	-1.70195400	-1.32937600	1.17727700	N	-6.52726600	3.05067500	0.44201900
H	-0.20338800	-0.78607400	-0.77006100	C	-6.62646300	1.76514000	0.85872800
H	-0.97061600	0.78353300	-0.92425700	O	-5.83037400	0.89368300	0.50324000
H	1.22515300	1.99263700	-0.57797800	C	-7.78315700	1.44843200	1.78379000
H	6.24865200	2.22526200	-1.26624900	H	-5.69740300	-3.57894600	1.91938100
C	-2.96158000	-1.09101800	-0.55552400	H	-4.88925800	-0.80478300	0.28940200
H	-3.19699400	-0.32303300	-1.29880600	H	-6.43013400	-2.16421800	1.12339800
H	-2.53320100	-1.94498100	-1.08228000	H	-7.38767800	1.02534300	2.70942000
C	4.82725700	-2.89381000	1.28785200	H	-8.39905700	2.31676400	2.02311500
C	3.91526600	-3.19218100	0.09023800	H	-7.19663900	3.71698700	0.79491300
C	2.66630800	-3.98696600	0.48465100	H	-8.41008300	0.68756000	1.31397600
C	1.71810100	-4.25476200	-0.69037500	H	-6.41583000	-3.75272400	0.32012200
C	0.41865100	-4.95291000	-0.27690500				
N	5.96050000	-2.04407000	0.94784000				
C	7.20983700	-2.52395800	0.74108200				
O	7.50460200	-3.71662900	0.83294000				
C	8.25819700	-1.48201700	0.38904800				
H	7.85494900	-0.46958200	0.33792600				
H	9.05178600	-1.51711400	1.13903800				
H	4.25260400	-2.39376700	2.07458000				
H	5.78660700	-1.04911300	0.83821400				
H	5.22362700	-3.82271900	1.70111100				
H	4.48916600	-3.74149500	-0.66415000				
H	2.96504000	-4.94163300	0.93513900				
H	2.12247100	-3.43858100	1.26533700				
H	-0.09230300	-4.35293900	0.48576600				
H	0.64123200	-5.92183800	0.18329000				
H	2.23642300	-4.85883800	-1.44541200				
H	1.47431000	-3.30124300	-1.17782900				
H	3.61526200	-2.24361600	-0.37110700				
H	8.70425600	-1.74430600	-0.57297300				
C	-0.53590200	-5.17172000	-1.45858200				
H	-0.71459700	-4.21979300	-1.97046200				
H	-0.09218400	-5.85984000	-2.17989200				
C	0.22518600	6.51788100	-0.03031900				
C	-0.90519200	5.81329600	-0.79074800				
C	-2.05642000	5.39719000	0.13141200				
C	-3.20096100	4.69415900	-0.60847400				
C	-4.32591300	4.23005600	0.32323000				
N	1.34427100	6.90243900	-0.88665600				
C	2.48208700	6.17672000	-1.00685100				
O	2.66925100	5.13514400	-0.37448600				
C	3.52678000	6.72214000	-1.95821700				
H	3.22303800	7.64453200	-2.45560300				
H	4.44725500	6.90638300	-1.40017000				
H	-0.15177100	7.42024100	0.46019800				
H	1.24739000	7.73071300	-1.45355200				
H	0.62625100	5.86182900	0.74307800				
H	-0.49436000	4.93152000	-1.29396500				
H	-1.66992900	4.73206700	0.91347700				
H	-2.44966300	6.28162800	0.64868800				
H	-4.72755000	5.08868000	0.87504000				
H	-3.92657100	3.53509800	1.06967000				
H	-2.80206100	3.82848800	-1.15143700				

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Gibbs Free Energy= -2077.083084

C	-5.22786200	-3.45334200	-0.95913500	H	2.69746600	-0.27524100	0.33339700
C	-4.07792600	-3.80030100	-0.00378400	H	1.97974400	-1.88026200	0.28545800
C	-2.92401400	-4.51929900	-0.71042800	C	-1.75736400	6.53065100	-0.28409400
C	-1.75814200	-4.86203600	0.22403400	C	-0.58464300	5.86919500	0.44948300
C	-0.58687800	-5.55030100	-0.48658800	C	0.58579000	5.54796800	-0.48613400
N	-6.31378000	-2.72443300	-0.31782100	C	1.75715700	4.85969600	0.22431000
C	-7.39413800	-3.34127200	0.21592500	C	2.92317400	4.51763000	-0.71021700
O	-7.55466000	-4.56305600	0.19641200	N	-2.88740200	6.83873100	0.59098100
C	-8.42613600	-2.42285600	0.84735900	C	-3.93029800	5.99931200	0.78911100
H	-8.15532400	-1.36806600	0.78332300	O	-4.02261400	4.91477700	0.20871300
H	-9.38594400	-2.58076300	0.35018900	C	-4.99463900	6.46738100	1.76008100
H	-4.85460100	-2.83771900	-1.78310600	H	-4.79808000	7.45587200	2.17807100
H	-6.23266900	-1.71358500	-0.25045000	H	-5.95702100	6.48373400	1.24458200
H	-5.64464200	-4.36797400	-1.38589800	H	-1.43519300	7.46404600	-0.75411900
H	-4.46952700	-4.42690400	0.80465000	H	-2.85706500	7.69367700	1.12468500
H	-3.29910700	-5.44020900	-1.17467100	H	-2.12913900	5.87336000	-1.07137600
H	-2.55423300	-3.89186100	-1.53210700	H	-0.94270300	4.95024400	0.92599800
H	-0.23169700	-4.90772800	-1.30225700	H	0.23057600	4.90550500	-1.30187400
H	-0.94251900	-6.47494400	-0.95899700	H	0.94135900	6.47269300	-0.95843400
H	-2.12116500	-5.50677700	1.03410600	H	3.29794400	5.43882000	-1.17416400
H	-1.39748900	-3.94322500	0.70386300	H	2.55364500	3.89031300	-1.53210200
H	-3.70952000	-2.87756800	0.45993300	H	1.39671200	3.94062200	0.70379400
H	-8.55018100	-2.70214700	1.89617600	H	2.11997900	5.50423700	1.03463100
C	0.58362900	-5.87162300	0.44890700	H	-0.24311000	6.52993200	1.25532200
C	1.75649600	-6.53252400	-0.28493200	H	-5.06872300	5.74544900	2.57628600
N	2.88712400	-6.83975600	0.58972500	C	4.07734100	3.79886000	-0.00376400
C	3.92764100	-5.99790600	0.78996600	C	5.22754700	3.45288500	-0.95914800
O	4.01660200	-4.91156500	0.21242300	N	6.31379400	2.72429400	-0.31803400
C	4.99352200	-6.46544700	1.75948800	C	7.39389500	3.34147800	0.21584500
H	5.95553700	-6.47949000	1.24320900	O	7.55361600	4.56337600	0.19708600
H	5.06701400	-5.74449700	2.57659800	C	8.42656100	2.42331800	0.84655700
H	4.79900300	-7.45485400	2.17625500	H	9.38625900	2.58237100	0.34954500
H	2.85914500	-7.69618900	1.12115600	H	8.55036900	2.70183000	1.89561100
H	2.12741800	-5.87517000	-1.07258600	H	8.15654700	1.36837800	0.78161800
H	1.43481800	-7.46627200	-0.75456200	H	6.23362000	1.71330700	-0.25172800
H	0.94149900	-4.95273100	0.92564900	H	5.64387400	4.36792400	-1.38548800
H	0.24230500	-6.53270200	1.25454600	H	4.85468300	2.83740500	-1.78340900
C	-3.50424600	1.55089200	-1.20190700	H	4.46857000	4.42529700	0.80497900
C	-2.33159200	1.05785800	-0.34467900	H	3.70933100	2.87575200	0.45952200
C	-1.17256100	0.51761100	-1.18836400				
C	0.00106200	0.00146500	-0.34827300				
C	1.17468900	-0.51512000	-1.18809300				
N	-4.60087400	2.10212300	-0.41341500				
C	-5.65393400	1.36624300	-0.00753600				
O	-5.78431900	0.16758000	-0.28619700				
C	-6.69956100	2.09579900	0.81268600				
H	-6.44466900	3.14037500	0.99467800				
H	-7.65589500	2.04599600	0.28690000				
H	-3.16539300	2.33219200	-1.88822100				
H	-4.53478600	3.07597600	-0.12932700				
H	-3.90289900	0.72913400	-1.79963500				
H	-2.69519900	0.27791800	0.33327100				
H	-1.53792100	-0.29166600	-1.83353700				
H	-0.81524000	1.30669100	-1.86289900				
H	1.54029100	0.29388400	-1.83347000				
H	0.81727700	-1.30433200	-1.86242400				
H	-0.35286400	-0.80067300	0.31179300				
H	0.35496800	0.80391400	0.31143000				
H	-1.97827600	1.88327900	0.28438700				
H	-6.82151900	1.58124200	1.76837400				
C	2.33347700	-1.05540500	-0.34410300				
C	3.50590200	-1.54958500	-1.20098300				
N	4.60192800	-2.10130100	-0.41200100				
C	5.65634200	-1.36654900	-0.00760500				
O	5.78887800	-0.16862100	-0.28839100				
C	6.70090200	-2.09654300	0.81360200				
H	6.82473400	-1.57998400	1.76795800				
H	6.44377500	-3.14010000	0.99828100				
H	7.65697100	-2.05019400	0.28700500				
H	4.53424200	-3.07458700	-0.12632100				
H	3.90533900	-0.72837700	-1.79893100				
H	3.16657900	-2.33090100	-1.88705600				

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Gibbs Free Energy= -2077.083132

C	-3.86343300	0.03904100	1.52491700	H	2.98482200	3.27002900	-0.18551100
C	-2.60577400	-0.17961600	0.67466000	H	3.24833000	4.77933100	-1.04985800
C	-1.31991600	-0.18170000	1.50766600	C	-4.46946000	-5.33089900	0.49923100
C	-0.06041300	-0.42642900	0.66918400	C	-3.23924500	-5.32675900	-0.41640300
C	1.23256000	-0.45963100	1.49171100	C	-1.94361000	-5.62296800	0.34697200
N	-5.09544100	-0.00802100	0.74500600	C	-0.69667300	-5.60213600	-0.54494200
C	-5.69427100	1.09365600	0.25062700	C	0.60123100	-5.88994700	0.21887400
O	-5.26602200	2.23775500	0.44525600	N	-5.71815600	-5.05300300	-0.20689700
C	-6.95142800	0.85821200	-0.56383300	C	-6.27156800	-3.82014800	-0.29557500
H	-7.23095300	-0.19439600	-0.62115400	O	-5.76701300	-2.83190500	-0.99208800
H	-7.77095100	1.42526400	-0.11711600	C	-7.55981700	-3.72010600	-1.08613800
H	-3.93094500	-0.73022100	2.29990800	H	-7.89365200	-4.67471900	-1.49590700
H	-5.47167000	-0.92426200	0.51595700	H	-8.34078900	-3.32105300	-0.43554600
H	-3.82058100	1.01070000	2.01966600	H	-4.57247500	-6.30156800	0.99294900
H	-2.55509700	0.60558100	-0.08748100	H	-6.16781100	-5.81134300	-0.69593300
H	-1.22476000	0.77537000	2.03570100	H	-4.36400700	-4.57220800	1.27588700
H	-1.39187300	-0.95335400	2.28554000	H	-3.16818900	-4.34964300	-0.90590400
H	1.14874600	-1.13478200	2.26483600	H	-1.82244000	-4.88847800	1.15292300
H	1.34853600	0.49190700	2.02556100	H	-2.02370600	-6.60253600	0.83575000
H	0.01967100	0.35249300	-0.09934500	H	0.53317700	-6.87969900	0.68852900
H	-0.16705900	-1.37613900	0.12894200	H	0.70484700	-5.16889700	1.03923400
H	-2.70026500	-1.13248200	0.14063500	H	-0.61884000	-4.62269400	-1.03298700
H	-6.79549500	1.24415900	-1.57394900	H	-0.81434400	-6.33700300	-1.35131500
C	2.47948500	-0.72241000	0.64126400	H	-3.37737900	-6.06909500	-1.21186200
C	3.76471100	-0.78634100	1.47566800	H	-7.41714600	-3.01214500	-1.90532000
N	4.94849100	-1.07378100	0.67335800	C	1.85136300	-5.82862800	-0.66582100
C	5.81824200	-0.12445300	0.27322500	C	3.13660500	-6.11786300	0.11922300
O	5.70496800	1.06887600	0.57891600	N	4.34412400	-6.03520500	-0.69934000
C	6.97696000	-0.60341800	-0.57980200	C	5.13334100	-4.93613100	-0.76269500
H	6.94662300	-0.08428400	-1.54051900	O	4.90346100	-3.92072600	-0.10210700
H	7.91238000	-0.32979100	-0.08684000	C	6.32994800	-5.02293100	-1.68712300
H	6.96321900	-1.68015100	-0.75226900	H	6.26112800	-4.22332400	-2.42766000
H	5.07745900	-2.03009200	0.35304000	H	7.23751900	-4.85620200	-1.10319200
H	3.67652700	-1.56564300	2.23909700	H	6.41174400	-5.98008000	-2.20430500
H	3.93499200	0.16354100	1.98424100	H	4.57521700	-6.81980600	-1.28903000
H	2.36228100	-1.66713400	0.09729200	H	3.09589100	-7.11775900	0.56118000
H	2.58785200	0.06367900	-0.11429000	H	3.25218900	-5.39961800	0.93173500
C	-3.22994200	5.38862500	0.48342300	H	1.75860700	-6.54844800	-1.48819000
C	-1.97785000	4.86174100	-0.23021800	H	1.93472200	-4.83692400	-1.12314100
C	-0.68453400	5.20379800	0.51703700				
C	0.57401100	4.64745300	-0.15900200				
C	1.86649700	4.94062000	0.61157400				
N	-4.47248800	5.01611100	-0.18049900				
C	-5.13147100	5.84332900	-1.02585300				
O	-4.75073700	6.98342500	-1.29660300				
C	-6.40480000	5.27805400	-1.63219700				
H	-6.62674800	4.26558900	-1.29249100				
H	-7.23737600	5.93666400	-1.37455800				
H	-3.26519000	5.00041900	1.50637400				
H	-4.83376400	4.07926100	-0.02135000				
H	-3.19909000	6.47817500	0.53890600				
H	-1.94656500	5.27928600	-1.24256800				
H	-0.59462300	6.29334200	0.61123700				
H	-0.74438700	4.81275200	1.54154300				
H	1.77441300	4.54245300	1.63093400				
H	1.98816400	6.02591300	0.71802200				
H	0.65385000	5.05977200	-1.17265000				
H	0.46678500	3.56133900	-0.27931200				
H	-2.06279300	3.77383000	-0.33911800				
H	-6.30764900	5.28279200	-2.72039600				
C	3.11623300	4.35045700	-0.05028100				
C	4.39117200	4.59782400	0.76647400				
N	5.57832900	3.99643000	0.17311300				
C	6.50177000	4.70877800	-0.51529800				
O	6.43052400	5.92590100	-0.69242600				
C	7.66675000	3.90451900	-1.06715500				
H	7.69513200	4.02809900	-2.15232900				
H	8.59617000	4.31521500	-0.66607000				
H	7.60635400	2.84295500	-0.82378000				
H	5.69791400	2.99089400	0.26344300				
H	4.26976300	4.19028500	1.77574700				
H	4.57808200	5.66899400	0.85790100				

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Gibbs Free Energy= -2194.976702

C	4.73386500	4.56529600	-0.97149800	C	-7.86180200	0.63258200	-0.62313500
C	3.56744200	4.58015700	0.02552300	O	-6.43196900	-1.16869000	0.05981000
C	2.25150800	5.03251900	-0.61558300	H	-7.97936100	0.25549000	-1.64155200
C	1.06962800	5.04461900	0.36067100	H	-7.86624600	1.72304200	-0.63871000
C	-0.25978100	5.43809000	-0.29298900	H	-5.85775800	1.94156800	0.26122700
N	5.98584500	4.09702800	-0.39245000	H	-4.15337900	1.29411500	1.74873300
C	6.90356000	4.93783800	0.14018800	H	-4.52308000	-0.40591500	1.44720500
O	6.76304500	6.16187000	0.16982500	H	-8.71387100	0.27604600	-0.03998000
C	8.14839000	4.27519900	0.70444300	C	4.05186700	-5.72662900	-0.71585600
H	8.14014300	3.18980400	0.59631300	C	2.85421400	-5.68530100	-2.04733100
H	9.02384900	4.68333000	0.19426200	C	1.53985600	-5.37012000	-0.48160600
H	4.49356600	3.91365400	-1.81722800	C	0.32657500	-5.32860000	0.45481200
H	6.15221700	3.09479300	-0.36243100	C	-0.98262400	-4.97263200	-0.25876100
H	4.90255200	5.57156600	-1.36059300	N	5.31836800	-6.00545900	-0.04235600
H	3.82600400	5.24364900	0.85785400	C	6.20876000	-5.04990000	0.31485800
H	2.37962000	6.03587200	-1.04118300	O	6.03510400	-3.85460600	0.06646500
H	2.01383600	4.37136900	-1.45971600	C	7.45241000	-5.52864000	1.03510200
H	-0.47451300	4.74537100	-1.11692600	H	7.46824400	-6.60592800	1.20758400
H	-0.16173700	6.43180200	-0.74823400	H	8.32864800	-5.24997900	0.44579100
H	1.28864500	5.73462500	1.18539500	H	3.90003100	-6.49270100	-1.48200800
H	0.96646200	4.05056600	0.81467800	H	5.51561600	-6.95871200	0.22072700
H	3.44622800	3.57534900	0.44735800	H	4.16487600	-4.76823600	-1.22394500
H	8.23525100	4.53336600	1.76237900	H	3.04521500	-4.93144000	1.01227700
C	-1.44323700	5.44181300	0.68158500	H	1.63331700	-4.40454000	-0.99486300
C	-2.78072800	5.77158100	0.01012700	H	1.36568400	-6.11707500	-1.26666500
H	-2.98827400	5.04276300	-0.78088900	H	-1.17110800	-5.70160100	-1.05699000
H	-2.71935600	6.75355800	-0.47472100	H	-0.86937500	-4.00007100	-0.75499600
H	-1.51625600	4.45913600	1.16482200	H	0.51242300	-4.59951700	1.25396700
H	-1.24875600	6.16332800	1.48542600	H	0.21755800	-6.30193900	0.94978100
C	-3.95038900	5.76750700	1.00148400	H	2.76988000	-6.64935500	0.75701600
N	-5.24062700	6.04107300	0.37181900	H	7.52217900	-5.01280700	1.99489600
C	-6.10971800	5.07591700	-0.01008800	C	-2.19668700	-4.92332100	0.67619600
C	-7.38332100	5.54770900	-0.68090300	C	-3.49644400	-4.53238800	-0.03492400
O	-5.89196000	3.87699800	0.18046600	H	-3.71333900	-5.24791900	-0.83524600
H	-7.45718200	5.07786300	-1.66380900	H	-3.37727800	-3.55173200	-0.51099100
H	-7.43698800	6.63098300	-0.79974300	H	-2.32456800	-5.90257700	1.15465700
H	-5.47198300	6.99913200	0.15887900	H	-1.99778900	-4.21095000	1.48801400
H	-3.79037800	6.51602600	1.78303700	C	-4.69862600	-4.48287300	0.91786100
H	-4.03184400	4.79391100	1.48630700	N	-5.93862300	-4.08261800	0.26678100
H	-8.23759900	5.21236000	-0.08892900	C	-6.81432900	-4.97758300	-0.24996600
C	4.24174800	-0.73289000	-1.16038800	C	-8.05363300	-4.38143700	-0.89413800
C	3.10443700	-0.62345800	-0.13665700	O	-6.64004700	-6.19667200	-0.20356100
C	1.74948200	-0.33405900	-0.79033300	H	-8.10464100	-4.71560400	-1.93296600
C	0.59754700	-0.24443700	0.21692100	H	-8.06672600	-3.29134400	-0.86121900
C	-0.75624600	0.07461100	-0.42659700	H	-6.13503100	-3.09007000	0.17681800
N	5.53764800	-1.00939800	-0.55146700	H	-4.50371900	-3.77473000	1.72935800
C	6.41382300	-0.03909800	-0.22138100	H	-4.85815500	-5.46665900	1.36412900
O	6.19849200	1.16075800	-0.43441800	H	-8.93603500	-4.77077000	-0.38089200
C	7.70465700	-0.50077100	0.42492700				
H	7.74882900	-1.58189900	0.56007600				
H	8.54338900	-0.17954900	-0.19702600				
H	4.02956100	-1.53481600	-1.87394200				
H	5.76177900	-1.97387400	-0.32432500				
H	4.33087800	0.19866000	-1.72203800				
H	3.35006500	0.17054400	0.57693400				
H	1.81226000	0.60582600	-1.35341100				
H	1.52443100	-1.11581000	-1.52779400				
H	-0.98668300	-0.68478000	-1.18474700				
H	-0.68468600	1.02874900	-0.96430100				
H	0.83172800	0.52319300	0.96559500				
H	0.52365700	-1.19158600	0.76662600				
H	3.04823800	-1.55587200	0.43756900				
H	7.80736500	-0.00968700	1.39532600				
C	-1.90878400	0.14773500	0.58122900				
C	-3.25520300	0.50158300	-0.05808400				
H	-3.51234700	-0.23866100	-0.82365100				
H	-3.17929500	1.46898400	-0.56812200				
H	-1.99457200	-0.81424100	1.10265200				
H	-1.66683300	0.89066000	1.35267900				
C	-4.39349400	0.56624500	0.96808700				
N	-5.67357800	0.94997800	0.38474400				
C	-6.59106400	0.05487000	-0.03182100				

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Gibbs Free Energy= -2194.977035

C	-3.31523400	-0.13016900	0.31727800	O	-6.26341400	-3.01051300	0.28642700
C	-1.94060300	-0.10031000	-0.35843700	C	-7.88978800	-4.14398700	1.63926500
C	-0.77410900	-0.23320600	0.62756800	H	-8.74827700	-3.73266300	1.10387400
C	0.59854800	-0.27405200	-0.05298000	H	-8.13219500	-5.15360600	1.97426300
C	1.76673500	-0.42149000	0.92894300	H	-6.46220400	-6.10124300	0.86113400
H	-3.42772000	-1.06411900	0.88028200	H	-4.87593600	-4.50801800	-1.04862000
H	-3.39542000	0.68659000	1.04291300	H	-5.03409400	-6.26548700	-1.04883000
H	-1.83091400	0.83286200	-0.92528100	H	-7.71025900	-3.51225300	2.51153200
H	-0.80417700	0.60072700	1.33987800	C	-2.78332600	4.88780700	-0.34885600
H	-0.90788800	-1.14621100	1.22245500	C	-1.35768100	4.79105400	-0.90192000
H	1.60438800	-1.31207600	1.55044500	C	-0.27273200	4.93256700	0.17200500
H	1.77302600	0.43291400	1.61731000	C	1.14852400	4.72788700	-0.36475100
H	0.73791200	0.63760400	-0.64741500	C	2.23613900	4.84455500	0.70947200
H	0.62145000	-1.10820800	-0.76638500	H	-2.93562300	4.11333400	0.411347800
H	-1.88264700	-0.91234900	-1.09529100	H	-2.92847400	5.85209800	0.15003000
C	3.12883300	-0.53195200	0.23640800	H	-1.21005200	5.56051600	-1.67030300
C	4.28554700	-0.69956100	1.23007100	H	-0.34969300	5.92295400	0.63784500
N	5.57447800	-0.89291300	0.57539100	H	-0.46144500	4.20465800	0.97205600
C	6.46580400	0.10073900	0.38725900	H	1.99663300	4.16427700	1.53782700
O	6.27936200	1.25858700	0.78062100	H	2.22234500	5.85673100	1.13295600
C	7.74215600	-0.28077800	-0.33704800	H	1.34635000	5.45504900	-1.16237200
H	7.83306100	0.33178700	-1.23691200	H	1.21362500	3.73725700	-0.83395000
H	8.59416900	-0.05035000	0.30635800	H	-1.23391100	3.82560500	-1.41097200
H	7.77618700	-1.33495700	-0.61459900	C	3.64114900	4.52497600	0.18841400
H	5.77505900	-1.81800300	0.20518000	C	4.71382300	4.61012000	1.28240900
H	4.10260500	-1.56662900	1.87210100	N	6.03458500	4.19852400	0.82504200
H	4.36705900	0.18036500	1.86981700	C	6.98055000	5.07549700	0.41375800
H	3.12386600	-1.38762700	-0.44902100	O	6.82003000	6.29706700	0.41024600
H	3.31304400	0.35906900	-0.37382700	C	8.28873700	4.45431200	-0.04639600
C	-4.46829200	-0.01687100	-0.68818900	H	8.47601000	4.75562200	-1.07959900
N	-5.78301500	-0.13210400	-0.06781100	H	9.10077300	4.85520000	0.56445100
C	-6.53662000	0.93142200	0.27622400	H	8.29096000	3.36534600	0.01943700
O	-6.18773100	2.10199300	0.08272600	H	6.22639500	3.20183500	0.77355400
C	-7.87181700	0.61883700	0.92337400	H	4.43553100	3.96914000	2.12514700
H	-8.66609700	1.06763400	0.32282000	H	4.79398500	5.63384200	1.65227200
H	-8.05822900	-0.45103400	1.02477200	H	3.65171000	3.51474300	-0.23801000
H	-6.11752500	-1.06913500	0.14013800	C	3.90758200	5.21237000	-0.62200200
H	-4.42704600	0.94281800	-1.20595300	H	-3.85016400	4.72957900	-1.44066600
H	-4.38547100	-0.80707500	-1.44036600	N	-5.21169000	4.71837000	-0.92297700
H	-7.90209600	1.08596000	1.91026400	C	-5.99600800	5.82253600	-0.89143300
C	-3.59821100	-5.50400900	0.39125000	O	-5.63361800	6.92233500	-1.31214200
C	-2.36451400	-5.57946300	-0.51504600	C	-7.38140200	5.62199100	-0.30206400
C	-1.04821000	-5.71255700	0.25997200	H	-8.12475300	5.90140400	-1.05232300
C	0.19139200	-5.71980600	-0.64206000	H	-7.56170500	4.59687900	0.02398600
C	1.50761000	-5.86790000	0.13037000	H	-5.57132900	3.84499700	-0.54951900
H	-3.64209400	-6.39263300	1.03270500	H	-3.77472400	5.54858900	-2.15829600
H	-3.51703000	-4.63838900	1.05744900	H	-3.68874200	3.79243700	-1.98361400
H	-2.32481000	-4.68088600	-1.14344300	H	-7.50199400	6.29930300	0.54659000
H	-0.96652500	-4.88626900	0.97739300				
H	-1.07043900	-6.63342500	0.85662000				
H	1.49990000	-6.81804800	0.67987200				
H	1.57302100	-5.07732500	0.88840900				
H	0.21766000	-4.79041400	-1.22481900				
H	0.10605600	-6.53502700	-1.37192900				
H	-2.46628100	-6.42872200	-1.20303100				
C	2.74790900	-5.80539200	-0.76812400				
C	4.05155000	-5.97337400	0.02188400				
N	5.24847300	-5.86410500	-0.80924200				
C	5.97713900	-4.72835200	-0.92749500				
O	5.69648200	-3.69818200	-0.31089500				
C	7.17203600	-4.79146700	-1.85586400				
H	7.06110100	-4.02357700	-2.62426900				
H	8.07324900	-4.55977800	-1.28426900				
H	7.29755600	-5.76195100	-2.33827000				
H	5.51927700	-6.66188900	-1.36332000				
H	4.07240800	-6.94751000	0.51933300				
H	4.12854200	-5.20506700	0.79214100				
H	2.68740500	-6.58411500	-1.53830000				
H	2.77665700	-4.84485700	-1.29365300				
C	-4.90259300	-5.38941200	-0.40689600				
N	-6.08860100	-5.26579500	0.43770600				
C	-6.67741400	-4.08239300	0.73364400				

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Gibbs Free Energy= -2312.871612

C	-3.01665700	4.91229600	-0.67809400	C	-3.76810900	-0.72578800	-0.53948600
C	-1.82116100	4.86073000	0.28017300	C	-5.02070700	-1.00986000	-1.37784100
C	-0.51893100	5.38857000	-0.33282000	N	-6.21650900	-1.21994800	-0.56857300
C	0.68306700	5.29914700	0.61432500	C	-7.06354600	-0.22339400	-0.24477400
C	1.98986500	5.80988200	-0.00359100	O	-6.90693900	0.94350800	-0.62651800
H	-3.17241100	5.94706600	-1.00859000	C	-8.25030700	-0.61073300	0.61554900
H	-2.77764100	4.33633900	-1.58198300	H	-6.37602000	-2.15147800	-0.19321000
H	-1.66962700	3.82508500	0.61130000	H	-4.87114100	-1.90586400	-1.98683300
H	-0.29734000	4.82657600	-1.24944700	H	-3.60726300	-1.55914300	0.15459900
H	-0.66107300	6.43177500	-0.64278600	H	-3.95090900	0.16388700	0.07298800
H	1.86610600	6.86033800	-0.29671600	H	-5.21773400	-0.17442900	-2.05208100
H	2.19171500	5.25672400	-0.92968800	H	-8.25436500	-1.66758000	0.88427000
H	0.81777300	4.25605100	0.92821100	H	-8.24067400	-0.00574800	1.52491100
H	0.46797400	5.86659400	1.52879600	H	-9.16885200	-0.37567900	-0.07284400
H	-2.05656700	5.43736800	1.18373000	C	-1.99199900	-5.81520800	-0.01034800
C	3.19582600	5.67864200	0.93305300	C	-0.68596500	-5.29560200	0.60172600
C	4.49373800	6.17843900	0.28796700	C	0.51684200	-5.39144900	-0.34383700
N	5.66421800	6.03469500	1.15222800	C	1.81695100	-4.85567500	-0.26675300
C	6.47432200	4.95067700	1.13846600	C	3.01486200	-4.91170800	-0.68824200
O	6.29807900	4.00720600	0.36371900	H	-2.19635000	-5.27133400	-0.94137800
C	7.62582200	4.96009700	2.12236300	H	-1.86617500	-6.86820200	-0.29338000
H	7.54663500	4.08157300	2.76606900	H	-0.46945700	-5.85363500	1.52164400
H	8.56279600	4.88051400	1.56705900	H	0.66116800	-6.43725100	-0.64392000
H	7.65772700	5.85533000	2.74519800	H	0.29532100	-4.83822100	-1.26579500
H	5.84585800	6.75526400	1.83371400	H	2.77848900	-4.34025600	-1.59567800
H	4.40455000	7.23510100	0.02066400	H	3.17175500	-5.94815100	-1.01296200
H	4.69835400	5.62079500	-0.62715900	H	2.05219300	-5.42471300	1.17518200
H	3.01046000	6.23985700	1.85699200	H	1.66230900	-3.81794100	0.58972100
H	3.32903900	4.63055100	1.22186000	H	-0.82300100	-4.24984300	0.90552300
C	-4.31393400	4.37697200	-0.06285800	C	4.31006200	-4.37351000	-0.07108000
C	-5.48718300	4.39644500	-1.05175200	C	5.48672900	-4.39483500	-1.05593200
N	-6.72962200	3.88480800	-0.48790700	N	6.72828900	-3.88744700	-0.48693100
C	-7.66216300	4.69040200	0.07287100	C	7.65318500	-4.69646000	0.08179800
O	-7.54380000	5.91503600	0.14586100	O	7.52921500	-5.92040800	0.15421900
C	-8.89566000	3.98716600	0.61261700	C	8.88486100	-3.99780400	0.63137000
H	-6.87996100	2.87926000	-0.49442900	H	8.96854600	-4.21978500	1.69780600
H	-5.24438600	3.79114000	-1.93045200	H	9.76915800	-4.41025900	0.14020100
H	-4.16034700	3.34961900	0.28846500	H	8.86261000	-2.91690700	0.48655500
H	-4.58447400	4.97430700	0.81455600	H	6.87952600	-2.88225900	-0.48521000
H	-5.67169400	5.41842500	-1.38877700	H	5.24887200	-3.78860500	-1.93538200
H	-8.86962300	2.90675200	0.46476600	H	5.67023400	-5.41710100	-1.39263600
H	-8.98703000	4.20599600	1.67906800	H	4.15474300	-3.34555800	0.27767900
H	-9.77788300	4.39856000	0.11676900	H	4.57873300	-4.96871100	0.80836900
C	-2.51574300	-0.51780000	-1.39704500	C	-3.19632000	-5.67769600	0.92748800
C	-1.25745900	-0.23599300	-0.56833000	C	-4.49543800	-6.18751000	0.29255300
C	0.00322900	-0.01747900	-1.41213200	N	-5.66253200	-6.03591400	1.16033100
C	1.25624400	0.25253600	-0.57182800	C	-6.46544800	-4.94655400	1.14895800
C	2.52135900	0.48752300	-1.40482600	O	-6.28815300	-4.00621500	0.37042700
H	-2.68528200	0.31399400	-2.09264300	C	-7.61032800	-4.94536800	2.14050600
H	-2.34750400	-1.40617300	-2.01971700	H	-5.84691000	-6.75559200	1.84199600
H	-1.08793900	-1.07011400	0.12487800	H	-4.40574600	-7.24711000	0.03747000
H	0.17425800	-0.89808500	-2.04465600	H	-3.00697600	-6.22882700	1.85657700
H	-0.16175400	0.82269100	-2.09900300	H	-3.33140100	-4.62710800	1.20612900
H	2.36036300	1.34355800	-2.07309200	H	-4.70433600	-5.64103300	-0.62838000
H	2.69311700	-0.37903900	-2.05593800	H	-7.65750200	-5.84813100	2.75131900
H	1.42417600	-0.59307600	0.10745400	H	-7.50724200	-4.07803100	2.79614800
H	1.07977500	1.12589300	0.06931000	H	-8.54886400	-4.83697600	1.59299800
H	-1.43005100	0.64842300	0.05829500				
C	3.76860300	0.73432500	-0.55009300				
C	5.02456000	0.98827200	-1.39314200				
N	6.21868900	1.22153800	-0.58766800				
C	7.06551600	0.23448200	-0.23525600				
O	6.91002400	-0.94211100	-0.58595900				
C	8.25033500	0.64555900	0.61653700				
H	8.24168700	0.06133200	1.53938600				
H	9.17010600	0.40128200	0.08007500				
H	8.24985800	1.70831000	0.86083700				
H	6.37507600	2.16106600	-0.23171300				
H	4.87863300	1.86409400	-2.03181700				
H	5.22214400	0.13107200	-2.03929100				
H	3.60210100	1.59439700	0.10917600				
H	3.95091000	-0.12965800	0.09824100				

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Gibbs Free Energy= -2312.870467

C	-2.54308600	-0.39554200	1.37516000	C	-3.50476500	-5.79311800	-0.66278300
C	-1.24397800	-0.36250100	0.56235000	C	-4.80615800	-5.90630600	0.14055800
C	0.02265000	-0.26185600	1.41947300	N	-6.00691200	-5.79713100	-0.68527200
C	1.31263800	-0.26111600	0.59182500	C	-6.70799400	-4.64888300	-0.84160800
C	2.59081200	-0.17451500	1.43347800	O	-6.39633400	-3.60281100	-0.26810900
H	-2.50634600	-1.23555300	2.08129000	C	-7.91157600	-4.71760900	-1.75847700
H	-2.61344900	0.51335200	1.98593700	H	-8.07748900	-5.70780900	-2.18540300
H	-1.27629700	0.48343500	-0.13581600	H	-7.77695600	-3.99886800	-2.56961000
H	-0.02051600	0.65036700	2.02797000	H	-4.85978100	-5.11240000	0.88645700
H	0.04773500	-1.09973800	2.12852400	H	-3.50912000	-4.84242400	-1.20670100
H	2.60491100	-1.00122300	2.15594300	H	-3.47424100	-6.58820800	-1.41782300
H	2.57387100	0.74853700	2.02659200	H	-6.30335500	-6.60862200	-1.20528300
H	1.28889700	0.57815000	-0.11466400	H	-8.79875200	-4.41955100	-1.19596300
H	1.34693400	-1.17166900	-0.02064200	H	-4.84535700	-6.86352800	0.66878100
H	-1.18679400	-1.26591800	-0.05893300	C	-2.83440900	5.05603300	0.64825900
C	3.86839200	-0.21677200	0.58888300	C	-1.56811100	4.74507300	-0.15807100
C	5.14462600	-0.13287200	1.43549400	C	-0.27405400	5.18961900	0.53331100
N	6.36436100	-0.23750500	0.64168400	C	0.99414400	4.82896000	-0.24882300
C	7.01733100	0.83581000	0.15437200	C	2.29081300	5.24864900	0.45345500
O	6.65505500	1.99902300	0.37035300	H	-2.75504600	4.58351100	1.63647200
C	8.24928900	0.54293800	-0.67980400	H	-2.89264300	6.13648100	0.83118300
H	8.10373600	0.95411200	-1.68146200	H	-1.63745300	5.22534300	-1.14238400
H	9.10540500	1.05436700	-0.23454800	H	-0.30406200	6.27442500	0.69693100
H	8.46751600	-0.52276800	-0.75841600	H	-0.22363700	4.73317500	1.53072000
H	6.68526500	-1.17066900	0.39783300	H	2.31525000	4.80560900	1.45797200
H	5.15995900	-0.94081800	2.17257200	H	2.28780300	6.33620300	0.59989800
H	5.17751000	0.81506400	1.97527500	H	0.95368000	5.29422000	-1.24184400
H	3.89176200	-1.14349000	0.00361600	H	1.01365000	3.74475900	-0.42143000
H	3.86782800	0.61005200	-0.12949900	H	-1.52131700	3.66483500	-0.34936200
C	-3.79458700	-0.52207600	0.50051100	C	3.55561900	4.84141200	-0.30975400
C	-5.08982400	-0.58296800	1.31951900	C	4.84319500	5.25141000	0.41765100
N	-6.27770100	-0.75963300	0.49128200	N	6.05574100	4.81905400	-0.26559700
C	-7.06220100	0.26459900	0.10109400	C	6.73983800	5.61590400	-1.11969600
O	-6.85879900	1.43683400	0.44028900	O	6.41049400	6.77466200	-1.37891900
C	-8.24065000	-0.09866100	-0.78127100	C	7.97237700	4.99231400	-1.75266300
H	-8.28431700	-1.16217900	-1.01874500	H	7.84911900	4.99542400	-2.83828000
H	-8.17786000	0.47580100	-1.70806100	H	8.83891900	5.61500200	-1.51936100
H	-5.21956400	0.33628900	1.89259000	H	8.15866900	3.97263900	-1.41291400
H	-3.85371500	0.32603700	-0.19046800	H	6.36874000	3.86320200	-0.11621400
H	-3.72290300	-1.42593300	-0.11589200	H	4.85477100	4.82134500	1.42394700
H	-6.47396100	-1.69678500	0.14971000	H	4.88703200	6.33768400	0.51613400
H	-9.16311200	0.19343100	-0.27406900	H	3.56281000	3.75494000	-0.45811300
H	-5.04745800	-1.41750300	2.02586200	H	3.55324500	5.29689500	-1.30595700
C	-2.25950100	-5.87669100	0.22716300	C	-4.12297100	4.58589200	-0.03479600
C	-0.94573900	-5.75509100	-0.55408400	C	-5.37204800	4.84595700	0.81747400
C	0.30119300	-5.79513500	0.33715200	N	-6.60100000	4.36832000	0.19751900
C	1.61379600	-5.65219600	-0.44206900	C	-7.46150400	5.18490700	-0.45530300
C	2.85993400	-5.66287400	0.45134400	O	-7.29282000	6.40020700	-0.56947900
H	-2.26669600	-6.82537100	0.77930000	C	-8.68409200	4.50489500	-1.04825200
H	-2.30398400	-5.08293300	0.98341500	H	-8.70932500	3.43077000	-0.85982300
H	-0.95148400	-4.81733400	-1.12393600	H	-8.69806900	4.68481500	-2.12572100
H	0.23598700	-4.99319200	1.08353500	H	-5.48948900	5.91604400	0.99597800
H	0.31443000	-6.73634100	0.90177300	H	-4.24155700	5.09281200	-0.99891700
H	2.89079700	-6.60149200	1.01960200	H	-4.05634400	3.51234100	-0.24857800
H	2.77830700	-4.85905300	1.19377900	H	-6.79155900	3.37015300	0.22966700
H	1.59184400	-4.71815800	-1.01758300	H	-9.57990500	4.96672700	-0.62695500
H	1.68899000	-6.46231300	-1.17872800	H	-5.26732400	4.35226100	1.78922600
H	-0.88850700	-6.56214100	-1.29566400				
C	4.16733000	-5.49665200	-0.33115600				
C	5.40030600	-5.49301300	0.58062100				
N	6.65704300	-5.33689100	-0.14891800				
C	7.28065600	-4.14751500	-0.32306100				
O	6.84226200	-3.09799100	0.15313700				
C	8.56279900	-4.17420400	-1.12911900				
H	8.46119700	-3.49099500	-1.97475200				
H	9.37878400	-3.80708100	-0.50292200				
H	8.82116500	-5.16627600	-1.50257300				
H	7.05569400	-6.15150000	-0.58960800				
H	5.45566100	-6.42561900	1.14962300				
H	5.34009400	-4.67074100	1.29471700				
H	4.26338600	-6.30556300	-1.06570300				
H	4.14584300	-4.55896300	-0.89671900				