

Supporting Information

Mechanistic Study and Ligand Design for the Formation of Zinc Formate Complexes from Zinc Hydride Complexes and Carbon Dioxide

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Table S1. Solvent effect corrected absolute free energies (Hartree) and Cartesian coordinates (Å) of all optimized structures.

CO₂

$G_{\text{solv}} = -188.533858$

C	-0.84178500	-0.86206900	0.00000000
O	0.32310600	-0.86206900	0.00000000
O	-2.00667600	-0.86206900	0.00000000

1a

$G_{\text{solv}} = -2704.427120$

Zn	1.98511500	11.47915200	2.02373700
H	0.75000800	11.40506200	3.00879300
O	3.04965100	10.14433600	1.08318700
C	3.97217900	9.59261700	1.86721500
C	4.95947900	10.42506700	2.45195900
C	5.93829200	9.90254100	3.29596500
H	6.68655800	10.55068000	3.74681000
C	5.95480700	8.54314200	3.56559500
C	5.00029200	7.70986200	2.98464400
H	5.04996400	6.65499600	3.23241600
C	4.00293500	8.19284100	2.13435400
C	4.95347500	11.88549800	2.09265500
H	5.85897200	12.38057400	2.47554900
H	4.96039600	11.97127100	1.00337800
N	3.75894700	12.61798600	2.58951800
C	3.60456400	13.91009700	1.89802100
H	4.56225800	14.45191400	1.86138500
H	2.91222900	14.52097200	2.48516000
C	3.07134500	13.73402900	0.47773300
H	2.95346400	14.72181800	0.00782900
H	3.78981000	13.17562400	-0.12639400
N	1.79694900	12.99195600	0.45582100
C	3.84099300	12.80583700	4.04238000

H	4.69432600	13.44503100	4.31691400
H	3.95911600	11.83458200	4.52743900
H	2.91729000	13.26195300	4.40727600
C	0.66296500	13.86927500	0.77223300
H	0.54709800	14.65801400	0.01342100
H	0.80417200	14.33489800	1.75019000
H	-0.25393500	13.27765900	0.81719000
C	1.58978200	12.33860700	-0.84354800
H	1.56272700	13.07224500	-1.66322000
H	0.64087000	11.79630400	-0.82715200
H	2.39199300	11.61850200	-1.01864400
C	2.96324300	7.24973100	1.50744900
C	3.05299100	7.33121600	-0.02942600
H	2.30343600	6.67435200	-0.48827200
H	4.04162900	7.00769500	-0.37594700
H	2.88122800	8.35273000	-0.37524600
C	1.54591400	7.64217300	1.96874600
H	1.46916000	7.61042100	3.06154600
H	0.80789300	6.94202400	1.55760500
H	1.28526500	8.64900100	1.63820100
C	3.18995600	5.78410700	1.91027300
H	3.09041500	5.63175200	2.99089100
H	4.17408700	5.41698600	1.59768300
H	2.43671300	5.15585000	1.42202400
O	6.89672300	8.02168700	4.43264500
C	8.01851300	7.45076400	3.78077900
H	8.68671200	7.07796300	4.56075800
H	7.72497400	6.61553200	3.13080000
H	8.54943800	8.19953400	3.17677500

2a

$G_{\text{solv}} = -2892.953121$

Zn	1.52368700	0.14937700	0.42268500
H	1.84015200	0.99158300	1.72446500
O	0.13660400	0.24893500	-0.94093200
C	-0.99867600	-0.34069900	-0.57807900
C	-0.97808500	-1.71564800	-0.23491000
C	-2.13742200	-2.37616900	0.16932900
H	-2.11160200	-3.42975000	0.43864200
C	-3.33562000	-1.68217800	0.23008300
C	-3.37462900	-0.33444300	-0.12418700
H	-4.33355300	0.16801400	-0.05492900
C	-2.23681500	0.36423000	-0.53326300
C	0.31977100	-2.46185200	-0.38519000
H	0.16129500	-3.54251100	-0.24845400
H	0.68824000	-2.30437200	-1.40170700
N	1.38526800	-2.00967300	0.54802500
C	2.71254800	-2.47969300	0.11151600
H	2.68662200	-3.55147600	-0.13878800
H	3.39902600	-2.36229100	0.95585300
C	3.22751500	-1.69396500	-1.09305000
H	4.22858200	-2.06048300	-1.36452800
H	2.58103000	-1.86449000	-1.95682500

N	3.25717000	-0.24129800	-0.83348100
C	1.09441200	-2.45746300	1.91527100
H	1.11404500	-3.55550600	1.99072400
H	0.10500800	-2.10276900	2.21125000
H	1.83024800	-2.03628900	2.60478500
C	4.47076700	0.14494400	-0.10240900
H	5.37350000	-0.04860200	-0.70141700
H	4.54102400	-0.41027900	0.83574400
H	4.42507100	1.20828800	0.14285400
C	3.15274000	0.51910400	-2.08661400
H	3.97901900	0.27818000	-2.77218200
H	3.18251500	1.58843900	-1.86339400
H	2.19641500	0.29748700	-2.56516600
C	-2.30634500	1.85123000	-0.91639100
C	-1.82376500	2.03749100	-2.36870900
H	-1.86050100	3.09846400	-2.64578600
H	-2.46641700	1.48469300	-3.06403500
H	-0.79820600	1.68113400	-2.48600000
C	-1.41692300	2.67521600	0.03554600
H	-1.74325500	2.55454100	1.07444700
H	-1.47349600	3.74102600	-0.21913100
H	-0.37687800	2.35415800	-0.04356500
C	-3.73319500	2.41297100	-0.82283400
H	-4.13309400	2.36108500	0.19604900
H	-4.42646800	1.89297100	-1.49370300
H	-3.72415700	3.46854100	-1.11666100
O	-4.47993400	-2.32043100	0.67010100
C	-5.33428800	-2.74802200	-0.37705100
H	-6.19052800	-3.24036700	0.09011300
H	-5.69069900	-1.90024900	-0.97731300
H	-4.82298500	-3.46084900	-1.03862200
C	1.46976100	3.76778500	1.56984700
O	0.91995300	3.72147300	2.59503700
O	2.02845700	3.86206800	0.55041700

TS_{2a,3a}

$G_{\text{solv}} = -2892.933776$

Zn	1.88865700	0.14576400	-0.13725400
H	2.07809700	1.22610300	1.09455100
O	0.50888700	0.09079000	-1.46150100
C	-0.60036700	-0.48711800	-0.98822200
C	-0.52954400	-1.82036400	-0.51929000
C	-1.66019600	-2.46909500	-0.02285100
H	-1.60024200	-3.49205000	0.34102100
C	-2.87185300	-1.79820500	0.01469000
C	-2.94930600	-0.47933700	-0.43132900
H	-3.91203100	0.01397100	-0.35458000
C	-1.84204800	0.20585500	-0.93550300
C	0.79744600	-2.52757200	-0.57560900
H	0.68112600	-3.59032200	-0.31896900
H	1.19170100	-2.46724700	-1.59314400
N	1.81795400	-1.92785100	0.33392300
C	3.17378600	-2.41954800	0.01319600

H	3.16473900	-3.50605300	-0.15386500
H	3.80960100	-2.23274400	0.88323800
C	3.75311300	-1.72495500	-1.21874500
H	4.77697200	-2.08344100	-1.39373000
H	3.16561100	-1.97630100	-2.10515900
N	3.73791800	-0.25194500	-1.07916500
C	1.47715400	-2.19710400	1.73936400
H	1.50109900	-3.27518600	1.95444300
H	0.47562800	-1.81757100	1.94940600
H	2.18530700	-1.68410200	2.39454400
C	4.85659500	0.22508500	-0.24834000
H	5.82080900	-0.00595500	-0.72247700
H	4.82516700	-0.24201700	0.73830500
H	4.77270700	1.30507800	-0.11222600
C	3.77595100	0.39987300	-2.39992900
H	4.68216000	0.11873000	-2.95450100
H	3.76589000	1.48397600	-2.26541000
H	2.89187700	0.11337900	-2.97374200
C	-1.94604800	1.67146600	-1.38871100
C	-1.56290800	1.78646100	-2.87731700
H	-1.61138300	2.83410200	-3.19879000
H	-2.25546800	1.20975800	-3.50169100
H	-0.55009700	1.41643000	-3.04975200
C	-1.00780000	2.55312000	-0.53900600
H	-1.23129000	2.44997600	0.52860500
H	-1.13512900	3.60823500	-0.80876400
H	0.03854700	2.29092300	-0.70192000
C	-3.36944500	2.22759900	-1.22799500
H	-3.69813900	2.22493800	-0.18272200
H	-4.10163700	1.67145000	-1.82442000
H	-3.38950800	3.26696600	-1.57336400
O	-3.98471500	-2.42564600	0.53700300
C	-4.90212800	-2.88106000	-0.44432900
H	-5.72344600	-3.36485000	0.08915700
H	-5.30145500	-2.05001400	-1.04046600
H	-4.42921000	-3.60765800	-1.11907300
C	2.02207100	2.54732100	1.70412000
O	1.42586800	2.38419400	2.73223000
O	2.61290600	3.30705900	0.98480500

3a

$G_{\text{solv}} = -2892.976989$

Zn	1.54095900	0.35015800	0.04519400
H	-0.26828000	1.09047300	2.13056500
O	0.14932300	0.31129800	-1.25054400
C	-0.93819900	-0.34356600	-0.81967500
C	-0.80999100	-1.68151200	-0.36946400
C	-1.91194700	-2.39656800	0.08745200
H	-1.80370900	-3.42080900	0.43508900
C	-3.16969900	-1.80329300	0.10095600
C	-3.30893300	-0.49042700	-0.34688200
H	-4.28905100	-0.03370000	-0.33286100
C	-2.21927000	0.26184700	-0.80813100

C	0.54559500	-2.33791000	-0.41303700
H	0.46116800	-3.40904000	-0.17978800
H	0.95535000	-2.24549000	-1.42254400
N	1.52681200	-1.71970700	0.52404900
C	2.90508300	-2.16381300	0.23096500
H	2.93341900	-3.24424800	0.03054000
H	3.50882900	-1.98602400	1.12504600
C	3.50136200	-1.41559500	-0.96063200
H	4.54098700	-1.73692300	-1.11325800
H	2.94763500	-1.65644400	-1.87184100
N	3.43742700	0.05363900	-0.78186500
C	1.16614000	-2.00825300	1.92025400
H	1.23377500	-3.08486900	2.13347600
H	0.14233200	-1.67968500	2.10747400
H	1.83378800	-1.46475700	2.59286300
C	4.48298800	0.53349800	0.14049600
H	5.48286900	0.32776200	-0.26643500
H	4.38485100	0.04956500	1.11357000
H	4.36831000	1.60816100	0.29072300
C	3.56129700	0.73634800	-2.08219400
H	4.51500700	0.48930800	-2.56889600
H	3.51363600	1.81646600	-1.92683600
H	2.73505500	0.44149700	-2.73275800
C	-2.40969700	1.71121900	-1.28900400
C	-1.96313500	1.83187900	-2.75976700
H	-2.08669900	2.86473400	-3.10821000
H	-2.57197700	1.18491700	-3.40225100
H	-0.91542300	1.54735600	-2.87512100
C	-1.58377500	2.67215000	-0.41032400
H	-1.89815200	2.61400000	0.63793500
H	-1.72914000	3.70660300	-0.74465100
H	-0.51772500	2.44580700	-0.46698900
C	-3.87551700	2.16712600	-1.21197900
H	-4.26022100	2.15507200	-0.18585200
H	-4.53341500	1.55430700	-1.83871900
H	-3.94943700	3.19836800	-1.57394400
O	-4.19926300	-2.57634000	0.56553500
C	-5.48078500	-1.99258400	0.65270000
H	-6.13702100	-2.76124700	1.06456500
H	-5.48569700	-1.12352600	1.32385800
H	-5.86030500	-1.69343000	-0.33320600
C	0.65456000	1.65580700	2.38527400
O	0.66746700	2.36616800	3.37830500
O	1.65371600	1.48886000	1.57207800

TS_{3a,4a}

$G_{\text{solv}} = -2892.972530$

Zn	1.43826700	0.43702600	0.08950900
H	2.24430900	3.42249900	1.60569000
O	0.02908800	0.38072400	-1.18131200
C	-1.04174100	-0.32779000	-0.79669000
C	-0.87467700	-1.66037400	-0.34352600
C	-1.96416300	-2.42647000	0.05715900

H	-1.82578900	-3.44602400	0.40773600
C	-3.24751100	-1.89374100	0.00635600
C	-3.42491400	-0.58705400	-0.44480500
H	-4.42475000	-0.17656900	-0.47950800
C	-2.34866300	0.21689100	-0.84642700
C	0.50512000	-2.26601700	-0.33340000
H	0.45068800	-3.33697900	-0.08983600
H	0.93884300	-2.17207100	-1.33288200
N	1.43555100	-1.60288600	0.62232400
C	2.83237200	-2.02644300	0.39905000
H	2.89775800	-3.11893600	0.29250500
H	3.40587800	-1.75072100	1.28857300
C	3.43537500	-1.36483700	-0.83887100
H	4.48602300	-1.66860700	-0.94111200
H	2.91246600	-1.70017200	-1.73768200
N	3.33264600	0.11319500	-0.78792300
C	1.02657900	-1.85273600	2.01304000
H	1.09114100	-2.92296600	2.25697200
H	-0.00316900	-1.51963800	2.15300900
H	1.66690200	-1.28275000	2.68921900
C	4.40350300	0.68993600	0.04569000
H	5.39061800	0.44976100	-0.37312600
H	4.34242300	0.31243600	1.06766800
H	4.29129800	1.77512000	0.08456600
C	3.39284600	0.67897800	-2.14722500
H	4.33828000	0.41781000	-2.64280600
H	3.31440100	1.76719800	-2.09016100
H	2.55585300	0.30276100	-2.73928500
C	-2.58109400	1.66294200	-1.31844800
C	-2.07114300	1.83123700	-2.76368200
H	-2.21973700	2.86554400	-3.09802800
H	-2.62243100	1.17487700	-3.44718400
H	-1.00867200	1.59036200	-2.83349600
C	-1.84035400	2.64077800	-0.38430600
H	-2.18912300	2.53333600	0.64913100
H	-2.02574600	3.67560600	-0.69777800
H	-0.76343000	2.46532700	-0.40008200
C	-4.06806200	2.05265600	-1.30541000
H	-4.50035000	2.00625700	-0.29940900
H	-4.66756900	1.42132400	-1.97119200
H	-4.17159600	3.08531300	-1.65627000
O	-4.26227400	-2.71530900	0.41835100
C	-5.58306200	-2.22637200	0.34086900
H	-6.22588500	-3.03078400	0.70248600
H	-5.72836000	-1.34283300	0.97619600
H	-5.86470800	-1.98157800	-0.69182000
C	2.35586700	2.42529000	2.08284100
O	3.18852300	2.27097800	2.96624800
O	1.53521100	1.52795600	1.64292000

4a

$G_{\text{solv}} = -2892.983702$

Zn	1.39012900	0.58633500	0.22151600
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H	2.25812800	2.72991400	3.19029500
O	-0.01915800	0.49263200	-1.06705100
C	-1.08973700	-0.21672400	-0.69404200
C	-0.91742000	-1.53713000	-0.20783400
C	-2.00424800	-2.30523600	0.19584800
H	-1.86048300	-3.31480400	0.57241900
C	-3.29210600	-1.78722000	0.11218100
C	-3.47685000	-0.49761800	-0.38361600
H	-4.48101300	-0.10187800	-0.45209200
C	-2.40328900	0.30677400	-0.79196800
C	0.46925900	-2.12448600	-0.18334100
H	0.42921300	-3.19391700	0.06960300
H	0.90193600	-2.03270500	-1.18270700
N	1.38642900	-1.44133400	0.77124400
C	2.79372700	-1.83940800	0.55626900
H	2.88661900	-2.93492300	0.52410100
H	3.36216100	-1.47696700	1.41716400
C	3.36558600	-1.24798200	-0.73164900
H	4.42153500	-1.53514100	-0.82422600
H	2.84676500	-1.65606600	-1.60191000
N	3.22866500	0.22740800	-0.77339700
C	0.97886500	-1.71783300	2.15822700
H	1.04250100	-2.79403300	2.37590600
H	-0.05315900	-1.39226900	2.30294500
H	1.62559100	-1.16160800	2.83820900
C	4.36027100	0.88029800	-0.09140100
H	5.29847500	0.68658100	-0.63067900
H	4.43887800	0.51598300	0.93332500
H	4.18785400	1.95844200	-0.05438300
C	3.13692400	0.70488700	-2.16399900
H	4.02826800	0.41920900	-2.74037600
H	3.05192700	1.79426100	-2.16408800
H	2.24359200	0.29124900	-2.63697400
C	-2.64369500	1.72555700	-1.33540600
C	-2.09179900	1.82969800	-2.77135300
H	-2.25277700	2.84052500	-3.16634200
H	-2.60600400	1.12297500	-3.43346800
H	-1.02239300	1.61142200	-2.79464100
C	-1.94512100	2.75787000	-0.42853600
H	-2.33464100	2.70345900	0.59461600
H	-2.12356000	3.77323800	-0.80388300
H	-0.86764900	2.58983300	-0.39287000
C	-4.13605400	2.09006700	-1.38834300
H	-4.60082800	2.08529100	-0.39578200
H	-4.70334800	1.41671700	-2.04112900
H	-4.24425500	3.10265000	-1.79250000
O	-4.30527100	-2.60758700	0.53349800
C	-5.62822900	-2.13015800	0.43232500
H	-6.26905100	-2.92891300	0.80988000
H	-5.78413700	-1.23098300	1.04295000
H	-5.90365600	-1.91380300	-0.60844700
C	2.22498900	1.87589100	2.49007300
O	2.86036300	0.84948600	2.74331000

O	1.49267600	2.07975900	1.45239700
TS_{4a,5a}			
$G_{\text{solv}} = -2892.982732$			
Zn	1.40845100	0.58636200	0.20949500
H	2.21535800	3.11172400	2.66829800
O	-0.01929900	0.46192900	-1.07001700
C	-1.09039300	-0.24636400	-0.70435200
C	-0.92196800	-1.57723000	-0.24759300
C	-2.00713300	-2.34905700	0.15296600
H	-1.86321400	-3.36614200	0.50896600
C	-3.29281200	-1.82227600	0.09752500
C	-3.47576300	-0.52099300	-0.36770800
H	-4.47823800	-0.11762900	-0.41311000
C	-2.40282100	0.28681000	-0.77169600
C	0.46478800	-2.16016100	-0.23721600
H	0.42861200	-3.23518900	-0.00593200
H	0.89844900	-2.04612000	-1.23394900
N	1.37658700	-1.49259600	0.73144000
C	2.77578200	-1.91294100	0.52296000
H	2.84663900	-3.00892800	0.45479700
H	3.34439100	-1.60238800	1.40423300
C	3.38084100	-1.29271800	-0.73478200
H	4.42953400	-1.60698300	-0.82782100
H	2.85887300	-1.65447700	-1.62354900
N	3.28271500	0.18310800	-0.72361800
C	0.95578300	-1.78332600	2.10992300
H	1.00981400	-2.86274500	2.31604500
H	-0.07375300	-1.45028700	2.25271100
H	1.59375300	-1.23898200	2.80643100
C	4.39184700	0.78244800	0.03601400
H	5.35532000	0.56434900	-0.44660600
H	4.40377300	0.39793500	1.05716900
H	4.25412300	1.86463800	0.08210800
C	3.26719800	0.71913600	-2.09502900
H	4.17996000	0.44068200	-2.64120800
H	3.19817600	1.80866900	-2.05476100
H	2.39252900	0.33958600	-2.62787200
C	-2.64192200	1.72385500	-1.26587000
C	-2.10045900	1.87989600	-2.70100500
H	-2.25552700	2.90733200	-3.05313000
H	-2.62579000	1.20569300	-3.38788300
H	-1.03314700	1.65443000	-2.74059300
C	-1.93115900	2.72075500	-0.32896700
H	-2.31119000	2.62882500	0.69561900
H	-2.11347700	3.74971900	-0.66351000
H	-0.85300100	2.55395900	-0.31254800
C	-4.13338300	2.09514800	-1.29324100
H	-4.58868000	2.06128400	-0.29676800
H	-4.70981800	1.44417000	-1.96067300
H	-4.24153600	3.12018400	-1.66478100
O	-4.30563700	-2.64523100	0.51684800
C	-5.62596000	-2.15589600	0.44856500

H	-6.26645400	-2.95631800	0.82334900
H	-5.76410400	-1.26660500	1.07780600
H	-5.91858800	-1.91861800	-0.58293800
C	1.99043800	2.26044400	2.00622900
O	2.10984500	1.09277600	2.43149600
O	1.61671800	2.52437100	0.82078700

5a

$$G_{\text{solv}} = -2892.986289$$

Zn	1.43444500	0.51530100	0.18107700
H	1.66049800	3.43194000	2.26415100
O	0.00544200	0.40213100	-1.07223400
C	-1.06238700	-0.29391500	-0.67338100
C	-0.90041900	-1.62990800	-0.23008200
C	-1.98886200	-2.39059600	0.18390100
H	-1.85262500	-3.41344500	0.52615600
C	-3.26803400	-1.84617000	0.15938700
C	-3.44163200	-0.53422900	-0.27879200
H	-4.43816400	-0.11422100	-0.29195700
C	-2.36567800	0.26338000	-0.69353100
C	0.47837400	-2.23430600	-0.24068700
H	0.42595800	-3.30886900	-0.00902000
H	0.90443200	-2.12805700	-1.24241000
N	1.41665700	-1.58308600	0.71373600
C	2.80135600	-2.03414600	0.48508300
H	2.84136400	-3.12392100	0.33975700
H	3.37824100	-1.80874200	1.38655200
C	3.42931700	-1.34192900	-0.72327100
H	4.47369300	-1.66676700	-0.83203000
H	2.90311100	-1.62886300	-1.63710200
N	3.35354000	0.12968400	-0.60988700
C	1.00417500	-1.83395200	2.10107900
H	1.04393200	-2.90734800	2.34043000
H	-0.01695400	-1.47831000	2.24722500
H	1.65829300	-1.28502900	2.78158300
C	4.39472200	0.65377200	0.28977400
H	5.39705700	0.43304100	-0.10433000
H	4.29906200	0.21105600	1.28346700
H	4.27342000	1.73423800	0.38284900
C	3.47197400	0.76717400	-1.93214400
H	4.43789500	0.52967600	-2.40029700
H	3.38521700	1.84910600	-1.81366500
H	2.66231700	0.42337600	-2.57987600
C	-2.59045600	1.71578600	-1.14846800
C	-2.11395500	1.88845400	-2.60452500
H	-2.25408700	2.92779200	-2.92681700
H	-2.69132900	1.24561100	-3.27954900
H	-1.05664700	1.63401700	-2.70021000
C	-1.81006300	2.67744000	-0.22917200
H	-2.10751300	2.54334900	0.81757500
H	-2.01797500	3.71754700	-0.50936600
H	-0.73426400	2.51488700	-0.30856300
C	-4.07118100	2.12454200	-1.09372100

H	-4.47735500	2.07683200	-0.07673500
H	-4.69683300	1.50593200	-1.74748800
H	-4.17016000	3.16082300	-1.43515900
O	-4.28439900	-2.66183400	0.58422900
C	-5.59967500	-2.15632700	0.53963100
H	-6.24499100	-2.95496200	0.90993100
H	-5.72041000	-1.27515200	1.18365000
H	-5.90169100	-1.90020600	-0.48467300
C	1.65108300	2.60441400	1.53711000
O	1.35265600	1.44653700	1.97949000
O	1.92721600	2.81899000	0.34083200

1b

$$G_{\text{solv}} = -2723.831997$$

Zn	1.96971900	11.49757900	2.00853000
H	0.72758100	11.48028000	2.98927400
O	2.98111500	10.12006400	1.07899700
C	3.89419100	9.54203000	1.85967400
C	4.91157600	10.34412600	2.43700300
C	5.86953800	9.79985000	3.28398100
H	6.61231800	10.45143400	3.74012100
C	5.88173800	8.43266900	3.56498600
C	4.89561900	7.63846700	2.97079300
H	4.90472000	6.57586200	3.17506300
C	3.89494500	8.15010000	2.13437400
C	4.94885500	11.80429800	2.07768900
H	5.86961600	12.27207100	2.45894700
H	4.95689800	11.88829100	0.98844400
N	3.77855700	12.57394000	2.57504500
C	3.66508600	13.87190100	1.88686000
H	4.63760100	14.38757200	1.85957800
H	2.98473100	14.49907200	2.47110800
C	3.13817000	13.71650500	0.46172500
H	3.04988800	14.70953000	-0.00368400
H	3.84682000	13.14352300	-0.14035300
N	1.84468300	13.00871100	0.42690300
C	3.86582400	12.75640800	4.02822100
H	4.73878000	13.36797500	4.30414100
H	3.95402100	11.78105300	4.51136300
H	2.95674900	13.24063200	4.39365800
C	0.73064100	13.91878700	0.71964200
H	0.64262300	14.70021200	-0.05045300
H	0.87376400	14.39357100	1.69291300
H	-0.20144200	13.35112700	0.76248000
C	1.63886900	12.34923500	-0.86949000
H	1.64567100	13.07549600	-1.69622700
H	0.67454400	11.83453800	-0.86292200
H	2.42195300	11.60387000	-1.02430000
C	2.82629300	7.22941700	1.52081500
C	2.89505600	7.30907700	-0.01722700
H	2.12462400	6.66905100	-0.46549200
H	3.87135100	6.96441500	-0.37809800
H	2.74100300	8.33464200	-0.35932300

C	1.42556600	7.65691700	2.00168000
H	1.36008000	7.61633500	3.09504800
H	0.66234200	6.98327100	1.59185300
H	1.19163700	8.67459000	1.68417100
C	3.01997900	5.75717400	1.91797200
H	2.93400800	5.60463000	2.99990700
H	3.98817800	5.36357200	1.58837400
H	2.24192300	5.15067400	1.44103100
N	6.87403100	7.91118600	4.44906800
C	6.62755300	6.58432300	4.97781500
H	6.72799400	5.78232200	4.22290800
H	7.35110100	6.38156500	5.77379200
H	5.62495100	6.52891600	5.41052700
C	8.24097300	8.03937700	3.96100900
H	8.43836400	9.05932300	3.62572100
H	8.94102200	7.81007100	4.77126900
H	8.44903800	7.35531400	3.11777800

1c

$G_{\text{solv}} = -2665.166216$

Zn	1.99665800	11.47607500	2.02464100
H	0.77386200	11.39710500	3.02618200
O	3.05603700	10.15385100	1.06983000
C	3.99340000	9.60795200	1.84721200
C	4.98350100	10.44403900	2.41849000
C	5.97946500	9.93402200	3.24932300
H	6.73095100	10.58943300	3.68226500
C	6.01585000	8.57410600	3.51731400
C	5.06008800	7.73473200	2.94860900
H	5.11710900	6.67333000	3.17341100
C	4.04231400	8.21247300	2.11549700
C	4.96464700	11.90475800	2.05873100
H	5.87163600	12.40584300	2.42974600
H	4.95721400	11.98862300	0.96928800
N	3.77162500	12.62900300	2.57053500
C	3.60040700	13.91999500	1.88084300
H	4.55517900	14.46562400	1.82813300
H	2.91564400	14.52867500	2.47900200
C	3.04500900	13.74133100	0.46938500
H	2.91780600	14.72857700	0.00058800
H	3.75533300	13.18380500	-0.14511500
N	1.77223500	12.99638800	0.46719500
C	3.87082500	12.81794100	4.02203400
H	4.72405700	13.46171900	4.28606000
H	4.00014300	11.84755800	4.50598600
H	2.94913500	13.26913000	4.39809300
C	0.64145800	13.86863700	0.80652400
H	0.51150200	14.66159700	0.05428500
H	0.79643100	14.32869000	1.78498100
H	-0.27306500	13.27425500	0.86212000
C	1.54483000	12.34609400	-0.83023000
H	1.50270500	13.08153600	-1.64771200
H	0.59735000	11.80189500	-0.79933200

H	2.34552300	11.62799200	-1.02012300
C	3.00653500	7.25666100	1.50126200
C	3.07890200	7.33929500	-0.03643600
H	2.32937500	6.67694000	-0.48744000
H	4.06624600	7.02387600	-0.39369800
H	2.89551100	8.35998600	-0.37856900
C	1.59114900	7.63662300	1.97857600
H	1.52491300	7.59828600	3.07192400
H	0.85395600	6.93393700	1.57032100
H	1.32150900	8.64369400	1.65634900
C	3.24943600	5.79274900	1.90106400
H	3.16389100	5.63936200	2.98300300
H	4.23140000	5.43170900	1.57457200
H	2.49425500	5.15914200	1.42299800
O	7.01047200	8.10514500	4.34089300
H	6.91840300	7.15303000	4.44451500

1d

$$G_{\text{solv}} = -2747.088728$$

Zn	1.97569900	11.51980400	2.04051300
H	0.75210700	11.46986200	3.04221500
O	3.00463600	10.15886000	1.09783900
C	3.94092200	9.61418300	1.86974700
C	4.94031300	10.44219800	2.43056600
C	5.92527400	9.92248300	3.27159000
H	6.66176700	10.61118800	3.67719100
C	5.97331900	8.56598900	3.57844600
C	4.99316000	7.75199400	2.98992000
H	5.02344800	6.69113400	3.21224500
C	3.98371400	8.21781500	2.14864000
C	4.94569600	11.89641500	2.04754300
H	5.86166500	12.38811000	2.40989800
H	4.93875900	11.96621300	0.95703100
N	3.76669000	12.65315700	2.54792300
C	3.61164700	13.93069000	1.82982400
H	4.57362900	14.46210500	1.76355400
H	2.93567600	14.56192200	2.41471000
C	3.05210800	13.72698000	0.42311300
H	2.93561300	14.70476900	-0.06763700
H	3.75525600	13.14766500	-0.17932500
N	1.77077100	12.99680500	0.43909500
C	3.87705800	12.87253800	3.99427800
H	4.74042400	13.51049900	4.23901300
H	3.99692200	11.91075500	4.49762400
H	2.96401200	13.34409800	4.36653800
C	0.64947100	13.89167200	0.75036600
H	0.52752800	14.66142900	-0.02683600
H	0.81000500	14.38128900	1.71349900
H	-0.27124500	13.30905000	0.82501100
C	1.53833200	12.31163700	-0.83940700
H	1.50781800	13.02349300	-1.67799800
H	0.58368200	11.78098800	-0.79517600
H	2.32959900	11.57729800	-1.00492600

C	2.94591400	7.26381400	1.53459000
C	3.02207300	7.33987500	-0.00344900
H	2.27450400	6.67521500	-0.45450600
H	4.01082800	7.02381600	-0.35640700
H	2.83888600	8.35864600	-0.35160400
C	1.52958700	7.64838700	2.00582500
H	1.46053000	7.61369900	3.09917400
H	0.79158800	6.94604700	1.59808400
H	1.26300700	8.65513000	1.67954400
C	3.18386700	5.80025600	1.93930700
H	3.09380000	5.64969000	3.02117100
H	4.16724700	5.43707700	1.61971200
H	2.42969400	5.16693700	1.45883400
C	7.02799700	7.94327700	4.50383500
C	7.99549100	8.99338400	5.06746100
C	6.33191500	7.25124800	5.69202400
C	7.85389800	6.90094700	3.72485100
H	8.55509400	9.50080700	4.27386000
H	7.47227300	9.75290900	5.65930800
H	8.72528400	8.50817900	5.72516400
H	5.66638900	6.44753600	5.36076500
H	7.07343900	6.81102200	6.36984900
H	5.73050300	7.96719300	6.26308700
H	8.61249700	6.44666600	4.37399400
H	7.22452000	6.09446400	3.33490400
H	8.36564000	7.36532900	2.87457800

1e

$G_{\text{solv}} = -2589.967189$

Zn	1.98122400	11.49453100	2.05006600
H	0.74877700	11.42435600	3.03795200
O	3.03684800	10.14774000	1.11244400
C	3.96241400	9.59416600	1.88717100
C	4.95292400	10.42744800	2.47056400
C	5.93272500	9.89734500	3.30653900
H	6.67888600	10.55911100	3.74276600
C	5.96213600	8.53392000	3.57137700
C	5.00366300	7.70773500	2.98137500
H	5.05148200	6.64608200	3.19829400
C	3.99811500	8.19169300	2.14067500
C	4.95034200	11.88649800	2.10574100
H	5.85765300	12.37975000	2.48696900
H	4.95887000	11.96881200	1.01622500
N	3.75899500	12.62849800	2.59790200
C	3.60651100	13.91361000	1.89266100
H	4.56504300	14.45351100	1.85034800
H	2.91465000	14.53162000	2.47299700
C	3.07355900	13.72272100	0.47398400
H	2.95744200	14.70529400	-0.00699000
H	3.79161700	13.15655200	-0.12333400
N	1.79788200	12.98221500	0.45935500
C	3.84530000	12.83125000	4.04833600
H	4.70103300	13.47094500	4.31410800

H	3.96220600	11.86432700	4.54239200
H	2.92387800	13.29349300	4.41137500
C	0.66417600	13.86639500	0.75726100
H	0.54972700	14.64047500	-0.01665600
H	0.80483800	14.35096800	1.72609900
H	-0.25325700	13.27645600	0.81244900
C	1.59465300	12.30774000	-0.82997300
H	1.57400800	13.02772800	-1.66180000
H	0.64371700	11.76907800	-0.80898200
H	2.39493000	11.58164600	-0.98827500
C	2.96032300	7.25405600	1.50231200
C	3.04640900	7.35300000	-0.03391600
H	2.29990000	6.69667700	-0.49863900
H	4.03632100	7.03920600	-0.38552300
H	2.86783100	8.37696500	-0.36878200
C	1.54188700	7.63550300	1.96993200
H	1.46516000	7.58472700	3.06210300
H	0.80495500	6.94115200	1.54697800
H	1.27910400	8.64738700	1.65685300
C	3.19111100	5.78380600	1.88583800
H	3.09483400	5.61750700	2.96475300
H	4.17513300	5.42271000	1.56620800
H	2.43766000	5.16023300	1.39172900
H	6.72154200	8.11084100	4.22189700

If

$$G_{\text{solv}} = -3049.559875$$

Zn	1.97620300	11.49872200	2.04408600
H	0.74717700	11.41903700	3.03416800
O	3.03548000	10.14652500	1.11012000
C	3.95917900	9.59492600	1.88325800
C	4.95029300	10.42684900	2.46630100
C	5.93299400	9.90544100	3.30348500
H	6.68278400	10.55747000	3.74313700
C	5.94357700	8.54426600	3.55575700
C	4.99806300	7.70244600	2.97879600
H	5.05356600	6.64412300	3.20309000
C	3.99638200	8.19254300	2.13875900
C	4.95003400	11.88672100	2.10412200
H	5.85782300	12.37848800	2.48503700
H	4.95888500	11.96731200	1.01458000
N	3.75870200	12.62545100	2.59752500
C	3.60759600	13.91289000	1.89508600
H	4.56623200	14.45245100	1.85544700
H	2.91557000	14.52917000	2.47684300
C	3.07557100	13.72571300	0.47579600
H	2.95966900	14.70943600	-0.00246600
H	3.79352900	13.16127800	-0.12332400
N	1.79933200	12.98557200	0.45925500
C	3.84448700	12.82523800	4.04892300
H	4.70082100	13.46311000	4.31627000
H	3.95883700	11.85769100	4.54231300
H	2.92348300	13.28828900	4.41161600

C	0.66607800	13.87088700	0.75823100
H	0.55391800	14.64655300	-0.01416000
H	0.80650300	14.35310300	1.72824300
H	-0.25219000	13.28207800	0.81100200
C	1.59581100	12.31532200	-0.83266600
H	1.57550700	13.03833200	-1.66164100
H	0.64468800	11.77701800	-0.81357200
H	2.39606200	11.58988600	-0.99404200
C	2.96126400	7.24967500	1.50448000
C	3.04881200	7.34630700	-0.03166700
H	2.30435800	6.68662200	-0.49419000
H	4.03951400	7.03406600	-0.38206200
H	2.86687000	8.36853600	-0.36977400
C	1.54356900	7.63202100	1.97316700
H	1.46812400	7.58465000	3.06546300
H	0.80809400	6.93461900	1.55348000
H	1.27826500	8.64206700	1.65647300
C	3.19658500	5.78184300	1.89336000
H	3.10046100	5.61860500	2.97273500
H	4.18087200	5.42150100	1.57375200
H	2.44442400	5.15522000	1.40181100
Cl	7.17460600	7.86388900	4.61734400

1g

$G_{\text{solv}} = -2703.262461$

Zn	1.94949100	11.54218900	2.05552700
H	0.70275100	11.47968300	3.02326600
O	2.99145300	10.12226800	1.18358200
C	3.93091900	9.58215300	1.92341200
C	4.92933800	10.42555000	2.49429300
C	5.92199800	9.89449100	3.30026300
H	6.67857800	10.55101500	3.73000200
C	5.97024800	8.52166500	3.55348100
C	5.00312100	7.68678500	2.96667200
H	5.08376400	6.62697300	3.18145100
C	3.98685200	8.16702700	2.15571500
C	4.92341700	11.88297800	2.12461700
H	5.83462100	12.37438100	2.49805000
H	4.92866300	11.95820500	1.03465600
N	3.73789600	12.63173400	2.61613600
C	3.60342800	13.92352300	1.91702900
H	4.56386500	14.46076600	1.89907500
H	2.90070600	14.53729300	2.48867900
C	3.09824100	13.74432500	0.48685200
H	2.98572200	14.73064300	0.01403900
H	3.82958700	13.18908700	-0.10471800
N	1.82514200	12.99829500	0.44376300
C	3.82047100	12.82774400	4.06869700
H	4.68396000	13.45410300	4.33947200
H	3.92063000	11.85804100	4.56083700
H	2.90440200	13.30241800	4.42862300
C	0.68179600	13.88522700	0.70126900
H	0.58490000	14.64563600	-0.08778900

H	0.80023900	14.38655300	1.66449300
H	-0.23570700	13.29453300	0.74507700
C	1.65726700	12.31463400	-0.84669800
H	1.65553300	13.02974400	-1.68245300
H	0.70824900	11.77242000	-0.84682500
H	2.46398600	11.59124000	-0.98240700
C	2.94716400	7.23067700	1.52047400
C	3.00210500	7.35706700	-0.01534200
H	2.26117500	6.69103600	-0.47411500
H	3.99089400	7.06864100	-0.39061800
H	2.79369500	8.38018100	-0.33455800
C	1.53519700	7.58720400	2.02613600
H	1.48007100	7.50172900	3.11733500
H	0.79758800	6.89806800	1.59689800
H	1.25536900	8.60491300	1.74829100
C	3.20882200	5.75872900	1.87468700
H	3.13976800	5.57337700	2.95226700
H	4.19139600	5.41899200	1.52878600
H	2.45445600	5.13198800	1.38654300
C	7.02507000	7.98134500	4.40593400
O	7.17667800	6.80474800	4.69949900
H	7.73312600	8.73988700	4.80408400

1h

$G_{\text{solv}} = -2794.424872$

Zn	1.93661700	11.56194300	2.04810200
H	0.67959000	11.49265000	3.00189000
O	2.97386800	10.11419400	1.20137200
C	3.91826100	9.57984700	1.93029300
C	4.92020000	10.42744900	2.49609500
C	5.92190700	9.91131700	3.29558300
H	6.68177200	10.55591700	3.72400800
C	5.95594200	8.54040600	3.53212900
C	5.00740500	7.68555400	2.96300600
H	5.09591300	6.62876300	3.17650600
C	3.98503900	8.16569400	2.15918800
C	4.91273900	11.88427900	2.12227700
H	5.82520800	12.37544200	2.49128100
H	4.91548900	11.95315200	1.03193900
N	3.72858200	12.63322800	2.61428300
C	3.60151700	13.92867300	1.91878300
H	4.56366100	14.46253200	1.90793900
H	2.89817500	14.54190500	2.49012100
C	3.10191400	13.75685700	0.48584500
H	2.99132400	14.74560100	0.01815200
H	3.83494500	13.20493900	-0.10683300
N	1.82797600	13.01173700	0.43530400
C	3.81113400	12.82645100	4.06815200
H	4.67762100	13.44746800	4.34011000
H	3.90597400	11.85607100	4.55982300
H	2.89717300	13.30551100	4.42733300
C	0.68461000	13.90092200	0.68832700
H	0.59344700	14.66175400	-0.10074100

H	0.79978300	14.40147900	1.65230300
H	-0.23424100	13.31203900	0.72733200
C	1.66434200	12.33178600	-0.85792900
H	1.66456600	13.04973000	-1.69104800
H	0.71574900	11.78895200	-0.86255200
H	2.47220400	11.60999400	-0.99520100
C	2.94963800	7.22096300	1.53040600
C	2.99193200	7.35296600	-0.00536800
H	2.25465600	6.68025200	-0.45968500
H	3.98061300	7.07606700	-0.38928700
H	2.76963700	8.37422400	-0.32076700
C	1.53954600	7.56476300	2.04993100
H	1.49264500	7.46784200	3.14048800
H	0.80343900	6.87541900	1.61901600
H	1.25147000	8.58332100	1.78393800
C	3.22877900	5.75089300	1.87831200
H	3.16968400	5.56104600	2.95580600
H	4.21117100	5.42107200	1.52199500
H	2.47637500	5.11854800	1.39497300
N	6.99699000	7.99163700	4.36668500
O	7.02869500	6.77537800	4.54886700
O	7.81568100	8.76394100	4.86705400

li

$G_{\text{solv}} = -2704.429800$

Zn	2.06966900	11.49880000	2.05972100
H	0.94164200	11.36979900	3.16025000
O	3.03538600	10.14008300	1.02730500
C	4.00934500	9.58269800	1.73284000
C	5.04024800	10.41803300	2.22930800
C	6.06561100	9.89173100	3.02563300
C	6.09449200	8.53017600	3.31022200
C	5.09035800	7.71094600	2.78181700
C	4.04220000	8.17986900	1.99722500
C	5.01656300	11.86522500	1.82743600
H	5.95720800	12.36304200	2.09280500
H	4.89855200	11.91077900	0.74227900
N	3.88341300	12.62449500	2.42654900
C	3.68009600	13.90673600	1.72940700
H	4.63906900	14.42389800	1.57223400
H	3.07231800	14.54650700	2.37658200
C	2.98541600	13.71496200	0.38285300
H	2.82880100	14.69547700	-0.09095400
H	3.62186600	13.13233100	-0.28677100
N	1.70642300	12.99294500	0.52205000
C	4.11344900	12.83877700	3.86050500
H	4.99597800	13.47162300	4.03580000
H	4.27132300	11.87495500	4.34861900
H	3.23416700	13.31071700	4.30691100
C	0.62870200	13.88751500	0.96221300
H	0.43454000	14.67245000	0.21553400
H	0.88936300	14.35781500	1.91295800
H	-0.28335500	13.30740300	1.11810600

C	1.33805100	12.33078600	-0.73659900
H	1.22565000	13.05687700	-1.55579300
H	0.38977800	11.80395100	-0.60250800
H	2.10374700	11.59657100	-0.99686300
C	2.95802400	7.24565900	1.43900500
C	2.93331700	7.33666100	-0.09983600
H	2.15245000	6.68176900	-0.50696700
H	3.89419700	7.01781300	-0.52074100
H	2.73462200	8.36018100	-0.42472000
C	1.57728000	7.63432300	2.00301500
H	1.57397500	7.57725100	3.09758800
H	0.80722200	6.94979700	1.62510400
H	1.30426600	8.65113200	1.71540900
C	3.21244900	5.77683600	1.81245800
H	3.18988300	5.61540000	2.89627600
H	4.17290900	5.41408100	1.42888600
H	2.42740000	5.15096700	1.37336200
H	6.87281100	8.09006700	3.92164900
H	5.14915400	6.65394400	3.01827200
O	6.99857100	10.78227000	3.47813700
C	8.03895700	10.29722700	4.30064800
H	8.65870000	11.16173500	4.54547300
H	7.64863800	9.86161700	5.22909400
H	8.65373400	9.55342000	3.77871700

Ij

$G_{\text{solv}} = -2704.418705$

Zn	2.05334300	11.45722700	2.10710700
H	0.90696500	11.31984000	3.18697200
O	3.07954300	10.13345700	1.09781700
C	4.04723500	9.57928800	1.81698000
C	5.03822800	10.44664800	2.35654200
C	6.03968400	9.93550700	3.16269700
H	6.79416700	10.60113700	3.57768500
C	6.09496700	8.57710800	3.44722500
C	5.14218100	7.71315600	2.89090500
C	4.10854400	8.17128900	2.04024800
C	4.99762100	11.89937200	1.97737100
H	5.91922100	12.40544800	2.30439400
H	4.94450900	11.97530000	0.88852200
N	3.82823300	12.63604700	2.52974800
C	3.61778800	13.90938500	1.81869700
H	4.56913500	14.44744400	1.68725500
H	2.97673700	14.53929400	2.44276200
C	2.96918500	13.69323200	0.45277600
H	2.80809000	14.66690500	-0.03353600
H	3.63761900	13.11818800	-0.19205900
N	1.70146800	12.94647500	0.55711300
C	3.99517100	12.85760600	3.97039500
H	4.85726000	13.50969300	4.17968600
H	4.15021600	11.89808400	4.46812100
H	3.09055100	13.31406100	4.38026200
C	0.59378000	13.81958100	0.96467900

H	0.40679600	14.60102200	0.21248000
H	0.81545200	14.29419700	1.92306800
H	-0.31104100	13.22163200	1.09258200
C	1.38227800	12.27585200	-0.71080800
H	1.27767900	12.99902600	-1.53354500
H	0.44189600	11.72937200	-0.60253600
H	2.17028100	11.55795300	-0.94867400
C	3.04875700	7.27220100	1.34918000
C	3.10407900	7.51512700	-0.17631000
H	2.33754400	6.91075100	-0.67745400
H	4.08001400	7.21116100	-0.57308900
H	2.93624300	8.56378900	-0.42328000
C	1.64641200	7.62058400	1.89072900
H	1.59437000	7.43565000	2.96974100
H	0.88986700	6.99049900	1.40579200
H	1.38968900	8.66455400	1.70815500
C	3.21775800	5.75030000	1.53196400
H	3.09777900	5.43412700	2.56970800
H	4.18790400	5.39261700	1.17824200
H	2.43964700	5.25548000	0.93723000
O	5.18388300	6.37988100	3.17424900
H	6.87925700	8.20093500	4.09084600
C	6.17862700	5.87793700	4.03641000
H	6.10909500	6.31594000	5.04042900
H	5.99320600	4.80416600	4.10649500
H	7.18773500	6.03732700	3.63517000

1k

$G_{\text{solv}} = -2704.427636$

Zn	1.97337200	11.44155800	1.85536600
H	0.67024900	11.29266000	2.73793400
O	3.14132000	10.18390300	0.93789700
C	4.07008500	9.68496300	1.73644800
C	4.99071600	10.50448900	2.41176400
C	5.96590400	9.96467200	3.26349300
C	6.07443200	8.59545100	3.47010000
C	5.16117600	7.76672900	2.78837200
C	4.18482700	8.28158500	1.94622500
C	4.92587100	11.98388800	2.15027800
H	5.77459800	12.49889900	2.62644500
H	4.99921400	12.14908700	1.07227900
N	3.66008300	12.61323100	2.61098500
C	3.47792200	13.94566000	2.00986800
H	4.40044100	14.54165400	2.08930600
H	2.70691200	14.46676300	2.58581600
C	3.06113900	13.85439200	0.54367700
H	2.92163900	14.86843900	0.14024400
H	3.85390500	13.38463100	-0.04271100
N	1.83758100	13.05033000	0.36812600
C	3.63172000	12.69309300	4.07569700
H	4.42288200	13.35676900	4.45789200
H	3.77705000	11.69588500	4.49639700
H	2.65894900	13.06670100	4.40538100

C	0.63286200	13.84480700	0.63752500
H	0.53065400	14.66986900	-0.08397100
H	0.66943600	14.25864100	1.64771300
H	-0.24819500	13.20255700	0.57454200
C	1.77782500	12.47330500	-0.98144200
H	1.78856900	13.25609400	-1.75500500
H	0.85835000	11.89143900	-1.08436800
H	2.62479600	11.79895400	-1.12504000
H	5.21912800	6.69355900	2.93351700
H	6.64396200	10.65491600	3.75698800
O	3.27844100	7.52209800	1.27298700
C	3.34770500	6.12315700	1.41917100
H	3.17520500	5.81238900	2.45856800
H	2.55361600	5.71339500	0.79225100
H	4.31259400	5.72473200	1.07708200
C	7.12420100	7.96008700	4.39204000
C	8.03361500	9.01080400	5.04445900
C	6.42070000	7.17465800	5.51573500
C	8.01271600	6.99649200	3.58151800
H	8.59173500	9.58710700	4.29837000
H	7.46553000	9.71127000	5.66656000
H	8.76504800	8.51452800	5.69197500
H	5.79356800	6.37017400	5.11801200
H	7.15842400	6.71963100	6.18786700
H	5.77873800	7.83440700	6.10996100
H	8.77542500	6.54243400	4.22575700
H	7.42974600	6.18419200	3.13537600
H	8.52209700	7.52596000	2.76884000

II

$G_{\text{solv}} = -3027.404151$

Zn	1.89482700	11.59239800	1.82587400
H	0.81834000	11.48785000	2.99390900
C	4.09969800	9.49565500	1.51791200
C	5.00121400	10.44473900	2.06287100
C	6.00818500	10.06540300	2.94273000
H	6.69157300	10.80266300	3.35455700
C	6.14925500	8.73242800	3.30679500
C	5.26711100	7.79208300	2.78651300
H	5.38305200	6.76030400	3.08104200
C	4.23279600	8.13515600	1.89957300
C	4.91373000	11.90979000	1.70779900
H	5.84541000	12.41589300	2.00264200
H	4.79702400	12.00981600	0.62679100
N	3.77344400	12.61159700	2.35022100
C	3.63782700	13.97509400	1.80172300
H	4.62566800	14.44311800	1.67532100
H	3.09283800	14.57878100	2.53229600
C	2.90307200	13.98414900	0.46527300
H	2.83675700	15.01840500	0.09320300
H	3.46453300	13.40510900	-0.27299600
N	1.56324800	13.37988000	0.57199500
C	3.94204300	12.65659400	3.80848500

H	4.84986300	13.21084000	4.09303500
H	4.01148800	11.64176900	4.20325400
H	3.07046900	13.13682500	4.25955700
C	0.61161300	14.27042800	1.24726200
H	0.47763800	15.20862300	0.68691700
H	0.95158500	14.50431500	2.25784600
H	-0.35221900	13.76468500	1.33534700
C	1.05120700	13.02225700	-0.75641800
H	0.92859000	13.91237300	-1.39208300
H	0.08117500	12.52961600	-0.65078700
H	1.74152600	12.32812500	-1.24122100
C	3.29731100	7.00027200	1.41166600
C	3.37893500	6.85026300	-0.12066900
H	2.73946300	6.02113100	-0.44680300
H	4.40645300	6.62464100	-0.42893000
H	3.05456300	7.75188000	-0.64032200
C	1.85005400	7.27811000	1.86613100
H	1.79640600	7.32448300	2.96000600
H	1.19206200	6.46764300	1.53012100
H	1.46761100	8.21691500	1.46495700
C	3.67698500	5.62660100	1.99827600
H	3.61139200	5.60464500	3.09183000
H	4.68048300	5.30381300	1.69837300
H	2.97195300	4.87915100	1.61936500
O	7.16186700	8.44441900	4.17181500
C	7.33391100	7.10159700	4.57755500
H	8.18096400	7.10112600	5.26522600
H	6.44875800	6.72124300	5.10293000
H	7.56408500	6.44800000	3.72667900
S	2.86954300	10.09576600	0.35165000

1m

$G_{\text{solv}} = -3277.664265$

Zn	1.71532400	11.18226200	1.99505600
H	0.36559600	10.78989100	2.72237500
O	3.07597100	10.00055700	1.18338100
C	4.00485400	9.43960900	1.94924500
C	5.02390400	10.25816500	2.50597200
C	6.00995700	9.72272400	3.33431600
H	6.78026300	10.35948100	3.76364100
C	6.01261100	8.36421100	3.60848400
C	5.04250900	7.54141100	3.04128600
H	5.09047000	6.48475400	3.28066200
C	4.03601700	8.03655700	2.20773400
C	5.02591700	11.72534300	2.16788400
H	5.94541400	12.21395600	2.50887300
H	4.95738000	11.84905500	1.08116500
C	3.51978300	14.20226800	1.98080100
H	4.49485300	14.69862100	2.05423900
H	2.79563700	14.84407700	2.49705200
C	3.12713600	14.03108400	0.50394200
H	2.98255800	15.01118100	0.03426400
H	3.93352500	13.53378200	-0.04678700

C	4.08765900	13.04185900	4.57596300
H	4.99545100	13.65432000	4.56472900
H	4.28417100	12.12642500	5.14179500
H	3.28883300	13.58851600	5.08503800
C	0.24429100	14.18928400	0.54164800
H	0.32833100	15.05964300	-0.11741200
H	0.25215900	14.52469800	1.58304700
H	-0.71387300	13.69296400	0.36294800
C	1.58300000	12.70676900	-1.53581400
H	1.69321600	13.64033100	-2.09739000
H	0.63778300	12.23182400	-1.81388700
H	2.39398800	12.02376000	-1.80371500
C	2.99850200	7.09135500	1.57758500
C	3.06027500	7.20795600	0.04145300
H	2.31322800	6.54868600	-0.41818600
H	4.04780900	6.90785300	-0.32873600
H	2.86644100	8.23407000	-0.27757000
C	1.58196400	7.44331200	2.06951200
H	1.52485700	7.39553500	3.16294500
H	0.85319600	6.73154200	1.66159300
H	1.28579800	8.44629700	1.76006100
C	3.25652400	5.61988800	1.94015600
H	3.17083600	5.43721800	3.01725600
H	4.24355300	5.27860500	1.60793200
H	2.50891000	4.99132500	1.44362500
O	6.96625400	7.83278100	4.45755000
C	8.07311700	7.25805000	3.78439900
H	8.75237800	6.87758500	4.55116300
H	7.76355000	6.42767300	3.13561800
H	8.59856300	8.00600100	3.17447900
P	1.60792200	12.99639400	0.26988300
P	3.55901000	12.58695300	2.88584000

1n

$G_{\text{solv}} = -2665.136262$

Zn	1.92091400	11.40694100	2.16133900
H	0.58931900	11.37947400	2.99559100
O	3.00504200	10.11699200	1.20247900
C	3.95801400	9.55848500	1.94656400
C	4.97032600	10.38383500	2.49719400
C	5.99274200	9.85047100	3.28030300
H	6.76261400	10.49342600	3.70121100
C	6.02614300	8.48658100	3.52489000
C	5.04115900	7.66182600	2.98466400
H	5.10462000	6.60336400	3.21295300
C	3.99969900	8.15580800	2.19536100
C	4.92940800	11.85224100	2.17819000
H	5.84262200	12.35163500	2.53461600
H	4.88611000	11.97684500	1.09398500
N	3.74034600	12.53416400	2.75162600
C	3.32123400	13.70955700	1.97588100
H	4.16588500	14.15925400	1.43533700
H	2.91766200	14.45236400	2.66625600

N	2.24974700	13.30652900	1.04297000
C	3.92299800	12.80931300	4.17905100
H	4.72984400	13.53573800	4.35948800
H	4.17445100	11.87742200	4.69040000
H	2.99200200	13.19083600	4.60586300
C	1.10518800	14.22299100	1.07664300
H	1.37001500	15.22759000	0.71453400
H	0.72049500	14.29717400	2.09659600
H	0.30836500	13.82228400	0.44549700
C	2.71116100	13.09880300	-0.33507600
H	3.10339300	14.02704400	-0.77680100
H	1.87171700	12.74907200	-0.94076900
H	3.47868800	12.32450000	-0.36297300
C	2.92904800	7.21873800	1.61272400
C	2.93992600	7.31375100	0.07411300
H	2.16791100	6.65986600	-0.35040400
H	3.90943600	6.99346400	-0.32523400
H	2.74984000	8.33761300	-0.25407800
C	1.53705200	7.60564700	2.14957400
H	1.51518300	7.56045700	3.24449800
H	0.77926200	6.91048400	1.76743300
H	1.25809600	8.61514100	1.84313000
C	3.17507300	5.74941600	1.99004100
H	3.13502000	5.58744400	3.07313300
H	4.13972000	5.38351200	1.62060800
H	2.39534000	5.12644800	1.53808700
O	7.01655300	7.95093200	4.32611400
C	8.10638300	7.40715500	3.59993800
H	8.81384500	7.01264800	4.33310900
H	7.78268400	6.59271100	2.93816200
H	8.60348600	8.17811300	2.99525100

1o

$G_{\text{solv}} = -2743.705956$

Zn	2.03876800	11.78804500	2.05922300
H	0.75542400	11.98144800	2.97607000
O	2.91095800	10.21426400	1.33504200
C	3.91881500	9.65075900	1.98295100
C	5.00455600	10.44806400	2.42232200
C	6.08774500	9.88162100	3.09503300
H	6.91350400	10.50197400	3.43587400
C	6.11172500	8.51845200	3.33928000
C	5.04802700	7.72205300	2.91726500
H	5.09924800	6.66339200	3.14797400
C	3.94508000	8.24734600	2.24266600
C	4.99526100	11.92556700	2.13012300
H	5.94519300	12.37527900	2.46009000
H	4.91192700	12.08007000	1.05164500
N	3.87152500	12.66117900	2.76875200
C	3.94023100	14.10398300	2.45662000
H	4.92184100	14.48824800	2.78007200
H	3.18216700	14.60042700	3.07231600
C	3.71443500	14.50019000	0.99676400

H	3.93345900	15.57255000	0.94161600
H	4.44414800	14.02445800	0.33497800
N	1.85894500	12.93760300	0.22059100
C	3.91840100	12.49225600	4.23035200
H	4.85453900	12.89718500	4.64483000
H	3.85427200	11.43318400	4.48492500
H	3.06994700	13.01017500	4.68334100
C	0.42661600	12.93620400	-0.11740700
H	0.23402600	13.52333600	-1.02852300
H	-0.14880100	13.35684900	0.71027900
H	0.09090000	11.90932900	-0.28155600
C	2.60716600	12.32149400	-0.88435300
H	2.47432400	12.89672100	-1.81363500
H	2.25340200	11.30039300	-1.03260200
H	3.66932300	12.26092000	-0.65002900
C	2.77455800	7.35064800	1.80761500
C	2.59031900	7.43104900	0.27904700
H	1.75174200	6.79648100	-0.03414300
H	3.49099900	7.07887200	-0.23772400
H	2.38974600	8.45745200	-0.03368700
C	1.48186200	7.80425700	2.51457200
H	1.58952400	7.72842100	3.60274100
H	0.64191300	7.16534300	2.21451600
H	1.23484100	8.83792600	2.26522900
C	3.00492100	5.87494100	2.16924300
H	3.10245200	5.72376900	3.25021000
H	3.89519200	5.46336600	1.67988100
H	2.14535600	5.28392300	1.83388600
O	7.16825200	7.96225300	4.03591800
C	8.09975700	7.27889000	3.21471400
H	8.87347300	6.87845500	3.87417700
H	7.62770800	6.44924800	2.67175400
H	8.56003200	7.96167700	2.48714900
C	2.29204300	14.32911500	0.46418200
H	1.58891600	14.76190800	1.18509300
H	2.18976200	14.90032700	-0.47335500

1p

$G_{\text{solv}} = -2940.096983$

Zn	2.10149500	11.54216000	1.96062000
H	0.93473000	11.05316400	2.90359700
O	3.19857000	10.24166000	0.96498400
C	4.00924800	9.62371600	1.81673400
C	4.95153400	10.40434800	2.53070900
C	5.81464400	9.82650200	3.46034500
H	6.53461900	10.43348100	4.00515600
C	5.75436700	8.46036400	3.68822000
C	4.84468500	7.67712600	2.97847400
H	4.83441200	6.61407100	3.19507800
C	3.96551600	8.21686500	2.03690400
C	5.04028200	11.86198000	2.17899500
H	5.95978200	12.29880500	2.58604100
H	5.10182000	11.93729400	1.09138600

N	3.86301700	12.68025500	2.60000700
C	3.81406100	13.91872800	1.80081600
H	4.81655100	14.35800600	1.69559900
H	3.20345700	14.65297200	2.32948600
C	3.25506400	13.68371600	0.39773900
H	3.29053800	14.63773500	-0.14370000
H	3.90856000	12.99317000	-0.13967100
N	1.89231800	13.10025000	0.38577600
C	2.97728300	7.33135200	1.26180200
C	3.23100700	7.47412300	-0.25222900
H	2.51515500	6.86111600	-0.81419500
H	4.24087900	7.13416900	-0.51099600
H	3.12364200	8.51424200	-0.56722800
C	1.52968300	7.74903800	1.58459900
H	1.33071100	7.66915400	2.65916600
H	0.82232500	7.09596500	1.05796800
H	1.33969800	8.78025000	1.28276700
C	3.12452700	5.84461300	1.61999500
H	2.90681400	5.64955700	2.67610800
H	4.12784600	5.46402100	1.39720100
H	2.41361500	5.25905900	1.02638400
O	6.58215500	7.87952600	4.63148900
C	7.73697300	7.27376600	4.07626600
H	8.30570000	6.84790800	4.90635800
H	7.47279900	6.47167300	3.37402000
H	8.35881300	8.01284000	3.55237400
C	3.88002600	12.93297100	4.07630500
C	2.54631700	13.48349900	4.57922500
C	5.02466400	13.84127200	4.53972600
H	4.01899800	11.94145500	4.51964200
H	1.70577600	12.86080300	4.26377700
H	2.55692100	13.49883800	5.67340700
H	2.36841800	14.51248400	4.24689800
H	6.01115900	13.47736200	4.24138500
H	4.90716800	14.86274100	4.16093900
H	5.01888300	13.89419100	5.63247700
C	1.70981300	12.28320000	-0.86660900
C	1.97339700	12.99697000	-2.20060200
C	0.37196800	11.55214200	-0.91278600
H	2.48197600	11.51427400	-0.76159700
H	2.89006300	13.59330100	-2.18912600
H	2.10070400	12.23233300	-2.97394900
H	1.14816100	13.64050600	-2.51243900
H	0.13512400	11.06231400	0.03653400
H	-0.45541000	12.21637700	-1.18053500
H	0.42765400	10.77376500	-1.67996900
C	0.88383400	14.16106700	0.72470400
C	-0.41176900	13.63878400	1.34719900
C	0.56064200	15.14943900	-0.40161500
H	1.37619500	14.73360800	1.51686900
H	-0.21797900	12.92651900	2.15170300
H	-0.95650800	14.48839300	1.77267200
H	-1.07062500	13.16268400	0.61884300

H	1.45058800	15.51187300	-0.92330200
H	-0.11823700	14.71039100	-1.13807900
H	0.05445000	16.01988000	0.02825300

TS_{2b,3b}

$G_{\text{solv}} = -2912.339197$

Zn	1.91073300	0.16330700	-0.14408600
H	2.20170300	1.19300100	1.11750700
O	0.52162200	0.17618900	-1.45511300
C	-0.60421300	-0.38407300	-0.99144000
C	-0.56879000	-1.72694100	-0.54261800
C	-1.70611400	-2.34814700	-0.03997200
H	-1.63900500	-3.36781900	0.33368800
C	-2.92659800	-1.67303600	0.00888200
C	-2.95647500	-0.34837600	-0.43958900
H	-3.89712200	0.18501300	-0.39881900
C	-1.82869400	0.32446700	-0.92669800
C	0.73915000	-2.46845200	-0.60761400
H	0.59423200	-3.53148200	-0.36656300
H	1.13472400	-2.40353200	-1.62430300
N	1.77484800	-1.90955100	0.30958000
C	3.11598300	-2.43782900	-0.01289300
H	3.07805000	-3.52491600	-0.17372300
H	3.75922600	-2.26234400	0.85419900
C	3.71000600	-1.76629500	-1.25069600
H	4.72198200	-2.15638600	-1.42755100
H	3.11252900	-2.00665700	-2.13331400
N	3.73946400	-0.29260400	-1.11999900
C	1.42448600	-2.18111900	1.71187800
H	1.41830400	-3.26138900	1.91749100
H	0.43372500	-1.77552000	1.92414400
H	2.14586300	-1.69364600	2.37212000
C	4.88529800	0.15429200	-0.31053200
H	5.83445800	-0.11301300	-0.79619900
H	4.85255700	-0.30161400	0.68129800
H	4.84030200	1.23781800	-0.18453300
C	3.77530100	0.35003500	-2.44486000
H	4.66519900	0.04157600	-3.01145700
H	3.79662600	1.43484700	-2.31721000
H	2.87486500	0.08527800	-3.00341800
C	-1.90914500	1.79642700	-1.36629700
C	-1.51644100	1.92212300	-2.85166500
H	-1.54407800	2.97418500	-3.16150400
H	-2.21576800	1.36516800	-3.48631700
H	-0.50959500	1.53543000	-3.02258600
C	-0.95997300	2.65242400	-0.50282700
H	-1.19307000	2.54392400	0.56222800
H	-1.06289100	3.71244900	-0.76418500
H	0.08172100	2.36887200	-0.66081000
C	-3.32300300	2.37755500	-1.20735400
H	-3.65877400	2.36779500	-0.16423200
H	-4.06221400	1.84406700	-1.81568900
H	-3.32078800	3.42174800	-1.53889600

C	2.03085200	2.48431600	1.79608600
O	1.38982200	2.23717300	2.77902100
O	2.62186900	3.30223400	1.14550500
N	-4.07053600	-2.34513300	0.53125500
C	-5.19408800	-1.50740600	0.90264100
H	-5.72152600	-1.06679900	0.03665500
H	-5.91733800	-2.11358100	1.45699000
H	-4.86188500	-0.69644500	1.55636100
C	-4.50246500	-3.49140500	-0.25823200
H	-3.66171400	-4.15469800	-0.47001500
H	-5.24811900	-4.06241800	0.30448300
H	-4.95098900	-3.18816900	-1.22178100

TS_{2c,3c}

$G_{\text{solv}} = -2853.674317$

Zn	1.89545000	0.14095600	-0.12751800
H	2.09263600	1.20735400	1.11598000
O	0.52515700	0.09444300	-1.45655300
C	-0.58598300	-0.50241500	-1.00174700
C	-0.51033600	-1.83893500	-0.54579300
C	-1.63672600	-2.50921100	-0.07072700
H	-1.56654500	-3.53545100	0.28011100
C	-2.86051800	-1.85800500	-0.05094600
C	-2.94688800	-0.53846800	-0.49084900
H	-3.91696800	-0.05174800	-0.45027000
C	-1.83628300	0.16889900	-0.96250100
C	0.82261900	-2.53646200	-0.59625500
H	0.71193800	-3.60223700	-0.35026900
H	1.22249600	-2.46410800	-1.61071000
N	1.83242800	-1.93789900	0.32518000
C	3.19334700	-2.41807200	0.00871200
H	3.19369200	-3.50432500	-0.16061700
H	3.82401500	-2.22757700	0.88179200
C	3.77212600	-1.71632400	-1.21936500
H	4.79852500	-2.06860400	-1.39232100
H	3.18895000	-1.96877300	-2.10821700
N	3.74799800	-0.24405400	-1.07541300
C	1.48453700	-2.22183300	1.72571400
H	1.51407700	-3.30158000	1.93176200
H	0.47904000	-1.85093200	1.93227100
H	2.18507100	-1.70987800	2.38987000
C	4.86618600	0.23680900	-0.24666500
H	5.83047200	0.01440600	-0.72496700
H	4.84119100	-0.23492800	0.73797300
H	4.77570400	1.31561300	-0.10533300
C	3.77757800	0.41223900	-2.39397600
H	4.68348100	0.13855000	-2.95288200
H	3.76159400	1.49585000	-2.25575000
H	2.89282300	0.12275300	-2.96519200
C	-1.95603300	1.63722700	-1.40296400
C	-1.53715800	1.77806200	-2.87972900
H	-1.59464900	2.82918400	-3.18818400
H	-2.20363700	1.19891500	-3.52958200

H	-0.51453600	1.42624200	-3.02990500
C	-1.05200700	2.51967900	-0.51776000
H	-1.30807400	2.40648800	0.54145100
H	-1.17789700	3.57595500	-0.78373600
H	0.00047200	2.26432300	-0.64970900
C	-3.39085100	2.17160700	-1.27223700
H	-3.74638100	2.15339800	-0.23569600
H	-4.09935100	1.61316600	-1.89472400
H	-3.41669000	3.21453800	-1.60601100
C	1.98221900	2.54103000	1.72519700
O	1.34143100	2.36650500	2.72318600
O	2.59539900	3.30404000	1.02989600
O	-3.94979900	-2.54949300	0.41500200
H	-4.72494600	-1.97941700	0.39751800

TS_{2d,3d}

$G_{\text{solv}} = -2935.596175$

Zn	1.92919200	0.15128900	-0.13536200
H	2.20145100	1.18694200	1.12515200
O	0.52278800	0.14904100	-1.42921900
C	-0.57882300	-0.45303900	-0.96845700
C	-0.50355500	-1.79294700	-0.53048700
C	-1.63131100	-2.45750600	-0.04482600
H	-1.51409900	-3.48709800	0.28182500
C	-2.87028800	-1.82907400	0.01711300
C	-2.92508200	-0.49618800	-0.41834900
H	-3.88240200	0.00984000	-0.36363300
C	-1.83070900	0.21843700	-0.90317500
C	0.82202000	-2.49981800	-0.61039800
H	0.70601900	-3.56847900	-0.37814200
H	1.21199800	-2.41739400	-1.62813500
N	1.84976900	-1.92380300	0.30647100
C	3.20147100	-2.41826900	-0.02550300
H	3.18812000	-3.50454400	-0.19482600
H	3.84441000	-2.23423000	0.84006900
C	3.77354800	-1.72322800	-1.26069000
H	4.79492100	-2.08497300	-1.44356800
H	3.17938900	-1.97280800	-2.14299400
N	3.76423700	-0.25023800	-1.11935500
C	1.51124900	-2.21223000	1.70819000
H	1.52693300	-3.29389500	1.90604600
H	0.51350600	-1.82744700	1.92676900
H	2.22567700	-1.71558100	2.36914900
C	4.89954800	0.22065100	-0.30840900
H	5.85415300	-0.01574500	-0.79929200
H	4.88252200	-0.24605500	0.67874700
H	4.82494400	1.30113500	-0.17119500
C	3.78116600	0.40309000	-2.43947400
H	4.67769700	0.12207600	-3.00977100
H	3.77458300	1.48708500	-2.30354000
H	2.88721400	0.11904400	-2.99897800
C	-1.95585300	1.68914300	-1.33426000
C	-1.57568800	1.83234700	-2.82130100

H	-1.63848700	2.88385800	-3.12777000
H	-2.26047300	1.25499200	-3.45360900
H	-0.55797900	1.47884000	-2.99977000
C	-1.02783300	2.56953900	-0.47186700
H	-1.24978200	2.44720000	0.59405700
H	-1.16724500	3.62723600	-0.72556500
H	0.02133500	2.32062100	-0.63845500
C	-3.38563100	2.22654400	-1.16486000
H	-3.71487300	2.20212000	-0.11988000
H	-4.11163000	1.67292200	-1.77113300
H	-3.41702300	3.27152900	-1.49223100
C	2.02322500	2.48402300	1.79040200
O	1.37985700	2.24272900	2.77321800
O	2.61363700	3.29913500	1.13550200
C	-4.14171100	-2.51706500	0.53234200
C	-5.20746000	-2.52987500	-0.58025100
H	-6.12017700	-3.02844300	-0.23217900
H	-5.48069800	-1.51656600	-0.89202200
H	-4.84148900	-3.06381400	-1.46422800
C	-4.68954300	-1.74983300	1.75104400
H	-5.60058600	-2.22860700	2.12974400
H	-3.95268700	-1.72839600	2.56149300
H	-4.93867900	-0.71383200	1.50025600
C	-3.88201100	-3.96836400	0.96016500
H	-3.51967200	-4.58100700	0.12705900
H	-3.15299200	-4.02826900	1.77609100
H	-4.81382600	-4.41951000	1.31857700

TS_{2e,3e}

$G_{\text{solv}} = -2778.474263$

Zn	1.88906100	0.14105100	-0.12937500
H	2.07692400	1.21848500	1.10625500
O	0.50491900	0.09071500	-1.45005700
C	-0.60326400	-0.48455200	-0.97728900
C	-0.53060300	-1.81947000	-0.50603200
C	-1.66203800	-2.46023100	-0.00480300
H	-1.58275000	-3.48446000	0.35448500
C	-2.88043600	-1.79538500	0.03076400
C	-2.95131400	-0.47880200	-0.42767900
H	-3.91180500	0.02183700	-0.37552500
C	-1.84445900	0.20948000	-0.93118500
C	0.79540200	-2.52749200	-0.57058900
H	0.67873100	-3.59057100	-0.31495500
H	1.18544500	-2.46716900	-1.58977100
N	1.82286900	-1.93191200	0.33485900
C	3.17654500	-2.42250300	0.00306100
H	3.16542900	-3.50778800	-0.17140500
H	3.81772300	-2.24225100	0.87056900
C	3.74944800	-1.72023000	-1.22764300
H	4.77230800	-2.07775400	-1.41026900
H	3.15712800	-1.96582900	-2.11247600
N	3.73534600	-0.24802200	-1.07877300
C	1.49135900	-2.20643300	1.74128700

H	1.51688800	-3.28536700	1.95214400
H	0.49106300	-1.82768400	1.95864600
H	2.20345300	-1.69580400	2.39406800
C	4.85640800	0.22333100	-0.24793300
H	5.81926800	-0.00653000	-0.72534600
H	4.82652800	-0.24878900	0.73636500
H	4.77427000	1.30274800	-0.10624200
C	3.77023100	0.41207100	-2.39557300
H	4.67548600	0.13492900	-2.95365100
H	3.75976200	1.49528800	-2.25420400
H	2.88528400	0.12856400	-2.96948400
C	-1.94441700	1.67180500	-1.39653300
C	-1.56175700	1.77625400	-2.88609000
H	-1.60985500	2.82154200	-3.21547600
H	-2.25472500	1.19513900	-3.50579500
H	-0.54917000	1.40474200	-3.05684200
C	-1.00478700	2.55953800	-0.55426100
H	-1.22493200	2.46256900	0.51472600
H	-1.13389400	3.61309900	-0.82952500
H	0.04154000	2.29778900	-0.71813100
C	-3.36656500	2.23292200	-1.24023500
H	-3.69601700	2.23717000	-0.19514800
H	-4.10004300	1.67552500	-1.83370600
H	-3.38327700	3.27044200	-1.59156200
C	2.01298400	2.53360400	1.72558300
O	1.41003400	2.36153700	2.74846700
O	2.60722200	3.30016600	1.01635100
H	-3.76837900	-2.28589000	0.41754200

TS_{2f,3f}

$G_{\text{solv}} = -3238.066874$

Zn	1.47058200	0.09015200	0.24612800
H	1.71660800	1.11040600	1.51500600
O	0.06451100	0.22098000	-1.05633900
C	-1.05225700	-0.37979400	-0.65434700
C	-1.00915500	-1.75611900	-0.31712300
C	-2.15014900	-2.42991700	0.11255700
H	-2.10217400	-3.48441900	0.36961100
C	-3.34338100	-1.73468200	0.20057800
C	-3.41116600	-0.38410000	-0.12712900
H	-4.36768600	0.11540700	-0.03354200
C	-2.28622800	0.32383600	-0.55394900
C	0.29768000	-2.48825700	-0.45989400
H	0.15353100	-3.56883400	-0.31759000
H	0.68189000	-2.33030900	-1.47072200
N	1.34262800	-2.01637400	0.49442400
C	2.68113900	-2.50720100	0.10373400
H	2.63998300	-3.57136300	-0.16872200
H	3.33339800	-2.42226800	0.97752600
C	3.26124200	-1.70785100	-1.06226400
H	4.27161400	-2.07543700	-1.28909300
H	2.65541600	-1.85572000	-1.95967700
N	3.29065400	-0.25690300	-0.77486100

C	1.01128000	-2.42713400	1.86734000
H	1.01376300	-3.52219400	1.96666000
H	0.02086100	-2.05133600	2.13096900
H	1.73904700	-2.00265200	2.56309400
C	4.44206600	0.09954400	0.07164000
H	5.38698000	-0.11928700	-0.44531800
H	4.41322600	-0.45976500	1.00964400
H	4.39676000	1.16444600	0.30588600
C	3.32432300	0.52546100	-2.02392900
H	4.21332100	0.27716000	-2.62045800
H	3.34264000	1.58859500	-1.77671700
H	2.42384200	0.31997100	-2.60706600
C	-2.36937700	1.82125100	-0.89218100
C	-1.97976200	2.04214800	-2.36717600
H	-2.01469000	3.11151800	-2.60818600
H	-2.67653000	1.52236500	-3.03506800
H	-0.96978600	1.67677900	-2.56399500
C	-1.41812200	2.62146100	0.02122600
H	-1.63131000	2.43011900	1.07884300
H	-1.54148900	3.69585800	-0.15772800
H	-0.37652600	2.36630500	-0.17676900
C	-3.78560400	2.38186300	-0.69124500
H	-4.11895200	2.30015800	0.34953300
H	-4.52341000	1.88690300	-1.33264600
H	-3.78966900	3.44563000	-0.95163700
C	1.97919300	2.61481400	1.49406200
O	1.55545100	2.96375000	2.55364400
O	2.52873400	2.89136900	0.46226200
Cl	-4.79695400	-2.56674000	0.74348700

TS_{2g,3g}

$G_{\text{solv}} = -2891.768131$

Zn	1.84486400	0.25867500	-0.06715900
H	1.98435900	1.31254800	1.18954500
O	0.43492400	0.17085800	-1.38820400
C	-0.65874200	-0.42745300	-0.95430200
C	-0.55918900	-1.75245700	-0.44310300
C	-1.68281000	-2.40332600	0.04086000
H	-1.59469000	-3.41579400	0.43416500
C	-2.92784700	-1.77313200	0.02068400
C	-3.02608400	-0.47221400	-0.50005300
H	-4.01163500	-0.02054500	-0.49684800
C	-1.93282700	0.22513100	-0.99251200
C	0.78095000	-2.43572900	-0.47895100
H	0.67887600	-3.49444300	-0.20051200
H	1.17029400	-2.39517700	-1.49927800
N	1.79267600	-1.80310300	0.41332200
C	3.15717300	-2.27229300	0.09146400
H	3.17261500	-3.36400600	-0.03657200
H	3.79644000	-2.03650500	0.94672900
C	3.70208100	-1.60839200	-1.17200600
H	4.72847800	-1.95502800	-1.35371700
H	3.10524800	-1.89766300	-2.04041600

N	3.66573300	-0.13043200	-1.07884400
C	1.46993500	-2.06273800	1.82604800
H	1.52437900	-3.13763200	2.05118100
H	0.45833500	-1.71006800	2.03608100
H	2.16618100	-1.51680700	2.46565200
C	4.81654000	0.38479700	-0.31632800
H	5.75886800	0.15094900	-0.83092700
H	4.83922400	-0.05182400	0.68377900
H	4.72881400	1.46831900	-0.21260200
C	3.64166500	0.47582300	-2.42182600
H	4.53040800	0.18967500	-3.00121200
H	3.62026400	1.56392800	-2.32550900
H	2.74142900	0.15658600	-2.95129200
C	-2.06830500	1.65006100	-1.55183600
C	-1.60871900	1.67775600	-3.02297500
H	-1.70678800	2.69212200	-3.42820700
H	-2.22796300	1.01058100	-3.63375500
H	-0.56657700	1.36641000	-3.11766700
C	-1.21970500	2.63027700	-0.71750900
H	-1.52360200	2.61140100	0.33519400
H	-1.35530000	3.65343500	-1.08788200
H	-0.15671200	2.38895500	-0.77296300
C	-3.52188900	2.14607700	-1.50784700
H	-3.91000600	2.20004700	-0.48475700
H	-4.19312500	1.51351100	-2.09902800
H	-3.56877000	3.15624600	-1.92863800
C	3.01861700	1.73023000	2.23668400
O	3.25970100	0.75523300	2.89065500
O	3.18822100	2.89232100	2.02066300
C	-4.10258400	-2.47605200	0.53659500
O	-5.24011200	-2.03399500	0.56845700
H	-3.89959800	-3.49746400	0.92383300

TS_{2h,3h}

$G_{\text{solv}} = -2982.929839$

Zn	1.48760300	0.07622900	0.25602400
H	1.68028900	1.11129800	1.52452700
O	0.05053300	0.22710400	-1.02886200
C	-1.05607800	-0.36962400	-0.64112400
C	-1.00931300	-1.75469900	-0.30174700
C	-2.14388900	-2.42081900	0.12498300
H	-2.11064300	-3.47317500	0.38567700
C	-3.34066300	-1.71892100	0.20919800
C	-3.41308800	-0.36528600	-0.12728600
H	-4.37397600	0.12268000	-0.03323400
C	-2.29563700	0.33895600	-0.55245400
C	0.29643500	-2.48685300	-0.45455300
H	0.14820200	-3.56684700	-0.31610300
H	0.67415700	-2.32705700	-1.46757000
N	1.34764600	-2.02163200	0.49580000
C	2.68350400	-2.51533800	0.09416400
H	2.63547900	-3.57624900	-0.18792000
H	3.33899600	-2.44188300	0.96641300

C	3.26274500	-1.70713500	-1.06618500
H	4.27276900	-2.07253100	-1.29618200
H	2.65677500	-1.84727200	-1.96490800
N	3.29307000	-0.25734800	-0.76692100
C	1.02387200	-2.44097300	1.86916900
H	1.02401600	-3.53627400	1.95993800
H	0.03660700	-2.06452500	2.14310800
H	1.75776900	-2.02351500	2.56251600
C	4.44510400	0.09157800	0.08396200
H	5.38909000	-0.12440100	-0.43505200
H	4.41567600	-0.47541600	1.01731200
H	4.40099400	1.15497900	0.32531000
C	3.33235900	0.53478600	-2.01100900
H	4.22372900	0.28888000	-2.60422000
H	3.34973800	1.59576700	-1.75535200
H	2.43537300	0.33342800	-2.60089800
C	-2.37419300	1.83416000	-0.89752900
C	-1.98184000	2.04879700	-2.37265900
H	-2.01828600	3.11702100	-2.61693100
H	-2.67649700	1.52611400	-3.04028500
H	-0.97038000	1.68693900	-2.56867500
C	-1.42478900	2.63754000	0.01495400
H	-1.63508800	2.44523800	1.07291400
H	-1.55494300	3.71095000	-0.16315800
H	-0.38189000	2.39069600	-0.18548300
C	-3.79188800	2.39157300	-0.70030800
H	-4.12587500	2.31306300	0.34042500
H	-4.52806800	1.89183300	-1.33969400
H	-3.79828900	3.45400300	-0.96511200
C	1.93735800	2.58146700	1.46326200
O	1.54256500	2.96308800	2.52461900
O	2.45866400	2.84861400	0.41105000
N	-4.53205200	-2.40423900	0.66061400
O	-5.58777800	-1.77782900	0.71199200
O	-4.43875100	-3.58960600	0.97763000

TS_{2i,3i}

$G_{\text{solv}} = -2892.940483$

Zn	1.87114300	0.11086000	-0.10272500
H	2.09369300	1.15234500	1.16161600
O	0.50534900	0.13937500	-1.44809200
C	-0.61676800	-0.44904700	-1.03410400
C	-0.55215800	-1.79542600	-0.60363900
C	-1.70140400	-2.44710400	-0.13407800
C	-2.92013200	-1.77777400	-0.11785700
C	-2.96696500	-0.45082300	-0.55792600
H	-3.93242600	0.04167700	-0.51976900
C	-1.85647000	0.25253200	-1.01292300
C	0.76978600	-2.50609000	-0.68041200
H	0.64948700	-3.57919000	-0.49466000
H	1.17803100	-2.37452100	-1.68530700
N	1.77923500	-1.96453400	0.28053800
C	3.13489200	-2.45632900	-0.03949000

H	3.11896400	-3.53731500	-0.23908600
H	3.76195600	-2.29893900	0.84300300
C	3.73328400	-1.73009600	-1.24399200
H	4.75851900	-2.08682700	-1.41435600
H	3.15800600	-1.95651500	-2.14473400
N	3.72034600	-0.26148800	-1.06329700
C	1.40947100	-2.30451100	1.66318600
H	1.42881200	-3.39128900	1.82392800
H	0.40288000	-1.93606300	1.86880300
H	2.10314000	-1.82353600	2.35744500
C	4.84067700	0.18742600	-0.21965300
H	5.80392300	-0.02531500	-0.70441500
H	4.81231100	-0.31587200	0.74918800
H	4.75650900	1.26188000	-0.04448600
C	3.75832100	0.42900800	-2.36387100
H	4.66293500	0.16235800	-2.92823300
H	3.75129100	1.50864400	-2.19689800
H	2.87227500	0.16268400	-2.94420900
C	-1.93914700	1.72620400	-1.44039600
C	-1.48931100	1.88108800	-2.90678500
H	-1.52873900	2.93630200	-3.20459700
H	-2.14822700	1.31668300	-3.57709900
H	-0.46746500	1.52045800	-3.04201700
C	-1.04107500	2.58893600	-0.52974900
H	-1.31480200	2.46450100	0.52389300
H	-1.15074800	3.65025600	-0.78341100
H	0.01106300	2.32415900	-0.64746200
C	-3.36977500	2.27676700	-1.33235100
H	-3.74517400	2.25307200	-0.30305700
H	-4.07255800	1.72932600	-1.97081600
H	-3.37858100	3.32260000	-1.65858100
C	1.95768900	2.45955100	1.80196000
O	1.29471200	2.25630800	2.78073100
O	2.58212300	3.24762500	1.14440800
H	-3.82790100	-2.25326400	0.23286000
O	-1.53483100	-3.73468900	0.28859100
C	-2.66375200	-4.42662300	0.78302100
H	-2.30662000	-5.41555100	1.07529200
H	-3.08965800	-3.92552000	1.66113200
H	-3.43714200	-4.53818900	0.01335200

TS_{2j,3j}

$G_{\text{solv}} = -2892.926141$

Zn	1.85271900	0.12546300	-0.09741200
H	2.05063800	1.18582100	1.14862000
O	0.47367600	0.05958900	-1.42097300
C	-0.63399000	-0.54000000	-0.98186000
C	-0.51225900	-1.88154200	-0.52883600
C	-1.62876900	-2.55316100	-0.06091400
H	-1.53827800	-3.58034800	0.28641700
C	-2.86904700	-1.93084000	-0.03873200
C	-2.99216100	-0.60777000	-0.48329300
C	-1.88734200	0.13570700	-0.96326600

C	0.83122600	-2.55132800	-0.59524300
H	0.73739400	-3.62145700	-0.35925600
H	1.22865800	-2.46596900	-1.60963600
N	1.84229800	-1.95145700	0.32753300
C	3.20855200	-2.39912000	-0.01231100
H	3.22822700	-3.48237100	-0.19908500
H	3.84624500	-2.20961100	0.85595900
C	3.75886800	-1.66711600	-1.23647400
H	4.79125000	-1.99363200	-1.42399200
H	3.17278000	-1.92033800	-2.12318900
N	3.70269500	-0.19785200	-1.07234700
C	1.51460500	-2.26518800	1.72583600
H	1.56812800	-3.34753200	1.91366600
H	0.50340400	-1.91861400	1.94668800
H	2.21049400	-1.75015600	2.39252300
C	4.81570800	0.29734200	-0.24519400
H	5.78115400	0.10488300	-0.73402800
H	4.80953900	-0.18988900	0.73222300
H	4.70015600	1.37143900	-0.08698800
C	3.70650700	0.47741700	-2.38150300
H	4.61465500	0.23377600	-2.95057400
H	3.66536000	1.55823900	-2.22753500
H	2.82512300	0.17465500	-2.95096800
C	-1.93345800	1.61651100	-1.42928900
C	-1.44895900	1.70909100	-2.89295900
H	-1.43122900	2.75902700	-3.21088900
H	-2.13398600	1.17066400	-3.55841200
H	-0.44743700	1.29432800	-3.01197500
C	-1.01880900	2.46462200	-0.51693000
H	-1.32785800	2.38092000	0.53095100
H	-1.08336900	3.52181100	-0.80100500
H	0.02594000	2.16506500	-0.59711800
C	-3.31462800	2.30160400	-1.39559200
H	-3.72771500	2.36347000	-0.38655800
H	-4.04741100	1.80177700	-2.03245700
H	-3.18578000	3.32484800	-1.76937200
C	1.97174400	2.51944600	1.76011800
O	1.35172900	2.35131900	2.77203400
O	2.57817700	3.27522400	1.05133400
O	-4.20604000	0.00752400	-0.45844000
C	-5.31266800	-0.64381500	0.12353600
H	-5.12617400	-0.90202100	1.17362700
H	-6.13402500	0.07380400	0.07601000
H	-5.59847700	-1.54580500	-0.43238800
H	-3.73038100	-2.47736100	0.32222400

TS_{2k,3k}

$G_{\text{solv}} = -2892.935703$

Zn	1.80030400	0.35027100	-0.25042700
H	2.00269500	1.51314100	0.88539800
O	0.42846200	0.08684800	-1.56114500
C	-0.64219800	-0.54229900	-1.08891300
C	-0.55351300	-1.78550600	-0.43355000

C	-1.69528700	-2.42638600	0.05658800
H	-1.56800300	-3.38327500	0.55867800
C	-2.96774200	-1.87927100	-0.09298700
C	-3.06170100	-0.64414000	-0.75272200
H	-4.03228100	-0.18404200	-0.88494100
C	-1.93572300	0.01725300	-1.23840100
C	0.80085600	-2.43085000	-0.31337100
H	0.70843000	-3.44516300	0.10249300
H	1.23652000	-2.51929500	-1.31214800
N	1.75680800	-1.65531400	0.52342800
C	3.13987800	-2.13319700	0.33518200
H	3.18292200	-3.23158500	0.37937500
H	3.73820300	-1.75368300	1.16866000
C	3.72705900	-1.66099000	-0.99398400
H	4.76360400	-2.01521400	-1.08159000
H	3.16773400	-2.09326200	-1.82714100
N	3.67174800	-0.18859300	-1.13284500
C	1.36785300	-1.71055000	1.94045400
H	1.43373700	-2.73760500	2.32939700
H	0.33879300	-1.36084400	2.04576700
H	2.01661100	-1.05443300	2.52510100
C	4.78868700	0.45244100	-0.41902400
H	5.75279400	0.15210500	-0.85363700
H	4.77664000	0.17373000	0.63680700
H	4.69016400	1.53744800	-0.48484800
C	3.69154200	0.20420400	-2.55205700
H	4.60156200	-0.15743400	-3.05158600
H	3.66041300	1.29400500	-2.62361100
H	2.81065000	-0.19936900	-3.05580500
C	2.99215000	2.10832400	1.95819900
O	2.97316600	1.33561600	2.86944700
O	3.37728800	3.12106400	1.46063100
C	-4.19808200	-2.62118200	0.45184300
C	-4.30720600	-4.00379200	-0.22013100
C	-4.05601900	-2.80973500	1.97454200
C	-5.50557100	-1.86087200	0.18756800
H	-4.40386400	-3.90414700	-1.30677300
H	-3.42730200	-4.62317500	-0.01849400
H	-5.18617800	-4.54317100	0.15296200
H	-3.97595000	-1.84225800	2.48231200
H	-4.92815000	-3.33685200	2.37996000
H	-3.16667800	-3.39513200	2.22943700
H	-6.35022000	-2.43230600	0.58791300
H	-5.51359100	-0.87943500	0.67466100
H	-5.68584800	-1.71770100	-0.88362800
O	-1.97647300	1.22018400	-1.87274900
C	-3.23247900	1.82970900	-2.06475100
H	-3.72960800	2.04947900	-1.11042500
H	-3.03588000	2.76908800	-2.58463800
H	-3.89467600	1.21180900	-2.68606300

TS_{21,31}
 $G_{\text{solv}} = -3215.915609$

Zn	2.07751400	0.35979300	-0.23550100
H	2.24143500	1.23097400	1.14740100
C	-0.68933600	-0.39330300	-1.31693800
C	-0.45733300	-1.69637500	-0.80895000
C	-1.49221400	-2.46271900	-0.28647000
H	-1.30295700	-3.45914400	0.10211100
C	-2.78514500	-1.95685100	-0.24983300
C	-3.02274900	-0.67351700	-0.72824300
H	-4.02979000	-0.28829800	-0.68337100
C	-2.00509400	0.13546500	-1.26144000
C	0.91793800	-2.32092900	-0.80301000
H	0.82884000	-3.39886800	-0.60522900
H	1.37896400	-2.19158900	-1.78436400
N	1.83024400	-1.73253600	0.21362600
C	3.18840700	-2.29899100	0.08165600
H	3.14044800	-3.38835500	-0.06203800
H	3.71244800	-2.12207200	1.02466700
C	3.96198400	-1.67163900	-1.07306500
H	4.96329000	-2.12309000	-1.12999200
H	3.45864300	-1.87732500	-2.02106100
N	4.06193800	-0.20446400	-0.93200600
C	1.31824200	-1.95326500	1.57575300
H	1.24553300	-3.02710200	1.80353200
H	0.32818900	-1.50580500	1.67485200
H	1.98622300	-1.47111500	2.29190400
C	5.09229400	0.17258700	0.04824400
H	6.08756400	-0.15784400	-0.28327600
H	4.87776000	-0.26792900	1.02292200
H	5.10171800	1.25885000	0.16303900
C	4.36673600	0.41793400	-2.22951500
H	5.33250900	0.06689400	-2.62145200
H	4.41032000	1.50314900	-2.10900500
H	3.57893700	0.17834000	-2.94724800
C	-2.39535000	1.55677100	-1.74222700
C	-2.13403100	1.70906600	-3.25433100
H	-2.45414100	2.70352600	-3.58753800
H	-2.70769300	0.96421400	-3.81802700
H	-1.08019300	1.59286300	-3.50768300
C	-1.62613100	2.62123600	-0.93356500
H	-1.86436900	2.53580700	0.13310000
H	-1.92183700	3.62397200	-1.26412900
H	-0.54636600	2.52960500	-1.05203300
C	-3.89231900	1.85990700	-1.53501300
H	-4.18686400	1.82015900	-0.48053100
H	-4.54043700	1.18844100	-2.10919900
H	-4.09296300	2.87742600	-1.88605800
O	-3.73896300	-2.77448300	0.27280800
C	-5.06553700	-2.29225500	0.35885000
H	-5.64917600	-3.09807400	0.80606100
H	-5.13150600	-1.40440600	1.00031100
H	-5.47608200	-2.06027900	-0.63183900
C	3.10490000	1.57439100	2.47603400
O	3.27225300	0.52620000	3.02068200

O	3.23123600	2.75352700	2.39779900
S	0.70201700	0.48481400	-2.05243100
TS_{2m,3m}			
$G_{\text{solv}} = -3466.176809$			
Zn	1.76169300	0.42919600	0.02835800
H	1.78468400	1.70998400	1.05634700
O	0.38586500	0.08221800	-1.30723200
C	-0.74526800	-0.49663000	-0.90309700
C	-0.71641300	-1.86023900	-0.51210000
C	-1.87386000	-2.50933100	-0.08128900
H	-1.84640800	-3.55357100	0.22114700
C	-3.07353800	-1.81709400	-0.03992300
C	-3.11821100	-0.48123100	-0.43296300
H	-4.07748200	0.02083500	-0.37343000
C	-1.98392400	0.20682900	-0.87102700
C	0.59536400	-2.60038500	-0.56825700
H	0.45721300	-3.67361100	-0.39896800
H	1.05700400	-2.46916300	-1.55328200
C	3.44023300	-2.55820400	0.09778800
H	3.39579700	-3.64375100	-0.04794200
H	4.15291500	-2.37392600	0.91066900
C	3.91510300	-1.87832000	-1.19874000
H	4.93430000	-2.20011900	-1.44198000
H	3.27857700	-2.17986300	-2.03857700
C	1.45233000	-2.83404900	2.21007100
H	1.57058500	-3.91375300	2.07341500
H	0.42527300	-2.62264000	2.52107900
H	2.12461800	-2.49309500	3.00211600
C	5.38186900	0.44901600	-0.26021400
H	6.27017100	0.04834700	-0.75880300
H	5.35113000	0.08303700	0.77023000
H	5.44972600	1.53992500	-0.22358400
C	4.12588200	0.47610700	-2.86593700
H	5.02097400	0.00386100	-3.28327300
H	4.24035500	1.56281000	-2.90814700
H	3.25504400	0.20366600	-3.46837300
C	-2.07074300	1.68133100	-1.30362800
C	-1.62574700	1.81971600	-2.77333300
H	-1.65652000	2.87318700	-3.07804200
H	-2.29266200	1.25691100	-3.43702000
H	-0.60761400	1.44818700	-2.90771200
C	-1.17151800	2.55842700	-0.40993100
H	-1.39931500	2.40843300	0.65114500
H	-1.32742700	3.61874000	-0.64221500
H	-0.11663000	2.33477500	-0.57035200
C	-3.50121900	2.23356600	-1.19608700
H	-3.87220400	2.22259000	-0.16502100
H	-4.20772200	1.68110800	-1.82577700
H	-3.50909500	3.27544300	-1.53443400
O	-4.21238000	-2.44966100	0.41976200
C	-5.09528600	-2.86144700	-0.61056600
H	-5.94139600	-3.35476300	-0.12651800

H	-5.46325400	-2.00611100	-1.19244900
H	-4.60371900	-3.56919700	-1.29212900
C	2.01791200	3.17996400	1.50148900
O	1.46108300	3.22643300	2.55531400
O	2.66980600	3.69400400	0.64222900
P	1.79485200	-1.92573200	0.66391000
P	3.84914700	-0.02947200	-1.13397400

TS_{2n,3n}

$G_{\text{solv}} = -2853.642388$

Zn	1.71680300	0.61303500	-0.00133500
H	2.01621100	1.74822900	1.15635700
O	0.35645200	0.46242800	-1.32258800
C	-0.70622400	-0.25481800	-0.93874300
C	-0.52075700	-1.59482200	-0.52222300
C	-1.60306700	-2.38478500	-0.13470800
H	-1.45412700	-3.41378900	0.18361200
C	-2.88149300	-1.85148900	-0.15444200
C	-3.07450000	-0.53052100	-0.55633400
H	-4.08930500	-0.14905800	-0.53700600
C	-2.01911700	0.29375400	-0.95306900
C	0.87005900	-2.16668100	-0.54378500
H	0.84797000	-3.24468600	-0.33092900
H	1.29562900	-2.03610100	-1.54101400
N	1.78395000	-1.49783300	0.42581800
C	3.20171000	-1.57571100	0.03150900
H	3.40095100	-2.45747500	-0.59100100
H	3.80836900	-1.63718800	0.93609600
N	3.55422000	-0.32502200	-0.68389300
C	1.52834700	-1.95788300	1.79720000
H	1.75431900	-3.02692100	1.91578000
H	0.47410300	-1.79662600	2.03143600
H	2.13011200	-1.37981100	2.50190000
C	4.82114100	0.25468700	-0.20812500
H	5.67766800	-0.38378400	-0.46480300
H	4.78669700	0.39226600	0.87410800
H	4.96167200	1.23271100	-0.67372300
C	3.58226900	-0.46717700	-2.14962400
H	4.35513000	-1.18104600	-2.46634400
H	3.79919900	0.50691900	-2.59336300
H	2.60957100	-0.79046800	-2.52189800
C	-2.26362600	1.75226000	-1.37539700
C	-1.77783100	1.96976600	-2.82212200
H	-1.94033800	3.01289500	-3.11977500
H	-2.33476600	1.33129100	-3.51776600
H	-0.71462700	1.74201900	-2.91816700
C	-1.51493500	2.70616800	-0.42343900
H	-1.83382500	2.55156400	0.61392600
H	-1.72798500	3.74853100	-0.68865400
H	-0.43449800	2.55991100	-0.47891300
C	-3.75313500	2.12819800	-1.32499700
H	-4.16796500	2.04833200	-0.31389900
H	-4.35819400	1.51028300	-1.99809900

H	-3.87146600	3.16936000	-1.64402800
O	-3.94807300	-2.62023900	0.26366800
C	-4.77627800	-3.08335300	-0.79103100
H	-5.57311100	-3.67317900	-0.33267900
H	-5.22341000	-2.25150200	-1.35057300
H	-4.20998900	-3.71684000	-1.48719500
C	3.09953700	2.50262600	1.77958100
O	3.49883800	1.82552300	2.68973100
O	3.18713500	3.53608700	1.17717700

TS_{20,30}

$G_{\text{solv}} = -2932.216205$

Zn	2.00640200	0.10623000	-0.01116300
H	2.30639700	1.07115700	1.30487100
O	0.53492400	0.25678000	-1.23613200
C	-0.57937200	-0.38659100	-0.89483900
C	-0.51304500	-1.76546600	-0.58549300
C	-1.66272400	-2.48233700	-0.25161900
H	-1.60752300	-3.54055500	-0.00768100
C	-2.88752600	-1.83639100	-0.21679700
C	-2.96077600	-0.47205500	-0.49658900
H	-3.93611000	-0.00332300	-0.42356400
C	-1.83528300	0.28217600	-0.83204900
C	0.82478300	-2.45589500	-0.61951000
H	0.69491100	-3.53678700	-0.46213900
H	1.28844500	-2.31155400	-1.59955500
N	1.78600100	-1.94367300	0.40457300
C	3.07404500	-2.67026700	0.32085500
H	2.86800100	-3.75075600	0.36888400
H	3.64571700	-2.41266100	1.21893800
C	3.93872600	-2.37903900	-0.90671100
H	4.75657700	-3.10752800	-0.87908500
H	3.40000700	-2.58640500	-1.83598200
N	3.69322000	0.12997200	-1.27446800
C	1.22753700	-2.11712600	1.75892300
H	1.04445600	-3.17997400	1.97391500
H	0.28567800	-1.57383900	1.84646300
H	1.92866700	-1.71666800	2.49444100
C	4.41026200	1.40059000	-1.05267200
H	5.30931700	1.45625800	-1.68325600
H	4.69981700	1.48595600	-0.00342300
H	3.75333000	2.23826000	-1.29489300
C	3.24590000	0.06696900	-2.67784100
H	4.10994500	0.06704000	-3.35804700
H	2.61299900	0.92909600	-2.89199600
H	2.64537700	-0.82602600	-2.85065400
C	-1.93173500	1.79486100	-1.08965500
C	-1.46128300	2.11469500	-2.52223900
H	-1.51676500	3.19492200	-2.70555700
H	-2.09986800	1.61429400	-3.25977400
H	-0.43123300	1.78733100	-2.67702200
C	-1.05860300	2.55470800	-0.06938700
H	-1.36285600	2.32013700	0.95672000

H	-1.16369100	3.63665900	-0.21345800
H	-0.00368100	2.30008100	-0.18372600
C	-3.36954200	2.31710500	-0.94407900
H	-3.76380900	2.16627800	0.06704700
H	-4.05528800	1.84694800	-1.65814000
H	-3.38183500	3.39464700	-1.14127100
O	-4.02123800	-2.53665800	0.14538400
C	-4.85875000	-2.87623300	-0.94725800
H	-5.71383500	-3.41854500	-0.53723200
H	-5.22025200	-1.98206400	-1.47195700
H	-4.33073100	-3.51961500	-1.66438000
C	2.10174000	2.30546800	2.15709100
O	1.45219300	1.93053200	3.08873900
O	2.68565600	3.18780100	1.59666600
C	4.59502100	-0.99891200	-0.94712000
H	5.03818100	-0.78493300	0.03193600
H	5.41652600	-1.00914300	-1.67990900

TS_{2p,3p}

$G_{\text{solv}} = -3128.613538$

Zn	1.64088300	-0.06399100	0.04209500
H	1.65535000	1.12225600	1.16736000
O	0.19603200	0.06141100	-1.25278500
C	-0.94692600	-0.38200500	-0.73063600
C	-1.00052500	-1.71365300	-0.25364200
C	-2.16798200	-2.23563800	0.30251900
H	-2.20091800	-3.25973100	0.66805100
C	-3.29724700	-1.43719000	0.38886200
C	-3.25645500	-0.12349800	-0.07668600
H	-4.16178900	0.46419900	0.02981800
C	-2.10724800	0.43746500	-0.63786700
C	0.22463400	-2.56720200	-0.42101500
H	-0.01160000	-3.61914700	-0.22469200
H	0.54858600	-2.49800700	-1.46078200
N	1.38297100	-2.15013400	0.43387500
C	2.63562300	-2.72966700	-0.09767800
H	2.50226400	-3.79382400	-0.33678500
H	3.40543400	-2.66573600	0.67434800
C	3.10666000	-2.01537300	-1.36504500
H	3.98833700	-2.53770200	-1.74419200
H	2.34324100	-2.11047800	-2.13961300
N	3.35072600	-0.56286900	-1.18159900
C	-2.07935700	1.89708000	-1.11898900
C	-1.71473500	1.95066200	-2.61583700
H	-1.68236400	2.99288900	-2.95678100
H	-2.46431800	1.42305000	-3.21748600
H	-0.73916500	1.49390400	-2.79557800
C	-1.04002400	2.69327700	-0.30542800
H	-1.27157300	2.65855900	0.76489100
H	-1.03890400	3.74447100	-0.61814900
H	-0.03626800	2.29343400	-0.45444600
C	-3.43803200	2.59276500	-0.94397500
H	-3.74324200	2.64439900	0.10705700

H	-4.23315100	2.09718700	-1.51294200
H	-3.36498300	3.62181400	-1.31300200
O	-4.45182400	-1.93057100	0.96520300
C	-5.39167400	-2.42267800	0.02444100
H	-6.26134200	-2.76509900	0.59007600
H	-5.70427100	-1.63804800	-0.67753300
H	-4.97667100	-3.26471800	-0.54660400
C	1.66225600	2.36002400	2.08937700
O	1.01110800	2.02395500	3.03121400
O	2.32833100	3.16957900	1.51665800
C	1.12220400	-2.50167700	1.86979000
C	2.03983900	-1.75069800	2.82915400
C	1.18010200	-4.00558800	2.15328700
H	0.10104300	-2.15203300	2.04857200
H	2.01329200	-0.67123400	2.65959200
H	1.70254100	-1.92705400	3.85469200
H	3.07737100	-2.09646400	2.76802900
H	0.53426400	-4.59201800	1.49423900
H	2.20113900	-4.39396300	2.06967800
H	0.84446200	-4.18726400	3.17825100
C	3.07435700	0.17057200	-2.47198900
C	4.05008200	-0.16268200	-3.60116200
C	2.97564300	1.67997700	-2.26262700
H	2.07529300	-0.16907500	-2.76073800
H	4.12393700	-1.23937600	-3.78281100
H	3.69498300	0.30138900	-4.52630200
H	5.05359000	0.22845900	-3.40313900
H	2.30808400	1.94021900	-1.43535200
H	3.94565100	2.15297300	-2.07967400
H	2.55696000	2.13368400	-3.16565300
C	4.71194800	-0.22526400	-0.61374800
C	5.82188700	-1.22730800	-0.94402400
C	4.67259900	0.02992100	0.88997500
H	4.98770100	0.72131700	-1.08181000
H	5.88392400	-1.46200100	-2.00942200
H	6.77879900	-0.78574900	-0.65019500
H	5.71523300	-2.16367900	-0.38531100
H	3.98498400	0.84028300	1.14231300
H	4.38366600	-0.86234600	1.45214600
H	5.66873400	0.32516700	1.23488500

A text file of all computed molecule Cartesian coordinates in an .xyz format for convenient visualization in the Supporting Information.