

Supplementary Materials: Reaction Mechanisms of CO₂ Reduction to Formaldehyde Catalyzed by Hourglass Ru, Fe, and Os Complexes: A Density Functional Theory Study

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

Ru-1cyp			
$G_{\text{solv}} = -1955.921603$; $E_{\text{solv}} = -1956.70639802$			
C	11.07314000	4.92736400	8.15168400
H	11.15644800	5.32178000	9.17175300
C	10.92655900	3.37682200	8.23346500
H	11.67245900	2.85101200	7.63151100
H	11.06414200	3.04799700	9.26880400
C	9.49828900	3.05918400	7.74773000
H	9.51469200	2.82560600	6.67517400
H	9.05967400	2.20009100	8.26551600
C	8.72310400	4.36112900	7.96508300
H	8.46832600	4.47994400	9.02666400
H	7.79266900	4.41145600	7.38998900
C	9.74245200	5.42284900	7.54508200
H	9.48373700	6.43505500	7.87380500
H	9.80656800	5.43359200	6.44914800
C	13.94326200	5.13831600	8.42515200
H	13.65536400	5.61035900	9.37343100
C	14.20778900	3.64215200	8.69561600
H	13.54296600	3.23248000	9.46244200
H	14.06555700	3.06121100	7.77623800
C	15.68646700	3.59769000	9.09274400
H	15.81295100	3.96304200	10.12081200
H	16.11021500	2.58894400	9.04328000
C	16.32974000	4.56971500	8.09995900
H	16.44275400	4.06892100	7.13043500
H	17.32060400	4.91592500	8.41196600
C	15.31285400	5.72051600	7.96285100
H	15.27535400	6.07807300	6.92926500
H	15.59045100	6.57031400	8.59651100
C	12.52067200	7.34934700	7.33568100
H	13.54550800	7.63678400	7.06892500
C	12.20559500	7.98444000	8.70323800
H	11.33136700	7.51161200	9.16904300
H	13.04033500	7.90569400	9.40737600
C	11.86018000	9.43109900	8.33829800
H	11.36077000	9.97287400	9.14840000
H	12.77916400	9.97749600	8.08890500
C	10.98226400	9.27265400	7.08991900
H	10.94991900	10.17841000	6.47641900
H	9.95179200	9.05565200	7.39843200
C	11.57049600	8.06018400	6.32977900
H	12.13395200	8.36500700	5.44319000
H	10.77182700	7.40489000	5.97390900
C	13.29995100	4.66586100	1.49983200

H	13.87690300	4.19858100	0.69135800
C	13.49676000	6.19336000	1.41384100
H	14.50975600	6.46620900	1.10284200
H	13.31255900	6.65436400	2.39263400
C	12.41911300	6.64430900	0.42387800
H	12.23345500	7.72300000	0.45623900
H	12.71804200	6.38750000	−0.60122800
C	11.20304000	5.81365100	0.84540900
H	10.73652700	6.27944500	1.72294800
H	10.43665500	5.74341700	0.06674200
C	11.78273000	4.43629700	1.23430700
H	11.65066900	3.70750000	0.42736700
H	11.26484000	4.03566400	2.11325100
C	13.54257800	2.10556500	2.72832700
H	12.46263600	2.09425600	2.53376900
C	13.81264100	1.12151600	3.90846500
H	14.40948300	1.57080100	4.70512200
H	12.86167900	0.82884200	4.36580900
C	14.51896900	−0.10046200	3.28471800
H	15.60508500	−0.01335100	3.41429800
H	14.21331500	−1.04382900	3.74804300
C	14.18060200	−0.02757500	1.79181100
H	13.16359300	−0.40250500	1.61619400
H	14.86325000	−0.61133400	1.16536800
C	14.23699800	1.47568700	1.50240200
H	13.75095300	1.75203800	0.56084300
H	15.28655700	1.78767300	1.43665800
C	15.72232700	4.06980500	2.93686800
H	15.96878600	3.78589100	1.90651600
C	16.25520800	5.51380500	3.18753200
H	16.67766600	5.91419200	2.25898500
H	15.46874800	6.19710400	3.51528500
C	17.34776900	5.37518900	4.26298600
H	18.14610900	6.11632100	4.15077800
H	16.90098300	5.51188000	5.25502600
C	17.83479400	3.93106000	4.12569000
H	18.38589600	3.57513200	5.00281900
H	18.49455100	3.83243000	3.25296900
C	16.52865300	3.16597600	3.89579000
H	16.00532900	3.07337400	4.85419900
H	16.67565600	2.15853400	3.49233900
P	12.57785600	5.49487500	7.21824400
P	13.87706900	3.90104200	3.09155600
Ru	12.91477100	4.68263100	5.06008200
H	14.29814200	4.12348200	5.67604200
H	13.77793900	6.04346200	4.86138400
H	11.76714900	5.40373100	3.97299700
H	11.48750500	5.63124200	4.76823400
H	11.77908900	3.35989200	5.11573500
H	12.50139800	3.08667600	5.53665800
H₂			
$G_{\text{solv}} = -1.176234; E_{\text{solv}} = -1.17487290$			
H	−0.55660100	0.40462400	0.00000000
H	−1.30004700	0.40462400	0.00000000
1Ru			
$G_{\text{solv}} = -1954.728561; E_{\text{solv}} = -1955.49581633$			
C	11.18942800	4.83258200	8.16025100
H	11.14421400	5.29312000	9.15555800

C	11.20464900	3.28218500	8.32792700
H	12.00718300	2.81233700	7.75137200
H	11.37076600	3.02176100	9.37810600
C	9.82302500	2.78590500	7.84797700
H	9.89552200	2.43492700	6.81073100
H	9.44370000	1.95328200	8.44878500
C	8.92390200	4.02474000	7.89675900
H	8.59840000	4.22020400	8.92710100
H	8.02722600	3.93102500	7.27509700
C	9.86641200	5.13428200	7.42547100
H	9.49294900	6.14364500	7.62689100
H	10.00761800	5.04118800	6.34035700
C	13.98969700	5.40385300	8.60671900
H	13.57565400	5.91269400	9.48663800
C	14.37805200	3.96060100	9.00677900
H	13.74062000	3.56402300	9.80314800
H	14.28919900	3.29305100	8.14147000
C	15.85379900	4.06106500	9.40522800
H	15.94924500	4.50170100	10.40690100
H	16.35602000	3.08775000	9.41860600
C	16.41495700	5.01753300	8.35127800
H	16.52679600	4.48076500	7.40095100
H	17.39099200	5.43679400	8.61691900
C	15.32678900	6.09490600	8.20128600
H	15.30473100	6.48255700	7.17857400
H	15.52258400	6.93961600	8.87213600
C	12.40344700	7.33322800	7.20185100
H	13.41302400	7.73321600	7.04876500
C	11.80041600	8.05825700	8.41960900
H	10.96181400	7.49454700	8.84664100
H	12.53443700	8.21295300	9.21732400
C	11.27538800	9.36704200	7.81962300
H	10.57699400	9.89301500	8.47900500
H	12.11531000	10.04393700	7.61561400
C	10.63027600	8.91415900	6.50292000
H	10.51999700	9.72924200	5.78087700
H	9.62499100	8.52470400	6.70672100
C	11.54124000	7.77843500	5.98273800
H	12.19492600	8.12827800	5.17642600
H	10.94548800	6.95799900	5.56884300
C	13.34594400	4.86278900	1.67517200
H	13.78552900	4.43035200	0.76739900
C	13.70383500	6.36526900	1.72601100
H	14.69476400	6.57249100	1.31200900
H	13.70151200	6.72281100	2.76478000
C	12.56993800	7.04448800	0.95416300
H	12.51858100	8.12396300	1.13146600
H	12.70234200	6.88810500	−0.12470400
C	11.33181700	6.29304300	1.44879900
H	11.05369900	6.67139800	2.44126600
H	10.46015200	6.41491100	0.79790900
C	11.78998400	4.82358500	1.55887800
H	11.49570400	4.25341200	0.67101100
H	11.31968800	4.33584800	2.42038500
C	13.41110500	2.17569500	2.65742900
H	12.33114400	2.29686400	2.50502200
C	13.60425200	1.09415500	3.76397400
H	14.30813300	1.40746700	4.53813000

H	12.65185300	0.91451800	4.27380900
C	14.09142300	−0.17520800	3.03127000
H	15.18148800	−0.26402200	3.12100700
H	13.65820100	−1.09191500	3.44379300
C	13.72391500	0.05169200	1.56001200
H	12.65943000	−0.16376600	1.39763100
H	14.29907900	−0.57566700	0.87090100
C	13.98549500	1.54896100	1.37090900
H	13.52606200	1.95766000	0.46461200
H	15.06730400	1.71451200	1.29674600
C	15.80052100	3.86040400	2.86133200
H	15.96427600	3.56269800	1.81858200
C	16.51106900	5.22716600	3.09660200
H	16.88874000	5.61411000	2.14344700
H	15.83817700	5.97835700	3.51609000
C	17.67084000	4.93833300	4.06945200
H	18.54866900	5.56354300	3.87509200
H	17.33989100	5.13723200	5.09619600
C	17.94643300	3.44095600	3.90953200
H	18.50599500	3.01353200	4.74846600
H	18.52141700	3.25370300	2.99233500
C	16.53698500	2.85861600	3.77832200
H	16.06632000	2.84214000	4.76868600
H	16.52017600	1.83808700	3.38029000
P	12.68886800	5.49817000	7.28515200
P	13.96389100	3.88851900	3.13444500
Ru	13.19126400	4.63947800	5.19362800
H	14.15073000	3.60880300	5.85347200
H	14.46179400	5.68462500	5.23116500
H	11.72818300	3.72958600	4.99914400
H	12.30201400	3.22834500	5.46916400
2Ru			
$G_{\text{solv}} = -2143.264129$; $E_{\text{solv}} = -2144.04734419$			
C	−2.05990400	−0.06004600	2.99291600
H	−1.96934400	0.24307200	4.04289200
C	−2.01720200	−1.61897100	2.92360600
H	−1.27408300	−1.98531300	2.20962300
H	−1.74474000	−2.02500900	3.90280000
C	−3.43948100	−2.06477400	2.52383000
H	−3.48917200	−2.23154200	1.43954200
H	−3.73693600	−2.99942400	3.00933000
C	−4.33484200	−0.87889100	2.89242500
H	−4.52740300	−0.86866900	3.97322700
H	−5.30237200	−0.89295600	2.38042500
C	−3.47142100	0.32270600	2.50146600
H	−3.81724200	1.26908100	2.92755500
H	−3.48567900	0.42932100	1.40858900
C	0.75731400	0.53482500	3.22170600
H	0.44437100	0.97833100	4.17466000
C	1.16658400	−0.92965000	3.49545100
H	0.58729300	−1.37552400	4.31004500
H	1.01705300	−1.54567000	2.60169400
C	2.66649200	−0.84335500	3.79473600
H	2.83107100	−0.45670200	4.80936400
H	3.16944200	−1.81333200	3.72073700
C	3.15046400	0.16887300	2.75490100
H	3.19628200	−0.32395200	1.77616400
H	4.14332600	0.57764100	2.96802800

C	2.05445000	1.24968900	2.73388500
H	1.95028700	1.69084900	1.73736100
H	2.30424800	2.06571600	3.42128700
C	-0.96316200	2.59655300	2.28777000
H	-0.01605000	3.02857300	1.94295700
C	-1.20947300	3.09801600	3.72891300
H	-1.86583800	2.41453200	4.28309900
H	-0.28045800	3.19914200	4.29881300
C	-1.93412200	4.43221600	3.52576200
H	-2.42930900	4.79140100	4.43395300
H	-1.21632400	5.20016900	3.20935900
C	-2.90791100	4.12226000	2.38549800
H	-3.29016400	5.02037700	1.89052900
H	-3.77387500	3.57940700	2.78627500
C	-2.10524100	3.22099500	1.42669500
H	-1.66396800	3.81153000	0.61938100
H	-2.73730900	2.47496000	0.94159100
C	0.05146300	-0.33349500	-3.73576800
H	0.43556900	-1.03534500	-4.48743000
C	0.59517700	1.06428100	-4.09521300
H	1.62693100	1.02584600	-4.45636200
H	0.56842200	1.73748100	-3.23361600
C	-0.39444700	1.55675000	-5.15501700
H	-0.32324000	2.63443800	-5.33257100
H	-0.20367300	1.04675300	-6.10906000
C	-1.75304400	1.13363500	-4.58552900
H	-2.07292000	1.86503800	-3.83613000
H	-2.53518300	1.07307300	-5.34917300
C	-1.49300800	-0.22605500	-3.89705800
H	-1.86892800	-1.06085000	-4.49882900
H	-2.00645600	-0.26544400	-2.93035100
C	-0.05412300	-2.77332900	-2.27937900
H	-1.11683300	-2.64154900	-2.52657800
C	0.02462400	-3.66072400	-1.00169100
H	0.75917200	-3.28953600	-0.28430500
H	-0.93883600	-3.65384900	-0.48171900
C	0.39700400	-5.07894300	-1.49406500
H	1.45823400	-5.27408900	-1.29581000
H	-0.17431900	-5.86282600	-0.98740500
C	0.16137300	-5.05481000	-3.00926000
H	-0.90258600	-5.20932300	-3.23191500
H	0.72755800	-5.82425000	-3.54392600
C	0.56822600	-3.63118900	-3.39884500
H	0.22161200	-3.34275100	-4.39625800
H	1.66282300	-3.55474600	-3.39095600
C	2.39197000	-1.13212100	-2.20520700
H	2.61660000	-1.58944400	-3.17700400
C	3.11587500	0.24626700	-2.12642600
H	3.50848100	0.51388100	-3.11242800
H	2.45118400	1.05476300	-1.81407800
C	4.26062600	0.06699200	-1.10778800
H	5.16763800	0.60499400	-1.40079700
H	3.94759000	0.46226100	-0.13477600
C	4.46792000	-1.44704900	-1.00458200
H	4.97594500	-1.74934500	-0.08264000
H	5.06790000	-1.80890800	-1.85023500
C	3.04079300	-1.99310300	-1.10088100
H	2.52899800	-1.82786000	-0.14520300

H	2.99676000	−3.06450200	−1.32575400
P	−0.67849300	0.77277400	2.07292100
P	0.54849400	−1.02232700	−2.08926600
Ru	−0.30160300	−0.00940000	−0.12787300
H	0.34686000	−1.24307600	0.61577500
H	1.21056300	0.23801100	0.20025000
H	−1.72334600	−1.04227400	−0.59513900
H	−1.94113800	−0.75080900	0.14767300
C	0.08691300	1.89543700	−0.71861400
O	−1.07190100	1.78854400	−1.17908200
O	0.95135200	2.74614500	−0.65857500
TS_{2,3}-Ru			
$G_{\text{solv}} = -2143.255352; E_{\text{solv}} = -2144.03527333$			
C	10.87380400	5.18149900	7.76658200
H	10.88560600	5.45737400	8.82773700
C	10.92714900	3.62443700	7.67449000
H	11.72002500	3.26350800	7.01374100
H	11.13268100	3.20571000	8.66456000
C	9.53709600	3.18107100	7.17160000
H	9.56047100	3.03140900	6.08388000
H	9.21086800	2.23823000	7.62171000
C	8.61417500	4.35905000	7.49541700
H	8.34760400	4.35158900	8.56048000
H	7.68414600	4.34975000	6.91820800
C	9.49743200	5.56957900	7.18468600
H	9.11816600	6.50653800	7.60387300
H	9.56241900	5.69763700	6.09637400
C	13.69035800	5.77432200	8.16121400
H	13.36480300	6.19570400	9.11985500
C	14.06236500	4.28927500	8.38747100
H	13.49651200	3.84241400	9.21107100
H	13.86141700	3.69987500	7.48624200
C	15.57567100	4.30828100	8.62840800
H	15.79745700	4.64410300	9.65029800
H	16.03662200	3.32405500	8.49250600
C	16.05496700	5.34881900	7.61519500
H	16.02343800	4.91128700	6.60945400
H	17.07581000	5.70110600	7.79537000
C	15.01244100	6.47375200	7.71687700
H	14.91650100	7.02036100	6.77456300
H	15.31228600	7.20241600	8.47896400
C	11.95390600	7.87681300	7.32111200
H	12.92658600	8.34829000	7.13903100
C	11.50972200	8.26472500	8.74825500
H	10.77837800	7.55260200	9.15062000
H	12.34903500	8.30793600	9.44971700
C	10.82372300	9.61986200	8.54725800
H	10.21071700	9.91935800	9.40388200
H	11.58016700	10.39880500	8.38711800
C	10.01000200	9.40528700	7.26692900
H	9.71033500	10.34238800	6.78779500
H	9.09053700	8.85684100	7.50958900
C	10.92137100	8.54831300	6.36454800
H	11.45221100	9.17082600	5.63942300
H	10.34826900	7.82428400	5.77963100
C	12.92139000	4.90028900	1.13524400
H	13.30001700	4.17655200	0.40078800
C	13.41573800	6.29634100	0.71185700

H	14.45423300	6.28634200	0.36793300
H	13.33340300	7.00058000	1.54609700
C	12.42588200	6.68738200	−0.38927800
H	12.45712200	7.75494800	−0.62879800
H	12.65459100	6.13210800	−1.30888400
C	11.07113900	6.24409900	0.17864200
H	10.67692400	7.02946500	0.83232000
H	10.32534900	6.06287800	−0.60173900
C	11.37353500	4.97400600	1.01213400
H	10.98413600	4.06908200	0.53298900
H	10.89869100	5.04617000	1.99732700
C	12.79218400	2.56614700	2.74899900
H	11.71847400	2.72993500	2.58582800
C	12.94432300	1.72558300	4.05269200
H	13.70681000	2.12446700	4.72374800
H	12.00473900	1.74294400	4.61493900
C	13.29528800	0.29294000	3.59254900
H	14.37462300	0.12384000	3.69306200
H	12.79154100	−0.47467300	4.18801700
C	12.91373200	0.24658700	2.10877800
H	11.83225600	0.09256800	1.99863500
H	13.42129400	−0.55245100	1.55888100
C	13.28991400	1.64627700	1.61552900
H	12.84579400	1.89554300	0.64665400
H	14.38021300	1.70776200	1.50747600
C	15.30199100	4.12386200	2.60750600
H	15.46915400	3.59541100	1.66159100
C	16.05994300	5.48752500	2.55198700
H	16.53976600	5.59626500	1.57334400
H	15.40472600	6.35317400	2.67865900
C	17.11803500	5.42514100	3.66645600
H	18.01670700	5.99986400	3.42153800
H	16.70231500	5.84072600	4.59276100
C	17.38291300	3.92941500	3.85086400
H	17.87561000	3.69234900	4.79965900
H	18.01968200	3.55335800	3.03892800
C	15.97780700	3.32843600	3.74937000
H	15.45293100	3.50715700	4.69475300
H	15.97375500	2.24918200	3.56163900
P	12.29422000	6.08205200	6.97685900
P	13.46790900	4.29924600	2.79988200
Ru	12.75548400	5.43381800	4.74430600
H	13.52913600	4.28105400	5.48952100
H	14.21216300	6.13156100	4.58907100
H	11.25750000	4.60118300	4.43861200
H	11.56289800	4.25886900	5.16261600
C	13.39202200	7.45580200	4.43913100
O	12.39857800	7.42141200	3.69157500
O	14.15215400	8.29801200	4.87112500
3Ru			
$G_{\text{solv}} = -2143.269743$; $E_{\text{solv}} = -2144.04797961$			
C	−1.63795900	−0.44106100	3.09479400
H	−1.82203700	0.00141900	4.08114100
C	−0.93462000	−1.81965200	3.29973200
H	0.00560800	−1.90259600	2.74904800
H	−0.69699000	−1.95627900	4.35997700
C	−1.94737400	−2.88174300	2.82979000
H	−1.76061600	−3.13152100	1.77727400

H	−1.87839900	−3.81031400	3.40515000
C	−3.30792300	−2.19095200	2.94949200
H	−3.63035100	−2.16502700	3.99878500
H	−4.09484800	−2.68400700	2.36946100
C	−3.00280100	−0.77542100	2.45303300
H	−3.77343800	−0.04219500	2.71205000
H	−2.91675400	−0.79698100	1.36027700
C	0.67542300	1.26185100	3.38695500
H	0.15062500	1.47126700	4.32743800
C	1.72585600	0.15383700	3.64272500
H	1.41309100	−0.54315600	4.42583000
H	1.89419500	−0.42974500	2.72831800
C	3.00720400	0.91851300	3.98801900
H	2.95844800	1.29279900	5.01927200
H	3.90614800	0.29969100	3.89940000
C	2.97630300	2.08596000	3.00024000
H	3.27486800	1.73338400	2.00441600
H	3.64932300	2.90545000	3.26952800
C	1.50058500	2.52124800	2.97758000
H	1.22846300	2.92557500	1.99902900
H	1.32323900	3.32319400	3.70237700
C	−1.66042100	2.32939400	2.07808000
H	−0.94494600	3.09978300	1.76862900
C	−2.32145000	2.80832500	3.38508300
H	−2.78568300	1.97406800	3.92686500
H	−1.60798100	3.28905900	4.06244200
C	−3.41773300	3.75540400	2.88763200
H	−4.16171900	3.99162000	3.65544100
H	−2.96731100	4.69998800	2.55655300
C	−4.00672600	3.00200400	1.68845700
H	−4.55246800	3.65642000	1.00176000
H	−4.71715300	2.24717100	2.04971800
C	−2.79839900	2.31435600	1.01412000
H	−2.46585200	2.85673400	0.12500500
H	−3.05208000	1.30598600	0.67956400
C	0.25393800	0.13278000	−3.59546600
H	0.28146700	−0.55146800	−4.45319700
C	1.32254100	1.21500300	−3.84530700
H	2.22997700	0.80390300	−4.29914700
H	1.61204100	1.71846500	−2.91905400
C	0.59469300	2.21619300	−4.74745800
H	1.10846100	3.18083300	−4.80648900
H	0.51627400	1.81397400	−5.76677900
C	−0.79258300	2.31647200	−4.10269200
H	−0.74309200	2.99727200	−3.24687500
H	−1.55524300	2.69592700	−4.79046100
C	−1.10702600	0.88834200	−3.60114300
H	−1.81778200	0.37722200	−4.26007400
H	−1.55530000	0.92383300	−2.60256400
C	−0.77721000	−2.25451200	−2.46631600
H	−1.70339700	−1.68116600	−2.60411900
C	−1.04070700	−3.29863700	−1.33964200
H	−0.23810200	−3.33393000	−0.60002000
H	−1.95079900	−3.02688000	−0.79517300
C	−1.19525100	−4.66127100	−2.05167500
H	−0.26208000	−5.23266500	−1.97064600
H	−1.98863500	−5.27546800	−1.61450700
C	−1.44941000	−4.31315300	−3.52244300

H	-2.50134600	-4.03605100	-3.67058600
H	-1.22321900	-5.13821300	-4.20550000
C	-0.55777300	-3.08864800	-3.74546000
H	-0.81021700	-2.53741400	-4.65655800
H	0.48720800	-3.41281000	-3.83165400
C	2.12749100	-1.70660400	-2.34789700
H	2.18177000	-2.00777400	-3.40088600
C	3.31541800	-0.74200300	-2.03887700
H	3.89305900	-0.56724600	-2.95244200
H	2.99242600	0.23987900	-1.68252500
C	4.17762900	-1.46341200	-0.98757700
H	5.23838200	-1.20634600	-1.06856700
H	3.84609300	-1.18544100	0.02185300
C	3.88814800	-2.94743800	-1.22378400
H	4.18657300	-3.58658300	-0.38634500
H	4.41632000	-3.29870500	-2.12008300
C	2.37568000	-2.95030400	-1.46231100
H	1.87357800	-2.83678700	-0.49379700
H	2.00250000	-3.87060500	-1.92340300
P	-0.62836000	0.79376000	2.15022800
P	0.46698400	-0.92401800	-2.09018900
Ru	0.07877900	0.05797100	0.02445200
H	0.81394900	-1.17559200	0.66409700
H	1.72711500	1.20443900	0.05428600
H	-1.41594200	-0.28822100	-0.25629100
H	-0.46984400	-1.32961400	0.45541800
C	1.30573800	2.17492800	-0.46481300
O	0.07218900	2.12449100	-0.73317200
O	2.14890000	3.04093600	-0.64380900
TS_{3,4-Ru}			
$G_{\text{solv}} = -2143.267578; E_{\text{solv}} = -2144.04765806$			
C	-1.52908100	-0.46600200	3.14421500
H	-1.73412600	-0.00123200	4.11591100
C	-0.80699700	-1.82757600	3.39538800
H	0.15413600	-1.90417500	2.88074000
H	-0.60290200	-1.94194400	4.46530900
C	-1.78418700	-2.91646000	2.91322300
H	-1.57197000	-3.16969700	1.86606600
H	-1.70520800	-3.83894600	3.49705100
C	-3.16131600	-2.25476200	3.00101100
H	-3.50166500	-2.22334500	4.04444100
H	-3.92716000	-2.77241900	2.41429600
C	-2.87867500	-0.83949100	2.49057800
H	-3.66782900	-0.11940300	2.72974900
H	-2.77791000	-0.87341200	1.39951600
C	0.76300100	1.26607600	3.41907800
H	0.23254900	1.45840300	4.36021300
C	1.84469200	0.18991000	3.67560700
H	1.54197300	-0.53316000	4.43862600
H	2.05127600	-0.37009000	2.75327300
C	3.08990300	0.99284600	4.06206900
H	3.00094400	1.35148900	5.09616100
H	4.01205300	0.40680700	3.99009900
C	3.04435500	2.17126700	3.08763400
H	3.39193200	1.84260100	2.09942500
H	3.67532500	3.01248900	3.38936500
C	1.55350800	2.54978800	3.01629700
H	1.29624700	2.92813700	2.02363600

H	1.32320100	3.35561400	3.72132500
C	-1.57311600	2.28152800	2.06692600
H	-0.86507500	3.05176000	1.74097800
C	-2.24375500	2.78424500	3.35974900
H	-2.70535000	1.95911700	3.91771400
H	-1.53693100	3.28476500	4.02980600
C	-3.34353500	3.71278200	2.83567200
H	-4.09305300	3.96150800	3.59414500
H	-2.89720600	4.65244100	2.48568900
C	-3.92154100	2.92879600	1.65071500
H	-4.46625000	3.56465500	0.94600700
H	-4.63079100	2.17928200	2.02525000
C	-2.70626000	2.23126100	0.99917400
H	-2.37171200	2.75133000	0.09768000
H	-2.95269100	1.21311500	0.69037400
C	0.34948400	0.11964100	-3.55031900
H	0.35335100	-0.55260000	-4.41782800
C	1.44033400	1.18091300	-3.79524800
H	2.33034600	0.75702500	-4.27153900
H	1.75532000	1.65825500	-2.86360400
C	0.72442300	2.21856800	-4.66498400
H	1.26056700	3.17166500	-4.70993800
H	0.62173400	1.84073500	-5.69159900
C	-0.64985500	2.33760100	-3.99663900
H	-0.56766800	2.99040400	-3.12183800
H	-1.41208700	2.75714300	-4.66130900
C	-0.99496200	0.90484100	-3.53112100
H	-1.71745400	0.42652400	-4.20204800
H	-1.43953500	0.92478700	-2.53066700
C	-0.70559500	-2.27286800	-2.45191300
H	-1.62322400	-1.68503300	-2.58804400
C	-0.98787500	-3.31852100	-1.33289300
H	-0.16386800	-3.40471100	-0.62112600
H	-1.86516000	-3.01132800	-0.75491500
C	-1.22435400	-4.66379400	-2.05842800
H	-0.33172500	-5.29559800	-1.97281900
H	-2.05998700	-5.22808400	-1.63309000
C	-1.44380300	-4.29300700	-3.53008400
H	-2.48104400	-3.97113500	-3.69047400
H	-1.24349100	-5.12227700	-4.21609000
C	-0.50002700	-3.10463900	-3.73371900
H	-0.71830500	-2.53867400	-4.64465500
H	0.53279600	-3.46884500	-3.80700800
C	2.20732300	-1.76157800	-2.34300300
H	2.25949900	-2.04281300	-3.40166000
C	3.40236500	-0.81238400	-2.01297300
H	3.97994800	-0.61800900	-2.92244400
H	3.08386900	0.16280600	-1.63299100
C	4.26151700	-1.56316600	-0.97961800
H	5.32416700	-1.31328500	-1.05765400
H	3.93528600	-1.30451100	0.03692500
C	3.95890000	-3.03929800	-1.24654000
H	4.25456500	-3.69884300	-0.42408500
H	4.48134800	-3.37540400	-2.15183400
C	2.44603400	-3.02385100	-1.48126800
H	1.94772200	-2.92425900	-0.50895600
H	2.06271800	-3.93232900	-1.95706900
P	-0.52526500	0.75940300	2.17916100

P	0.55682000	−0.96348500	−2.06353500
Ru	0.19458200	−0.01157500	0.06971100
H	0.80616000	−1.34479400	0.71289000
H	1.95622200	1.36871800	0.07681100
H	−1.29320900	−0.35076200	−0.20947700
H	−0.23708700	−1.45488000	0.55947400
C	1.41025600	2.24096100	−0.44239700
O	0.18042100	2.01779200	−0.67668800
O	2.09001100	3.23006100	−0.68656600
4Ru			
$G_{\text{solv}} = -2143.272023; E_{\text{solv}} = -2144.05278249$			
C	−1.76752900	−0.36046400	3.15364400
H	−1.85387900	0.09485700	4.14764800
C	−1.28953600	−1.83466900	3.33275900
H	−0.42739300	−2.07921200	2.70691000
H	−0.98265600	−1.99891000	4.37064700
C	−2.50077000	−2.72018800	2.97067700
H	−2.41828300	−3.05509900	1.92864100
H	−2.56689100	−3.61551500	3.59659500
C	−3.71335100	−1.79518100	3.10621200
H	−3.98666500	−1.67650900	4.16298600
H	−4.59597000	−2.16075000	2.57154600
C	−3.18367400	−0.47180500	2.54999800
H	−3.81071100	0.39147900	2.79426800
H	−3.12698700	−0.54411600	1.45560400
C	0.81861400	0.94610300	3.30959500
H	0.40639300	1.29962600	4.26274300
C	1.64970900	−0.33459900	3.56845800
H	1.28550700	−0.89793800	4.43280100
H	1.60831500	−0.99836100	2.69671800
C	3.08772800	0.16816100	3.73457600
H	3.22733700	0.60113700	4.73394000
H	3.83010400	−0.62700700	3.60821400
C	3.18370500	1.26171700	2.66949400
H	3.27694000	0.79708400	1.67914300
H	4.03915100	1.93086000	2.80449600
C	1.83699900	1.99612000	2.76845700
H	1.54587600	2.41416500	1.80187800
H	1.90596700	2.83654300	3.46778300
C	−1.39775400	2.39132200	2.16809200
H	−0.58180600	3.05079800	1.85069800
C	−1.94341600	2.93464700	3.50390600
H	−2.48763600	2.16010700	4.05922700
H	−1.14969000	3.31401600	4.15586900
C	−2.93222000	4.01802400	3.06058500
H	−3.61291000	4.32945400	3.85987200
H	−2.38236900	4.90564200	2.72297000
C	−3.65232800	3.36287700	1.87624300
H	−4.15164200	4.08851700	1.22694100
H	−4.42408500	2.67991900	2.25465400
C	−2.55334400	2.57121900	1.13656500
H	−2.17531600	3.11796600	0.26957100
H	−2.93709500	1.61942100	0.75612900
C	0.23801600	0.04397100	−3.60527300
H	0.34103500	−0.62451400	−4.46808900
C	1.22088900	1.21809300	−3.80540100
H	2.13313400	0.90414100	−4.32296000
H	1.51711200	1.65184900	−2.84742300

C	0.40211400	2.24790600	-4.59023500
H	0.84196800	3.24931900	-4.55459000
H	0.32911100	1.94644800	-5.64431900
C	-0.97115800	2.17837700	-3.91559800
H	-0.93323300	2.73303600	-2.97218800
H	-1.77274600	2.60396000	-4.52807200
C	-1.18497400	0.67947700	-3.62433100
H	-1.79451500	0.20513100	-4.40183500
H	-1.71574000	0.54128300	-2.67392100
C	-0.49125700	-2.49268800	-2.55944100
H	-1.48737300	-2.07078600	-2.75070100
C	-0.64825400	-3.58467100	-1.45761500
H	0.08872800	-3.48801600	-0.65732800
H	-1.63143400	-3.49058200	-0.98468000
C	-0.50486900	-4.94184200	-2.18047100
H	0.51264500	-5.33053100	-2.04745600
H	-1.19266200	-5.69880500	-1.79127600
C	-0.73562400	-4.62590800	-3.66192500
H	-1.81055900	-4.53986800	-3.86861800
H	-0.32771600	-5.38830200	-4.33343200
C	-0.06531100	-3.25960800	-3.82999500
H	-0.36462200	-2.74841100	-4.74991600
H	1.02346900	-3.39281200	-3.86352200
C	2.27910100	-1.51315400	-2.22024800
H	2.47090000	-1.77468700	-3.26851500
C	3.28250100	-0.40014800	-1.78876500
H	3.77572300	0.02334200	-2.66873600
H	2.78118300	0.42544500	-1.27468200
C	4.30076800	-1.08639300	-0.85156300
H	5.32055800	-0.71792400	-0.99940200
H	4.03021200	-0.89159000	0.19396300
C	4.15088900	-2.58372000	-1.13641200
H	4.53330300	-3.21587600	-0.32838500
H	4.68603900	-2.85436400	-2.05617200
C	2.64202400	-2.72994100	-1.34459900
H	2.14275400	-2.65805200	-0.36968500
H	2.35036200	-3.68022900	-1.80358600
P	-0.62036000	0.70880000	2.16500400
P	0.50642200	-0.99142800	-2.09324100
Ru	-0.11022300	-0.06627200	-0.00150000
H	1.31230100	-0.39352600	0.50601600
H	1.98120200	2.52624700	-0.46891600
H	-0.96765600	-1.38554400	0.30772200
H	0.04136900	-1.54037200	0.57639700
C	0.94014800	2.83040500	-0.71304900
O	0.07159800	1.89139000	-0.64393800
O	0.71656600	3.99795300	-1.02694000
TS _{4,5-Ru}			
G _{solv} = -2143.270082; E _{solv} = -2144.05152607			
C	-1.57476400	-0.44840400	3.20596600
H	-1.61327200	-0.00616200	4.20941500
C	-0.91623000	-1.85768500	3.31856100
H	-0.11837200	-2.00667300	2.58708400
H	-0.46695700	-1.97890100	4.30942400
C	-2.05404200	-2.87764800	3.09585100
H	-2.04668800	-3.21844900	2.05274000
H	-1.95199100	-3.76370400	3.73020000
C	-3.34136800	-2.09087100	3.35736600

H	-3.51676400	-1.99208600	4.43676700
H	-4.22811700	-2.55700000	2.91576900
C	-3.02313400	-0.72335300	2.74917500
H	-3.71554100	0.06625400	3.05736400
H	-3.07007700	-0.80037500	1.65557800
C	0.80555200	1.21964600	3.17380100
H	0.41237800	1.58639300	4.12926500
C	1.78374400	0.04224700	3.43673500
H	1.60379900	-0.43470000	4.40503500
H	1.67186600	-0.72904600	2.66678000
C	3.18642600	0.65026700	3.31149000
H	3.46467700	1.16939600	4.23803700
H	3.95416300	-0.10369400	3.10822200
C	3.01275000	1.66293500	2.17918300
H	2.94139500	1.13285000	1.21958300
H	3.83433400	2.38253000	2.10381400
C	1.66981500	2.32989800	2.50325700
H	1.20711900	2.75796200	1.61067800
H	1.81892700	3.15356200	3.21093600
C	-1.67554000	2.30967700	2.18235700
H	-0.98482100	3.08193200	1.82263700
C	-2.22378300	2.78182000	3.54295700
H	-2.64125500	1.94572900	4.11833900
H	-1.45610800	3.25981300	4.16064000
C	-3.35688100	3.73253400	3.14288900
H	-4.03488000	3.96324500	3.97138500
H	-2.93408200	4.67851200	2.78158500
C	-4.04375000	2.98995400	1.98974600
H	-4.63917700	3.65312000	1.35486900
H	-4.72615000	2.23430300	2.40019000
C	-2.89538200	2.30898100	1.21262900
H	-2.62865200	2.86559000	0.31050800
H	-3.17732900	1.30268400	0.88961400
C	0.48570500	0.12839100	-3.61520600
H	0.68573300	-0.53066600	-4.47025200
C	1.56885600	1.22442100	-3.61061100
H	2.55552700	0.83390700	-3.88013800
H	1.64327600	1.68469200	-2.62074600
C	1.03049700	2.24591900	-4.61731400
H	1.52486700	3.21992000	-4.54010800
H	1.18410900	1.87517100	-5.63974600
C	-0.46736100	2.31214900	-4.29155700
H	-0.63261400	3.00275900	-3.45837600
H	-1.06644600	2.66909600	-5.13523000
C	-0.85475400	0.87807200	-3.85899500
H	-1.44054700	0.36512500	-4.62961100
H	-1.47010900	0.91055300	-2.95285200
C	-0.76285900	-2.25586200	-2.69366600
H	-1.65667800	-1.67217600	-2.95001200
C	-1.18541800	-3.32079000	-1.63540200
H	-0.53967000	-3.32601400	-0.75509200
H	-2.19395700	-3.09539000	-1.27320900
C	-1.14725500	-4.67968800	-2.36525500
H	-0.19723200	-5.18878900	-2.15824100
H	-1.95039600	-5.35054400	-2.04492700
C	-1.21719500	-4.32573300	-3.85414500
H	-2.25157000	-4.09268000	-4.13911200
H	-0.86558400	-5.13165700	-4.50643100

C	-0.35712000	-3.06182400	-3.94679900
H	-0.51799600	-2.50208000	-4.87348900
H	0.70322700	-3.34283000	-3.90941800
C	2.09976000	-1.73980500	-2.09328100
H	2.34978500	-2.00747400	-3.12706900
C	3.20419200	-0.78430900	-1.53823200
H	3.91456100	-0.53858700	-2.33435300
H	2.79638300	0.16296100	-1.17178000
C	3.90444700	-1.56203100	-0.40788000
H	4.96657400	-1.31167700	-0.32180600
H	3.43007200	-1.32569100	0.55408800
C	3.64945000	-3.03262600	-0.74703700
H	3.81091600	-3.70662800	0.10055500
H	4.30980200	-3.35465800	-1.56303800
C	2.19324000	-3.01102400	-1.21950200
H	1.54573700	-2.91949700	-0.33956300
H	1.89144900	-3.91246600	-1.76278200
P	-0.66358700	0.76073300	2.13478900
P	0.42271200	-0.94873300	-2.11315400
Ru	-0.15475800	0.03113000	-0.03900500
H	1.05065300	-0.72206000	0.57169000
H	1.17485000	3.62035300	-0.65254500
H	-1.40095800	-0.89663600	0.03813000
H	-0.23216900	-1.43804800	0.48839300
C	0.13986800	3.23053300	-0.75926700
O	0.06891400	1.95249300	-0.75551900
O	-0.78929700	4.02260400	-0.90048100
5_{Ru}			
$G_{\text{solv}} = -2143.275915; E_{\text{solv}} = -2144.05601824$			
C	-0.99223400	-0.50475900	3.32781300
H	-1.14182000	-0.01302800	4.29631200
C	0.05147500	-1.65042500	3.51644500
H	0.89398800	-1.57369400	2.82402000
H	0.46639300	-1.60660100	4.52896300
C	-0.72168800	-2.96618200	3.30108700
H	-0.62728300	-3.28588900	2.25483900
H	-0.34654200	-3.78077700	3.92863700
C	-2.18082700	-2.60144200	3.58406300
H	-2.35241500	-2.53218200	4.66649900
H	-2.89366900	-3.32621300	3.17760500
C	-2.30590000	-1.21932800	2.93850800
H	-3.19176100	-0.66394400	3.26229900
H	-2.36708900	-1.34103900	1.84988400
C	0.90601800	1.67162600	3.05424200
H	0.55145900	1.85103700	4.07821400
C	2.22890600	0.88463600	3.13757500
H	2.21128300	0.10470600	3.90441200
H	2.44600000	0.39883000	2.17472800
C	3.26933100	1.97318800	3.41247000
H	3.19530500	2.29503700	4.45961900
H	4.29705100	1.63639700	3.24123800
C	2.84528400	3.10970300	2.47467800
H	3.26648500	2.93741600	1.47679200
H	3.20045400	4.08884700	2.81012600
C	1.30053200	3.03146400	2.40724500
H	0.97065700	3.08862600	1.36646500
H	0.82554500	3.85848500	2.94494000
C	-1.79591700	2.08773700	2.16651000

H	-1.34950800	2.93296400	1.62805100
C	-2.25134500	2.60083200	3.54743400
H	-2.37057800	1.77401900	4.25995600
H	-1.54361100	3.31383100	3.98350600
C	-3.62536700	3.21146000	3.25494700
H	-4.21715700	3.38889000	4.15928000
H	-3.50057600	4.17376000	2.74178700
C	-4.26107900	2.18770800	2.30678800
H	-5.09069600	2.60306700	1.72646300
H	-4.66344200	1.35244900	2.89529000
C	-3.10213400	1.70038600	1.41056900
H	-3.10282100	2.18902500	0.43349300
H	-3.17591000	0.62866700	1.21386700
C	1.09649900	0.08530600	-3.51606200
H	1.35376400	-0.59566200	-4.33926000
C	2.31971100	0.97786900	-3.23890300
H	3.26221600	0.42150300	-3.25856400
H	2.22086100	1.45642500	-2.25758800
C	2.22761800	2.03507700	-4.34373500
H	2.85007400	2.91375800	-4.14513000
H	2.56146600	1.60222600	-5.29611300
C	0.72912000	2.36707200	-4.40465900
H	0.49617200	3.15963100	-3.68491200
H	0.42124800	2.73021200	-5.38999700
C	-0.00543600	1.06373000	-4.00282300
H	-0.55482500	0.63020600	-4.84502400
H	-0.73825500	1.27087000	-3.21597400
C	-0.90027500	-1.83926800	-2.84269000
H	-1.56320400	-1.00834500	-3.11271500
C	-1.69881000	-2.78039900	-1.89060300
H	-1.14802700	-3.03425900	-0.98220500
H	-2.61296800	-2.27566700	-1.56231600
C	-2.02054200	-4.04184400	-2.72055800
H	-1.29762100	-4.83533600	-2.49160500
H	-3.01697700	-4.44115200	-2.50773600
C	-1.84855800	-3.60750300	-4.18044200
H	-2.73410800	-3.05272200	-4.51669300
H	-1.70219100	-4.44861700	-4.86591000
C	-0.64168000	-2.66656600	-4.11885700
H	-0.53946900	-2.03758000	-5.00904000
H	0.27626800	-3.26154100	-4.02665700
C	1.92054300	-2.23060200	-2.01468600
H	2.17845200	-2.50449600	-3.04488000
C	3.19743500	-1.67182500	-1.31060300
H	4.00671500	-1.56194000	-2.03971800
H	3.03416000	-0.68160800	-0.86929700
C	3.57274300	-2.70701800	-0.23123900
H	4.65462400	-2.78903500	-0.08695900
H	3.13273100	-2.41710600	0.73191300
C	2.92300200	-4.00805000	-0.71015200
H	2.82350000	-4.75732200	0.08210800
H	3.51493800	-4.45301500	-1.52089100
C	1.57274700	-3.52318900	-1.24485900
H	0.92064200	-3.30178400	-0.39204300
H	1.05779900	-4.25604100	-1.87445600
P	-0.45727700	0.81054800	2.13475900
P	0.55803000	-0.97199300	-2.09603500
Ru	0.12072200	0.03411300	-0.00680500

H	0.72950400	−1.26262300	0.67124700
H	0.09523700	3.88604500	−1.25687600
H	−1.37512700	−0.24469200	−0.24716700
H	−0.40447700	−1.37962900	0.43677600
C	−0.43228900	2.91828100	−1.12459900
O	0.34177000	1.98920900	−0.70322000
O	−1.63252200	2.84290100	−1.38517000
6Ru			
$G_{\text{solv}} = -2554.892522; E_{\text{solv}} = -2555.85853832$			
C	−1.18313200	−0.99547400	3.38121300
H	−1.46066000	−0.53782500	4.33855200
C	0.15887500	−1.77030500	3.57512700
H	0.93463700	−1.44973100	2.87301000
H	0.54785200	−1.59074900	4.58273100
C	−0.18343900	−3.26091900	3.38988000
H	−0.02281700	−3.55492500	2.34387900
H	0.43618600	−3.91466400	4.01209300
C	−1.67693800	−3.34856900	3.71342700
H	−1.83231900	−3.31073500	4.79969200
H	−2.14762300	−4.26373200	3.33903900
C	−2.23069000	−2.08314600	3.05345500
H	−3.23287900	−1.80916600	3.39801100
H	−2.29169200	−2.25385600	1.97229900
C	−0.26395100	1.70282000	3.18988600
H	−0.92750700	1.85273300	4.05317000
C	1.14213700	1.37495900	3.72927100
H	1.09187300	0.75130800	4.62694000
H	1.72119500	0.82993600	2.97887200
C	1.80629300	2.74852900	4.00493000
H	2.01179500	2.89568800	5.07032600
H	2.76465100	2.80479200	3.48007600
C	0.82818900	3.81584200	3.46728400
H	1.34088500	4.66085700	2.99482600
H	0.22432100	4.22276800	4.28827300
C	−0.08069900	3.05857000	2.49191600
H	0.42884700	2.91223700	1.53410100
H	−1.02761500	3.57560800	2.30299400
C	−2.78693400	1.10132700	2.04768200
H	−2.62777400	2.02351500	1.47825600
C	−3.47993200	1.46849700	3.37639900
H	−3.35587800	0.67508500	4.12632200
H	−3.09383100	2.39694600	3.80910900
C	−4.95697700	1.56992500	2.98484100
H	−5.63238500	1.56369500	3.84699800
H	−5.12653100	2.50333600	2.43275000
C	−5.15117700	0.36790400	2.05511400
H	−6.03076900	0.46541700	1.41091800
H	−5.29149700	−0.53800700	2.65966100
C	−3.83716400	0.27187300	1.25025500
H	−3.93903300	0.70645000	0.25211100
H	−3.54194000	−0.76909800	1.10667000
C	−0.16976500	−0.39694800	−3.61703900
H	−0.18535400	−1.10260700	−4.45900200
C	1.05206100	0.52063100	−3.78070300
H	1.94824500	−0.01927700	−4.10268000
H	1.27505200	1.00749900	−2.82815900
C	0.57509800	1.55406500	−4.80457600
H	1.20932900	2.44751200	−4.83789600

H	0.57826100	1.11054300	−5.80938000
C	−0.86156300	1.86355300	−4.36091500
H	−0.85066400	2.65703900	−3.60554100
H	−1.48974300	2.21524800	−5.18537900
C	−1.39434600	0.55255600	−3.73244500
H	−2.17503800	0.09470000	−4.34960800
H	−1.83871800	0.75815500	−2.75272700
C	−1.79485900	−2.33553500	−2.34032900
H	−2.52843200	−1.52359700	−2.42164600
C	−2.27710100	−3.26605600	−1.18888300
H	−1.45923100	−3.60279400	−0.54761500
H	−2.97401800	−2.72221000	−0.54381000
C	−2.95775300	−4.47327400	−1.87743300
H	−2.29484200	−5.34671400	−1.84173900
H	−3.89429900	−4.76030800	−1.38942900
C	−3.15469200	−4.04671700	−3.33779200
H	−4.05879400	−3.43174900	−3.43561600
H	−3.25401700	−4.89509300	−4.02264900
C	−1.91782600	−3.18870300	−3.61671200
H	−2.01224700	−2.58067900	−4.52220100
H	−1.04511000	−3.84275400	−3.74309200
C	1.11873700	−2.68259600	−2.38170600
H	0.95942700	−3.05763500	−3.39954000
C	2.56615000	−2.11388400	−2.27840800
H	3.06852000	−2.21934600	−3.24705800
H	2.59618300	−1.05438100	−2.02080900
C	3.27758300	−2.96987500	−1.21664600
H	4.35477200	−3.05162300	−1.39483800
H	3.13965500	−2.52108500	−0.22361200
C	2.54605000	−4.31267700	−1.27111500
H	2.72432100	−4.94208500	−0.39268500
H	2.85851900	−4.87807900	−2.15918400
C	1.08234500	−3.88129500	−1.40329200
H	0.72896400	−3.56014500	−0.41587300
H	0.41723500	−4.68004900	−1.74803800
P	−1.06990500	0.39698200	2.14837600
P	−0.19940200	−1.41186100	−2.06859000
Ru	−0.26678700	−0.32585900	0.02802900
H	0.14794000	−1.73288200	0.69534200
H	−0.43008700	3.53532200	−1.20768500
H	−1.78484800	−0.40613100	−0.27148500
H	−0.86677500	−1.70986900	0.52066900
C	−0.89773600	2.57040300	−0.91502700
O	−0.04213500	1.62918500	−0.77580700
O	−2.11967600	2.52152300	−0.77473200
C	3.71482700	2.21718900	−1.08152600
C	3.67445900	2.61841400	0.44069900
H	1.69700400	−0.16334600	0.33809000
C	5.11209000	2.06877300	−1.66456700
H	5.03944900	1.76197700	−2.71204100
H	5.64608400	3.02411100	−1.62789500
H	5.69978300	1.31795600	−1.13261800
C	4.91316400	2.17895500	1.21987800
H	5.79572500	2.75683300	0.92985000
H	4.73579500	2.33834900	2.28724100
H	5.12463200	1.11607500	1.06914400
C	2.86776700	3.12184900	−1.97425000
H	3.27503600	4.13627100	−2.01234200

H	2.86639000	2.71903900	−2.99048900
H	1.83250900	3.15950100	−1.62591500
C	3.38068000	4.08821300	0.69991600
H	3.37859300	4.27947200	1.77646700
H	4.15129500	4.72053700	0.24654700
H	2.40705200	4.37884500	0.29989700
O	3.08058800	0.91189400	−1.07352600
O	2.56940800	1.83181800	0.95006500
B	2.32927700	0.83425700	0.05924700
TS_{6,7-Ru}			
$G_{\text{solv}} = -2554.890853; E_{\text{solv}} = -2555.85615589$			
C	−0.76419900	−0.45194900	3.21557400
H	−1.05512400	0.00073800	4.17098600
C	0.55060000	−1.26554000	3.43554600
H	1.35671900	−0.95305600	2.76488500
H	0.91068900	−1.11627700	4.45884600
C	0.17452700	−2.74222200	3.21096700
H	0.35497400	−3.01925200	2.16378700
H	0.76017800	−3.42438400	3.83564700
C	−1.32862400	−2.79628200	3.49448800
H	−1.51104300	−2.77516900	4.57704600
H	−1.81285400	−3.69152400	3.09036100
C	−1.83314600	−1.50461000	2.84544900
H	−2.83469500	−1.20922600	3.17441100
H	−1.87566700	−1.65448800	1.76047700
C	0.27223600	2.20207700	3.09563800
H	−0.34689000	2.28078300	4.00090700
C	1.71061800	1.85770200	3.53009100
H	1.72073700	1.16583700	4.37765000
H	2.25098500	1.38158800	2.70660600
C	2.37240700	3.21681800	3.87452200
H	2.61662000	3.29107700	4.93941300
H	3.30874300	3.32346300	3.31966400
C	1.36521200	4.30884600	3.45230200
H	1.85216200	5.17663300	2.99405600
H	0.81090500	4.67259200	4.32671700
C	0.40112700	3.60698900	2.48875800
H	0.85629200	3.53952800	1.49712600
H	−0.55904700	4.12467000	2.39514400
C	−2.25645200	1.73217100	1.89457200
H	−2.05032500	2.65564100	1.34252400
C	−2.95044000	2.10818400	3.21943700
H	−2.88109200	1.29329200	3.95310100
H	−2.52155300	3.00477500	3.67859300
C	−4.41300000	2.29339000	2.80576300
H	−5.10294300	2.30885500	3.65612100
H	−4.52437800	3.24293000	2.26636000
C	−4.65306900	1.11627300	1.85444100
H	−5.51326000	1.26957300	1.19524300
H	−4.85376000	0.21158900	2.44325400
C	−3.32987800	0.95739900	1.07341500
H	−3.39463300	1.39561600	0.07340900
H	−3.08261900	−0.09643200	0.93294700
C	0.30058400	0.16854200	−3.73615100
H	0.20954900	−0.53298600	−4.57628900
C	1.52401100	1.06139900	−4.00102500
H	2.37690400	0.49945800	−4.39570000
H	1.84261000	1.54732400	−3.07616800

C	0.98295100	2.10210600	−4.98494600
H	1.63310200	2.97941800	−5.08017000
H	0.88358100	1.65565400	−5.98359300
C	−0.39905500	2.44658900	−4.41393200
H	−0.29793800	3.22651200	−3.65064100
H	−1.08633000	2.83042500	−5.17439900
C	−0.91271500	1.14067500	−3.75973900
H	−1.74078000	0.70249000	−4.32757600
H	−1.28546900	1.34475500	−2.75007000
C	−1.21620500	−1.84408700	−2.45103200
H	−1.98013500	−1.05821400	−2.50543900
C	−1.63595200	−2.80920200	−1.30118600
H	−0.80275300	−3.08273800	−0.65027800
H	−2.37938400	−2.31882500	−0.66475500
C	−2.22123600	−4.06242400	−1.99129800
H	−1.47703200	−4.86876600	−1.99433700
H	−3.11048200	−4.44590300	−1.48124600
C	−2.49982500	−3.62783900	−3.43438100
H	−3.44659100	−3.07453400	−3.48809200
H	−2.56532500	−4.46881900	−4.13228600
C	−1.33355900	−2.68374600	−3.73846400
H	−1.50316700	−2.06828800	−4.62760500
H	−0.42619800	−3.27691600	−3.91130300
C	1.71154800	−2.07663500	−2.53434700
H	1.54962000	−2.46246000	−3.54769500
C	3.13799300	−1.45281900	−2.45722000
H	3.62861700	−1.54885700	−3.43293400
H	3.13368600	−0.39169900	−2.20557200
C	3.89612100	−2.27256700	−1.39955400
H	4.97316800	−2.31438100	−1.59272600
H	3.75440100	−1.81951800	−0.40917700
C	3.21645000	−3.64296800	−1.43312600
H	3.43063500	−4.25766800	−0.55224900
H	3.53794200	−4.20357100	−2.32105500
C	1.73565100	−3.26879200	−1.54721000
H	1.38575000	−2.95082300	−0.55736500
H	1.09586800	−4.09486200	−1.87527500
P	−0.57321900	0.95547700	2.01044300
P	0.34906200	−0.86203700	−2.19735800
Ru	0.24564300	0.22416700	−0.10202600
H	0.62709500	−1.17008400	0.56715800
H	0.49389100	4.15170500	−1.15672700
H	−1.27460500	0.17323300	−0.44260800
H	−0.45019900	−1.10975600	0.35204400
C	−0.07920800	3.22665900	−0.95038900
O	0.65740500	2.17017700	−0.90351600
O	−1.29517700	3.28748500	−0.81148200
C	4.14944600	2.81985400	−1.32101800
C	4.10715200	3.24983200	0.19250600
H	2.10971100	0.55385500	0.19692700
C	5.54004900	2.51452300	−1.86157600
H	5.46306400	2.20261000	−2.90756700
H	6.17715400	3.40438500	−1.81915700
H	6.02414100	1.70912900	−1.30572900
C	5.25832800	2.66248700	1.01044600
H	6.21749700	3.11469400	0.74059600
H	5.07682100	2.85489800	2.07136800
H	5.33004200	1.57929100	0.87350300

C	3.44248500	3.79865800	−2.25799900
H	3.98622300	4.74570200	−2.32566800
H	3.39365200	3.36170200	−3.25915100
H	2.42086700	4.00260000	−1.93228900
C	4.00602800	4.74942500	0.42950400
H	3.97506000	4.94930900	1.50487200
H	4.87626500	5.26863500	0.01389800
H	3.10150200	5.16757700	−0.01770400
O	3.39488000	1.59110200	−1.30541700
O	2.89650900	2.62743300	0.67054900
B	2.56430400	1.62280100	−0.21002000
7Ru			
$G_{\text{solv}} = -2554.902088; E_{\text{solv}} = -2555.86949078$			
C	−1.33992300	−1.10010200	3.30427900
H	−1.60054700	−0.70069300	4.29121100
C	−0.04164700	−1.95600300	3.44761300
H	0.76967500	−1.60615400	2.80275100
H	0.32091200	−1.90148400	4.48013700
C	−0.45159600	−3.39748000	3.09743400
H	−0.30123300	−3.57430300	2.02412000
H	0.13450900	−4.14574900	3.64056900
C	−1.94839800	−3.45028900	3.41173600
H	−2.10617400	−3.52104000	4.49603000
H	−2.45874500	−4.29814600	2.94269400
C	−2.44360200	−2.09901500	2.88810800
H	−3.42701500	−1.81120300	3.27424600
H	−2.52400000	−2.15981600	1.79748100
C	−0.18265200	1.51057100	3.31529700
H	−0.67081100	1.44803900	4.29890500
C	1.30527500	1.17906200	3.49705500
H	1.47199300	0.29277000	4.11690300
H	1.76337600	1.00724000	2.51837400
C	1.87148200	2.45424700	4.13554900
H	1.69145600	2.43165000	5.21777500
H	2.95403600	2.54790300	3.99303500
C	1.08713000	3.61648700	3.48916900
H	1.67976600	4.09745300	2.70661200
H	0.83432500	4.38373000	4.22839700
C	−0.17965000	2.98553300	2.86339300
H	−0.11019100	3.04441700	1.77448800
H	−1.09711100	3.50241200	3.16182500
C	−2.77989900	1.22853700	2.19289800
H	−2.55471400	2.20007900	1.73525200
C	−3.42815300	1.49881000	3.56527000
H	−3.40091900	0.60189600	4.19830400
H	−2.93408200	2.30711700	4.11394500
C	−4.88097000	1.81725000	3.20321500
H	−5.55654100	1.78548000	4.06435900
H	−4.93929700	2.82390300	2.76965300
C	−5.21071400	0.76303500	2.13960300
H	−6.05352200	1.05140200	1.50381800
H	−5.48619300	−0.17668700	2.63500700
C	−3.90261300	0.57290400	1.33659600
H	−3.94998800	1.06418400	0.36083500
H	−3.71861000	−0.48494800	1.14004800
C	−0.26959500	−0.47886000	−3.64704000
H	−0.52212000	−1.22970600	−4.40488100
C	1.01957900	0.22101800	−4.11885300

H	1.71573200	−0.47957000	−4.59335000
H	1.53523600	0.69928800	−3.28298900
C	0.49755500	1.29788800	−5.07454700
H	1.24835000	2.06163400	−5.30640600
H	0.17871600	0.84558400	−6.02373000
C	−0.71280800	1.85803500	−4.32029800
H	−0.36257400	2.55347700	−3.54757000
H	−1.40818100	2.40793300	−4.96255000
C	−1.36779500	0.62602600	−3.65705300
H	−2.23669500	0.28651100	−4.23192200
H	−1.72465300	0.86728300	−2.65067200
C	−1.67868800	−2.50862800	−2.28011000
H	−2.48789300	−1.78021900	−2.42380800
C	−2.08581000	−3.42537900	−1.08372400
H	−1.29700100	−3.52934200	−0.33631900
H	−2.94655800	−2.98839400	−0.56687500
C	−2.44922400	−4.79404900	−1.69625400
H	−1.59520000	−5.47859800	−1.61742600
H	−3.29335200	−5.26992200	−1.18732400
C	−2.72525100	−4.49831400	−3.17271600
H	−3.72996400	−4.07184300	−3.29195200
H	−2.66221500	−5.38576600	−3.81080000
C	−1.67063000	−3.44155700	−3.51179200
H	−1.88996500	−2.91199800	−4.44369000
H	−0.69587900	−3.93145300	−3.63065100
C	1.27329700	−2.51927100	−2.24483800
H	1.22932400	−2.91483300	−3.26672000
C	2.63942900	−1.79412700	−2.04010100
H	3.22224100	−1.85042000	−2.96680100
H	2.53405700	−0.73551500	−1.79638300
C	3.35315800	−2.56186300	−0.91432100
H	4.44399600	−2.52760200	−1.00772400
H	3.08830100	−2.12359400	0.05725300
C	2.77767500	−3.97671000	−1.00427100
H	2.95384300	−4.57704200	−0.10523300
H	3.21649400	−4.51088400	−1.85770000
C	1.29095400	−3.70645400	−1.25180300
H	0.83432700	−3.41248200	−0.29935400
H	0.74148100	−4.57496000	−1.62967300
P	−1.12913100	0.37607600	2.19119100
P	−0.19265500	−1.40109700	−2.03704900
Ru	−0.39704300	−0.25098400	0.02035600
H	0.14969600	−1.56363500	0.65860700
H	0.10333700	3.82007000	−0.71954700
H	−1.93016800	−0.31966200	−0.32470400
H	−1.28525600	−1.46410300	0.36144000
C	−0.59732900	2.97398100	−0.76864900
O	0.00112900	1.79549400	−0.74600400
O	−1.79617800	3.11094800	−0.84695400
C	3.37606700	2.41156800	−1.32133700
C	3.35702200	2.66453400	0.22531000
H	1.34843200	0.32562100	0.18164200
C	4.67877000	1.83093700	−1.85987900
H	4.59794600	1.68654800	−2.94217000
H	5.52024000	2.50660300	−1.66989500
H	4.89842900	0.86039600	−1.40937500
C	4.16319600	1.61368900	0.99665100
H	5.23932100	1.73220500	0.83529700

H	3.96573100	1.72813400	2.06611200
H	3.87887500	0.59760500	0.70555100
C	2.99194700	3.65173200	-2.13435600
H	3.78756700	4.40397500	-2.13292700
H	2.80534500	3.35170600	-3.16997900
H	2.07932700	4.11673500	-1.75091200
C	3.79642700	4.06045800	0.64545000
H	3.81082000	4.13666400	1.73709000
H	4.80804500	4.27325900	0.28235900
H	3.11894600	4.82642900	0.26039400
O	2.34761400	1.43566100	-1.47349900
O	1.97163100	2.49458500	0.53832000
B	1.45046600	1.52664800	-0.37006500
TS_{7,8-Ru}			
$G_{\text{solv}} = -2554.882555; E_{\text{solv}} = -2555.84640032$			
C	-2.03531900	-0.96797600	3.17291900
H	-2.22850800	-0.49845900	4.14552700
C	-1.20227300	-2.26388500	3.41637500
H	-0.34132000	-2.33130900	2.74423900
H	-0.81178000	-2.27017200	4.43955100
C	-2.17410400	-3.44159200	3.18464200
H	-2.03415400	-3.84278500	2.17279400
H	-2.01097700	-4.26579500	3.88618500
C	-3.57228100	-2.82513400	3.29464300
H	-3.84935800	-2.69591200	4.34924600
H	-4.34898600	-3.43265500	2.81858900
C	-3.39228400	-1.45769300	2.62870100
H	-4.20501200	-0.75711800	2.84699100
H	-3.35738100	-1.59301500	1.54133800
C	0.09451900	0.88429100	3.44056500
H	-0.41133400	0.82378000	4.41587700
C	1.39120700	0.06136200	3.49780800
H	1.25124100	-0.93609600	3.92488000
H	1.76798800	-0.06810900	2.47677400
C	2.35306900	0.92888900	4.33075400
H	2.29782000	0.64604800	5.38786200
H	3.39393800	0.78653200	4.01988300
C	1.87205500	2.39166100	4.14184100
H	2.64241400	3.02603800	3.68889000
H	1.62551700	2.83947600	5.11069500
C	0.61788700	2.31455000	3.24657900
H	0.89429300	2.46542800	2.19919600
H	-0.12413600	3.07627800	3.50906000
C	-2.30272700	1.72785100	2.04879400
H	-1.66542900	2.57153900	1.75228800
C	-3.07464300	2.16733400	3.30335300
H	-3.53501000	1.30643300	3.80431200
H	-2.43771100	2.67608100	4.03482700
C	-4.17094300	3.06405700	2.71950000
H	-4.98204300	3.26775400	3.42630900
H	-3.73759500	4.02755800	2.42286000
C	-4.64149600	2.29200800	1.47644300
H	-5.07946700	2.94955800	0.72011300
H	-5.41338200	1.56794700	1.76475800
C	-3.38725300	1.54938200	0.95058900
H	-3.04036300	1.96802000	0.00096100
H	-3.61171600	0.49467700	0.76745500
C	-0.60424400	-0.79865200	-3.54385500

H	-0.58184200	-1.55703600	-4.33542100
C	0.25415400	0.39695200	-3.99945700
H	1.11004100	0.08015700	-4.60535200
H	0.64960700	0.94758800	-3.14292100
C	-0.72906900	1.28720700	-4.76527200
H	-0.35753300	2.30930800	-4.89478300
H	-0.92356200	0.87000200	-5.76298300
C	-1.99352500	1.22111500	-3.90340300
H	-1.87829400	1.89587600	-3.04855900
H	-2.89892900	1.51964000	-4.44192300
C	-2.05505000	-0.24136500	-3.41369000
H	-2.74173400	-0.83659200	-4.02608400
H	-2.42993800	-0.29300300	-2.38247800
C	-1.07093100	-3.18117000	-2.09847500
H	-2.09547200	-2.79047700	-2.16112400
C	-1.01709200	-4.15108800	-0.87575700
H	-0.19357200	-3.93070100	-0.19204400
H	-1.93883300	-4.05297500	-0.29224500
C	-0.90135600	-5.57254400	-1.46345300
H	0.14863100	-5.89094900	-1.47729300
H	-1.45592400	-6.31372800	-0.87932700
C	-1.40776700	-5.43795300	-2.90244600
H	-2.50545900	-5.40884200	-2.91567800
H	-1.08844700	-6.25974500	-3.55176800
C	-0.84772200	-4.08000800	-3.33497200
H	-1.33444200	-3.68666000	-4.23271600
H	0.22100600	-4.18746400	-3.55895400
C	1.67825100	-2.17203300	-2.34688500
H	1.68337000	-2.57025600	-3.36965800
C	2.72413800	-1.02775300	-2.24487200
H	3.02530800	-0.69767800	-3.24412800
H	2.30920500	-0.15380100	-1.73741800
C	3.92324000	-1.61362400	-1.46172400
H	4.88898300	-1.30460800	-1.87622500
H	3.88944600	-1.27068100	-0.41999300
C	3.72043600	-3.13201800	-1.49764600
H	4.25049200	-3.65569800	-0.69511000
H	4.07112800	-3.54175200	-2.45429800
C	2.20021900	-3.26874400	-1.39759100
H	1.88822800	-3.05498300	-0.36726500
H	1.83352900	-4.26563900	-1.66264200
P	-1.12202300	0.30448600	2.16157600
P	-0.05026900	-1.61985000	-1.97570900
Ru	-0.47764900	-0.47924600	0.04154600
H	0.68494200	-1.28319700	0.68415600
H	-0.38943100	4.29020000	0.33136200
H	-1.78811100	-1.51681600	0.14915900
H	-1.05496900	-1.92609500	0.56319400
C	-0.96942600	3.83355000	-0.48484000
O	-0.33159300	2.86909100	-1.14357900
O	-2.08826600	4.18451400	-0.77401400
C	3.14961200	2.90416800	-1.50956200
C	3.06117900	2.96565800	0.05307200
H	0.63757900	0.78669400	-0.23951500
C	4.31095600	2.08499600	-2.04781800
H	4.26442800	2.05137600	-3.14046800
H	5.26270600	2.54572800	-1.76208800
H	4.29561600	1.06143300	-1.67528700

C	3.49785400	1.66626300	0.72795700
H	4.57757100	1.51521800	0.63408700
H	3.25486200	1.72220700	1.79134000
H	2.97469800	0.80390200	0.30706500
C	3.14051500	4.28771200	−2.16399600
H	4.08493600	4.81649100	−2.00230100
H	2.99318100	4.16742400	−3.24109000
H	2.32458000	4.90840300	−1.78049400
C	3.76826400	4.15326400	0.68672000
H	3.64459100	4.11857400	1.77348700
H	4.84084400	4.12350600	0.46747500
H	3.36371100	5.10307100	0.33042700
O	1.90076500	2.26757200	−1.85900200
O	1.63855000	3.11867800	0.25555000
B	1.01498100	2.54439500	−0.83563500
8Ru			
$G_{\text{solv}} = -2554.897573; E_{\text{solv}} = -2555.85685161$			
C	−2.04609700	−1.14278400	3.48445300
H	−2.16125800	−0.61146700	4.43749800
C	−1.17860800	−2.41681500	3.72907800
H	−0.33768600	−2.48295800	3.03205300
H	−0.76018800	−2.39321600	4.74100200
C	−2.13265500	−3.61754900	3.56032600
H	−2.05619300	−4.01004600	2.53809400
H	−1.89929400	−4.43968400	4.24451700
C	−3.53177900	−3.03222700	3.77219900
H	−3.72623100	−2.88961300	4.84351600
H	−4.32978000	−3.66492500	3.36946900
C	−3.43328800	−1.67593100	3.06858100
H	−4.24120300	−0.98507800	3.33133900
H	−3.47670700	−1.83831200	1.98508800
C	0.03361200	0.80805800	3.37741600
H	−0.44343500	1.00504800	4.34933700
C	1.28570400	−0.06172500	3.59796200
H	1.11299200	−0.87409200	4.30944100
H	1.57152000	−0.51628200	2.64249500
C	2.38466900	0.91869000	4.07820700
H	2.59010100	0.79629200	5.14661500
H	3.32650000	0.72684700	3.55239400
C	1.84431700	2.33830300	3.78063700
H	2.59583500	2.99727700	3.33178400
H	1.51431900	2.81887500	4.70942200
C	0.63493100	2.12131400	2.86104500
H	0.96427600	1.98276200	1.82371800
H	−0.06507400	2.96353700	2.89125500
C	−2.48389000	1.43877700	2.14258000
H	−1.89368200	2.25626000	1.71330600
C	−3.14931000	1.98322900	3.41929300
H	−3.48857000	1.16759800	4.07024400
H	−2.47370400	2.61555700	4.00562600
C	−4.36638500	2.73773900	2.87421000
H	−5.10778000	2.97260100	3.64524500
H	−4.04165100	3.68375500	2.42214700
C	−4.90584300	1.79445200	1.79069400
H	−5.53472800	2.30845600	1.05755100
H	−5.52183800	1.01710100	2.26037000
C	−3.65010400	1.15965600	1.14946600
H	−3.42162700	1.61931000	0.18289000

H	-3.79922100	0.09155200	0.96623100
C	-0.59584000	-0.82334700	-3.34552000
H	-0.43964300	-1.45903900	-4.22613400
C	0.21536300	0.47122200	-3.53551000
H	1.18261000	0.29596100	-4.01629800
H	0.40767700	0.94098900	-2.56566700
C	-0.71722800	1.36819500	-4.35136200
H	-0.41128400	2.41882000	-4.33421400
H	-0.73952700	1.03662900	-5.39877100
C	-2.07803300	1.13584600	-3.68670600
H	-2.14230300	1.75245700	-2.78328700
H	-2.92261200	1.40809000	-4.32796500
C	-2.08403700	-0.36258000	-3.30520600
H	-2.68311400	-0.95348500	-4.00670900
H	-2.53119800	-0.50827900	-2.31229100
C	-1.09665200	-3.37772300	-2.21767100
H	-2.12585400	-3.01120200	-2.32883600
C	-1.10418800	-4.45696600	-1.09005700
H	-0.34971600	-4.27337400	-0.32114300
H	-2.07284200	-4.44565400	-0.57944400
C	-0.87806900	-5.80936500	-1.79627700
H	0.18408900	-6.08246000	-1.75424000
H	-1.44054600	-6.62536500	-1.33145300
C	-1.27646000	-5.55571900	-3.25346600
H	-2.37007800	-5.56265600	-3.35257600
H	-0.87417100	-6.30066000	-3.94794100
C	-0.74003700	-4.14423900	-3.51012400
H	-1.16780500	-3.67872300	-4.40378400
H	0.34648600	-4.19680100	-3.65388600
C	1.62255200	-2.26795600	-2.14127300
H	1.70311200	-2.59228700	-3.18590300
C	2.61501600	-1.09010200	-1.90920600
H	3.08265800	-0.80932000	-2.85940300
H	2.11157500	-0.20113100	-1.52202400
C	3.66654000	-1.61676100	-0.91393900
H	4.66094800	-1.18708100	-1.07990100
H	3.36137900	-1.36344700	0.10941700
C	3.62769900	-3.13687500	-1.08884600
H	4.08211800	-3.67982400	-0.25329100
H	4.15542000	-3.42845400	-2.00706700
C	2.12777200	-3.40837200	-1.22938000
H	1.66416900	-3.33132900	-0.23824200
H	1.89618800	-4.39953900	-1.63336400
P	-1.26290000	0.04783700	2.28665000
P	-0.15065500	-1.81357800	-1.84217400
Ru	-0.71543100	-0.84264000	0.20839800
H	0.51015000	-1.56832200	0.83394700
H	-0.24678500	3.15303400	0.40267700
H	-1.96864600	-2.00012000	0.34140100
H	-1.23129400	-2.34054200	0.74805800
C	-0.68271900	3.32696400	-0.58984700
O	0.21196800	3.31568200	-1.59337600
O	-1.85352200	3.51718200	-0.78767800
C	3.77421600	3.12974000	-1.76044700
C	3.52322400	3.15679500	-0.20547200
H	0.31049200	0.44089100	-0.07362500
C	4.72177300	2.03780700	-2.22675400
H	4.81743100	2.07383400	-3.31579100

H	5.71646800	2.18247900	−1.79248600
H	4.35827100	1.04770700	−1.94912600
C	3.62104400	1.78222200	0.45025500
H	4.64586600	1.40107400	0.42526800
H	3.31480700	1.86511800	1.49486800
H	2.95945200	1.05795800	−0.03070100
C	4.19630500	4.48264600	−2.33112000
H	5.21399000	4.74428500	−2.02702000
H	4.16767700	4.43009800	−3.42307700
H	3.52145100	5.28407100	−2.01464200
C	4.36517900	4.16868100	0.55390500
H	4.11646000	4.12996100	1.61827300
H	5.42964300	3.93511200	0.44761500
H	4.19338800	5.18805100	0.20277600
O	2.45046400	2.85009000	−2.28830200
O	2.12786000	3.56245000	−0.12806700
B	1.56931800	3.22691200	−1.32638600
9_{Ru}			
$G_{\text{solv}} = -2554.886694; E_{\text{solv}} = -2555.85192620$			
C	−2.55791900	−1.17665900	2.79986700
H	−2.59857700	−1.43148000	3.86759000
C	−3.09412000	−2.39084200	1.98704100
H	−2.49262400	−2.56233300	1.09070000
H	−3.04449000	−3.30284800	2.58980100
C	−4.55496500	−2.04242900	1.61115100
H	−4.60585400	−1.75826100	0.55377700
H	−5.23754600	−2.88602800	1.75487600
C	−4.91778400	−0.83350000	2.48170300
H	−5.21727700	−1.16031600	3.48651600
H	−5.73676600	−0.23506400	2.06859200
C	−3.59725100	−0.06473600	2.56348500
H	−3.58430000	0.69863600	3.34836800
H	−3.42240900	0.43736100	1.60516000
C	0.08541100	−1.92562400	3.58684600
H	−0.32971800	−1.72559200	4.58263800
C	−0.13534200	−3.42034300	3.26078900
H	−1.03585000	−3.81673600	3.74073600
H	−0.24161200	−3.56206300	2.17953600
C	1.14803900	−4.10716000	3.74017200
H	1.13322700	−4.22213300	4.83252300
H	1.28569500	−5.10110700	3.30140100
C	2.23764100	−3.11350400	3.33085300
H	2.41722400	−3.20155400	2.25196500
H	3.19270600	−3.27981500	3.84023500
C	1.63122700	−1.73367800	3.64411000
H	1.99019900	−0.97725900	2.93955900
H	1.92454300	−1.40520200	4.64800300
C	−0.46032800	0.83812400	3.35165800
H	0.63768300	0.88077300	3.36080200
C	−0.95810500	0.95486500	4.81903500
H	−1.80118000	0.28821700	5.02717300
H	−0.16010000	0.67541900	5.51476700
C	−1.37690200	2.43511500	5.00492900
H	−2.47069400	2.51655400	4.99998900
H	−1.02819200	2.85384700	5.95413400
C	−0.80980000	3.17204600	3.78255000
H	0.24694300	3.42394000	3.94588600
H	−1.34429100	4.10314100	3.56380500

C	-0.92517300	2.13372200	2.66368300
H	-0.33126900	2.36146900	1.77600500
H	-1.97328800	2.06747300	2.34847000
C	0.98150800	-0.48880900	-3.31660500
H	1.73727800	-0.87775000	-4.01317800
C	1.06712600	1.04287600	-3.36049800
H	2.09708700	1.41146700	-3.32813400
H	0.53623600	1.46858100	-2.50158200
C	0.35544300	1.39453200	-4.67083100
H	0.03552600	2.44035500	-4.70881000
H	1.04236500	1.22185300	-5.50969600
C	-0.82950400	0.41358000	-4.74179100
H	-1.72705300	0.88168300	-4.32697200
H	-1.05837100	0.12962100	-5.77414600
C	-0.42530700	-0.80845000	-3.87573100
H	-0.41415400	-1.73937000	-4.45284400
H	-1.13931100	-0.94408700	-3.05697400
C	1.30026500	-3.06748800	-2.20510400
H	0.26085400	-3.19954300	-2.53224500
C	1.57352200	-4.12533900	-1.09173900
H	2.00075200	-3.68993300	-0.18690100
H	0.62882200	-4.58437900	-0.78581000
C	2.52347200	-5.16580200	-1.72033100
H	3.56250900	-4.94066700	-1.44615200
H	2.31326700	-6.18550600	-1.38171300
C	2.35277000	-4.98682200	-3.23204400
H	1.42888100	-5.47577100	-3.56853300
H	3.18147100	-5.40377300	-3.81424700
C	2.21796200	-3.46875300	-3.37999800
H	1.81111200	-3.16860800	-4.35114000
H	3.21030600	-3.00919800	-3.28087100
C	3.12184800	-0.86408600	-1.45921400
H	3.59725800	-1.02173200	-2.43511600
C	3.37115800	0.61440500	-1.02162900
H	3.89586900	1.15080200	-1.82043200
H	2.44048700	1.15182000	-0.81913800
C	4.25336500	0.53773200	0.23759200
H	4.93453000	1.39071200	0.32676700
H	3.61725200	0.52508700	1.13229700
C	4.97497800	-0.80624400	0.11199800
H	5.40277000	-1.15794700	1.05701700
H	5.79058800	-0.73259300	-0.62008300
C	3.86755500	-1.72335800	-0.41403300
H	3.20102500	-1.97191700	0.41878500
H	4.23905100	-2.66273100	-0.83715100
P	-0.77933000	-0.74693500	2.43291800
P	1.31846100	-1.28273700	-1.67224000
Ru	0.04109600	-0.85171500	0.24269400
H	1.33210200	-0.23460500	0.86265400
H	0.22541800	0.80280800	0.03589200
H	-0.43113600	-2.42145500	0.20513700
H	1.06427800	-1.85090800	0.84399400
C	-1.00497500	4.91727500	-2.32813900
C	-0.50435500	4.65090400	-0.85944400
C	0.04877200	5.49333900	-3.25961300
H	-0.37710100	5.63132500	-4.25757700
H	0.38814700	6.46925300	-2.89706900
H	0.91344300	4.83273100	-3.34826500

C	0.97616600	4.27941000	−0.78115200
H	1.61338800	5.14677100	−0.97713100
H	1.19602900	3.90682800	0.22293900
H	1.23367800	3.48885700	−1.49233200
C	−2.28741800	5.74427500	−2.38954800
H	−2.10101000	6.78722800	−2.11754100
H	−2.67689700	5.72049600	−3.41108400
H	−3.05862000	5.34347500	−1.72443700
C	−0.83017500	5.74984400	0.13690200
H	−0.44765500	5.47528400	1.12394300
H	−0.35355200	6.68889700	−0.16226100
H	−1.90606200	5.91493200	0.22264400
O	−1.34210700	3.58075800	−2.78882200
O	−1.24885400	3.45602400	−0.49858500
B	−1.52914400	2.82842100	−1.67434300
O	−1.94572900	1.51102700	−1.76983400
C	−1.96938300	0.73541700	−0.67505400
H	−2.03854800	1.27756200	0.27220200
O	−2.06793100	−0.47729800	−0.77851300
TS_{9,10-Ru}			
$G_{\text{solv}} = -2554.885907; E_{\text{solv}} = -2555.85123331$			
C	10.62332500	4.25481200	7.98065700
H	10.58448500	3.98940500	9.04597900
C	10.10733500	3.04071700	7.15480600
H	10.70620100	2.89445500	6.25229600
H	10.17842600	2.12180800	7.74474400
C	8.63811200	3.36606300	6.79010500
H	8.57627600	3.65384800	5.73456800
H	7.97117200	2.51024300	6.93502300
C	8.25963700	4.56486900	7.66829300
H	7.96697200	4.22847200	8.67198300
H	7.43117700	5.15321600	7.25978700
C	9.56847900	5.35335800	7.75163500
H	9.57175800	6.11250000	8.54077600
H	9.73426100	5.86248300	6.79560600
C	13.27713800	3.53922500	8.76523700
H	12.86456100	3.73673100	9.76252700
C	13.06754200	2.04188000	8.44373100
H	12.17449000	1.63850800	8.93158200
H	12.95361800	1.89566500	7.36394900
C	14.36093600	1.36773700	8.91424400
H	14.35495400	1.25340300	10.00668800
H	14.50484300	0.37485400	8.47517200
C	15.43796200	2.37149300	8.49659600
H	15.60923600	2.28560000	7.41621500
H	16.39869000	2.21379200	8.99794700
C	14.82125600	3.74519500	8.81596800
H	15.17060900	4.50721300	8.11272100
H	15.11584200	4.07290400	9.81972400
C	12.69826400	6.29623700	8.54024200
H	13.79592600	6.34924900	8.55064100
C	12.19823400	6.40438900	10.00735100
H	11.35729500	5.73349500	10.21051100
H	12.99612400	6.12504500	10.70323400
C	11.77305700	7.88238200	10.19818300
H	10.67892000	7.95841000	10.19766500
H	12.12349300	8.30024400	11.14710600
C	12.33209500	8.62538400	8.97558100

H	13.38760500	8.88404000	9.13656600
H	11.79115200	9.55327600	8.75960900
C	12.22052500	7.58843700	7.85518800
H	12.80749700	7.82477900	6.96510500
H	11.17161700	7.51311000	7.54501800
C	14.15565600	4.97035700	1.84347200
H	14.89330600	4.54160600	1.15128100
C	14.30276700	6.49632400	1.76811400
H	15.34825600	6.82010200	1.77330100
H	13.80621000	6.96435400	2.62471400
C	13.58126600	6.85135800	0.46425300
H	13.30643500	7.90922900	0.40976500
H	14.24232800	6.63015100	−0.38421300
C	12.35361700	5.92358100	0.44065600
H	11.49637400	6.43327600	0.88987300
H	12.07199200	5.64810500	−0.58089800
C	12.73518200	4.68791900	1.29686400
H	12.72188000	3.76085400	0.71326800
H	12.02451200	4.56421300	2.11998800
C	14.44496300	2.40290200	2.98225400
H	13.40404400	2.27753500	2.65683300
C	14.71199300	1.35152400	4.10353100
H	15.12938400	1.79239200	5.01014400
H	13.76581800	0.89032000	4.40232100
C	15.66755500	0.30903600	3.48798200
H	16.70543000	0.54306100	3.75887100
H	15.46270300	−0.70748000	3.83915200
C	15.49460300	0.46973900	1.97479800
H	14.57061100	−0.02402800	1.64571200
H	16.32271600	0.04685400	1.39611500
C	15.35848100	1.98578200	1.80883000
H	14.94754100	2.27281100	0.83562200
H	16.35092500	2.44727400	1.89782700
C	16.28324300	4.60539800	3.71205000
H	16.75537200	4.45559300	2.73329400
C	16.53305700	6.08072800	4.16076300
H	17.05996200	6.62258700	3.36724400
H	15.60311500	6.61938500	4.36408400
C	17.41353300	5.99410800	5.42029500
H	18.09237900	6.84793300	5.51823700
H	16.77703600	5.97064300	6.31441800
C	18.13854700	4.65329100	5.28147100
H	18.56760000	4.29352900	6.22286100
H	18.95362800	4.73605900	4.54981500
C	17.03311300	3.73835000	4.74738300
H	16.36955800	3.47919100	5.57896900
H	17.40634500	2.80422200	4.31460900
P	12.39440400	4.71096400	7.61915400
P	14.47857300	4.19305800	3.49755000
Ru	13.19785600	4.63320300	5.42088200
H	14.45770800	5.34698900	6.01987200
H	13.18425300	6.29571200	5.11462300
H	12.86559400	3.04266600	5.45506600
H	14.29881100	3.72329700	6.03799300
C	12.21725100	10.32156100	2.85967400
C	12.74593300	10.08194600	4.32293800
C	13.23930700	10.92524600	1.90992600
H	12.79589300	11.04321300	0.91697200

H	13.55291300	11.91381500	2.26145400
H	14.12322000	10.29161000	1.81302100
C	14.23961100	9.76150400	4.38398300
H	14.84628900	10.64889900	4.18038600
H	14.48252800	9.39789200	5.38622000
H	14.51498700	8.97932900	3.67011300
C	10.91003700	11.11027900	2.81249200
H	11.06839400	12.15998900	3.07655200
H	10.50634600	11.06875900	1.79699800
H	10.16140300	10.68944000	3.49084400
C	12.39811500	11.17722500	5.31667600
H	12.80354800	10.92313500	6.30016300
H	12.83737700	12.13023100	5.00449600
H	11.31850100	11.30563300	5.41738100
O	11.91545600	8.97473600	2.41324400
O	12.04811400	8.86810400	4.70206600
B	11.76317100	8.21896600	3.53555800
O	11.37793300	6.90029500	3.45673300
C	11.33485900	6.12993900	4.57442300
H	11.09463900	6.68386000	5.48531200
O	11.15769900	4.91073100	4.45226800
10Ru			
$G_{\text{solv}} = -2554.896516; E_{\text{solv}} = -2555.86617861$			
C	-2.56727400	-1.27646700	2.77160200
H	-2.66157300	-1.55528600	3.82978900
C	-2.98867500	-2.49805400	1.90010600
H	-2.29536100	-2.65854800	1.07062900
H	-2.99433200	-3.40888100	2.50755800
C	-4.40079700	-2.16891100	1.36430000
H	-4.32069400	-1.82223800	0.32854400
H	-5.06709700	-3.03744700	1.37781100
C	-4.90210500	-1.01855800	2.24373000
H	-5.28309000	-1.40132400	3.20049300
H	-5.70167100	-0.43604900	1.77417700
C	-3.63052800	-0.20038000	2.47852100
H	-3.72161000	0.53164900	3.28803500
H	-3.38790500	0.33882400	1.55759400
C	0.07329100	-1.93681700	3.66707800
H	-0.37841700	-1.76938900	4.65267900
C	-0.09166100	-3.43189000	3.30386500
H	-0.97969000	-3.87158800	3.76814600
H	-0.19077300	-3.55566600	2.21972100
C	1.21463800	-4.08526200	3.76815000
H	1.19892600	-4.23701000	4.85571600
H	1.39144400	-5.05799900	3.29743800
C	2.26667800	-3.03743100	3.39919400
H	2.44520200	-3.07324200	2.31672500
H	3.22899200	-3.18941400	3.89898900
C	1.60969600	-1.69776300	3.77357600
H	1.96173900	-0.88806300	3.12731000
H	1.86665500	-1.42242000	4.80286700
C	-0.56527400	0.81797200	3.45748700
H	0.52890900	0.88321700	3.53775700
C	-1.15777200	0.91145200	4.89000100
H	-2.01770400	0.24761600	5.02478100
H	-0.41079400	0.61205700	5.63233500
C	-1.58076400	2.39207200	5.07238600
H	-2.67320200	2.47563200	5.02950000

H	-1.26534400	2.80059800	6.03732800
C	-0.96591900	3.14149500	3.88034100
H	0.07912600	3.40425800	4.09333700
H	-1.49846100	4.06763700	3.63944500
C	-1.01726400	2.10926600	2.75167400
H	-0.38709200	2.36313900	1.89471000
H	-2.04746300	2.02410800	2.38874000
C	0.99896400	-0.43972500	-3.27167000
H	1.71522400	-0.88371300	-3.97719000
C	1.18407500	1.08271700	-3.33551500
H	2.23721900	1.38141100	-3.34044500
H	0.71114500	1.55369800	-2.46741800
C	0.45416900	1.46873500	-4.62696300
H	0.18609800	2.52953900	-4.65689000
H	1.10956600	1.26317500	-5.48355100
C	-0.78387500	0.55288100	-4.66654300
H	-1.64618400	1.07354200	-4.24146900
H	-1.04178400	0.27107300	-5.69275800
C	-0.43815200	-0.67976100	-3.79193900
H	-0.49516200	-1.61744700	-4.35601300
H	-1.13752900	-0.75348600	-2.95332200
C	1.19185500	-3.01815200	-2.12607000
H	0.13852100	-3.09625400	-2.42466300
C	1.44035600	-4.07706900	-1.00739300
H	1.91906500	-3.65741300	-0.12072900
H	0.48074200	-4.48380000	-0.67276800
C	2.31336600	-5.17530100	-1.64999300
H	3.37006900	-5.00777100	-1.40412200
H	2.05376700	-6.17794300	-1.29568700
C	2.11310400	-4.99995600	-3.15843200
H	1.15634100	-5.44149400	-3.46688900
H	2.90327800	-5.46568900	-3.75663100
C	2.05560600	-3.47869400	-3.31993500
H	1.63850500	-3.16678800	-4.28253600
H	3.07253200	-3.06994200	-3.25135200
C	3.14707000	-0.89564000	-1.44021800
H	3.59652000	-1.04795200	-2.42918600
C	3.45530900	0.56340400	-0.97555300
H	3.95401100	1.11160000	-1.78199200
H	2.54935400	1.12069600	-0.71775300
C	4.39098000	0.42937500	0.24059300
H	5.10824300	1.25366500	0.31109500
H	3.79861100	0.42405400	1.16468900
C	5.05302600	-0.93893300	0.05963700
H	5.50705000	-1.32491000	0.97848200
H	5.83797200	-0.88409600	-0.70664200
C	3.88800400	-1.80118200	-0.43332600
H	3.24417400	-2.03053800	0.42281900
H	4.20013400	-2.75099200	-0.87972300
P	-0.79910700	-0.76565300	2.51719600
P	1.32611000	-1.23021700	-1.62814100
Ru	0.07224100	-0.77687000	0.33780900
H	1.35706100	-0.11392100	0.97268000
H	-0.49385100	0.99103800	-0.08270400
H	-0.05538700	-2.33215900	0.44642100
H	1.24546900	-1.58341100	0.95986100
C	-1.11430200	4.94299800	-2.37333000
C	-0.25413800	4.70201800	-1.07801700

C	-0.37865200	5.65573000	-3.49769500
H	-1.04481400	5.77409700	-4.35732200
H	-0.05719200	6.65253700	-3.17737900
H	0.49884000	5.09423700	-3.82491100
C	1.23315800	4.50143100	-1.37105900
H	1.71188200	5.43938400	-1.66817500
H	1.72587500	4.13492700	-0.46579100
H	1.39289800	3.76473200	-2.16382400
C	-2.44605400	5.63831100	-2.08816600
H	-2.30265800	6.68930300	-1.81937700
H	-3.06679100	5.59490500	-2.98762600
H	-2.99209000	5.14322000	-1.27894700
C	-0.43588600	5.74398500	0.01489200
H	0.19014200	5.48699600	0.87482200
H	-0.13319500	6.73423700	-0.34155900
H	-1.47200700	5.79531900	0.35577400
O	-1.42216200	3.59752500	-2.79921400
O	-0.76721300	3.43844200	-0.60261300
B	-1.31947500	2.79488600	-1.68964900
O	-1.70979600	1.49889200	-1.68348000
C	-1.60572800	0.75476400	-0.46052400
H	-2.22632800	1.27853100	0.28515300
O	-1.84975200	-0.52834000	-0.60353700
11Ru			
$G_{\text{solv}} = -2554.905918; E_{\text{solv}} = -2555.87736495$			
C	-2.54151300	-1.33388600	2.60086300
H	-2.76386300	-1.09896600	3.64925500
C	-2.28281600	-2.86949700	2.47404700
H	-1.29001200	-3.10380100	2.08390800
H	-2.35965000	-3.33557700	3.46319100
C	-3.37679100	-3.40644600	1.53506900
H	-3.01801700	-3.37264500	0.49834300
H	-3.65335200	-4.44170100	1.76179700
C	-4.52895200	-2.41519100	1.69751500
H	-5.05546100	-2.59725300	2.64484900
H	-5.26454700	-2.47189900	0.88835300
C	-3.80256200	-1.06829200	1.73772400
H	-4.42205000	-0.26441800	2.14743200
H	-3.50896600	-0.78206100	0.72042900
C	0.20687200	-0.65569900	3.37825300
H	-0.26060600	-0.45869400	4.34983000
C	0.78319300	-2.08731100	3.43276100
H	0.16201900	-2.76110600	4.03064300
H	0.86448300	-2.51552700	2.42730200
C	2.19100400	-1.89570700	4.00538700
H	2.13818100	-1.70836600	5.08637200
H	2.83551300	-2.76725200	3.84837900
C	2.67912100	-0.64365600	3.27379000
H	2.97102300	-0.91803200	2.25185700
H	3.54552100	-0.17086300	3.74835400
C	1.44775700	0.28127200	3.22521800
H	1.43128900	0.85710500	2.29430100
H	1.46922400	1.00420700	4.04936700
C	-1.52569400	1.43654700	2.59004300
H	-0.57203100	1.96526100	2.47807600
C	-2.03268400	1.62091400	4.05202600
H	-1.95433700	0.71950800	4.66677500
H	-1.42765900	2.38989500	4.54860700

C	-3.48314800	2.10252900	3.93058700
H	-4.15489300	1.24358500	3.80842500
H	-3.81742500	2.65951100	4.81210700
C	-3.47273700	2.93967700	2.65122400
H	-3.01393800	3.91708400	2.85743300
H	-4.47230700	3.12473300	2.24447400
C	-2.58648700	2.13316300	1.69196200
H	-2.11741100	2.77942300	0.94684600
H	-3.18193800	1.40471800	1.13756000
C	0.39904500	-0.82479600	-3.75596800
H	0.99456900	-1.42444600	-4.45817200
C	0.72937900	0.65010900	-4.03921300
H	1.80051300	0.81425800	-4.19155900
H	0.41492400	1.29027300	-3.20789000
C	-0.09393400	0.95151700	-5.29775700
H	-0.24234900	2.02450700	-5.45924700
H	0.43454400	0.55992500	-6.17641100
C	-1.41836300	0.19003400	-5.09552300
H	-2.17704900	0.85104300	-4.66194800
H	-1.82285900	-0.17308900	-6.04566800
C	-1.09990800	-0.96998200	-4.11513300
H	-1.29993200	-1.94963900	-4.56247600
H	-1.71600700	-0.89328000	-3.21161100
C	0.51566000	-3.27549200	-2.34546200
H	-0.55255000	-3.31768400	-2.59545600
C	0.74457300	-4.21210100	-1.11930300
H	1.30697000	-3.73132000	-0.31682400
H	-0.22115700	-4.49256000	-0.68717200
C	1.49565800	-5.44646300	-1.66231300
H	2.57170800	-5.34514100	-1.47055100
H	1.16971600	-6.37775600	-1.18856800
C	1.24825100	-5.42338500	-3.17374800
H	0.25004600	-5.82101500	-3.39936600
H	1.97714300	-6.01261700	-3.74006400
C	1.29494000	-3.92948400	-3.50606000
H	0.86154600	-3.69848400	-4.48426000
H	2.34005400	-3.59254500	-3.51835500
C	2.62575700	-1.21360000	-1.98568900
H	3.02859600	-1.50112200	-2.96495900
C	3.01615000	0.27198300	-1.69980800
H	3.48206900	0.71237600	-2.58772900
H	2.14994100	0.88856000	-1.44705600
C	4.01304100	0.23187900	-0.52624200
H	4.78380000	1.00682000	-0.60308300
H	3.47390800	0.39497300	0.41480700
C	4.58629900	-1.18760500	-0.55635500
H	5.05384800	-1.48446500	0.38875400
H	5.34397800	-1.27488500	-1.34676900
C	3.35911500	-2.03533500	-0.90302600
H	2.73810800	-2.12792200	-0.00525600
H	3.60632300	-3.04592300	-1.24514500
P	-1.08510300	-0.30675600	2.08293300
P	0.78262300	-1.45689600	-2.05375600
Ru	-0.31666300	-0.69784600	-0.10642100
H	1.11870000	-0.53211100	0.50377300
H	-2.38789200	2.10172100	-1.12573100
H	-0.87721300	-2.14352900	0.05532700
H	0.53650800	-1.82082800	0.53092200

C	0.47066000	4.81630300	0.10241000
C	1.75887400	3.98640200	0.45402200
C	0.72780600	6.07826900	−0.70495600
H	−0.21698900	6.59635600	−0.89426100
H	1.38347300	6.75977900	−0.15279700
H	1.18903400	5.85222000	−1.66859100
C	2.83791500	4.06465400	−0.62696600
H	3.31828700	5.04755300	−0.64671900
H	3.60230100	3.31135800	−0.41664100
H	2.42662500	3.85901800	−1.62043400
C	−0.38439100	5.13580700	1.32919800
H	0.08479600	5.90334200	1.95210500
H	−1.35722300	5.50922000	0.99705800
H	−0.55322500	4.24673000	1.94430800
C	2.35763200	4.28134700	1.82042500
H	3.23664600	3.64936600	1.97907300
H	2.67338300	5.32772000	1.88822700
H	1.64733100	4.07642900	2.62430400
O	−0.28048700	3.88459300	−0.71337500
O	1.25766800	2.63464200	0.45269600
B	0.15103100	2.62633400	−0.36367900
O	−0.40756600	1.46724900	−0.76732900
C	−1.75411100	1.24863600	−1.42353200
H	−1.52644100	1.33228500	−2.50066100
O	−2.17391700	0.05961200	−1.01482000
TS_{11,12-Ru}			
$G_{\text{solv}} = -2554.899776$; $E_{\text{solv}} = -2555.87005802$			
C	−2.41575500	−1.47998200	2.81630600
H	−2.56330200	−1.26101500	3.88084800
C	−2.13704800	−3.00916700	2.65613400
H	−1.16190200	−3.22361500	2.21363200
H	−2.15518800	−3.48757400	3.64215500
C	−3.27247100	−3.55387200	1.77405500
H	−2.98233300	−3.48542900	0.71739600
H	−3.50635700	−4.60163000	1.99068000
C	−4.43733400	−2.59969700	2.03817200
H	−4.89079500	−2.81719800	3.01486600
H	−5.22605800	−2.66014700	1.28087100
C	−3.74573400	−1.23363800	2.05926300
H	−4.35142400	−0.45451700	2.53244200
H	−3.54177900	−0.92175600	1.02947900
C	0.31098100	−0.71671900	3.48913400
H	−0.14999300	−0.52010100	4.46470000
C	0.91375100	−2.13692100	3.54782000
H	0.30509500	−2.82350300	4.14395100
H	1.00789700	−2.56242800	2.54186800
C	2.31541200	−1.91488100	4.12343500
H	2.25440000	−1.71897300	5.20247800
H	2.97644200	−2.77584200	3.97676500
C	2.78145800	−0.66097200	3.38092900
H	3.08448400	−0.94169700	2.36424700
H	3.63615700	−0.16586400	3.85384300
C	1.53247800	0.23983100	3.31454400
H	1.50451600	0.79907300	2.37473100
H	1.54110800	0.97826500	4.12514300
C	−1.48328400	1.32501900	2.69655500
H	−0.54017500	1.86440100	2.55239900
C	−1.96067600	1.53885400	4.16549100

H	-1.94565700	0.62891600	4.77274000
H	-1.29398800	2.25459500	4.66169900
C	-3.37609500	2.12571100	4.06343500
H	-4.11419200	1.31629900	3.99464900
H	-3.64112200	2.73844900	4.93137200
C	-3.34799700	2.90982500	2.75064200
H	-2.80818400	3.85554200	2.89766800
H	-4.34532300	3.15543300	2.37060900
C	-2.56187300	1.99534900	1.80348400
H	-2.10627300	2.54467600	0.97686900
H	-3.23095900	1.25403800	1.35907700
C	0.53526700	-0.88682300	-3.62523300
H	1.22025500	-1.41666000	-4.30120600
C	0.76082500	0.62048800	-3.84036600
H	1.82188900	0.87022100	-3.93440500
H	0.36472500	1.20070300	-2.99960100
C	-0.02194400	0.90687500	-5.12750500
H	-0.23781100	1.97161400	-5.26458400
H	0.56913100	0.57897800	-5.99241600
C	-1.29665500	0.05221300	-5.00628200
H	-2.10181100	0.63676900	-4.54588200
H	-1.66550300	-0.27336900	-5.98391200
C	-0.91832700	-1.14656800	-4.09709300
H	-0.98529000	-2.09992400	-4.63180500
H	-1.60236300	-1.21814800	-3.24304900
C	0.63397400	-3.35663800	-2.24632200
H	-0.42155900	-3.41391200	-2.54348000
C	0.82355700	-4.30840500	-1.02636800
H	1.39456800	-3.84809000	-0.21749000
H	-0.15260200	-4.56490700	-0.60303600
C	1.55065600	-5.55812200	-1.57187200
H	2.61920300	-5.50631300	-1.32704900
H	1.16627700	-6.48801800	-1.14124500
C	1.37765900	-5.48761500	-3.09309400
H	0.38463700	-5.85813900	-3.37975900
H	2.12256800	-6.07592700	-3.63896200
C	1.46838700	-3.98661300	-3.37997600
H	1.09673200	-3.71910100	-4.37429400
H	2.51752800	-3.66825900	-3.32079700
C	2.70448700	-1.28886100	-1.79226400
H	3.13856700	-1.58858900	-2.75432900
C	3.08583200	0.19887400	-1.51248900
H	3.55056200	0.63771000	-2.40178000
H	2.21430400	0.80900100	-1.26358700
C	4.07811900	0.16936500	-0.33351900
H	4.86265400	0.92836600	-0.42661700
H	3.53630100	0.36898500	0.59848000
C	4.63126300	-1.25845900	-0.32300600
H	5.07538500	-1.54132200	0.63767600
H	5.40394700	-1.37310500	-1.09514100
C	3.40207300	-2.09923300	-0.67842700
H	2.75856600	-2.16743600	0.20600100
H	3.64588100	-3.11875800	-0.99620100
P	-1.01581100	-0.41468500	2.21853800
P	0.86723700	-1.53900200	-1.91873100
Ru	-0.28625000	-0.80983000	0.00974600
H	1.13888400	-0.65888600	0.61315100
H	-2.61590600	1.82288400	-1.15959000

H	−0.85184400	−2.26620200	0.14426900
H	0.40246900	−2.04251800	0.63094200
C	0.63294500	4.62546800	0.25253400
C	1.89526200	3.79048100	0.67232400
C	0.93830300	5.87445000	−0.56183200
H	0.00822700	6.40245000	−0.79441300
H	1.58346500	6.55738700	0.00163600
H	1.42972100	5.62697600	−1.50540700
C	3.01143700	3.83367700	−0.37432300
H	3.50092600	4.81220100	−0.40763800
H	3.76196800	3.08083500	−0.11834400
H	2.62874700	3.60149100	−1.37332500
C	−0.26004800	4.98325000	1.44375800
H	0.19327900	5.75664600	2.07199700
H	−1.21655100	5.36015600	1.06973100
H	−0.46250000	4.10650600	2.06632100
C	2.45770600	4.12087900	2.04772400
H	3.31965800	3.47865400	2.25452900
H	2.79059600	5.16342600	2.09556900
H	1.71937000	3.95263800	2.83501200
O	−0.09079800	3.69373300	−0.56639400
O	1.37928000	2.45418100	0.69406900
B	0.28322000	2.40575700	−0.16943100
O	−0.31565700	1.29651800	−0.56169100
C	−2.08580500	0.89445700	−1.41872500
H	−1.56762600	0.90527400	−2.38169100
O	−2.36341500	−0.17106100	−0.83995800
12Ru			
$G_{\text{solv}} = -2554.912091$; $E_{\text{solv}} = -2555.88040484$			
C	−2.50460700	−1.37240300	2.63807400
H	−2.66784600	−1.13868600	3.69693600
C	−2.20372600	−2.90029100	2.51071900
H	−1.23400300	−3.10783100	2.05370200
H	−2.19473900	−3.35449700	3.50791700
C	−3.34559900	−3.48590500	1.66289600
H	−3.06765700	−3.45473600	0.60120100
H	−3.56870500	−4.52657200	1.92029500
C	−4.51667800	−2.53293300	1.90494500
H	−4.95932200	−2.71825600	2.89293300
H	−5.31236500	−2.62562100	1.15812100
C	−3.83454000	−1.16237800	1.87485800
H	−4.44398800	−0.36692000	2.31519200
H	−3.63334700	−0.89753500	0.83109400
C	0.16752900	−0.54520100	3.37439600
H	−0.34287200	−0.34807200	4.32554500
C	0.79390900	−1.95522600	3.46402600
H	0.18841000	−2.64308700	4.06209500
H	0.90710700	−2.39207200	2.46514500
C	2.18574000	−1.70628700	4.05278300
H	2.11149100	−1.50564600	5.13025600
H	2.86175400	−2.55743800	3.91698600
C	2.63746300	−0.44769800	3.30984100
H	2.94702900	−0.72162700	2.29285900
H	3.48236700	0.06073700	3.78641300
C	1.37576000	0.43281100	3.24035200
H	1.35898900	1.01182200	2.31364500
H	1.35939600	1.15163200	4.06868300
C	−1.63264500	1.44707500	2.44739600

H	-0.69660200	2.00264000	2.31994500
C	-2.17522500	1.71495300	3.88406900
H	-2.26156300	0.81220500	4.49644400
H	-1.48801600	2.38482900	4.41401600
C	-3.54200200	2.39572000	3.69509500
H	-4.33458900	1.63776500	3.64696200
H	-3.79070000	3.07645500	4.51567200
C	-3.42326600	3.09441800	2.33894300
H	-2.82387000	4.00885400	2.44182000
H	-4.39138600	3.37985200	1.91341000
C	-2.67368200	2.06882800	1.48188300
H	-2.18890100	2.50741000	0.60625500
H	-3.38294900	1.31706400	1.12060900
C	0.37712700	-0.72179700	-3.73778400
H	1.09046200	-1.14568400	-4.45785700
C	0.44711300	0.81408000	-3.84190700
H	1.47217600	1.17672300	-3.96472800
H	0.04075200	1.27336500	-2.93378000
C	-0.44127200	1.12369300	-5.04980300
H	-0.72858700	2.17881700	-5.10965100
H	0.08710800	0.86922700	-5.97853000
C	-1.64119800	0.18813600	-4.85497000
H	-2.36569700	0.66602400	-4.18179000
H	-2.17291200	-0.02570100	-5.78749600
C	-1.06311700	-1.08776000	-4.19772000
H	-1.03409400	-1.92338600	-4.90501600
H	-1.68912900	-1.40897900	-3.35851100
C	0.59892000	-3.23590300	-2.43037000
H	-0.45771000	-3.30982800	-2.71831000
C	0.81540900	-4.20336900	-1.22832700
H	1.40035500	-3.75107000	-0.42454300
H	-0.15134300	-4.46796000	-0.78874800
C	1.53467300	-5.44292400	-1.80807300
H	2.60571000	-5.39854900	-1.57310400
H	1.15301200	-6.38125900	-1.39349300
C	1.34646100	-5.34163100	-3.32676900
H	0.35197600	-5.70988100	-3.61159900
H	2.08815300	-5.91627400	-3.89133600
C	1.42949700	-3.83440000	-3.58263000
H	1.05139100	-3.54275700	-4.56800800
H	2.47778800	-3.51483100	-3.52138900
C	2.64442200	-1.15534300	-2.01642400
H	3.04576100	-1.44888600	-2.99448200
C	3.03141800	0.33037900	-1.74116100
H	3.45295400	0.77872000	-2.64748400
H	2.16741200	0.93036300	-1.44839200
C	4.07363000	0.29369100	-0.60516200
H	4.85532900	1.05067400	-0.73004200
H	3.57092500	0.49222600	0.34897700
C	4.62277700	-1.13552100	-0.62052800
H	5.10369000	-1.42260200	0.32095800
H	5.36405600	-1.25071800	-1.42301400
C	3.37810400	-1.97075100	-0.93020600
H	2.76443100	-2.03592600	-0.02417700
H	3.60597000	-2.99108600	-1.25733200
P	-1.11001100	-0.29352500	2.04432100
P	0.80892200	-1.42213700	-2.07433900
Ru	-0.32749100	-0.70794800	-0.13716200

H	1.09071100	−0.58643100	0.49779700
H	−3.78433500	0.74864100	−2.02354000
H	−0.94971100	−2.15520400	−0.03999800
H	0.29458500	−1.97974800	0.48764200
C	0.73491100	4.67327400	0.08299500
C	1.95401300	3.85222600	0.63733600
C	1.11387900	5.89130400	−0.74873600
H	0.20857200	6.40932400	−1.08106000
H	1.71107000	6.59669000	−0.16026200
H	1.68280100	5.60694400	−1.63690700
C	3.15784200	3.86505100	−0.30848600
H	3.63978100	4.84751600	−0.34397900
H	3.89042600	3.13555100	0.04719100
H	2.86670100	3.58199600	−1.32499600
C	−0.24824000	5.08234400	1.18475000
H	0.15596600	5.87538200	1.82227500
H	−1.16803300	5.44886800	0.71891800
H	−0.50871100	4.22838600	1.81762300
C	2.39907700	4.23457900	2.04347600
H	3.24005600	3.60271200	2.34651200
H	2.72768300	5.27916200	2.08160200
H	1.59648300	4.09402700	2.77132000
O	0.07479000	3.71774800	−0.75080400
O	1.43777300	2.52022000	0.66147800
B	0.39082800	2.42810900	−0.27221700
O	−0.22521300	1.34098100	−0.65490500
C	−2.75873100	0.67840300	−1.62838500
H	−2.08835200	1.54834900	−1.65388000
O	−2.37907400	−0.37630000	−1.14945300
13Ru			
$G_{\text{solv}} = -2440.451472$; $E_{\text{solv}} = -2441.38796780$			
C	−2.10613400	−1.79104400	3.01944500
H	−2.36537400	−1.46878000	4.03468400
C	−1.43317300	−3.19824600	3.10061500
H	−0.42869400	−3.21384100	2.66929700
H	−1.33574700	−3.49752900	4.14997800
C	−2.37311600	−4.15912800	2.35053900
H	−2.07063700	−4.22516500	1.29750200
H	−2.35433700	−5.17261400	2.76401700
C	−3.74620400	−3.49063600	2.44022700
H	−4.17437700	−3.63729900	3.44074100
H	−4.46447000	−3.87652200	1.70935300
C	−3.41202100	−2.01230500	2.22114300
H	−4.21155000	−1.33635500	2.54049600
H	−3.23877600	−1.84123900	1.15052900
C	0.22326500	−0.19519400	3.65638100
H	−0.36662900	−0.01117900	4.56492400
C	1.20608500	−1.34301000	3.95567900
H	0.75738800	−2.13303100	4.56566000
H	1.55688400	−1.79742100	3.02038500
C	2.37317800	−0.63670100	4.65191800
H	2.09241200	−0.38603100	5.68356200
H	3.27878900	−1.25101800	4.69460100
C	2.55254000	0.64100400	3.82387600
H	3.16026000	0.42358200	2.93769500
H	3.06045300	1.43788800	4.37697900
C	1.12602900	1.04135700	3.38114900
H	1.13443200	1.31765900	2.32391800

H	0.75644600	1.90878400	3.94022200
C	-1.94277200	1.09513800	2.34269700
H	-1.16558800	1.84103900	2.13229700
C	-2.63824800	1.48935900	3.67042800
H	-2.92738300	0.61373000	4.26138600
H	-1.96102900	2.07976400	4.29692100
C	-3.89489500	2.29974300	3.25636900
H	-4.79845200	1.70920800	3.44939900
H	-3.99518800	3.23178200	3.82167200
C	-3.75079800	2.53879100	1.74456300
H	-3.13370300	3.42661500	1.55475500
H	-4.71353900	2.69248700	1.24583900
C	-3.00732500	1.29553800	1.24942300
H	-2.54647800	1.42211100	0.26665800
H	-3.70001100	0.44775400	1.20073400
C	0.66043600	-0.42914200	-3.31873000
H	1.00735000	-0.96512400	-4.21029500
C	1.40551700	0.92364200	-3.26430700
H	2.41543500	0.85161700	-3.68186000
H	1.49938200	1.27313700	-2.23459300
C	0.49538400	1.87566200	-4.04749200
H	0.71103600	2.93084400	-3.84447200
H	0.61687500	1.71121800	-5.12689100
C	-0.90967400	1.46245300	-3.59900100
H	-1.10982000	1.88506700	-2.60906500
H	-1.69525400	1.80525200	-4.28082200
C	-0.84662600	-0.07431800	-3.49748900
H	-1.23519900	-0.54715900	-4.40673800
H	-1.46053600	-0.43347300	-2.66236300
C	0.33486900	-3.16075500	-2.61628000
H	-0.68446300	-2.91039700	-2.94092700
C	0.23173900	-4.36995900	-1.63812300
H	0.80834000	-4.22194200	-0.72242300
H	-0.80925000	-4.50260800	-1.32627400
C	0.74130100	-5.59773900	-2.42430700
H	1.78176100	-5.81212400	-2.14964600
H	0.16013900	-6.50110500	-2.21456300
C	0.68376000	-5.17690000	-3.89665200
H	-0.34238100	-5.26606300	-4.27694800
H	1.33092000	-5.77940000	-4.54241000
C	1.09076300	-3.70148200	-3.84893800
H	0.84072900	-3.16087200	-4.76708700
H	2.17664400	-3.63034400	-3.70755600
C	2.77605400	-1.71095800	-1.77776500
H	3.15465900	-1.81254100	-2.80275100
C	3.45468200	-0.47526500	-1.10686200
H	4.01267800	0.09373200	-1.85814200
H	2.73361200	0.21220300	-0.65714200
C	4.40218000	-1.04700100	-0.03208000
H	5.32468200	-0.46565200	0.06711500
H	3.89883000	-1.03422900	0.94303300
C	4.64203400	-2.49871000	-0.45498300
H	5.01301200	-3.13110100	0.35860900
H	5.37178900	-2.54306000	-1.27471900
C	3.26025100	-2.92522000	-0.95642600
H	2.60626700	-3.08130800	-0.08943300
H	3.26949200	-3.85121000	-1.54115700
P	-0.99538400	-0.49712400	2.29044300

P	0.93197500	−1.56146200	−1.87535000
Ru	−0.10020800	−0.98552000	0.16616800
H	1.25199000	−1.26466300	0.85709500
H	−0.91193700	−2.34503400	0.15555800
H	0.17378800	−2.46843900	0.63570000
C	0.65592600	4.42717300	0.16845900
C	2.08029500	3.76644200	0.13856000
C	0.52446100	5.69466900	−0.66395900
H	−0.49252400	6.09015100	−0.57824200
H	1.21940400	6.46553800	−0.31275600
H	0.72156200	5.50048300	−1.72071000
C	2.78629800	3.93736600	−1.20940500
H	3.13228500	4.96492000	−1.36169200
H	3.65494600	3.27237400	−1.23978400
H	2.12758500	3.66610800	−2.03997600
C	0.15692900	4.68423500	1.59441700
H	0.68855800	5.51400800	2.07138000
H	−0.90778300	4.93367500	1.55578700
H	0.27352200	3.79367700	2.22075900
C	3.00666100	4.19437200	1.26922200
H	3.97216300	3.68908000	1.16563200
H	3.18434700	5.27522900	1.24402700
H	2.59420100	3.92813900	2.24522500
O	−0.17064000	3.40264300	−0.39515400
O	1.77187500	2.37835400	0.29102400
B	0.45306300	2.16974900	−0.14577000
O	−0.10927900	0.99823900	−0.29927900
14Ru			
$G_{\text{solv}} = -2852.074642$; $E_{\text{solv}} = -2853.19707293$			
C	−1.09924200	−1.45606200	3.46507800
H	−1.15368900	−1.12463100	4.50877300
C	−0.40984400	−2.85761700	3.42662500
H	0.53458100	−2.86039500	2.87908800
H	−0.18668100	−3.18097400	4.44992100
C	−1.42967000	−3.80798100	2.78115200
H	−1.31385300	−3.78755100	1.68917700
H	−1.30630900	−4.84502800	3.11078000
C	−2.78136000	−3.20081600	3.15672100
H	−3.00884400	−3.40929700	4.21093100
H	−3.61212400	−3.58106000	2.55268400
C	−2.53856500	−1.70345700	2.94581100
H	−3.27402800	−1.07191300	3.45310000
H	−2.60785300	−1.48564700	1.87512800
C	1.31125600	0.14819100	3.62202600
H	0.91160500	0.36089800	4.62079000
C	2.31012900	−1.02257100	3.76033000
H	2.02673400	−1.71948200	4.55534500
H	2.36941300	−1.59179000	2.82641500
C	3.66007500	−0.34103400	4.00422500
H	3.72522000	0.01146500	5.04252800
H	4.50983600	−1.00874700	3.82409700
C	3.60968100	0.84890600	3.04424400
H	3.79591300	0.49692900	2.02132000
H	4.35380500	1.62053200	3.26897600
C	2.16459000	1.36779700	3.15262400
H	1.82445700	1.78297200	2.20031100
H	2.09735300	2.16921700	3.89859200
C	−1.09428500	1.43811800	2.86714000

H	-0.39383600	2.19890000	2.50392600
C	-1.43728100	1.74438900	4.35785600
H	-1.12928700	0.95820900	5.05370200
H	-0.91492700	2.65627500	4.67092500
C	-2.95868500	1.96399600	4.40100300
H	-3.47054300	1.00817200	4.57229900
H	-3.26274100	2.64594200	5.20202400
C	-3.29581000	2.47829500	2.99971000
H	-3.01072100	3.53602800	2.91407800
H	-4.36212900	2.40464800	2.75797000
C	-2.42194500	1.60923200	2.08953400
H	-2.25430100	2.04014200	1.10131600
H	-2.91783900	0.65388100	1.91514100
C	1.87323200	-0.11138800	-3.00418300
H	2.43594300	-0.65069800	-3.77981800
C	2.73903200	1.07635900	-2.55270000
H	3.78783700	0.80478600	-2.39940800
H	2.35539400	1.49285400	-1.61237600
C	2.54252000	2.07204400	-3.69939600
H	2.90092600	3.08009200	-3.46512800
H	3.09966100	1.72583900	-4.58080900
C	1.03195500	2.00742400	-3.96522600
H	0.50428000	2.68232500	-3.28064300
H	0.77234100	2.30940000	-4.98568100
C	0.62574500	0.54363800	-3.65629600
H	0.33813600	-0.00198100	-4.56227800
H	-0.22595200	0.51971800	-2.97405600
C	0.50968600	-2.58988100	-2.73360300
H	-0.31322400	-1.98130900	-3.12173500
C	-0.13277400	-3.76983600	-1.94621600
H	0.31491400	-3.91734700	-0.96037000
H	-1.19308300	-3.55579200	-1.77516900
C	0.04907700	-5.01786700	-2.83773900
H	0.90993200	-5.60399800	-2.49120500
H	-0.82178100	-5.68084300	-2.81760900
C	0.34717900	-4.46262900	-4.23541300
H	-0.58457200	-4.14360500	-4.72188800
H	0.83463700	-5.19012600	-4.89302700
C	1.21930900	-3.23884700	-3.93837700
H	1.30550400	-2.55457700	-4.78911400
H	2.23119500	-3.57502900	-3.67864400
C	3.11464300	-2.17337100	-1.44362300
H	3.53518100	-2.34140100	-2.44234300
C	4.12674800	-1.30783700	-0.63059800
H	4.96263200	-1.01824200	-1.27692200
H	3.68044800	-0.38610100	-0.24837700
C	4.62216600	-2.20726000	0.51585800
H	5.65667100	-1.99239700	0.80309300
H	3.99595200	-2.05261700	1.40353700
C	4.41721400	-3.63216300	-0.00472600
H	4.42904500	-4.38821500	0.78769700
H	5.20492000	-3.88936800	-0.72548500
C	3.06214900	-3.53384500	-0.71207400
H	2.27062000	-3.53743900	0.04607100
H	2.86408200	-4.36458900	-1.39775000
P	-0.16806200	-0.14218400	2.52769000
P	1.46028300	-1.36712700	-1.70887500
Ru	0.42261200	-0.69106600	0.29709200

H	1.76424400	0.03290300	0.62634900
H	0.47675900	−2.20833300	0.75729000
H	1.50900400	−1.58403800	0.97102200
C	−0.37736600	4.59606300	−0.37830800
C	1.05367600	4.23164200	0.16117300
C	−0.40863400	5.72661400	−1.39842000
H	−1.44249700	5.91996100	−1.70193300
H	−0.00268600	6.65036000	−0.97142200
H	0.16290900	5.47454400	−2.29456000
C	2.14980000	4.45897200	−0.88026500
H	2.35046100	5.52403200	−1.03633200
H	3.07212200	3.97908600	−0.53912000
H	1.87037200	4.01553700	−1.83860200
C	−1.36942100	4.88930500	0.75039600
H	−1.18074300	5.86134800	1.21785400
H	−2.38441600	4.89193100	0.34142500
H	−1.32103000	4.11983500	1.52475000
C	1.43782000	4.90804300	1.47176300
H	2.44833500	4.60232300	1.76098600
H	1.43051500	5.99880100	1.36769600
H	0.75965600	4.63056000	2.28228800
O	−0.78664200	3.38114100	−1.01252700
O	0.94853000	2.82354400	0.38206100
B	−0.09548800	2.31227300	−0.40834400
O	−0.40922700	1.04916000	−0.56193600
C	−3.37663600	−0.45193600	−2.67133600
C	−4.01310900	0.22181700	−1.39551600
H	−1.30029200	−1.44806500	−0.15998400
C	−3.20681200	0.47906200	−3.86307200
H	−2.73516700	−0.06422600	−4.68749100
H	−4.17955400	0.84342900	−4.20996500
H	−2.57657100	1.33566100	−3.61628300
C	−3.78480800	1.72904300	−1.32591200
H	−4.34023900	2.24845400	−2.11326900
H	−4.14321300	2.09684000	−0.35993400
H	−2.72565000	1.98368400	−1.40795300
C	−4.07684200	−1.74170300	−3.09871200
H	−5.07006400	−1.54429700	−3.51333200
H	−3.47415200	−2.23253200	−3.86901200
H	−4.18021100	−2.43640100	−2.25952400
C	−5.48436500	−0.09792300	−1.17511100
H	−5.82945800	0.39283100	−0.26023500
H	−6.08811600	0.27744700	−2.00806100
H	−5.66007800	−1.17073800	−1.07046400
O	−2.06337000	−0.84169800	−2.20843800
O	−3.25207100	−0.37812600	−0.31498700
B	−2.07844200	−0.81566000	−0.84749300
TS _{14,15-Ru}			
G _{solv} = −2852.072033; E _{solv} = −2853.19694451			
C	−1.64786500	−1.39646800	3.24117800
H	−1.70437300	−1.07350300	4.28732000
C	−0.94978800	−2.79310400	3.19143300
H	−0.00289000	−2.78417800	2.64823100
H	−0.73012700	−3.12579400	4.21253600
C	−1.96061300	−3.74231700	2.53061600
H	−1.84064600	−3.70750500	1.43955000
H	−1.83132500	−4.78242400	2.84816500
C	−3.31791600	−3.14928400	2.90846100

H	-3.54816300	-3.37287600	3.95900400
H	-4.14351200	-3.52757300	2.29619900
C	-3.08560100	-1.64740700	2.71792900
H	-3.82536100	-1.02867900	3.23508400
H	-3.15627200	-1.41441000	1.65012000
C	0.75094400	0.23275200	3.40281900
H	0.35213400	0.44884100	4.40095500
C	1.75604800	-0.93217600	3.54534200
H	1.48097300	-1.62190500	4.34957400
H	1.81069400	-1.51161400	2.61767200
C	3.10522900	-0.24300700	3.77202200
H	3.17843100	0.11763900	4.80695300
H	3.95604700	-0.90856800	3.58902900
C	3.04134300	0.93970700	2.80380800
H	3.21728100	0.58064300	1.78148800
H	3.78566400	1.71499400	3.01484700
C	1.59613600	1.45491900	2.92468600
H	1.24460000	1.86842600	1.97564300
H	1.53376700	2.25648600	3.67090100
C	-1.66696300	1.50162900	2.66873900
H	-0.97785400	2.27144400	2.30257900
C	-1.99412200	1.79357300	4.16655900
H	-1.69872600	0.99029300	4.84805500
H	-1.45107600	2.68931400	4.49039200
C	-3.51142900	2.04013800	4.22396600
H	-4.03784500	1.09260200	4.39780900
H	-3.79650200	2.72544800	5.02903300
C	-3.85319800	2.56134100	2.82662900
H	-3.54797700	3.61329600	2.73785800
H	-4.92292800	2.50832800	2.59491200
C	-3.00490900	1.67386100	1.91083400
H	-2.85319700	2.08852100	0.91299000
H	-3.51317100	0.72136500	1.75965300
C	1.34492600	-0.04243700	-3.21015200
H	1.92263100	-0.58410800	-3.97313100
C	2.20538200	1.14032300	-2.73567500
H	3.24818500	0.86343200	-2.55399900
H	1.79880200	1.55802000	-1.80524000
C	2.04577600	2.13881800	-3.88554600
H	2.40119800	3.14505400	-3.63845900
H	2.62726800	1.79226600	-4.75082700
C	0.54331400	2.08095800	-4.19622100
H	-0.00196900	2.76292600	-3.53271100
H	0.31659300	2.37849000	-5.22567400
C	0.11819400	0.62157000	-3.89180300
H	-0.15409400	0.07569700	-4.80224300
H	-0.75035600	0.60667600	-3.23104300
C	-0.07309100	-2.49636600	-2.95378700
H	-0.87994800	-1.86995400	-3.34724100
C	-0.74722400	-3.66047100	-2.16989600
H	-0.30245600	-3.82371500	-1.18521600
H	-1.80066200	-3.41698200	-1.99630600
C	-0.60007600	-4.90996900	-3.06631200
H	0.23855200	-5.52565300	-2.71661500
H	-1.49248600	-5.54384100	-3.05505100
C	-0.27465500	-4.35966800	-4.46010800
H	-1.19273500	-4.01242400	-4.95317400
H	0.19694200	-5.09927000	-5.11580000

C	0.62981200	−3.16222700	−4.15258600
H	0.74467200	−2.47888400	−5.00078200
H	1.62868900	−3.52807600	−3.88266800
C	2.53408100	−2.13586500	−1.65084300
H	2.95519500	−2.31421900	−2.64758900
C	3.55986600	−1.28928700	−0.83502400
H	4.39932100	−1.00857400	−1.48057100
H	3.12703600	−0.36298100	−0.44849500
C	4.04170200	−2.20050800	0.30828000
H	5.08141700	−2.00711700	0.59179100
H	3.42212100	−2.03440700	1.19859500
C	3.80582700	−3.62059900	−0.21244800
H	3.80313800	−4.37668000	0.58002200
H	4.58677100	−3.89433200	−0.93451500
C	2.45188200	−3.49357400	−0.91734900
H	1.66167000	−3.47735400	−0.15803800
H	2.23438400	−4.32064700	−1.60159300
P	−0.72870100	−0.06900700	2.31229000
P	0.89784800	−1.29645200	−1.92321000
Ru	−0.13517500	−0.60942500	0.08013700
H	1.19053500	0.15692800	0.39145300
H	−0.06991700	−2.11811900	0.54142500
H	1.01103500	−1.41758300	0.74977700
C	−1.02144100	4.64867400	−0.66569900
C	0.39362800	4.29219900	−0.08067700
C	−1.02484300	5.76540900	−1.70080400
H	−2.04972900	5.95256800	−2.03672800
H	−0.63331000	6.69520500	−1.27362100
H	−0.42659400	5.50337200	−2.57645200
C	1.52001600	4.50849400	−1.09115500
H	1.72445000	5.57203300	−1.25224800
H	2.43196300	4.03345900	−0.71709600
H	1.27057800	4.05460400	−2.05266500
C	−2.04598000	4.95206200	0.43019600
H	−1.87595400	5.93175200	0.88849300
H	−3.04943100	4.94184600	−0.00603400
H	−2.01370500	4.19395100	1.21642500
C	0.73842700	4.98372500	1.23297900
H	1.74002000	4.68207900	1.55553000
H	0.73410900	6.07308600	1.11537500
H	0.03639000	4.71582400	2.02629000
O	−1.41147200	3.42408500	−1.29645100
O	0.28242700	2.88587600	0.15347300
B	−0.73935700	2.36734100	−0.65721400
O	−1.04516000	1.09747700	−0.79764600
C	−3.91324300	−0.30654300	−2.87826900
C	−4.55875200	0.34905400	−1.59475000
H	−1.83908400	−1.31197400	−0.39005900
C	−3.78170000	0.63149400	−4.07022600
H	−3.30170100	0.10326000	−4.89969700
H	−4.76683700	0.96995900	−4.40860800
H	−3.17278800	1.50456300	−3.82694900
C	−4.41185400	1.86777700	−1.54232200
H	−5.01554300	2.34845800	−2.31896100
H	−4.76651800	2.22257800	−0.56976900
H	−3.37257100	2.18349000	−1.65344100
C	−4.58298200	−1.61365700	−3.30348300
H	−5.58703600	−1.44429700	−3.70450500

H	-3.97607200	-2.08323200	-4.08381700
H	-4.65416800	-2.31496400	-2.46655300
C	-6.00977700	-0.03983500	-1.34619400
H	-6.36291800	0.44270900	-0.42986200
H	-6.64653800	0.29571700	-2.17161200
H	-6.12999900	-1.11873700	-1.22701700
O	-2.58751000	-0.66181900	-2.43322200
O	-3.75678200	-0.20393900	-0.52415300
B	-2.56968100	-0.60270600	-1.06813800
15Ru			
$G_{\text{solv}} = -2852.094360; E_{\text{solv}} = -2853.21961275$			
C	-1.36343000	-2.03160800	3.06884100
H	-1.70993300	-1.82526000	4.08787800
C	0.00891300	-2.76862000	3.16851600
H	0.80539000	-2.25597700	2.62381600
H	0.31882200	-2.82384400	4.21821500
C	-0.23182500	-4.18033000	2.60335500
H	-0.00090200	-4.19350900	1.53014000
H	0.39450400	-4.93886700	3.08408400
C	-1.73140300	-4.41686200	2.79637800
H	-1.94480000	-4.66045200	3.84588400
H	-2.12290300	-5.23115000	2.17741600
C	-2.33256600	-3.05509700	2.43531100
H	-3.35922900	-2.92434700	2.79301000
H	-2.34476300	-2.95044000	1.34441900
C	-0.44154700	0.64959000	3.48735800
H	-0.89072800	0.36997500	4.45162200
C	1.07950900	0.44560900	3.59564300
H	1.34984000	-0.49671200	4.08161000
H	1.53218200	0.45876300	2.59681300
C	1.53571300	1.67448400	4.38616800
H	1.28258400	1.54947400	5.44754300
H	2.61628500	1.84362200	4.32015700
C	0.71857100	2.81776200	3.76880900
H	1.26216900	3.20888400	2.90444800
H	0.56227500	3.64916300	4.46441300
C	-0.61117400	2.18062400	3.29266400
H	-0.80856200	2.43201700	2.24741400
H	-1.46891200	2.54469100	3.86887100
C	-3.01881700	0.28339100	2.30047400
H	-2.86875800	1.34438400	2.07742500
C	-3.78734100	0.15764000	3.64595300
H	-3.36604500	-0.59879600	4.31511100
H	-3.74687800	1.10893600	4.18773300
C	-5.24161700	-0.20309500	3.26134500
H	-5.40238100	-1.28172000	3.38312000
H	-5.98153300	0.30622900	3.88708000
C	-5.35781100	0.15877900	1.77537200
H	-5.51114600	1.24078000	1.66222200
H	-6.18867800	-0.35058200	1.27509400
C	-3.98667300	-0.22594400	1.21438200
H	-3.76308900	0.23187000	0.24734600
H	-3.92950300	-1.31317400	1.08836500
C	0.75236400	-0.28247400	-3.49335200
H	1.31352500	-0.87761700	-4.22894400
C	1.46459500	1.06815900	-3.33015100
H	2.54732300	0.96484200	-3.20481700
H	1.06265100	1.60030400	-2.46613100

C	1.08751300	1.82526700	−4.60933000
H	1.17761000	2.90929900	−4.48411800
H	1.75935000	1.53043200	−5.42572600
C	−0.36038000	1.38711100	−4.92280600
H	−1.06800500	2.16317300	−4.62038000
H	−0.49954700	1.21492600	−5.99548300
C	−0.61329900	0.10075700	−4.09900500
H	−1.02718100	−0.70920300	−4.70919300
H	−1.32502200	0.31385000	−3.29477700
C	−0.30993800	−2.77838400	−2.67069900
H	−1.26817100	−2.33409100	−2.96781500
C	−0.62572900	−3.94729200	−1.68878800
H	−0.02219000	−3.91207600	−0.78026400
H	−1.66936500	−3.88231700	−1.36473800
C	−0.36371800	−5.24739800	−2.47875100
H	0.62889400	−5.64323200	−2.22860500
H	−1.09162000	−6.03201000	−2.24937500
C	−0.38038500	−4.82344200	−3.95084600
H	−1.41516600	−4.71573000	−4.30213800
H	0.12293200	−5.53713800	−4.61134200
C	0.29939200	−3.45204500	−3.91799100
H	0.13502000	−2.86993400	−4.83040700
H	1.38261900	−3.58912900	−3.80339000
C	2.36477800	−1.90632700	−1.76268400
H	2.73743500	−2.16453700	−2.76147100
C	3.27935000	−0.79948900	−1.15724000
H	3.97277000	−0.42813200	−1.91980100
H	2.70772300	0.05882200	−0.79516300
C	4.04348700	−1.46696500	0.00363600
H	5.06679000	−1.08952500	0.10568500
H	3.52136900	−1.26744100	0.94755800
C	3.98160200	−2.96551100	−0.30591200
H	4.18048100	−3.59489800	0.56806100
H	4.71491300	−3.22557200	−1.08121000
C	2.55854200	−3.13280200	−0.84645200
H	1.85975100	−3.09519500	−0.00305600
H	2.39842600	−4.07805200	−1.37608000
P	−1.29451200	−0.38570400	2.20370700
P	0.61292100	−1.32473400	−1.96458500
Ru	−0.36306600	−0.55162700	0.04532200
H	0.94606600	−1.08193400	0.76633200
H	−1.47801600	−1.60984000	−0.22363100
H	−0.20866100	−2.04824500	0.41848200
C	2.54019200	4.31542000	−0.19239400
C	3.39232500	3.13270100	0.41329500
C	3.19399500	5.02978300	−1.36765600
H	2.53205700	5.82326800	−1.72696100
H	4.14078500	5.48938000	−1.06484400
H	3.38293600	4.34875100	−2.20007100
C	4.34128700	2.49480300	−0.60116900
H	5.16742700	3.16614100	−0.85437900
H	4.75891100	1.58113700	−0.16905400
H	3.81741600	2.22220500	−1.52178200
C	2.08465000	5.34165100	0.84564700
H	2.92707000	5.92056600	1.23616200
H	1.38210800	6.03456900	0.37361400
H	1.56853500	4.86728600	1.68444200
C	4.14972100	3.48161800	1.68645200

H	4.68515500	2.59831500	2.04735200
H	4.88511600	4.27044500	1.49585200
H	3.47701800	3.81670700	2.47868000
O	1.35982100	3.64131800	−0.66963300
O	2.38899300	2.14712800	0.73204200
B	1.27096500	2.43548700	−0.01559000
O	0.21775800	1.59610500	−0.08496300
C	−2.40709900	3.18491000	−1.93622300
C	−2.61215100	3.56638300	−0.42693300
H	−1.58047000	0.49213100	−0.75614100
C	−2.19258400	4.37859700	−2.85900100
H	−2.11578400	4.04256000	−3.89786400
H	−3.03306500	5.07912100	−2.79479900
H	−1.27110400	4.90812700	−2.60764500
C	−1.80254200	4.80015500	−0.01343400
H	−2.22039900	5.72301000	−0.43061500
H	−1.81878800	4.88116400	1.07876900
H	−0.76135300	4.70463800	−0.33279000
C	−3.53679100	2.30277700	−2.48229900
H	−4.47369400	2.85849800	−2.59556300
H	−3.24325000	1.92473700	−3.46664200
H	−3.71962500	1.44168700	−1.83154000
C	−4.06762400	3.73290900	−0.00456400
H	−4.11497600	3.99109500	1.05872700
H	−4.55497900	4.53627300	−0.56872400
H	−4.63132000	2.80843200	−0.15174500
O	−1.21282000	2.40941800	−1.89727500
O	−2.07297200	2.43455700	0.24818700
B	−1.14947200	1.77274300	−0.62356100
TS _{15,16-Ru}			
$G_{\text{solv}} = -2852.087273$; $E_{\text{solv}} = -2853.20850495$			
C	−1.33874200	−1.88221600	3.03253900
H	−1.71115800	−1.68723000	4.04494400
C	0.03600900	−2.61164300	3.15673000
H	0.83208600	−2.09626100	2.61435300
H	0.33260400	−2.65865600	4.21095100
C	−0.18698700	−4.02804500	2.59533100
H	0.07297100	−4.04579700	1.52915900
H	0.42775300	−4.78233200	3.09768600
C	−1.69039900	−4.26844500	2.74807100
H	−1.93237800	−4.51174900	3.79172100
H	−2.06299800	−5.08426000	2.11915600
C	−2.28457200	−2.90852500	2.36948100
H	−3.32192300	−2.78420600	2.69713900
H	−2.26226600	−2.80157400	1.27903500
C	−0.40970800	0.77795700	3.50710500
H	−0.89801600	0.49471700	4.45032100
C	1.10313900	0.54699900	3.67298400
H	1.33337700	−0.38974000	4.18883800
H	1.58875500	0.52163700	2.69008000
C	1.56325100	1.78230800	4.45073700
H	1.26480500	1.69683400	5.50444600
H	2.65009600	1.92117900	4.42321200
C	0.80120200	2.92321400	3.76753200
H	1.36179000	3.22872300	2.87907900
H	0.68435500	3.80621900	4.40535100
C	−0.55353800	2.31584000	3.33085100
H	−0.78404300	2.59044900	2.29891400

H	-1.38132600	2.68991000	3.94360900
C	-2.96563700	0.45874600	2.29697100
H	-2.81525000	1.51597400	2.05407400
C	-3.70458800	0.36448700	3.66438000
H	-3.21741900	-0.30880000	4.37622900
H	-3.72980000	1.35149700	4.13993800
C	-5.13318100	-0.12094600	3.33722300
H	-5.19507000	-1.20968000	3.46083000
H	-5.89065200	0.32299900	3.99150100
C	-5.32781200	0.22926200	1.85819900
H	-5.55009900	1.30075100	1.75464100
H	-6.14641100	-0.32740300	1.38868700
C	-3.95911500	-0.08091900	1.24617400
H	-3.79314300	0.38499200	0.27221700
H	-3.85463300	-1.16151200	1.10299800
C	0.85937700	-0.11614300	-3.46706700
H	1.40172400	-0.72236600	-4.20733400
C	1.62171200	1.20431600	-3.28797400
H	2.69854000	1.06036800	-3.15602600
H	1.23715200	1.73714900	-2.41469800
C	1.27908800	1.98923300	-4.55933900
H	1.42915200	3.06699000	-4.43490700
H	1.92931200	1.65929600	-5.37966500
C	-0.19117300	1.62735200	-4.86269400
H	-0.85503100	2.42772600	-4.52485500
H	-0.35582300	1.49663200	-5.93758700
C	-0.48756700	0.32887400	-4.07159100
H	-0.92573800	-0.45138600	-4.70313700
H	-1.19400800	0.53559600	-3.26125100
C	-0.30342700	-2.57255700	-2.67890100
H	-1.24220200	-2.08538900	-2.97059700
C	-0.67026700	-3.74007700	-1.71279400
H	-0.06964600	-3.73930200	-0.80183000
H	-1.71111000	-3.63460300	-1.39052500
C	-0.46144200	-5.04014700	-2.51839600
H	0.51318100	-5.48103700	-2.27206000
H	-1.22196800	-5.79680100	-2.30052900
C	-0.45711200	-4.59751500	-3.98520100
H	-1.48602600	-4.44183100	-4.33623800
H	0.01665700	-5.32362700	-4.65435700
C	0.27979200	-3.25634200	-3.93270900
H	0.14408900	-2.65689200	-4.83887500
H	1.35573500	-3.44170400	-3.81740500
C	2.39942300	-1.82380400	-1.76623700
H	2.74681200	-2.10588000	-2.76796100
C	3.37405300	-0.75953600	-1.18050700
H	4.07024300	-0.41875100	-1.95557400
H	2.84138800	0.11857200	-0.80629400
C	4.12554000	-1.45642600	-0.02843300
H	5.16949800	-1.13283400	0.05203700
H	3.62769500	-1.22161600	0.92041900
C	3.98086500	-2.95294200	-0.32105500
H	4.15709400	-3.58221100	0.55809200
H	4.69035400	-3.26021600	-1.10161000
C	2.54431800	-3.05030800	-0.84237200
H	1.85807700	-2.96532700	0.00746300
H	2.33067100	-3.99094000	-1.36166500
P	-1.24247500	-0.22790700	2.17801200

P	0.66874900	−1.16409700	−1.94182900
Ru	−0.29697200	−0.38643100	0.04198800
H	1.13240500	−0.67043300	0.79107000
H	−1.44002400	−1.40408400	−0.24469300
H	−0.08582400	−1.87255800	0.43747000
C	2.73127900	4.42969600	−0.07971300
C	3.51658300	3.16063200	0.44935300
C	3.40235900	5.14736500	−1.24277200
H	2.78601300	5.99621400	−1.55270700
H	4.38312400	5.53214900	−0.94481400
H	3.52904100	4.49048900	−2.10575300
C	4.43829700	2.53753700	−0.59733200
H	5.29004200	3.18798700	−0.81697900
H	4.81993800	1.58832500	−0.21232400
H	3.90552500	2.33087700	−1.52979700
C	2.37307500	5.43728600	1.01164100
H	3.26452300	5.93731200	1.40188400
H	1.71143400	6.19780800	0.58695900
H	1.84579300	4.96493200	1.84425000
C	4.27761700	3.38283400	1.74803200
H	4.75147400	2.44661300	2.05700300
H	5.06293800	4.13373100	1.61201700
H	3.61820500	3.71020400	2.55422700
O	1.48956200	3.86161300	−0.55382200
O	2.46071300	2.20360600	0.70111600
B	1.36529900	2.61797800	0.00564600
O	0.23097500	1.87028100	−0.12297500
C	−2.50510000	3.31988300	−1.97895900
C	−2.77049000	3.75877700	−0.48996400
H	−1.60350500	0.30730500	−0.75629700
C	−2.48742900	4.47065400	−2.97467000
H	−2.32843800	4.08627900	−3.98623100
H	−3.44588900	5.00072700	−2.96474500
H	−1.68887500	5.18182400	−2.75349100
C	−2.25070400	5.16199300	−0.17346600
H	−2.85200000	5.93658600	−0.65894100
H	−2.29689300	5.31892200	0.90843300
H	−1.20807200	5.27634700	−0.48569600
C	−3.44886600	2.22008500	−2.46390900
H	−4.47272800	2.59244700	−2.56621800
H	−3.11425700	1.87178900	−3.44521000
H	−3.44627800	1.36257500	−1.78567500
C	−4.21216400	3.60933400	−0.02930200
H	−4.29736900	3.91580200	1.01772700
H	−4.87640200	4.24618400	−0.62335600
H	−4.55308500	2.57541400	−0.11042800
O	−1.17822400	2.75443400	−1.90026100
O	−1.94817300	2.84106400	0.25775000
B	−0.98665800	2.36468000	−0.60121500
16Ru			
$G_{\text{solv}} = -2852.088112$; $E_{\text{solv}} = -2853.20856201$			
C	−1.25446900	−2.38817400	3.06734600
H	−1.63083700	−2.19674800	4.07901200
C	0.12203300	−3.11407200	3.19324200
H	0.91726700	−2.59501100	2.65290800
H	0.41678300	−3.16210100	4.24795100
C	−0.09567500	−4.53001700	2.62844200
H	0.16835500	−4.54514300	1.56325100

H	0.51885900	−5.28382700	3.13179200
C	−1.59910000	−4.77439100	2.77500400
H	−1.84441100	−5.02107200	3.81710200
H	−1.96739600	−5.58943900	2.14254300
C	−2.19522400	−3.41490700	2.39787900
H	−3.23422000	−3.29425000	2.72178600
H	−2.16863300	−3.30455200	1.30787300
C	−0.32727100	0.27065500	3.55134600
H	−0.81790400	−0.01591000	4.49234500
C	1.18536800	0.04338400	3.72216900
H	1.41636700	−0.89495500	4.23477800
H	1.67427600	0.02366600	2.74081100
C	1.63851800	1.27651700	4.50745700
H	1.33549000	1.18586500	5.55942200
H	2.72509200	1.41862000	4.48572900
C	0.87644600	2.41829100	3.82569300
H	1.44040600	2.72969500	2.94141800
H	0.75353000	3.29800900	4.46690600
C	−0.47396100	1.80858000	3.37900400
H	−0.69820700	2.08566600	2.34636300
H	−1.30677500	2.17909400	3.98708200
C	−2.87846400	−0.04301800	2.33550400
H	−2.72714700	1.01443600	2.09326100
C	−3.61684300	−0.13701300	3.70355400
H	−3.12359000	−0.80198200	4.41899800
H	−3.65120000	0.85229000	4.17383700
C	−5.04094300	−0.63608100	3.37913200
H	−5.09112200	−1.72582700	3.49930000
H	−5.80121100	−0.20193200	4.03675000
C	−5.24196400	−0.28319700	1.90179900
H	−5.47149400	0.78721900	1.80201500
H	−6.05809200	−0.84377000	1.43263700
C	−3.87283300	−0.58317800	1.28564600
H	−3.71246600	−0.11333300	0.31267400
H	−3.76256400	−1.66245800	1.13738300
C	0.94077700	−0.59599500	−3.42381100
H	1.47981300	−1.19709400	−4.17065600
C	1.70299100	0.72377300	−3.23945800
H	2.78051200	0.57999600	−3.11342800
H	1.32250200	1.24894700	−2.35976000
C	1.35449400	1.51853200	−4.50330500
H	1.49881300	2.59581900	−4.36865500
H	2.00616400	1.20022700	−5.32698000
C	−0.11412800	1.15164800	−4.81039500
H	−0.78231800	1.95063300	−4.47753100
H	−0.27404200	1.01782900	−5.88562600
C	−0.40880400	−0.14665100	−4.01861800
H	−0.85430200	−0.92473500	−4.64773800
H	−1.10864000	0.06081300	−3.20264900
C	−0.21288500	−3.06028700	−2.64670700
H	−1.15400700	−2.57431200	−2.93266800
C	−0.57346500	−4.23415500	−1.68583700
H	0.02822000	−4.23538900	−0.77560400
H	−1.61433900	−4.13455300	−1.36177300
C	−0.36082600	−5.52926500	−2.49828000
H	0.61670000	−5.96657700	−2.25706100
H	−1.11700100	−6.29069400	−2.28179100
C	−0.36314200	−5.07942000	−3.96290000

H	-1.39388500	-4.92632900	-4.30971300
H	0.11143700	-5.80024600	-4.63720700
C	0.36841500	-3.73547500	-3.90606500
H	0.22710100	-3.13191200	-4.80868700
H	1.44548000	-3.91723300	-3.79567800
C	2.48996300	-2.31014100	-1.73767900
H	2.83400700	-2.58810000	-2.74170000
C	3.46516100	-1.24651900	-1.15200600
H	4.15915100	-0.90325100	-1.92803300
H	2.93214200	-0.37028700	-0.77390500
C	4.22007700	-1.94527300	-0.00345600
H	5.26355700	-1.61981700	0.07633700
H	3.72267900	-1.71431900	0.94659100
C	4.07778600	-3.44113600	-0.30038200
H	4.25734500	-4.07279100	0.57639300
H	4.78599500	-3.74458100	-1.08362300
C	2.64010400	-3.53953300	-0.81837200
H	1.95598100	-3.45866200	0.03362000
H	2.42692400	-4.47886700	-1.34023000
P	-1.15552900	-0.73228400	2.21639200
P	0.75693600	-1.65313500	-1.90347400
Ru	-0.20764500	-0.88794400	0.08205300
H	1.23684000	-1.12348500	0.83022800
H	-1.34225300	-1.91431900	-0.20132300
H	0.02841300	-2.36872400	0.47978100
C	2.81586700	3.93881900	-0.01495400
C	3.59327700	2.66278000	0.50883300
C	3.49463600	4.66148000	-1.17034100
H	2.88300800	5.51489500	-1.47708200
H	4.47569600	5.04023800	-0.86578200
H	3.62218100	4.00988300	-2.03718200
C	4.51698800	2.04315600	-0.53797300
H	5.37146200	2.69249100	-0.75012100
H	4.89432700	1.09056800	-0.15728300
H	3.98734600	1.84391200	-1.47382000
C	2.45659000	4.94048100	1.08142800
H	3.34815200	5.43536500	1.47787900
H	1.79869400	5.70555600	0.65904200
H	1.92500700	4.46461100	1.90929200
C	4.34937800	2.87260300	1.81237600
H	4.81729200	1.93203300	2.11705000
H	5.13874500	3.62073500	1.68486300
H	3.68799600	3.19764300	2.61783100
O	1.57396100	3.37855000	-0.49818500
O	2.53202200	1.70808200	0.74977700
B	1.44182900	2.13211700	0.05377500
O	0.29718700	1.39872000	-0.08540400
C	-2.44136500	2.85255200	-1.93269200
C	-2.70909100	3.29433100	-0.44422500
H	-1.53777800	-0.26286000	-0.71796600
C	-2.44194000	3.99834100	-2.93389200
H	-2.27523600	3.61111800	-3.94306700
H	-3.40927000	4.51194300	-2.92755500
H	-1.65613700	4.72451800	-2.71596200
C	-2.21870600	4.70977100	-0.13648400
H	-2.83798400	5.46797000	-0.62503900
H	-2.26607200	4.87204500	0.94447900
H	-1.17957000	4.84622900	-0.45174500

C	-3.36802900	1.73566200	-2.41006400
H	-4.39890600	2.08967200	-2.50629500
H	-3.03351700	1.39151500	-3.39278900
H	-3.34534500	0.87941900	-1.73053500
C	-4.14414400	3.11420300	0.02532600
H	-4.22987200	3.42236300	1.07172600
H	-4.82550300	3.73414800	-0.56705700
H	-4.46255300	2.07279300	-0.05031000
O	-1.10518000	2.30435800	-1.85573600
O	-1.86196600	2.39815700	0.30510400
B	-0.89839600	1.94127000	-0.55532600
1Ru-HBpin			
$G_{\text{solv}} = -2366.374469$; $E_{\text{solv}} = -2367.32746861$			
C	16.10271100	3.76966500	6.99581900
H	17.02262600	4.17613900	7.43392200
C	16.48912700	2.97599300	5.70922100
H	15.92171000	3.29591400	4.83226000
H	17.54835300	3.13628300	5.48261400
C	16.22231500	1.49224600	6.03257200
H	15.21989800	1.20816300	5.68361100
H	16.93788100	0.82082200	5.54718500
C	16.25775500	1.41863600	7.56119100
H	17.29601300	1.43338800	7.91829500
H	15.77873500	0.51934600	7.96238600
C	15.54222200	2.70880900	7.96929800
H	15.69742500	2.98310600	9.01757900
H	14.46328400	2.57840600	7.82097600
C	16.13668000	6.47876000	5.99150400
H	16.95486500	6.59207700	6.71299700
C	16.73783200	6.09497100	4.61700800
H	17.70187400	5.58573900	4.71640900
H	16.06005500	5.42408200	4.07885400
C	16.82854100	7.41892200	3.84875000
H	17.70445300	7.99493000	4.17684500
H	16.91109800	7.27233500	2.76643200
C	15.54298500	8.13509000	4.26731200
H	14.68859100	7.67429000	3.75539200
H	15.54036000	9.20508800	4.03249800
C	15.44355300	7.85701300	5.77470500
H	14.40713900	7.86430600	6.11889600
H	15.97786100	8.62986800	6.34120300
C	14.75352800	5.93253600	8.42869500
H	14.37975600	6.94037100	8.22310500
C	15.98899800	6.06628500	9.34145900
H	16.61394000	5.16475300	9.31607000
H	16.62276200	6.91583300	9.06567500
C	15.37239400	6.20823300	10.73724000
H	16.09555600	6.05283600	11.54494900
H	14.95221400	7.21608400	10.85416000
C	14.24692000	5.16672200	10.72443200
H	13.48780000	5.34974900	11.49186800
H	14.67153900	4.17380500	10.92140000
C	13.67001600	5.22426100	9.29323600
H	12.74872800	5.81206500	9.25120200
H	13.41468000	4.22756700	8.92388000
C	9.88346900	3.36086400	4.17886900
H	9.51374300	2.83007000	3.29351900
C	8.86801600	4.47108100	4.51954500

H	8.41354400	4.90086700	3.62036200
H	9.35292300	5.28138500	5.06975800
C	7.85853000	3.77169100	5.43468400
H	7.22863700	4.47583500	5.99032300
H	7.19475900	3.11978600	4.85024400
C	8.76166100	2.93124400	6.34105400
H	9.22142300	3.58313700	7.09469600
H	8.22827200	2.13517700	6.87104300
C	9.85300400	2.38839100	5.39666300
H	9.61240300	1.37345300	5.06010700
H	10.81840300	2.33810800	5.91233300
C	12.26503600	2.27274700	3.13615500
H	12.15888200	1.61795100	4.01159200
C	13.76304600	2.22994100	2.70103800
H	14.18711200	3.22292700	2.55048300
H	14.36314600	1.76335800	3.48949400
C	13.80795500	1.39331400	1.40523800
H	13.83055600	2.05764600	0.53188600
H	14.69549300	0.75523400	1.34788300
C	12.49705900	0.60201900	1.40383000
H	12.57790500	−0.26560100	2.07216200
H	12.21508700	0.23301500	0.41220800
C	11.49252200	1.60506900	1.97727300
H	10.56384900	1.13088100	2.30925900
H	11.23191500	2.33696300	1.20210300
C	11.38270200	4.94364900	2.25221300
H	10.69579400	4.39009200	1.60091300
C	10.77369100	6.35297000	2.53253700
H	9.79755400	6.42899400	2.03942300
H	10.61738200	6.54983600	3.59364300
C	11.76011800	7.36383400	1.92166600
H	11.26328100	8.27117100	1.56156000
H	12.49396100	7.66592900	2.68042600
C	12.46855300	6.57923400	0.81575700
H	13.40240300	7.04449500	0.48230200
H	11.81136500	6.47988400	−0.05874200
C	12.69166100	5.21459000	1.47378400
H	13.53340700	5.29671300	2.17078500
H	12.92193700	4.41690800	0.75934000
P	14.97662600	5.22650300	6.72591000
P	11.61539100	3.90811500	3.77535600
Ru	13.06359600	4.71784400	5.45718100
H	14.12082200	4.63946500	4.24930800
H	12.78370500	6.34183100	5.07840400
H	13.06101200	3.15810800	6.09916300
H	13.67827100	3.15143200	5.43377400
C	10.14883100	7.88872600	6.59893800
C	11.48256100	8.49528800	7.14426100
H	11.88009000	5.12983800	6.69566400
C	9.29337300	8.84361400	5.77705100
H	8.38740500	8.32963700	5.44021400
H	8.98922000	9.71017300	6.37451100
H	9.82765200	9.19654500	4.89208100
C	12.10090600	9.51533300	6.18268600
H	11.51310100	10.43798200	6.13949100
H	13.10667200	9.77125700	6.52877700
H	12.18389400	9.10706300	5.17030300
C	9.29876700	7.23354200	7.69241200

H	8.84080300	7.97553300	8.35470500
H	8.49764200	6.65878800	7.21753400
H	9.89516900	6.54387800	8.29789800
C	11.39369200	9.08895200	8.54368400
H	12.37157700	9.48077200	8.84175400
H	10.67432000	9.91492200	8.57302600
H	11.09474500	8.33811700	9.27868100
O	10.63085700	6.85250800	5.74356400
O	12.33274200	7.34581600	7.18647700
B	11.89096400	6.41281600	6.21593000
CO₂			
$G_{\text{solv}} = -188.533929; E_{\text{solv}} = -188.52494603$			
C	-0.09485100	0.31165300	0.00000000
O	1.07004300	0.31165300	0.00000000
O	-1.25974500	0.31165300	0.00000000
HBpin			
$G_{\text{solv}} = -411.620745; E_{\text{solv}} = -411.78003159$			
C	-0.54961800	0.72578900	-0.07263700
C	-1.03444400	2.22004500	-0.09845400
H	2.36067000	2.49325800	-0.23609000
C	-1.25527200	-0.19040300	-1.06042900
H	-0.84995300	-1.20298900	-0.97761300
H	-2.32744400	-0.23555800	-0.84225300
H	-1.12240300	0.14399000	-2.09125800
C	-1.53316200	2.67101100	-1.47137300
H	-2.49285700	2.20783100	-1.71917100
H	-1.66915300	3.75610100	-1.46067700
H	-0.81545800	2.42859300	-2.26098800
C	-0.56795400	0.10659700	1.32494800
H	-1.59084500	-0.07308600	1.66884900
H	-0.04288100	-0.85226800	1.29466600
H	-0.06195800	0.74530200	2.05536200
C	-2.05362700	2.57905700	0.97204800
H	-2.32530900	3.63493100	0.88241500
H	-2.96429800	1.98351700	0.84919800
H	-1.66147800	2.41590100	1.97792500
O	0.84550500	0.84580600	-0.45694600
O	0.19440600	2.94906100	0.15931400
B	1.23026300	2.12729800	-0.18260600
pinBOCHO			
$G_{\text{solv}} = -600.170716; E_{\text{solv}} = -600.34076123$			
C	-0.53975000	0.61542900	-0.13281500
C	-0.83273800	2.16185400	-0.11463400
C	-1.43792400	-0.18712100	-1.05960600
H	-1.16695800	-1.24549100	-1.01078400
H	-2.48452500	-0.09097100	-0.75278100
H	-1.34548000	0.13858200	-2.09749600
C	-1.35171800	2.69483400	-1.44833800
H	-2.37674100	2.36306600	-1.63590000
H	-1.34588800	3.78812500	-1.42104700
H	-0.72448400	2.37258400	-2.28529400
C	-0.51739800	-0.01095200	1.26012600
H	-1.52329800	-0.06695800	1.68588900
H	-0.11977200	-1.02678500	1.18615500
H	0.12060900	0.55240700	1.94807300
C	-1.72205100	2.62845800	1.02530200
H	-1.86429800	3.71115600	0.96374100
H	-2.70625800	2.15393000	0.95735400

H	−1.28848300	2.39754300	2.00022100
O	0.82214400	0.56250300	−0.64050400
O	0.49851300	2.72317300	0.07098800
B	1.37264100	1.77543900	−0.37648400
O	2.72815000	1.99739200	−0.55937600
C	3.25720900	3.23254200	−0.44791500
H	2.52133700	4.02556200	−0.24937200
O	4.43556000	3.42779700	−0.56358700
(pinBO) ₂ CH ₂			
G _{solv} = −1011.826229; E _{solv} = −1012.18183779			
H	−3.90642900	1.79489600	0.41510900
C	−0.53443200	3.66308200	−2.00491900
C	−0.81617300	3.81626500	−0.46572100
C	0.92265500	3.41388000	−2.36180700
H	1.02546400	3.32269800	−3.44707600
H	1.54855400	4.24925400	−2.03057100
H	1.29656900	2.49338100	−1.90866800
C	0.11127600	2.96196200	0.39720800
H	1.13043200	3.36039300	0.40880700
H	−0.26882800	2.95271900	1.42273500
H	0.13805700	1.92962500	0.03987800
C	−1.09088500	4.82123000	−2.83328000
H	−0.51477500	5.73835900	−2.67768200
H	−1.03667400	4.55751800	−3.89326200
H	−2.13854400	5.02358300	−2.58932500
C	−0.84243100	5.24968600	0.03930700
H	−1.04423600	5.25819100	1.11458900
H	0.12566700	5.73366800	−0.12735200
H	−1.61776400	5.83838800	−0.45522100
O	−1.30502600	2.48665400	−2.34274100
O	−2.14327600	3.25189400	−0.34393400
B	−2.29023500	2.37931100	−1.39548300
O	−3.32645900	1.50945000	−1.54498600
C	−4.18829100	1.22139800	−0.47502200
H	−5.20838300	1.46590700	−0.77841200
O	−4.17495400	−0.15417600	−0.20547700
C	−1.66834300	−2.38482600	0.97506800
C	−1.11151200	−0.99094500	1.44008500
C	−1.66091300	−3.46005100	2.05013400
H	−2.05539900	−4.39424600	1.63985600
H	−0.63979200	−3.64729200	2.39891800
H	−2.27830000	−3.18032500	2.90630500
C	−1.39957900	−0.68571200	2.90987300
H	−0.78083600	−1.29715100	3.57339700
H	−1.17340600	0.36688300	3.10328300
H	−2.45119200	−0.85791000	3.15932200
C	−0.99538300	−2.90146900	−0.29728000
H	0.03300400	−3.22147600	−0.10497400
H	−1.55840000	−3.76143300	−0.67060600
H	−0.98184900	−2.13956600	−1.08290600
C	0.36261500	−0.77187900	1.13819600
H	0.68873100	0.19161500	1.53972700
H	0.96610300	−1.55340300	1.61219700
H	0.56070100	−0.78202600	0.06432500
O	−3.03819000	−2.07061100	0.63412500
O	−1.90644300	−0.06886700	0.65332200
B	−3.06731700	−0.73366900	0.33561500
HCHO			

$G_{\text{solv}} = -114.465363; E_{\text{solv}} = -114.47076963$			
C	-0.28089900	0.90851400	0.00000000
H	0.24416300	-0.06478600	0.00000000
H	-1.38647400	0.87640700	0.00000000
O	0.32293800	1.95511600	0.00000000
pinBOBpin			
$G_{\text{solv}} = -897.360742; E_{\text{solv}} = -897.68427029$			
C	-0.95732600	1.21594800	0.16352800
C	-2.21104900	0.36017500	-0.24930500
C	3.63870400	-3.32754000	0.54295800
C	3.87897200	-1.84715600	0.06823400
C	-1.21000500	2.21278800	1.28376200
H	-0.29023200	2.76251300	1.50429600
H	-1.97455500	2.93808800	0.98606000
H	-1.53586600	1.71694100	2.20035100
C	-3.16063200	0.08334700	0.91683400
H	-3.70262600	0.98578700	1.21478300
H	-3.89113800	-0.66937400	0.60737400
H	-2.62605000	-0.30444400	1.78967800
C	-0.28594700	1.90979400	-1.02180100
H	-0.89608800	2.73511200	-1.40081100
H	0.67687300	2.31365500	-0.69649100
H	-0.09629900	1.21072700	-1.84215000
C	-2.98516300	0.90366100	-1.44008400
H	-3.83572200	0.25068700	-1.65678900
H	-3.37277200	1.90419300	-1.22126400
H	-2.36386000	0.95733200	-2.33644400
C	4.43509800	-3.73699100	1.77195500
H	4.20260200	-4.77352500	2.03296700
H	5.50986800	-3.67018700	1.57284400
H	4.19900900	-3.11004300	2.63411100
C	3.82553100	-4.35461900	-0.57389600
H	4.88006600	-4.46355600	-0.84441100
H	3.45818100	-5.32505100	-0.22819900
H	3.26233500	-4.08123100	-1.47165800
C	4.18876400	-0.88872600	1.21835100
H	5.18672100	-1.06635800	1.63013000
H	4.14792100	0.13802800	0.84390700
H	3.45617700	-0.97913600	2.02638900
C	4.91095400	-1.69393700	-1.03780500
H	5.01349300	-0.63778700	-1.30383600
H	5.88879100	-2.05560600	-0.70267800
H	4.62418800	-2.24310000	-1.93689000
O	-0.03789200	0.20203900	0.63389500
O	-1.61254000	-0.90495800	-0.61703900
O	2.57837600	-1.47818600	-0.44804100
O	2.23117100	-3.31817000	0.87941800
O	0.31517200	-2.12525900	0.09285600
B	-0.40649200	-0.97306500	0.02844100
B	1.66449700	-2.28580900	0.18029500
Fe-1cyp			
$G_{\text{solv}} = -3124.537937; E_{\text{solv}} = -3125.32568092$			
C	11.12639600	4.86396600	8.06568500
H	11.16434000	5.29703500	9.07285600
C	11.04227500	3.31124600	8.19838000
H	11.83533400	2.79604000	7.64941800
H	11.14882300	3.02478900	9.24985500
C	9.65078200	2.91317000	7.66840500

H	9.71897200	2.65256700	6.60399900
H	9.23268700	2.04791000	8.19284300
C	8.80945700	4.18272500	7.82016900
H	8.51421400	4.31967200	8.86895000
H	7.89768500	4.17273000	7.21403300
C	9.79379600	5.27751400	7.40195600
H	9.47826600	6.28623500	7.68898400
H	9.89539600	5.25853600	6.30868400
C	13.98109400	5.21767500	8.36859000
H	13.67319400	5.74401600	9.28115900
C	14.27461000	3.74874000	8.74113900
H	13.61338100	3.37802600	9.53066500
H	14.14974900	3.10536500	7.86191200
C	15.75188400	3.75965100	9.14462900
H	15.86794100	4.19925000	10.14447300
H	16.19484700	2.75815700	9.16651600
C	16.37738600	4.67199800	8.08642400
H	16.48885600	4.10912500	7.15140000
H	17.36597600	5.05012300	8.36684500
C	15.34383600	5.79758900	7.88223600
H	15.30586200	6.09887100	6.83103700
H	15.60525700	6.68305700	8.47275000
C	12.47652400	7.31012400	7.16339600
H	13.49529500	7.63246400	6.91236600
C	12.09369800	7.99229000	8.49058400
H	11.23353700	7.49604500	8.95813100
H	12.91287500	7.98988400	9.21708500
C	11.68431000	9.40079400	8.05048800
H	11.13696800	9.95222900	8.82216300
H	12.58010500	9.98273100	7.79713400
C	10.84844800	9.13937100	6.79118700
H	10.77904600	10.01443100	6.13754500
H	9.82492000	8.87553700	7.08582500
C	11.52474100	7.93230000	6.09949200
H	12.10313800	8.23991500	5.22230300
H	10.77578900	7.22235300	5.74085700
C	13.26205600	4.76768500	1.66236000
H	13.76215800	4.29408000	0.80804300
C	13.55133800	6.28455100	1.61199100
H	14.54640900	6.50454500	1.21406200
H	13.49471800	6.71859200	2.61829800
C	12.41795900	6.85041000	0.75149700
H	12.30902000	7.93577800	0.84844300
H	12.59999600	6.62569100	−0.30792200
C	11.19701200	6.07486600	1.25287900
H	10.86407700	6.50505100	2.20659400
H	10.34742000	6.10961600	0.56348000
C	11.71849900	4.64134700	1.48053300
H	11.49457300	4.00359900	0.61843200
H	11.23292200	4.18426400	2.35005000
C	13.47169300	2.15030900	2.77531500
H	12.39335900	2.18008600	2.57137400
C	13.69786900	1.12702500	3.93087600
H	14.33387500	1.52588300	4.72482100
H	12.73881200	0.88121400	4.39932200
C	14.32456300	−0.12153500	3.27267000
H	15.41294300	−0.11250100	3.41190700
H	13.95187100	−1.05588300	3.70415600

C	14.00518500	0.01841400	1.77980100
H	12.96989600	−0.29055600	1.58297400
H	14.65933500	−0.58425600	1.14097800
C	14.15134300	1.52420900	1.54018200
H	13.69996900	1.85784200	0.59995300
H	15.21799900	1.77765200	1.50265700
C	15.70814100	4.03001600	3.00987300
H	15.92646400	3.75185300	1.97127100
C	16.30877700	5.44510100	3.26865900
H	16.67800600	5.86536700	2.32660800
H	15.57053400	6.14158200	3.67252200
C	17.46810800	5.23769500	4.26296700
H	18.30110900	5.92619400	4.08666400
H	17.10816500	5.40697400	5.28468500
C	17.85560600	3.76536400	4.10363900
H	18.42729500	3.37588100	4.95280300
H	18.46305900	3.62630900	3.19903500
C	16.49604500	3.08129200	3.93898400
H	16.00572500	3.02585500	4.91779000
H	16.56381300	2.06462800	3.53702500
P	12.62037100	5.45515800	7.12764000
P	13.86276600	3.92046700	3.20499100
Fe	12.99618100	4.62321500	5.11156400
H	14.22034200	3.96929800	5.71988900
H	13.94266900	5.80504700	5.00713800
H	12.26130700	5.81722800	4.38163400
H	11.63694100	5.23102800	4.49813300
H	11.90815600	3.43518500	5.13269200
H	12.59702300	3.16692500	5.58310800
1_{Fe}			
$G_{\text{solv}} = -3123.343910$; $E_{\text{solv}} = -3124.11177177$			
C	11.23524400	4.79942500	8.11456000
H	11.20379200	5.26678100	9.10734900
C	11.25051200	3.24939100	8.29181000
H	12.04369200	2.77455500	7.70624000
H	11.43426900	2.99531200	9.34054600
C	9.85991100	2.75192400	7.83884200
H	9.91393900	2.38929400	6.80440800
H	9.48833900	1.92663400	8.45427400
C	8.96464500	3.99347600	7.88979300
H	8.65533300	4.19863600	8.92321700
H	8.05843200	3.89677400	7.28266300
C	9.90238900	5.09738500	7.39592000
H	9.53313300	6.10873300	7.59455000
H	10.02687000	4.99670200	6.30923400
C	14.04210500	5.37226400	8.51043600
H	13.63898100	5.90318200	9.38252400
C	14.42496400	3.93500600	8.93959800
H	13.79863800	3.56516500	9.75750600
H	14.31521200	3.24843700	8.09241000
C	15.90879100	4.03082500	9.30854600
H	16.02813100	4.49363700	10.29772000
H	16.40216800	3.05331800	9.33431200
C	16.45665700	4.95742500	8.22183000
H	16.53174300	4.40012600	7.27979000
H	17.44582600	5.36708300	8.45176200
C	15.38030600	6.04656400	8.08044200
H	15.34748300	6.43043200	7.05693500

H	15.59595700	6.89088100	8.74591100
C	12.44234400	7.28019400	7.08682900
H	13.45199300	7.67293800	6.91734600
C	11.84934000	8.03263000	8.29325800
H	11.02512900	7.47114100	8.74997200
H	12.59440600	8.21723600	9.07419600
C	11.29855500	9.31887400	7.66787200
H	10.60161200	9.85166700	8.32331800
H	12.12604700	10.00185200	7.43538500
C	10.64311100	8.82405200	6.37185100
H	10.50330500	9.62005100	5.63384900
H	9.65022100	8.41681500	6.60031300
C	11.57205800	7.69877100	5.86315200
H	12.22011600	8.05503100	5.05513700
H	10.99171200	6.86453200	5.45394500
C	13.32783300	4.92912400	1.80005800
H	13.79395600	4.53598900	0.88694800
C	13.64579800	6.43545000	1.89538400
H	14.66349600	6.67121200	1.57226400
H	13.54331800	6.78138000	2.93335600
C	12.57182300	7.08788700	1.02182600
H	12.48040000	8.16633700	1.18830600
H	12.81270000	6.93402400	−0.03839200
C	11.30324000	6.31397400	1.39592500
H	10.88200200	6.73320000	2.31797900
H	10.52449300	6.37277800	0.62906900
C	11.77810300	4.86334200	1.64834300
H	11.50553100	4.20115300	0.81990800
H	11.29914200	4.45733000	2.54758800
C	13.36912400	2.22513500	2.73001300
H	12.28919800	2.35368700	2.58226300
C	13.56123000	1.11751600	3.81051500
H	14.26959000	1.41021800	4.58838300
H	12.61020500	0.93035700	4.32062600
C	14.03931100	−0.13682200	3.04637300
H	15.12914800	−0.23310700	3.13124200
H	13.60250000	−1.06081400	3.43823400
C	13.67027600	0.12684400	1.58171400
H	12.60445800	−0.07937600	1.41599700
H	14.24114500	−0.48670900	0.87673800
C	13.93915700	1.62683600	1.42846700
H	13.48184800	2.06073700	0.53274700
H	15.02186800	1.78892700	1.35866500
C	15.76714700	3.89420900	2.99777400
H	15.94509700	3.58483300	1.96070800
C	16.47521700	5.26389100	3.22340600
H	16.83852400	5.65270700	2.26544400
H	15.80233600	6.01039300	3.65115700
C	17.64845200	4.98097900	4.18298100
H	18.52882000	5.59404600	3.96316200
H	17.33666800	5.20177500	5.21075000
C	17.90938100	3.47820400	4.04833300
H	18.46935600	3.06186300	4.89251700
H	18.47881600	3.26933900	3.13227400
C	16.49484200	2.90471100	3.93393800
H	16.02266000	2.91395100	4.92358100
H	16.47003100	1.87685700	3.55502500
P	12.72277400	5.44707300	7.20687100

P	13.92819900	3.92448000	3.24529600
Fe	13.17095800	4.60317600	5.21463100
H	13.97658300	3.50151100	5.84837200
H	14.38340800	5.56230700	5.26845900
H	11.77358100	3.79672500	5.00622100
H	12.30934600	3.30212800	5.46536900
2_{Fe}			
$G_{\text{solv}} = -3311.886840; E_{\text{solv}} = -3312.66848983$			
C	-2.02317600	-0.11436200	2.85332900
H	-1.92432300	0.14838700	3.91328400
C	-1.98393700	-1.67023000	2.72506600
H	-1.23421000	-2.01171900	2.00565300
H	-1.72300700	-2.11316900	3.69127100
C	-3.40424900	-2.09580400	2.29917000
H	-3.45223700	-2.20617900	1.20756500
H	-3.70248800	-3.05409700	2.73553500
C	-4.29963100	-0.92952800	2.72540100
H	-4.48779300	-0.96972800	3.80633500
H	-5.26904400	-0.92081800	2.21696800
C	-3.43834500	0.28957100	2.38688000
H	-3.78195200	1.21522900	2.85828000
H	-3.46008200	0.44809200	1.30040600
C	0.79262800	0.45848000	3.08188800
H	0.48219100	0.86634900	4.05191700
C	1.20142500	-1.01157900	3.31046800
H	0.58294300	-1.50162300	4.06881000
H	1.11140800	-1.58504000	2.38089900
C	2.67882800	-0.91638400	3.70207000
H	2.77428600	-0.55748700	4.73556800
H	3.19965000	-1.87722300	3.63243000
C	3.21324500	0.13031500	2.72186500
H	3.35375700	-0.34359400	1.74333200
H	4.17480300	0.55906000	3.02096300
C	2.09374700	1.18710000	2.62846700
H	2.01821800	1.59597200	1.61574200
H	2.29683200	2.03075400	3.29732200
C	-0.92444500	2.56139900	2.24769200
H	0.02376400	3.00486100	1.92007500
C	-1.16818300	3.00404800	3.70792000
H	-1.83075600	2.30330600	4.23236100
H	-0.23915200	3.07345800	4.28263700
C	-1.88168700	4.35140700	3.56010200
H	-2.37420700	4.67692800	4.48237700
H	-1.15748000	5.12577800	3.27578300
C	-2.85807000	4.09661300	2.40834000
H	-3.23091000	5.01745600	1.94915600
H	-3.72974100	3.54750200	2.78764000
C	-2.06611900	3.22354700	1.41469400
H	-1.62475800	3.83693100	0.62446200
H	-2.70639100	2.49796300	0.90978900
C	0.02308500	-0.32835400	-3.67545400
H	0.41127600	-1.05325100	-4.40255800
C	0.56231900	1.05968800	-4.07946400
H	1.59014200	1.01058400	-4.45042800
H	0.54575300	1.75677900	-3.23663100
C	-0.43815200	1.52501500	-5.14138400
H	-0.36836400	2.59767300	-5.34794100
H	-0.25865600	0.98986600	-6.08387000

C	-1.78944900	1.11717300	-4.54532200
H	-2.09370500	1.86036700	-3.80086000
H	-2.58459300	1.04892800	-5.29469600
C	-1.52243500	-0.23250200	-3.84197100
H	-1.89031000	-1.07542400	-4.43745500
H	-2.03949900	-0.26639400	-2.87696700
C	-0.10144700	-2.71317200	-2.13803600
H	-1.16392800	-2.58538400	-2.38948200
C	-0.02674400	-3.56386400	-0.83541200
H	0.71396700	-3.17900100	-0.13175100
H	-0.98793700	-3.53302900	-0.31238300
C	0.33024000	-4.99956600	-1.28748400
H	1.38921800	-5.20063600	-1.08317200
H	-0.24961600	-5.76256400	-0.75915200
C	0.09513000	-5.01587300	-2.80290900
H	-0.97014400	-5.16670300	-3.02183500
H	0.65430800	-5.80519000	-3.31560700
C	0.51502800	-3.60745500	-3.23171100
H	0.17301200	-3.34383000	-4.23753500
H	1.61035100	-3.54056000	-3.22382800
C	2.35193200	-1.08733200	-2.10735000
H	2.57445900	-1.59573600	-3.05364400
C	3.08592300	0.28796800	-2.10293400
H	3.47825900	0.49942200	-3.10264500
H	2.42831500	1.11689200	-1.83333800
C	4.23088600	0.15595100	-1.07762500
H	5.14209200	0.66831700	-1.40166600
H	3.92336600	0.60941800	-0.12845900
C	4.42634400	-1.35156900	-0.88971900
H	4.92955800	-1.60511900	0.04952600
H	5.02709800	-1.76356600	-1.71147900
C	2.99648900	-1.89447100	-0.96025800
H	2.48364400	-1.68061100	-0.01504000
H	2.94820500	-2.97549100	-1.13217500
P	-0.64755600	0.74778900	1.95048400
P	0.50865300	-0.95843600	-2.00186100
Fe	-0.30562000	0.08398600	-0.17650400
H	0.32660800	-1.07153100	0.52139700
H	1.10636400	0.33987100	0.10151900
H	-1.55653300	-0.92115700	-0.59662300
H	-1.78337300	-0.61146600	0.12604200
C	0.09169600	1.86653400	-0.70700800
O	-1.06901500	1.69649600	-1.14547700
O	0.91422400	2.75907400	-0.67488600
TS _{2,3-Fe}			
G _{solv} = -3311.886091; E _{solv} = -3312.66749341			
C	10.95755800	5.09970200	7.67913000
H	11.06241400	5.30567500	8.75110200
C	11.02033300	3.55401000	7.46454200
H	11.78547000	3.26422700	6.73972900
H	11.27168500	3.06182700	8.40927000
C	9.61293500	3.13442000	6.99591200
H	9.57564500	3.10423300	5.89859300
H	9.32918700	2.14147700	7.35849900
C	8.69397600	4.25060800	7.49940500
H	8.50561100	4.13100900	8.57435800
H	7.72498400	4.27611800	6.99057100
C	9.53115400	5.50739100	7.24810500

H	9.17135500	6.39022100	7.78510500
H	9.49874800	5.74362200	6.17635300
C	13.75679300	5.73774700	7.94537100
H	13.44374400	6.12448300	8.92344100
C	14.17577000	4.26740800	8.14591500
H	13.55085200	3.75283800	8.88264700
H	14.10568100	3.71721600	7.20047800
C	15.64527900	4.36925100	8.56422300
H	15.71893400	4.70669500	9.60676200
H	16.17728200	3.41534800	8.48361900
C	16.18721100	5.44186400	7.61599300
H	16.36487300	4.98732800	6.63470000
H	17.13246500	5.88103500	7.94989600
C	15.05308800	6.48291000	7.50797300
H	14.98290600	6.89020300	6.49469500
H	15.23596100	7.33137200	8.17643500
C	11.98043800	7.82744200	7.20145300
H	12.93345600	8.30841200	6.94882400
C	11.64407000	8.19608900	8.66346000
H	10.96907600	7.45915200	9.11685300
H	12.53650900	8.25759900	9.29444800
C	10.90951500	9.53436900	8.53478800
H	10.35630600	9.80611400	9.43997500
H	11.63136600	10.33534000	8.32981500
C	10.00712700	9.31553300	7.31664000
H	9.64605000	10.25050300	6.87695900
H	9.12447900	8.73722700	7.61861000
C	10.87057800	8.49836000	6.33448500
H	11.33755400	9.14945400	5.59041800
H	10.27339900	7.77764600	5.77132300
C	12.92941600	4.92223300	1.19590900
H	13.30004000	4.17044300	0.48696500
C	13.48226900	6.29008900	0.74584900
H	14.51200200	6.22237100	0.38323900
H	13.45867500	7.01342600	1.56643100
C	12.49056500	6.72434000	−0.33711800
H	12.57255700	7.78720600	−0.58572900
H	12.66701200	6.15044900	−1.25716300
C	11.13285500	6.35543100	0.27044800
H	10.82960800	7.13686700	0.97514300
H	10.34134200	6.25803600	−0.47942700
C	11.38473800	5.03796400	1.03915400
H	10.99366800	4.17214800	0.49349400
H	10.87926100	5.06271200	2.01085800
C	12.76531600	2.59740300	2.81649700
H	11.70702500	2.73962600	2.55373000
C	12.81113800	1.79277800	4.14621100
H	13.61063800	2.13827300	4.80476200
H	11.87849800	1.92929600	4.70257500
C	13.03064400	0.31435300	3.73889400
H	14.05287400	0.00723000	3.99000200
H	12.35407500	−0.36844400	4.26186000
C	12.84539200	0.27617000	2.21507000
H	11.78090300	0.18483300	1.96241300
H	13.37081200	−0.55895600	1.74067500
C	13.36267900	1.64486800	1.76438700
H	13.06837200	1.90001700	0.74136500
H	14.45941400	1.65049000	1.80837200

C	15.25561000	4.17109800	2.76919600
H	15.45742200	3.61058000	1.84843300
C	16.01269900	5.53350300	2.69224400
H	16.46470800	5.64438900	1.70115700
H	15.36070700	6.39682200	2.84234500
C	17.09789400	5.47642700	3.78292300
H	18.01036300	6.00664800	3.49302800
H	16.72011900	5.94966700	4.69698800
C	17.31804600	3.98233300	4.03136000
H	17.80710900	3.77164200	4.98848500
H	17.94166300	3.55234500	3.23618900
C	15.89730900	3.41646000	3.95534500
H	15.36666000	3.65865000	4.88361500
H	15.86669100	2.32947400	3.82293800
P	12.31323400	6.03850000	6.82107600
P	13.41582400	4.34051900	2.88776300
Fe	12.64709700	5.46480900	4.67533700
H	13.27405300	4.30355100	5.38326700
H	14.05362600	5.92922800	4.75482700
H	11.36020900	4.51668500	4.26614300
H	11.13212900	4.87212100	4.96963700
C	13.16425000	7.29123400	4.25739300
O	12.07173400	7.14862500	3.67122600
O	13.96521900	8.18162800	4.45325400
3_{Fe}			
$G_{\text{solv}} = -3311.893623; E_{\text{solv}} = -3312.67854045$			
C	-1.56458100	-0.48461900	3.01505200
H	-1.84435700	0.00619000	3.95458200
C	-0.79202800	-1.79690800	3.36307500
H	0.20243000	-1.84256800	2.91098600
H	-0.64676700	-1.85912700	4.44675600
C	-1.68448000	-2.95242900	2.87219700
H	-1.40237700	-3.23382500	1.84920400
H	-1.59232900	-3.84718000	3.49572400
C	-3.09580800	-2.36031800	2.85886100
H	-3.49502400	-2.30978900	3.88049500
H	-3.80029500	-2.93884600	2.25240600
C	-2.85796000	-0.95094900	2.30966900
H	-3.69327200	-0.26502400	2.48448400
H	-2.69909900	-1.01373700	1.22718400
C	0.61125200	1.36469900	3.36970500
H	0.01860600	1.52013300	4.28080600
C	1.75767200	0.38800600	3.70634000
H	1.44884000	-0.40215200	4.39707100
H	2.12779900	-0.09507200	2.79098500
C	2.84849200	1.29485600	4.28216400
H	2.58292100	1.58859300	5.30648500
H	3.82959400	0.81021200	4.31888700
C	2.81284200	2.51016000	3.35106900
H	3.37261400	2.28904700	2.43519900
H	3.25766000	3.40500200	3.79700600
C	1.32012100	2.70500500	3.00550400
H	1.20801300	2.97491900	1.95196900
H	0.87751400	3.52373400	3.58266000
C	-1.65827300	2.22060300	1.83216700
H	-0.96035200	3.00241400	1.51190700
C	-2.40657800	2.74694100	3.07161400
H	-2.88524900	1.92900400	3.62600200

H	-1.74648600	3.27750700	3.76581700
C	-3.48903000	3.64176800	2.46067000
H	-4.28278600	3.90149900	3.16879100
H	-3.03707500	4.57771500	2.10763900
C	-3.99089900	2.81360700	1.27068500
H	-4.49306300	3.42192700	0.51217500
H	-4.72088100	2.07543100	1.62707300
C	-2.73817900	2.09380200	0.71902800
H	-2.36819200	2.56117300	-0.19784300
H	-2.96000800	1.05594600	0.46407800
C	0.20587500	0.24858700	-3.42111800
H	0.12127800	-0.38929900	-4.31028600
C	1.30818900	1.28734500	-3.71306100
H	2.14272100	0.85661000	-4.27531100
H	1.70987400	1.71775300	-2.79210300
C	0.55722200	2.37546100	-4.48659300
H	1.11763600	3.31381100	-4.54680200
H	0.35861900	2.03661700	-5.51268300
C	-0.75466200	2.51012600	-3.70527400
H	-0.58178800	3.12631000	-2.81686700
H	-1.55314700	2.97916000	-4.28938800
C	-1.10819700	1.07073900	-3.26838400
H	-1.89397900	0.64194200	-3.90056500
H	-1.47373100	1.05736600	-2.23682000
C	-0.84842700	-2.14983600	-2.32764000
H	-1.75060700	-1.52573400	-2.37037000
C	-1.08262100	-3.21870400	-1.21985700
H	-0.20276500	-3.37223300	-0.59022500
H	-1.88833300	-2.88980200	-0.55619800
C	-1.45027700	-4.52588100	-1.96153300
H	-0.59114000	-5.20802000	-1.96462600
H	-2.28057600	-5.05743500	-1.48652400
C	-1.76297100	-4.09739800	-3.40068800
H	-2.79209100	-3.72183100	-3.47072300
H	-1.65746200	-4.91298000	-4.12334400
C	-0.77927200	-2.94917400	-3.64325300
H	-1.03591700	-2.34499100	-4.51907200
H	0.22536200	-3.36035200	-3.80513300
C	2.06662100	-1.76436100	-2.43779900
H	1.99990600	-2.05190300	-3.49410800
C	3.34186100	-0.88720800	-2.23901200
H	3.79552300	-0.67272000	-3.21182900
H	3.13289900	0.07915300	-1.77393900
C	4.29937800	-1.72332200	-1.36690300
H	5.35024200	-1.55139200	-1.61847700
H	4.16870900	-1.45820900	-0.30956800
C	3.84900100	-3.16954000	-1.58580100
H	4.20968200	-3.85797300	-0.81461700
H	4.20575900	-3.53627700	-2.55736100
C	2.32413500	-3.03835800	-1.60119900
H	1.97689400	-2.89643300	-0.56902700
H	1.80888900	-3.91616300	-2.00507300
P	-0.55856500	0.74978200	2.06273900
P	0.48673500	-0.89825300	-1.99610500
Fe	0.26272700	-0.00190000	0.08991400
H	0.74161900	-1.37591100	0.72496000
H	1.87257800	0.61018200	0.32051300
H	-1.18619900	-0.28205400	-0.18575900

H	−0.10394600	−1.44338000	0.57920200
C	1.68841500	1.66635900	−0.20890000
O	0.49540700	1.89981100	−0.54713200
O	2.71931900	2.31606000	−0.30356900
TS_{3,4}-Fe			
$G_{\text{solv}} = -3311.893108; E_{\text{solv}} = -3312.67441254$			
C	−1.52010200	−0.48769700	3.06967900
H	−1.76699700	0.01067400	4.01451100
C	−0.78014800	−1.82189500	3.40366900
H	0.18620200	−1.91242300	2.89993500
H	−0.57898200	−1.87132700	4.47889800
C	−1.73643500	−2.95255500	2.97529700
H	−1.49458200	−3.27813800	1.95481700
H	−1.66471700	−3.83071100	3.62436900
C	−3.12253900	−2.30278700	2.97939500
H	−3.49572700	−2.21165300	4.00796700
H	−3.86382100	−2.86583300	2.40315100
C	−2.84046700	−0.91739700	2.39251700
H	−3.64592200	−0.19596000	2.56377900
H	−2.70177400	−1.01009800	1.30882100
C	0.76398500	1.24199200	3.34791700
H	0.23703800	1.32640600	4.30732600
C	1.92123600	0.23184900	3.51958000
H	1.66044100	−0.59975900	4.18048300
H	2.20046500	−0.19643500	2.54528000
C	3.07730300	1.08121300	4.05379600
H	2.91445500	1.30128000	5.11705200
H	4.04868800	0.58405500	3.96243300
C	2.97589600	2.36312100	3.22305900
H	3.44011000	2.20391700	2.24216800
H	3.48337400	3.21575500	3.68390000
C	1.46184800	2.60552900	3.04912300
H	1.25110600	2.99081100	2.04878500
H	1.09962400	3.36270500	3.75219900
C	−1.54844200	2.22647400	1.91228800
H	−0.83761700	2.98523000	1.56740400
C	−2.23139900	2.76844000	3.18174600
H	−2.71599700	1.96294100	3.74903300
H	−1.52775200	3.27159700	3.85333300
C	−3.30672300	3.70107300	2.61650200
H	−4.06408000	3.98224600	3.35565300
H	−2.83864200	4.62367300	2.25001600
C	−3.87988100	2.89542000	1.44312700
H	−4.39277600	3.52332400	0.70817300
H	−4.61712600	2.17715800	1.82460500
C	−2.67200200	2.14294600	0.83818200
H	−2.31928900	2.60865700	−0.08600200
H	−2.93479200	1.11509300	0.58050600
C	0.30118400	0.15666200	−3.44257700
H	0.25619800	−0.49732900	−4.32257800
C	1.39555600	1.20874900	−3.71678700
H	2.24912400	0.78515600	−4.25609800
H	1.76613300	1.65424600	−2.79088300
C	0.64980500	2.28491500	−4.51137600
H	1.20129500	3.22906900	−4.55914400
H	0.47601800	1.94229000	−5.54097500
C	−0.67709100	2.40484000	−3.75468700
H	−0.51955800	3.00522700	−2.85273200

H	-1.46701600	2.87943200	-4.34606300
C	-1.03134900	0.95857400	-3.34626600
H	-1.77739700	0.52397200	-4.02156100
H	-1.44850000	0.93211900	-2.33487100
C	-0.72185500	-2.26515600	-2.37536700
H	-1.63891100	-1.67057800	-2.48437100
C	-0.99181200	-3.32434100	-1.26878700
H	-0.12352300	-3.48384600	-0.62496300
H	-1.80545200	-2.98414300	-0.61986800
C	-1.35431300	-4.63382700	-2.01260300
H	-0.52442000	-5.34686300	-1.93889200
H	-2.23621400	-5.12428000	-1.58947800
C	-1.55102300	-4.22891700	-3.48004000
H	-2.57053500	-3.85425100	-3.63817300
H	-1.39108800	-5.05776400	-4.17701000
C	-0.55110100	-3.08465600	-3.66826300
H	-0.74160100	-2.49755700	-4.57205100
H	0.46446100	-3.49460100	-3.74381800
C	2.18967100	-1.76711800	-2.33357100
H	2.20917000	-2.05532100	-3.39152500
C	3.40153700	-0.82535100	-2.04455800
H	3.93107300	-0.60879600	-2.97750500
H	3.10472300	0.14140700	-1.62819800
C	4.31390400	-1.59595500	-1.07105900
H	5.37284800	-1.36265000	-1.21724500
H	4.06136900	-1.33642900	-0.03379200
C	3.97196700	-3.06663800	-1.32015800
H	4.30189200	-3.73169300	-0.51550600
H	4.43658600	-3.41137900	-2.25324200
C	2.44947400	-3.02556100	-1.47307600
H	2.00436400	-2.90669800	-0.47575700
H	2.02443800	-3.93169800	-1.91686900
P	-0.50158900	0.71296700	2.08829800
P	0.55254600	-0.96516600	-1.99248100
Fe	0.21918500	-0.08040200	0.08507500
H	0.53620800	-1.52448500	0.69439300
H	2.24204300	1.29833600	0.30503500
H	-1.22053700	-0.27859600	-0.24036600
H	-0.30618800	-1.48100900	0.55285200
C	1.68191200	2.08343900	-0.28491500
O	0.47183700	1.77917400	-0.55991100
O	2.29282300	3.10497300	-0.58764800
4_{Fe}			
$G_{\text{solv}} = -3311.898398; E_{\text{solv}} = -3312.68174625$			
C	-1.72151500	-0.40455900	3.07040700
H	-1.78171200	0.02388000	4.07944600
C	-1.25576900	-1.88455700	3.19949800
H	-0.54240000	-2.15636000	2.41580700
H	-0.74588500	-2.03961100	4.15493300
C	-2.53714100	-2.74817000	3.08717900
H	-2.56815100	-3.24216300	2.10828500
H	-2.57724100	-3.53582400	3.84564900
C	-3.70501200	-1.75979000	3.19606400
H	-3.92860800	-1.54668000	4.24936700
H	-4.62387400	-2.13011000	2.73033500
C	-3.15794700	-0.50021000	2.52140900
H	-3.74914200	0.39648300	2.73052200
H	-3.14769000	-0.64433900	1.43294200

C	0.82386100	0.94784800	3.27375600
H	0.36851200	1.27314700	4.21646800
C	1.67070000	−0.34206100	3.49839300
H	1.50951500	−0.76448000	4.49510000
H	1.40022000	−1.11094600	2.76923700
C	3.13489400	0.06637800	3.25933800
H	3.58847900	0.43886700	4.18686100
H	3.74551500	−0.77066700	2.90509900
C	3.02319300	1.20722300	2.24736700
H	2.77180300	0.80097500	1.25904700
H	3.93817100	1.80119500	2.15169900
C	1.84064300	2.01464000	2.78434700
H	1.43577900	2.71533200	2.05036800
H	2.16724400	2.61482600	3.64277000
C	−1.41034300	2.34343500	2.06101600
H	−0.61124700	3.02515900	1.75073400
C	−2.00381300	2.89046800	3.37330800
H	−2.54536800	2.11111500	3.92466000
H	−1.23546300	3.29509100	4.04045900
C	−2.99971300	3.94848300	2.88616700
H	−3.71115900	4.25640700	3.65959800
H	−2.45588700	4.84257400	2.55606400
C	−3.67148000	3.26855000	1.68658200
H	−4.15320600	3.98074300	1.00980100
H	−4.45154900	2.58568200	2.04731600
C	−2.54204700	2.47264800	0.99670600
H	−2.15157600	3.00134500	0.12338600
H	−2.90001300	1.50279600	0.63728500
C	0.23228300	0.10326400	−3.50746300
H	0.28726800	−0.56357900	−4.37588200
C	1.24717300	1.24927000	−3.72786800
H	2.11585500	0.91835200	−4.30664300
H	1.61381600	1.63905000	−2.77535800
C	0.42837700	2.33758400	−4.42976600
H	0.90587400	3.32106000	−4.37820300
H	0.28986000	2.08244700	−5.48934600
C	−0.90967800	2.28631400	−3.68734400
H	−0.79646700	2.78256800	−2.71733300
H	−1.72311000	2.78020100	−4.22878400
C	−1.17053300	0.78333200	−3.47420600
H	−1.80117000	0.37557900	−4.27265300
H	−1.69743500	0.60659800	−2.52786800
C	−0.48260400	−2.44314900	−2.45869400
H	−1.48052100	−2.02345500	−2.64529200
C	−0.62618300	−3.52877600	−1.34645800
H	0.08687700	−3.39546900	−0.52868600
H	−1.62534600	−3.46821100	−0.90171500
C	−0.42387300	−4.88695600	−2.05058000
H	0.61154200	−5.22574000	−1.92163900
H	−1.07286900	−5.66943700	−1.64527400
C	−0.68256300	−4.59961100	−3.53302700
H	−1.76245000	−4.55296500	−3.72659100
H	−0.25752500	−5.35714300	−4.19936200
C	−0.06058100	−3.21387000	−3.72925900
H	−0.39731100	−2.72223900	−4.64694700
H	1.03077300	−3.31055100	−3.78813800
C	2.29090400	−1.44944700	−2.13777500
H	2.49869500	−1.65061700	−3.19669700

C	3.27361200	−0.35166500	−1.62968300
H	3.73340000	0.16764100	−2.47571900
H	2.75385100	0.40318300	−1.03285100
C	4.33082700	−1.08652600	−0.77362700
H	5.34332400	−0.70706800	−0.94242200
H	4.10340700	−0.94955000	0.29041600
C	4.17552900	−2.56740400	−1.13477300
H	4.57062600	−3.24024300	−0.36666300
H	4.69685000	−2.78984800	−2.07522400
C	2.66406000	−2.70710600	−1.32831700
H	2.17691700	−2.68292300	−0.34563300
H	2.36990300	−3.63419200	−1.83059700
P	−0.58616200	0.68633700	2.08827200
P	0.51430900	−0.94118800	−2.00353400
Fe	−0.08181700	−0.03977600	−0.00179300
H	0.90458700	−0.98654500	0.60284400
H	2.23700200	2.59236500	−0.29083900
H	−1.35113400	−0.98229000	0.02347600
H	−0.68942400	−1.42899700	0.36692800
C	1.16456700	2.75953200	−0.52378400
O	0.44700700	1.70132800	−0.49047000
O	0.77640100	3.89323600	−0.79802300
5_{Fe}			
$G_{\text{solv}} = -3311.901540; E_{\text{solv}} = -3312.68278301$			
C	−1.08239000	−0.52158500	3.22636500
H	−1.25606600	−0.03326700	4.19261600
C	−0.05925900	−1.67989200	3.44693800
H	0.78598600	−1.63583700	2.75362900
H	0.35920600	−1.61605800	4.45671600
C	−0.85503700	−2.98899600	3.26381400
H	−0.73553300	−3.35815500	2.23660800
H	−0.51671600	−3.78331100	3.93643200
C	−2.31585600	−2.58768200	3.48531800
H	−2.52313500	−2.48680800	4.55886200
H	−3.02800200	−3.31031500	3.07393700
C	−2.39394400	−1.21902700	2.80432000
H	−3.27902600	−0.64057100	3.08743300
H	−2.42627500	−1.35901700	1.71641400
C	0.85323300	1.59943600	3.05923800
H	0.48730000	1.65161500	4.09203600
C	2.17442700	0.78697300	3.03436100
H	2.22335900	0.04378900	3.83564200
H	2.26966900	0.24774000	2.08134700
C	3.28311500	1.84018900	3.12110200
H	3.39181400	2.18882000	4.15681500
H	4.25567500	1.45863200	2.79317400
C	2.74437100	2.96724500	2.23862300
H	2.85601100	2.68853200	1.18367500
H	3.25667300	3.92265800	2.39129300
C	1.25128000	3.03656600	2.59729400
H	0.65724900	3.40800700	1.75993600
H	1.09253500	3.73599400	3.42579000
C	−1.83376500	2.07055400	2.06185900
H	−1.37028700	2.92674700	1.56241100
C	−2.35850800	2.54588700	3.42921500
H	−2.55871800	1.69918100	4.09914900
H	−1.65487100	3.21348900	3.93820600
C	−3.68340300	3.22323300	3.06530200

H	-4.32962400	3.39861200	3.93199600
H	-3.48243800	4.19423100	2.59501900
C	-4.29579800	2.25763800	2.04189600
H	-5.05007400	2.73455900	1.40839500
H	-4.79365000	1.43628700	2.57387100
C	-3.09847900	1.71453800	1.22795900
H	-3.01593300	2.18885000	0.24670300
H	-3.20005000	0.64317700	1.04386700
C	0.92697700	0.13435900	-3.45289800
H	0.98807200	-0.52799100	-4.32709000
C	2.24694100	0.92379500	-3.38533500
H	3.11973500	0.29771100	-3.59816600
H	2.37630900	1.36730200	-2.39313300
C	2.03496800	2.02262700	-4.43220600
H	2.74952900	2.84670300	-4.33430600
H	2.15534000	1.59970300	-5.43855600
C	0.58014900	2.46438100	-4.21137500
H	0.53928400	3.24559900	-3.44497900
H	0.13023300	2.88265200	-5.11722100
C	-0.16877300	1.20345600	-3.71075900
H	-0.89134200	0.84018300	-4.44928200
H	-0.72781500	1.43015200	-2.79640500
C	-0.90192800	-1.89935900	-2.68219500
H	-1.61682500	-1.10177600	-2.92128900
C	-1.61176200	-2.87460700	-1.69450800
H	-0.99755900	-3.12612400	-0.82720100
H	-2.51905400	-2.40288800	-1.30474700
C	-1.93983500	-4.14195400	-2.51459600
H	-1.18900100	-4.91807600	-2.31950500
H	-2.91594200	-4.56571800	-2.25939900
C	-1.84222300	-3.70195700	-3.97934800
H	-2.75882300	-3.17760800	-4.27923500
H	-1.69568800	-4.53807200	-4.67079700
C	-0.66710700	-2.72008000	-3.96732300
H	-0.62586300	-2.09266600	-4.86325100
H	0.27543200	-3.28050300	-3.91116800
C	1.97820000	-2.12607300	-1.99237300
H	2.22303900	-2.37630900	-3.03194700
C	3.23510800	-1.49428900	-1.31263000
H	4.02109000	-1.33604900	-2.05765700
H	3.02450000	-0.51509700	-0.86826100
C	3.69514600	-2.50890700	-0.24636200
H	4.78241300	-2.52252200	-0.12243700
H	3.25728500	-2.25453900	0.72785500
C	3.11971400	-3.84534100	-0.72209800
H	3.08595500	-4.60633300	0.06450600
H	3.71958900	-4.24447300	-1.55059900
C	1.73024600	-3.44208100	-1.22205400
H	1.08831300	-3.26635000	-0.34988500
H	1.24375300	-4.20271500	-1.84109900
P	-0.49522000	0.79651000	2.05688700
P	0.54185000	-0.94979800	-2.00624300
Fe	0.12059800	0.00723800	0.01770700
H	0.22179200	-1.44694800	0.63531300
H	1.36476400	3.57032200	-0.89854300
H	-1.31970200	-0.02205100	-0.35329400
H	-0.60984400	-1.30822000	0.40398200
C	0.51476300	2.87642200	-0.73144400

O	0.89495500	1.67270000	−0.51376000
O	−0.63632600	3.30884300	−0.77682900
6Fe			
$G_{\text{solv}} = -3723.528569; E_{\text{solv}} = -3724.49795783$			
C	−1.32991500	−1.23890400	3.19923600
H	−1.64147900	−0.87425500	4.18467200
C	−0.06844700	−2.14080400	3.39061100
H	0.79657000	−1.79397400	2.81687300
H	0.23124800	−2.13178200	4.44403200
C	−0.49510000	−3.55898500	2.96716400
H	−0.26569300	−3.72112700	1.90530700
H	0.02266000	−4.33951900	3.53352500
C	−2.01317700	−3.57223500	3.16194700
H	−2.25561100	−3.68643900	4.22673800
H	−2.51014400	−4.38199400	2.61717300
C	−2.43040500	−2.18398200	2.66807800
H	−3.42768500	−1.88525700	3.00690600
H	−2.44275600	−2.18209200	1.57379700
C	−0.08073600	1.31143800	3.40486500
H	−0.59046700	1.17531400	4.36980700
C	1.39777700	0.94178400	3.59563900
H	1.53539500	0.00882900	4.15102300
H	1.87999700	0.83773500	2.61862400
C	1.96503000	2.15387600	4.34438600
H	1.72960800	2.06507300	5.41263900
H	3.05543900	2.22801800	4.26078900
C	1.23885100	3.37203700	3.73887300
H	1.85839000	3.84753600	2.97419300
H	1.02135100	4.12783900	4.50062800
C	−0.05157200	2.82236700	3.08329200
H	−0.00051000	2.98398100	2.00375600
H	−0.95240600	3.32492100	3.44961200
C	−2.63423400	1.19090600	2.15992700
H	−2.35756600	2.19080600	1.80232100
C	−3.35253100	1.37089600	3.50900400
H	−3.48387000	0.40467800	4.01466400
H	−2.81899900	2.03685700	4.19508700
C	−4.71826900	1.91763500	3.08429700
H	−5.46985800	1.86317000	3.87905200
H	−4.61293200	2.97225400	2.79978800
C	−5.08240900	1.06903900	1.85422700
H	−5.73194700	1.60973300	1.15915800
H	−5.62997200	0.17393500	2.17264100
C	−3.73381000	0.66499200	1.20256000
H	−3.59685200	1.10235500	0.21136200
H	−3.67990300	−0.41825300	1.07643300
C	−0.38317900	−0.28069900	−3.53578500
H	−0.64957200	−1.00841700	−4.31116600
C	0.84851700	0.48970600	−4.05014400
H	1.53665900	−0.16074000	−4.60118600
H	1.39995500	0.93987000	−3.22191200
C	0.23081200	1.59004800	−4.91806100
H	0.93712500	2.39445200	−5.15307000
H	−0.12623200	1.17242200	−5.86962100
C	−0.95250900	2.06335300	−4.06825600
H	−0.58188200	2.73162700	−3.28115000
H	−1.70274900	2.62037600	−4.63834100
C	−1.52424500	0.77546300	−3.43684500

H	-2.40413000	0.42767600	-3.98967500
H	-1.84418300	0.95043700	-2.40523000
C	-1.69329800	-2.36715200	-2.17484700
H	-2.50420000	-1.62806300	-2.19559300
C	-2.00511000	-3.35869200	-1.01056700
H	-1.16568900	-3.50582700	-0.32700300
H	-2.82816400	-2.96095100	-0.41007500
C	-2.40887600	-4.69030100	-1.67566800
H	-1.54504400	-5.36567500	-1.72401200
H	-3.19696700	-5.21171700	-1.12320200
C	-2.82383900	-4.29887600	-3.09591100
H	-3.83483400	-3.87069400	-3.08977600
H	-2.82286900	-5.14122100	-3.79533800
C	-1.80468100	-3.21632000	-3.46158400
H	-2.11295600	-2.62612100	-4.32966100
H	-0.84761000	-3.69303800	-3.70902600
C	1.23607600	-2.40482900	-2.39087200
H	1.08081500	-2.75368300	-3.41902100
C	2.63460500	-1.71932100	-2.30150600
H	3.09382900	-1.70136600	-3.29653500
H	2.58241700	-0.68556300	-1.95551300
C	3.46857000	-2.59228000	-1.34565000
H	4.53530200	-2.58717000	-1.59371600
H	3.36696900	-2.21896100	-0.31760000
C	2.82799100	-3.97844100	-1.44454800
H	3.10010100	-4.64574900	-0.61986500
H	3.12252700	-4.46622200	-2.38325300
C	1.33439300	-3.64402400	-1.46968300
H	1.02232700	-3.39434600	-0.44829800
H	0.70301400	-4.47029400	-1.81200800
P	-1.01568100	0.28075600	2.16931600
P	-0.18541400	-1.27794500	-1.98258700
Fe	-0.22899200	-0.26761100	0.08981900
H	0.35000400	-1.60507800	0.68765400
H	0.03929800	3.66133600	-0.54405800
H	-1.69438800	-0.55507500	-0.08930600
H	-0.49500400	-1.72279500	0.57057000
C	-0.65579100	2.81040300	-0.58482700
O	-0.04244800	1.64018500	-0.58875500
O	-1.85721700	2.94276300	-0.63260400
C	3.28585700	2.37751100	-1.25095200
C	3.29644900	2.63694100	0.29481400
H	1.37649300	0.19654300	0.28111500
C	4.60075900	1.85834400	-1.82254100
H	4.49567500	1.69971800	-2.90078700
H	5.41273000	2.57665400	-1.66309300
H	4.88166300	0.90405900	-1.37126900
C	4.18657800	1.64366400	1.04971400
H	5.24914900	1.82635600	0.86061900
H	4.00822600	1.75441200	2.12329100
H	3.95684400	0.61025700	0.77170200
C	2.82160100	3.59233600	-2.06185500
H	3.58211100	4.37946800	-2.09046900
H	2.61937800	3.27418400	-3.08935200
H	1.90051000	4.02082700	-1.65682600
C	3.66843200	4.06055100	0.68824100
H	3.73571500	4.14783700	1.77677500
H	4.64478800	4.33341200	0.27244100

H	2.92551500	4.78008500	0.33572300
O	2.30682900	1.35142000	−1.37094300
O	1.93602400	2.38475900	0.65283000
B	1.42674200	1.39774900	−0.24884500
TS_{6,7}-Fe			
$G_{\text{solv}} = -3723.495355; E_{\text{solv}} = -3724.46110883$			
C	−2.05409700	−0.99264600	3.07133200
H	−2.24495500	−0.52172200	4.04413700
C	−1.26639800	−2.31253300	3.32495600
H	−0.45520500	−2.44570800	2.60253400
H	−0.80685900	−2.29100400	4.31859900
C	−2.30254700	−3.45535500	3.20529700
H	−2.18714200	−3.96073400	2.23850900
H	−2.18041900	−4.21590700	3.98260600
C	−3.67079200	−2.76486500	3.25731500
H	−3.95575900	−2.56170100	4.29799600
H	−4.46973200	−3.36164900	2.80520800
C	−3.42023000	−1.44507800	2.52214800
H	−4.20512600	−0.70052000	2.69007700
H	−3.37343400	−1.63636300	1.44339400
C	0.15821300	0.74944900	3.36289900
H	−0.32368000	0.61628900	4.34324200
C	1.45393700	−0.07715700	3.32910100
H	1.31723300	−1.10744700	3.67113300
H	1.81140800	−0.12254100	2.29479800
C	2.42944100	0.71762700	4.21751400
H	2.39899200	0.34115400	5.24599900
H	3.46390300	0.61075400	3.87270600
C	1.93845400	2.18932800	4.17074900
H	2.70478500	2.87151500	3.78527100
H	1.68640100	2.53785600	5.17829700
C	0.68327900	2.18935900	3.27389800
H	0.95435800	2.41906900	2.23980500
H	−0.05471800	2.93106900	3.59710400
C	−2.22639100	1.71831800	1.98742000
H	−1.56827300	2.54813000	1.69577800
C	−2.98945300	2.16611800	3.24555200
H	−3.45401900	1.31038800	3.75132200
H	−2.34564400	2.67110900	3.97332700
C	−4.08408600	3.06904900	2.66844100
H	−4.88766800	3.28024800	3.38164300
H	−3.64769200	4.02895000	2.36451600
C	−4.56873600	2.29442800	1.43351500
H	−5.02587400	2.94657600	0.68393200
H	−5.32888600	1.56346500	1.73610500
C	−3.31630200	1.56457200	0.88840700
H	−2.97355100	2.00451300	−0.05217100
H	−3.54054000	0.51403100	0.67989500
C	−0.61023800	−0.78672800	−3.48445100
H	−0.60828700	−1.56225700	−4.25947300
C	0.25393200	0.38569300	−3.98545500
H	1.10617700	0.04082700	−4.58115500
H	0.65394800	0.96678000	−3.15184300
C	−0.72880100	1.24855100	−4.78270700
H	−0.35260000	2.26189600	−4.95942300
H	−0.93122100	0.78934400	−5.76011800
C	−1.98890400	1.22759100	−3.91142500
H	−1.86798300	1.94151700	−3.09000100

H	-2.89621300	1.50196300	-4.45926300
C	-2.05210600	-0.20941600	-3.34939200
H	-2.75973800	-0.82736800	-3.91351000
H	-2.40049700	-0.20566700	-2.30763800
C	-1.05834100	-3.15031500	-2.00673000
H	-2.08598700	-2.76739300	-2.07409000
C	-0.99492600	-4.10066300	-0.76856300
H	-0.17131600	-3.86261800	-0.09103300
H	-1.91676800	-4.00200100	-0.18498900
C	-0.86999700	-5.53052000	-1.33353500
H	0.18204300	-5.84169400	-1.34405800
H	-1.41834700	-6.26583800	-0.73629600
C	-1.38014900	-5.42251500	-2.77339900
H	-2.47808700	-5.40200300	-2.78490900
H	-1.05588500	-6.25212400	-3.41022700
C	-0.83159500	-4.06738200	-3.22907500
H	-1.32385900	-3.69254300	-4.13165600
H	0.23742300	-4.16941700	-3.45417200
C	1.68274500	-2.12460800	-2.27390800
H	1.68691800	-2.51928600	-3.29820000
C	2.72290800	-0.97498800	-2.17244800
H	3.02347200	-0.64508700	-3.17213700
H	2.30138500	-0.10335400	-1.66781100
C	3.92351400	-1.55412300	-1.38751500
H	4.88859100	-1.23343500	-1.79502500
H	3.88016700	-1.21913500	-0.34372600
C	3.73361300	-3.07379400	-1.43424300
H	4.26912300	-3.59878300	-0.63630200
H	4.08616800	-3.47374900	-2.39448500
C	2.21461000	-3.22280900	-1.33143300
H	1.90318700	-3.01663500	-0.30004700
H	1.85543800	-4.22078900	-1.60277700
P	-1.09022400	0.25760600	2.07802200
P	-0.04797400	-1.57951100	-1.90471800
Fe	-0.47622700	-0.48691400	0.03561700
H	0.53093300	-1.39102100	0.68194900
H	-0.39449900	4.39563500	0.21519400
H	-1.76688200	-1.43243100	0.10330700
H	-1.11047200	-1.84124800	0.49069400
C	-0.99705600	3.86865600	-0.53997900
O	-0.38591700	2.83059700	-1.10887100
O	-2.11654300	4.20555100	-0.84096300
C	3.09181100	2.95004100	-1.51291600
C	3.01674200	3.01345000	0.05018900
H	0.59100700	0.69683700	-0.20020200
C	4.26461200	2.15529200	-2.06216900
H	4.20718300	2.11907600	-3.15417100
H	5.20889500	2.63737600	-1.78719000
H	4.27549900	1.13228000	-1.68807400
C	3.48710600	1.72528500	0.72195100
H	4.56560100	1.58655400	0.60094500
H	3.27217100	1.78452100	1.79057600
H	2.96186800	0.85528200	0.31986100
C	3.04350200	4.33104500	-2.17081500
H	3.97663100	4.88213500	-2.01920000
H	2.88857500	4.20459300	-3.24609000
H	2.21677600	4.93357500	-1.78074400
C	3.70092700	4.21871700	0.67503900

H	3.58066300	4.18740100	1.76210300
H	4.77330100	4.20920000	0.45315200
H	3.27666300	5.15840000	0.31490800
O	1.85259900	2.28562700	−1.84788100
O	1.59123800	3.13401100	0.26613200
B	0.97259300	2.55465100	−0.82146200
7_{Fe}			
$G_{\text{solv}} = -3723.508931; E_{\text{solv}} = -3724.47147899$			
C	−2.18271200	−1.17322900	3.44032900
H	−2.30494900	−0.61216100	4.37548900
C	−1.39778800	−2.48599000	3.74858300
H	−0.55653600	−2.63204600	3.06396000
H	−0.98386800	−2.44386500	4.76145100
C	−2.42265700	−3.63415100	3.61968700
H	−2.33939200	−4.09704200	2.62804400
H	−2.26474400	−4.42343400	4.36142900
C	−3.78944400	−2.95362000	3.74491700
H	−4.01539400	−2.74418200	4.79892000
H	−4.60969700	−3.55644000	3.34123000
C	−3.57950000	−1.64229500	2.98353000
H	−4.35549500	−0.89401800	3.17533300
H	−3.58369100	−1.85344600	1.90688600
C	0.02984300	0.63347000	3.33031500
H	−0.46115800	0.89427200	4.27922100
C	1.20594400	−0.33058900	3.62356600
H	1.00050600	−0.94814100	4.50300900
H	1.35488400	−1.00594400	2.77562500
C	2.45542300	0.56933300	3.82260100
H	2.95971600	0.37962700	4.77555800
H	3.18395300	0.36998900	3.02789700
C	1.94364200	2.01575700	3.71630600
H	2.69800500	2.71505000	3.33802100
H	1.62906800	2.38153300	4.70238500
C	0.72043600	1.90028800	2.80320800
H	1.03800800	1.74450700	1.76410900
H	0.07843800	2.78742300	2.84192000
C	−2.41694600	1.38985100	2.01747600
H	−1.75832100	2.16128400	1.60423900
C	−3.10906400	1.99840100	3.24999500
H	−3.52497800	1.21852800	3.90040800
H	−2.42534900	2.60349600	3.85549200
C	−4.25323900	2.80965100	2.63277700
H	−5.01656000	3.10055200	3.36221800
H	−3.85392100	3.72677700	2.18131900
C	−4.79374500	1.87825000	1.53926000
H	−5.35315000	2.41414300	0.76674800
H	−5.47778500	1.14753400	1.98908300
C	−3.54778100	1.15848900	0.97299500
H	−3.24630100	1.58387300	0.01042500
H	−3.75150400	0.09634200	0.80297300
C	−0.70483100	−0.81857100	−3.17459300
H	−0.52328500	−1.41395300	−4.07810300
C	0.03347300	0.52581100	−3.32503700
H	0.99228900	0.42402800	−3.84227600
H	0.23188000	0.95886900	−2.33894000
C	−0.96923000	1.41153100	−4.06730600
H	−0.71562200	2.47433400	−4.01014300
H	−1.01307500	1.12660100	−5.12761100

C	-2.29100100	1.07581500	-3.37034300
H	-2.33932900	1.62144000	-2.42061100
H	-3.17321400	1.35718300	-3.95408000
C	-2.21697700	-0.44373300	-3.10348800
H	-2.78105400	-1.00741100	-3.85475300
H	-2.65933600	-0.69268400	-2.12930000
C	-1.04898500	-3.43507400	-2.12690700
H	-2.09750100	-3.12588200	-2.23387500
C	-0.99609200	-4.53407100	-1.01949000
H	-0.24990500	-4.32446200	-0.24865300
H	-1.96289800	-4.58558300	-0.50736100
C	-0.69824400	-5.85875800	-1.75180500
H	0.37621600	-6.07745600	-1.71016900
H	-1.21929600	-6.71183100	-1.30579600
C	-1.10451000	-5.59797700	-3.20579500
H	-2.19556300	-5.66422100	-3.31057900
H	-0.65886000	-6.30583400	-3.91243200
C	-0.64790800	-4.15370500	-3.43320000
H	-1.10115800	-3.69465300	-4.31769900
H	0.43991700	-4.13962700	-3.57545200
C	1.60202800	-2.16590000	-2.02456900
H	1.70053800	-2.42504000	-3.08615700
C	2.52218500	-0.94594100	-1.72294800
H	2.93457700	-0.55135800	-2.65795800
H	1.96717100	-0.13621100	-1.24342400
C	3.63989900	-1.47741700	-0.80297400
H	4.60541400	-0.99147800	-0.98391900
H	3.36842100	-1.29586600	0.24475600
C	3.66731800	-2.98593500	-1.06319100
H	4.17063800	-3.55133700	-0.27184800
H	4.18233800	-3.20030000	-2.00969500
C	2.17934600	-3.32396900	-1.18204300
H	1.73581700	-3.31604300	-0.17939400
H	1.98720500	-4.30419800	-1.63103300
P	-1.29418100	-0.06958400	2.23611900
P	-0.19400100	-1.83137500	-1.70879400
Fe	-0.77310500	-0.97771000	0.27433600
H	0.36928700	-1.73591000	0.89869200
H	-0.13597900	3.11943800	0.41506900
H	-1.92797000	-2.10178800	0.42534900
H	-1.20489700	-2.40959500	0.77702400
C	-0.57855600	3.41128500	-0.54686000
O	0.29443400	3.43443800	-1.56945500
O	-1.73841000	3.68774900	-0.69934500
C	3.84939600	3.25137300	-1.85249700
C	3.65028500	3.29713500	-0.28907100
H	0.10874700	0.28902500	-0.00273800
C	4.77970700	2.15173100	-2.33660200
H	4.83631700	2.17298800	-3.42874400
H	5.78931800	2.30103300	-1.94008400
H	4.42629100	1.16503800	-2.03311800
C	3.79345900	1.93530400	0.38330200
H	4.82530900	1.57516000	0.34195200
H	3.50772000	2.02942900	1.43249800
H	3.14111400	1.18941200	-0.07521400
C	4.25429100	4.59627000	-2.45349000
H	5.27942400	4.86280300	-2.18031200
H	4.19649800	4.52863700	-3.54341200

H	3.58722900	5.40153400	−2.13037700
C	4.49916900	4.33320000	0.42935500
H	4.28292900	4.30507400	1.50123000
H	5.56364100	4.11584600	0.29347000
H	4.29920900	5.34447800	0.06998200
O	2.50947200	2.96679900	−2.33524800
O	2.25222000	3.68104000	−0.16665100
B	1.65868900	3.34469700	−1.34726600
8Fe			
$G_{\text{solv}} = -3723.526347; E_{\text{solv}} = -3724.49768633$			
C	−2.07980600	−1.39995100	2.76333300
H	−2.14046800	−1.63352000	3.83445700
C	−2.20320500	−2.73120800	1.96011500
H	−1.41875000	−2.81713400	1.20537900
H	−2.10847400	−3.58575900	2.63859400
C	−3.59796200	−2.69834600	1.30147800
H	−3.49830400	−2.34375200	0.27028400
H	−4.07489300	−3.68380700	1.27913100
C	−4.38813500	−1.66863900	2.11445100
H	−4.73539300	−2.10847600	3.05961500
H	−5.26445600	−1.28068200	1.58452200
C	−3.33877800	−0.58930000	2.39261700
H	−3.63013000	0.11195400	3.18235000
H	−3.17658500	−0.01801400	1.47408800
C	0.60442900	−1.46379500	3.73926300
H	0.09999100	−1.33320400	4.70470800
C	0.74801800	−2.98122700	3.48390100
H	−0.07773000	−3.55129000	3.92025100
H	0.76441300	−3.18816600	2.40796900
C	2.10896900	−3.33592000	4.09149600
H	2.03442500	−3.39344700	5.18577700
H	2.49707600	−4.29474800	3.73203700
C	2.97810800	−2.14509000	3.68280000
H	3.24375800	−2.24860500	2.62453400
H	3.91051900	−2.06570900	4.25111400
C	2.06063500	−0.92291600	3.87048600
H	2.29440800	−0.13372600	3.14855900
H	2.20199800	−0.48607000	4.86556300
C	−0.56763800	1.08055000	3.40251300
H	0.48725300	1.38229800	3.48322800
C	−1.17510700	1.09350500	4.83197300
H	−1.89278900	0.27994900	4.97866200
H	−0.39073300	0.96043900	5.58416300
C	−1.87868900	2.46805000	4.97855300
H	−2.96668000	2.33472800	4.95495000
H	−1.63743900	2.96235700	5.92473200
C	−1.43852300	3.28536600	3.75407800
H	−0.47013400	3.76734500	3.94541900
H	−2.15297900	4.07202100	3.48865900
C	−1.28023600	2.22591800	2.66131400
H	−0.72566100	2.57595600	1.78652600
H	−2.27291700	1.91621900	2.31608400
C	1.58207300	−0.04835500	−3.04738900
H	2.44010900	−0.43574100	−3.61684300
C	1.85286400	1.42991400	−2.72631500
H	2.85211100	1.60875200	−2.31733200
H	1.12865400	1.77778300	−1.97893400
C	1.63450500	2.13635800	−4.07081600

H	1.38295600	3.19579800	−3.95102200
H	2.55918100	2.08810800	−4.65919400
C	0.50669400	1.34516000	−4.77084100
H	−0.43232000	1.90425800	−4.74041400
H	0.74974200	1.16872300	−5.82394800
C	0.36271600	0.01433000	−3.99170200
H	0.32354600	−0.85126900	−4.65996500
H	−0.56010700	0.02666200	−3.40734100
C	0.58191100	−2.63427400	−2.30127000
H	−0.33694400	−2.22467700	−2.73885800
C	0.15624400	−3.75343700	−1.32420100
H	0.88218200	−3.87073600	−0.51526600
H	−0.79638800	−3.49931800	−0.85432400
C	0.08609100	−5.04684400	−2.18003100
H	0.79337600	−5.79129100	−1.79688700
H	−0.90614600	−5.50739900	−2.15031000
C	0.48109400	−4.63180100	−3.61154900
H	−0.41229600	−4.36506100	−4.19000600
H	1.00017800	−5.42664200	−4.15741700
C	1.34219900	−3.38142000	−3.40849000
H	1.47090400	−2.79274000	−4.32269700
H	2.34062400	−3.67749100	−3.05935600
C	3.16678900	−1.64164100	−1.30629400
H	3.53727100	−1.94795300	−2.29191800
C	4.06461100	−0.47110700	−0.79709300
H	4.73041900	−0.13806700	−1.60056700
H	3.48290200	0.40252900	−0.48896000
C	4.87185200	−1.03895500	0.38786600
H	5.88620800	−0.63084600	0.44004400
H	4.37045600	−0.78748900	1.33141600
C	4.84055200	−2.55703700	0.18819900
H	5.06641000	−3.11474400	1.10358600
H	5.57485200	−2.85353100	−0.57250700
C	3.41903100	−2.80547200	−0.32510000
H	2.71320900	−2.75928900	0.51157200
H	3.29754100	−3.78251600	−0.80465900
P	−0.44979300	−0.54831500	2.50850700
P	1.38895700	−1.14670300	−1.54722200
Fe	0.36919300	−0.51395800	0.38358100
H	1.62557500	0.31473800	0.86971800
H	−0.28488600	1.00207700	−0.04120600
H	0.72763500	−1.92953600	0.72143800
H	1.79572900	−0.52654100	1.02529900
C	−1.60855700	4.68333000	−2.52313200
C	−0.92697000	4.69302800	−1.10480900
C	−0.90140800	5.52838200	−3.57128200
H	−1.43185500	5.45249400	−4.52494700
H	−0.88834800	6.58189400	−3.27227500
H	0.12685400	5.19703900	−3.73005200
C	0.59138100	4.86130600	−1.16420200
H	0.87132600	5.88118400	−1.44476300
H	1.00852300	4.64967000	−0.17525000
H	1.04527800	4.16665800	−1.87668300
C	−3.09542700	5.03739900	−2.47509300
H	−3.24999200	6.09635800	−2.24685200
H	−3.54124300	4.82742700	−3.45147600
H	−3.62671700	4.43967900	−1.72782500
C	−1.52331200	5.68159900	−0.11423100

H	-0.98744100	5.61631700	0.83751600
H	-1.42903900	6.70673900	-0.48743600
H	-2.57796500	5.47371400	0.07794200
O	-1.51639400	3.29304000	-2.90543900
O	-1.18605800	3.35412200	-0.63379800
B	-1.40482300	2.56650800	-1.74468200
O	-1.49652600	1.21680200	-1.70101200
C	-1.34465600	0.57631300	-0.41785500
H	-2.05543600	1.06901600	0.26436800
O	-1.40944200	-0.73547300	-0.45966700
9_{Fe}			
$G_{\text{solv}} = -3723.531326; E_{\text{solv}} = -3724.50603350$			
C	-2.53760900	-1.35739600	2.50984300
H	-2.75597500	-1.15861200	3.56645600
C	-2.28809400	-2.88929600	2.33528600
H	-1.29474000	-3.11529200	1.94439700
H	-2.38158900	-3.38633400	3.30836400
C	-3.37601500	-3.38440200	1.36848000
H	-3.01075300	-3.30178400	0.33734200
H	-3.65259500	-4.42925800	1.54673200
C	-4.52977300	-2.40284000	1.57281500
H	-5.05420400	-2.62473500	2.51307200
H	-5.26703600	-2.42709000	0.76340600
C	-3.80452000	-1.05757000	1.66592300
H	-4.42304400	-0.27421500	2.11613000
H	-3.50967100	-0.73503100	0.66007500
C	0.18862200	-0.72569700	3.34994200
H	-0.30609100	-0.61076700	4.32118900
C	0.78745700	-2.14982800	3.30706400
H	0.16327200	-2.87454000	3.83779400
H	0.88952000	-2.50062800	2.27343200
C	2.17640500	-1.98580200	3.93167400
H	2.09127600	-1.89057300	5.02246700
H	2.84030300	-2.83129600	3.72181800
C	2.66580000	-0.66983200	3.32348400
H	3.00310000	-0.85637200	2.29548900
H	3.50619600	-0.22381700	3.86532300
C	1.41934100	0.23719000	3.30836100
H	1.41982900	0.89138300	2.42944800
H	1.40509900	0.89189000	4.18725100
C	-1.53236700	1.40457600	2.64807500
H	-0.58509300	1.95054900	2.56234400
C	-2.03980600	1.52073000	4.11840600
H	-2.03308700	0.57313900	4.66471400
H	-1.38692800	2.20450600	4.67470900
C	-3.45462700	2.10878900	4.02719000
H	-4.18532700	1.30443400	3.87271400
H	-3.74628000	2.65022600	4.93313300
C	-3.39468200	2.99267000	2.78093100
H	-2.85334700	3.92126800	3.01152700
H	-4.38129400	3.27176600	2.39649000
C	-2.59053700	2.14606900	1.78747000
H	-2.12636200	2.75995700	1.01226100
H	-3.25437300	1.44404700	1.27777400
C	0.45085400	-0.73417000	-3.64652800
H	1.09736500	-1.30271000	-4.32996700
C	0.74555200	0.75535000	-3.89528600
H	1.81640000	0.95886600	-3.99142900

H	0.36598100	1.37451200	-3.07567700
C	-0.02318200	1.04571700	-5.18988900
H	-0.18717900	2.11590700	-5.35509600
H	0.55302500	0.66793200	-6.04451200
C	-1.33711200	0.25573500	-5.04663700
H	-2.11674900	0.89317800	-4.61432000
H	-1.71208100	-0.08728400	-6.01620700
C	-1.02247800	-0.92452900	-4.08972400
H	-1.15321200	-1.89354600	-4.58341300
H	-1.68847200	-0.91254300	-3.22012700
C	0.43665600	-3.19662500	-2.25847900
H	-0.64367500	-3.19591400	-2.45042700
C	0.70155000	-4.16883300	-1.06680100
H	1.24971800	-3.70198000	-0.24690600
H	-0.25469100	-4.49182400	-0.64459600
C	1.47217400	-5.36479100	-1.65991700
H	2.55290100	-5.21759700	-1.53343300
H	1.21587900	-6.31197700	-1.17465500
C	1.13214700	-5.33882500	-3.15228400
H	0.12752700	-5.75038800	-3.31637300
H	1.83250800	-5.91342400	-3.76783400
C	1.13844900	-3.84187200	-3.47459100
H	0.63686600	-3.60625100	-4.41860300
H	2.17788500	-3.49716800	-3.55911300
C	2.63796700	-1.24030700	-1.87413100
H	3.03065800	-1.55722000	-2.84805600
C	3.08417400	0.23482800	-1.61558300
H	3.55903600	0.64354200	-2.51371900
H	2.24217400	0.88822100	-1.37016100
C	4.08908700	0.18084700	-0.44902600
H	4.88966800	0.92193600	-0.54947200
H	3.56998000	0.39017700	0.49459100
C	4.60607900	-1.26067900	-0.45132000
H	5.06401300	-1.55664700	0.49859600
H	5.35919600	-1.38983400	-1.23986900
C	3.35096700	-2.07326900	-0.78462100
H	2.73608900	-2.15614400	0.11904300
H	3.56905800	-3.09174500	-1.12174400
P	-1.07682100	-0.30781900	2.04521900
P	0.78187800	-1.39707600	-1.94111800
Fe	-0.24789200	-0.59236400	-0.05544100
H	1.18335800	-0.25338900	0.56427500
H	-2.51419800	1.79086100	-0.93435500
H	-0.42631400	-2.04969000	0.28799500
H	1.06711500	-1.09475400	0.63815000
C	0.40537700	4.76366900	-0.03632200
C	1.71469300	3.96133400	0.29918500
C	0.61546900	5.98590400	-0.91508100
H	-0.34137300	6.48799200	-1.08587500
H	1.28960800	6.69816700	-0.42775300
H	1.03441200	5.71521800	-1.88650500
C	2.74008700	3.98425200	-0.83541400
H	3.21485300	4.96564600	-0.92965100
H	3.51714500	3.24452200	-0.62272900
H	2.28309400	3.72595100	-1.79621400
C	-0.39703600	5.13553900	1.21083900
H	0.09178700	5.93650300	1.77357500
H	-1.38781600	5.48400600	0.90571400

H	−0.52775700	4.27599200	1.87560500
C	2.37573100	4.33522600	1.61654500
H	3.26922000	3.72118300	1.76498800
H	2.68239000	5.38642500	1.61228600
H	1.70724400	4.16808600	2.46393500
O	−0.37240100	3.78716800	−0.77213100
O	1.22248700	2.60925000	0.39656000
B	0.08428500	2.55227900	−0.37701200
O	−0.46631200	1.36781900	−0.69883400
C	−1.80006200	1.04099900	−1.31720600
H	−1.64708700	1.21870700	−2.39710900
O	−2.03882400	−0.21605700	−0.96540300
TS_{9,10}-Fe			
$G_{\text{solv}} = -3723.526300; E_{\text{solv}} = -3724.49582350$			
C	−2.42593700	−1.47632900	2.79858600
H	−2.52632500	−1.26328700	3.86968300
C	−2.19622600	−3.01329400	2.62305900
H	−1.23121200	−3.26324500	2.17686800
H	−2.22032600	−3.49814300	3.60571300
C	−3.35993200	−3.51764900	1.75580200
H	−3.09925500	−3.42994900	0.69215000
H	−3.60643800	−4.56632000	1.95225900
C	−4.49851900	−2.54911100	2.07551600
H	−4.92245400	−2.78009700	3.06211100
H	−5.31299500	−2.58139200	1.34432900
C	−3.78202900	−1.19557000	2.10050200
H	−4.35569700	−0.41774000	2.61380300
H	−3.61516500	−0.86543800	1.07024700
C	0.32128900	−0.80187500	3.40328000
H	−0.12285900	−0.64434100	4.39433500
C	0.91172700	−2.22680700	3.39183700
H	0.28725200	−2.94511700	3.93140500
H	1.03171000	−2.58338700	2.36115800
C	2.29500400	−2.04662600	4.02355300
H	2.19542800	−1.91429400	5.10935200
H	2.95653400	−2.90279300	3.85204900
C	2.79738900	−0.75615900	3.37132700
H	3.17529200	−0.98829700	2.36867700
H	3.61220000	−0.28001300	3.92677200
C	1.54974000	0.14535900	3.25167700
H	1.55125500	0.67824100	2.29707400
H	1.53243600	0.90585200	4.04134900
C	−1.43204300	1.30396300	2.65886200
H	−0.48559400	1.82748900	2.48401800
C	−1.85554700	1.52580200	4.14285700
H	−1.84493100	0.61460900	4.74831800
H	−1.15423700	2.22203600	4.61840800
C	−3.25755400	2.15087700	4.08903900
H	−4.01924100	1.36167900	4.04829500
H	−3.47572100	2.77161500	4.96435100
C	−3.25562600	2.93184900	2.77379600
H	−2.68690400	3.86358700	2.89885300
H	−4.25940300	3.20239200	2.42877300
C	−2.52787500	1.99412400	1.80286800
H	−2.09118100	2.52250100	0.95251800
H	−3.23436400	1.26580700	1.39575200
C	0.54123800	−0.81420500	−3.56568900
H	1.25819800	−1.32314600	−4.22424200

C	0.73982700	0.70066000	−3.76342200
H	1.79740500	0.97085100	−3.83836800
H	0.32264800	1.26688600	−2.92309800
C	−0.02940900	0.98584300	−5.05853100
H	−0.25742200	2.04842200	−5.19235600
H	0.57467200	0.66880200	−5.91859500
C	−1.29298600	0.11483800	−4.95392800
H	−2.09728000	0.67767000	−4.46494800
H	−1.67179800	−0.18321800	−5.93648400
C	−0.89043900	−1.10680800	−4.08744900
H	−0.90353400	−2.03569500	−4.66730000
H	−1.59607100	−1.24795000	−3.26011400
C	0.63472500	−3.28635500	−2.18787100
H	−0.41963500	−3.35841400	−2.48619600
C	0.84222300	−4.24243300	−0.96959200
H	1.34103000	−3.75701200	−0.12709800
H	−0.13043100	−4.58567100	−0.60045700
C	1.67378500	−5.42977500	−1.49810900
H	2.73544900	−5.27575600	−1.26743700
H	1.37895300	−6.38192400	−1.04606400
C	1.47732800	−5.39674500	−3.01651000
H	0.50411800	−5.83054700	−3.28177200
H	2.24853400	−5.94912000	−3.56329000
C	1.47946000	−3.89754800	−3.32665700
H	1.07483900	−3.66441900	−4.31667900
H	2.51131100	−3.52493900	−3.29600600
C	2.68175400	−1.21818600	−1.71343600
H	3.11184400	−1.50357700	−2.68175400
C	3.07359900	0.26015900	−1.41289000
H	3.51124800	0.71985900	−2.30551200
H	2.20897700	0.85848500	−1.12365800
C	4.09850100	0.20449300	−0.26245700
H	4.89354800	0.95031700	−0.37186900
H	3.58406100	0.40621500	0.68365800
C	4.62909100	−1.23206000	−0.27628500
H	5.08484600	−1.53147600	0.67391400
H	5.38745100	−1.35109800	−1.06207000
C	3.38200400	−2.05081100	−0.61943500
H	2.74675100	−2.11452100	0.27120700
H	3.60750000	−3.06996600	−0.95166800
P	−1.01439700	−0.44057700	2.15809000
P	0.84410900	−1.46250700	−1.84997800
Fe	−0.35409200	−0.80238000	−0.00964500
H	0.98741800	−0.95853500	0.63207900
H	−2.77837000	1.67768600	−1.17116200
H	−0.97228300	−2.27769500	0.04248100
H	−0.22960400	−2.30170800	0.44558500
C	0.63094000	4.53679500	0.15830500
C	1.91702400	3.78469400	0.65410300
C	0.90063900	5.73659900	−0.73990800
H	−0.04605500	6.20792100	−1.02272800
H	1.50914900	6.48523700	−0.22050300
H	1.41581000	5.44165700	−1.65685300
C	3.04616800	3.80049400	−0.37984400
H	3.49492300	4.79451300	−0.47656100
H	3.82388500	3.10075800	−0.06199100
H	2.68829100	3.48170700	−1.36396600
C	−0.28953000	4.94713200	1.31192300

H	0.12338900	5.78418100	1.88411000
H	−1.25675600	5.25365100	0.90227900
H	−0.46209700	4.11166100	1.99709900
C	2.44750400	4.24225700	2.00629600
H	3.33873500	3.66242700	2.26637300
H	2.72639500	5.30148800	1.98135000
H	1.70958500	4.09257300	2.79796200
O	−0.04291300	3.52370900	−0.59599100
O	1.45348300	2.43671400	0.77068500
B	0.36338300	2.27047000	−0.09734500
O	−0.21619700	1.14030500	−0.41439400
C	−2.20504700	0.76744300	−1.40897700
H	−1.55819000	0.82082600	−2.28726300
O	−2.41156500	−0.28195500	−0.80762900
10Fe			
$G_{\text{solv}} = -3723.533359; E_{\text{solv}} = -3724.50567104$			
C	−2.53180100	−1.34010600	2.60731300
H	−2.67675500	−1.09511700	3.66628800
C	−2.28794000	−2.88051300	2.49074100
H	−1.31820400	−3.13584400	2.05858900
H	−2.31283900	−3.32899200	3.49020900
C	−3.44040800	−3.42884300	1.63363300
H	−3.16319300	−3.39862900	0.57105400
H	−3.69177800	−4.46525100	1.88140600
C	−4.58371500	−2.44516200	1.88318600
H	−5.02665200	−2.62419000	2.87212700
H	−5.38480500	−2.51314200	1.13969700
C	−3.86460500	−1.09328200	1.85686300
H	−4.45050700	−0.28612200	2.30720600
H	−3.66868900	−0.82478200	0.81308300
C	0.18491700	−0.63395000	3.29568200
H	−0.29864400	−0.45414800	4.26428900
C	0.77825400	−2.05929600	3.33158500
H	0.15745000	−2.75778800	3.90099300
H	0.88895800	−2.45274400	2.31402600
C	2.17006500	−1.86297600	3.94012200
H	2.08772200	−1.70278100	5.02375000
H	2.82851800	−2.72371800	3.77967100
C	2.65978400	−0.58858200	3.24935200
H	2.99585300	−0.83645400	2.23495300
H	3.49697900	−0.10878700	3.76740400
C	1.41444900	0.31602000	3.16384600
H	1.41604600	0.88067300	2.22879700
H	1.40400600	1.04815500	3.98054000
C	−1.55811200	1.43935300	2.42520400
H	−0.61159600	1.96900500	2.27256700
C	−2.04422100	1.70394400	3.88249100
H	−2.08820200	0.80415300	4.50345000
H	−1.34664200	2.38923500	4.37843900
C	−3.42652500	2.36286000	3.74979200
H	−4.20681300	1.59166700	3.71042200
H	−3.66178000	3.02284400	4.59116000
C	−3.35756800	3.09095600	2.40594900
H	−2.76960500	4.01234300	2.51307300
H	−4.34143600	3.37119900	2.01430800
C	−2.61897500	2.09610400	1.50302100
H	−2.15163000	2.56850500	0.63543000
H	−3.33398600	1.35797500	1.12616500

C	0.39036000	−0.66326300	−3.66773900
H	1.12144900	−1.08327800	−4.37199500
C	0.46066400	0.87364200	−3.77005100
H	1.48713600	1.23594200	−3.88121100
H	0.04631300	1.33247800	−2.86622600
C	−0.41551100	1.18662000	−4.98581400
H	−0.70194300	2.24199400	−5.04567200
H	0.12106200	0.93366500	−5.91032600
C	−1.61652200	0.25100300	−4.80273600
H	−2.33733700	0.72095600	−4.12008400
H	−2.15144000	0.05031200	−5.73637200
C	−1.03714100	−1.03341200	−4.16495800
H	−0.98306000	−1.84878900	−4.89425000
H	−1.67749800	−1.38507600	−3.34928800
C	0.59427600	−3.18014000	−2.36285800
H	−0.46459900	−3.26349600	−2.64017700
C	0.83759800	−4.15358100	−1.16606100
H	1.35921500	−3.67940600	−0.33112000
H	−0.12355800	−4.50380500	−0.77394300
C	1.65609300	−5.33074900	−1.73770600
H	2.72286100	−5.18217500	−1.52762700
H	1.37080100	−6.29213500	−1.29919500
C	1.42722100	−5.26715900	−3.25120100
H	0.44942200	−5.69772500	−3.50481100
H	2.18783900	−5.80680600	−3.82497800
C	1.42004900	−3.76163700	−3.52976400
H	0.99721700	−3.50573200	−4.50665800
H	2.45150500	−3.38791000	−3.50850100
C	2.62794400	−1.10718200	−1.92243000
H	3.02644200	−1.39812000	−2.90255300
C	3.03186200	0.37135100	−1.64314600
H	3.44086800	0.82401400	−2.55324000
H	2.17675700	0.97093900	−1.33078500
C	4.09216600	0.31951500	−0.52441400
H	4.88428500	1.06327900	−0.66368700
H	3.60729800	0.52757500	0.43626600
C	4.61892400	−1.11823900	−0.54580700
H	5.10262400	−1.41340100	0.39179000
H	5.35269400	−1.24397100	−1.35374400
C	3.35980500	−1.93514000	−0.84568000
H	2.75069900	−1.99105300	0.06377200
H	3.57252400	−2.95696900	−1.17842900
P	−1.10248500	−0.31236400	1.98947600
P	0.78979900	−1.36215000	−1.99336800
Fe	−0.38565400	−0.71233300	−0.14531400
H	0.94993500	−0.87800200	0.52782500
H	−3.69357200	0.70644600	−1.94538000
H	−0.99651300	−2.19549200	−0.07374500
H	−0.24678900	−2.20285100	0.32277600
C	0.67510700	4.59488000	−0.01321400
C	1.92828300	3.85925100	0.58333700
C	1.00125000	5.77196500	−0.92339600
H	0.07428100	6.23078700	−1.28243400
H	1.57137100	6.53775700	−0.38563900
H	1.57752900	5.45463400	−1.79540600
C	3.12693100	3.86361900	−0.36955000
H	3.57041500	4.86057100	−0.46233000
H	3.88849800	3.18391100	0.02210300

H	2.84301100	3.51286000	−1.36675500
C	−0.31534900	5.03662700	1.06956100
H	0.06157200	5.88705300	1.64709500
H	−1.25397200	5.33364800	0.59163200
H	−0.53364700	4.21805400	1.76189900
C	2.36358600	4.34873400	1.95914100
H	3.23986000	3.78215400	2.28994700
H	2.63519900	5.40996900	1.93246300
H	1.57522700	4.20733800	2.70240500
O	0.04999900	3.56389700	−0.77881200
O	1.46678100	2.51256000	0.69609100
B	0.41940800	2.31468800	−0.22487200
O	−0.15803500	1.19202600	−0.54225600
C	−2.66797100	0.65022500	−1.54884700
H	−2.01453200	1.53213100	−1.55972100
O	−2.26783400	−0.40333200	−1.08333000
11_{re}			
$G_{\text{solv}} = -3609.081715$; $E_{\text{solv}} = -3610.01807364$			
C	−2.04542100	−1.78670900	2.92627600
H	−2.26698500	−1.50205500	3.96181800
C	−1.42225700	−3.21933900	2.93164700
H	−0.45378100	−3.25864700	2.42431500
H	−1.25425000	−3.54328200	3.96417100
C	−2.45533900	−4.13140400	2.24073600
H	−2.21846600	−4.22259400	1.17272600
H	−2.46817700	−5.14262200	2.65942500
C	−3.78584100	−3.39138500	2.40023200
H	−4.17067800	−3.51914800	3.42063800
H	−4.55893000	−3.73620100	1.70577300
C	−3.38414300	−1.93233500	2.16875800
H	−4.13396100	−1.21235400	2.51224100
H	−3.23902100	−1.76908400	1.09304600
C	0.29623400	−0.25108900	3.61336800
H	−0.30457300	−0.08519700	4.51884700
C	1.25231400	−1.42708000	3.88618400
H	0.77539300	−2.23911400	4.44386500
H	1.62037600	−1.83779900	2.93782000
C	2.40647000	−0.77172500	4.64982700
H	2.09708800	−0.56377500	5.68287000
H	3.30143500	−1.40126000	4.69250700
C	2.63154000	0.53909300	3.88621600
H	3.27526500	0.35348500	3.01886800
H	3.12148200	1.30557700	4.49551600
C	1.22881400	0.97424900	3.39947200
H	1.28005400	1.26888300	2.34988800
H	0.85347700	1.83760900	3.96074900
C	−1.83610100	1.10179900	2.28436700
H	−1.03971600	1.84572500	2.16131800
C	−2.62880800	1.45068900	3.57372100
H	−2.86107500	0.56834100	4.17909700
H	−2.03848300	2.11891200	4.21029300
C	−3.92953800	2.13723300	3.08983400
H	−4.76617400	1.42988900	3.14494400
H	−4.19970700	3.00266300	3.70327100
C	−3.66968900	2.50119100	1.62155600
H	−3.09591900	3.43510600	1.55670400
H	−4.59210300	2.63862300	1.04740900
C	−2.81078900	1.34042500	1.11418100

H	-2.26975900	1.56476800	0.19162600
H	-3.44643400	0.46616500	0.93255500
C	0.62258800	-0.41614200	-3.23901200
H	0.90812400	-0.97552100	-4.13796400
C	1.41282000	0.91357800	-3.23950400
H	2.39035400	0.80888100	-3.72194000
H	1.58526600	1.26139300	-2.21891400
C	0.48285800	1.89464100	-3.96109400
H	0.74707400	2.94254600	-3.77941700
H	0.51969400	1.72382900	-5.04582400
C	-0.89678700	1.52557800	-3.40949800
H	-0.99811600	1.93695900	-2.39936000
H	-1.72212200	1.91199700	-4.01695400
C	-0.87990000	-0.01320400	-3.34578900
H	-1.31915500	-0.44773600	-4.25128300
H	-1.46890000	-0.37695800	-2.49479600
C	0.28591300	-3.13475900	-2.48903400
H	-0.73838100	-2.87558500	-2.79031900
C	0.19661600	-4.32503600	-1.48329900
H	0.74092100	-4.13645100	-0.55448000
H	-0.84952900	-4.48853500	-1.20229600
C	0.75573900	-5.55443800	-2.22862700
H	1.81103500	-5.70385700	-1.96855200
H	0.22562600	-6.47691600	-1.97181600
C	0.64463500	-5.19175200	-3.71280300
H	-0.38854800	-5.32871500	-4.05830000
H	1.29270300	-5.79748100	-4.35460600
C	1.00522200	-3.70318600	-3.73280100
H	0.69911300	-3.20374800	-4.65727900
H	2.09305500	-3.59273200	-3.64377400
C	2.76550000	-1.69692100	-1.73130800
H	3.12268300	-1.76533000	-2.76722400
C	3.46202900	-0.48746600	-1.03296400
H	3.96496900	0.13637900	-1.77934600
H	2.75156600	0.15409300	-0.50718100
C	4.47739900	-1.09787700	-0.04232600
H	5.40956400	-0.52601100	0.00854700
H	4.04347400	-1.10931700	0.96475900
C	4.67788100	-2.53897700	-0.51992300
H	5.08187800	-3.19898300	0.25502300
H	5.36560600	-2.56695200	-1.37595400
C	3.26883100	-2.93763300	-0.96479400
H	2.65235900	-3.10683300	-0.07363300
H	3.24162200	-3.84777100	-1.57280500
P	-0.90822500	-0.50072000	2.22475500
P	0.92069500	-1.53265600	-1.78820100
Fe	-0.05831600	-0.95034800	0.17077400
H	0.89242000	-1.91461700	0.81535500
H	-1.22707100	-1.97024000	-0.11020800
H	-0.58522200	-2.41254100	0.29790900
C	0.63027200	4.37299100	0.17434300
C	2.12923800	3.90513000	0.13962100
C	0.30833500	5.55355900	-0.73112700
H	-0.75057100	5.81443200	-0.63665800
H	0.90076600	6.43234300	-0.45324900
H	0.50298500	5.31762300	-1.77974700
C	2.77726700	4.08618800	-1.23568300
H	2.98012700	5.13942100	-1.45564600

H	3.72591800	3.54109400	−1.25213100
H	2.14395500	3.68033200	−2.03031000
C	0.13618500	4.65559600	1.59671300
H	0.57165000	5.57306800	2.00536300
H	−0.95153900	4.77113800	1.57677000
H	0.37693200	3.82756200	2.27159600
C	3.01426300	4.52139300	1.21505900
H	4.03863300	4.15162400	1.10577500
H	3.03570300	5.61325700	1.12705000
H	2.66913000	4.25576500	2.21700000
O	−0.06479500	3.21334000	−0.29845900
O	2.01387400	2.49947700	0.38092300
B	0.72758500	2.09311800	−0.00498000
O	0.32769300	0.85048700	−0.07573500
12_{Fe}			
$G_{\text{solv}} = -4020.719808; E_{\text{solv}} = -4021.84656114$			
C	−1.30993500	−1.97807200	2.95071300
H	−1.56751100	−1.75207400	3.99178400
C	0.02260100	−2.78968800	2.96254900
H	0.78768800	−2.34329200	2.32390500
H	0.42384100	−2.81996000	3.98151900
C	−0.34484100	−4.20757300	2.48704100
H	−0.19277500	−4.28636100	1.40278900
H	0.26764600	−4.98245900	2.95906200
C	−1.83796400	−4.34053000	2.79582300
H	−1.98772600	−4.52567500	3.86788600
H	−2.32397700	−5.15302300	2.24539600
C	−2.38105100	−2.95876600	2.42041000
H	−3.36977400	−2.75190900	2.84204300
H	−2.47344400	−2.89869300	1.32980000
C	−0.27475900	0.64802800	3.34743200
H	−0.69570900	0.38345800	4.33010300
C	1.23710700	0.37123200	3.36324000
H	1.48584600	−0.60470200	3.78979500
H	1.61563500	0.39471100	2.33672900
C	1.83521500	1.53365300	4.17947600
H	2.00141500	1.23076700	5.21941900
H	2.80619000	1.83311200	3.77412700
C	0.79532400	2.68139600	4.11291400
H	1.23017700	3.61528100	3.74063500
H	0.40232400	2.89560700	5.11358700
C	−0.33950100	2.17785700	3.20097300
H	−0.16523800	2.45938200	2.15898600
H	−1.31434200	2.58954800	3.48196300
C	−2.92952800	0.38397400	2.31497700
H	−2.76800100	1.43931500	2.07601600
C	−3.60816600	0.27964300	3.70923300
H	−3.15942900	−0.48226600	4.35422500
H	−3.51033200	1.23209100	4.24224500
C	−5.09269600	−0.05074100	3.42631900
H	−5.26902300	−1.12492700	3.56530200
H	−5.77730100	0.47735800	4.09778700
C	−5.30312500	0.30812700	1.94994100
H	−5.44563200	1.39197500	1.84320900
H	−6.17551800	−0.18745600	1.51007000
C	−3.98039700	−0.10214900	1.29694400
H	−3.81362500	0.35606100	0.31859300
H	−3.95838900	−1.19001500	1.16491900

C	0.82652700	−0.26246400	−3.49399500
H	1.41890200	−0.89390700	−4.17207900
C	1.55998800	1.08057600	−3.36052600
H	2.63208700	0.96037500	−3.17306300
H	1.12556900	1.67306400	−2.55280800
C	1.25977300	1.76307000	−4.69887500
H	1.43653900	2.84357200	−4.66624200
H	1.90680100	1.34438200	−5.48132000
C	−0.21531700	1.41432500	−4.97576200
H	−0.85848400	2.20865800	−4.58943800
H	−0.41626900	1.31177800	−6.04756600
C	−0.49964100	0.10452600	−4.19777300
H	−0.83495600	−0.70419400	−4.85617800
H	−1.28371100	0.28018200	−3.45458400
C	−0.30919900	−2.71360500	−2.66856100
H	−1.25035400	−2.26701000	−3.01410300
C	−0.67509500	−3.87442200	−1.69194500
H	−0.10801100	−3.83801800	−0.75980700
H	−1.73313300	−3.80730100	−1.41666800
C	−0.38586500	−5.18409100	−2.45581900
H	0.59381300	−5.57994200	−2.15986000
H	−1.12617000	−5.96297800	−2.24798800
C	−0.33943000	−4.77407100	−3.93054000
H	−1.35789900	−4.66378100	−4.32584400
H	0.18687400	−5.49680400	−4.56255000
C	0.34773800	−3.40730300	−3.88120100
H	0.22849100	−2.83459500	−4.80603600
H	1.42348800	−3.55073300	−3.71707700
C	2.33072500	−1.86404300	−1.66210100
H	2.74046500	−2.13722900	−2.64234100
C	3.23517800	−0.76488200	−1.02989100
H	3.97227700	−0.41998100	−1.76372300
H	2.66389000	0.10828200	−0.70932300
C	3.92681500	−1.42505700	0.17862800
H	4.94907400	−1.06144600	0.33013300
H	3.35694800	−1.20268400	1.08867300
C	3.85926300	−2.92718600	−0.11247000
H	4.00134700	−3.54611900	0.77995400
H	4.63026600	−3.20966000	−0.84218000
C	2.46517400	−3.08444200	−0.72725100
H	1.72216600	−3.02953700	0.07631800
H	2.32556100	−4.03296400	−1.25727600
P	−1.23095400	−0.32282100	2.08999300
P	0.59901800	−1.25369900	−1.94060900
Fe	−0.43117600	−0.47371700	−0.04406100
H	0.74464400	−1.12149600	0.65196200
H	−1.49138300	−1.61114700	−0.23260300
H	−0.77559100	−1.97498300	0.11656300
C	2.38121800	4.29152800	−0.11013100
C	3.29942900	3.13647100	0.43327300
C	3.00905100	5.14332500	−1.20319000
H	2.30052300	5.91425400	−1.52056800
H	3.91178800	5.64245900	−0.83495200
H	3.26950500	4.54544500	−2.07908200
C	4.26325200	2.59224900	−0.62149800
H	5.05362400	3.31361400	−0.85041300
H	4.72943800	1.67970600	−0.23976100
H	3.73979700	2.34179700	−1.54883300

C	1.81800000	5.18534500	0.99531100
H	2.59922200	5.79412500	1.46036200
H	1.07073200	5.85800000	0.56518400
H	1.32510500	4.59274800	1.77165600
C	4.05732300	3.47637200	1.70714200
H	4.65743500	2.61677700	2.02049800
H	4.73614000	4.31885100	1.53651200
H	3.37885000	3.73488100	2.52261400
O	1.27301400	3.56368500	−0.67237700
O	2.34524000	2.09372500	0.72031600
B	1.22958200	2.33662700	−0.04968500
O	0.21863300	1.45433300	−0.17331800
C	−2.42813700	3.04800900	−2.00962100
C	−2.61105100	3.46566400	−0.50632000
H	−1.61700500	0.39065700	−0.79579700
C	−2.23844600	4.22388100	−2.96156800
H	−2.20525700	3.87285600	−3.99770800
H	−3.07021700	4.93271900	−2.87748100
H	−1.30412500	4.74979300	−2.75293800
C	−1.82095300	4.72696700	−0.14332100
H	−2.26685600	5.62959600	−0.57595900
H	−1.81638500	4.83681400	0.94668900
H	−0.78596600	4.63982600	−0.48077600
C	−3.56467000	2.15179100	−2.52004600
H	−4.50572000	2.70157500	−2.62829000
H	−3.28495800	1.75722800	−3.50214300
H	−3.73402400	1.30175800	−1.85133500
C	−4.06274900	3.62400400	−0.06460600
H	−4.09602700	3.91313900	0.99126900
H	−4.56954700	4.40531900	−0.64267500
H	−4.61870200	2.69015400	−0.17633200
O	−1.23334700	2.27676600	−1.97319200
O	−2.03986300	2.36541900	0.19017100
B	−1.15954800	1.64890900	−0.68982500
1Fe-HBpin			
$G_{\text{solv}} = -3534.999725$; $E_{\text{solv}} = -3535.95692874$			
C	16.00303700	3.74368300	6.95059200
H	16.94480200	4.14085800	7.34874000
C	16.33271400	2.90696600	5.67609600
H	15.74853900	3.21958000	4.80854200
H	17.38835700	3.03452000	5.41461400
C	16.04027900	1.43927000	6.04637300
H	15.01899900	1.17229600	5.74098000
H	16.72079000	0.73714100	5.55422900
C	16.12734000	1.40493200	7.57412000
H	17.17759900	1.40733300	7.89462100
H	15.64449200	0.52716600	8.01610000
C	15.45329100	2.72074400	7.97095100
H	15.65009100	3.01781600	9.00581400
H	14.36734400	2.60886000	7.86435400
C	16.06318300	6.42590300	5.87275900
H	16.90486500	6.54105000	6.56616300
C	16.61279700	5.99272400	4.48995800
H	17.57950100	5.48527100	4.57077400
H	15.91421500	5.30461400	4.00351900
C	16.67441900	7.28600400	3.66784300
H	17.56755000	7.86884400	3.93128300
H	16.70449300	7.09687700	2.58938000

C	15.41366900	8.02538900	4.11880400
H	14.53365500	7.54395800	3.67355400
H	15.39928700	9.08385600	3.83681700
C	15.39353100	7.81339200	5.63899800
H	14.38095100	7.86697300	6.04412400
H	15.98340600	8.59281900	6.13739500
C	14.76856700	5.96507300	8.37558100
H	14.42444700	6.98221800	8.16589900
C	16.03520200	6.07128900	9.24783400
H	16.62369300	5.14557800	9.22941600
H	16.69369300	6.88770500	8.93231100
C	15.46477000	6.27318900	10.65588100
H	16.20468800	6.11232900	11.44724600
H	15.08604800	7.29906000	10.75647500
C	14.30103700	5.27532700	10.70421900
H	13.56962200	5.51256700	11.48366900
H	14.69216800	4.27365300	10.92448400
C	13.68970400	5.31008000	9.28607800
H	12.78290000	5.91981600	9.24844200
H	13.40096200	4.31013400	8.95050000
C	9.94024100	3.42711800	4.16622700
H	9.62211900	2.87718300	3.27312900
C	8.88510500	4.51952100	4.43910100
H	8.46564900	4.92420200	3.51190600
H	9.32706400	5.34635600	4.99865800
C	7.84711300	3.81350300	5.31646500
H	7.17774900	4.51409600	5.82926100
H	7.22455900	3.13844600	4.71326200
C	8.72254200	3.00767500	6.27915000
H	9.13515300	3.68308700	7.03946600
H	8.18117700	2.21111200	6.80006900
C	9.86589900	2.47024100	5.39562500
H	9.65846400	1.44674000	5.06279200
H	10.80569600	2.44207500	5.95820700
C	12.35944000	2.32020200	3.26585100
H	12.29685600	1.70429200	4.17246800
C	13.84191600	2.29436000	2.77703200
H	14.28160100	3.28859200	2.69402000
H	14.45484800	1.74849600	3.50202700
C	13.83216700	1.55325200	1.42817900
H	13.72664700	2.27105600	0.60401200
H	14.75376600	0.98928100	1.25217400
C	12.58351900	0.67199100	1.49307200
H	12.77347300	−0.20303100	2.12933400
H	12.25580900	0.30743200	0.51386400
C	11.55645700	1.59044400	2.16159200
H	10.69931500	1.04258700	2.56522100
H	11.17127300	2.29822200	1.41652700
C	11.56120500	4.99653600	2.30961200
H	10.98022200	4.40483400	1.59217900
C	10.83703900	6.36425500	2.52075800
H	9.90112600	6.37013500	1.95043600
H	10.58472700	6.55731700	3.56349700
C	11.80009000	7.43834200	1.98461200
H	11.27453300	8.29988100	1.55876900
H	12.42989000	7.80749600	2.80413200
C	12.67342700	6.69800200	0.97036300
H	13.60304400	7.22608800	0.73185100

H	12.12192100	6.54880100	0.03213600
C	12.92061000	5.35485700	1.66287800
H	13.68144800	5.49018400	2.44007500
H	13.27269300	4.57607200	0.97863400
P	14.90052200	5.21943900	6.67848000
P	11.69543400	3.97228500	3.85414300
Fe	13.02177600	4.74856300	5.51917500
H	14.02877800	4.61645700	4.40232400
H	12.81599200	6.26518700	5.08990700
H	12.95884800	3.30019400	6.19088500
H	13.54691600	3.25345700	5.56919000
C	10.16253000	7.77477400	6.61210800
C	11.47854600	8.41488400	7.16004100
H	11.94179600	5.08305900	6.66104400
C	9.25281300	8.72428300	5.84395300
H	8.36036000	8.18837700	5.50486300
H	8.92776700	9.55558000	6.47943000
H	9.75506100	9.13095100	4.96317300
C	12.04300300	9.48971500	6.22522600
H	11.42511600	10.39366800	6.22460900
H	13.04666900	9.76612400	6.56221000
H	12.12048200	9.11906200	5.19831100
C	9.36049800	7.04322300	7.69447600
H	8.87980000	7.74045700	8.38869300
H	8.57899200	6.44752000	7.21216800
H	9.99828700	6.36335900	8.26811900
C	11.38572200	8.95989900	8.57930300
H	12.35252400	9.37751700	8.87880100
H	10.63747400	9.75781000	8.64389200
H	11.12367100	8.17537900	9.29291000
O	10.67382500	6.79691900	5.70956800
O	12.37129200	7.30114300	7.15345600
B	11.94854900	6.36725800	6.16663700
Os-1cyp			
$G_{\text{solv}} = -1951.770462$; $E_{\text{solv}} = -1952.55525331$			
C	11.12287100	4.83807100	8.06758500
H	11.14911300	5.16570100	9.11411300
C	11.08483100	3.27973200	8.03492900
H	11.85699200	2.86054600	7.38528100
H	11.25077200	2.88506900	9.04286900
C	9.68110600	2.90289500	7.52017400
H	9.72632200	2.72644900	6.43834600
H	9.29125100	1.99395400	7.98991400
C	8.82240100	4.14083300	7.79178700
H	8.54051500	4.18643500	8.85237000
H	7.90179400	4.16615400	7.19951200
C	9.78028400	5.28512400	7.45183400
H	9.45133700	6.25999500	7.82763500
H	9.87080300	5.35446400	6.36040000
C	13.96548300	5.22378700	8.45568500
H	13.61413200	5.62599900	9.41389400
C	14.30884300	3.73003400	8.65783400
H	13.67856200	3.26065900	9.41918800
H	14.17298000	3.17609000	7.72255500
C	15.79699800	3.73341600	9.02135400
H	15.93436000	4.04533200	10.06555200
H	16.26386100	2.75001500	8.90232800
C	16.36683900	4.79083300	8.07396400

H	16.44040100	4.36538300	7.06502700
H	17.36285400	5.14426100	8.36019400
C	15.31368700	5.91319400	8.08128400
H	15.27380800	6.41827600	7.11148400
H	15.56083800	6.67074600	8.83367600
C	12.42959900	7.40567800	7.45756800
H	13.43538000	7.77503600	7.22181200
C	12.06048500	7.92945200	8.85897000
H	11.22933500	7.35711800	9.29069600
H	12.89871500	7.87872800	9.56129500
C	11.59511600	9.36187800	8.58137800
H	11.04953900	9.80759600	9.41966700
H	12.46517800	9.99840100	8.37358700
C	10.73826200	9.20756500	7.31866400
H	10.62191300	10.14512700	6.76624700
H	9.73247800	8.87349700	7.60290900
C	11.44078800	8.11136300	6.48458300
H	11.99361500	8.53413000	5.64079200
H	10.70814600	7.42226600	6.05729600
C	13.34794400	4.62902700	1.44946100
H	13.87149700	4.07803000	0.65815800
C	13.64573800	6.13189200	1.27045500
H	14.66241200	6.31463000	0.91012400
H	13.53008000	6.65836200	2.22597300
C	12.56356000	6.60458000	0.29567600
H	12.45511800	7.69399400	0.27537200
H	12.80247300	6.27314800	−0.72374100
C	11.31230700	5.88560100	0.80736100
H	10.92179500	6.42161000	1.68201600
H	10.50730500	5.83716700	0.06715100
C	11.81054800	4.48861200	1.23369900
H	11.61111900	3.74336300	0.45622300
H	11.29210200	4.15225200	2.13826700
C	13.43899100	2.12394700	2.80190700
H	12.35830300	2.18133300	2.62200800
C	13.65269900	1.17317100	4.01582500
H	14.38301100	1.56091100	4.72836000
H	12.71564500	1.07042900	4.57018500
C	14.12201200	−0.17341300	3.41752700
H	15.20545000	−0.28413600	3.55095100
H	13.64941900	−1.03449400	3.90021800
C	13.80434700	−0.08296900	1.91954400
H	12.74636100	−0.31590400	1.74048400
H	14.40316200	−0.76828400	1.31052300
C	14.06754000	1.39145400	1.60073200
H	13.64117300	1.70855500	0.64322600
H	15.15091800	1.56212000	1.55617500
C	15.75492600	3.93720900	2.90371600
H	15.99143900	3.54412900	1.90779600
C	16.36522300	5.36656900	3.03369400
H	16.81529500	5.66099200	2.07922700
H	15.61500500	6.11780400	3.29024600
C	17.43796700	5.26686100	4.13295600
H	18.28239700	5.94167400	3.95867000
H	16.99308500	5.53303300	5.09970400
C	17.83623700	3.78913800	4.14756700
H	18.34672300	3.48947400	5.06914100
H	18.50577800	3.56672300	3.30584100

C	16.49177100	3.08044600	3.95893000
H	15.94814800	3.10122200	4.91057800
H	16.58752800	2.03401900	3.64986400
P	12.60923000	5.57071100	7.23531100
P	13.90704600	3.90201900	3.06221300
Os	13.04959400	4.87503800	5.03127600
H	14.60482700	4.87917700	5.51332200
H	13.79300900	6.34616400	4.72355800
H	11.96554300	5.58828200	3.90092900
H	11.69514700	5.89792600	4.75596500
H	11.78111100	3.77587800	5.03979300
H	13.49251600	3.46113200	5.70719400
1Os			
$G_{\text{solv}} = -1950.572520; E_{\text{solv}} = -1951.33787136$			
C	11.09172400	4.89447200	8.02305800
H	11.00289000	5.31308700	9.03378600
C	11.02102500	3.34026100	8.11434400
H	11.83360500	2.86086100	7.56195900
H	11.10323200	3.02369600	9.15922400
C	9.65485000	2.93967100	7.51765000
H	9.78968600	2.63779200	6.47211600
H	9.19370300	2.10081200	8.04913400
C	8.81504500	4.21949000	7.56540900
H	8.42375500	4.38499800	8.57825300
H	7.96390600	4.20108100	6.87660700
C	9.84143000	5.29877700	7.21449600
H	9.50398600	6.31617300	7.43883600
H	10.05752100	5.24035300	6.14006400
C	13.88506700	5.29656500	8.68611600
H	13.44391500	5.77895500	9.56743000
C	14.17832200	3.81602900	9.02595600
H	13.46825300	3.40801400	9.75156000
H	14.12031800	3.20117500	8.12006200
C	15.62458100	3.82451700	9.52967300
H	15.66714700	4.20852300	10.55790100
H	16.08082900	2.82896600	9.52530800
C	16.30358400	4.80462000	8.57078000
H	16.46884400	4.30825500	7.60595300
H	17.27258100	5.16625200	8.93013100
C	15.27619300	5.93696300	8.39312500
H	15.33919600	6.36098400	7.38653800
H	15.46524800	6.74817600	9.10541800
C	12.48974300	7.36990600	7.27399500
H	13.52470200	7.72457800	7.19720800
C	11.85043800	8.07228800	8.48597400
H	10.95628200	7.53926100	8.83157000
H	12.53886500	8.14901400	9.33402000
C	11.43853000	9.43442100	7.91753800
H	10.73069300	9.97111900	8.55774200
H	12.32643500	10.06873100	7.79703100
C	10.85266300	9.07815600	6.54482200
H	10.83765100	9.92758400	5.85518400
H	9.81522600	8.74406800	6.66885900
C	11.72376300	7.90925300	6.02889400
H	12.43983000	8.24637300	5.27144700
H	11.10155600	7.14288800	5.55560900
C	13.22819300	4.74799200	1.69821900
H	13.63616800	4.31842300	0.77541900

C	13.50691300	6.27379700	1.71309400
H	14.40524100	6.53758500	1.14741300
H	13.65993100	6.62593300	2.74262200
C	12.22838100	6.90928200	1.16006300
H	12.14559300	7.97425300	1.40145500
H	12.19569500	6.80954500	0.06698600
C	11.13227000	6.05422900	1.79617500
H	11.02277800	6.32956800	2.85485000
H	10.15192300	6.17387900	1.32397300
C	11.67190900	4.61863400	1.68640100
H	11.34913300	4.16132900	0.74447400
H	11.28741600	3.99420600	2.49815800
C	13.50176000	2.09673600	2.77689900
H	12.40837900	2.16023500	2.73545700
C	13.85605400	1.06565000	3.89081900
H	14.62752800	1.42839200	4.57349100
H	12.97050400	0.87610000	4.50478600
C	14.31476400	−0.20941300	3.14885700
H	15.41105700	−0.25843900	3.13010900
H	13.95897800	−1.12608300	3.62941100
C	13.79444800	−0.04376200	1.71592600
H	12.72804800	−0.30085300	1.66803400
H	14.32162200	−0.67241600	0.99065200
C	13.97760900	1.45525300	1.45906000
H	13.41688400	1.81764600	0.59093400
H	15.04025700	1.65901700	1.27649100
C	15.81533200	3.89887000	2.71937600
H	15.91826100	3.57148100	1.67783100
C	16.46986800	5.30626600	2.86136700
H	16.76043700	5.67921700	1.87301100
H	15.79067600	6.03798800	3.30388700
C	17.70599700	5.10813900	3.76010200
H	18.53382000	5.77166900	3.48969200
H	17.43458000	5.32110800	4.80148800
C	18.04879600	3.62288900	3.62235000
H	18.68911800	3.25064500	4.42907300
H	18.56447200	3.43589600	2.67069300
C	16.66572900	2.96772900	3.61210600
H	16.27069100	2.96470800	4.63555300
H	16.67218400	1.93377000	3.25097000
P	12.67921100	5.52258600	7.29557700
P	14.00481600	3.84852300	3.13005400
Os	13.33008200	4.68565500	5.20967800
H	14.69231400	4.19504000	5.86111400
H	14.54581700	5.85201500	5.18414900
H	11.83566500	3.91344900	4.99267600
H	13.37639300	3.21540000	5.79460400
2Os			
$G_{\text{solv}} = -2139.105703$; $E_{\text{solv}} = -2139.88894656$			
C	−2.07604400	−0.03858800	3.01601700
H	−1.99135900	0.28575900	4.05988900
C	−2.04061100	−1.59902600	2.97745000
H	−1.28662900	−1.98465100	2.28572800
H	−1.79119800	−1.98690800	3.97005200
C	−3.45675400	−2.04381900	2.55752200
H	−3.48792000	−2.21913600	1.47379000
H	−3.76563700	−2.97335400	3.04566000
C	−4.35319000	−0.85138000	2.89997400

H	−4.55894100	−0.82703300	3.97813900
H	−5.31429300	−0.86875900	2.37620400
C	−3.48094300	0.34187500	2.50364900
H	−3.82837500	1.29520100	2.91238000
H	−3.48168500	0.43249300	1.40932200
C	0.74804000	0.53636900	3.24631400
H	0.43239500	0.99043500	4.19317500
C	1.15088800	−0.92770700	3.53390900
H	0.57238400	−1.36173800	4.35536200
H	0.99493800	−1.55165300	2.64738900
C	2.65257100	−0.84719100	3.82516100
H	2.82522500	−0.45217900	4.83522600
H	3.14929100	−1.82074900	3.75713700
C	3.13615100	0.15259500	2.77349600
H	3.16685600	−0.34769700	1.79788300
H	4.13461300	0.55406900	2.97371200
C	2.04961900	1.24224000	2.75642600
H	1.94772200	1.68667500	1.76135400
H	2.30748700	2.05418700	3.44560500
C	−0.95059200	2.59809800	2.26977300
H	−0.00413500	3.01332700	1.90359100
C	−1.17357900	3.12979500	3.70375800
H	−1.82541000	2.46150300	4.28139200
H	−0.23590000	3.23711000	4.25808700
C	−1.89404000	4.46357800	3.48385200
H	−2.37487200	4.84328500	4.39136500
H	−1.17656000	5.22103800	3.14250600
C	−2.88433200	4.13643000	2.36294200
H	−3.27027600	5.02667300	1.85682000
H	−3.74655000	3.60389600	2.78536200
C	−2.09749200	3.21551000	1.41023400
H	−1.65960300	3.78994000	0.58972100
H	−2.73835500	2.46639800	0.94244700
C	0.04510900	−0.33799100	−3.73458800
H	0.43294900	−1.02950100	−4.49352800
C	0.58089700	1.06719700	−4.07813800
H	1.60849600	1.03604300	−4.45177600
H	0.56457300	1.72703600	−3.20642400
C	−0.42178500	1.57504100	−5.11805800
H	−0.35599300	2.65616600	−5.27547800
H	−0.23998200	1.08392100	−6.08373900
C	−1.77202100	1.13626400	−4.54144600
H	−2.08109800	1.84692400	−3.76810500
H	−2.56469000	1.09395700	−5.29541800
C	−1.50067800	−0.23980200	−3.89242100
H	−1.86775600	−1.05983500	−4.51949400
H	−2.01506300	−0.31274200	−2.92823200
C	−0.03156900	−2.79781700	−2.30919900
H	−1.09627700	−2.67310300	−2.55155500
C	0.06096700	−3.70150200	−1.04471800
H	0.80895000	−3.34273400	−0.33536300
H	−0.89344200	−3.69469100	−0.50846600
C	0.42083200	−5.11491500	−1.56096400
H	1.47906100	−5.32402000	−1.36163600
H	−0.16018400	−5.90163600	−1.07003600
C	0.19098200	−5.06414900	−3.07675500
H	−0.87183000	−5.21599300	−3.30646900
H	0.76005200	−5.82354300	−3.62254600

C	0.59675400	−3.63355900	−3.44108600
H	0.25297300	−3.32961700	−4.43484700
H	1.69114600	−3.55407600	−3.42719400
C	2.39660200	−1.12796500	−2.21316600
H	2.62632500	−1.57119800	−3.19020400
C	3.10187300	0.25924800	−2.11768100
H	3.50306100	0.53625700	−3.09762100
H	2.42439500	1.05831000	−1.80919800
C	4.23627500	0.08723300	−1.08723500
H	5.13630300	0.64698700	−1.36032200
H	3.90246600	0.46167800	−0.11286800
C	4.47088000	−1.42379800	−1.00383700
H	4.97800000	−1.73020200	−0.08278200
H	5.08304900	−1.76238500	−1.85038900
C	3.05467600	−1.99412100	−1.11756000
H	2.53514300	−1.85341800	−0.16234100
H	3.03133400	−3.06238800	−1.35961100
P	−0.68375100	0.76902500	2.09209300
P	0.55267700	−1.04443600	−2.09971100
Os	−0.29651400	−0.05471800	−0.10916900
H	0.32444800	−1.34427900	0.64465900
H	1.25361500	0.18808600	0.24373800
H	−1.69497600	−1.08122400	−0.59513900
H	−1.92422800	−0.76740700	0.18174500
C	0.05251700	1.86175200	−0.73727000
O	−1.12732900	1.72851900	−1.16778100
O	0.88110900	2.75270800	−0.73555900
TS _{2,3-Os}			
$G_{\text{solv}} = -2139.090906$; $E_{\text{solv}} = -2139.87210141$			
C	10.89552200	5.17109100	7.73562700
H	10.85475100	5.47734800	8.78718500
C	11.00865800	3.61466100	7.69312700
H	11.87013100	3.26140300	7.12121300
H	11.13015000	3.23102600	8.71126700
C	9.68701500	3.11222000	7.08025500
H	9.80246400	2.98021800	5.99594500
H	9.37287900	2.14910200	7.49473600
C	8.69002300	4.24316300	7.34356400
H	8.35903400	4.22105000	8.39017400
H	7.79905400	4.19053600	6.70979100
C	9.53236200	5.49435800	7.08315600
H	9.08921100	6.41125900	7.48347300
H	9.64715800	5.62851600	6.00007100
C	13.68136500	5.85917000	8.21531500
H	13.30890800	6.27001900	9.16133700
C	14.10801000	4.39263600	8.45941200
H	13.52530200	3.91902600	9.25579600
H	13.97659300	3.79725500	7.54965000
C	15.60602200	4.48166100	8.76890400
H	15.76467200	4.83280200	9.79732000
H	16.11628900	3.51841500	8.66187200
C	16.08494000	5.53697700	7.77053800
H	16.12930400	5.09105600	6.76877700
H	17.07618400	5.94033900	8.00100900
C	14.98572800	6.61165800	7.80585600
H	14.90077900	7.12926700	6.84621300
H	15.21875300	7.37245200	8.55957700
C	11.90516800	7.89247100	7.28796500

H	12.86391700	8.39456900	7.11670000
C	11.42028600	8.28518500	8.70059300
H	10.71199700	7.55045500	9.10334900
H	12.24474300	8.37547100	9.41504900
C	10.68201100	9.60673600	8.46473900
H	10.04272200	9.89452200	9.30594200
H	11.40804000	10.41374800	8.30308200
C	9.90086500	9.33600600	7.17516300
H	9.56477300	10.25060100	6.67707800
H	9.00475400	8.74748100	7.41136300
C	10.86831100	8.51255300	6.30147800
H	11.39068400	9.15391400	5.58697600
H	10.34266600	7.76214200	5.70586000
C	12.89206600	4.91916600	1.16206400
H	13.18999800	4.18454900	0.40244300
C	13.45702500	6.29083700	0.74035800
H	14.45672700	6.21296200	0.30245000
H	13.50712000	6.96491900	1.60112800
C	12.40501200	6.81180100	−0.24264500
H	12.50575200	7.88319300	−0.44270700
H	12.49084800	6.28158600	−1.20103500
C	11.08530000	6.45528900	0.44966600
H	10.86971500	7.20510000	1.21816600
H	10.23442200	6.42812200	−0.23832100
C	11.34451600	5.08786900	1.12202100
H	10.89067400	4.26765700	0.55499900
H	10.90658600	5.06801400	2.12595600
C	12.73801700	2.56376200	2.75405900
H	11.66865900	2.77522900	2.62218400
C	12.89273300	1.71602300	4.05396400
H	13.66236200	2.10397300	4.72316200
H	11.95593400	1.74013000	4.62092200
C	13.22110700	0.28246900	3.58490000
H	14.30277900	0.10912000	3.64536500
H	12.73633800	−0.48181200	4.20007500
C	12.78388800	0.23802900	2.11692800
H	11.69647500	0.10299000	2.04862100
H	13.25612000	−0.57142100	1.55101100
C	13.16731000	1.62906700	1.60427200
H	12.68710300	1.88556100	0.65473400
H	14.25264500	1.66685000	1.44811900
C	15.30316800	4.02285100	2.52385000
H	15.41163000	3.51508300	1.55850300
C	16.11876500	5.35309600	2.47782700
H	16.59974300	5.44820400	1.49826600
H	15.50395700	6.24596200	2.61577900
C	17.17703500	5.23022100	3.58534100
H	18.08844900	5.79176400	3.35740500
H	16.77061700	5.62251700	4.52624100
C	17.40427500	3.72307800	3.71626300
H	17.90524800	3.44068300	4.64799500
H	18.01669100	3.35786800	2.88104300
C	15.98084500	3.16557300	3.62076200
H	15.48393600	3.32158100	4.58452700
H	15.94135800	2.09511100	3.39221200
P	12.31497200	6.10575300	6.98521600
P	13.48604900	4.26499300	2.78718000
Os	12.87237800	5.42749400	4.76473000

H	13.76742500	4.33014700	5.52239800
H	14.32634800	6.17487200	4.43635300
H	11.39014700	4.62554300	4.53515800
H	11.86003800	4.17633500	5.26514700
C	13.41575400	7.49539900	4.48359300
O	12.44231100	7.41859200	3.70146700
O	14.12741400	8.37378200	4.92329100
3Os			
$G_{\text{solv}} = -2139.107002; E_{\text{solv}} = -2139.88964865$			
C	-1.53778700	-0.46988900	3.13067400
H	-1.68699100	-0.04376500	4.12987200
C	-0.76692000	-1.81897500	3.28291800
H	0.15072600	-1.85252100	2.69184200
H	-0.48093200	-1.96029800	4.33060600
C	-1.75115900	-2.91671500	2.83706500
H	-1.60501700	-3.13276300	1.77079800
H	-1.61150800	-3.85319600	3.38649300
C	-3.13376100	-2.29272600	3.03885900
H	-3.40324200	-2.30048500	4.10345100
H	-3.92603400	-2.81090900	2.48879400
C	-2.91878200	-0.85626900	2.55583800
H	-3.70691000	-0.16414800	2.86950600
H	-2.88945700	-0.85615300	1.46030000
C	0.69960000	1.34752700	3.32689200
H	0.19991900	1.56665600	4.27826300
C	1.78971200	0.27211800	3.56676500
H	1.55196700	-0.37681900	4.41488100
H	1.89429400	-0.36643100	2.68150200
C	3.08583500	1.06733800	3.75439300
H	3.13128300	1.49107800	4.76630000
H	3.98134500	0.45438400	3.60808400
C	2.94157500	2.18618100	2.72203900
H	3.12630800	1.78412900	1.71693300
H	3.63612500	3.01785900	2.87363500
C	1.47236600	2.61583500	2.85082800
H	1.09876300	3.03500300	1.91273400
H	1.37231500	3.40562700	3.60356600
C	-1.74180900	2.30425000	2.14269700
H	-1.08025100	3.11057700	1.80457700
C	-2.35613200	2.74222900	3.48641300
H	-2.74454400	1.88174000	4.04634100
H	-1.63429300	3.25786700	4.12817600
C	-3.52712400	3.63119900	3.05667100
H	-4.24009200	3.82196100	3.86544000
H	-3.14661100	4.60087000	2.71036300
C	-4.13809500	2.85450800	1.88394500
H	-4.75673500	3.48175500	1.23468700
H	-4.78417300	2.05790600	2.27485600
C	-2.93155100	2.24242000	1.13831000
H	-2.67513800	2.81510900	0.24319400
H	-3.14720700	1.22699700	0.79859800
C	0.39670700	0.12388700	-3.64798200
H	0.47918200	-0.57670900	-4.48819600
C	1.52447300	1.16258700	-3.80773400
H	2.44735200	0.71505400	-4.19040500
H	1.76531500	1.64612800	-2.85624300
C	0.91490800	2.20049600	-4.75459000
H	1.46845300	3.14467300	-4.75838700

H	0.90718800	1.81061400	−5.78161400
C	−0.51625700	2.34870500	−4.22687000
H	−0.51170300	3.00859700	−3.35314500
H	−1.20165100	2.77614600	−4.96575400
C	−0.93059500	0.92579600	−3.78997600
H	−1.57697900	0.44948800	−4.53554100
H	−1.49057700	0.96180200	−2.84969400
C	−0.83459200	−2.18227900	−2.54844200
H	−1.72401700	−1.56894800	−2.74406000
C	−1.20897100	−3.20470500	−1.43334300
H	−0.45124200	−3.26989100	−0.65031700
H	−2.13273500	−2.88737000	−0.93944500
C	−1.38474000	−4.56405100	−2.14626200
H	−0.48654700	−5.17798400	−2.00480700
H	−2.23139400	−5.13656200	−1.75499200
C	−1.53253400	−4.21794400	−3.63190900
H	−2.56025000	−3.89667400	−3.84629200
H	−1.30142900	−5.05789300	−4.29495300
C	−0.57639600	−3.03505000	−3.80776600
H	−0.75075600	−2.48111400	−4.73542600
H	0.45708000	−3.40409900	−3.82965100
C	2.08333700	−1.76608500	−2.24525300
H	2.20508400	−2.06600300	−3.29304500
C	3.28216800	−0.85192700	−1.84023400
H	3.92365500	−0.67771800	−2.71018200
H	2.96598900	0.13208300	−1.48134700
C	4.04685000	−1.62230000	−0.74846900
H	5.12114700	−1.41336400	−0.76288000
H	3.66639500	−1.33797900	0.24137700
C	3.70610000	−3.08981900	−1.01742000
H	3.92052900	−3.74684300	−0.16827300
H	4.27491300	−3.45936700	−1.88092900
C	2.21378700	−3.02195300	−1.35309000
H	1.65533100	−2.88672700	−0.41975000
H	1.83003700	−3.92251000	−1.84363500
P	−0.63501400	0.81779000	2.14833200
P	0.44543900	−0.90750600	−2.11062100
Os	0.01761200	0.11048600	−0.01358400
H	1.04105600	−0.94168700	0.62333700
H	1.51583000	1.38258800	−0.09749800
H	−1.49568500	−0.34218500	−0.24952500
H	−0.43595400	−1.33552500	0.45523000
C	0.97574400	2.33547400	−0.58476900
O	−0.25198300	2.16832500	−0.81824900
O	1.73780800	3.27048500	−0.75078700
TS _{3,4-Os}			
G _{solv} = −2139.105693; E _{solv} = −2139.88748115			
C	−1.47261000	−0.46409900	3.18548200
H	−1.60992000	−0.01756800	4.17741500
C	−0.73260200	−1.82733100	3.36162600
H	0.17133200	−1.90148200	2.75386400
H	−0.42782500	−1.94623200	4.40672300
C	−1.75148300	−2.91284200	2.96439800
H	−1.62158000	−3.17109400	1.90532100
H	−1.63175200	−3.83282200	3.54534900
C	−3.11502600	−2.24498900	3.15448300
H	−3.37708900	−2.21028700	4.22039300
H	−3.92503200	−2.75874900	2.62666900

C	-2.86394900	-0.83177100	2.62363200
H	-3.63321000	-0.10952700	2.91431500
H	-2.83595900	-0.86818700	1.52820400
C	0.81815900	1.29948700	3.32101900
H	0.33898600	1.55828300	4.27246300
C	1.87588800	0.18851700	3.56364400
H	1.66808000	-0.38842200	4.46967700
H	1.88875100	-0.51571500	2.72378800
C	3.22241500	0.92017100	3.60622500
H	3.37869500	1.38202000	4.58971100
H	4.06900600	0.25349600	3.41180200
C	3.04626700	2.00597800	2.54456300
H	3.10612800	1.55219500	1.54467900
H	3.80034500	2.79770500	2.59089200
C	1.62666600	2.52727900	2.80165900
H	1.20005100	2.99891000	1.91247400
H	1.64941300	3.29967600	3.57849600
C	-1.62185100	2.30252200	2.16344000
H	-0.95557100	3.08130900	1.77504100
C	-2.17078600	2.79001200	3.51999700
H	-2.51501400	1.95000000	4.13696300
H	-1.42205400	3.34056200	4.09882700
C	-3.37796500	3.64579100	3.12333100
H	-4.05027000	3.85258600	3.96254900
H	-3.03394900	4.60844300	2.72359400
C	-4.03318000	2.81890000	2.01174900
H	-4.71626500	3.40496600	1.38915700
H	-4.61952500	2.00754800	2.46278800
C	-2.85156200	2.24105600	1.20628800
H	-2.63876900	2.84133800	0.31842600
H	-3.06293700	1.23159900	0.84587200
C	0.54898300	0.09331300	-3.60590200
H	0.70931100	-0.58979100	-4.44957100
C	1.64761700	1.17265600	-3.67174700
H	2.60818800	0.76628700	-4.00463000
H	1.80949900	1.63596400	-2.69310000
C	1.06468000	2.21414400	-4.63163000
H	1.57825700	3.17868600	-4.56948300
H	1.14808100	1.85349500	-5.66594200
C	-0.40618700	2.29514800	-4.20706200
H	-0.49422400	2.94331300	-3.32941500
H	-1.05194100	2.70412300	-4.99074700
C	-0.79406200	0.85143200	-3.81721200
H	-1.37732400	0.36278700	-4.60570500
H	-1.40765700	0.85623800	-2.91057900
C	-0.71393100	-2.23166700	-2.57209400
H	-1.60123600	-1.62281200	-2.78843300
C	-1.11200800	-3.26595000	-1.47634400
H	-0.38654500	-3.31860000	-0.66227100
H	-2.06226800	-2.96923000	-1.02089800
C	-1.23146400	-4.62438100	-2.20164300
H	-0.32141800	-5.21515100	-2.03832500
H	-2.07337900	-5.22177800	-1.83839700
C	-1.34611100	-4.27122200	-3.68865100
H	-2.37407000	-3.96913800	-3.92812900
H	-1.08076700	-5.10208000	-4.35030500
C	-0.40944600	-3.06816200	-3.83195700
H	-0.57318400	-2.50733700	-4.75754300

H	0.63160500	−3.41616900	−3.83368700
C	2.19429500	−1.79574400	−2.16347900
H	2.37775300	−2.05711800	−3.21272600
C	3.35138500	−0.87481800	−1.66299900
H	4.01102800	−0.61772800	−2.49783200
H	2.98722300	0.07325200	−1.25079800
C	4.10954300	−1.68933700	−0.59664600
H	5.18171300	−1.46970100	−0.58609200
H	3.71447500	−1.45665300	0.40072300
C	3.78983700	−3.14704100	−0.93730200
H	3.98883100	−3.83697600	−0.11092000
H	4.38507200	−3.47472200	−1.79969900
C	2.30681000	−3.07926600	−1.31137200
H	1.72055800	−2.98049200	−0.39058500
H	1.94523500	−3.96510000	−1.84340600
P	−0.55304600	0.78838300	2.17272300
P	0.54268500	−0.95598700	−2.08199400
Os	0.06839200	0.03819300	0.01174900
H	1.06553400	−1.05081800	0.63786700
H	1.58318900	2.07219500	−0.24821500
H	−1.41110500	−0.44676900	−0.22565900
H	−0.34376700	−1.40363700	0.52572600
C	0.71358700	2.67092600	−0.66735500
O	−0.36892800	2.00662400	−0.80764100
O	0.91956600	3.85038500	−0.92719600
4Os			
$G_{\text{solv}} = -2139.112004; E_{\text{solv}} = -2139.89433461$			
C	−1.69072800	−0.37973100	3.14916000
H	−1.75302600	0.05394700	4.15445100
C	−1.18629500	−1.85060000	3.27686800
H	−0.31358400	−2.05291300	2.65173000
H	−0.89406300	−2.05015900	4.31317900
C	−2.37423600	−2.74073000	2.86231500
H	−2.28959300	−2.99390500	1.79788700
H	−2.41043000	−3.68011400	3.42292500
C	−3.60717100	−1.85878000	3.07330800
H	−3.86140700	−1.80739500	4.14040700
H	−4.49128400	−2.21615900	2.53547400
C	−3.12215900	−0.49375700	2.57954100
H	−3.76122600	0.33985400	2.88772400
H	−3.09608900	−0.50673100	1.48263000
C	0.86661900	0.99126500	3.28334300
H	0.46402600	1.35423200	4.23702300
C	1.71599400	−0.27286500	3.55318300
H	1.34809500	−0.84424200	4.41062500
H	1.70137100	−0.93698500	2.68102200
C	3.13874100	0.26178300	3.74488200
H	3.24648700	0.70615400	4.74316000
H	3.90117200	−0.51749300	3.64197100
C	3.23640700	1.34780400	2.67161700
H	3.37994000	0.87743300	1.69034000
H	4.06673100	2.04313500	2.82928600
C	1.86487100	2.04467900	2.71249300
H	1.57987400	2.39955800	1.71815500
H	1.89187800	2.92302000	3.36627800
C	−1.39402700	2.39269400	2.19676400
H	−0.59371400	3.07641700	1.88776300
C	−1.93610700	2.90149700	3.54750100

H	-2.46109100	2.10642400	4.09193900
H	-1.14324500	3.28198700	4.19996300
C	-2.94742800	3.97552900	3.13338700
H	-3.62526600	4.26058100	3.94484700
H	-2.41605400	4.87840400	2.80681900
C	-3.66754000	3.32991200	1.94392300
H	-4.18332600	4.05906800	1.31178200
H	-4.42491200	2.62808700	2.31663000
C	-2.56326000	2.56899400	1.18020100
H	-2.20571700	3.13701000	0.31757800
H	-2.93440200	1.61649300	0.79017200
C	0.33670800	0.02630100	-3.62739700
H	0.51369200	-0.63716500	-4.48269100
C	1.31037000	1.21793600	-3.74792800
H	2.27137000	0.92079200	-4.18009300
H	1.50662400	1.65917700	-2.76721600
C	0.54377900	2.22323800	-4.61346800
H	0.95779400	3.23479600	-4.55333500
H	0.57378100	1.90958500	-5.66591600
C	-0.88568100	2.13319300	-4.06915800
H	-0.95997800	2.72093100	-3.14835300
H	-1.63391800	2.51540700	-4.77097200
C	-1.09094000	0.63825800	-3.74725200
H	-1.64910600	0.12991800	-4.54146800
H	-1.67147300	0.52026900	-2.82397900
C	-0.54458700	-2.45910200	-2.57238500
H	-1.51713500	-1.98809100	-2.76652800
C	-0.75975500	-3.54357100	-1.47247700
H	-0.06575800	-3.44603300	-0.63560500
H	-1.76421600	-3.43736800	-1.04993800
C	-0.60236300	-4.90320600	-2.18378200
H	0.41849300	-5.28247500	-2.04746600
H	-1.28489000	-5.66332100	-1.79125400
C	-0.83272200	-4.59506300	-3.66646100
H	-1.90720800	-4.49576600	-3.86972700
H	-0.43704300	-5.36648800	-4.33510100
C	-0.14351600	-3.23905300	-3.84380400
H	-0.44185500	-2.72428800	-4.76225500
H	0.94228100	-3.39144400	-3.88759000
C	2.27033400	-1.60746200	-2.19918700
H	2.46208800	-1.88294300	-3.24329000
C	3.31546000	-0.53133800	-1.76542800
H	3.90898000	-0.22158400	-2.63150700
H	2.84649500	0.37017600	-1.36011800
C	4.20673200	-1.21380300	-0.70925500
H	5.24318500	-0.86382200	-0.74492800
H	3.82058800	-1.00012100	0.29606000
C	4.05737800	-2.71021800	-0.99271800
H	4.36930000	-3.34182300	-0.15459500
H	4.65522200	-2.99409900	-1.86893000
C	2.56461300	-2.83326200	-1.30670900
H	2.00370500	-2.76329400	-0.36699200
H	2.29088800	-3.77618500	-1.79080900
P	-0.58190700	0.72615100	2.15848000
P	0.51931800	-1.00789700	-2.10317300
Os	-0.05681900	-0.03569900	-0.01692300
H	1.40357600	-0.33188800	0.49405000
H	1.58504300	3.12088400	-0.42630600

H	−1.12256200	−1.20558800	0.21050700
H	0.27951100	−1.47228300	0.59821000
C	0.51311400	3.08355100	−0.70994200
O	0.02092000	1.89776400	−0.75626900
O	−0.08243900	4.12147800	−0.97896400
TS_{4,5-Os}			
$G_{\text{solv}} = -2139.111903; E_{\text{solv}} = -2139.89420676$			
C	−1.59491000	−0.43033800	3.20903600
H	−1.64382200	0.01861400	4.20855900
C	−0.94240000	−1.84187200	3.33679400
H	−0.08928000	−1.97479800	2.66785300
H	−0.57590900	−1.98604200	4.35863200
C	−2.05820700	−2.85316700	3.00791200
H	−2.01016300	−3.12181400	1.94508200
H	−1.96982000	−3.77826200	3.58630100
C	−3.35801500	−2.09055500	3.27467700
H	−3.55562800	−2.03872600	4.35366800
H	−4.23166000	−2.54447500	2.79565500
C	−3.03814300	−0.69775100	2.72733900
H	−3.73746100	0.07708000	3.05708200
H	−3.07346800	−0.73472800	1.63179800
C	0.79281500	1.22454800	3.20376000
H	0.38825300	1.60649700	4.14864100
C	1.75915500	0.05147800	3.50641700
H	1.51201800	−0.45594000	4.44376900
H	1.71724400	−0.69638100	2.70659900
C	3.15378500	0.68698800	3.50835100
H	3.33254800	1.21492700	4.45430500
H	3.95346400	−0.04998600	3.38042000
C	3.06350000	1.69082500	2.35803900
H	3.10660900	1.15415500	1.40083900
H	3.86757700	2.43372200	2.36043700
C	1.67399600	2.32274500	2.53382900
H	1.27240500	2.66622700	1.57674700
H	1.73092800	3.20002400	3.18776800
C	−1.65903800	2.32779900	2.18397300
H	−0.95641700	3.09203800	1.82854900
C	−2.20799100	2.80774800	3.54181900
H	−2.62908300	1.97505600	4.11930300
H	−1.43964400	3.28496900	4.15915700
C	−3.33819300	3.76040300	3.13864200
H	−4.01569100	3.99541000	3.96630400
H	−2.91341200	4.70427200	2.77395600
C	−4.02585500	3.01498400	1.98840400
H	−4.62546200	3.67469100	1.35390600
H	−4.70366400	2.25666000	2.40130400
C	−2.87621100	2.33873600	1.21019500
H	−2.60947400	2.90354500	0.31327500
H	−3.15899900	1.33630300	0.87609000
C	0.47743400	0.10837800	−3.62252700
H	0.69753300	−0.54995200	−4.47290000
C	1.53564400	1.22885100	−3.61308500
H	2.53030900	0.86205700	−3.88605400
H	1.60345400	1.68344900	−2.61998000
C	0.97456900	2.24669400	−4.61106500
H	1.44540100	3.23143900	−4.52395200
H	1.13934000	1.88909700	−5.63641600
C	−0.52489700	2.27372900	−4.28870300

H	-0.70849600	2.94829400	-3.44629900
H	-1.13014200	2.62830700	-5.12894100
C	-0.87884700	0.82529100	-3.87856200
H	-1.43706400	0.30511400	-4.66462600
H	-1.51125800	0.82979500	-2.98360000
C	-0.77093500	-2.26387800	-2.67636100
H	-1.67006600	-1.67702900	-2.90463500
C	-1.16652700	-3.33672600	-1.61620200
H	-0.50327500	-3.34184900	-0.74935500
H	-2.16833500	-3.11686900	-1.23281200
C	-1.14019800	-4.69027300	-2.35578500
H	-0.18275300	-5.19625300	-2.17697000
H	-1.93147100	-5.36743100	-2.01953200
C	-1.25055200	-4.32638000	-3.83986500
H	-2.29287700	-4.09495200	-4.09577000
H	-0.91355300	-5.12631300	-4.50715000
C	-0.39735200	-3.05884500	-3.94609200
H	-0.58426900	-2.49207900	-4.86367200
H	0.66416300	-3.33760900	-3.93963800
C	2.10105800	-1.76922400	-2.13235800
H	2.31048400	-2.05690800	-3.16970900
C	3.23993000	-0.82265000	-1.63612900
H	3.91648000	-0.59270300	-2.46570700
H	2.86070400	0.13227000	-1.25964000
C	3.98025300	-1.59958800	-0.53068000
H	5.04946800	-1.36744200	-0.49888200
H	3.55708700	-1.34372900	0.44958500
C	3.68420400	-3.06962400	-0.83692100
H	3.87263500	-3.73438100	0.01232600
H	4.30109500	-3.41463600	-1.67727100
C	2.20893600	-3.02786600	-1.24324200
H	1.60179800	-2.90869200	-0.33837500
H	1.86728300	-3.93126900	-1.75887600
P	-0.66033900	0.76721700	2.14544100
P	0.43107900	-0.96351200	-2.11512500
Os	-0.13184600	0.02321400	-0.03306300
H	1.24074000	-0.51273500	0.53163100
H	1.11629200	3.55255900	-0.58123600
H	-1.34434500	-0.99674700	0.09424200
H	-0.00610300	-1.45953500	0.56620500
C	0.07603000	3.21692100	-0.76906200
O	-0.05638700	1.93898700	-0.80068200
O	-0.80632600	4.04579500	-0.96327900
5Os			
$G_{\text{solv}} = -2139.116007; E_{\text{solv}} = -2139.89726613$			
C	-1.06580500	-0.50090000	3.32279600
H	-1.20619600	-0.01330500	4.29481800
C	-0.06500700	-1.68457100	3.50643300
H	0.78640300	-1.62658200	2.82415600
H	0.33625900	-1.67161000	4.52542800
C	-0.88131200	-2.96764200	3.25952400
H	-0.78770100	-3.26755400	2.20786800
H	-0.54068500	-3.80680200	3.87437900
C	-2.32918800	-2.55761700	3.53752500
H	-2.50747800	-2.49957400	4.61965900
H	-3.06338600	-3.25053300	3.11382400
C	-2.40074400	-1.16211400	2.91291200
H	-3.26926000	-0.58018100	3.23754700

H	−2.45522200	−1.26662400	1.82258000
C	0.89519800	1.62214600	3.10646800
H	0.51507500	1.81497800	4.11783800
C	2.18152500	0.77525400	3.22471100
H	2.13323200	0.04928500	4.04138300
H	2.35780100	0.21478400	2.29563700
C	3.28907600	1.81618700	3.40450300
H	3.26310000	2.21579900	4.42691900
H	4.29034000	1.40817800	3.23143100
C	2.89782300	2.90246300	2.39968300
H	3.20628700	2.59278300	1.39296900
H	3.37012400	3.86861800	2.60262300
C	1.35735000	2.96946500	2.47057000
H	0.94061800	3.12108200	1.47191900
H	1.02265300	3.80705500	3.09142200
C	−1.78097000	2.12365100	2.18180800
H	−1.30248200	2.96582400	1.66721000
C	−2.25402400	2.62588600	3.56033800
H	−2.41123400	1.79121900	4.25602100
H	−1.53785200	3.31293200	4.02351100
C	−3.60410400	3.27818500	3.24672300
H	−4.21200700	3.45705700	4.13997400
H	−3.44137100	4.24469600	2.75262100
C	−4.24494700	2.28801600	2.26692300
H	−5.04977700	2.73536900	1.67557100
H	−4.68230200	1.45371300	2.83112200
C	−3.07901800	1.78476600	1.38892900
H	−3.04326200	2.29234600	0.42200600
H	−3.17732900	0.71897000	1.17180900
C	1.02168100	0.08619400	−3.53052900
H	1.24525400	−0.59105800	−4.36626200
C	2.24491300	0.99605300	−3.32145700
H	3.19188200	0.45092200	−3.38613800
H	2.19266500	1.48000600	−2.33961600
C	2.08320400	2.04291400	−4.42853500
H	2.69917000	2.93341700	−4.26533400
H	2.38178000	1.60781700	−5.39142600
C	0.57750800	2.35089300	−4.42671500
H	0.36256800	3.16045700	−3.72080300
H	0.21964000	2.68121700	−5.40677300
C	−0.11785200	1.04852500	−3.95621300
H	−0.72281600	0.59845800	−4.75031900
H	−0.79452800	1.26336600	−3.12170000
C	−0.87504900	−1.90432100	−2.79825400
H	−1.57750500	−1.09939800	−3.04781900
C	−1.61090000	−2.88344000	−1.83439200
H	−1.02705200	−3.12003600	−0.94297900
H	−2.53618000	−2.41897000	−1.47896800
C	−1.90150800	−4.15142600	−2.66548100
H	−1.14111100	−4.91553100	−2.45939700
H	−2.87504000	−4.59314000	−2.43161500
C	−1.78192800	−3.70209400	−4.12577100
H	−2.69680200	−3.18178100	−4.43795800
H	−1.61737600	−4.53238900	−4.82022200
C	−0.61314700	−2.71336100	−4.08546200
H	−0.55726300	−2.07651300	−4.97411200
H	0.32999900	−3.27109100	−4.01746300
C	1.97706900	−2.18027500	−2.02473500

H	2.22030700	−2.45547100	−3.05802000
C	3.24778200	−1.56716900	−1.35539400
H	4.04049400	−1.44819600	−2.10117400
H	3.06210800	−0.57315200	−0.93193600
C	3.67373500	−2.56720700	−0.26245700
H	4.75959400	−2.60670300	−0.13018900
H	3.23316100	−2.27648800	0.69991300
C	3.06640700	−3.89919900	−0.71023200
H	3.00681500	−4.63813600	0.09560900
H	3.66242400	−4.33547800	−1.52281800
C	1.69090000	−3.47307800	−1.23007500
H	1.04542000	−3.25905000	−0.37053600
H	1.19398200	−4.23457800	−1.83992700
P	−0.47608500	0.81082600	2.15336200
P	0.56557900	−0.97776500	−2.08654400
Os	0.10285200	0.03796700	−0.00316000
H	0.86153900	−1.19974400	0.66892800
H	0.38219600	3.91637600	−1.19583600
H	−1.42281300	−0.19085700	−0.31070400
H	−0.57425600	−1.34619800	0.41209300
C	−0.24798300	3.01457100	−1.06216600
O	0.42996200	1.99226400	−0.68455100
O	−1.45512500	3.07179600	−1.28179700
6Os			
$G_{\text{solv}} = -2550.734533; E_{\text{solv}} = -2551.70098720$			
C	−1.12590900	−1.01615800	3.38801800
H	−1.38886100	−0.56172200	4.35087400
C	0.23081600	−1.77138500	3.55109900
H	0.99593200	−1.41879000	2.85358700
H	0.62057900	−1.61522300	4.56272600
C	−0.08811100	−3.25970400	3.32427900
H	0.04210600	−3.50810900	2.26281600
H	0.56349300	−3.92263400	3.90296900
C	−1.56811900	−3.38564600	3.69240400
H	−1.68988500	−3.37667500	4.78373500
H	−2.03296700	−4.30068100	3.31036400
C	−2.16559100	−2.11691400	3.07818300
H	−3.15961000	−1.86638600	3.46229900
H	−2.25777500	−2.26943200	1.99748300
C	−0.25292100	1.69408900	3.18915800
H	−0.90495000	1.83543500	4.06242900
C	1.16354900	1.37867200	3.70701000
H	1.13340200	0.74649700	4.59947100
H	1.73847500	0.84696800	2.94425800
C	1.81459900	2.75757900	3.98460700
H	2.01708900	2.90441400	5.05061400
H	2.77365200	2.82388500	3.46218500
C	0.82671200	3.81774700	3.44931600
H	1.33197000	4.65989000	2.96383600
H	0.23224200	4.23039300	4.27413600
C	−0.09284800	3.05189300	2.49032900
H	0.40083700	2.91069700	1.52377200
H	−1.04712400	3.56089000	2.31794100
C	−2.78896400	1.06454500	2.09585700
H	−2.64912900	1.99171100	1.52911100
C	−3.46035200	1.41555200	3.44011400
H	−3.29662800	0.62713700	4.18740500
H	−3.08801400	2.35440300	3.86228200

C	-4.94926300	1.47745200	3.08673300
H	-5.60144000	1.45127500	3.96617800
H	-5.15877900	2.40666200	2.54113600
C	-5.13357000	0.27232900	2.15958700
H	-6.03639200	0.34087400	1.54428800
H	-5.22182000	-0.63987900	2.76445600
C	-3.84409000	0.22514100	1.31360700
H	-3.99104500	0.67903300	0.32929700
H	-3.52842200	-0.80441500	1.13611500
C	-0.13627200	-0.40845800	-3.64351500
H	-0.16575400	-1.12146600	-4.47834600
C	1.11929700	0.46248400	-3.80299900
H	1.99849700	-0.11306500	-4.11028800
H	1.35208400	0.95212000	-2.85415100
C	0.68941900	1.50274700	-4.84029100
H	1.36102000	2.36799400	-4.88417800
H	0.67344400	1.04737800	-5.83967300
C	-0.73250900	1.87533400	-4.39977700
H	-0.68467200	2.66031300	-3.63676600
H	-1.34192800	2.26315200	-5.22207900
C	-1.32455300	0.58376100	-3.78497900
H	-2.10546400	0.15429300	-4.42179300
H	-1.78611200	0.80237200	-2.81595400
C	-1.83396000	-2.29503900	-2.39892000
H	-2.54614900	-1.46662600	-2.50057100
C	-2.37320700	-3.22161800	-1.26758800
H	-1.59590200	-3.53460800	-0.56823200
H	-3.11988000	-2.68073800	-0.67768200
C	-2.99425600	-4.44393600	-1.98130400
H	-2.30162300	-5.29386900	-1.93702100
H	-3.93219900	-4.76778500	-1.51950500
C	-3.16549600	-4.00843800	-3.44091800
H	-4.07267800	-3.39997000	-3.55180800
H	-3.24277000	-4.85112000	-4.13569800
C	-1.92953600	-3.13898900	-3.68535100
H	-2.01015900	-2.52370200	-4.58714400
H	-1.05058700	-3.78661600	-3.80093100
C	1.08022200	-2.69902300	-2.34223000
H	0.96650700	-3.06171200	-3.37024200
C	2.52742400	-2.15257700	-2.15597800
H	3.10391200	-2.33476000	-3.07076400
H	2.56490200	-1.07909500	-1.96693500
C	3.12623800	-2.95598200	-0.99173200
H	4.21753300	-3.02861800	-1.04729200
H	2.87085900	-2.47495800	-0.03778600
C	2.41660300	-4.30826500	-1.08221000
H	2.51227800	-4.91262200	-0.17375800
H	2.82287100	-4.89157600	-1.91932800
C	0.96808700	-3.89763000	-1.36671400
H	0.51397100	-3.57736300	-0.42266700
H	0.35239100	-4.70687900	-1.77327000
P	-1.06119300	0.38124600	2.15857900
P	-0.22590700	-1.40528100	-2.08418700
Os	-0.31513200	-0.30493700	0.00296000
H	0.24334900	-1.66167100	0.66295200
H	-0.43690500	3.59153800	-1.20308100
H	-1.85273800	-0.22115000	-0.36339000
H	-1.21667800	-1.54451900	0.37947400

C	−0.90060600	2.62537800	−0.91409600
O	−0.04152800	1.67894000	−0.80117500
O	−2.11776400	2.56854700	−0.75409100
C	3.69810700	2.24029400	−1.10501700
C	3.66898900	2.63073000	0.41973200
H	1.64096200	−0.11224500	0.29976400
C	5.08996000	2.07711800	−1.69548100
H	5.00847600	1.78063900	−2.74522100
H	5.63728200	3.02453200	−1.65255300
H	5.66902400	1.31355700	−1.17233800
C	4.89620300	2.15345000	1.19388200
H	5.79124500	2.71534900	0.91106000
H	4.72194400	2.30306600	2.26309800
H	5.08410500	1.08823100	1.02909000
C	2.85586400	3.16031700	−1.98634700
H	3.27821200	4.16842100	−2.02511700
H	2.83731200	2.76118200	−3.00373200
H	1.82491400	3.21295200	−1.62768400
C	3.40982000	4.10449700	0.69067800
H	3.41415300	4.28824100	1.76850000
H	4.19425200	4.72145300	0.23999100
H	2.44274400	4.42077100	0.29447200
O	3.04639700	0.94189200	−1.10183400
O	2.54384500	1.86583900	0.92305900
B	2.29076400	0.88060800	0.02588300
TS _{6,7-Os}			
$G_{\text{solv}} = -2550.731561$; $E_{\text{solv}} = -2551.69934453$			
C	−0.66524900	−0.45519600	3.23083000
H	−0.94197300	−0.00437600	4.19132300
C	0.68459400	−1.21833700	3.41408900
H	1.46162900	−0.87127500	2.72695800
H	1.06091500	−1.06306000	4.43089900
C	0.35968700	−2.70521400	3.18519800
H	0.50960700	−2.95807000	2.12758700
H	0.99530000	−3.37065300	3.77850800
C	−1.12805800	−2.82115100	3.52445600
H	−1.27096700	−2.81206100	4.61321000
H	−1.59123800	−3.73304200	3.13300200
C	−1.70612600	−1.54824300	2.90008900
H	−2.70515000	−1.29212300	3.26736600
H	−1.77993000	−1.69866400	1.81775300
C	0.26328200	2.23367700	3.06720000
H	−0.35440500	2.32281800	3.97204900
C	1.70679300	1.92205800	3.50732500
H	1.72832200	1.24699400	4.36789900
H	2.25542200	1.43941800	2.69359600
C	2.34489000	3.29820700	3.82489800
H	2.57421600	3.40172900	4.89065400
H	3.28753800	3.40395700	3.28045500
C	1.32765100	4.36621500	3.36472100
H	1.80754400	5.22159600	2.87647300
H	0.77097500	4.75569400	4.22629600
C	0.36886900	3.62444400	2.42566400
H	0.81929100	3.53668100	1.43383600
H	−0.59927600	4.12522000	2.32217700
C	−2.27801100	1.66945100	1.94631400
H	−2.11806900	2.59194200	1.37731500
C	−2.93779700	2.03853000	3.29149200

H	-2.78385700	1.25086200	4.04162900
H	-2.54552800	2.97212500	3.70752100
C	-4.42716100	2.12177000	2.94542900
H	-5.07515700	2.11065800	3.82817600
H	-4.62584400	3.05052800	2.39495500
C	-4.63344000	0.91319000	2.02740000
H	-5.54041400	0.98756300	1.41896300
H	-4.72662800	0.00611300	2.63912800
C	-3.35121200	0.84558900	1.17166000
H	-3.50411700	1.29922300	0.18787500
H	-3.05164000	-0.18824100	0.99137600
C	0.35638700	0.15484600	-3.78617000
H	0.25974600	-0.56016100	-4.61364600
C	1.62693800	0.98446300	-4.03180200
H	2.46107900	0.37593200	-4.39700400
H	1.94737800	1.46871200	-3.10685600
C	1.16113200	2.03790500	-5.03999500
H	1.85840000	2.87854400	-5.13479100
H	1.05433900	1.58392500	-6.03450000
C	-0.20950800	2.45987900	-4.49578700
H	-0.07449200	3.22268200	-3.72020800
H	-0.85729100	2.89322200	-5.26430100
C	-0.81096900	1.17925700	-3.86888900
H	-1.62627900	0.77708400	-4.48005800
H	-1.22886000	1.39901400	-2.88059400
C	-1.27781000	-1.77361800	-2.53140500
H	-2.01131100	-0.96130700	-2.60960600
C	-1.77205300	-2.73191400	-1.40386000
H	-0.99104200	-2.98504100	-0.68527200
H	-2.56850600	-2.24208000	-0.83445200
C	-2.29621000	-3.99507200	-2.11980300
H	-1.52768700	-4.77849700	-2.10605600
H	-3.18934600	-4.40910500	-1.64118100
C	-2.53883600	-3.55257200	-3.56576400
H	-3.48678000	-3.00327100	-3.63957700
H	-2.58133000	-4.38769100	-4.27258500
C	-1.36875700	-2.60148800	-3.83052600
H	-1.51994100	-1.97641600	-4.71616200
H	-0.45629900	-3.19045100	-3.99097200
C	1.65138600	-2.10114100	-2.48999300
H	1.54440900	-2.46790400	-3.51732700
C	3.08419900	-1.51552200	-2.30785700
H	3.66070500	-1.67849000	-3.22625300
H	3.09436400	-0.44277800	-2.11155600
C	3.70970800	-2.30647000	-1.14907700
H	4.80213400	-2.35200300	-1.21159700
H	3.44896000	-1.83177000	-0.19342300
C	3.03372900	-3.67601500	-1.23687700
H	3.14933700	-4.27878700	-0.32967000
H	3.44937100	-4.24839000	-2.07695900
C	1.57407500	-3.30103600	-1.51274000
H	1.11898500	-2.99011600	-0.56595700
H	0.97498600	-4.12517700	-1.91408400
P	-0.56592600	0.95062300	2.01328300
P	0.31150400	-0.84490900	-2.22537100
Os	0.19299500	0.25790700	-0.13609600
H	0.69942200	-1.10550300	0.53974600
H	0.42298100	4.20109700	-1.21018900

H	-1.34088000	0.38070500	-0.53860200
H	-0.76868800	-0.94770300	0.20851400
C	-0.12735700	3.26756000	-0.98570700
O	0.63688300	2.22670400	-0.94095400
O	-1.34067200	3.29769300	-0.82908600
C	4.13878000	2.84054400	-1.32555200
C	4.10483200	3.24649800	0.19400200
H	2.06626400	0.57738500	0.15531700
C	5.52434900	2.53882400	-1.87829400
H	5.44115000	2.24679100	-2.92943500
H	6.16479200	3.42541000	-1.82229700
H	6.00778100	1.72199700	-1.33875000
C	5.24658400	2.62840400	1.00131600
H	6.21075100	3.07579700	0.74175300
H	5.06572800	2.80089900	2.06573700
H	5.30687300	1.54769800	0.84118700
C	3.42456300	3.83398600	-2.24062200
H	3.97571800	4.77661800	-2.30855500
H	3.35289900	3.40709600	-3.24469400
H	2.41113400	4.04346900	-1.89375600
C	4.02298700	4.74289500	0.45501600
H	4.00389900	4.92766800	1.53319300
H	4.89631500	5.25689800	0.03959300
H	3.12029800	5.17853700	0.02135800
O	3.37813300	1.61247500	-1.32374700
O	2.88353200	2.63127500	0.66177800
B	2.54818000	1.64751900	-0.23358600
7Os			
$G_{\text{solv}} = -2550.743580$; $E_{\text{solv}} = -2551.71326484$			
C	-1.33861400	-1.09944900	3.31994200
H	-1.59626100	-0.69170600	4.30399700
C	-0.04366300	-1.95941400	3.46768500
H	0.77977600	-1.59862300	2.84531100
H	0.29942100	-1.92735200	4.50800300
C	-0.45033000	-3.39185500	3.08309000
H	-0.30604400	-3.53931100	2.00461900
H	0.14060000	-4.15216200	3.60397900
C	-1.94489600	-3.45443800	3.40523100
H	-2.09513600	-3.54523700	4.48917500
H	-2.45610600	-4.29526900	2.92457400
C	-2.44719300	-2.09585800	2.90755000
H	-3.42489500	-1.81362900	3.31188500
H	-2.54273900	-2.14153800	1.81795900
C	-0.17818200	1.50970000	3.31521800
H	-0.66384900	1.45385000	4.30016100
C	1.30938300	1.17730500	3.49450800
H	1.47638900	0.29672100	4.12231500
H	1.76262900	0.99249100	2.51580100
C	1.88166600	2.45703600	4.11809400
H	1.70658000	2.44443900	5.20124400
H	2.96384800	2.54729600	3.97024600
C	1.09667400	3.61507700	3.46519700
H	1.68603500	4.08718800	2.67488200
H	0.84983400	4.38980300	4.19860500
C	-0.17482600	2.98121100	2.85259400
H	-0.11289600	3.03107600	1.76265700
H	-1.08932200	3.50231600	3.15245600
C	-2.77704900	1.22743100	2.20744500

H	-2.55169500	2.19463500	1.74099200
C	-3.41116100	1.50948100	3.58446300
H	-3.36910000	0.62076000	4.22803600
H	-2.91718700	2.32813800	4.11757500
C	-4.87149100	1.81120700	3.23872300
H	-5.53464700	1.78463700	4.10965900
H	-4.94497700	2.81146100	2.79257800
C	-5.20400500	0.74025000	2.19369100
H	-6.06655300	1.00354200	1.57357600
H	-5.44793400	-0.19953200	2.70549300
C	-3.91024900	0.56977700	1.36551400
H	-3.98082200	1.07270200	0.39712900
H	-3.71972500	-0.48298700	1.15080800
C	-0.25977100	-0.48443100	-3.65473900
H	-0.50425100	-1.23761300	-4.41236600
C	1.02846700	0.21997500	-4.12142000
H	1.72960100	-0.47795700	-4.59256000
H	1.53840400	0.70043400	-3.28398800
C	0.50757200	1.29612300	-5.07852100
H	1.25708200	2.06226600	-5.30678200
H	0.19321000	0.84418800	-6.02933400
C	-0.70720500	1.85159600	-4.32810800
H	-0.36117800	2.54416100	-3.55067400
H	-1.40023100	2.40359700	-4.97107400
C	-1.36302000	0.61535500	-3.67440700
H	-2.22350500	0.27309400	-4.26006200
H	-1.73444900	0.85167500	-2.67207600
C	-1.67879500	-2.50819000	-2.29907000
H	-2.48357900	-1.77449900	-2.43981300
C	-2.09861800	-3.43579200	-1.11524800
H	-1.31959900	-3.54571300	-0.35918200
H	-2.96473800	-3.00268700	-0.60460900
C	-2.45380100	-4.79912300	-1.74329900
H	-1.59752500	-5.48123400	-1.66669300
H	-3.29908700	-5.28318500	-1.24402300
C	-2.72205700	-4.48898900	-3.21787300
H	-3.72626200	-4.06142300	-3.33795300
H	-2.65544400	-5.36962600	-3.86510300
C	-1.66622000	-3.42843900	-3.54052900
H	-1.88245000	-2.89021500	-4.46814400
H	-0.69072000	-3.91672800	-3.66071600
C	1.27722300	-2.52290400	-2.24855800
H	1.24639800	-2.90559300	-3.27549300
C	2.63596100	-1.79381700	-2.01454300
H	3.25617100	-1.88589900	-2.91404900
H	2.52535300	-0.72734400	-1.81147100
C	3.29974400	-2.52566100	-0.83758600
H	4.39326400	-2.46731900	-0.86788900
H	2.96633800	-2.07985900	0.10924700
C	2.76072800	-3.95356700	-0.94210200
H	2.90507500	-4.54251000	-0.02989700
H	3.25406600	-4.48414300	-1.76746900
C	1.28174400	-3.71865600	-1.26347100
H	0.77228900	-3.44596700	-0.33266700
H	0.77427900	-4.59793800	-1.67373200
P	-1.12750800	0.37063000	2.19779500
P	-0.19013200	-1.40573100	-2.04243900
Os	-0.39352800	-0.26125400	0.02576500

H	0.27873900	−1.53979400	0.69214400
H	0.06689400	3.83035900	−0.76492500
H	−1.96223800	−0.28630400	−0.34048700
H	−1.25178100	−1.53832700	0.38408700
C	−0.62647600	2.97778100	−0.78245700
O	−0.00982200	1.80411100	−0.75691400
O	−1.82676400	3.09514000	−0.83560300
C	3.37655200	2.41670300	−1.33154600
C	3.35388100	2.66692100	0.21497500
H	1.34181000	0.34384300	0.17862400
C	4.67354400	1.82115000	−1.86623200
H	4.59480100	1.67900400	−2.94888700
H	5.52187200	2.48689800	−1.67235500
H	4.88028700	0.84775800	−1.41592000
C	4.14023000	1.60270200	0.98752500
H	5.21838700	1.70539000	0.82956100
H	3.94138700	1.71836300	2.05635700
H	3.84204300	0.59134400	0.69375500
C	3.00646700	3.66086200	−2.14416200
H	3.80889700	4.40568700	−2.13875500
H	2.82083900	3.36381500	−3.18073700
H	2.09670300	4.13362100	−1.76302900
C	3.80902400	4.05567800	0.64027900
H	3.81973500	4.12948900	1.73205500
H	4.82502800	4.25497600	0.28204100
H	3.14395600	4.83148300	0.25338900
O	2.33605300	1.45227800	−1.48836100
O	1.96255200	2.51455900	0.51970300
B	1.44150400	1.55535400	−0.39037200
TS _{7,8-Os}			
$G_{\text{solv}} = -2550.727641$; $E_{\text{solv}} = -2551.69064369$			
C	−2.01358900	−0.99618700	3.18106900
H	−2.25048000	−0.51246300	4.13666800
C	−1.14178200	−2.25556200	3.47553500
H	−0.23509000	−2.28605900	2.86439200
H	−0.82269500	−2.24925300	4.52348800
C	−2.04310900	−3.47162500	3.17798100
H	−1.84418500	−3.83581200	2.16279600
H	−1.86709600	−4.30416100	3.86669500
C	−3.47127600	−2.92335200	3.24556900
H	−3.79071500	−2.82080000	4.29126000
H	−4.20107100	−3.56071100	2.73527000
C	−3.33222100	−1.54242300	2.59805600
H	−4.18090700	−0.88039700	2.80029600
H	−3.25265800	−1.66412500	1.51213600
C	0.05806700	0.92560900	3.45868400
H	−0.47010200	0.89255900	4.42310100
C	1.36262200	0.12145900	3.57666300
H	1.22544800	−0.85852800	4.04249800
H	1.76645400	−0.04444200	2.57095600
C	2.29698200	1.03348000	4.39253300
H	2.21737400	0.79619800	5.45920200
H	3.34622300	0.88687100	4.11358100
C	1.80935100	2.48161500	4.12795500
H	2.58197400	3.09774500	3.65478100
H	1.54834100	2.97422000	5.07084200
C	0.56797500	2.35394200	3.22048400
H	0.85698500	2.46931200	2.17164600

H	-0.18651000	3.11567400	3.44472900
C	-2.33421600	1.68695800	2.03072700
H	-1.70793300	2.54245400	1.74482800
C	-3.13505300	2.11026100	3.27107300
H	-3.61193000	1.24224500	3.74370300
H	-2.51592400	2.60482200	4.02727000
C	-4.20963900	3.02181800	2.67011300
H	-5.04065400	3.21608900	3.35596100
H	-3.76280700	3.98869700	2.40677100
C	-4.64811500	2.27783000	1.39695200
H	-5.02496000	2.96010000	0.62997300
H	-5.45861700	1.57979400	1.63742600
C	-3.39840400	1.49426000	0.91825200
H	-3.02596600	1.87508400	-0.03834900
H	-3.63999900	0.43844800	0.76867700
C	-0.63475500	-0.78378500	-3.53302200
H	-0.60223600	-1.53382000	-4.33205600
C	0.20985700	0.42819100	-3.97110400
H	1.06699700	0.13142400	-4.58498000
H	0.60403200	0.96627800	-3.10605600
C	-0.78419900	1.32451500	-4.71524700
H	-0.42285200	2.35257400	-4.82330700
H	-0.97802800	0.92681100	-5.72100100
C	-2.04442400	1.22786400	-3.85080200
H	-1.92910900	1.88375800	-2.98153900
H	-2.95453200	1.53340400	-4.37707500
C	-2.09335000	-0.24640500	-3.39827600
H	-2.76665100	-0.83287700	-4.03328500
H	-2.48016100	-0.33169700	-2.37412400
C	-1.10590800	-3.16408600	-2.08291900
H	-2.12464300	-2.75781300	-2.12886300
C	-1.04810100	-4.12884200	-0.85932800
H	-0.18972100	-3.94126900	-0.21080400
H	-1.93711800	-3.98072200	-0.23879200
C	-1.00895700	-5.55612300	-1.44508000
H	0.02458600	-5.92467600	-1.46770300
H	-1.59273200	-6.26870500	-0.85391100
C	-1.52147400	-5.40439000	-2.88079200
H	-2.61731700	-5.33447700	-2.88606200
H	-1.23789700	-6.23829100	-3.53136100
C	-0.91594700	-4.06805700	-3.31969200
H	-1.39221200	-3.65961400	-4.21648900
H	0.14785300	-4.21311800	-3.54668300
C	1.65077000	-2.18762300	-2.38053400
H	1.63181700	-2.59356700	-3.39978400
C	2.71029800	-1.05273700	-2.30706900
H	3.01055800	-0.74908200	-3.31493100
H	2.31216200	-0.16102600	-1.81708800
C	3.90641200	-1.63779700	-1.51978000
H	4.87315700	-1.33633900	-1.93716500
H	3.87516600	-1.28631500	-0.48043200
C	3.69586900	-3.15511100	-1.54439000
H	4.23007900	-3.67695600	-0.74351600
H	4.03606800	-3.57183300	-2.50170900
C	2.17604900	-3.28280200	-1.43044100
H	1.87550000	-3.06283400	-0.39796000
H	1.79932600	-4.27861000	-1.68593300
P	-1.12459300	0.29171300	2.17306600

P	−0.06541400	−1.62092300	−1.98036300
Os	−0.41386400	−0.46191800	0.05257700
H	0.93165400	−1.06161800	0.62069000
H	−0.39289500	4.22544300	0.36950500
H	−1.78385200	−1.35067000	0.06480500
H	−0.45598600	−1.90594200	0.70884000
C	−0.94439600	3.82352700	−0.49396600
O	−0.27568700	2.91952300	−1.20394300
O	−2.05984100	4.18258100	−0.78784300
C	3.20582900	2.88557200	−1.49521100
C	3.09126900	2.94902500	0.06551900
H	0.66821600	0.89149700	−0.28627300
C	4.36490000	2.04953800	−2.01262800
H	4.33871900	2.01856400	−3.10606100
H	5.31874500	2.49340300	−1.70776600
H	4.32508600	1.02537600	−1.64299900
C	3.49438200	1.64164900	0.74781300
H	4.57434200	1.47743200	0.68258900
H	3.22313500	1.69788300	1.80460300
H	2.97343100	0.78586400	0.31066500
C	3.22773800	4.26931500	−2.14910900
H	4.17699900	4.78472300	−1.97258400
H	3.09590600	4.15114400	−3.22847300
H	2.41451500	4.90101100	−1.77836500
C	3.81026700	4.12338600	0.71023500
H	3.67137600	4.09089800	1.79510000
H	4.88503100	4.07559900	0.50522700
H	3.42651600	5.07997300	0.34911200
O	1.95699500	2.26455100	−1.86579000
O	1.66950400	3.12829300	0.24331300
B	1.05447200	2.54635200	−0.85359000
8Os			
$G_{\text{solv}} = -2550.738691$; $E_{\text{solv}} = -2551.70088119$			
C	−1.93350800	−1.16617200	3.41153000
H	−2.07515300	−0.66928900	4.37879400
C	−0.98129300	−2.38631900	3.61727900
H	−0.08815200	−2.33576900	2.98845600
H	−0.64310200	−2.41665600	4.65936300
C	−1.82239800	−3.63254900	3.28789600
H	−1.71141800	−3.87895700	2.22440700
H	−1.52010600	−4.51002100	3.86899500
C	−3.26396600	−3.19267800	3.55341700
H	−3.46234500	−3.16927800	4.63369200
H	−4.00794400	−3.84963100	3.09055200
C	−3.28373800	−1.77517000	2.97377400
H	−4.13703900	−1.17575100	3.30867700
H	−3.32767700	−1.84796000	1.88185400
C	0.01299300	0.92119600	3.36844800
H	−0.47860700	1.07667100	4.34049600
C	1.31012800	0.12378900	3.58815300
H	1.17565400	−0.74035700	4.24420400
H	1.66395300	−0.24714000	2.61837100
C	2.30880800	1.15014900	4.16900500
H	2.37350100	1.05325200	5.25787600
H	3.31829400	0.98248400	3.77778100
C	1.75549300	2.54548200	3.78117600
H	2.50177300	3.17711300	3.28723200
H	1.42681900	3.08503400	4.67663500

C	0.55111600	2.26721600	2.86771100
H	0.88788100	2.14921100	1.83096900
H	-0.18939000	3.07403600	2.89967700
C	-2.54010500	1.44480400	2.18192900
H	-2.00685600	2.30118600	1.75182700
C	-3.16918300	1.91739700	3.50629600
H	-3.41836300	1.06595000	4.15197400
H	-2.50463300	2.57897300	4.07235900
C	-4.46225700	2.60095400	3.05145800
H	-5.17137000	2.76551300	3.86962500
H	-4.22845500	3.57789800	2.60875900
C	-4.99606800	1.64865100	1.97449900
H	-5.71161600	2.12793100	1.29951400
H	-5.51458800	0.81060600	2.45718200
C	-3.73912300	1.13698900	1.23576200
H	-3.59484100	1.66535200	0.28813800
H	-3.82586200	0.07440900	0.99638500
C	-0.54735300	-0.82431700	-3.45013900
H	-0.37720600	-1.50165300	-4.29618200
C	0.29981300	0.44339000	-3.66317400
H	1.27437800	0.22920700	-4.11237400
H	0.48041200	0.94024000	-2.70464600
C	-0.58894000	1.33678500	-4.53007700
H	-0.25801600	2.38017100	-4.53554400
H	-0.59079900	0.97548400	-5.56777700
C	-1.97179500	1.15598100	-3.89623300
H	-2.04451900	1.79749600	-3.01090200
H	-2.79224600	1.43148400	-4.56668700
C	-2.02611800	-0.33121200	-3.47795100
H	-2.60735100	-0.92674800	-4.19026600
H	-2.51875300	-0.44391600	-2.50332800
C	-1.18086600	-3.28889600	-2.18354700
H	-2.18957400	-2.87610100	-2.31281800
C	-1.24412900	-4.29959600	-0.99781900
H	-0.45412600	-4.13819900	-0.26176900
H	-2.18813700	-4.17163700	-0.45987500
C	-1.14390000	-5.70246400	-1.63392600
H	-0.11186300	-6.07073700	-1.56917500
H	-1.78106400	-6.43794800	-1.13266300
C	-1.51191900	-5.49350000	-3.10669600
H	-2.60190400	-5.41992000	-3.21761200
H	-1.16489800	-6.30239800	-3.75827100
C	-0.86642400	-4.14263500	-3.42967200
H	-1.24823400	-3.69473600	-4.35289600
H	0.21500400	-4.28345000	-3.55272700
C	1.59200500	-2.31256200	-2.16226200
H	1.66123800	-2.69007000	-3.18947100
C	2.63950200	-1.17416300	-1.97560500
H	3.13888300	-0.97063300	-2.92942900
H	2.17680500	-0.23979800	-1.64835900
C	3.64576200	-1.69906200	-0.93437400
H	4.66080100	-1.31855400	-1.09467600
H	3.32976900	-1.38981600	0.07055000
C	3.54317000	-3.22205100	-1.04357200
H	3.96284000	-3.74696500	-0.17893400
H	4.06809400	-3.57636400	-1.94098000
C	2.03451500	-3.43194600	-1.19227300
H	1.56528600	-3.29020400	-0.21110800

H	1.76051000	−4.42899700	−1.55270400
P	−1.24108800	0.11790400	2.25628900
P	−0.15860600	−1.76030100	−1.89883200
Os	−0.63373400	−0.68058300	0.13688400
H	0.79482700	−1.11648500	0.66527300
H	−0.30567700	3.15682700	0.38595800
H	−2.04634400	−1.57631100	0.13363800
H	−0.50836700	−2.11039600	0.80960600
C	−0.71762200	3.22054700	−0.62919200
O	0.20647900	3.21751500	−1.60432700
O	−1.89331300	3.29742700	−0.87340500
C	3.77199500	3.04805700	−1.68112300
C	3.48255000	3.05696200	−0.13350000
H	0.46258200	0.59202500	−0.14657100
C	4.73282700	1.96320100	−2.13673500
H	4.86178400	2.01714900	−3.22160300
H	5.71398200	2.10008800	−1.67029300
H	4.36101300	0.96864500	−1.88727100
C	3.55749300	1.67272500	0.50491700
H	4.58319600	1.29293900	0.50847500
H	3.21481200	1.73920900	1.53961900
H	2.91263700	0.95745000	−0.01035600
C	4.20517600	4.40853000	−2.22467700
H	5.21576200	4.66674100	−1.89511400
H	4.20006200	4.37065800	−3.31759500
H	3.52286700	5.20502200	−1.91181400
C	4.31143400	4.05397900	0.65867600
H	4.04825500	3.99258000	1.71839700
H	5.37752500	3.82333000	0.56278200
H	4.14355900	5.08020800	0.32598100
O	2.46202900	2.77221300	−2.24371800
O	2.08680900	3.46837500	−0.08707100
B	1.55723700	3.13815400	−1.29964200
9Os			
$G_{\text{solv}} = -2550.735469$; $E_{\text{solv}} = -2551.69979891$			
C	−2.56616200	−1.13716400	2.80083800
H	−2.60878200	−1.37977400	3.87100400
C	−3.12021400	−2.35305400	2.00217500
H	−2.51081200	−2.55840100	1.11842700
H	−3.10188200	−3.25359100	2.62369000
C	−4.56617200	−1.97692300	1.59941300
H	−4.59164400	−1.69072500	0.54143400
H	−5.26752400	−2.80734200	1.72867300
C	−4.92013300	−0.76169100	2.46420500
H	−5.23256800	−1.08269600	3.46693500
H	−5.72711600	−0.15249500	2.04320200
C	−3.58924700	−0.01214300	2.55501700
H	−3.57051500	0.75314600	3.33784500
H	−3.40187800	0.48749000	1.59796200
C	0.05955300	−1.91992800	3.60105400
H	−0.36411600	−1.70966200	4.59108400
C	−0.17577800	−3.41294500	3.27500400
H	−1.08333700	−3.79930200	3.74987300
H	−0.27680200	−3.55336400	2.19304500
C	1.09749800	−4.11401100	3.76045400
H	1.07594300	−4.23006900	4.85263100
H	1.22661100	−5.10890000	3.32120100
C	2.19972400	−3.13168400	3.35795800

H	2.38187700	−3.21807200	2.27936300
H	3.15078400	−3.30997700	3.87078000
C	1.60699400	−1.74670900	3.67343600
H	1.98169600	−0.99045200	2.97728800
H	1.89426300	−1.42848200	4.68238300
C	−0.44148800	0.85279300	3.33007500
H	0.65668200	0.87743100	3.34680100
C	−0.94850600	0.99805700	4.79180000
H	−1.79392900	0.33730900	5.00870500
H	−0.15486300	0.73028400	5.49711600
C	−1.36437400	2.48239800	4.94752000
H	−2.45760900	2.56802400	4.92110700
H	−1.03140100	2.91467600	5.89630500
C	−0.77263700	3.19705300	3.72387600
H	0.28381600	3.44189500	3.89981500
H	−1.29539900	4.12981500	3.48404600
C	−0.88081600	2.14444700	2.61792200
H	−0.26988300	2.35307000	1.73761300
H	−1.92325500	2.08576100	2.28352200
C	0.98408700	−0.50647300	−3.32886300
H	1.75267700	−0.86633400	−4.02706100
C	1.01809300	1.02745200	−3.35813000
H	2.03467000	1.43100600	−3.32081400
H	0.47283200	1.42461600	−2.49446300
C	0.29493200	1.36938000	−4.66446400
H	−0.06043300	2.40409100	−4.68995300
H	0.98748700	1.23084200	−5.50494400
C	−0.85506800	0.34837200	−4.74811400
H	−1.77038300	0.78116500	−4.33368900
H	−1.06990200	0.06515800	−5.78366300
C	−0.41176800	−0.86624000	−3.89066300
H	−0.37192500	−1.79252800	−4.47378500
H	−1.12058300	−1.02920500	−3.07253100
C	1.34549100	−3.08297100	−2.21853400
H	0.30725700	−3.22863100	−2.54353300
C	1.63296400	−4.13187700	−1.10103300
H	2.06603400	−3.68729300	−0.20343000
H	0.69307300	−4.59200500	−0.78256700
C	2.58404500	−5.17080800	−1.73097500
H	3.62292200	−4.94245900	−1.45892600
H	2.37749600	−6.19081100	−1.39109000
C	2.41057800	−4.99436200	−3.24291600
H	1.48929600	−5.48911200	−3.57804400
H	3.24121900	−5.40714200	−3.82535200
C	2.26640700	−3.47722800	−3.39231000
H	1.85857100	−3.17939500	−4.36384400
H	3.25569600	−3.01145500	−3.29189900
C	3.14207000	−0.85690500	−1.48685400
H	3.61496500	−1.01697200	−2.46346500
C	3.37559500	0.62789600	−1.06224400
H	3.88295300	1.16610500	−1.87096500
H	2.43975600	1.15301000	−0.85167700
C	4.27292300	0.57182400	0.18746600
H	4.94677900	1.43206700	0.26110200
H	3.64638100	0.56128900	1.08866200
C	5.00603800	−0.76637500	0.06750000
H	5.44716800	−1.10412600	1.01139200
H	5.81326100	−0.69252500	−0.67387400

C	3.90203600	−1.69882900	−0.43790500
H	3.24347300	−1.94244400	0.40268900
H	4.27779300	−2.63989200	−0.85357800
P	−0.77971400	−0.73914700	2.43007100
P	1.34361600	−1.29889200	−1.68837500
Os	0.06485000	−0.87842500	0.24003100
H	1.39758800	−0.26261700	0.86475600
H	0.19590700	0.80324600	0.00135700
H	−0.47753000	−2.45872200	0.15627700
H	1.09260300	−1.90739600	0.87589200
C	−1.01809100	4.91768600	−2.27110900
C	−0.54162100	4.60283300	−0.80355700
C	0.06128600	5.48685600	−3.17680100
H	−0.34948200	5.66049300	−4.17547900
H	0.42269200	6.44396500	−2.78661800
H	0.90843000	4.80496600	−3.27244100
C	0.92659300	4.18679700	−0.71772800
H	1.59032500	5.04042200	−0.88347600
H	1.12243500	3.78166700	0.27873300
H	1.17076900	3.40804000	−1.44627900
C	−2.27785700	5.77868900	−2.32710300
H	−2.06765100	6.80919400	−2.02649600
H	−2.65450300	5.79116600	−3.35364600
H	−3.06776300	5.38218000	−1.68169900
C	−0.84902600	5.68378600	0.21763300
H	−0.49034100	5.36889300	1.20186600
H	−0.33881400	6.61536400	−0.04746900
H	−1.92064300	5.87921900	0.29246700
O	−1.38406700	3.60021200	−2.76859000
O	−1.32318400	3.42068400	−0.48085200
B	−1.59707600	2.82783200	−1.67462800
O	−2.02157300	1.51212500	−1.79881700
C	−2.00734700	0.72151200	−0.71968700
H	−2.07447500	1.24330800	0.23867800
O	−2.03951200	−0.49353500	−0.83931400
TS_{9,10-Os}			
$G_{\text{solv}} = -2550.733888$; $E_{\text{solv}} = -2551.69862618$			
C	10.60721400	4.25349500	7.98153500
H	10.56131700	4.00312200	9.04990100
C	10.09893700	3.02648100	7.16959400
H	10.71602400	2.85287500	6.28436500
H	10.14819600	2.12064900	7.78165000
C	8.64143000	3.35567500	6.76605100
H	8.60780900	3.64023800	5.70835800
H	7.96765600	2.50293900	6.89675100
C	8.24702500	4.55954900	7.62955500
H	7.93797300	4.22943100	8.63044700
H	7.42528400	5.14474200	7.20330100
C	9.55429900	5.34869000	7.72850400
H	9.54533600	6.11373800	8.51187600
H	9.73445300	5.85081900	6.77155300
C	13.25575200	3.53986600	8.78251400
H	12.82825700	3.73116300	9.77461300
C	13.06079500	2.04290300	8.44875900
H	12.16813200	1.62858700	8.92801900
H	12.95511100	1.90453900	7.36729600
C	14.35670700	1.37512000	8.92135800
H	14.34411500	1.24878900	10.01245900

H	14.51216700	0.38825500	8.47271300
C	15.42822100	2.39216400	8.52246400
H	15.60733200	2.32110600	7.44234000
H	16.38657900	2.23659000	9.02906900
C	14.79767700	3.75653400	8.85332100
H	15.14890800	4.53032400	8.16435300
H	15.07810700	4.07208100	9.86498500
C	12.67526100	6.29720100	8.54664000
H	13.77257600	6.35020200	8.56649800
C	12.16240000	6.41161900	10.00821600
H	11.31572900	5.74613700	10.20498300
H	12.95189400	6.12924300	10.71237100
C	11.74325200	7.89268300	10.19090200
H	10.64950100	7.97376200	10.18575500
H	12.09170300	8.31301600	11.13944800
C	12.31096500	8.62843200	8.96765700
H	13.36605400	8.88574800	9.13342800
H	11.77326600	9.55635200	8.74381000
C	12.20427300	7.58620400	7.85180800
H	12.79744700	7.81668000	6.96440800
H	11.15714100	7.51110700	7.53561000
C	14.13886100	4.95275100	1.83643300
H	14.87504600	4.53174400	1.13814700
C	14.26475200	6.48031900	1.75984300
H	15.30572600	6.81810000	1.75220000
H	13.77344500	6.93963000	2.62417400
C	13.52150200	6.82804800	0.46642400
H	13.23084000	7.88204900	0.41853000
H	14.17499300	6.61884700	−0.39084100
C	12.30750400	5.88200500	0.45495600
H	11.44685000	6.37801400	0.91282200
H	12.01995100	5.60279800	−0.56389700
C	12.71618900	4.65156300	1.30621200
H	12.70840800	3.72443200	0.72268000
H	12.01715200	4.51789200	2.13767300
C	14.45937200	2.39263500	2.98683100
H	13.41483600	2.25783700	2.67747300
C	14.75034600	1.35161100	4.11195900
H	15.17229900	1.80315200	5.01103900
H	13.81257700	0.88217600	4.42389000
C	15.71009200	0.31603600	3.49188300
H	16.74861300	0.56537600	3.74610200
H	15.52320300	−0.69997800	3.85423600
C	15.51403200	0.46222700	1.98008200
H	14.59058200	−0.04380400	1.66853600
H	16.33813800	0.04311000	1.39299100
C	15.35993500	1.97547900	1.80390700
H	14.93204800	2.25065100	0.83454400
H	16.34883600	2.44759300	1.87489500
C	16.28960100	4.61227900	3.68321000
H	16.75311100	4.45551100	2.70154200
C	16.53307100	6.09359900	4.11501900
H	17.04814200	6.63167300	3.31127100
H	15.60120700	6.62714600	4.32247000
C	17.42577300	6.02529100	5.36678600
H	18.09924000	6.88487000	5.45063700
H	16.79719000	6.00483400	6.26629500
C	18.15890000	4.68846000	5.23370900

H	18.60044800	4.34154400	6.17405200
H	18.96571300	4.76959400	4.49268800
C	17.05442400	3.76071600	4.72055000
H	16.39974800	3.50675900	5.56060600
H	17.42972000	2.82474300	4.29366500
P	12.38052700	4.70910300	7.62809700
P	14.48626400	4.18550100	3.48988300
Os	13.21108100	4.62480800	5.42749700
H	14.49320500	5.37756100	6.03099900
H	13.13707400	6.30662200	5.06982000
H	12.82269600	3.01436000	5.41212500
H	14.33691400	3.70112400	6.07437200
C	12.24182700	10.33671400	2.88668200
C	12.78120400	10.07416200	4.34230800
C	13.26448500	10.93168300	1.93217900
H	12.81321400	11.06572000	0.94483100
H	13.59800800	11.91171300	2.28923100
H	14.13662400	10.28428600	1.82074000
C	14.26936200	9.72681600	4.38518700
H	14.88955100	10.60560300	4.18519000
H	14.51545900	9.34765900	5.38086200
H	14.52395400	8.94827300	3.65978700
C	10.94746400	11.14715400	2.85995400
H	11.12590400	12.19155800	3.13200400
H	10.53339600	11.12184500	1.84814200
H	10.19852100	10.73254100	3.54179500
C	12.46204400	11.16504600	5.35025800
H	12.87109500	10.89324400	6.32749700
H	12.91596700	12.11306300	5.04403300
H	11.38587100	11.31207800	5.46186700
O	11.91306300	8.99890100	2.43028100
O	12.06667900	8.86836900	4.71670500
B	11.76150600	8.23586600	3.54680600
O	11.36274600	6.92082000	3.46286400
C	11.33638400	6.14487400	4.57563400
H	11.07464700	6.68614600	5.48791200
O	11.17343300	4.91994900	4.44051800
10_{Os}			
$G_{\text{solv}} = -2550.739209; E_{\text{solv}} = -2551.71049320$			
C	-2.64408400	-1.29878800	2.77509100
H	-2.73584600	-1.56587000	3.83610900
C	-3.08126200	-2.52530200	1.91797300
H	-2.37776500	-2.72467900	1.10562400
H	-3.12233900	-3.42300400	2.54342700
C	-4.47422200	-2.17129100	1.35116600
H	-4.36551400	-1.82265800	0.31859800
H	-5.15520700	-3.02848500	1.34702900
C	-4.97345300	-1.01491800	2.22309700
H	-5.37120800	-1.39295900	3.17485100
H	-5.75985200	-0.42301500	1.74316100
C	-3.69483500	-0.21244000	2.47329600
H	-3.78590100	0.51949300	3.28287800
H	-3.43702000	0.32571900	1.55587100
C	0.00038900	-1.98966700	3.63902500
H	-0.45639200	-1.84210100	4.62549000
C	-0.15171700	-3.47889400	3.24966800
H	-1.04444300	-3.93018300	3.69348900
H	-0.23186800	-3.58472000	2.16240800

C	1.15076400	−4.13187000	3.72468700
H	1.11951900	−4.29763600	4.80996100
H	1.33927700	−5.09777600	3.24447100
C	2.20400100	−3.07532500	3.38450900
H	2.40402300	−3.10056200	2.30580300
H	3.15683000	−3.22731300	3.90220500
C	1.53462200	−1.74049000	3.75521500
H	1.88359600	−0.93094400	3.10734600
H	1.78349000	−1.46101400	4.78532100
C	−0.62107900	0.76907000	3.46109000
H	0.47397600	0.82466500	3.53226100
C	−1.19984800	0.84976800	4.89949100
H	−2.06748100	0.19570100	5.03229500
H	−0.45094100	0.52958700	5.63103500
C	−1.60179400	2.33305300	5.10686400
H	−2.69353400	2.43097600	5.07912800
H	−1.26902600	2.72464000	6.07300900
C	−0.99235300	3.09073200	3.91724800
H	0.05779900	3.33964000	4.12130100
H	−1.51733400	4.02567900	3.69420700
C	−1.06671300	2.07351600	2.77632100
H	−0.44077100	2.33181700	1.91768100
H	−2.10171200	2.00401200	2.42340000
C	0.82758600	−0.54289500	−3.33520800
H	1.51188000	−1.02537900	−4.04574300
C	0.99199800	0.97221000	−3.51601000
H	2.04000100	1.27191300	−3.61793900
H	0.57908600	1.50172200	−2.65288100
C	0.16541700	1.26820400	−4.77132100
H	−0.10184200	2.32627000	−4.85708700
H	0.75097300	0.99571400	−5.65969900
C	−1.06985000	0.35885600	−4.64276100
H	−1.87871300	0.90209400	−4.14646200
H	−1.44004800	0.03724300	−5.62178000
C	−0.63260500	−0.83799500	−3.75883400
H	−0.69267300	−1.79139300	−4.29591600
H	−1.27939800	−0.91117400	−2.87896200
C	1.27100600	−3.03371600	−2.08000400
H	0.22316700	−3.21483900	−2.35226900
C	1.63172700	−4.01661400	−0.92262800
H	2.05555500	−3.51365900	−0.05235900
H	0.72229800	−4.51514900	−0.57220700
C	2.62042100	−5.03513300	−1.52348600
H	3.65255000	−4.72718600	−1.31129900
H	2.49109100	−6.04022300	−1.10979800
C	2.37417600	−4.96644000	−3.03278800
H	1.46437900	−5.52394100	−3.29217900
H	3.19767700	−5.37739900	−3.62616000
C	2.15084600	−3.47066400	−3.27253600
H	1.67978800	−3.26154000	−4.23788500
H	3.12003400	−2.95437000	−3.25825400
C	3.03904400	−0.71315400	−1.52211800
H	3.48834200	−0.86864400	−2.51065000
C	3.21629100	0.78689600	−1.12501600
H	3.66464300	1.34044800	−1.95708800
H	2.26424300	1.27235800	−0.88980000
C	4.15965000	0.79245200	0.09175200
H	4.79676700	1.68263900	0.12496400

H	3.56946600	0.76974500	1.01675300
C	4.94665000	−0.51420900	−0.03573300
H	5.43750900	−0.81583700	0.89552000
H	5.72126800	−0.41796800	−0.80849600
C	3.86665000	−1.50221900	−0.48435400
H	3.24822300	−1.75408400	0.38372200
H	4.26612300	−2.43564900	−0.89432400
P	−0.87304400	−0.80352400	2.50583800
P	1.25357400	−1.21796000	−1.66173900
Os	−0.00645000	−0.80483700	0.31427800
H	1.29244900	−0.07175500	0.93043900
H	−0.54759900	0.98357700	−0.04274000
H	−0.21576600	−2.39397700	0.33728200
H	1.16341000	−1.68462000	0.94073700
C	−0.86056500	4.94147300	−2.29621300
C	0.00073600	4.60355300	−1.02277600
C	−0.08852400	5.60976100	−3.42330600
H	−0.75825100	5.79889100	−4.26747200
H	0.32039000	6.57032200	−3.09237900
H	0.73241000	4.98289500	−3.77738200
C	1.46142100	4.28813600	−1.34583900
H	2.00946400	5.19070300	−1.63310900
H	1.93779700	3.86581600	−0.45639200
H	1.54778100	3.55790100	−2.15538900
C	−2.12137200	5.74196100	−1.96925500
H	−1.88101800	6.76938300	−1.68010600
H	−2.76104900	5.77435700	−2.85573200
H	−2.69211700	5.27713000	−1.15924900
C	−0.07707100	5.63166600	0.09502700
H	0.54519900	5.30780700	0.93474500
H	0.29324000	6.60359800	−0.24758100
H	−1.09883000	5.75428000	0.46018700
O	−1.29280700	3.63494300	−2.73964500
O	−0.60752100	3.37618000	−0.56225100
B	−1.23325800	2.80674000	−1.64848500
O	−1.72948900	1.54486200	−1.65417100
C	−1.67072200	0.78288500	−0.44993700
H	−2.27933200	1.30854500	0.30303500
O	−1.94382900	−0.49244900	−0.61443100
11os			
$G_{\text{solv}} = -2550.749614; E_{\text{solv}} = -2551.72264469$			
C	−2.53972000	−1.33493800	2.61446300
H	−2.75949100	−1.09684400	3.66251500
C	−2.27584300	−2.86995000	2.49120300
H	−1.28460300	−3.10049100	2.09531100
H	−2.34519000	−3.33324400	3.48213300
C	−3.37277700	−3.41431400	1.55992100
H	−3.01864100	−3.38515100	0.52147400
H	−3.64586100	−4.44904000	1.79303100
C	−4.52705900	−2.42553500	1.72233600
H	−5.04963800	−2.60476600	2.67233300
H	−5.26564100	−2.48762300	0.91627200
C	−3.80421000	−1.07660000	1.75483300
H	−4.42442900	−0.27202500	2.16191900
H	−3.51568700	−0.79504100	0.73492700
C	0.20421100	−0.64203000	3.38668900
H	−0.26881000	−0.43944300	4.35424100
C	0.78378400	−2.07232900	3.45074800

H	0.16921300	−2.74059100	4.06164100
H	0.85529400	−2.50857900	2.44856500
C	2.19761600	−1.87470000	4.00608800
H	2.15827600	−1.68013900	5.08645600
H	2.84151000	−2.74627500	3.84666500
C	2.67389400	−0.62683200	3.26026600
H	2.94370200	−0.90570300	2.23361400
H	3.54981700	−0.15283000	3.71596300
C	1.44273300	0.29775200	3.23223300
H	1.41842700	0.88301500	2.30789700
H	1.47161500	1.01059600	4.06510400
C	−1.53435000	1.43831300	2.58639100
H	−0.58129400	1.96799500	2.47403100
C	−2.04508200	1.63014900	4.04566100
H	−1.96761500	0.73185700	4.66500400
H	−1.44205000	2.40198100	4.54024600
C	−3.49579600	2.10949700	3.91808000
H	−4.16627800	1.24902800	3.80031800
H	−3.83265000	2.67191400	4.79513400
C	−3.48406200	2.93852900	2.63340300
H	−3.02774800	3.91811700	2.83467600
H	−4.48308600	3.11904300	2.22326400
C	−2.59357100	2.12806000	1.68141600
H	−2.12318100	2.77171100	0.93461400
H	−3.18580900	1.39552400	1.12885800
C	0.40072400	−0.82906800	−3.76144500
H	0.99662600	−1.42718500	−4.46422000
C	0.72903600	0.64643100	−4.04301600
H	1.79952700	0.81156300	−4.19838500
H	0.41816600	1.28456100	−3.20868900
C	−0.09896200	0.95167600	−5.29748200
H	−0.24891400	2.02507700	−5.45516800
H	0.42675500	0.56331500	−6.17915800
C	−1.42190200	0.18825800	−5.09342900
H	−2.17968900	0.84680500	−4.65424100
H	−1.83010100	−0.17083100	−6.04349400
C	−1.09827300	−0.97581500	−4.11972600
H	−1.29662000	−1.95372900	−4.57147300
H	−1.71420600	−0.90596500	−3.21556200
C	0.51844600	−3.27921600	−2.35400500
H	−0.55090000	−3.32069200	−2.59933200
C	0.75344200	−4.22096500	−1.13301200
H	1.31835000	−3.74235900	−0.33147100
H	−0.21024100	−4.50277100	−0.69734100
C	1.50252200	−5.45245400	−1.68459100
H	2.57937000	−5.35132900	−1.49713200
H	1.17938500	−6.38612000	−1.21355000
C	1.24869700	−5.42305900	−3.19477400
H	0.24973200	−5.82032700	−3.41778700
H	1.97543700	−6.00929700	−3.76703300
C	1.29277300	−3.92768400	−3.52080200
H	0.85486600	−3.69330900	−4.49623400
H	2.33758200	−3.58996600	−3.53649400
C	2.62782400	−1.21652300	−1.99457100
H	3.02776400	−1.51050100	−2.97292200
C	3.02215200	0.26984600	−1.71836800
H	3.49890900	0.69965800	−2.60583300
H	2.15683600	0.89323200	−1.47947500

C	4.00699600	0.23596100	−0.53512900
H	4.77751600	1.01172200	−0.60732300
H	3.45737500	0.40129600	0.39931200
C	4.58213900	−1.18279600	−0.55469200
H	5.04269700	−1.47462100	0.39536900
H	5.34627500	−1.27209200	−1.33869400
C	3.35873200	−2.03369700	−0.90660800
H	2.73194900	−2.12547300	−0.01314800
H	3.61052900	−3.04414100	−1.24593600
P	−1.08735700	−0.30630600	2.08672100
P	0.78408400	−1.46049700	−2.05748200
Os	−0.31720100	−0.70805800	−0.10911800
H	1.14651500	−0.46608600	0.49146700
H	−2.38510600	2.11530400	−1.14796600
H	−0.95387300	−2.16390600	0.00890000
H	0.52821600	−1.88154900	0.54214000
C	0.48215100	4.81526100	0.10954900
C	1.76329400	3.97800000	0.47078500
C	0.75243900	6.07726800	−0.69292600
H	−0.18797700	6.60044200	−0.88970500
H	1.40635500	6.75418500	−0.13319300
H	1.22147200	5.85094000	−1.65270300
C	2.85268600	4.05286200	−0.59962400
H	3.33800200	5.03337100	−0.61256200
H	3.61105300	3.29524900	−0.38356500
H	2.44987400	3.85137200	−1.59738900
C	−0.38370000	5.13435300	1.32858700
H	0.08267400	5.89781900	1.95848600
H	−1.35160800	5.51304400	0.98824200
H	−0.56236300	4.24410500	1.93923000
C	2.34971300	4.26432400	1.84406600
H	3.22170100	3.62462300	2.00990600
H	2.67315300	5.30788700	1.91804100
H	1.62965000	4.06286200	2.63999900
O	−0.26668400	3.88809200	−0.71606900
O	1.25533300	2.62772600	0.46057000
B	0.15664600	2.63070100	−0.36175300
O	−0.40989600	1.47385000	−0.77109200
C	−1.74936100	1.26170400	−1.43542100
H	−1.51614600	1.33128200	−2.51113000
O	−2.17349200	0.07468000	−1.01465400
TS _{11,12-0s}			
G _{solv} = −2550.742116; E _{solv} = −2551.71474185			
C	−2.41274400	−1.49004000	2.82290700
H	−2.55900300	−1.27403900	3.88803300
C	−2.12556300	−3.01690300	2.65827500
H	−1.15458500	−3.22141200	2.20260800
H	−2.12950500	−3.49684600	3.64362900
C	−3.26604700	−3.56777900	1.78648700
H	−2.98296200	−3.50127300	0.72793600
H	−3.49502800	−4.61567600	2.00759100
C	−4.43289100	−2.61733700	2.05562400
H	−4.88002200	−2.83421000	3.03534000
H	−5.22597300	−2.68198400	1.30315800
C	−3.74582800	−1.24902600	2.07086800
H	−4.35179400	−0.47007300	2.54411800
H	−3.54691700	−0.93967400	1.03945500
C	0.30157100	−0.70023800	3.50463300

H	-0.16780200	-0.49246700	4.47369200
C	0.90342100	-2.12107200	3.57955500
H	0.30241300	-2.79462800	4.19802000
H	0.97822300	-2.56459300	2.58040800
C	2.31638800	-1.89516100	4.12531600
H	2.27867700	-1.68640600	5.20307700
H	2.97261500	-2.75910100	3.97466100
C	2.76817700	-0.65061700	3.35932100
H	3.03479900	-0.94041200	2.33498800
H	3.64072100	-0.15729500	3.80063000
C	1.52343600	0.25573700	3.32784400
H	1.48455600	0.83361900	2.40016100
H	1.54865700	0.97653000	4.15407400
C	-1.50506000	1.32133000	2.69532000
H	-0.56384000	1.86649100	2.55958900
C	-1.99756300	1.53662700	4.15888000
H	-2.00553100	0.62287800	4.76048100
H	-1.32587000	2.23816800	4.66820800
C	-3.40333500	2.14499400	4.04194600
H	-4.15303500	1.34633900	3.97326900
H	-3.66564800	2.76748100	4.90369400
C	-3.35549800	2.91928000	2.72380100
H	-2.80311100	3.85822100	2.86703700
H	-4.34694200	3.17593800	2.33564800
C	-2.57623300	1.98593500	1.79016300
H	-2.11492000	2.51813700	0.95533500
H	-3.25121000	1.24308700	1.35724300
C	0.53314600	-0.89679900	-3.63110600
H	1.21646100	-1.42912800	-4.30628600
C	0.76088000	0.60964000	-3.85038100
H	1.82179100	0.85591500	-3.95376800
H	0.37561600	1.19319300	-3.00660700
C	-0.03262600	0.89841100	-5.13031700
H	-0.24591700	1.96377800	-5.26679500
H	0.54905800	0.56711200	-6.00023200
C	-1.30870600	0.04845600	-4.99613500
H	-2.10432400	0.63425900	-4.52072200
H	-1.69396000	-0.26929000	-5.96994400
C	-0.92155500	-1.15719000	-4.10024300
H	-0.98625500	-2.10519200	-4.64450900
H	-1.60285500	-1.24250700	-3.24509000
C	0.62881400	-3.36160200	-2.24875200
H	-0.43023300	-3.41596400	-2.53350500
C	0.83099900	-4.31566900	-1.03257100
H	1.40156400	-3.85343900	-0.22504300
H	-0.14152100	-4.57798300	-0.60490500
C	1.56141300	-5.55947900	-1.58561600
H	2.63267700	-5.49866900	-1.35463600
H	1.19032400	-6.49222700	-1.14948800
C	1.36854800	-5.49125700	-3.10433100
H	0.37315700	-5.86571500	-3.37743500
H	2.10833900	-6.07707100	-3.65990500
C	1.44976800	-3.99003600	-3.39314800
H	1.06405900	-3.72501600	-4.38281000
H	2.49858900	-3.66823600	-3.34875700
C	2.70645700	-1.29739500	-1.80831300
H	3.13260200	-1.60512500	-2.77109500
C	3.09555600	0.19117200	-1.54223400

H	3.57652600	0.61408700	−2.43075700
H	2.22641200	0.81255800	−1.31328000
C	4.07153600	0.16871700	−0.35060500
H	4.85370300	0.93132000	−0.43442000
H	3.51573800	0.36660600	0.57354700
C	4.63038300	−1.25655900	−0.33206400
H	5.06930300	−1.53465700	0.63233100
H	5.40874300	−1.36964400	−1.09876600
C	3.40674500	−2.10330500	−0.69227900
H	2.76125600	−2.17612600	0.18979400
H	3.65695100	−3.12117500	−1.01029200
P	−1.02003100	−0.41609300	2.22402000
P	0.86688000	−1.54415900	−1.92166700
Os	−0.27485300	−0.81261100	0.01281800
H	1.18295300	−0.57805200	0.60253200
H	−2.63525900	1.80790800	−1.22174300
H	−0.91429900	−2.27739200	0.10517000
H	0.49336400	−2.02861900	0.66304500
C	0.64982700	4.63461400	0.27047400
C	1.90943800	3.79530700	0.68962300
C	0.95935900	5.88695800	−0.53654000
H	0.03080000	6.41725300	−0.76980400
H	1.60320100	6.56604900	0.03295000
H	1.45416000	5.64372300	−1.47943400
C	3.02775700	3.83930500	−0.35424800
H	3.52021300	4.81645000	−0.38216100
H	3.77530100	3.08314200	−0.09971700
H	2.64670900	3.61259300	−1.35513300
C	−0.24761300	4.98551700	1.46015400
H	0.20434700	5.75315800	2.09628600
H	−1.20157100	5.36712800	1.08449600
H	−0.45490900	4.10435000	2.07499700
C	2.46855300	4.11791000	2.06799800
H	3.32794900	3.47229700	2.27456000
H	2.80436000	5.15924300	2.12092100
H	1.72743200	3.94875900	2.85240600
O	−0.07325900	3.70732300	−0.55578200
O	1.38999900	2.45921600	0.70429500
B	0.29589600	2.42073500	−0.15757000
O	−0.31400200	1.31521500	−0.55101900
C	−2.07093400	0.88752800	−1.42923500
H	−1.52454400	0.87046400	−2.37470600
O	−2.33227400	−0.15833900	−0.80489000
12Os			
$G_{\text{solv}} = -2550.757038; E_{\text{solv}} = -2551.72757047$			
C	−2.50224000	−1.37053100	2.64030500
H	−2.67049500	−1.13519100	3.69792700
C	−2.19651400	−2.89737000	2.51491000
H	−1.22926900	−3.09903300	2.05040900
H	−2.18009100	−3.34985100	3.51274000
C	−3.33974500	−3.48847700	1.67246500
H	−3.06169800	−3.46401100	0.61075800
H	−3.56300200	−4.52736800	1.93684700
C	−4.51118900	−2.53431100	1.90789400
H	−4.95532300	−2.71359600	2.89635000
H	−5.30610500	−2.63112900	1.16068700
C	−3.82883700	−1.16417000	1.87133700
H	−4.43965500	−0.36557000	2.30401300

H	-3.62343800	-0.90657100	0.82651000
C	0.16450000	-0.53624400	3.38904600
H	-0.35310900	-0.33240000	4.33462000
C	0.78875600	-1.94703600	3.48951700
H	0.18577200	-2.62601600	4.10020200
H	0.89135900	-2.39489900	2.49491100
C	2.18699500	-1.69688700	4.06234700
H	2.12564600	-1.48833500	5.13919100
H	2.85972300	-2.55030100	3.92476700
C	2.63240100	-0.44431100	3.30597600
H	2.92045600	-0.72407800	2.28431700
H	3.48844100	0.06220400	3.76447600
C	1.37394000	0.44064700	3.25689200
H	1.35193200	1.03139700	2.33798300
H	1.36688100	1.14777600	4.09549300
C	-1.63439700	1.44962300	2.45134100
H	-0.69820700	2.00625300	2.32924500
C	-2.18809800	1.71962000	3.88283900
H	-2.27219400	0.81873900	4.49820000
H	-1.50934900	2.39649100	4.41485400
C	-3.55820700	2.39008900	3.68202300
H	-4.34489400	1.62639300	3.62888600
H	-3.81837100	3.07045200	4.49932200
C	-3.43365300	3.08753300	2.32576200
H	-2.84134100	4.00623900	2.43213400
H	-4.40025600	3.36572500	1.89211500
C	-2.66964800	2.06631400	1.47635800
H	-2.17920300	2.50888600	0.60583000
H	-3.36987000	1.30993100	1.10713900
C	0.37535500	-0.72974200	-3.74248700
H	1.08266500	-1.15772600	-4.46573900
C	0.45117100	0.80558400	-3.84941000
H	1.47694100	1.16365300	-3.97914500
H	0.05209100	1.26888000	-2.94015100
C	-0.44387400	1.11748800	-5.05169500
H	-0.72685400	2.17378300	-5.11162400
H	0.07747500	0.85908400	-5.98322100
C	-1.64642400	0.18743000	-4.84764900
H	-2.36456100	0.66968500	-4.17074100
H	-2.18526100	-0.02526800	-5.77630200
C	-1.06922000	-1.09008800	-4.19281600
H	-1.04825800	-1.92637900	-4.89951600
H	-1.69051300	-1.40899000	-3.34917400
C	0.59649400	-3.24207000	-2.43478600
H	-0.46294600	-3.31262800	-2.71299400
C	0.82166400	-4.21157600	-1.23636200
H	1.41347200	-3.76064300	-0.43742600
H	-0.14167400	-4.47282300	-0.78803000
C	1.53309900	-5.45155600	-1.82439500
H	2.60622000	-5.41036800	-1.59823300
H	1.15269300	-6.38991900	-1.40867600
C	1.33271100	-5.34707300	-3.34129600
H	0.33510200	-5.71265500	-3.61859800
H	2.06843700	-5.92205500	-3.91338400
C	1.41637600	-3.83948200	-3.59496200
H	1.03120900	-3.54566000	-4.57697800
H	2.46576100	-3.52192600	-3.54134000
C	2.64838600	-1.16364000	-2.03067200

H	3.04473300	−1.46176500	−3.00913100
C	3.03810200	0.32320100	−1.76308400
H	3.47540100	0.76081000	−2.66726600
H	2.17371900	0.93149700	−1.48878100
C	4.06331700	0.29147700	−0.61264200
H	4.84152200	1.05414600	−0.72438500
H	3.54488600	0.48371300	0.33433600
C	4.62106000	−1.13418200	−0.62421800
H	5.09676600	−1.41860900	0.32064900
H	5.36885100	−1.24436500	−1.42139100
C	3.38309300	−1.97609900	−0.94228900
H	2.76560100	−2.04731100	−0.03972900
H	3.61836600	−2.99421200	−1.27097300
P	−1.10660100	−0.29106200	2.05123500
P	0.81219300	−1.42934300	−2.07964000
Os	−0.31330200	−0.71014800	−0.13154700
H	1.13957700	−0.50990200	0.49341700
H	−3.76893100	0.72836900	−2.01358700
H	−1.01622500	−2.15944100	−0.06715500
H	0.38897100	−1.96858200	0.52578200
C	0.73799400	4.67509600	0.08913400
C	1.95465600	3.85291000	0.64722400
C	1.12036400	5.89362900	−0.73977100
H	0.21651400	6.41204000	−1.07529100
H	1.71494800	6.59813100	−0.14773100
H	1.69324500	5.61031200	−1.62569400
C	3.16227200	3.86577400	−0.29326400
H	3.64472600	4.84801900	−0.32549900
H	3.89280500	3.13557800	0.06499700
H	2.87560700	3.58378200	−1.31135200
C	−0.25053400	5.08168900	1.18670200
H	0.15087500	5.87340100	1.82750700
H	−1.16797100	5.44936900	0.71722200
H	−0.51412800	4.22671300	1.81691100
C	2.39279200	4.23161800	2.05625100
H	3.23278500	3.59961000	2.36146600
H	2.72041700	5.27629800	2.09832500
H	1.58689500	4.08862100	2.77990400
O	0.08088900	3.71987000	−0.74936600
O	1.43767700	2.52004900	0.66644500
B	0.39631200	2.43389900	−0.26910800
O	−0.22269300	1.34738500	−0.65661000
C	−2.74109700	0.69298800	−1.62439900
H	−2.09551600	1.57962900	−1.66268400
O	−2.33265200	−0.34856300	−1.13621500
13Os			
$G_{\text{solv}} = -2436.295427; E_{\text{solv}} = -2437.23236342$			
C	−2.08256900	−1.78607200	3.02384100
H	−2.33467800	−1.47032300	4.04277800
C	−1.40414200	−3.19090300	3.09048200
H	−0.39762300	−3.19574600	2.66595200
H	−1.31737500	−3.50574000	4.13646200
C	−2.33195000	−4.14234100	2.31572800
H	−2.02549400	−4.17544000	1.26254100
H	−2.30278600	−5.16591100	2.70327700
C	−3.71168500	−3.49077100	2.42097100
H	−4.13718500	−3.66296300	3.41862400
H	−4.42709000	−3.86811900	1.68278800

C	-3.39353100	-2.00468800	2.23214700
H	-4.19729700	-1.34446900	2.57321900
H	-3.23134000	-1.80933900	1.16426400
C	0.24449100	-0.18214900	3.65962500
H	-0.33924300	-0.00500300	4.57262900
C	1.22755500	-1.33899700	3.93547200
H	0.79831500	-2.10427300	4.58950700
H	1.51701800	-1.82603000	2.99636100
C	2.44887800	-0.64176800	4.54180200
H	2.24199600	-0.36202000	5.58356300
H	3.34402600	-1.27270300	4.53797600
C	2.59202300	0.61278100	3.67505100
H	3.08841800	0.35459200	2.73162500
H	3.18720000	1.39880600	4.15166900
C	1.14414900	1.05939000	3.38324100
H	1.06929800	1.41239400	2.35170500
H	0.84390600	1.88899100	4.03417600
C	-1.94612200	1.10491400	2.37887500
H	-1.18009000	1.86038400	2.16137700
C	-2.62144900	1.48437500	3.72071400
H	-2.90022600	0.60141200	4.30556500
H	-1.93580500	2.06866900	4.34368600
C	-3.88621600	2.29630800	3.33486300
H	-4.78557600	1.70479000	3.54346000
H	-3.97534800	3.22601200	3.90581100
C	-3.77251600	2.54205800	1.82145000
H	-3.16441700	3.43413700	1.62290100
H	-4.74548600	2.69226800	1.34194200
C	-3.03221900	1.30516500	1.30664800
H	-2.59297100	1.43857000	0.31510600
H	-3.72061600	0.45396000	1.26744100
C	0.74300500	-0.42689000	-3.32066700
H	1.12078200	-0.96431800	-4.19878600
C	1.49225000	0.92082500	-3.23731200
H	2.52454000	0.83983400	-3.59372000
H	1.52828500	1.28142000	-2.20707900
C	0.63393300	1.86552600	-4.08458400
H	0.84867400	2.92301600	-3.89277900
H	0.81169700	1.67773500	-5.15228300
C	-0.79709600	1.47243500	-3.70454500
H	-1.05181700	1.92487200	-2.74071200
H	-1.53999100	1.80113400	-4.43887100
C	-0.75307800	-0.06212000	-3.55621900
H	-1.12152100	-0.55987100	-4.46033500
H	-1.39316700	-0.38816100	-2.72745600
C	0.31386200	-3.13947000	-2.60575300
H	-0.70029800	-2.86039800	-2.92235900
C	0.18513700	-4.34782500	-1.62964000
H	0.74772400	-4.20544900	-0.70511500
H	-0.86147200	-4.46764600	-1.33242500
C	0.68777500	-5.58002800	-2.41157700
H	1.72908400	-5.79621500	-2.14100700
H	0.10492100	-6.48084100	-2.19542000
C	0.62478400	-5.16416400	-3.88480500
H	-0.40538900	-5.24200800	-4.25674900
H	1.25966700	-5.77624600	-4.53382000
C	1.05019100	-3.69359200	-3.84445600
H	0.79832800	-3.15159700	-4.76139300

H	2.13838000	−3.63643000	−3.71422600
C	2.79568900	−1.75875900	−1.75690100
H	3.17440800	−1.87436400	−2.78008600
C	3.50662300	−0.53797300	−1.09014100
H	4.10791300	−0.00833500	−1.83684900
H	2.80392400	0.18842200	−0.67266700
C	4.40310400	−1.12834100	0.01635800
H	5.33434500	−0.56740300	0.14699200
H	3.86713600	−1.10506600	0.97394400
C	4.62199600	−2.58511400	−0.39907600
H	4.96229900	−3.22333500	0.42319700
H	5.36811900	−2.64524400	−1.20290700
C	3.24196900	−2.98292200	−0.92799000
H	2.56858300	−3.12838300	−0.07469200
H	3.24386700	−3.90723900	−1.51526400
P	−0.98373900	−0.47884900	2.30017200
P	0.95651200	−1.55799000	−1.86711100
Os	−0.06945900	−0.95001600	0.17381300
H	1.33416300	−1.11684600	0.86950100
H	−0.97262200	−2.27062200	0.10477900
H	0.36635000	−2.40038100	0.72156600
C	0.56569500	4.44598700	0.15426300
C	1.98501400	3.77224000	0.14498500
C	0.45928400	5.71677300	−0.67635900
H	−0.55494300	6.12187100	−0.60527500
H	1.15604400	6.47939900	−0.31131700
H	0.67143000	5.52422300	−1.73041100
C	2.71882600	3.94783300	−1.18683000
H	3.07952400	4.97262700	−1.32167900
H	3.57996700	3.27286200	−1.20730300
H	2.07304600	3.69277200	−2.03232500
C	0.04575600	4.70334400	1.57221100
H	0.58036300	5.52482000	2.05983400
H	−1.01446200	4.96756500	1.51765700
H	0.14010600	3.81032800	2.19877800
C	2.89285700	4.17813900	1.29821900
H	3.85335900	3.66079400	1.20970500
H	3.08502000	5.25663300	1.28569700
H	2.45713100	3.90946800	2.26325300
O	−0.26291000	3.43016100	−0.42793400
O	1.66079300	2.38446100	0.27743400
B	0.35034900	2.19704000	−0.18143500
O	−0.21185500	1.02277500	−0.35394900
14os			
$G_{\text{solv}} = -2847.918071; E_{\text{solv}} = -2849.04309690$			
C	−1.07822400	−1.46688800	3.46578900
H	−1.13769300	−1.13742700	4.50965600
C	−0.38000500	−2.86376300	3.42627400
H	0.55574700	−2.85990500	2.86441100
H	−0.14260800	−3.18108900	4.44820000
C	−1.39986300	−3.82354700	2.79424400
H	−1.28518700	−3.81453200	1.70213500
H	−1.27334900	−4.85667200	3.13479900
C	−2.75327100	−3.21711800	3.16485600
H	−2.98086400	−3.41744800	4.22061300
H	−3.58300900	−3.60447200	2.56379700
C	−2.51450200	−1.72086500	2.94321100
H	−3.25373300	−1.08758900	3.44290500

H	-2.57953800	-1.51108200	1.87049300
C	1.31959600	0.15653300	3.63483900
H	0.91069100	0.37257900	4.62885600
C	2.32214800	-1.01106000	3.78303600
H	2.04827000	-1.69189200	4.59518400
H	2.36807400	-1.59875100	2.86058600
C	3.67605300	-0.32670000	3.99627200
H	3.76030000	0.03763500	5.02914900
H	4.52227500	-0.99667200	3.80819500
C	3.60895200	0.85306600	3.02514300
H	3.76736100	0.48956800	2.00155400
H	4.36160600	1.62374600	3.22342500
C	2.16997200	1.37829100	3.16529700
H	1.81505000	1.80947000	2.22574000
H	2.12216800	2.16899800	3.92425400
C	-1.09270300	1.42758400	2.87997700
H	-0.39586300	2.19609200	2.52600600
C	-1.44749900	1.72314600	4.36986700
H	-1.14767200	0.93009200	5.06141600
H	-0.92528600	2.63067400	4.69537700
C	-2.96912000	1.94521600	4.40250900
H	-3.48355500	0.98986800	4.56852200
H	-3.27805100	2.62612100	5.20250900
C	-3.29633900	2.46238700	2.99985400
H	-3.01008700	3.52014700	2.91814800
H	-4.36100900	2.38964200	2.75056700
C	-2.41596900	1.59459400	2.09505500
H	-2.24556300	2.02455200	1.10663500
H	-2.90846700	0.63754100	1.92020400
C	1.88878800	-0.12168500	-3.00895000
H	2.45435100	-0.66012800	-3.78277600
C	2.75312500	1.06423100	-2.54924500
H	3.80121500	0.79165700	-2.39316900
H	2.36645600	1.47605200	-1.60786400
C	2.56020000	2.06741900	-3.68969600
H	2.91667800	3.07419100	-3.44684200
H	3.12053200	1.72802000	-4.57164200
C	1.05069800	2.00348100	-3.96092800
H	0.52029300	2.67305700	-3.27319300
H	0.79377400	2.31293700	-4.97979500
C	0.64501200	0.53716900	-3.66443500
H	0.36335300	-0.00227100	-4.57593500
H	-0.21187400	0.50773100	-2.98893100
C	0.50730400	-2.59071200	-2.73930100
H	-0.30771600	-1.97533600	-3.13342100
C	-0.14987000	-3.76248900	-1.95358500
H	0.31111400	-3.92798600	-0.97719100
H	-1.20184800	-3.52610200	-1.76195000
C	-0.00873900	-5.00656800	-2.85917200
H	0.82860600	-5.62701400	-2.51526900
H	-0.90280100	-5.63816000	-2.84976500
C	0.31460100	-4.44926400	-4.25081300
H	-0.60458800	-4.10311800	-4.74270600
H	0.78860300	-5.18454700	-4.90961600
C	1.21454700	-3.24966400	-3.93891200
H	1.32799600	-2.56416100	-4.78553700
H	2.21423600	-3.61254600	-3.66810200
C	3.11266600	-2.19492200	-1.44618800

H	3.53034100	−2.37283700	−2.44430900
C	4.13327600	−1.33486800	−0.63771600
H	4.97572800	−1.06374300	−1.28366700
H	3.69887000	−0.40336400	−0.26666300
C	4.61087700	−2.22877200	0.52032500
H	5.64594400	−2.02306600	0.81241400
H	3.97951900	−2.05857300	1.40133900
C	4.39284100	−3.65581500	0.01148700
H	4.39153100	−4.40431900	0.81112300
H	5.18207100	−3.92872100	−0.70200000
C	3.04270100	−3.54886900	−0.70382900
H	2.24717000	−3.53351700	0.04951000
H	2.83993600	−4.38328200	−1.38381300
P	−0.15336600	−0.14520700	2.53438800
P	1.46577000	−1.37563200	−1.71344700
Os	0.44392000	−0.68014200	0.30046500
H	1.77650700	0.13922100	0.60286600
H	0.36520700	−2.23243200	0.72339000
H	1.64157300	−1.47314000	0.97268700
C	−0.39496100	4.60896800	−0.38442700
C	1.03357600	4.25037600	0.16443200
C	−0.42401400	5.73746500	−1.40618100
H	−1.45651600	5.92711400	−1.71641500
H	−0.02370300	6.66287900	−0.97765100
H	0.15423200	5.48593300	−2.29815200
C	2.13508300	4.47050400	−0.87256000
H	2.33588100	5.53444600	−1.03543000
H	3.05560000	3.99385900	−0.52234200
H	1.86172100	4.01926500	−1.82916900
C	−1.39558200	4.89592300	0.73779900
H	−1.21546500	5.86889700	1.20648000
H	−2.40810900	4.89247200	0.32285100
H	−1.34681300	4.12625600	1.51209600
C	1.40937600	4.93310800	1.47370800
H	2.41882900	4.63060900	1.76970400
H	1.40056500	6.02326400	1.36429700
H	0.72726500	4.65790300	2.28165200
O	−0.79510300	3.39020200	−1.02056000
O	0.92806600	2.84237600	0.39217600
B	−0.10423300	2.33093500	−0.40737600
O	−0.40969800	1.06319800	−0.56538200
C	−3.36709000	−0.44536500	−2.67278500
C	−4.00757200	0.23036300	−1.39997700
H	−1.29215800	−1.41654000	−0.14673200
C	−3.20411200	0.48064600	−3.86899100
H	−2.72986000	−0.06372300	−4.69111700
H	−4.17946500	0.83724000	−4.21645400
H	−2.57898100	1.34231700	−3.62678400
C	−3.78675200	1.73871400	−1.33543200
H	−4.34879600	2.25296000	−2.12139500
H	−4.14176800	2.10692600	−0.36838000
H	−2.72972700	1.99954600	−1.42395900
C	−4.05611300	−1.74344900	−3.09179500
H	−5.05019200	−1.55636400	−3.50902500
H	−3.44854600	−2.23475500	−3.85787000
H	−4.15558700	−2.43307400	−2.24802600
C	−5.47634500	−0.09751700	−1.17745700
H	−5.82483800	0.39683000	−0.26586500

H	-6.08212800	0.26842900	-2.01304400
H	-5.64478800	-1.17078300	-1.06608300
O	-2.04921500	-0.82197300	-2.20845500
O	-3.24177100	-0.36011900	-0.31632400
B	-2.06711200	-0.78737100	-0.85000900
TS_{14,15-Os}			
$G_{\text{solv}} = -2847.918200; E_{\text{solv}} = -2849.04300389$			
C	-1.64014500	-1.39791700	3.24700400
H	-1.70177400	-1.07218600	4.29185300
C	-0.93836000	-2.79270400	3.20290300
H	0.00361200	-2.78227100	2.65163600
H	-0.71170500	-3.11823700	4.22474500
C	-1.94943000	-3.74883500	2.55214100
H	-1.82783600	-3.72499400	1.46104300
H	-1.82040400	-4.78562500	2.88043600
C	-3.30759800	-3.15290400	2.92210200
H	-3.54020800	-3.36700000	3.97408300
H	-4.13204800	-3.53682200	2.31167700
C	-3.07508900	-1.65280500	2.71953100
H	-3.81748200	-1.02974000	3.22761000
H	-3.14034600	-1.42914600	1.64934000
C	0.75519700	0.23503400	3.41750300
H	0.34855900	0.45232300	4.41198200
C	1.76083700	-0.92970200	3.56622200
H	1.49084900	-1.60825800	4.38162500
H	1.80533000	-1.52064500	2.64587200
C	3.11384400	-0.24147000	3.77281900
H	3.20086200	0.12606400	4.80432000
H	3.96098300	-0.90997500	3.58369400
C	3.04071300	0.93533900	2.79841300
H	3.19566800	0.56893900	1.77534100
H	3.79265700	1.70799500	2.99162400
C	1.60124300	1.45803800	2.94297200
H	1.24086600	1.88640000	2.00410700
H	1.55467000	2.24983200	3.70079800
C	-1.66241800	1.49848400	2.67584300
H	-0.97316000	2.27065600	2.31494500
C	-2.00029400	1.78822700	4.17133600
H	-1.70340200	0.98698400	4.85452000
H	-1.46528800	2.68759700	4.49852200
C	-3.51948400	2.02469100	4.21998100
H	-4.04079500	1.07342400	4.38865000
H	-3.81415800	2.70651100	5.02453400
C	-3.85590300	2.54664900	2.82160600
H	-3.55695800	3.60077600	2.73707300
H	-4.92380600	2.48721700	2.58297500
C	-2.99589500	1.66684200	1.90939400
H	-2.84035600	2.08623000	0.91394200
H	-3.49768600	0.71208700	1.75132200
C	1.35254800	-0.04904300	-3.21415500
H	1.93224800	-0.58876500	-3.97662000
C	2.20983900	1.13481400	-2.73624000
H	3.25325100	0.86005500	-2.55542200
H	1.80248900	1.54835600	-1.80415500
C	2.04736000	2.13784100	-3.88148300
H	2.39994700	3.14397400	-3.62983700
H	2.62922800	1.79696500	-4.74870300
C	0.54507900	2.07711400	-4.19148000

H	-0.00166000	2.75335400	-3.52326100
H	0.31616900	2.38044100	-5.21874800
C	0.12555400	0.61450900	-3.89590200
H	-0.14249000	0.07273500	-4.81003200
H	-0.74519500	0.59277700	-3.23837000
C	-0.06780000	-2.50074400	-2.95959600
H	-0.86789800	-1.87154300	-3.36281700
C	-0.75523200	-3.65690600	-2.17898200
H	-0.27656200	-3.85873200	-1.21790400
H	-1.79093400	-3.38074800	-1.95611700
C	-0.68292500	-4.89122500	-3.10814400
H	0.10862100	-5.57050900	-2.76776400
H	-1.61539500	-5.46448500	-3.11929200
C	-0.31128300	-4.33340700	-4.48842900
H	-1.20529900	-3.94101300	-4.99173800
H	0.14002000	-5.08272000	-5.14734200
C	0.63521000	-3.17770700	-4.15002600
H	0.79551200	-2.49154800	-4.98857900
H	1.61233300	-3.58566300	-3.86098200
C	2.53694000	-2.14599100	-1.65379100
H	2.95362200	-2.33230000	-2.65090600
C	3.56733800	-1.29773400	-0.84529600
H	4.41042900	-1.03139300	-1.49236400
H	3.14137700	-0.36406500	-0.47008000
C	4.03921100	-2.19860000	0.30997400
H	5.07867300	-2.00736100	0.59612000
H	3.41548900	-2.01946800	1.19466600
C	3.79871500	-3.62269800	-0.19689500
H	3.78900000	-4.37030300	0.60352200
H	4.58169200	-3.90784400	-0.91248400
C	2.44819200	-3.49707200	-0.90848700
H	1.65476800	-3.46794600	-0.15332300
H	2.23170400	-4.32993400	-1.58608300
P	-0.71918300	-0.07066600	2.32006900
P	0.90276000	-1.30320200	-1.92634000
Os	-0.11996200	-0.60420800	0.08597400
H	1.20392900	0.24079600	0.37589400
H	-0.17407900	-2.15365400	0.51673000
H	1.09989700	-1.36518200	0.75780300
C	-1.02829600	4.66185200	-0.65835800
C	0.38926200	4.31030800	-0.07699900
C	-1.03808500	5.77727500	-1.69434900
H	-2.06431100	5.96091600	-2.02800500
H	-0.64856900	6.70849500	-1.26859100
H	-0.44082700	5.51646900	-2.57100200
C	1.51211200	4.52305300	-1.09188600
H	1.71491900	5.58602000	-1.25832200
H	2.42549200	4.05057300	-0.71827400
H	1.26037800	4.06431600	-2.05062800
C	-2.05132400	4.96016000	0.43996500
H	-1.88405700	5.94041600	0.89788700
H	-3.05581600	4.94601200	0.00631600
H	-2.01370300	4.20199600	1.22603700
C	0.73653700	5.00500300	1.23388500
H	1.73973800	4.70623400	1.55387800
H	0.72933100	6.09402100	1.11385700
H	0.03752300	4.73689500	2.02972500
O	-1.41556100	3.43429800	-1.28807500

O	0.28076700	2.90354200	0.16141400
B	−0.73692100	2.38566500	−0.64923900
O	−1.03629800	1.11185400	−0.79447400
C	−3.90162900	−0.31981400	−2.88267600
C	−4.55195800	0.34744300	−1.60809200
H	−1.83832500	−1.29211500	−0.36793100
C	−3.77346800	0.60397300	−4.08556200
H	−3.28995900	0.06817600	−4.90803500
H	−4.76017600	0.93295600	−4.42851200
H	−3.16958200	1.48323400	−3.85223000
C	−4.40355100	1.86605500	−1.56796000
H	−5.00744200	2.34087900	−2.34790100
H	−4.75670700	2.22879200	−0.59785400
H	−3.36424800	2.18043300	−1.68250200
C	−4.56109200	−1.63704200	−3.29101000
H	−5.56467400	−1.47922000	−3.69769700
H	−3.94871700	−2.11386000	−4.06253500
H	−4.63121800	−2.32670500	−2.44439200
C	−6.00284300	−0.04043100	−1.36004100
H	−6.35996300	0.45203700	−0.45063400
H	−6.63662000	0.28495700	−2.19172700
H	−6.12189100	−1.11808100	−1.22924000
O	−2.57280200	−0.66060100	−2.43073000
O	−3.75147400	−0.19490600	−0.52920400
B	−2.56391100	−0.59036400	−1.06885600
15o _s			
$G_{\text{solv}} = -2847.940379$; $E_{\text{solv}} = -2849.06578602$			
C	−1.37486400	−2.02601300	3.07909500
H	−1.72461600	−1.81801300	4.09658400
C	−0.00313000	−2.76372500	3.18283800
H	0.79452000	−2.25072300	2.64070500
H	0.30249700	−2.82066100	4.23374200
C	−0.24248300	−4.17438900	2.61479800
H	−0.00786300	−4.18485900	1.54255700
H	0.38163600	−4.93400000	3.09681100
C	−1.74275800	−4.41077800	2.80223400
H	−1.96006900	−4.65633500	3.85057000
H	−2.13222700	−5.22389900	2.18043100
C	−2.34238000	−3.04837500	2.44132300
H	−3.37012900	−2.91797300	2.79616700
H	−2.34962300	−2.94138200	1.35091500
C	−0.45725400	0.65535700	3.49937300
H	−0.92431400	0.38683100	4.45795200
C	1.06005700	0.43723900	3.63351900
H	1.31161900	−0.49785600	4.14274800
H	1.52724000	0.42270500	2.64133000
C	1.52124900	1.67767800	4.40250100
H	1.24913600	1.58293800	5.46235400
H	2.60504000	1.83065600	4.34952000
C	0.72987600	2.81379800	3.74209700
H	1.28278900	3.15547300	2.86284200
H	0.59168800	3.67663900	4.40249500
C	−0.61192900	2.18672500	3.28971600
H	−0.82184300	2.43194800	2.24557600
H	−1.45696100	2.56580200	3.87499600
C	−3.02489700	0.29061800	2.30385700
H	−2.87257400	1.35150400	2.08245000
C	−3.79578600	0.16582300	3.64812900

H	-3.37061800	-0.58387100	4.32225500
H	-3.76369300	1.12013100	4.18521400
C	-5.24647400	-0.20646000	3.26230100
H	-5.39765800	-1.28688000	3.38019400
H	-5.99114600	0.29419800	3.88942600
C	-5.36450000	0.15908100	1.77758400
H	-5.52330600	1.24075300	1.66792100
H	-6.19275200	-0.35281200	1.27555000
C	-3.99143100	-0.21751000	1.21593100
H	-3.77038700	0.24492500	0.25050900
H	-3.92873300	-1.30361100	1.08435200
C	0.75303400	-0.28579700	-3.49477400
H	1.31182100	-0.87686900	-4.23509500
C	1.46139200	1.06628900	-3.32819400
H	2.54533500	0.96599400	-3.21234400
H	1.06533400	1.58871100	-2.45554200
C	1.07182100	1.83429600	-4.59731800
H	1.14895400	2.91768200	-4.45845600
H	1.74592300	1.55839300	-5.41827600
C	-0.37137600	1.38284000	-4.91555400
H	-1.08806800	2.15363600	-4.62092800
H	-0.50295600	1.20530400	-5.98832200
C	-0.61676400	0.09659900	-4.09015000
H	-1.03605000	-0.71320100	-4.69672700
H	-1.32153700	0.30818200	-3.27937600
C	-0.30112500	-2.78443000	-2.67348000
H	-1.26220300	-2.34105200	-2.96260500
C	-0.60804000	-3.95864500	-1.69504200
H	-0.00050500	-3.92427700	-0.78950400
H	-1.64982200	-3.89757500	-1.36480900
C	-0.34667400	-5.25418900	-2.49228000
H	0.64865600	-5.64803700	-2.24981000
H	-1.07064500	-6.04229100	-2.26231500
C	-0.37327000	-4.82379500	-3.96233800
H	-1.41045200	-4.71731600	-4.30689200
H	0.12807400	-5.53301500	-4.62921500
C	0.30279000	-3.45061100	-3.92713600
H	0.13193900	-2.86510200	-4.83624600
H	1.38697400	-3.58561800	-3.81925700
C	2.37451100	-1.91069400	-1.77437200
H	2.73808300	-2.17807200	-2.77386900
C	3.29577900	-0.80018300	-1.18637300
H	3.99264500	-0.44624500	-1.95426600
H	2.72985400	0.06762600	-0.83871800
C	4.05363600	-1.45304800	-0.01396400
H	5.07652800	-1.07447200	0.08910600
H	3.52535500	-1.24213500	0.92397000
C	3.99273000	-2.95496600	-0.30600100
H	4.18969400	-3.57382000	0.57591600
H	4.72823500	-3.22387700	-1.07626400
C	2.57079200	-3.12900000	-0.84730400
H	1.87013600	-3.08517800	-0.00604700
H	2.41376700	-4.07880800	-1.36969400
P	-1.30100000	-0.38223300	2.21048800
P	0.62082600	-1.33037700	-1.96651700
Os	-0.35863700	-0.56129300	0.04726600
H	1.01853800	-1.01891200	0.77526100
H	-1.52950200	-1.59521300	-0.28205100

H	-0.20918900	-2.09292500	0.44215000
C	2.55100900	4.31388100	-0.17983800
C	3.40513200	3.12134400	0.40630000
C	3.19374900	5.03353100	-1.35790800
H	2.53102400	5.83232300	-1.70363100
H	4.14580900	5.48713000	-1.06292800
H	3.37031000	4.35771500	-2.19723300
C	4.34777200	2.49435700	-0.62033900
H	5.17129300	3.16930100	-0.87226300
H	4.76941200	1.57722200	-0.19987400
H	3.81843400	2.22963900	-1.54012000
C	2.11228400	5.33450900	0.87053700
H	2.96231500	5.90684100	1.25411700
H	1.40731600	6.03370700	0.41153100
H	1.60471900	4.85739800	1.71282500
C	4.16795900	3.45195600	1.68100100
H	4.70017400	2.56181200	2.02951100
H	4.90635400	4.23955900	1.49732800
H	3.49943600	3.78046600	2.47946300
O	1.36034500	3.64955900	-0.64905300
O	2.40222600	2.13139600	0.71800300
B	1.28089100	2.43650700	-0.01224700
O	0.21897000	1.60295300	-0.08326000
C	-2.41282900	3.18348400	-1.93843100
C	-2.62009100	3.57343500	-0.43176100
H	-1.58057300	0.49645800	-0.75208800
C	-2.20671300	4.37202800	-2.86893000
H	-2.12692500	4.02982500	-3.90541200
H	-3.05258700	5.06626700	-2.80935600
H	-1.28950900	4.91026500	-2.62047700
C	-1.81927100	4.81478400	-0.02548300
H	-2.24113500	5.73150000	-0.45169700
H	-1.83983200	4.90452000	1.06586500
H	-0.77596600	4.72294500	-0.33977400
C	-3.53274500	2.28598300	-2.47780800
H	-4.47478000	2.83181700	-2.59499600
H	-3.23536600	1.90345000	-3.45910500
H	-3.70745100	1.42805000	-1.82075300
C	-4.07613800	3.72777100	-0.00854300
H	-4.12474800	3.99175900	1.05313100
H	-4.57162900	4.52291000	-0.57704000
H	-4.63077400	2.79693600	-0.14965000
O	-1.21030000	2.41764700	-1.89336200
O	-2.06843700	2.44996300	0.25062800
B	-1.14401000	1.79800200	-0.61775200
TS _{15,16-Os}			
G _{solv} = -2847.934558; E _{solv} = -2849.05779747			
C	-1.35321500	-1.87864600	3.05560200
H	-1.72256300	-1.67605700	4.06749300
C	0.02193900	-2.60765500	3.17877400
H	0.81653200	-2.09117100	2.63536300
H	0.31914200	-2.65546700	4.23276500
C	-0.20128500	-4.02340800	2.61658800
H	0.05299400	-4.03845600	1.54904600
H	0.41709800	-4.77740500	3.11489200
C	-1.70351500	-4.26593300	2.77688400
H	-1.93994100	-4.50864200	3.82198800
H	-2.07796800	-5.08295300	2.15068200

C	-2.30143800	-2.90732500	2.39968100
H	-3.33711900	-2.78340100	2.73285700
H	-2.28442400	-2.80169300	1.30930300
C	-0.42401300	0.78231800	3.51430000
H	-0.91827100	0.50851500	4.45698600
C	1.08698400	0.54539800	3.68854700
H	1.31035100	-0.38707500	4.21487700
H	1.57615100	0.50723700	2.70779900
C	1.55128000	1.78648100	4.45423400
H	1.24878200	1.71459500	5.50776400
H	2.63900100	1.91903100	4.42871100
C	0.79785800	2.92334300	3.75525200
H	1.36209000	3.21306800	2.86386200
H	0.68576000	3.81558800	4.38101600
C	-0.55978000	2.31898900	3.32423800
H	-0.78954500	2.58550600	2.29026200
H	-1.38532900	2.70305500	3.93380800
C	-2.97606000	0.46077200	2.29746800
H	-2.82188700	1.51562800	2.04636900
C	-3.71803700	0.37829500	3.66356500
H	-3.23523200	-0.29348200	4.37979500
H	-3.73943300	1.36795000	4.13372900
C	-5.14820800	-0.10293000	3.33637200
H	-5.21581500	-1.19019400	3.46924200
H	-5.90538800	0.35040600	3.98451000
C	-5.33722800	0.23519400	1.85381200
H	-5.55512900	1.30656000	1.74033200
H	-6.15655300	-0.32245200	1.38678400
C	-3.96801000	-0.08536300	1.24862300
H	-3.79797600	0.37029100	0.27055600
H	-3.86603100	-1.16743100	1.11595900
C	0.85079300	-0.11842600	-3.47381400
H	1.39345600	-0.71774700	-4.21921400
C	1.60493200	1.20563800	-3.28855600
H	2.68323900	1.06839900	-3.16213800
H	1.22016600	1.72803500	-2.40935500
C	1.25192300	1.99921100	-4.55176900
H	1.38808800	3.07732500	-4.41529000
H	1.90661900	1.68692300	-5.37533200
C	-0.21371700	1.62223300	-4.86074100
H	-0.88748100	2.41698200	-4.52951400
H	-0.37114700	1.48648300	-5.93608800
C	-0.50113700	0.32277500	-4.06862100
H	-0.94249400	-0.45807100	-4.69714300
H	-1.20138700	0.52706200	-3.25223600
C	-0.29366200	-2.58622000	-2.69475500
H	-1.23843300	-2.10503000	-2.97664700
C	-0.64353800	-3.76411600	-1.73469700
H	-0.04466500	-3.75814000	-0.82285300
H	-1.68613600	-3.67574900	-1.41337300
C	-0.41534200	-5.05621200	-2.54694400
H	0.56902800	-5.47965800	-2.30873000
H	-1.16019000	-5.82801400	-2.32793400
C	-0.42840800	-4.60641100	-4.01138500
H	-1.46216200	-4.46441400	-4.35386900
H	0.05128100	-5.32176300	-4.68790800
C	0.28882500	-3.25466800	-3.95714400
H	0.13694800	-2.65214200	-4.85875300

H	1.36822000	−3.42522000	−3.85197900
C	2.40557500	−1.82375800	−1.78370800
H	2.74912400	−2.10522300	−2.78668000
C	3.37794500	−0.75406200	−1.20426700
H	4.07729800	−0.42106800	−1.97994100
H	2.84487000	0.12778900	−0.84022000
C	4.12484600	−1.44017200	−0.04358200
H	5.16570300	−1.10843200	0.04414500
H	3.61699900	−1.20521000	0.89988700
C	3.99275700	−2.93848300	−0.33171400
H	4.17039800	−3.56352200	0.55014700
H	4.70771400	−3.24268600	−1.10849500
C	2.55888000	−3.04810600	−0.85773500
H	1.86904100	−2.96821000	−0.01050700
H	2.35468300	−3.99082400	−1.37697100
P	−1.25465800	−0.23106600	2.18915900
P	0.67002400	−1.17434000	−1.95321800
Os	−0.30155500	−0.40980000	0.04509300
H	1.17194200	−0.64379500	0.78965700
H	−1.46480500	−1.45397400	−0.27327700
H	−0.08025300	−1.92643400	0.46932700
C	2.73521200	4.42136700	−0.07687300
C	3.52277800	3.15236600	0.44993800
C	3.40267400	5.13930100	−1.24179100
H	2.78489400	5.98765700	−1.55013900
H	4.38382700	5.52488200	−0.94623700
H	3.52776600	4.48258800	−2.10509500
C	4.44456200	2.53178400	−0.59797100
H	5.29576400	3.18329000	−0.81647400
H	4.82678500	1.58213400	−0.21469600
H	3.91197800	2.32638900	−1.53083300
C	2.37904000	5.42878000	1.01513000
H	3.27149600	5.92833600	1.40361400
H	1.71713100	6.18969500	0.59163300
H	1.85308700	4.95682800	1.84870200
C	4.28315100	3.37313500	1.74912800
H	4.75785800	2.43684000	2.05649800
H	5.06762700	4.12516200	1.61472400
H	3.62298800	3.69820200	2.55564200
O	1.49212500	3.85254300	−0.54842300
O	2.46829900	2.19285100	0.70077800
B	1.37286100	2.60852700	0.00834400
O	0.23719600	1.85943900	−0.12194300
C	−2.49869900	3.32196600	−1.97198000
C	−2.75686800	3.76699100	−0.48346800
H	−1.60134100	0.36879800	−0.74426800
C	−2.48201800	4.46933000	−2.97144200
H	−2.33147100	4.08157900	−3.98297100
H	−3.43814000	5.00347400	−2.95684800
H	−1.67907900	5.17769900	−2.75729800
C	−2.23239300	5.16973700	−0.17377900
H	−2.83382700	5.94426300	−0.65916700
H	−2.27356300	5.33017700	0.90779400
H	−1.19085500	5.28001800	−0.49086900
C	−3.44750600	2.22310700	−2.44940000
H	−4.47061300	2.59802200	−2.54945000
H	−3.11716000	1.87014300	−3.43041400
H	−3.44562700	1.36798900	−1.76836600

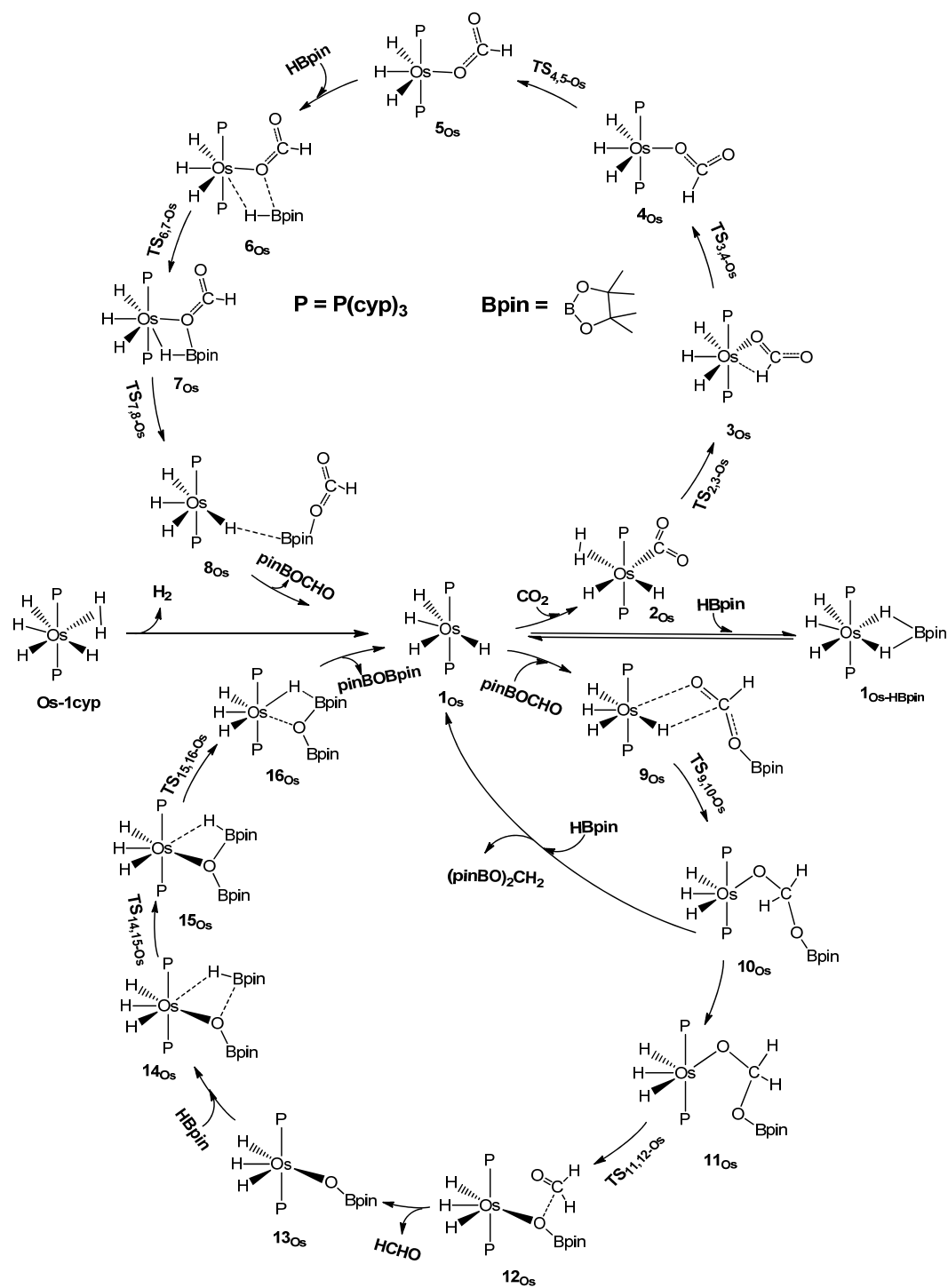
C	−4.19693100	3.62119700	−0.01666200
H	−4.27802100	3.93271200	1.02920400
H	−4.86303200	4.25554400	−0.61128400
H	−4.53845800	2.58690500	−0.09146500
O	−1.17328300	2.75224500	−1.89643100
O	−1.93425200	2.84990900	0.26445700
B	−0.98428300	2.35874400	−0.59834500
16os			
$G_{\text{solv}} = -2847.936142; E_{\text{solv}} = -2849.05786861$			
C	−1.25146200	−2.29384800	3.08596800
H	−1.62645200	−2.09231200	4.09603700
C	0.12548600	−3.01863600	3.21502900
H	0.92061200	−2.49879400	2.67529300
H	0.41816000	−3.06632600	4.27031500
C	−0.09053600	−4.43459200	2.65050200
H	0.16862400	−4.44777700	1.58413000
H	0.52791800	−5.18707300	3.15102500
C	−1.59268700	−4.68217500	2.80351200
H	−1.83328800	−4.92678400	3.84724200
H	−1.96156700	−5.49974200	2.17469200
C	−2.19327300	−3.32514600	2.42490900
H	−3.23091300	−3.20523100	2.75344400
H	−2.17151900	−3.21815800	1.33474900
C	−0.32415900	0.36639600	3.54956900
H	−0.82141700	0.09091300	4.49015400
C	1.18650500	0.13314000	3.73011800
H	1.40990200	−0.79950000	4.25613500
H	1.67940200	0.09744200	2.75118700
C	1.64424100	1.37405700	4.50003500
H	1.33704200	1.29994500	5.55205300
H	2.73175700	1.50935000	4.47992300
C	0.89131100	2.51023500	3.79945200
H	1.45886400	2.80311000	2.91115900
H	0.77378400	3.40112500	4.42617600
C	−0.46245400	1.90286800	3.36070000
H	−0.68669900	2.17005900	2.32576700
H	−1.29247200	2.28463600	3.96563100
C	−2.87058200	0.04809000	2.32455300
H	−2.71580300	1.10195400	2.06859400
C	−3.61075100	−0.02684600	3.69243700
H	−3.12173800	−0.68743700	4.41480400
H	−3.63959600	0.96732500	4.15265700
C	−5.03740500	−0.52187000	3.37220100
H	−5.09472400	−1.60933900	3.50833400
H	−5.79635000	−0.07334300	4.02165300
C	−5.23358700	−0.18963200	1.88949300
H	−5.45816000	0.88020200	1.77374900
H	−6.05120200	−0.75329000	1.42669800
C	−3.86458300	−0.50423400	1.28058100
H	−3.70145100	−0.05038900	0.30061300
H	−3.75740400	−1.58582900	1.14901600
C	0.94790100	−0.51544300	−3.43888800
H	1.48621700	−1.10939700	−4.19173900
C	1.70024300	0.80920500	−3.25043500
H	2.77970800	0.67403400	−3.13254900
H	1.32105000	1.32263900	−2.36360700
C	1.33750300	1.61313700	−4.50476800
H	1.46013500	2.69096200	−4.35431300

H	1.99725200	1.31999000	−5.33117800
C	−0.12335400	1.22229800	−4.82243100
H	−0.80757300	2.01539100	−4.50857700
H	−0.26822500	1.07282100	−5.89773000
C	−0.40812700	−0.07143300	−4.02078000
H	−0.86159500	−0.85276100	−4.64002600
H	−1.09702900	0.14004500	−3.19663600
C	−0.18109400	−2.99283200	−2.66542900
H	−1.12977000	−2.51499000	−2.93961600
C	−0.52000800	−4.17635400	−1.70810400
H	0.08008500	−4.16863700	−0.79708000
H	−1.56279600	−4.09684200	−1.38501800
C	−0.28454500	−5.46407700	−2.52494400
H	0.70483500	−5.87937300	−2.29325700
H	−1.02132300	−6.24312400	−2.30412100
C	−0.30958000	−5.01011600	−3.98793700
H	−1.34644600	−4.87496200	−4.32375600
H	0.17146900	−5.71981400	−4.66946600
C	0.39776200	−3.65312300	−3.93381100
H	0.23538100	−3.04885100	−4.83246300
H	1.47907200	−3.81607500	−3.83658400
C	2.51889600	−2.22138900	−1.76476100
H	2.85784700	−2.49930100	−2.77028800
C	3.49019100	−1.14892500	−1.18864500
H	4.18527900	−0.81312600	−1.96702800
H	2.95543600	−0.26947300	−0.82124600
C	4.24419200	−1.83321100	−0.03164300
H	5.28372000	−1.49652300	0.05349400
H	3.73746000	−1.60234300	0.91347500
C	4.11835400	−3.33156600	−0.32200900
H	4.30268800	−3.95742000	0.55791700
H	4.83139600	−3.63088600	−1.10246400
C	2.68268900	−3.44673400	−0.84186200
H	1.99666100	−3.37098100	0.00887200
H	2.48016600	−4.38955100	−1.36155700
P	−1.14909000	−0.64643900	2.21931800
P	0.77890800	−1.57937600	−1.92172100
Os	−0.18933700	−0.82672900	0.07906000
H	1.29816300	−1.00128400	0.82141600
H	−1.32840700	−1.90021200	−0.22030200
H	0.07771200	−2.33156900	0.51372600
C	2.84094900	4.02358300	−0.02615600
C	3.62120900	2.74770900	0.49448600
C	3.51587200	4.74782300	−1.18268400
H	2.90267600	5.60091600	−1.48709300
H	4.49723400	5.12728800	−0.88005700
H	3.64207800	4.09722400	−2.05043600
C	4.54457700	2.13110600	−0.55418500
H	5.39843900	2.78157900	−0.76520700
H	4.92267900	1.17792100	−0.17583000
H	4.01478100	1.93358000	−1.49032800
C	2.48289300	5.02379500	1.07178000
H	3.37503200	5.51893300	1.46655600
H	1.82360700	5.78875900	0.65141800
H	1.95353900	4.54699800	1.90045400
C	4.37702800	2.95570500	1.79838700
H	4.84653100	2.01515600	2.10062100
H	5.16498200	3.70561700	1.67288700

H	3.71478000	3.27723000	2.60456700
O	1.59797300	3.46204800	−0.50724800
O	2.56164000	1.79045300	0.73486600
B	1.47083000	2.21545600	0.04290500
O	0.32327000	1.48219100	−0.09588300
C	−2.41640800	2.94498300	−1.93736800
C	−2.67802300	3.39419700	−0.44985200
H	−1.51746800	−0.12363100	−0.71738500
C	−2.42187000	4.08564600	−2.94411400
H	−2.26099600	3.69357000	−3.95232200
H	−3.38907300	4.59937400	−2.93482600
H	−1.63484300	4.81277400	−2.73396600
C	−2.18961700	4.81200000	−0.15119900
H	−2.81266400	5.56632700	−0.64088600
H	−2.23278900	4.97947700	0.92912000
H	−1.15215100	4.94906000	−0.47154100
C	−3.34377700	1.82469800	−2.40520100
H	−4.37572200	2.17654700	−2.49722300
H	−3.01376300	1.47724600	−3.38822100
H	−3.31585000	0.97113400	−1.72271500
C	−4.11003900	3.21109700	0.02742800
H	−4.19230500	3.52495900	1.07239700
H	−4.79682400	3.82450400	−0.56543500
H	−4.42374600	2.16769000	−0.04076900
O	−1.07943100	2.39699100	−1.86326500
O	−1.82533300	2.50386700	0.30062400
B	−0.87160800	2.03709200	−0.56329900
1Os-HBpin			
$G_{\text{solv}} = -2362.223963$; $E_{\text{solv}} = -2363.17615466$			
C	16.04781400	3.72899800	7.04819200
H	16.91194900	4.10309500	7.61035100
C	16.57818700	2.99612600	5.77686500
H	16.17427200	3.40477800	4.84848700
H	17.66799200	3.09659500	5.72694700
C	16.18202100	1.51884400	5.95028300
H	15.20150900	1.34478800	5.48810500
H	16.89735000	0.83345000	5.48381200
C	16.05791300	1.33630900	7.46441000
H	17.05368100	1.26850800	7.92309000
H	15.49680100	0.43943200	7.74717800
C	15.36081700	2.63049900	7.89176100
H	15.42670200	2.82946700	8.96650200
H	14.29932600	2.55946300	7.62977400
C	16.22317600	6.47368400	6.16826400
H	16.98937300	6.51734100	6.95174900
C	16.90689600	6.14536800	4.81749700
H	17.84267100	5.59351400	4.95121400
H	16.24596000	5.53271700	4.19487200
C	17.09532800	7.50483800	4.13434200
H	17.96251700	8.03021000	4.55665100
H	17.25241900	7.41491400	3.05419000
C	15.80645000	8.24214900	4.50212700
H	14.97566800	7.84411600	3.90498500
H	15.85607000	9.32276000	4.32976100
C	15.59213200	7.88623000	5.98105100
H	14.53504900	7.91636000	6.25343700
H	16.11264500	8.60676400	6.62415900
C	14.58913800	5.84744300	8.43320100

H	14.27026200	6.87660800	8.24311200
C	15.72080000	5.89688200	9.47765100
H	16.30498100	4.96854300	9.48856200
H	16.41641800	6.72428800	9.30190600
C	14.95775400	6.02247300	10.80046900
H	15.57920600	5.81450800	11.67804200
H	14.56375700	7.04245000	10.90391600
C	13.80443700	5.02584900	10.62811200
H	12.96879100	5.22069500	11.30806700
H	14.16679000	4.01280400	10.84472100
C	13.39939300	5.13690000	9.14161700
H	12.49762400	5.74310200	9.01202900
H	13.17421900	4.15698100	8.71374000
C	10.00488200	3.23833600	4.33569800
H	9.53429100	2.72277200	3.49051000
C	9.04870500	4.34639300	4.84199000
H	8.38048300	4.70331400	4.05115000
H	9.61310300	5.20860700	5.20591600
C	8.30636000	3.71121800	6.02285300
H	7.85029200	4.45651200	6.68429600
H	7.50777500	3.04532900	5.66830400
C	9.40626500	2.89442400	6.70181800
H	10.08816400	3.57115000	7.23385600
H	9.02853600	2.16171300	7.42273500
C	10.14881500	2.24154400	5.52704300
H	9.67929300	1.28649900	5.26364200
H	11.19002800	2.02959600	5.78791600
C	12.34477900	2.24163200	3.06876900
H	12.38870500	1.61763600	3.96945000
C	13.78752100	2.29354400	2.47468200
H	14.13626300	3.31020000	2.28854500
H	14.49150300	1.85940600	3.19188000
C	13.74084000	1.45821600	1.17953300
H	13.59209400	2.11531800	0.31293200
H	14.66628200	0.89963500	1.00677300
C	12.51400900	0.55606600	1.34352300
H	12.75043000	−0.28677900	2.00672600
H	12.15010600	0.14342500	0.39661500
C	11.50100900	1.48299400	2.02174600
H	10.66244000	0.94336900	2.47332800
H	11.08720800	2.16832600	1.27148400
C	11.20455800	4.79978700	2.19272400
H	10.50885400	4.17075800	1.62505600
C	10.51906000	6.17292800	2.46754900
H	9.49829300	6.15483300	2.06828500
H	10.44795100	6.41610000	3.52702000
C	11.36739400	7.22105700	1.72538100
H	10.77307200	8.07118400	1.37396900
H	12.13955000	7.61239200	2.40107700
C	12.03569600	6.43511200	0.59599300
H	12.89795700	6.94929700	0.15812500
H	11.31468600	6.24131300	−0.20959100
C	12.41941400	5.12727500	1.29319000
H	13.30770500	5.30920500	1.91003700
H	12.65362900	4.31356900	0.59901100
P	14.97615900	5.21547300	6.73160800
P	11.65234800	3.84629700	3.72298200
Os	13.14642000	4.79111900	5.29633600

H	14.15623700	4.99059300	4.03372700
H	12.81462600	6.49261600	4.91787000
H	12.90555800	3.42260600	6.14593500
H	14.04033100	3.50942900	4.88963200
C	10.23708000	8.09411300	6.45940500
C	11.57234500	8.66423800	7.03869600
H	11.90375600	5.32806800	6.43630900
C	9.38636300	9.09678300	5.69374500
H	8.47612300	8.60854100	5.33187600
H	9.09059900	9.93067000	6.33973600
H	9.92124400	9.49413900	4.82833600
C	12.20618000	9.72569700	6.13468500
H	11.63146900	10.65733500	6.14001700
H	13.21480200	9.94702300	6.49606100
H	12.28716000	9.37104400	5.10224600
C	9.38737300	7.37670100	7.51220700
H	8.93648500	8.07996400	8.21964000
H	8.58133000	6.83741200	7.00589200
H	9.98056000	6.64770100	8.07364000
C	11.48500600	9.17787200	8.46860300
H	12.46396500	9.54869300	8.78862300
H	10.76875800	10.00351100	8.54286000
H	11.18265000	8.38770600	9.15958100
O	10.71891100	7.10549500	5.54315700
O	12.41711000	7.50715000	7.01767600
B	11.96613200	6.64069900	6.00343300



Scheme S1. Catalytic cycle for the reduction of carbon dioxide to formaldehyde catalyzed by **1_{os}**.