

Supporting Information

Mechanistic Insights into Ruthenium-Catalyzed Production of H₂ and CO₂ from Methanol and Water: A DFT Study

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1. Computational details

Experimental structures with the bis(2-(diisopropylphosphino)ethyl)amine (HPNP) and 2-(di-tertbutylphosphinomethyl)-6-(di-ethylaminomethyl)pyridine (PNN) ligands were employed without any simplification in calculations. All DFT calculations were performed using the Gaussian 09 suite of *ab initio* programs for a hybriide meta-GGA density functional M06 in conjunction with all-electron 6-31++G(d,p) basis set for H, C, N O and P atoms. Stuttgart relativistic effective core potential basis sets were used for Ru (ECP28MWB) ((8s7p6d2f1g) ->[6s5p3d2f1g]). The reliability of such computational method had been evaluated in our previous theoretical study of the dehydrogenation of ethanol catalyzed by the same aliphatic PNP piner ruthenium complex.¹

All structures studied in this paper were fully optimized with solvent corrections using the integral equation formalism polarizable continuum model (IEFPCM)² with radii and cavity-dispersion-solvent-structure terms in Truhlar and co-workers' SMD solvation model³ for methanol ($\epsilon = 32.613$). An ultrafine integration grid (99,590) was used for numerical integrations. The ground states of intermediates and transition states were confirmed as singlets through comparison with the optimized high-spin analogs. Thermal corrections were calculated within the harmonic potential approximation on optimized structures under T = 298.15 K and 1 atm pressure. Unless otherwise noted, the energies reported in the text are solvent corrected free energies. Calculating the harmonic vibrational frequencies for optimized structures and noting the number of imaginary frequencies (IFs) confirmed the nature of all intermediates (no IF) and transition state structures (only one IF). The latter were also confirmed to connect reactants and products by intrinsic reaction coordinate (IRC) calculations. The 3D molecular structure figures displayed in this paper were drawn by using the *JIMP2* molecular visualizing and manipulating program.⁴

2. Solvent corrected absolute free energies (Hartree) and Cartesian coordinates (Ångström) of all optimized geometric structures

H₂

G_{solv} = -1.170815

H	0.00000000	0.00000000	0.37170100
H	0.00000000	0.00000000	-0.37170100

CH₃OH

G_{solv} = -115.640898

O	-0.74756000	0.12416000	0.00000000
C	0.66554600	-0.02004400	0.00000000
H	1.01881300	-0.55162800	-0.89376000
H	1.09637300	0.98549100	0.00000000
H	1.01881300	-0.55162800	0.89376000
H	-1.14679600	-0.75525000	0.00000000

H₂O

G_{solv} = -76.407764

O	0.00000000	0.00000000	0.11791000
H	0.00000000	0.76431100	-0.47164000
H	0.00000000	-0.76431100	-0.47164000

CO₂

G_{solv} = -188.510114

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16436000
O	0.00000000	0.00000000	-1.16436000

HCOOH

G_{solv} = -189.679479

H	-0.10146000	1.50193400	0.00002300
C	-0.12351500	0.40240000	0.00000900
O	1.10751000	-0.09156000	-0.00001000
O	-1.13615200	-0.26462100	0.00000300
H	1.07168600	-1.06689000	-0.00002900

H₂CO

G_{solv} = -114.440442

C	0.00000000	0.00000000	-0.53368100
O	0.00000000	0.00000000	0.67917800
H	0.00000000	0.94220500	-1.11566700
H	0.00000000	-0.94220500	-1.11566700

H₂COOH⁻

G_{solv} = -190.370880

C	-0.14273500	0.48314100	0.04834800
O	-1.17665100	-0.35543700	-0.03702700
H	-0.09475000	1.25029800	-0.75934500
H	-0.08855800	1.03061700	1.02108900
O	1.15987500	-0.18071600	-0.10143700
H	1.17393400	-0.89053900	0.55588300

CH₃O⁻

G_{solv} = -154.374322

O	-0.00009200	0.81112800	0.00000000
C	-0.00009200	-0.57076600	0.00000000
H	0.51100500	-1.02124300	0.88390400
H	-1.02071600	-1.02194700	0.00000000
H	0.51100500	-1.02124300	-0.88390400

HCO₂⁻

G_{solv} = -189.236735

H	-0.00006000	1.45832500	0.00002900
C	-0.00006600	0.33955000	-0.00001500
O	1.12617700	-0.21845900	0.00000400
O	-1.12612000	-0.21849400	0.00000400

OH⁻

G_{solv} = -75.917828

O	0.00000000	0.00000000	0.10696300
H	0.00000000	0.00000000	-0.85570500

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G_{solv} = -1576.719638

Ru	0.00000000	0.13085200	-0.12568800
H	-0.00003300	-0.21400800	1.40903000
P	-2.33228100	-0.17519600	-0.20369100
P	2.33227900	-0.17521200	-0.20364500
O	-0.00005500	2.94673700	0.95643800
N	0.00001500	-1.70145900	-1.04534000
C	-2.47272500	-1.76361600	-1.14662500
H	-3.34733500	-2.34939800	-0.83245700
H	-2.62698000	-1.48040900	-2.19759100
C	-1.18399000	-2.55665100	-1.01203300
H	-1.20289400	-3.14777800	-0.07222500
H	-1.13526100	-3.30499200	-1.82566800
C	1.18399100	-2.55669000	-1.01192400
H	1.13529000	-3.30505700	-1.82553700
H	1.20280800	-3.14778400	-0.07209400
C	2.47276700	-1.76370900	-1.14645100
H	2.62717000	-1.48061000	-2.19742300
H	3.34731600	-2.34948800	-0.83210900
C	3.27027900	-0.46016600	1.37701700
H	4.30599300	-0.68791400	1.08037600
C	3.25809000	0.78199700	2.25929900
H	3.78324800	0.57817600	3.20240600
H	2.23007400	1.08029800	2.51075200
H	3.75157600	1.64058800	1.78854400
C	2.70903800	-1.66205200	2.12744700
H	3.26728400	-1.80926300	3.06191800
H	2.78407000	-2.59127400	1.54956900
H	1.65272000	-1.51083500	2.39296900
C	3.36751800	0.98667200	-1.23718000
H	3.01111200	0.75298800	-2.25378900

C	3.06521700	2.45682500	-0.97639000
H	3.67004700	3.08444100	-1.64526900
H	3.29910100	2.75588800	0.05375000
H	2.00992600	2.68978300	-1.16342800
C	4.86121100	0.69445800	-1.17204900
H	5.38925700	1.27752300	-1.93879100
H	5.09060700	-0.36455400	-1.34822300
H	5.28492200	0.97780900	-0.19923300
C	-3.36760100	0.98672500	-1.23710400
H	-3.01130000	0.75305300	-2.25375200
C	-4.86129400	0.69454200	-1.17183600
H	-5.38939600	1.27763900	-1.93851400
H	-5.28490800	0.97787800	-0.19897500
H	-5.09072700	-0.36446200	-1.34801800
C	-3.06524200	2.45687000	-0.97633400
H	-3.67010600	3.08450100	-1.64516900
H	-2.00996000	2.68980400	-1.16345400
H	-3.29904000	2.75594500	0.05382200
C	-3.27022400	-0.46029800	1.37698300
H	-4.30594700	-0.68802300	1.08035700
C	-2.70897300	-1.66224100	2.12731100
H	-3.26718100	-1.80949600	3.06179800
H	-1.65264100	-1.51106300	2.39279800
H	-2.78405200	-2.59142900	1.54938400
C	-3.25801400	0.78179600	2.25936600
H	-3.78316300	0.57790200	3.20246200
H	-3.75149800	1.64043200	1.78869200
H	-2.22999200	1.08006400	2.51083100
C	-0.00000300	1.85688200	0.48857900

TS_{1,2}

G_{solv} = -1692.358673

Ru	-0.00048500	-0.17205300	-0.12532800
H	-0.00118600	-1.29266400	0.97167900
P	2.33370000	0.00997000	0.14575300
P	-2.33473700	0.01406900	0.14245600
O	-0.00268900	-2.42913700	-2.10250800
N	0.00025900	1.45582700	1.28260100
C	2.47078500	1.46006500	1.29469100
H	3.36012100	1.38934500	1.93473700
H	2.59388000	2.34984200	0.66009900
C	1.20324600	1.59032900	2.12271400
H	1.17531900	0.82790600	2.91774200
H	1.19088600	2.57346800	2.62679700
C	-1.20572700	1.59716500	2.11708800
H	-1.19164500	2.58154600	2.61869300
H	-1.18430900	0.83667000	2.91413600
C	-2.47004400	1.46970800	1.28391600
H	-2.58516800	2.35688400	0.64429700
H	-3.36280200	1.40666300	1.91999900
C	-3.28874500	-1.34509600	0.97973700
H	-4.33176900	-0.99484400	1.02245900
C	-3.22187200	-2.64087500	0.18194500
H	-3.79906400	-3.42381200	0.69217900
H	-2.18600300	-2.99858600	0.09544500
H	-3.63017900	-2.53934800	-0.83060700
C	-2.79824500	-1.56610200	2.40558100

H	-3.37238700	-2.37968100	2.86880800
H	-2.92226100	-0.67833000	3.03696300
H	-1.73832700	-1.85724300	2.42524600
C	-3.33596900	0.55397700	-1.33717000
H	-2.97958400	1.58724300	-1.48300800
C	-2.99695300	-0.23080700	-2.59858600
H	-3.57494000	0.16168100	-3.44626800
H	-3.23949200	-1.29742800	-2.50385200
H	-1.93309400	-0.15029400	-2.85506400
C	-4.83694900	0.59107800	-1.08194500
H	-5.34516500	1.08895000	-1.91878700
H	-5.09512500	1.13907100	-0.16646400
H	-5.25604500	-0.42115200	-1.00308500
C	3.33688200	0.55567400	-1.33032000
H	2.99022600	1.59381100	-1.46404400
C	4.83865600	0.57692200	-1.07865000
H	5.34949200	1.07635700	-1.91295700
H	5.24911500	-0.43939500	-1.00762900
H	5.10335900	1.11624300	-0.15981600
C	2.98445200	-0.21071000	-2.59939800
H	3.56665900	0.18218600	-3.44399200
H	1.92119200	-0.11029000	-2.85233100
H	3.21043300	-1.28202000	-2.51654900
C	3.28476400	-1.35429700	0.97755000
H	4.32778200	-1.00458000	1.02440900
C	2.79124600	-1.58303500	2.40108600
H	3.36612900	-2.39731500	2.86216200
H	1.73198600	-1.87668200	2.41677800
H	2.91139700	-0.69782600	3.03686000
C	3.21902300	-2.64515200	0.17183900
H	3.79889500	-3.43002200	0.67601000
H	3.62466400	-2.53643500	-0.84112300
H	2.18368100	-3.00440100	0.08556900
C	-0.00141300	-1.52396500	-1.34482800
C	0.02522200	3.03367200	-1.47936800
H	-0.18432500	1.93108700	-1.56253900
H	0.99715500	3.18444500	-1.99180900
O	0.00827800	3.49770900	-0.17904300
H	0.00669600	2.42230200	0.57738800
H	-0.74599400	3.50572200	-2.11831500

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G_{solv} = -1692.360762

Ru	0.00159100	-0.11367000	-0.14109600
H	0.01599300	-1.46838000	0.67765600
P	2.33831900	-0.00276800	0.17060700
P	-2.33285000	-0.01727700	0.17234300
O	0.01804000	-1.78935100	-2.62670300
N	-0.00208100	1.07371800	1.69864700
C	2.47043000	1.06279800	1.68469900
H	3.36455600	0.82093200	2.27455200
H	2.58161700	2.09874300	1.33312900
C	1.21530400	0.93701000	2.52872000
H	1.17104300	-0.04034400	3.02855500
H	1.20923000	1.70698300	3.31687000
C	-1.21587100	0.92450700	2.53150400
H	-1.21409700	1.69180200	3.32229700

H	-1.16330700	-0.05459400	3.02724500
C	-2.47249400	1.04418000	1.68918800
H	-2.59090600	2.08075000	1.34199300
H	-3.36468900	0.79329600	2.27801700
C	-3.29890700	-1.55425800	0.57168400
H	-4.33527700	-1.21774000	0.73034300
C	-3.25613400	-2.54779200	-0.58202900
H	-3.84332700	-3.44045800	-0.32769300
H	-2.22591200	-2.87605300	-0.78056200
H	-3.66706500	-2.14018700	-1.51298900
C	-2.80357100	-2.20639700	1.85629200
H	-3.39609100	-3.10824700	2.06036000
H	-2.89854300	-1.55029000	2.72982100
H	-1.75220300	-2.51552200	1.77029500
C	-3.31890400	0.93844300	-1.08926300
H	-2.95288900	1.96532000	-0.92504600
C	-2.97695000	0.55298200	-2.52373700
H	-3.53647600	1.19141700	-3.22087100
H	-3.24146200	-0.48819300	-2.75019000
H	-1.90829200	0.68088100	-2.73830800
C	-4.82098100	0.91690600	-0.83814000
H	-5.31803900	1.63924300	-1.49942800
H	-5.07739800	1.18489300	0.19512100
H	-5.25199700	-0.07048300	-1.05158300
C	3.33176400	0.94607500	-1.09006000
H	2.97143600	1.97567400	-0.92773200
C	4.83373100	0.91564900	-0.83980200
H	5.33569900	1.63241500	-1.50343200
H	5.25780300	-0.07543000	-1.05028500
H	5.09229800	1.18475800	0.19265600
C	2.98493100	0.56000400	-2.52320900
H	3.54067600	1.19839200	-3.22336800
H	1.91476800	0.68605900	-2.73236500
H	3.24954000	-0.48121800	-2.74979900
C	3.30145000	-1.54026300	0.57836700
H	4.33867000	-1.20491500	0.73363500
C	2.80899300	-2.18640600	1.86723700
H	3.40144100	-3.08793200	2.07314200
H	1.75727300	-2.49535100	1.78592700
H	2.90739000	-1.52702300	2.73785800
C	3.25571100	-2.53989900	-0.57004100
H	3.84607800	-3.42996300	-0.31384000
H	3.66084900	-2.13640400	-1.50533700
H	2.22535200	-2.87160300	-0.76158300
C	0.01100400	-1.11659500	-1.65972100
C	-0.03198600	2.89410700	-0.89550400
H	-0.30290300	1.76741800	-0.87753000
H	0.93888000	2.93393600	-1.43639600
O	-0.03940800	3.47705300	0.32258300
H	-0.00708400	2.05260800	1.31025500
H	-0.80427100	3.27302300	-1.60209800

TS_{2,3}

G_{solv} = -1692.343985

Ru	-0.01157400	0.21099200	-0.12300000
H	-0.02447300	1.65162500	0.75800800
P	-2.33354500	0.01520100	0.15849000

P	2.31621000	0.06801400	0.15683100
O	-0.04275800	1.58019000	-2.78094400
N	0.00675300	-0.85089800	1.82729000
C	-2.44893100	-0.92032500	1.76132800
H	-3.37110700	-0.68322900	2.30813400
H	-2.48803800	-1.98983400	1.50407700
C	-1.22608400	-0.64858800	2.61775500
H	-1.21656200	0.38640400	2.98402200
H	-1.21633300	-1.31084100	3.49786100
C	1.22152600	-0.58458800	2.62713100
H	1.23074200	-1.23417600	3.51674400
H	1.16414200	0.45423200	2.97791700
C	2.46356800	-0.81653600	1.78677100
H	2.56230200	-1.88874000	1.56183700
H	3.36736100	-0.51478800	2.33191100
C	3.37763300	1.58660200	0.35960800
H	4.40501400	1.21367400	0.49252400
C	3.31278300	2.46715700	-0.88219200
H	3.95447800	3.34891800	-0.75096000
H	2.28811700	2.82704000	-1.05320700
H	3.64433100	1.94973500	-1.79047400
C	2.99780100	2.38681300	1.59840000
H	3.66066600	3.25805000	1.68844000
H	3.09299100	1.80697900	2.52454500
H	1.96683200	2.76097300	1.53305000
C	3.25668900	-1.06924300	-0.98736000
H	2.82677100	-2.04814400	-0.71612500
C	2.95357500	-0.82533800	-2.46053600
H	3.44606200	-1.59399700	-3.07185000
H	3.32516700	0.14947400	-2.80300100
H	1.87778600	-0.86814000	-2.67124200
C	4.75708500	-1.11310400	-0.72783300
H	5.20867800	-1.94005100	-1.29242000
H	4.99908100	-1.26727700	0.33164800
H	5.24895000	-0.18874700	-1.05949800
C	-3.27376200	-1.09627900	-1.01243100
H	-2.85399900	-2.08375400	-0.75923800
C	-4.77596400	-1.13887000	-0.76262200
H	-5.22627600	-1.95335900	-1.34596900
H	-5.26390500	-0.20699600	-1.07856800
H	-5.02397500	-1.31360200	0.29236400
C	-2.95796700	-0.82661400	-2.47853300
H	-3.46600100	-1.56913700	-3.10903000
H	-1.88216900	-0.89313000	-2.68380400
H	-3.30207300	0.16491300	-2.80119700
C	-3.41321500	1.51360300	0.40869800
H	-4.43618100	1.12504600	0.52805700
C	-3.04789600	2.28455100	1.67021300
H	-3.71938200	3.14716200	1.77819100
H	-2.02016000	2.66995600	1.62120400
H	-3.14509900	1.68036900	2.58052600
C	-3.35599900	2.42772600	-0.80939200
H	-4.01356300	3.29476300	-0.65972500
H	-3.67310000	1.92846700	-1.73299700
H	-2.33635200	2.80855900	-0.96499600
C	-0.02894200	1.04678900	-1.72514400
C	0.06951300	-3.31116800	-0.57896000

H	0.01337600	-1.36757900	-0.83886800
H	-0.95238000	-3.29025100	-1.00003700
O	0.27468300	-3.58727400	0.60411500
H	0.03564400	-1.84509400	1.56652000
H	0.89076300	-3.26992600	-1.31801200

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G_{solv} = -1692.346062

Ru	0.01220700	-0.21586800	-0.12110000
H	0.02467500	-1.64590000	0.77983100
P	2.33355400	-0.01374000	0.15760700
P	-2.31571100	-0.06791300	0.15681200
O	0.04784400	-1.61637600	-2.76267000
N	-0.00642700	0.86980700	1.81671200
C	2.44851900	0.94140800	1.74886500
H	3.37167500	0.71335400	2.29779100
H	2.48455000	2.00779100	1.47843000
C	1.22669200	0.67745200	2.60904100
H	1.21838700	-0.35346200	2.98653400
H	1.21632000	1.34951700	3.48167500
C	-1.22085700	0.61223300	2.61956200
H	-1.22995900	1.27143000	3.50208500
H	-1.16341500	-0.42276800	2.98125900
C	-2.46274700	0.83527400	1.77665300
H	-2.56058400	1.90507200	1.54002800
H	-3.36671500	0.54030700	2.32522700
C	-3.37869800	-1.58305800	0.37690600
H	-4.40537800	-1.20730600	0.50720700
C	-3.31641900	-2.47582600	-0.85629600
H	-3.95607200	-3.35744400	-0.71442900
H	-2.29161500	-2.83543500	-1.02739200
H	-3.65204600	-1.96786700	-1.76838200
C	-2.99886400	-2.37142900	1.62331400
H	-3.66502700	-3.23893000	1.72440600
H	-3.08946900	-1.78132800	2.54346500
H	-1.96953100	-2.75026400	1.55942200
C	-3.25647100	1.05656900	-1.00001500
H	-2.82599500	2.03833500	-0.74016700
C	-2.95430100	0.79601100	-2.47057300
H	-3.44551100	1.55886400	-3.09011600
H	-3.32776000	-0.18185100	-2.80214300
H	-1.87846600	0.83434300	-2.68214500
C	-4.75676400	1.10453600	-0.74036300
H	-5.20791600	1.92487600	-1.31484900
H	-4.99818400	1.27189500	0.31724700
H	-5.24961800	0.17659700	-1.06038900
C	3.27192400	1.08492800	-1.02700200
H	2.84865600	2.07436800	-0.78732900
C	4.77372400	1.13553900	-0.77624700
H	5.22215700	1.94320300	-1.37043900
H	5.26498800	0.20090300	-1.07862900
H	5.02000900	1.32566100	0.27650000
C	2.95870200	0.79551800	-2.48988300
H	3.46315300	1.53305800	-3.12903500
H	1.88266400	0.85354900	-2.69671900
H	3.30848500	-0.19786900	-2.80034800

C	3.41516300	-1.50788300	0.42497900
H	4.43818100	-1.11729900	0.53690700
C	3.05362900	-2.26334800	1.69703400
H	3.72604600	-3.12406900	1.81396300
H	2.02606000	-2.65001000	1.65534000
H	3.15289900	-1.64788900	2.59952400
C	3.35520200	-2.43764400	-0.78113000
H	4.01550400	-3.30117000	-0.62334000
H	3.66707400	-1.94978000	-1.71255400
H	2.33576100	-2.82282100	-0.92739900
C	0.03165500	-1.07089900	-1.71298600
C	-0.07259900	3.32826900	-0.60550100
H	-0.01219700	1.35170900	-0.85421100
H	0.95154600	3.29810900	-1.02088300
O	-0.28296600	3.60796300	0.57427800
H	-0.03567200	1.86074400	1.54499600
H	-0.89140800	3.27551400	-1.34685100

4

G_{solv} = -1577.909396

Ru	0.00435900	-0.20213400	0.00337500
H	0.02339900	0.86765700	1.33013100
H	-0.04551700	-1.06392200	-1.47501900
P	2.34916200	-0.00195100	-0.06788500
P	-2.29764000	0.16352300	-0.24369800
O	-0.13041700	-2.65895300	1.69846400
N	0.11534900	1.60846500	-1.30026600
H	0.11936500	1.22008500	-2.24629900
C	2.56622700	1.43397500	-1.22458100
H	3.50256700	1.97539600	-1.03591700
H	2.63108500	1.01481500	-2.24012400
C	1.37255900	2.36698800	-1.13795400
H	1.32828100	2.86716900	-0.16153900
H	1.43881500	3.14975900	-1.91010600
C	-1.07648200	2.47562800	-1.18915900
H	-1.03026700	3.27352700	-1.94701100
H	-1.03929800	2.95369900	-0.20137600
C	-2.34079200	1.65283800	-1.35767300
H	-2.39974200	1.27569900	-2.38947200
H	-3.23467600	2.26551900	-1.18337000
C	-3.36538600	0.63318000	1.21188000
H	-4.38760200	0.72310400	0.81365600
C	-3.32838800	-0.45518300	2.27788800
H	-3.99045700	-0.18895000	3.11303700
H	-2.31290200	-0.56775400	2.68404800
H	-3.64958500	-1.43401400	1.90213300
C	-2.97028000	1.97550600	1.81329700
H	-3.63285300	2.20481700	2.65900100
H	-3.05656000	2.80299100	1.09855900
H	-1.94060100	1.95583200	2.19563200
C	-3.29368600	-1.07865000	-1.22241100
H	-2.82554100	-0.99033600	-2.21674600
C	-3.09914100	-2.51425800	-0.75038000
H	-3.60884800	-3.20213000	-1.43884100
H	-3.52315900	-2.68270300	0.24815800
H	-2.03955500	-2.79610300	-0.72209700
C	-4.77236300	-0.73434800	-1.34765700

H	-5.24396700	-1.38721200	-2.09458100
H	-4.94186900	0.30344200	-1.66280500
H	-5.30323700	-0.89293800	-0.39906700
C	3.47377200	-1.32672600	-0.76232500
H	3.67187100	-1.97539600	0.10615500
C	4.80121400	-0.77607600	-1.27662700
H	5.48629600	-1.60540000	-1.49807300
H	5.30727100	-0.11790500	-0.56012400
H	4.66083300	-0.21478300	-2.21020300
C	2.79705600	-2.16509100	-1.83597700
H	3.49763700	-2.92225000	-2.21421000
H	2.48583500	-1.55024300	-2.69293100
H	1.90899900	-2.68327100	-1.45686400
C	3.27746000	0.44802500	1.48828500
H	4.34415900	0.37715200	1.22348200
C	2.99918500	1.86339700	1.97225900
H	3.57550600	2.06005400	2.88656500
H	1.93695000	2.00049900	2.21671700
H	3.28432800	2.62476300	1.23582800
C	2.97166500	-0.56496700	2.58603100
H	3.61635600	-0.38331900	3.45650500
H	3.13291500	-1.60332100	2.26696600
H	1.92870300	-0.47479400	2.91999500
C	-0.07990100	-1.68366000	1.02836500

TS_{4,5}

G_{solv} = -1577.862408

Ru	0.00000100	-0.13996700	-0.08857300
H	-0.00000700	0.45659900	1.42815400
P	2.33350800	0.17167100	-0.19002500
P	-2.33350100	0.17169100	-0.19006800
O	-0.00003800	-2.85942600	1.19093100
N	0.00002000	1.79785600	-1.11717300
C	2.46087800	1.77062800	-1.12197100
H	3.35865900	2.33601100	-0.83824900
H	2.56050400	1.50561400	-2.18471400
C	1.19660100	2.58954100	-0.91003000
H	1.20061700	3.01807500	0.11583900
H	1.20779300	3.45557400	-1.60011700
C	-1.19657700	2.58953700	-0.91010700
H	-1.20774400	3.45555200	-1.60021700
H	-1.20064600	3.01809800	0.11575000
C	-2.46083900	1.77060800	-1.12208400
H	-2.56041000	1.50555500	-2.18482300
H	-3.35863800	2.33599600	-0.83842800
C	-3.33692400	0.43071400	1.35497200
H	-4.36816300	0.60496500	1.01019400
C	-3.30207800	-0.80056400	2.25164400
H	-3.90123800	-0.62224700	3.15484400
H	-2.27499300	-1.02248100	2.57526100
H	-3.70296000	-1.69614000	1.76235900
C	-2.87611000	1.66251300	2.12346900
H	-3.50368400	1.79253700	3.01549800
H	-2.94968700	2.58385300	1.53300800
H	-1.83616000	1.55758400	2.46277400
C	-3.30517100	-1.00216200	-1.26813000
H	-2.91107300	-0.75618600	-2.26812200

C	-2.98599500	-2.46760800	-0.99831600
H	-3.55177400	-3.10363700	-1.69273200
H	-3.25858000	-2.77284000	0.02039400
H	-1.92020700	-2.68369700	-1.14145300
C	-4.80621500	-0.74267900	-1.26185800
H	-5.28912100	-1.33236700	-2.05271000
H	-5.05233500	0.31204700	-1.44046800
H	-5.26283300	-1.04328600	-0.30925100
C	3.30518200	-1.00212200	-1.26814500
H	2.91101800	-0.75614400	-2.26811000
C	4.80621400	-0.74256100	-1.26195500
H	5.28910000	-1.33219200	-2.05286100
H	5.26291500	-1.04318000	-0.30939300
H	5.05226700	0.31218400	-1.44054100
C	2.98609500	-2.46759000	-0.99834800
H	3.55186400	-3.10357400	-1.69281200
H	1.92031000	-2.68372900	-1.14142600
H	3.25876400	-2.77283000	0.02033700
C	3.33689800	0.43060600	1.35505200
H	4.36816200	0.60479000	1.01031400
C	2.87613700	1.66242900	2.12354200
H	3.50369000	1.79241100	3.01559100
H	1.83617000	1.55756100	2.46281500
H	2.94978500	2.58376700	1.53308800
C	3.30192500	-0.80067500	2.25171800
H	3.90110500	-0.62242200	3.15491800
H	3.70270400	-1.69629700	1.76243600
H	2.27481600	-1.02247700	2.57533400
C	-0.00002200	-1.80182600	0.66648900
H	0.00002600	0.51850400	-1.85648400
H	0.00001300	-0.41572900	-1.96026200

5

G_{solv} = -1577.881073

Ru	0.00000200	-0.17555400	-0.22907400
H	0.00000700	0.54198200	1.21763000
P	2.32717800	0.18676400	-0.20182500
P	-2.32718200	0.18677900	-0.20182400
O	0.00019700	-2.82521300	1.20708200
N	0.00000500	1.78529000	-1.12626500
C	2.46381000	1.82006900	-1.05516100
H	3.34505200	2.38453100	-0.72068000
H	2.59424100	1.59916800	-2.12503400
C	1.17167700	2.59161400	-0.83847600
H	1.15387700	2.98332000	0.20614100
H	1.18602100	3.49526300	-1.48229500
C	-1.17166400	2.59162500	-0.83849100
H	-1.18600400	3.49526400	-1.48232500
H	-1.15386000	2.98334700	0.20611900
C	-2.46379800	1.82008000	-1.05516900
H	-2.59421500	1.59916600	-2.12504100
H	-3.34504500	2.38454800	-0.72071000
C	-3.20521500	0.38535200	1.42668000
H	-4.26599400	0.53160700	1.17039600
C	-3.05840400	-0.86534900	2.28466300
H	-3.62737000	-0.74877500	3.21685800
H	-2.00664100	-1.02961000	2.55825200

H	-3.42137900	-1.77251600	1.78699800
C	-2.72986800	1.61180600	2.19485700
H	-3.28586000	1.68639100	3.13947100
H	-2.89042900	2.54634600	1.64457900
H	-1.66189600	1.54123600	2.44507900
C	-3.39691200	-0.92917700	-1.24709800
H	-3.03520500	-0.67985600	-2.25896200
C	-3.13817200	-2.41325200	-1.01914100
H	-3.69642100	-3.00353500	-1.75846700
H	-3.46953500	-2.74259500	-0.02580400
H	-2.07634200	-2.66853900	-1.12275300
C	-4.88374100	-0.60725600	-1.16949100
H	-5.42501700	-1.15410200	-1.95342400
H	-5.09271300	0.46137600	-1.30832500
H	-5.31003900	-0.91604900	-0.20536200
C	3.39690200	-0.92919200	-1.24710800
H	3.03524200	-0.67980500	-2.25897300
C	4.88374300	-0.60734300	-1.16943500
H	5.42502100	-1.15417000	-1.95338000
H	5.30998800	-0.91621400	-0.20530900
H	5.09277000	0.46128700	-1.30820100
C	3.13809700	-2.41327000	-1.01925000
H	3.69632000	-3.00352800	-1.75861400
H	2.07625600	-2.66850400	-1.12287900
H	3.46943400	-2.74268800	-0.02593000
C	3.20518700	0.38534900	1.42668900
H	4.26599200	0.53146500	1.17043100
C	2.72995300	1.61191600	2.19475400
H	3.28590500	1.68649800	3.13939100
H	1.66195700	1.54150000	2.44492300
H	2.89066400	2.54639500	1.64441500
C	3.05820600	-0.86526300	2.28477200
H	3.62711000	-0.74864900	3.21699900
H	3.42114200	-1.77250700	1.78721800
H	2.00640500	-1.02940200	2.55829500
C	0.00002100	-1.80863000	0.60870800
H	0.41366500	-0.80911600	-1.92167000
H	-0.41368200	-0.80910200	-1.92166700

TS_{5,1}

G_{solv} = -1577.882537

Ru	-0.00000500	-0.19363600	-0.22287100
H	-0.00015700	0.45843200	1.20910200
P	2.32784400	0.17829400	-0.20429900
P	-2.32788500	0.17821500	-0.20428200
O	0.00122200	-2.84609100	1.20349000
N	0.00012300	1.74466500	-1.13049500
C	2.46514000	1.78602400	-1.11022800
H	3.34705200	2.36032700	-0.79397000
H	2.59912000	1.52942600	-2.17167000
C	1.17580200	2.57219500	-0.92859000
H	1.17245400	3.04645300	0.07999600
H	1.17523200	3.42129400	-1.64264400
C	-1.17573200	2.57205400	-0.92894500
H	-1.17519500	3.42101600	-1.64316100
H	-1.17248600	3.04655200	0.07951600
C	-2.46502000	1.78577300	-1.11053100

H	-2.59881600	1.52886100	-2.17192100
H	-3.34697400	2.36019800	-0.79463200
C	-3.19572200	0.46126400	1.41862400
H	-4.24915600	0.64922000	1.15875600
C	-3.10803100	-0.76384300	2.31964000
H	-3.65425400	-0.58033300	3.25488200
H	-2.06359100	-0.98120900	2.58457500
H	-3.53467000	-1.66404300	1.86175300
C	-2.65970000	1.69013500	2.14302600
H	-3.19419800	1.81550700	3.09457900
H	-2.79395800	2.61333700	1.56731300
H	-1.59043000	1.58571400	2.37745900
C	-3.42716000	-0.95916600	-1.19760100
H	-3.09761000	-0.73442600	-2.22598500
C	-3.15157200	-2.43565700	-0.93917800
H	-3.75031100	-3.05079000	-1.62477600
H	-3.41985200	-2.73493900	0.08251400
H	-2.09611400	-2.69009000	-1.09686800
C	-4.91203300	-0.63918400	-1.08515500
H	-5.47614600	-1.21484900	-1.83160300
H	-5.12753900	0.42355100	-1.25644100
H	-5.30762500	-0.91320000	-0.09776900
C	3.42672800	-0.95916400	-1.19798200
H	3.09769400	-0.73354700	-2.22633500
C	4.91177000	-0.64017800	-1.08481300
H	5.47568200	-1.21500100	-1.83206100
H	5.30693800	-0.91587500	-0.09772300
H	5.12788200	0.42270100	-1.25443200
C	3.15007000	-2.43564900	-0.94055500
H	3.75019100	-3.05080000	-1.62493800
H	2.09490300	-2.68972400	-1.10069800
H	3.41593300	-2.73536300	0.08163700
C	3.19606900	0.46089500	1.41841800
H	4.24966900	0.64785500	1.15855800
C	2.66093500	1.69032500	2.14251300
H	3.19621900	1.81622700	3.09355300
H	1.59185100	1.58616700	2.37792800
H	2.79477000	2.61313800	1.56607400
C	3.10731000	-0.76385700	2.31971400
H	3.65542200	-0.58141000	3.25405700
H	3.53110800	-1.66514500	1.86130100
H	2.06283400	-0.97890100	2.58632200
C	-0.00001500	-1.82931000	0.59565100
H	0.38294700	-1.02199200	-2.31216800
H	-0.38166700	-1.02184400	-2.31355100

6_M

G_{solv} = -1693.544392

Ru	0.00234400	-0.25906800	-0.21876200
H	0.00777100	-1.64724500	0.74968500
H	-0.00404900	1.27200900	-1.01272900
P	2.34474500	-0.25785400	-0.00184900
P	-2.30069200	-0.05699500	0.18293800
O	-0.15155000	-1.75908600	-2.79867300
N	0.11830700	0.88120000	1.69996400
H	0.09880100	1.86628600	1.41697700
C	2.57567500	0.79294500	1.50995400

H	3.50905600	0.55532300	2.03709600
H	2.65552300	1.83358100	1.15989300
C	1.38078000	0.65633600	2.43553100
H	1.33073900	-0.35147700	2.86790500
H	1.45771000	1.37048300	3.27052300
C	-1.06292100	0.66691700	2.56476900
H	-1.01674400	1.34405100	3.43242000
H	-1.00601600	-0.36172600	2.94423500
C	-2.34442700	0.89172000	1.78249300
H	-2.44182300	1.95612300	1.52454000
H	-3.22082900	0.62492300	2.38743400
C	-3.35381500	-1.56103400	0.50782500
H	-4.37589100	-1.17761600	0.65006300
C	-3.32785200	-2.50927400	-0.68502300
H	-3.98848900	-3.36687600	-0.49873500
H	-2.31374300	-2.90150500	-0.84803800
H	-3.65824500	-2.03462000	-1.61664300
C	-2.94380300	-2.29773800	1.77638300
H	-3.61076500	-3.15699600	1.92985500
H	-3.00965600	-1.67040100	2.67368900
H	-1.91832300	-2.68461200	1.70222300
C	-3.31183600	1.03441300	-0.94748700
H	-2.84952600	2.01899800	-0.76600100
C	-3.12881400	0.70807300	-2.42458700
H	-3.64501700	1.46137100	-3.03526400
H	-3.55364800	-0.26902500	-2.68867400
H	-2.07219900	0.70967300	-2.71855100
C	-4.78766700	1.11656700	-0.57911300
H	-5.26877100	1.92463800	-1.14667300
H	-4.94817000	1.32269600	0.48706000
H	-5.31725800	0.18715900	-0.82923700
C	3.50145000	0.49037100	-1.26817600
H	3.69706600	-0.34384300	-1.96089600
C	4.82647200	0.94797800	-0.66523800
H	5.52932000	1.20889900	-1.46765600
H	5.30937200	0.18381000	-0.04420100
H	4.68964200	1.84709500	-0.04950900
C	2.86054200	1.62171100	-2.05731500
H	3.57883700	2.01941200	-2.78740300
H	2.56500800	2.45450600	-1.40203400
H	1.96921300	1.29223100	-2.60329300
C	3.22332100	-1.86895200	0.34192900
H	4.29772300	-1.63451200	0.28103300
C	2.93776700	-2.43810400	1.72387000
H	3.47966800	-3.38560100	1.84891900
H	1.86825400	-2.65184100	1.85647800
H	3.25933700	-1.76930600	2.53164300
C	2.87715100	-2.88647700	-0.74004900
H	3.48978400	-3.78969900	-0.61805200
H	3.04896000	-2.50644400	-1.75593400
H	1.82261300	-3.18738000	-0.66906300
C	-0.09244800	-1.17091200	-1.77348600
C	0.61581900	4.27738400	0.06566600
H	0.49041600	5.19070600	0.65579800
H	0.87464300	4.56188700	-0.96381700
O	-0.60271600	3.55538600	0.12184900
H	-0.49320900	2.73346500	-0.40304100

H	1.45259100	3.70277200	0.49435600
6w			
$G_{\text{solv}} = -1654.309473$			
Ru	-0.01541600	0.13531200	-0.21613200
H	-0.04337800	1.53858000	0.73596500
H	0.02909800	-1.39936000	-0.99337600
P	-2.35833100	0.07034600	-0.00059600
P	2.29016300	-0.04360700	0.17824800
O	0.09524400	1.60587900	-2.81535400
N	-0.10797000	-0.98379000	1.71750700
H	-0.08076200	-1.97219900	1.44415800
C	-2.55741400	-0.97489300	1.51990100
H	-3.50448400	-0.77337500	2.03732500
H	-2.58456200	-2.02240200	1.18195600
C	-1.37407300	-0.77492800	2.44880500
H	-1.35547200	0.24420100	2.85655800
H	-1.43157200	-1.47069000	3.30076100
C	1.07110900	-0.74360400	2.57532100
H	1.03489000	-1.40633800	3.45455800
H	1.00888600	0.29102500	2.93757100
C	2.34709000	-0.97497300	1.78711000
H	2.43879000	-2.04237100	1.53696200
H	3.22992800	-0.70618900	2.38161700
C	3.33889000	1.46907800	0.47415600
H	4.36623700	1.09500400	0.60312100
C	3.28561200	2.40666800	-0.72654200
H	3.94895200	3.26664400	-0.56219700
H	2.26761300	2.79608000	-0.87048100
H	3.59561300	1.92408900	-1.66127100
C	2.94158500	2.21361600	1.74217400
H	3.60266800	3.08025600	1.87853800
H	3.02527400	1.59475200	2.64380300
H	1.91171000	2.59086000	1.67890100
C	3.29769700	-1.15056200	-0.93881700
H	2.80670200	-2.12356500	-0.76963000
C	3.15469200	-0.81391800	-2.41769300
H	3.63360200	-1.59608700	-3.02234500
H	3.64430300	0.13469100	-2.67308100
H	2.10445200	-0.75028500	-2.72793700
C	4.76340600	-1.26851800	-0.54125000
H	5.23828900	-2.08303900	-1.10489200
H	4.89868200	-1.48474600	0.52632800
H	5.31815800	-0.34948200	-0.77454400
C	-3.48769600	-0.72340300	-1.26477300
H	-3.71291300	0.10098400	-1.96029100
C	-4.79621000	-1.22475800	-0.66049100
H	-5.48807600	-1.51597500	-1.46210500
H	-5.30751400	-0.47374400	-0.04615700
H	-4.62898200	-2.11399500	-0.03812400
C	-2.80715400	-1.83277200	-2.05178800
H	-3.51022200	-2.25501400	-2.78288700
H	-2.48412500	-2.65445700	-1.39592400
H	-1.92698400	-1.47275800	-2.59639000
C	-3.29133900	1.65304100	0.33125500
H	-4.35703300	1.38102800	0.27188600
C	-3.02719200	2.24387500	1.70834600

H	-3.59953600	3.17467800	1.82272100
H	-1.96549900	2.49314900	1.84187500
H	-3.32929900	1.57315300	2.52197800
C	-2.98062200	2.67362800	-0.75828500
H	-3.62672400	3.55438400	-0.64461900
H	-3.13604800	2.28012900	-1.77159200
H	-1.93831400	3.01436900	-0.68739300
C	0.05614900	1.02916700	-1.78250500
O	0.27880900	-3.71489200	0.24321300
H	0.17782300	-2.95939900	-0.37189200
H	-0.41317500	-4.33922200	-0.00940000

TS_{6,7-M}

G_{solv} = -1693.515547

Ru	0.00234400	-0.25906800	-0.21876200
H	0.00777100	-1.64724500	0.74968500
H	-0.00404900	1.27200900	-1.01272900
P	2.34474500	-0.25785400	-0.00184900
P	-2.30069200	-0.05699500	0.18293800
O	-0.15155000	-1.75908600	-2.79867300
N	0.11830700	0.88120000	1.69996400
H	0.09880100	1.86628600	1.41697700
C	2.57567500	0.79294500	1.50995400
H	3.50905600	0.55532300	2.03709600
H	2.65552300	1.83358100	1.15989300
C	1.38078000	0.65633600	2.43553100
H	1.33073900	-0.35147700	2.86790500
H	1.45771000	1.37048300	3.27052300
C	-1.06292100	0.66691700	2.56476900
H	-1.01674400	1.34405100	3.43242000
H	-1.00601600	-0.36172600	2.94423500
C	-2.34442700	0.89172000	1.78249300
H	-2.44182300	1.95612300	1.52454000
H	-3.22082900	0.62492300	2.38743400
C	-3.35381500	-1.56103400	0.50782500
H	-4.37589100	-1.17761600	0.65006300
C	-3.32785200	-2.50927400	-0.68502300
H	-3.98848900	-3.36687600	-0.49873500
H	-2.31374300	-2.90150500	-0.84803800
H	-3.65824500	-2.03462000	-1.61664300
C	-2.94380300	-2.29773800	1.77638300
H	-3.61076500	-3.15699600	1.92985500
H	-3.00965600	-1.67040100	2.67368900
H	-1.91832300	-2.68461200	1.70222300
C	-3.31183600	1.03441300	-0.94748700
H	-2.84952600	2.01899800	-0.76600100
C	-3.12881400	0.70807300	-2.42458700
H	-3.64501700	1.46137100	-3.03526400
H	-3.55364800	-0.26902500	-2.68867400
H	-2.07219900	0.70967300	-2.71855100
C	-4.78766700	1.11656700	-0.57911300
H	-5.26877100	1.92463800	-1.14667300
H	-4.94817000	1.32269600	0.48706000
H	-5.31725800	0.18715900	-0.82923700
C	3.50145000	0.49037100	-1.26817600
H	3.69706600	-0.34384300	-1.96089600
C	4.82647200	0.94797800	-0.66523800

H	5.52932000	1.20889900	-1.46765600
H	5.30937200	0.18381000	-0.04420100
H	4.68964200	1.84709500	-0.04950900
C	2.86054200	1.62171100	-2.05731500
H	3.57883700	2.01941200	-2.78740300
H	2.56500800	2.45450600	-1.40203400
H	1.96921300	1.29223100	-2.60329300
C	3.22332100	-1.86895200	0.34192900
H	4.29772300	-1.63451200	0.28103300
C	2.93776700	-2.43810400	1.72387000
H	3.47966800	-3.38560100	1.84891900
H	1.86825400	-2.65184100	1.85647800
H	3.25933700	-1.76930600	2.53164300
C	2.87715100	-2.88647700	-0.74004900
H	3.48978400	-3.78969900	-0.61805200
H	3.04896000	-2.50644400	-1.75593400
H	1.82261300	-3.18738000	-0.66906300
C	-0.09244800	-1.17091200	-1.77348600
C	0.61581900	4.27738400	0.06566600
H	0.49041600	5.19070600	0.65579800
H	0.87464300	4.56188700	-0.96381700
O	-0.60271600	3.55538600	0.12184900
H	-0.49320900	2.73346500	-0.40304100
H	1.45259100	3.70277200	0.49435600

TS_{6,7-w}

G_{solv} = -1654.282640

Ru	-0.01541600	0.13531200	-0.21613200
H	-0.04337800	1.53858000	0.73596500
H	0.02909800	-1.39936000	-0.99337600
P	-2.35833100	0.07034600	-0.00059600
P	2.29016300	-0.04360700	0.17824800
O	0.09524400	1.60587900	-2.81535400
N	-0.10797000	-0.98379000	1.71750700
H	-0.08076200	-1.97219900	1.44415800
C	-2.55741400	-0.97489300	1.51990100
H	-3.50448400	-0.77337500	2.03732500
H	-2.58456200	-2.02240200	1.18195600
C	-1.37407300	-0.77492800	2.44880500
H	-1.35547200	0.24420100	2.85655800
H	-1.43157200	-1.47069000	3.30076100
C	1.07110900	-0.74360400	2.57532100
H	1.03489000	-1.40633800	3.45455800
H	1.00888600	0.29102500	2.93757100
C	2.34709000	-0.97497300	1.78711000
H	2.43879000	-2.04237100	1.53696200
H	3.22992800	-0.70618900	2.38161700
C	3.33889000	1.46907800	0.47415600
H	4.36623700	1.09500400	0.60312100
C	3.28561200	2.40666800	-0.72654200
H	3.94895200	3.26664400	-0.56219700
H	2.26761300	2.79608000	-0.87048100
H	3.59561300	1.92408900	-1.66127100
C	2.94158500	2.21361600	1.74217400
H	3.60266800	3.08025600	1.87853800
H	3.02527400	1.59475200	2.64380300
H	1.91171000	2.59086000	1.67890100

C	3.29769700	-1.15056200	-0.93881700
H	2.80670200	-2.12356500	-0.76963000
C	3.15469200	-0.81391800	-2.41769300
H	3.63360200	-1.59608700	-3.02234500
H	3.64430300	0.13469100	-2.67308100
H	2.10445200	-0.75028500	-2.72793700
C	4.76340600	-1.26851800	-0.54125000
H	5.23828900	-2.08303900	-1.10489200
H	4.89868200	-1.48474600	0.52632800
H	5.31815800	-0.34948200	-0.77454400
C	-3.48769600	-0.72340300	-1.26477300
H	-3.71291300	0.10098400	-1.96029100
C	-4.79621000	-1.22475800	-0.66049100
H	-5.48807600	-1.51597500	-1.46210500
H	-5.30751400	-0.47374400	-0.04615700
H	-4.62898200	-2.11399500	-0.03812400
C	-2.80715400	-1.83277200	-2.05178800
H	-3.51022200	-2.25501400	-2.78288700
H	-2.48412500	-2.65445700	-1.39592400
H	-1.92698400	-1.47275800	-2.59639000
C	-3.29133900	1.65304100	0.33125500
H	-4.35703300	1.38102800	0.27188600
C	-3.02719200	2.24387500	1.70834600
H	-3.59953600	3.17467800	1.82272100
H	-1.96549900	2.49314900	1.84187500
H	-3.32929900	1.57315300	2.52197800
C	-2.98062200	2.67362800	-0.75828500
H	-3.62672400	3.55438400	-0.64461900
H	-3.13604800	2.28012900	-1.77159200
H	-1.93831400	3.01436900	-0.68739300
C	0.05614900	1.02916700	-1.78250500
O	0.27880900	-3.71489200	0.24321300
H	0.17782300	-2.95939900	-0.37189200
H	-0.41317500	-4.33922200	-0.00940000

7_M

G_{solv} = -1693.522924

Ru	-0.02349600	-0.17992800	-0.28956700
H	-0.07389600	-1.36183400	0.80767200
H	0.44159000	1.21794600	-1.39015600
P	2.31405300	-0.32975700	0.02808700
P	-2.33232200	0.04758500	0.15387500
O	-0.24085700	-2.25902400	-2.44155000
N	0.12587800	1.25997700	1.36470800
H	0.08197500	2.20802900	0.89921000
C	2.59417700	1.05584000	1.21846300
H	3.51359100	0.91611900	1.80232300
H	2.72694200	1.96024000	0.60488900
C	1.39097700	1.21810100	2.12914700
H	1.33036600	0.38517200	2.84301900
H	1.48591700	2.14529600	2.71844200
C	-1.02678500	1.23030900	2.29118300
H	-0.95676800	2.08362800	2.98608800
H	-0.95847500	0.31190600	2.89080300
C	-2.33870300	1.28787600	1.53043600
H	-2.46070700	2.27639500	1.06511600
H	-3.19137900	1.13564700	2.20473000

C	-3.27591500	-1.41883100	0.79748200
H	-4.31519100	-1.07007200	0.90011800
C	-3.22334600	-2.58302800	-0.18442100
H	-3.84519600	-3.40911300	0.18532500
H	-2.19682800	-2.96264500	-0.28477700
H	-3.58584800	-2.31976400	-1.18518100
C	-2.78355200	-1.86058100	2.16978100
H	-3.37643300	-2.72126800	2.50694100
H	-2.88301400	-1.07678900	2.92997500
H	-1.73201600	-2.17932500	2.13726900
C	-3.38828300	0.86255500	-1.14532500
H	-2.94887100	1.87423900	-1.17200000
C	-3.22466600	0.24799900	-2.52958200
H	-3.78209800	0.84456000	-3.26413500
H	-3.61981600	-0.77496100	-2.57499100
H	-2.17592000	0.22173400	-2.85023100
C	-4.85649900	0.97438600	-0.75575700
H	-5.37712800	1.63650100	-1.46018500
H	-4.99713600	1.38727900	0.25138600
H	-5.35651600	-0.00265700	-0.79879400
C	3.52084800	-0.03310700	-1.36009600
H	3.63059400	-1.02449900	-1.82763300
C	4.88497400	0.43049500	-0.85763200
H	5.60447700	0.43078500	-1.68698800
H	5.29588100	-0.21176400	-0.06916200
H	4.83591000	1.45650600	-0.46920500
C	2.97000100	0.93259900	-2.39867900
H	3.71463400	1.09598100	-3.18918500
H	2.74401600	1.91440200	-1.95591100
H	2.05664600	0.55331700	-2.87312500
C	2.98393600	-1.88181300	0.80222500
H	4.07915800	-1.77443400	0.75465900
C	2.57852800	-2.05176900	2.25946800
H	2.98140200	-2.99871400	2.64315300
H	1.48533200	-2.09183800	2.37210600
H	2.96361200	-1.24986400	2.90043500
C	2.56946600	-3.09729200	-0.01959600
H	3.08476600	-3.99232000	0.35296100
H	2.81290500	-2.99733600	-1.08551800
H	1.48882400	-3.27712400	0.06396600
C	-0.15498400	-1.43571100	-1.61025200
C	0.98607800	4.16632700	-0.37873200
H	0.99190100	5.23711000	-0.68212000
H	1.10513400	3.59564600	-1.33105700
O	-0.13278100	3.80709300	0.34490300
H	-0.38917200	1.26689100	-1.36042300
H	1.94513300	4.01990200	0.17325900

7_w

G_{solv} = -1654.289320

Ru	0.00800500	-0.11887300	-0.27688200
H	0.00415800	-1.05349100	1.04156600
H	0.42310900	1.02129000	-1.65066300
P	2.35587200	-0.10346700	0.02358500
P	-2.30739200	0.13399400	0.11733400
O	-0.13244300	-2.59198100	-1.96967700
N	0.11693900	1.63571700	1.04423200

H	0.08929100	2.46454700	0.39127200
C	2.58140100	1.49053000	0.93233700
H	3.50904400	1.50002400	1.51977700
H	2.66705400	2.27569100	0.16565000
C	1.37428400	1.76164200	1.81052700
H	1.33425000	1.05637400	2.65191100
H	1.43793200	2.77668200	2.23576000
C	-1.04553000	1.79029900	1.94431800
H	-0.99731900	2.77768800	2.43259600
H	-0.96789200	1.03011600	2.73437000
C	-2.34816900	1.65172600	1.17879200
H	-2.47470800	2.50614300	0.49851500
H	-3.20853300	1.64411300	1.86060600
C	-3.22514700	-1.16976900	1.07223600
H	-4.26940000	-0.82178700	1.10385700
C	-3.15983300	-2.51911100	0.36794800
H	-3.75832700	-3.25601700	0.91990500
H	-2.12687700	-2.89290600	0.33261800
H	-3.54254500	-2.48700900	-0.65907700
C	-2.71883800	-1.29181900	2.50390400
H	-3.28668900	-2.07528300	3.02325600
H	-2.84054100	-0.36560300	3.07787600
H	-1.65872500	-1.58080700	2.53221900
C	-3.37135900	0.61496400	-1.33302300
H	-2.96217700	1.61085200	-1.57391400
C	-3.17039800	-0.27656700	-2.55213200
H	-3.73722800	0.12873900	-3.40099100
H	-3.53124500	-1.29868400	-2.37989800
H	-2.11751100	-0.33360200	-2.85382900
C	-4.84648700	0.76272800	-0.98412700
H	-5.37809700	1.24348900	-1.81608700
H	-5.00873400	1.37713700	-0.08936100
H	-5.31929100	-0.21480600	-0.81862700
C	3.53040900	-0.01691300	-1.42058100
H	3.67939400	-1.07185800	-1.70020100
C	4.87893700	0.58893100	-1.04339900
H	5.58542200	0.46190900	-1.87410900
H	5.33018900	0.12501400	-0.15791100
H	4.79024000	1.66678800	-0.85397800
C	2.92492700	0.71425700	-2.60988300
H	3.65922900	0.76936900	-3.42451500
H	2.64510500	1.74674400	-2.35256600
H	2.03492000	0.20468600	-2.99808900
C	3.10831600	-1.44909500	1.06324700
H	4.19644100	-1.30397700	0.97353800
C	2.72961700	-1.35764000	2.53462600
H	3.18821600	-2.19227100	3.08163300
H	1.64178500	-1.43253400	2.67585600
H	3.07748300	-0.43000400	3.00458800
C	2.74113900	-2.81622300	0.49631300
H	3.31226900	-3.59940100	1.01202700
H	2.95131900	-2.90775800	-0.57741000
H	1.67412900	-3.02784700	0.65029200
C	-0.08093400	-1.61899600	-1.31633600
O	-0.04786100	3.96451500	-0.41023600
H	-0.40665200	1.07325900	-1.60754500
H	0.49196200	4.07352700	-1.20080600

TS_{7,8-M}

G_{solv} = -1693.521733

Ru	-0.02433500	-0.19601900	-0.29022600
H	-0.07292500	-1.31914200	0.86676800
H	0.44003600	1.15634500	-1.46156100
P	2.30984100	-0.32129700	0.03368600
P	-2.32337200	0.05610000	0.15167200
O	-0.25825700	-2.38824300	-2.34179100
N	0.12526700	1.30383200	1.25569400
H	-0.02839300	2.76616600	0.55474300
C	2.59146100	1.11097500	1.16259900
H	3.50221000	0.98781200	1.76431100
H	2.74024100	1.98527500	0.51027000
C	1.36023400	1.31036000	2.03188300
H	1.33800300	0.52667000	2.81755400
H	1.45731900	2.27169900	2.57773800
C	-0.99417200	1.33765900	2.19076600
H	-0.92327800	2.24125000	2.83050900
H	-0.95817300	0.47382200	2.88869700
C	-2.33087800	1.35638000	1.46636400
H	-2.47011000	2.31957000	0.95430600
H	-3.17318400	1.22764800	2.15916500
C	-3.27211200	-1.37900400	0.85949500
H	-4.31095900	-1.02479700	0.94854900
C	-3.22498800	-2.58603600	-0.06923600
H	-3.85077900	-3.39286600	0.33524900
H	-2.19993400	-2.97377800	-0.15276700
H	-3.58441100	-2.36531700	-1.08125300
C	-2.77965900	-1.76431900	2.24893700
H	-3.37923000	-2.60355800	2.62671300
H	-2.86569400	-0.94579900	2.97350300
H	-1.73103000	-2.09326000	2.22654800
C	-3.38836600	0.80668000	-1.18229700
H	-2.93789800	1.81048900	-1.26922000
C	-3.25094500	0.11887500	-2.53456500
H	-3.78957200	0.69580800	-3.29854600
H	-3.68293200	-0.89018500	-2.52782900
H	-2.20470000	0.03738500	-2.85525600
C	-4.85059400	0.95961800	-0.78475200
H	-5.37457800	1.58229300	-1.52227300
H	-4.97480700	1.43511400	0.19667100
H	-5.36167400	-0.01238100	-0.75928100
C	3.52378900	-0.09414500	-1.36524300
H	3.62528900	-1.10369200	-1.79425700
C	4.89207100	0.37709900	-0.88161300
H	5.61130800	0.34702900	-1.71090500
H	5.30001800	-0.24158700	-0.07296700
H	4.85047900	1.41503400	-0.52516800
C	2.98612400	0.83378700	-2.44481700
H	3.72994900	0.94893200	-3.24472900
H	2.77994100	1.83832600	-2.04617800
H	2.06422300	0.45042900	-2.89904600
C	2.98632900	-1.84051200	0.87001800
H	4.08136400	-1.73158000	0.82102200
C	2.58022500	-1.95845200	2.33214800
H	2.99523300	-2.88358700	2.75486800

H	1.48740100	-2.00795400	2.44395200
H	2.94988100	-1.12445900	2.94051800
C	2.57966500	-3.09012900	0.09687300
H	3.10335300	-3.96675900	0.50079700
H	2.81737300	-3.02963800	-0.97335900
H	1.50085300	-3.27504900	0.19165500
C	-0.16501300	-1.51029600	-1.56190100
C	1.03422900	4.19037000	-0.33986900
H	0.89776800	5.22504500	-0.67838500
H	1.36390100	3.59830000	-1.21107200
O	-0.17838600	3.71882700	0.19893500
H	-0.38570800	1.21456200	-1.42887900
H	1.84940800	4.18820300	0.40265400

TS_{7,8-w}

G_{solv} = -1654.289500

Ru	0.00566600	-0.12067300	-0.27663700
H	-0.00112600	-0.97245500	1.09668300
H	0.42505200	0.94220400	-1.70960600
P	2.34860300	-0.09848600	0.03099600
P	-2.30506200	0.15881900	0.10321700
O	-0.13214100	-2.69488800	-1.82088100
N	0.11826300	1.69959100	0.92197600
H	0.10708000	2.63368400	0.13661700
C	2.58334600	1.53561600	0.85792000
H	3.50269700	1.56514200	1.45805200
H	2.68928900	2.27513800	0.04992200
C	1.35796900	1.86027100	1.69451100
H	1.32344100	1.21781400	2.59007900
H	1.42897800	2.90187200	2.05980500
C	-1.03073900	1.91286100	1.81303700
H	-0.98327500	2.93381700	2.23582400
H	-0.97032400	1.21634000	2.66667200
C	-2.34541800	1.73403700	1.07370900
H	-2.47911300	2.54618700	0.34465800
H	-3.20132600	1.76423600	1.76105500
C	-3.22008700	-1.08584700	1.13801200
H	-4.26264900	-0.73216800	1.15888500
C	-3.16655700	-2.47422300	0.51308500
H	-3.77041300	-3.17335000	1.10690500
H	-2.13644000	-2.85710600	0.50008400
H	-3.54834100	-2.49971900	-0.51446200
C	-2.70250700	-1.13027100	2.57011700
H	-3.27764900	-1.87145500	3.14125400
H	-2.80222900	-0.16911800	3.08831600
H	-1.64681200	-1.43410500	2.60583200
C	-3.38268500	0.54911500	-1.36611900
H	-2.97688800	1.52891500	-1.67055300
C	-3.19264800	-0.41269200	-2.53238800
H	-3.76451900	-0.05689200	-3.39994300
H	-3.55364000	-1.42216900	-2.29729800
H	-2.14180100	-0.48998900	-2.83717700
C	-4.85524700	0.71699100	-1.01467100
H	-5.39565400	1.14328300	-1.87035900
H	-5.01158100	1.38599500	-0.15872700
H	-5.32417800	-0.24902100	-0.78328000
C	3.53039100	-0.09659700	-1.41171900

H	3.67983100	-1.16531800	-1.63247600
C	4.87910900	0.52750500	-1.06528100
H	5.59107700	0.34366300	-1.88068100
H	5.32212200	0.12205300	-0.14747500
H	4.79369400	1.61577600	-0.94743800
C	2.93030000	0.56759200	-2.64274800
H	3.66822700	0.57877800	-3.45602700
H	2.64784600	1.61180800	-2.44249100
H	2.04204900	0.03644400	-3.00566800
C	3.08894600	-1.39875600	1.13711900
H	4.17865200	-1.26415100	1.04869400
C	2.70195000	-1.23837700	2.60052200
H	3.15903200	-2.04481500	3.18965300
H	1.61339600	-1.30791000	2.73873400
H	3.04404100	-0.28761500	3.02649200
C	2.71854300	-2.78937000	0.63256500
H	3.28038700	-3.55125500	1.18900600
H	2.93664200	-2.93321100	-0.43395000
H	1.64870500	-2.98715000	0.78603000
C	-0.08304300	-1.67963800	-1.23094900
O	0.10379900	3.64486000	-0.66472400
H	-0.40513500	0.98714500	-1.67899700
H	0.19759500	4.43706300	-0.12314200

8_M

G_{solv} = -1693.521067

Ru	-0.02433500	-0.19601900	-0.29022600
H	-0.07292500	-1.31914200	0.86676800
H	0.44003600	1.15634500	-1.46156100
P	2.30984100	-0.32129700	0.03368600
P	-2.32337200	0.05610000	0.15167200
O	-0.25825700	-2.38824300	-2.34179100
N	0.12526700	1.30383200	1.25569400
H	-0.02839300	2.76616600	0.55474300
C	2.59146100	1.11097500	1.16259900
H	3.50221000	0.98781200	1.76431100
H	2.74024100	1.98527500	0.51027000
C	1.36023400	1.31036000	2.03188300
H	1.33800300	0.52667000	2.81755400
H	1.45731900	2.27169900	2.57773800
C	-0.99417200	1.33765900	2.19076600
H	-0.92327800	2.24125000	2.83050900
H	-0.95817300	0.47382200	2.88869700
C	-2.33087800	1.35638000	1.46636400
H	-2.47011000	2.31957000	0.95430600
H	-3.17318400	1.22764800	2.15916500
C	-3.27211200	-1.37900400	0.85949500
H	-4.31095900	-1.02479700	0.94854900
C	-3.22498800	-2.58603600	-0.06923600
H	-3.85077900	-3.39286600	0.33524900
H	-2.19993400	-2.97377800	-0.15276700
H	-3.58441100	-2.36531700	-1.08125300
C	-2.77965900	-1.76431900	2.24893700
H	-3.37923000	-2.60355800	2.62671300
H	-2.86569400	-0.94579900	2.97350300
H	-1.73103000	-2.09326000	2.22654800
C	-3.38836600	0.80668000	-1.18229700

H	-2.93789800	1.81048900	-1.26922000
C	-3.25094500	0.11887500	-2.53456500
H	-3.78957200	0.69580800	-3.29854600
H	-3.68293200	-0.89018500	-2.52782900
H	-2.20470000	0.03738500	-2.85525600
C	-4.85059400	0.95961800	-0.78475200
H	-5.37457800	1.58229300	-1.52227300
H	-4.97480700	1.43511400	0.19667100
H	-5.36167400	-0.01238100	-0.75928100
C	3.52378900	-0.09414500	-1.36524300
H	3.62528900	-1.10369200	-1.79425700
C	4.89207100	0.37709900	-0.88161300
H	5.61130800	0.34702900	-1.71090500
H	5.30001800	-0.24158700	-0.07296700
H	4.85047900	1.41503400	-0.52516800
C	2.98612400	0.83378700	-2.44481700
H	3.72994900	0.94893200	-3.24472900
H	2.77994100	1.83832600	-2.04617800
H	2.06422300	0.45042900	-2.89904600
C	2.98632900	-1.84051200	0.87001800
H	4.08136400	-1.73158000	0.82102200
C	2.58022500	-1.95845200	2.33214800
H	2.99523300	-2.88358700	2.75486800
H	1.48740100	-2.00795400	2.44395200
H	2.94988100	-1.12445900	2.94051800
C	2.57966500	-3.09012900	0.09687300
H	3.10335300	-3.96675900	0.50079700
H	2.81737300	-3.02963800	-0.97335900
H	1.50085300	-3.27504900	0.19165500
C	-0.16501300	-1.51029600	-1.56190100
C	1.03422900	4.19037000	-0.33986900
H	0.89776800	5.22504500	-0.67838500
H	1.36390100	3.59830000	-1.21107200
O	-0.17838600	3.71882700	0.19893500
H	-0.38570800	1.21456200	-1.42887900
H	1.84940800	4.18820300	0.40265400

8_w

G_{solv} = -1654.288713

Ru	0.00629300	-0.11693900	-0.27499100
H	-0.00095800	-1.04657000	1.04657400
H	0.42132000	1.04198100	-1.64705700
P	2.34675200	-0.09576500	0.03352600
P	-2.30120600	0.14575100	0.12024200
O	-0.12977700	-2.60518000	-1.96656100
N	0.11324200	1.61900900	1.00212100
H	0.06997400	2.94085100	0.06754700
C	2.57445700	1.50232400	0.92828500
H	3.49568800	1.51398600	1.52658000
H	2.67296300	2.27729800	0.15239800
C	1.34029100	1.77391100	1.77310700
H	1.34287300	1.10761500	2.66103400
H	1.40334300	2.80600700	2.17505700
C	-1.01883100	1.80778700	1.90043300
H	-0.96865300	2.81598900	2.36073900
H	-0.98107200	1.08999000	2.74756600
C	-2.34333600	1.66992400	1.16680200

H	-2.47996700	2.51561600	0.47716900
H	-3.19753300	1.66534800	1.85719600
C	-3.22295000	-1.15009400	1.08546200
H	-4.26644100	-0.79974000	1.11838800
C	-3.16439400	-2.50561300	0.39248100
H	-3.76285700	-3.23715300	0.95196100
H	-2.13242200	-2.88212000	0.35631900
H	-3.54969800	-2.48120200	-0.63385500
C	-2.71390700	-1.26479600	2.51688500
H	-3.28760700	-2.03769400	3.04605000
H	-2.82176600	-0.33128500	3.08177700
H	-1.65635700	-1.56319900	2.54406100
C	-3.37670900	0.60825100	-1.33093600
H	-2.96998800	1.60232500	-1.58415200
C	-3.18484200	-0.29249400	-2.54466600
H	-3.75550300	0.10625700	-3.39433100
H	-3.54610300	-1.31277400	-2.36226800
H	-2.13347300	-0.35511000	-2.85092900
C	-4.85015000	0.76082300	-0.97650900
H	-5.38708400	1.23464700	-1.80928500
H	-5.00721500	1.38254400	-0.08575700
H	-5.32294700	-0.21484700	-0.79974100
C	3.53016700	-0.03535400	-1.40817400
H	3.68312700	-1.09461500	-1.66871200
C	4.87663900	0.57984100	-1.03896700
H	5.58717100	0.43974200	-1.86439300
H	5.32565100	0.13383500	-0.14310300
H	4.78531400	1.66080100	-0.86868900
C	2.93029300	0.67078400	-2.61533000
H	3.66470500	0.70276300	-3.43135000
H	2.65717400	1.71089400	-2.38226400
H	2.03636800	0.15831500	-2.99087700
C	3.10067500	-1.43619400	1.08242000
H	4.18912300	-1.29032000	0.99563300
C	2.71885800	-1.33919700	2.55270500
H	3.18309800	-2.16635800	3.10674300
H	1.63124300	-1.42057500	2.69197200
H	3.05577300	-0.40432900	3.01612900
C	2.73882700	-2.80817400	0.52352200
H	3.30897500	-3.58764000	1.04630800
H	2.95280600	-2.90678300	-0.54890100
H	1.67135600	-3.02057100	0.67369800
C	-0.08100400	-1.61755100	-1.32652400
O	0.01419900	3.84685700	-0.42194400
H	-0.40570400	1.08341500	-1.61243700
H	0.54263800	3.74662900	-1.22249000

TS_{1,9}

G_{solv} = -1653.119705

Ru	-0.00079600	-0.14853800	-0.02039500
H	-0.01122000	0.48511800	1.43522700
P	2.33058000	0.17566700	-0.11134700
P	-2.33028200	0.17977800	-0.11405100
O	-0.00220200	-2.81035600	1.36931700
N	0.00128200	1.71896700	-1.09731500
C	2.46594400	1.72576400	-1.12301900
H	3.35800300	2.30768400	-0.85460500

H	2.58617200	1.40622600	-2.16814400
C	1.19576600	2.54940400	-0.97760600
H	1.19690500	3.07635800	-0.00297300
H	1.18730500	3.34243400	-1.74923700
C	-1.19169200	2.55118600	-0.97902600
H	-1.18153600	3.34426000	-1.75056800
H	-1.19232700	3.07824300	-0.00445800
C	-2.46415200	1.73103000	-1.12370500
H	-2.58874900	1.41429900	-2.16938000
H	-3.35427400	2.31487100	-0.85285600
C	-3.28992400	0.53431400	1.43924600
H	-4.32403300	0.72688600	1.11374000
C	-3.27032700	-0.66027300	2.38443100
H	-3.84058300	-0.42769800	3.29406900
H	-2.24320700	-0.90455100	2.69139200
H	-3.71292000	-1.56047900	1.94143600
C	-2.77026200	1.78315200	2.14049900
H	-3.36013500	1.96650700	3.04875100
H	-2.84434600	2.68141800	1.51548800
H	-1.72095300	1.66546000	2.44589600
C	-3.34771700	-1.03751000	-1.10082200
H	-3.01917400	-0.82670100	-2.13175500
C	-2.99062100	-2.48695200	-0.79375900
H	-3.58529500	-3.15883800	-1.42779700
H	-3.19698100	-2.75469500	0.25100400
H	-1.93043200	-2.69171500	-0.98975900
C	-4.84903800	-0.79238500	-1.02080800
H	-5.36919400	-1.42407100	-1.75355700
H	-5.11562300	0.25053700	-1.23649200
H	-5.24692400	-1.04899500	-0.02976200
C	3.33973800	-1.04493800	-1.10086400
H	2.98826400	-0.84943100	-2.12645100
C	4.83989100	-0.78538900	-1.04940000
H	5.35242800	-1.41650200	-1.78804100
H	5.25910500	-1.03195900	-0.06460400
H	5.09301200	0.25856600	-1.27621200
C	3.00147000	-2.49417600	-0.77273600
H	3.59171100	-3.16647000	-1.41053500
H	1.94057700	-2.71048000	-0.95074900
H	3.22761000	-2.75077900	0.27066800
C	3.29375900	0.53130800	1.43941600
H	4.32794200	0.72099700	1.11215700
C	2.77599600	1.78310400	2.13696000
H	3.36482200	1.96780700	3.04561000
H	1.72592400	1.66797100	2.44108000
H	2.85249500	2.67953500	1.50969500
C	3.27256100	-0.65957400	2.38928500
H	3.83856900	-0.42217900	3.30034100
H	3.71877300	-1.56073400	1.95218500
H	2.24459000	-0.90468800	2.69292700
C	-0.00165500	-1.77514400	0.79652400
O	0.08989500	-0.36100200	-2.43980300
H	0.01495900	0.69805200	-2.10921000
H	-0.76962900	-0.61772500	-2.79874700

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G_{solv} = -1653.135154

Ru	0.00868500	-0.22313000	0.05697100
H	0.04329200	1.10712200	0.98183700
P	2.35304700	0.03876700	-0.01332700
P	-2.30408700	0.12739400	-0.22918700
O	-0.10281700	-1.81392600	2.58165700
N	0.11064400	1.04744100	-1.75674600
H	0.07721800	0.28254300	-2.44219600
C	2.57148600	0.89794100	-1.64201400
H	3.50563400	1.47371300	-1.68383400
H	2.63992100	0.10510300	-2.40269700
C	1.37600100	1.78642300	-1.93748000
H	1.34859100	2.64926000	-1.25909300
H	1.43603600	2.18070600	-2.96389000
C	-1.06580100	1.91585500	-1.96550800
H	-1.02385700	2.37077600	-2.96768300
H	-1.00074100	2.73170300	-1.23293300
C	-2.35079600	1.12536000	-1.79627100
H	-2.45489500	0.40552200	-2.62147000
H	-3.22526100	1.78837800	-1.83219600
C	-3.26121200	1.13480800	1.00929900
H	-4.30137400	1.14103400	0.64836600
C	-3.20634300	0.49623100	2.39190100
H	-3.82102000	1.07399100	3.09529000
H	-2.17756400	0.49186400	2.77870900
H	-3.57417700	-0.53668100	2.40450900
C	-2.77056800	2.57574500	1.07601400
H	-3.35798500	3.12623300	1.82330700
H	-2.87801900	3.10617900	0.12223700
H	-1.71664600	2.62630500	1.38361100
C	-3.37123600	-1.33736800	-0.66744000
H	-2.94122200	-1.63975900	-1.63507800
C	-3.20565500	-2.50633100	0.29595000
H	-3.74475500	-3.38247700	-0.08947200
H	-3.61857000	-2.28361100	1.28831000
H	-2.15371300	-2.79074900	0.42133500
C	-4.83965100	-0.98952900	-0.87484500
H	-5.36569600	-1.84454800	-1.32089400
H	-4.98146400	-0.13047100	-1.54327900
H	-5.33765100	-0.76492500	0.07825800
C	3.56846800	-1.38003800	-0.05714900
H	3.75474300	-1.58908200	1.00840600
C	4.89266300	-1.02206500	-0.72311400
H	5.61325800	-1.83806200	-0.57708200
H	5.34746100	-0.10922200	-0.31942800
H	4.76957700	-0.88839200	-1.80607700
C	2.97154300	-2.63123600	-0.68444900
H	3.69255500	-3.45818200	-0.63120100
H	2.74304200	-2.47413400	-1.74868600
H	2.05758800	-2.95233500	-0.16851700
C	3.14775500	1.12986000	1.27382200
H	4.23191400	1.02722300	1.10797300
C	2.78230000	2.60134600	1.14130000
H	3.26848100	3.17304200	1.94353000
H	1.69864300	2.75816400	1.23888000
H	3.11070300	3.03433000	0.18867700
C	2.81154000	0.61704700	2.67041900
H	3.40530900	1.15562300	3.42103500

H	3.01627600	-0.45449200	2.79632000
H	1.75077200	0.78433000	2.90233900
C	-0.06407200	-1.20092700	1.56989400
O	-0.18287000	-1.74848200	-1.55773100
H	0.63951300	-2.24228300	-1.63239600

10

G_{solv} = -1577.197203

Ru	-0.00006200	-0.16581200	-0.18806700
H	0.00033600	0.42048900	1.25737500
P	2.34347600	0.17255400	-0.20417100
P	-2.34368000	0.17282800	-0.20384800
O	0.00030800	-2.83891900	1.14547300
N	-0.00023400	1.88604300	-1.07264000
C	2.47741300	1.84402600	-1.00330000
H	3.36678100	2.38781000	-0.65814900
H	2.60143000	1.66911200	-2.08189200
C	1.22339900	2.66092700	-0.75151800
H	1.14825800	2.95055000	0.30452000
H	1.24105600	3.58770600	-1.34452600
C	-1.22324000	2.66109900	-0.74960400
H	-1.24086200	3.58866700	-1.34139800
H	-1.14732700	2.94919900	0.30680400
C	-2.47760000	1.84485000	-1.00176800
H	-2.60198700	1.67083200	-2.08047400
H	-3.36673200	2.38849900	-0.65588500
C	-3.25920200	0.32600600	1.40588800
H	-4.30509500	0.53382800	1.13189300
C	-3.19031700	-0.97174900	2.20055800
H	-3.75453800	-0.86440000	3.13651000
H	-2.15249900	-1.21582200	2.46753500
H	-3.61085800	-1.82691000	1.65843200
C	-2.74070400	1.49265100	2.23761100
H	-3.29983500	1.54176300	3.18158200
H	-2.86479400	2.45960800	1.73575100
H	-1.67815600	1.36792000	2.49012100
C	-3.36745400	-0.91053000	-1.32308000
H	-3.03854100	-0.57923400	-2.32147100
C	-3.00956500	-2.38582400	-1.18448300
H	-3.59168800	-2.97824700	-1.90303300
H	-3.23360100	-2.77452900	-0.18270500
H	-1.94617900	-2.56768700	-1.38473000
C	-4.86723200	-0.67431700	-1.20514800
H	-5.39192200	-1.21040600	-2.00728800
H	-5.13296200	0.38752900	-1.28891100
H	-5.26061500	-1.04948200	-0.25085300
C	3.36816000	-0.91153000	-1.32213100
H	3.03996300	-0.58123600	-2.32107900
C	4.86782500	-0.67483000	-1.20365200
H	5.39310200	-1.21176000	-2.00484100
H	5.26065400	-1.04876400	-0.24863000
H	5.13341200	0.38697100	-1.28851200
C	3.01084000	-2.38692600	-1.18284000
H	3.59389100	-2.97946000	-1.90056200
H	1.94779100	-2.56954000	-1.38400600
H	3.23427700	-2.77481000	-0.18059900
C	3.25861400	0.32700700	1.40554400

H	4.30472400	0.53377300	1.13154900
C	2.74107800	1.49480000	2.23618200
H	3.29955100	1.54362100	3.18056800
H	1.67814700	1.37177200	2.48793900
H	2.86701600	2.46128600	1.73387600
C	3.18855400	-0.96989900	2.20147300
H	3.75364500	-0.86232300	3.13687900
H	3.60745000	-1.82621000	1.65992400
H	2.15058600	-1.21227700	2.46951800
C	-0.00019300	-1.79333800	0.60419900
H	-0.00115800	1.72169300	-2.08489600

11

G_{solv} = -1767.572673

Ru	0.05227200	-0.11007600	-0.23829600
H	0.09985300	-1.64798900	0.10082900
P	2.40344400	-0.20381900	-0.01155200
P	-2.25078200	-0.26020000	0.23579100
O	-0.05899600	-0.92460500	-3.11676300
N	0.15995700	0.43519300	1.89006800
H	0.12862800	1.47797100	1.81033700
C	2.63113600	0.43749500	1.71004500
H	3.55933400	0.06736900	2.16549200
H	2.72026800	1.53072000	1.62556100
C	1.42889900	0.08346500	2.56658000
H	1.40312400	-0.99345600	2.78008300
H	1.48568900	0.60606400	3.53436500
C	-1.00008000	0.00491200	2.70205200
H	-0.96880600	0.50371800	3.68372200
H	-0.89467600	-1.07357000	2.88267500
C	-2.30966300	0.31402300	1.99942600
H	-2.46948900	1.40237900	1.96922000
H	-3.15679000	-0.12470000	2.54339800
C	-3.04314000	-1.94373500	0.23975500
H	-4.09650900	-1.76939700	0.50737400
C	-2.97290400	-2.57741200	-1.14423000
H	-3.51438900	-3.53278200	-1.14666800
H	-1.93160500	-2.78681700	-1.42689400
H	-3.41306400	-1.94630400	-1.92593200
C	-2.43583500	-2.87016800	1.28543800
H	-2.92295700	-3.85285700	1.22591400
H	-2.57236200	-2.50099400	2.30884800
H	-1.36102500	-3.02624500	1.11374100
C	-3.45543100	0.88061500	-0.61512000
H	-3.20516200	1.85002900	-0.15777900
C	-3.19448600	0.99940400	-2.11143900
H	-3.86494300	1.75397300	-2.54505600
H	-3.37845900	0.05461400	-2.64008000
H	-2.16336300	1.30876500	-2.32311000
C	-4.91768500	0.57675500	-0.31700700
H	-5.54849200	1.39249500	-0.69498800
H	-5.11587000	0.47833400	0.75832700
H	-5.24882800	-0.34580400	-0.81226500
C	3.55117800	0.81571500	-1.06539100
H	3.68826500	0.20454600	-1.97166900
C	4.91105300	1.06188500	-0.42148100
H	5.58284800	1.53873100	-1.14771100

H	5.40183800	0.14287800	-0.07841500
H	4.82553800	1.74226900	0.43618900
C	2.89396600	2.12925100	-1.46353200
H	3.56611400	2.70816700	-2.11113600
H	2.67840600	2.74815200	-0.58042700
H	1.95458900	1.96824900	-2.00829200
C	3.19837500	-1.88515400	-0.06948600
H	4.28175300	-1.69526300	-0.01208400
C	2.80372700	-2.77540100	1.10086000
H	3.28593800	-3.75646900	0.99390500
H	1.71755900	-2.94583700	1.12836000
H	3.11377400	-2.36374800	2.06866500
C	2.88401300	-2.56967300	-1.39553400
H	3.46994300	-3.49388300	-1.48674600
H	3.11750300	-1.94497600	-2.26748100
H	1.82132800	-2.84285900	-1.45224700
C	-0.01955400	-0.58454900	-1.98965000
C	-0.15889200	3.09080200	-0.02605600
O	0.11399900	3.18968600	1.25952400
H	0.57095400	3.55877100	-0.72002400
H	-0.23254600	1.99264100	-0.40765200
O	-1.41625600	3.69242800	-0.40521100
H	-2.00154800	3.58095500	0.35882500

TS_{11,12}

G_{solv} = -1767.565523

Ru	0.03208600	-0.15897400	-0.23240900
H	0.08864600	-1.74896200	0.22744500
P	2.37820800	-0.22833800	-0.02034500
P	-2.26840300	-0.22213200	0.23099900
O	-0.10857000	-0.89285900	-3.12918100
N	0.15255700	0.40618100	1.90153300
H	0.15612800	1.43598300	1.84649400
C	2.61500200	0.37945600	1.71492200
H	3.54296700	-0.00435700	2.15888100
H	2.70821500	1.47405500	1.65881300
C	1.41424300	0.01160000	2.56730700
H	1.36979900	-1.07134900	2.74218300
H	1.48060900	0.50124500	3.55166500
C	-1.02317000	0.00180000	2.70372400
H	-0.98080600	0.48403900	3.69313400
H	-0.95173700	-1.08171000	2.86555500
C	-2.31439200	0.36476700	1.99296500
H	-2.42390300	1.45957200	1.95698600
H	-3.18323300	-0.03169300	2.53502100
C	-3.15466700	-1.86244600	0.23922100
H	-4.20166100	-1.63050000	0.48586100
C	-3.09221100	-2.50627200	-1.14088000
H	-3.65988800	-3.44658100	-1.14465200
H	-2.05436400	-2.74504300	-1.41412300
H	-3.50831500	-1.86678500	-1.92915800
C	-2.62212400	-2.81722800	1.29927700
H	-3.17656400	-3.76414200	1.24695600
H	-2.74024200	-2.42824400	2.31796300
H	-1.55988300	-3.04746100	1.13805100
C	-3.43063200	0.96464400	-0.62295500
H	-3.14231000	1.92637100	-0.17247500

C	-3.17158500	1.06808300	-2.12093300
H	-3.82500000	1.83607200	-2.55738000
H	-3.38070600	0.12530900	-2.64384800
H	-2.13406000	1.35091400	-2.33702400
C	-4.90477100	0.72294400	-0.32459900
H	-5.50003000	1.56625800	-0.70003600
H	-5.10816800	0.62957000	0.75027000
H	-5.27610300	-0.18246000	-0.82302000
C	3.54930700	0.79828600	-1.05098600
H	3.71309200	0.17779900	-1.94681600
C	4.89191600	1.04886200	-0.37174100
H	5.58715600	1.51094800	-1.08546600
H	5.36936300	0.13475700	0.00168500
H	4.78411700	1.74379600	0.47177600
C	2.92091100	2.11182800	-1.48951000
H	3.61694500	2.66345600	-2.13599900
H	2.70210600	2.75401300	-0.62428700
H	1.99047500	1.95385600	-2.04932000
C	3.22096100	-1.89122700	-0.10446700
H	4.29889800	-1.66675500	-0.08012700
C	2.89761500	-2.80248400	1.07078000
H	3.42449300	-3.75882200	0.94987500
H	1.82247300	-3.02469800	1.12190300
H	3.20905000	-2.37832000	2.03317400
C	2.89242500	-2.57973100	-1.42482800
H	3.50517900	-3.48403200	-1.53869400
H	3.08063900	-1.94233200	-2.29871600
H	1.83817500	-2.88717500	-1.45368000
C	-0.05587300	-0.59626500	-1.98593400
C	-0.02207100	3.18252300	-0.00639500
O	0.41067200	3.22081900	1.16351500
H	0.60907400	3.37667900	-0.88430200
H	-0.07792400	1.61238700	-0.45811100
O	-1.30395900	3.57064400	-0.27859300
H	-1.78990300	3.59929700	0.56325200

12

G_{solv} = -1767.580281

Ru	0.07190700	-0.37680200	-0.21432400
H	0.18433200	-1.83011800	0.67111600
P	2.41118500	-0.19507700	-0.01690100
P	-2.23670600	-0.31177900	0.19504200
O	0.01321100	-1.70403900	-2.89184000
N	0.14110500	0.66227500	1.75633600
H	0.11320100	1.65572400	1.50535600
C	2.58761900	0.73361800	1.58089600
H	3.53719600	0.50870000	2.08353300
H	2.59908000	1.80413600	1.32577100
C	1.40562100	0.44573700	2.48784200
H	1.41277100	-0.59535400	2.83702300
H	1.43664000	1.09427400	3.37801800
C	-1.04080500	0.39944300	2.60164900
H	-1.02124700	1.05715800	3.48542000
H	-0.96630200	-0.63598800	2.95940800
C	-2.31374000	0.61824600	1.80422000
H	-2.40827200	1.68572600	1.55133900
H	-3.19885600	0.34451800	2.39333500

C	-3.22709200	-1.86058900	0.51262600
H	-4.25842000	-1.51803500	0.68867400
C	-3.19926500	-2.78213900	-0.70086800
H	-3.79272000	-3.68479600	-0.50130000
H	-2.17227100	-3.10434500	-0.92527400
H	-3.60978800	-2.31306800	-1.60278200
C	-2.75826100	-2.60643900	1.75464700
H	-3.38006600	-3.50042300	1.89896900
H	-2.83783900	-2.00407700	2.66782800
H	-1.71687900	-2.94166600	1.65371000
C	-3.30126700	0.74401500	-0.91872800
H	-2.88740700	1.74687100	-0.72302000
C	-3.09787500	0.45094200	-2.39998400
H	-3.66599600	1.17382900	-3.00127000
H	-3.45056800	-0.55049000	-2.67863600
H	-2.04354100	0.53193800	-2.69077100
C	-4.77956700	0.74825900	-0.55175100
H	-5.29903100	1.53875400	-1.11037900
H	-4.95042000	0.93386200	0.51667200
H	-5.26322900	-0.20270000	-0.81309800
C	3.47568300	0.76472800	-1.21953000
H	3.68799700	0.03338300	-2.01607500
C	4.79792400	1.22708700	-0.61356200
H	5.44875000	1.62539500	-1.40353900
H	5.35147400	0.42537200	-0.11019100
H	4.64050800	2.03590600	0.11247100
C	2.74034500	1.94510700	-1.83685500
H	3.40345300	2.46992600	-2.53821000
H	2.43431800	2.67116000	-1.06878500
H	1.84364700	1.63371000	-2.38466700
C	3.42243800	-1.75347900	0.16884300
H	4.47398300	-1.43272300	0.10936200
C	3.21362900	-2.45714000	1.50167600
H	3.83071500	-3.36531000	1.53978700
H	2.16756900	-2.76613800	1.63270900
H	3.49785000	-1.83300500	2.35777500
C	3.12891800	-2.69779200	-0.99150700
H	3.82330500	-3.54856300	-0.97076500
H	3.22975500	-2.21327000	-1.97202500
H	2.10832500	-3.09826600	-0.91862500
C	0.03426800	-1.18283200	-1.82832000
C	-0.31583800	3.78950700	-0.15532100
O	0.09424300	3.63719500	0.97974200
H	0.31745600	3.79029900	-1.05399400
H	-0.09287700	1.19159900	-0.87607500
O	-1.58318200	4.01158500	-0.47062100
H	-2.12599600	4.01669100	0.34093000

13

G_{solv} = -1766.446639

Ru	0.00016300	0.12533600	-0.16362800
H	0.00208800	1.65577400	0.30135700
P	-2.33990200	0.10928000	0.17349900
P	2.33834400	0.11476500	0.17349000
O	0.00152100	1.08953100	-2.99288900
N	0.00244000	-0.41744100	1.98924300
C	-2.46044000	-0.42903700	1.94607800

H	-3.36842000	-0.04549800	2.42927800
H	-2.53220700	-1.52698100	1.93744500
C	-1.21953100	-0.00455100	2.70884100
H	-1.18068800	1.08679900	2.82704400
H	-1.22185800	-0.44238200	3.71962800
C	1.21792600	0.01495700	2.70895400
H	1.22249700	-0.41534400	3.72299300
H	1.16590500	1.10667400	2.81869600
C	2.46610800	-0.40022300	1.95268000
H	2.55781000	-1.49641400	1.96009300
H	3.36701900	0.00549500	2.43101600
C	3.31952100	1.69056300	0.04743700
H	4.36834500	1.40191000	0.21833900
C	3.17980700	2.30817900	-1.33855500
H	3.81180800	3.20301600	-1.41569400
H	2.14219900	2.62046300	-1.52213500
H	3.47295700	1.62657100	-2.14561800
C	2.91726100	2.69885100	1.11631900
H	3.51348300	3.61355400	0.99805500
H	3.08460300	2.32867800	2.13481800
H	1.85960800	2.98207000	1.02148100
C	3.32248100	-1.20976900	-0.69288400
H	2.84813500	-2.12265200	-0.29595800
C	3.13748900	-1.20836700	-2.20573700
H	3.55575100	-2.13112800	-2.63012400
H	3.66342100	-0.36974400	-2.68008300
H	2.08138000	-1.15587100	-2.49862000
C	4.79871800	-1.22461000	-0.31725200
H	5.27414500	-2.13394000	-0.70918000
H	4.96235000	-1.20903900	0.76788800
H	5.32916500	-0.36782100	-0.75430500
C	-3.32496600	-1.20814500	-0.70381400
H	-2.84964500	-2.12476700	-0.31683500
C	-4.80022900	-1.22867100	-0.32444800
H	-5.27492800	-2.13528000	-0.72356400
H	-5.33343700	-0.36898900	-0.75227300
H	-4.96132100	-1.22337900	0.76115000
C	-3.14510200	-1.19176000	-2.21727300
H	-3.56287300	-2.11128000	-2.64914900
H	-2.09039600	-1.13377500	-2.51385400
H	-3.67480900	-0.34967000	-2.68120700
C	-3.32491300	1.68373800	0.06501400
H	-4.37362900	1.39066500	0.22840400
C	-2.92903700	2.67984100	1.14756200
H	-3.52514200	3.59556500	1.03680800
H	-1.87100600	2.96486900	1.06226800
H	-3.10235500	2.29750300	2.16056500
C	-3.18150000	2.31730500	-1.31344700
H	-3.81498200	3.21170500	-1.38316700
H	-3.47049200	1.64410300	-2.12912100
H	-2.14382300	2.63333700	-1.48997800
C	0.00085600	0.69398400	-1.88187800
H	-0.06500400	-4.10015700	-0.62003200
C	-0.00887300	-3.14726000	-0.04689700
O	0.06278000	-3.22619800	1.20102300
O	-0.02336100	-2.10342200	-0.75754100
H	0.01246000	-1.44743000	1.93471800

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Ru	-0.04444800	-0.10618300	0.17713200
H	-0.12843000	-1.66224200	0.01384700
P	-2.39257400	-0.05726900	-0.15742100
P	2.27751300	-0.29290800	-0.16795800
O	-0.03597700	-0.65693000	3.11484400
N	-0.03831500	0.15821500	-2.02953500
C	-2.49745300	0.32281100	-1.97190600
H	-3.43178400	-0.04939800	-2.41247600
H	-2.50775700	1.41965600	-2.06126800
C	-1.29188800	-0.23838300	-2.70467000
H	-1.31665700	-1.33558700	-2.73479400
H	-1.27877600	0.11641600	-3.74687700
C	1.14932500	-0.40712300	-2.70604600
H	1.17051600	-0.07442500	-3.75545900
H	1.03312200	-1.49901200	-2.71284000
C	2.42598900	0.00728100	-1.99535700
H	2.59571300	1.08557300	-2.12939700
H	3.29426600	-0.51389300	-2.41965000
C	3.11573500	-1.92851100	0.11330700
H	4.17566400	-1.76131200	-0.13313000
C	2.99447200	-2.36531500	1.56742100
H	3.53917000	-3.30687400	1.71895100
H	1.94386300	-2.54379900	1.83622400
H	3.40338200	-1.63059800	2.27131800
C	2.57502400	-3.00919900	-0.81518600
H	3.08470100	-3.95866000	-0.60338900
H	2.74325700	-2.78094600	-1.87423000
H	1.49858300	-3.17260300	-0.66261100
C	3.37460200	1.02133300	0.57116800
H	3.07935900	1.91272900	-0.00683600
C	3.05502000	1.29812900	2.03581800
H	3.64693700	2.15440200	2.38655700
H	3.30017600	0.44412200	2.68113100
H	1.99620500	1.54248000	2.18930100
C	4.86175700	0.77445900	0.35560000
H	5.43304100	1.66331200	0.65503700
H	5.10554500	0.56365200	-0.69374000
H	5.22263900	-0.06496800	0.96502600
C	-3.35370000	1.33664700	0.62099200
H	-2.94196500	2.21454300	0.09541100
C	-4.85226300	1.27030500	0.35876200
H	-5.32906800	2.20147600	0.69272300
H	-5.32108400	0.44741400	0.91479300
H	-5.08753700	1.14103200	-0.70553100
C	-3.04776300	1.49868000	2.10555700
H	-3.59135600	2.36667500	2.50205700
H	-1.97868200	1.66322100	2.28862300
H	-3.35804600	0.62332800	2.69080000
C	-3.39696000	-1.60741200	0.06449100
H	-4.43120000	-1.32837200	-0.19069700
C	-2.95164100	-2.70961500	-0.88924300
H	-3.54424300	-3.61456800	-0.70007900
H	-1.89446600	-2.97217700	-0.73986000
H	-3.09674900	-2.44341100	-1.94265200

C	-3.34629400	-2.09848500	1.50547400
H	-3.95961300	-3.00353900	1.60994200
H	-3.72434900	-1.36078500	2.22281800
H	-2.31978400	-2.36091000	1.79758200
C	-0.04047300	-0.40985600	1.96340300
H	-0.09000600	2.25977500	0.19969000
C	0.47575900	3.07287300	-0.35846000
O	1.12692400	3.86048300	0.35980700
O	0.34483600	3.08083400	-1.60641200
H	0.03348000	1.18866200	-2.08538000

TS_{14,15} $G_{\text{solv}} = -1766.409398$

Ru	0.00003800	-0.24331200	-0.16919700
H	-0.00005400	-1.92171500	-0.11597600
P	2.32325000	-0.21571400	0.15399400
P	-2.32320800	-0.21569800	0.15400200
O	0.00006900	-0.16084100	-3.15832500
N	0.00005400	-0.28018300	2.05024700
C	2.45773600	-0.23170800	2.00978700
H	3.37210700	-0.73774800	2.34604000
H	2.52702200	0.81640000	2.33736900
C	1.22701500	-0.87704500	2.62078900
H	1.19514200	-1.95426400	2.41148400
H	1.22938900	-0.75093400	3.71494000
C	-1.22696900	-0.87687100	2.62083700
H	-1.22932700	-0.75068900	3.71498000
H	-1.19519500	-1.95410600	2.41160000
C	-2.45763400	-0.23146200	2.00979800
H	-2.52676200	0.81669600	2.33725300
H	-3.37206600	-0.73732800	2.34615500
C	-3.40456000	-1.62228300	-0.41173100
H	-4.43325100	-1.33942700	-0.13966500
C	-3.30632900	-1.80273800	-1.92166500
H	-3.97989500	-2.60626100	-2.24881500
H	-2.28563200	-2.08787300	-2.21397100
H	-3.57538200	-0.89820200	-2.48035900
C	-3.06166600	-2.92494700	0.29886800
H	-3.72427100	-3.72309500	-0.06250300
H	-3.18816000	-2.86274400	1.38655800
H	-2.02807600	-3.23332100	0.08973200
C	-3.22564500	1.35588700	-0.29561000
H	-2.77411400	2.07209800	0.41155300
C	-2.91577100	1.84357800	-1.70565700
H	-3.35617400	2.83834400	-1.85851600
H	-3.33850700	1.18019600	-2.47172500
H	-1.83668600	1.92518500	-1.88657000
C	-4.72656900	1.30463700	-0.04209800
H	-5.15734400	2.31007800	-0.14254500
H	-4.97400500	0.93908400	0.96300800
H	-5.23440200	0.66096900	-0.77306400
C	3.22546600	1.35604500	-0.29542100
H	2.77364100	2.07214000	0.41168100
C	4.72635500	1.30505400	-0.04164600
H	5.15696100	2.31057600	-0.14201100
H	5.23442800	0.66149800	-0.77254200
H	4.97369300	0.93951800	0.96349000

C	2.91578900	1.84371600	-1.70551800
H	3.35613600	2.83852000	-1.85829300
H	1.83673200	1.92523400	-1.88661800
H	3.33871100	1.18037800	-2.47152200
C	3.40470400	-1.62213300	-0.41195700
H	4.43337400	-1.33925500	-0.13983200
C	3.06183100	-2.92490900	0.29845100
H	3.72443200	-3.72299900	-0.06305200
H	2.02823600	-3.23324600	0.08928900
H	3.18834000	-2.86287100	1.38614800
C	3.30646600	-1.80238500	-1.92191500
H	3.97976700	-2.60610200	-2.24913200
H	3.57582900	-0.89787400	-2.48049800
H	2.28568600	-2.08715300	-2.21428200
C	0.00005300	-0.20222900	-1.97714700
H	0.00045200	1.48887400	0.00661800
C	-0.00023800	3.11124000	0.75280700
O	-0.00004800	2.84878000	1.90711200
O	-0.00049600	3.78063300	-0.22075000
H	0.00016500	0.71237700	2.30648000

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Ru	0.01409400	-0.37663300	-0.16172400
H	0.03909500	-2.06232200	0.16458100
P	2.32787800	-0.19230900	0.15514300
P	-2.30728200	-0.24909700	0.16148500
O	0.02857900	-0.70546100	-3.13202000
N	0.00963800	-0.05609200	2.04574900
C	2.45314600	0.08456500	1.99177500
H	3.39118300	-0.31175000	2.40107500
H	2.46221500	1.17345400	2.15196300
C	1.25181400	-0.51760500	2.69745000
H	1.26346200	-1.61447100	2.64714000
H	1.24533000	-0.23254200	3.76149300
C	-1.20764400	-0.57947100	2.69799000
H	-1.20850800	-0.30700500	3.76541900
H	-1.17073600	-1.67507800	2.63456500
C	-2.43952100	-0.02420400	2.00608300
H	-2.51014200	1.05735200	2.19553200
H	-3.35380100	-0.48282500	2.40410400
C	-3.45910700	-1.66758500	-0.20505000
H	-4.46274100	-1.32491800	0.09148800
C	-3.45104100	-2.00133500	-1.69138300
H	-4.13677500	-2.83497200	-1.89522000

H	-2.44786100	-2.31327800	-2.01651800
H	-3.76218100	-1.15880300	-2.32041900
C	-3.10992700	-2.90079300	0.61728700
H	-3.81961700	-3.70781600	0.38992400
H	-3.15637400	-2.71841200	1.69800900
H	-2.10255300	-3.26711900	0.37613400
C	-3.15962900	1.28781100	-0.47473200
H	-2.67726100	2.06832600	0.13830200
C	-2.84320900	1.59291800	-1.93341600
H	-3.25590500	2.57447800	-2.20460700
H	-3.28597100	0.85476500	-2.61493900
H	-1.76267100	1.62073800	-2.12071700
C	-4.65919900	1.32211900	-0.21099300
H	-5.05439700	2.32255000	-0.43341400
H	-4.91005000	1.09264400	0.83278900
H	-5.19688400	0.61192900	-0.85359500
C	3.15083200	1.34274300	-0.52120100
H	2.64647800	2.13027100	0.06505400
C	4.64766100	1.41582000	-0.24914500
H	5.02169000	2.42001900	-0.49001600
H	5.20438400	0.70500700	-0.87483000
H	4.89790200	1.21249100	0.80018500
C	2.84007600	1.59858800	-1.99065900
H	3.25649200	2.56959000	-2.29227700
H	1.75974500	1.62396500	-2.18171100
H	3.28403200	0.83762500	-2.64582500
C	3.49940700	-1.60191700	-0.18487700
H	4.50596500	-1.22234300	0.04906800
C	3.21819800	-2.80192200	0.70963100
H	3.93086600	-3.60550100	0.47923400
H	2.20766000	-3.19867600	0.53971500
H	3.32041900	-2.57106200	1.77701200
C	3.43717200	-2.00939100	-1.65173900
H	4.14490000	-2.82647100	-1.84700200
H	3.68573400	-1.18771300	-2.33421100
H	2.43308600	-2.37347400	-1.91314200
C	0.02113800	-0.58678200	-1.95401700
H	-0.00134300	1.31482300	-0.26271800
C	-0.12674900	3.58494900	0.58188300
O	-0.16335300	3.99235000	-0.50901400
O	-0.08857300	3.23790100	1.69515600
H	-0.01514700	0.96274600	2.14227500

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