

Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

**Mechanisms of Phosphine-Catalyzed [3+3] cycloaddition of ynones
and azomethine imines: A DFT Study**

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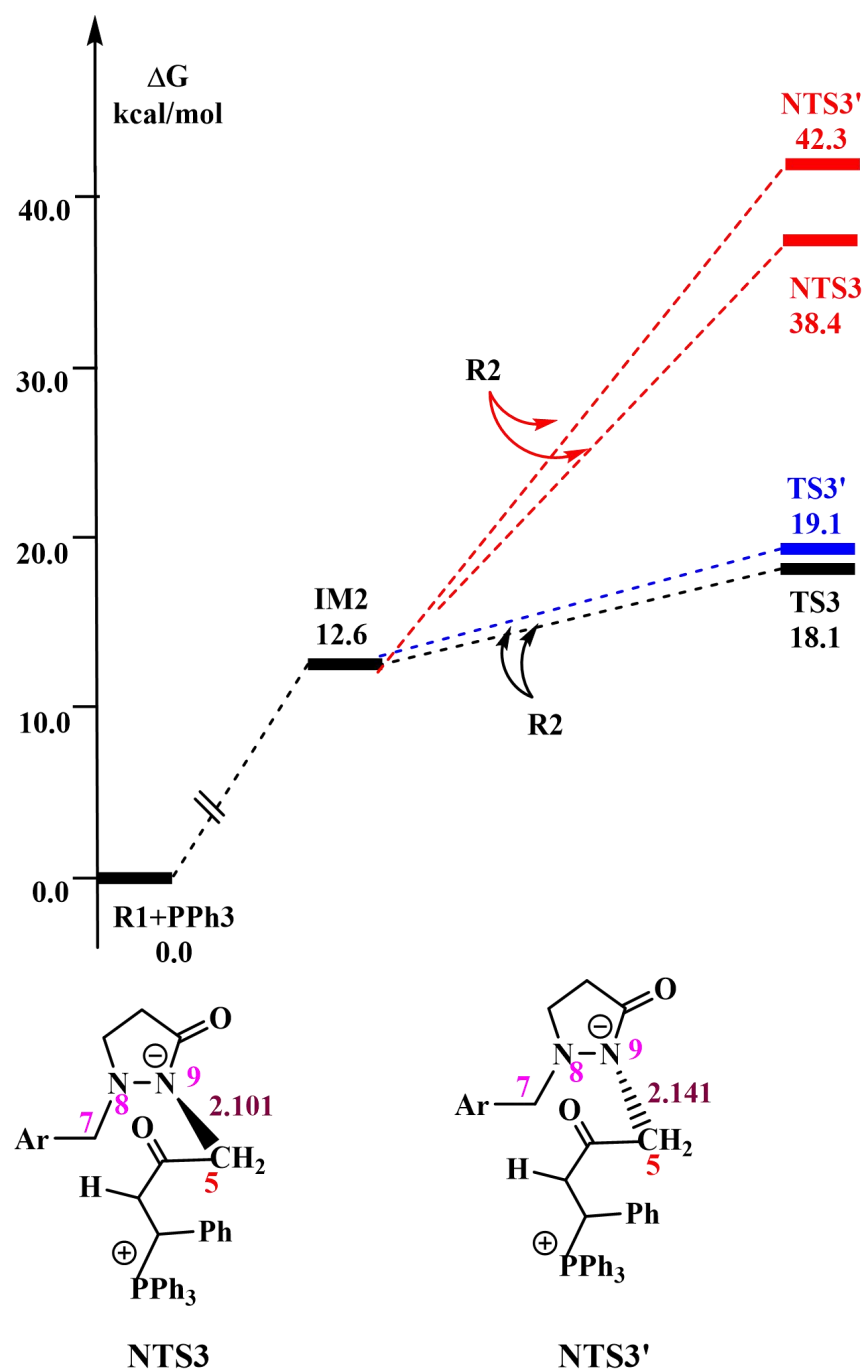
Content

Fig. S1 Free energy profile of the [3 + 3] cycloaddition reaction.

Fig. S2 Free energy profile of the addition of the N9 atom to the C5 atom.

Cartesian Coordinates

Fig. S2 Free energy profile and optimized structures for the addition of R2 to IM2 (the addition of the N9 atom to the C5 atom). The solvation-corrected relative free energies are given in kcal/mol. The bond lengths are given in Å.



Cartesian Coordinates

R1

C	0.50382000	-0.00021000	-0.09308700
C	1.71330300	-0.00031500	-0.14307900
C	-0.92919900	-0.00009000	-0.04034800
C	-1.63214900	1.21156400	-0.01591000
C	-1.63227700	-1.21162100	-0.01350100
C	-3.02065600	1.20649400	0.03508800
H	-1.08120800	2.14602400	-0.03951500
C	-3.02078300	-1.20630800	0.03751400
H	-1.08142200	-2.14617700	-0.03524100
C	-3.71693400	0.00015500	0.06199700
H	-3.56110200	2.14762000	0.05300300
H	-3.56131800	-2.14734500	0.05734800
H	-4.80169200	0.00025300	0.10148300
C	3.17833300	-0.00035300	-0.17136100
O	3.79031600	-0.00248400	-1.21471100
C	3.84932300	0.00240200	1.18119300
H	3.53772300	0.88487700	1.74884400
H	3.53805000	-0.87801200	1.75221600
H	4.93174900	0.00232900	1.04851500

R2

Br	-4.27470900	-0.30448500	0.09629800
O	6.10721500	0.06916700	0.08251500
N	2.76624000	0.34703200	-0.17058900
N	3.98517600	0.87671200	-0.28442300
C	-0.62049200	1.63518600	0.20951900
H	-0.26094300	2.62684800	0.46924100
C	-1.97485700	1.35724500	0.31076900
H	-2.67295500	2.11675900	0.64467200
C	-2.43321800	0.08675800	-0.02433200
C	-1.55180000	-0.89236900	-0.46747400
H	-1.92715800	-1.86907100	-0.75132300
C	-0.19593900	-0.60518400	-0.56254300
H	0.46190000	-1.37073700	-0.95412700
C	0.30103900	0.65935400	-0.20859700
C	1.69501600	1.08136800	-0.28436600
H	1.91132000	2.13665700	-0.41249300
C	4.90580200	-0.07701400	0.08699200
C	4.19262500	-1.35991100	0.55786700
H	4.28838300	-1.43600300	1.64408200
H	4.65651600	-2.23588800	0.10497400
C	2.76689100	-1.12721900	0.11338300
H	2.54243300	-1.64056000	-0.82389000

H	1.98727900	-1.33983900	0.84610100
<i>n</i>-BuOH			
C	-1.80217900	0.57328800	0.00068000
C	-0.28485900	0.56482700	0.00162400
H	-2.17353400	0.03842600	-0.88807600
H	-2.17464900	0.03581500	0.88739600
C	0.29574500	-0.84704600	-0.00023200
H	0.06542200	1.11977200	-0.87768200
H	0.06428700	1.11695500	0.88315300
C	1.82215600	-0.84537400	0.00113400
H	-0.07247400	-1.39473200	0.87726000
H	-0.07092600	-1.39178300	-0.88019800
H	2.22595900	-1.86191700	-0.00050600
H	2.21106600	-0.32649000	-0.88129500
H	2.20948000	-0.32996200	0.88628600
O	-2.22977900	1.92213700	0.00239300
H	-3.19572300	1.93532900	0.00192800
PPh₃			
P	-1.33636600	0.71643300	0.02324700
C	-0.48079000	1.43956800	1.48969200
C	-0.99851100	2.63180400	2.00855600
C	0.64540700	0.87242600	2.09491200
C	-0.39733600	3.25228700	3.09996900
H	-1.88250800	3.07364500	1.55451800
C	1.24207400	1.48849200	3.19211600
H	1.05629600	-0.05560800	1.70663700
C	0.72379700	2.67944300	3.69509000
H	-0.80885100	4.17818000	3.49040000
H	2.11469800	1.03686100	3.65466200
H	1.19013100	3.15756700	4.55118000
C	-0.65544100	-0.99938700	0.03815000
C	0.40526600	-1.43333000	-0.76195900
C	-1.25374600	-1.90999300	0.91817000
C	0.86031500	-2.74812400	-0.67780600
H	0.88070800	-0.74302300	-1.45297700
C	-0.79115500	-3.21819200	1.01111100
H	-2.08836000	-1.58792000	1.53717300
C	0.26740200	-3.64114000	0.20946300
H	1.68491200	-3.07201300	-1.30599600
H	-1.26094800	-3.91027700	1.70361100
H	0.62589700	-4.66395700	0.27510300
C	-0.37927700	1.46656000	-1.36421900
C	-0.91381200	1.32472300	-2.65064100
C	0.83519600	2.14132900	-1.20892900

C	-0.24191600	1.82881000	-3.75984300
H	-1.86554600	0.81447600	-2.78138600
C	1.50145100	2.65754400	-2.31821900
H	1.26389400	2.26361300	-0.21824200
C	0.96780100	2.49935800	-3.59448600
H	-0.66704200	1.70599300	-4.75145400
H	2.44365000	3.18072800	-2.18388500
H	1.49046800	2.90098900	-4.45743000
P₁			
C	3.62077400	1.19811400	-0.37471100
C	2.33451800	1.13599100	0.02358500
C	4.61405300	0.14447600	-0.56280100
C	5.95654700	0.52422400	-0.69601500
C	4.28710200	-1.21493300	-0.68724900
C	6.94978000	-0.42233100	-0.91696700
H	6.21731400	1.57644500	-0.61723700
C	5.27686100	-2.15697700	-0.92755900
H	3.25008600	-1.52709500	-0.62308500
C	6.61148700	-1.76743000	-1.03325200
H	7.98536000	-0.10896800	-1.00434000
H	5.00812900	-3.20389800	-1.02919700
H	7.38295100	-2.51070400	-1.20942000
C	1.49738700	2.37602000	0.02944000
O	1.91710600	3.46249000	-0.29975900
C	0.04887000	2.12542700	0.41522100
H	-0.54859900	2.98557900	0.10504500
H	-0.02874900	2.01931900	1.50558600
Br	-6.39706200	-0.60197400	-0.34544100
O	3.28755400	-0.66459300	2.10412200
N	0.33956900	-0.34678800	0.23451400
N	1.70281000	0.00715300	0.57410700
C	-2.76016600	1.17155700	0.56087600
H	-2.41306600	1.93896700	1.24679000
C	-4.11368500	0.83988800	0.54954500
H	-4.81287600	1.33760200	1.21234400
C	-4.56224100	-0.14260700	-0.32292500
C	-3.68479800	-0.79598100	-1.18335300
H	-4.05577800	-1.55822300	-1.85924900
C	-2.33999400	-0.45091800	-1.16276700
H	-1.64175900	-0.95660900	-1.82471000
C	-1.86311900	0.53512300	-0.29393200
C	-0.38006300	0.83383300	-0.29283000
H	-0.06576300	0.92140700	-1.34279100
C	2.17603800	-0.73896000	1.63455800

C	1.02583500	-1.64446200	2.04732800
H	1.02234100	-1.79101800	3.12713300
H	1.14710300	-2.61535300	1.55387900
C	-0.18046300	-0.89120200	1.50289700
H	-1.04926800	-1.51630300	1.29580000
H	-0.47304600	-0.09218500	2.20434400
H	3.95051400	2.21129700	-0.60023600
P_{1a}			
C	-2.85651600	0.29677600	-0.73635300
C	-1.91471300	0.92478000	0.00365700
C	-3.93514200	-0.62854700	-0.36369700
C	-5.08373600	-0.62605500	-1.16808000
C	-3.84385900	-1.57357400	0.66670900
C	-6.13369300	-1.50261500	-0.92109900
H	-5.15021900	0.07899400	-1.99279200
C	-4.88369000	-2.46285600	0.90028700
H	-2.95271300	-1.61359200	1.28052400
C	-6.03607400	-2.42501200	0.11647100
H	-7.02024800	-1.47452500	-1.54686100
H	-4.79329500	-3.19300200	1.69847500
H	-6.84780200	-3.12042500	0.30691500
C	-1.84765300	0.98434500	1.49582300
O	-2.72599500	0.54137200	2.20426000
C	-0.66501900	1.69443000	2.15053000
H	-0.29932500	1.04828800	2.95403900
H	-1.09808900	2.58250500	2.62351100
Br	4.83924700	-2.00817900	-0.21288100
O	-0.51520700	0.18101400	-2.45487300
N	-0.20861400	2.66797100	0.00788000
N	-0.87005200	1.60223300	-0.66616000
C	2.86898200	1.44844800	0.93533300
H	3.15102700	2.46592100	1.19736400
C	3.86323000	0.53770300	0.59410200
H	4.90825300	0.82724200	0.58798800
C	3.49828500	-0.76149600	0.25967300
C	2.16653700	-1.16036200	0.27923100
H	1.90060900	-2.17900400	0.02028900
C	1.18600400	-0.23838400	0.63106700
H	0.14919800	-0.56724600	0.63921300
C	1.52001500	1.08335800	0.94714900
C	0.46527100	2.13784700	1.21892000
H	0.96227900	3.00452000	1.66838900
C	-0.18864600	1.13051500	-1.77938000
C	0.99752800	2.05872000	-1.98963200

H	1.04251900	2.36650300	-3.03562300
H	1.91267300	1.50752200	-1.75088100
C	0.70129100	3.20834000	-1.02460400
H	1.58842100	3.62164700	-0.54037800
H	0.17455200	4.01741100	-1.53818400
H	-2.79162100	0.48484600	-1.80494500
TS1			
C	0.36744200	-1.70309600	-0.52084300
C	-0.69736900	-2.39381200	-0.53246700
C	1.81638900	-1.93045600	-0.62411800
C	2.36903600	-3.05581400	-0.00086200
C	2.65189700	-1.07901100	-1.35256000
C	3.73133500	-3.31385700	-0.09819700
H	1.71185100	-3.71578400	0.55656600
C	4.01606200	-1.33858000	-1.44773300
H	2.22709800	-0.21416000	-1.85584500
C	4.56015300	-2.45456600	-0.81773600
H	4.14961700	-4.18722600	0.39313900
H	4.65157600	-0.67146500	-2.02254900
H	5.62451400	-2.65649600	-0.88947300
C	-2.09729100	-2.56317100	-0.40945100
O	-2.66441900	-2.72453200	0.67579200
C	-2.89513000	-2.59732600	-1.70108500
H	-2.27644900	-2.39959100	-2.57932400
H	-3.36701800	-3.57960600	-1.80021300
H	-3.68902400	-1.84635500	-1.63435100
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C	-0.30082800	0.35968800	1.81922300
C	-0.91638600	-0.73850700	2.43743800
C	0.09107700	1.45931200	2.59367200
C	-1.13138800	-0.72335400	3.81304200
H	-1.26110600	-1.59408300	1.86015100
C	-0.11684200	1.45586300	3.96928600
H	0.55570400	2.32125300	2.12586200
C	-0.72683800	0.36435400	4.58187800
H	-1.61830200	-1.57354900	4.28020300
H	0.19274100	2.31245100	4.56018700
H	-0.89088000	0.36473100	5.65530600
C	0.91695500	1.85285100	-0.33708400
C	0.38464600	2.95499300	-1.01294500
C	2.25985900	1.88007200	0.06850700
C	1.18438000	4.06466900	-1.27934500
H	-0.65544500	2.95311400	-1.32398400
C	3.04997400	2.99339700	-0.19130600

H	2.68526600	1.02441400	0.58878800
C	2.51416000	4.08691300	-0.87046600
H	0.76073900	4.91673400	-1.80223000
H	4.08646800	3.00506900	0.13136000
H	3.13306100	4.95380700	-1.08049300
C	-1.66231000	0.58941800	-0.76096000
C	-1.71775200	0.59876200	-2.16090600
C	-2.83541600	0.74639500	-0.02243700
C	-2.92828400	0.80166100	-2.81265900
H	-0.80779500	0.44574300	-2.73823000
C	-4.05034300	0.93352100	-0.67958800
H	-2.80449600	0.70994400	1.06225600
C	-4.09670300	0.97021300	-2.07009300
H	-2.96351900	0.81349500	-3.89755700
H	-4.96140800	1.04784600	-0.10078700
H	-5.04494900	1.11944700	-2.57749200
TS1a			
C	-0.03497600	-1.48959300	-0.97186200
C	1.01944500	-2.14939400	-1.22469200
C	-1.49365700	-1.65209700	-1.13407100
C	-2.14180500	-2.69757100	-0.46762700
C	-2.25328000	-0.74743800	-1.88550400
C	-3.52532700	-2.82721800	-0.53922500
H	-1.54494900	-3.39471300	0.11229400
C	-3.63720900	-0.88150800	-1.95847600
H	-1.75508800	0.06232500	-2.41118200
C	-4.27712500	-1.91619400	-1.27845300
H	-4.01869600	-3.63806000	-0.01179600
H	-4.21629600	-0.17825600	-2.54955800
H	-5.35708600	-2.01617800	-1.33093100
C	2.37235200	-2.53885400	-1.27148200
O	2.90258800	-3.28958500	-0.44670600
C	3.18837500	-1.95466300	-2.41510000
H	2.56260300	-1.56148400	-3.22023500
H	3.80013800	-1.13976200	-2.00827800
H	3.86257300	-2.72128700	-2.80452500
P	0.15654000	0.29104500	0.18449400
C	-0.27964900	1.80681400	-0.71884600
C	0.29222600	1.98269100	-1.98789700
C	-1.18547700	2.75313600	-0.23386300
C	-0.03224300	3.09759400	-2.75160800
H	0.98766100	1.23968700	-2.37409000
C	-1.51342500	3.86401800	-1.00810700
H	-1.63204400	2.62463300	0.74746000

C	-0.93887300	4.03875700	-2.26353600
H	0.41659900	3.22934900	-3.73117000
H	-2.21750400	4.59585300	-0.62443900
H	-1.19710000	4.90570600	-2.86355000
C	-0.80108600	0.29431300	1.72890600
C	-0.18168500	0.39018900	2.97964300
C	-2.19165600	0.11625700	1.65738600
C	-0.94376200	0.31984500	4.14254200
H	0.89462700	0.52014300	3.04286200
C	-2.94565500	0.05653700	2.82414000
H	-2.68526000	0.02555000	0.69229700
C	-2.32407700	0.15528300	4.06730600
H	-0.45577400	0.39799300	5.10912900
H	-4.02084800	-0.07844500	2.75939200
H	-2.91516500	0.10212600	4.97639900
C	1.90658600	0.43453700	0.60180200
C	2.55712200	-0.71834800	1.05722800
C	2.63420000	1.61579600	0.41167300
C	3.92827100	-0.69440100	1.29808700
H	2.01611400	-1.65113200	1.18400400
C	3.99954400	1.63789500	0.67304900
H	2.13539100	2.51274200	0.05641400
C	4.64749600	0.48156400	1.10725400
H	4.42564600	-1.60791700	1.60605300
H	4.55990800	2.55634300	0.52800100
H	5.71784500	0.49810400	1.28968500
IMI			
C	0.98124100	-0.73360700	-0.56682100
C	0.74197800	-2.04780200	-0.60742600
C	2.26662700	0.01959000	-0.56736400
C	3.36277300	-0.51914800	0.12029600
C	2.42394800	1.23084600	-1.25036100
C	4.58599500	0.14329400	0.11912000
H	3.23955800	-1.46418600	0.64338700
C	3.64727900	1.89445900	-1.24329000
H	1.58391100	1.65303300	-1.79769300
C	4.73147600	1.35299600	-0.55742600
H	5.42855300	-0.28542100	0.65381600
H	3.75451900	2.83274100	-1.77983300
H	5.68636200	1.87022000	-0.55268100
C	1.59816400	-3.17740200	-0.60602400
O	2.05785600	-3.64855600	0.44386000
C	1.81560300	-3.89533400	-1.92891800
H	1.36514400	-3.36313800	-2.77091700

H	2.89213700	-3.99897400	-2.09200600
H	1.38873800	-4.90083400	-1.86742300
P	-0.53823500	0.02646800	-0.00861100
C	-0.81184900	-0.36996400	1.74993500
C	-0.20423200	-1.48992900	2.32792200
C	-1.64234100	0.45380200	2.52209100
C	-0.44152500	-1.77904400	3.66985000
H	0.45294600	-2.13287600	1.74582700
C	-1.87929100	0.14957100	3.85805600
H	-2.09227000	1.34092100	2.08293500
C	-1.27860700	-0.96902400	4.43175500
H	0.03575600	-2.64503900	4.11687300
H	-2.52460900	0.78959400	4.45151500
H	-1.45927600	-1.20389800	5.47642000
C	-0.57855800	1.84753000	-0.06768000
C	-1.33912600	2.53022100	-1.02011800
C	0.26689300	2.56342000	0.79014500
C	-1.25539400	3.91802500	-1.11248300
H	-1.99576200	1.98115500	-1.68920900
C	0.34790500	3.94673700	0.69199900
H	0.86782100	2.03507000	1.52672800
C	-0.41303000	4.62471100	-0.25976900
H	-1.85000000	4.44497800	-1.85209100
H	1.00791200	4.49677000	1.35516600
H	-0.34771300	5.70582800	-0.33549400
C	-1.95843500	-0.53790900	-0.98066900
C	-1.78151900	-0.86788200	-2.32757100
C	-3.23560900	-0.55035500	-0.41867200
C	-2.88408900	-1.19791700	-3.10731500
H	-0.78044400	-0.88502900	-2.74737300
C	-4.33529300	-0.88727700	-1.20417500
H	-3.37466300	-0.31426500	0.63237500
C	-4.16061100	-1.20727000	-2.54686700
H	-2.74510500	-1.45795700	-4.15187900
H	-5.32660800	-0.90650100	-0.76257200
H	-5.01847100	-1.47279600	-3.15689400
IM1a			
C	-0.96285200	-0.87290600	-0.20634200
C	-0.64598500	-2.17547800	-0.24662700
C	-2.29909700	-0.21582100	-0.13688500
C	-2.62255300	0.73031500	0.84238900
C	-3.28523000	-0.58756900	-1.05731600
C	-3.89300500	1.29451600	0.89491800
H	-1.87624100	1.01771100	1.58001800

C	-4.55819500	-0.02937200	-1.00252800
H	-3.03893600	-1.32229400	-1.81968100
C	-4.86513200	0.91816500	-0.02892600
H	-4.12714800	2.02226500	1.66611800
H	-5.31104700	-0.33185400	-1.72437300
H	-5.85729000	1.35687300	0.01317300
C	-1.54949200	-3.27812100	-0.09454700
O	-1.91413100	-3.67441000	1.01095200
C	-1.93350100	-4.04223100	-1.35579400
H	-3.02558700	-4.07392700	-1.41865900
H	-1.52619100	-3.58398100	-2.26172000
H	-1.57492700	-5.07310200	-1.28083200
P	0.55109500	0.06621500	-0.03622500
C	0.24857300	1.85923900	-0.02974300
C	-0.47702700	2.38084500	-1.10933300
C	0.63498800	2.69915900	1.01605300
C	-0.79702300	3.73189500	-1.14624700
H	-0.80441200	1.72293200	-1.91143400
C	0.30827800	4.05356400	0.97548900
H	1.17959100	2.29941500	1.86584900
C	-0.40352400	4.56930700	-0.10278700
H	-1.36308800	4.12962800	-1.98218800
H	0.60873600	4.70316200	1.79140100
H	-0.65946400	5.62393100	-0.12903700
C	1.38106700	-0.36048600	1.51887800
C	2.66689900	0.13341400	1.76776300
C	0.74022200	-1.17014100	2.46046600
C	3.29973800	-0.15709000	2.97102300
H	3.17408800	0.73686700	1.01772100
C	1.38454300	-1.45791600	3.66162600
H	-0.23065800	-1.60664000	2.23917100
C	2.65488100	-0.95023500	3.91924400
H	4.29742100	0.22430000	3.16368400
H	0.89193300	-2.09238300	4.39105500
H	3.15179300	-1.18325300	4.85601000
C	1.75880900	-0.21740900	-1.37176400
C	2.07762000	-1.52828700	-1.74946200
C	2.40668900	0.86209400	-1.98218200
C	3.02384500	-1.74524400	-2.74516300
H	1.56128000	-2.35338000	-1.26666500
C	3.35672700	0.63196600	-2.97430000
H	2.17205600	1.88135800	-1.69200600
C	3.66363400	-0.66965300	-3.35820400
H	3.26450300	-2.76164600	-3.04037800

H	3.85338900	1.47355100	-3.44672300
H	4.40345800	-0.84659400	-4.13293800
TS2₁			
C	-0.85298300	1.13562100	0.41465700
C	-0.22304400	1.97855000	1.24606000
C	-2.16940900	1.40209600	-0.23527700
C	-3.26244200	1.77069100	0.55784000
C	-2.33864400	1.31809400	-1.62187300
C	-4.49722600	2.03997900	-0.02631900
H	-3.13092000	1.84698700	1.63317000
C	-3.57314300	1.58228200	-2.20315900
H	-1.49872700	1.03024200	-2.24990000
C	-4.65805900	1.94010600	-1.40512800
H	-5.33660900	2.32381200	0.60109800
H	-3.68893100	1.50764800	-3.28018800
H	-5.62396600	2.14152400	-1.85823200
C	-0.73747600	3.31341400	1.60186500
O	-1.40146600	3.51360700	2.60158300
C	-0.32562200	4.42737400	0.66194500
H	0.75558500	4.40626200	0.49286400
H	-0.81604200	4.27104000	-0.30652600
H	-0.62813300	5.38960700	1.07817800
P	-0.08023600	-0.51860200	0.16730900
C	0.14840100	-1.52305000	1.67294500
C	0.32190000	-0.94489300	2.93290700
C	0.07280800	-2.91617000	1.55263300
C	0.43211100	-1.76013500	4.05458600
H	0.38045000	0.13055700	3.03698000
C	0.21055800	-3.72469100	2.67630300
H	-0.10934100	-3.37519100	0.58478200
C	0.38775900	-3.14601200	3.92945600
H	0.56104700	-1.30498500	5.03121200
H	0.16276700	-4.80389400	2.57087400
H	0.48169000	-3.77491500	4.80963600
C	-1.43052000	-1.46677400	-0.65207000
C	-1.33684500	-1.92815900	-1.96541000
C	-2.61912100	-1.66851900	0.06133800
C	-2.42049800	-2.57384900	-2.56116900
H	-0.42461100	-1.78015800	-2.53547800
C	-3.70019600	-2.30113800	-0.53661700
H	-2.70125900	-1.31426800	1.08674200
C	-3.60168000	-2.75482100	-1.85237200
H	-2.33702100	-2.93026600	-3.58322100
H	-4.62091200	-2.44026800	0.02105600

H	-4.44692400	-3.24972000	-2.32076100
C	1.26158800	-0.64147600	-1.04189700
C	1.45882200	0.38335300	-1.96802500
C	2.03667600	-1.80236200	-1.10445900
C	2.44654100	0.25236500	-2.94305800
H	0.86178600	1.29004000	-1.91445900
C	3.00825800	-1.93331300	-2.09007700
H	1.90029200	-2.59037600	-0.37057500
C	3.21855800	-0.90412400	-3.00719700
H	2.61059500	1.05776900	-3.65213800
H	3.61371300	-2.83326000	-2.13095100
H	3.98526200	-1.00392300	-3.76919800
C	6.29154700	0.98917700	-0.96335100
C	5.03435800	1.71695100	-0.49446000
H	6.95852100	1.64680700	-1.52953200
H	6.85322900	0.59185100	-0.11105100
H	6.02511800	0.14198800	-1.60602200
C	4.09015100	0.80559300	0.28376100
H	5.31227600	2.58149300	0.12302300
H	4.50109500	2.12095000	-1.36679000
C	2.80125700	1.50068900	0.70739300
H	3.83578300	-0.06222000	-0.33461900
H	4.58842300	0.41310500	1.17988700
H	3.06262800	2.33461000	1.39005200
H	2.36672000	1.99389700	-0.19043700
O	1.90144800	0.63125100	1.31539000
H	0.90379200	1.46233200	1.53449800
TS2a₁			
C	-0.60784600	1.14834700	-0.39495900
C	0.55646900	1.70566700	-0.75717100
C	-1.90823200	1.85556600	-0.22664700
C	-2.62554200	2.30851600	-1.33682500
C	-2.42047000	2.07252500	1.05862800
C	-3.85252500	2.94271000	-1.16383800
H	-2.20266000	2.17202800	-2.32682100
C	-3.64945400	2.70444600	1.22781000
H	-1.84898900	1.74246600	1.92337200
C	-4.37175800	3.13133100	0.11511200
H	-4.40416200	3.29121500	-2.03158300
H	-4.04004100	2.86840900	2.22762600
H	-5.33152400	3.62191300	0.24576600
C	0.66389700	3.14637400	-1.09324300
O	0.18369500	3.62610100	-2.10187000
C	1.46911500	3.93637000	-0.08706900

H	0.82335700	4.15220100	0.77328500
H	2.30382500	3.32983900	0.28014500
H	1.80675100	4.87699400	-0.52568200
P	-0.58149800	-0.61722600	0.02162800
C	-2.08124400	-1.40098600	-0.66921900
C	-3.36225200	-0.94797800	-0.31606600
C	-1.95766300	-2.47480000	-1.55817700
C	-4.49008900	-1.55545000	-0.85565300
H	-3.48706400	-0.12812500	0.38371400
C	-3.09318700	-3.07670600	-2.09461900
H	-0.97730600	-2.84551800	-1.83747100
C	-4.35875500	-2.61719800	-1.74809000
H	-5.47435100	-1.19324900	-0.57667800
H	-2.98234100	-3.90623800	-2.78555200
H	-5.24285100	-3.08588500	-2.16924000
C	0.80772400	-1.46149700	-0.76036600
C	1.47929000	-2.48097400	-0.08459400
C	1.10802500	-1.18208900	-2.09799600
C	2.44945200	-3.22353000	-0.75093400
H	1.25731200	-2.68228100	0.95920400
C	2.07421000	-1.93457100	-2.75688100
H	0.59225600	-0.37975400	-2.61707000
C	2.74126400	-2.95777100	-2.08592000
H	2.98087000	-4.00799200	-0.22191300
H	2.31067400	-1.71488100	-3.79304000
H	3.49932100	-3.53913400	-2.60143000
C	-0.58357700	-0.91847700	1.80902300
C	0.45312000	-0.35868900	2.57215500
C	-1.59270900	-1.67747500	2.41174500
C	0.44936000	-0.56316100	3.94952700
H	1.26108900	0.19155000	2.06627400
C	-1.57754800	-1.86731200	3.79030500
H	-2.38431300	-2.12095700	1.81639400
C	-0.56029300	-1.30684500	4.55803300
H	1.24767100	-0.13798500	4.55005500
H	-2.36024900	-2.45345600	4.26143000
H	-0.55184500	-1.45531500	5.63391100
C	7.30817800	1.17308700	-0.03240900
C	6.10655800	0.23085800	-0.01334400
H	8.23877200	0.64518400	-0.26455900
H	7.17192700	1.96027100	-0.78183200
H	7.43269800	1.66267300	0.93956200
C	4.79570500	0.94205800	0.31035100
H	6.01546000	-0.26858000	-0.98777100

H	6.27637100	-0.56624500	0.72306800
C	3.57484300	0.01512700	0.30510400
H	4.85846000	1.42204600	1.29662500
H	4.61897500	1.74790500	-0.41683100
H	3.78968300	-0.82598200	1.00346600
H	3.52293400	-0.45855900	-0.70138300
O	2.41221300	0.66798700	0.64065400
H	1.57009500	1.14630800	-0.42235600
IM2₁			
C	-0.10518300	-0.20266500	-1.08480200
C	0.06693700	-1.37893900	-1.72755000
C	0.75880300	1.00956000	-1.16406200
C	0.49819800	2.02193600	-2.09015200
C	1.80695600	1.16423800	-0.25057900
C	1.27296000	3.17836700	-2.09919600
H	-0.31198900	1.89539500	-2.80274500
C	2.58166300	2.32119900	-0.26277100
H	2.03745300	0.34765100	0.42895200
C	2.31004300	3.33317500	-1.18107400
H	1.06920100	3.95838800	-2.82635800
H	3.40694900	2.42163500	0.43710300
H	2.91423600	4.23530600	-1.19127000
C	1.05225000	-1.80888500	-2.80129800
O	0.56035000	-2.66450000	-3.57013500
C	2.34244700	-1.29541800	-2.73682600
H	2.56352100	-0.38132300	-2.20030100
H	2.51675600	-1.96195000	-0.82465300
H	3.06190700	-1.63224400	-3.47606900
P	-1.41237800	-0.07387800	0.13399400
C	-2.19365800	1.56346900	0.08961000
C	-1.43885100	2.68794000	0.45482600
C	-3.52133200	1.71570400	-0.31873100
C	-2.01371400	3.95137500	0.39726500
H	-0.40584000	2.57683800	0.77516000
C	-4.08934300	2.98608800	-0.37007000
H	-4.11318500	0.84794200	-0.59236400
C	-3.33673800	4.10139900	-0.01595700
H	-1.42467200	4.82002500	0.67265600
H	-5.12081600	3.10055200	-0.68724800
H	-3.78120000	5.09092300	-0.06040500
C	-2.69606200	-1.31685000	-0.14809700
C	-3.22790100	-2.03583000	0.92476300
C	-3.18356700	-1.52147900	-1.44626200
C	-4.24990700	-2.95439100	0.69963300

H	-2.83982200	-1.88838000	1.92810500
C	-4.20319900	-2.44081500	-1.66076300
H	-2.74868400	-0.98477100	-2.28534000
C	-4.73600800	-3.15528600	-0.58854700
H	-4.65841700	-3.51835900	1.53188700
H	-4.57050900	-2.60938300	-2.66753100
H	-5.52608100	-3.87929000	-0.76125900
C	-0.75736200	-0.29471300	1.80531800
C	0.33594700	-1.14826300	1.98174000
C	-1.36041900	0.33052200	2.90343500
C	0.82699100	-1.36707800	3.26627900
H	0.83859000	-1.61736400	1.13731600
C	-0.86671100	0.09476400	4.18186300
H	-2.20329700	1.00132800	2.75806200
C	0.22729300	-0.75161200	4.36171900
H	1.68634400	-2.01721600	3.39695600
H	-1.32985700	0.57824300	5.03606200
H	0.61608300	-0.92399200	5.36081200
C	6.75740400	0.73330100	0.70950600
C	6.19412300	-0.68143300	0.59748900
H	7.84436000	0.73001800	0.83340000
H	6.52154800	1.31525200	-0.18800700
H	6.32298000	1.25730200	1.56845600
C	4.67959000	-0.68656900	0.41043800
H	6.66571700	-1.19996800	-0.24689900
H	6.45531100	-1.25553300	1.49652300
C	4.08628200	-2.08813200	0.31199300
H	4.20068700	-0.16304200	1.25165400
H	4.41403800	-0.13063300	-0.49927200
H	4.55982600	-2.62875900	-0.52084600
H	4.30681100	-2.64854400	1.23037200
O	2.68432300	-2.06473800	0.14865000
H	-0.64724300	-2.18206200	-1.54576800
IM2a₁			
C	-0.73590300	1.02007100	-0.69486100
C	0.32597100	1.39124300	-1.43226300
C	-1.86492400	1.90348100	-0.28308800
C	-2.18051900	2.10076100	1.06765100
C	-2.66020600	2.51627300	-1.26200300
C	-3.27301300	2.88438400	1.42870700
H	-1.56071600	1.65770600	1.84030700
C	-3.74786200	3.30174500	-0.89407700
H	-2.40700400	2.37829700	-2.30655200
C	-4.06278900	3.48206300	0.45092500

H	-3.50068900	3.03205600	2.47977300
H	-4.35075100	3.77374700	-1.66360400
H	-4.91471100	4.09204400	0.73499800
C	0.55496200	2.78195600	-1.95840600
O	-0.23413500	3.31539300	-2.71052300
C	1.83945700	3.41709500	-1.50672400
H	1.85184400	3.46274600	-0.41383500
H	2.67893600	2.76195200	-1.75932900
H	1.93915200	4.40344400	-1.96192600
P	-0.66923200	-0.66492700	-0.03746800
C	0.57126700	-1.63001800	-0.93160300
C	0.21485600	-2.19353500	-2.16528600
C	1.87038400	-1.76502800	-0.43769000
C	1.15683100	-2.90762400	-2.89368400
H	-0.79395900	-2.07788200	-2.55195000
C	2.80522000	-2.48740500	-1.17706100
H	2.16370500	-1.25254200	0.46993200
C	2.45108100	-3.05831100	-2.39433000
H	0.88292900	-3.34392000	-3.84867200
H	3.81912900	-2.58073000	-0.80145400
H	3.18720200	-3.61643800	-2.96496700
C	-0.36028200	-0.64969400	1.75092000
C	-1.18910700	-1.36674500	2.62239800
C	0.68464500	0.15184500	2.23627700
C	-0.95918500	-1.30028000	3.99254100
H	-2.01482400	-1.96140700	2.24569100
C	0.89546400	0.20098700	3.61322000
H	1.32531500	0.69824700	1.50857800
C	0.08271700	-0.51830800	4.48685600
H	-1.59930900	-1.85359800	4.67222800
H	1.70356900	0.81313800	4.00139200
H	0.25605400	-0.46600700	5.55776300
C	-2.22923200	-1.56564100	-0.30071400
C	-3.43921100	-0.92922900	-0.58907200
C	-2.19582700	-2.96248200	-0.16708700
C	-4.59944400	-1.68593600	-0.74633100
H	-3.48855100	0.14773000	-0.69573800
C	-3.35842100	-3.70792100	-0.31684500
H	-1.25646600	-3.46565800	0.04720300
C	-4.56291000	-3.06888400	-0.60846200
H	-5.53366500	-1.18457500	-0.97711400
H	-3.32273800	-4.78736600	-0.21152200
H	-5.47046000	-3.65182900	-0.73031800
C	7.15262300	-0.26218000	0.31704600

C	6.07880400	0.76870300	0.65885000
H	8.14914600	0.06253800	0.63313600
H	6.94195800	-1.22016600	0.80585500
H	7.18585800	-0.44413900	-0.76290300
C	4.68043500	0.34236900	0.22277900
H	6.07874700	0.95397200	1.74159000
H	6.32661000	1.72812500	0.18613100
C	3.57056900	1.34400200	0.58966600
H	4.64972000	0.19105400	-0.86633800
H	4.43992400	-0.63161500	0.67850100
H	3.58160400	1.42923300	1.70832800
H	3.92289300	2.34858800	0.24164800
O	2.34778500	1.00708500	0.09064900
H	1.16011000	0.71078600	-1.58530900
TS2₂			
C	-0.25283800	-0.07044700	-1.22056000
C	-0.08788400	-1.18593100	-1.94932200
C	0.45149200	1.23958800	-1.33047000
C	-0.15104900	2.29679700	-2.01691400
C	1.66757500	1.43854000	-0.66607100
C	0.45174300	3.55103000	-2.03736200
H	-1.09803700	2.13516300	-2.52612200
C	2.26096100	2.69785300	-0.68636800
H	2.15861600	0.57529700	-0.21478900
C	1.65287700	3.75540700	-1.36184100
H	-0.01871900	4.36750800	-2.57659800
H	3.21223600	2.84606200	-0.18336800
H	2.12207100	4.73483900	-1.37467000
C	0.86464700	-1.47595600	-3.10686100
O	0.47250100	-2.36132800	-3.85767100
C	2.17102100	-0.85562900	-3.06300700
H	2.15132400	0.22987500	-2.95717900
H	2.55481200	-1.21935000	-1.85936000
H	2.79895500	-1.18244400	-3.89166800
P	-1.37208100	-0.16041900	0.19877800
C	-2.25675900	1.40462700	0.43524900
C	-1.52416100	2.53305100	0.83216300
C	-3.63338600	1.50452500	0.21925400
C	-2.17173700	3.75082100	0.99653200
H	-0.45158000	2.46233200	0.99804300
C	-4.27384200	2.72980200	0.38902200
H	-4.20934000	0.63183700	-0.07206600
C	-3.54442200	3.85032500	0.77361900
H	-1.60063800	4.62391100	1.29456800

H	-5.34355300	2.80420400	0.22242000
H	-4.04532600	4.80462100	0.90380600
C	-2.58965500	-1.47585600	-0.03854000
C	-2.83016300	-2.40736100	0.97334400
C	-3.29980200	-1.54347500	-1.24516900
C	-3.78748200	-3.40067300	0.78011900
H	-2.26630100	-2.36403100	1.90027400
C	-4.25477800	-2.53566000	-1.42761100
H	-3.08922700	-0.83550300	-2.04306400
C	-4.49801800	-3.46281300	-0.41432600
H	-3.96877300	-4.13085800	1.56186300
H	-4.79841500	-2.59407200	-2.36469900
H	-5.23891200	-4.24187800	-0.56324200
C	-0.43894900	-0.46946600	1.70796300
C	0.78799300	-1.13553100	1.62773600
C	-0.97892900	-0.08284600	2.94386400
C	1.47323300	-1.40801800	2.81279800
H	1.26911300	-1.41113500	0.67839500
C	-0.28736400	-0.37711500	4.11107500
H	-1.92637700	0.44870200	2.98976000
C	0.94071100	-1.03906000	4.04313700
H	2.43595200	-1.90657800	2.75158800
H	-0.69792400	-0.08137500	5.07129000
H	1.48356600	-1.25834400	4.95778000
C	6.89088200	0.39069200	1.38103700
C	6.21092400	-0.80469500	0.71702200
H	7.93729900	0.18211100	1.62534700
H	6.86785800	1.26598400	0.72254300
H	6.37663700	0.66358800	2.30933700
C	4.75089900	-0.53860700	0.36276800
H	6.75852600	-1.08069700	-0.19359200
H	6.26829300	-1.67665000	1.38265600
C	4.04131700	-1.72837600	-0.29704700
H	4.18984300	-0.26172300	1.26941900
H	4.68320700	0.32224300	-0.31943200
H	4.60223500	-1.97979900	-1.22211600
H	4.16648800	-2.60891500	0.36807300
O	2.71142900	-1.47285800	-0.56263700
H	-0.70446200	-2.05841700	-1.73579800
TS2a₂			
C	-0.93606500	0.99250900	-0.77784800
C	-0.07320700	1.35086700	-1.74682500
C	-1.98502200	1.86073500	-0.16712100
C	-2.11767900	2.03285700	1.21478900

C	-2.91381500	2.47769700	-1.01773800
C	-3.16021400	2.79912400	1.73205100
H	-1.39259700	1.60004100	1.89481100
C	-3.95323700	3.23643000	-0.49741800
H	-2.79442700	2.36984500	-2.09016500
C	-4.08350100	3.39559400	0.88142800
H	-3.24099700	2.93350400	2.80629900
H	-4.65761200	3.71349500	-1.17166800
H	-4.89529300	3.99124300	1.28775400
C	0.24517900	2.77878700	-2.17680100
O	-0.59091200	3.66758900	-2.10800800
C	1.66994000	2.89231500	-2.43065300
H	2.20209000	2.38033800	-1.32911700
H	2.03459400	2.14696500	-3.14575900
H	1.97843900	3.90509500	-2.68709700
P	-0.73591600	-0.68134600	-0.10988400
C	0.43805900	-1.64599400	-1.10438600
C	-0.00557600	-2.71915300	-1.88560100
C	1.79567900	-1.29233900	-1.09045600
C	0.91215600	-3.45934700	-2.62466100
H	-1.05784000	-2.98010300	-1.92461200
C	2.70034000	-2.04511000	-1.83334900
H	2.13590100	-0.38739600	-0.57869800
C	2.26437900	-3.13084900	-2.58949700
H	0.56689400	-4.29179400	-3.22936200
H	3.74974400	-1.76672400	-1.82275100
H	2.97738000	-3.71358700	-3.16483400
C	-0.11043900	-0.54507900	1.58790100
C	-0.75000400	-1.17245900	2.66276300
C	1.00978600	0.27159100	1.79885600
C	-0.24939400	-1.00890900	3.95056100
H	-1.64647500	-1.76369800	2.50982600
C	1.49948600	0.41628600	3.09424800
H	1.51116700	0.81528100	0.98572000
C	0.87844100	-0.22079300	4.16588400
H	-0.74820900	-1.49213700	4.78461400
H	2.36995200	1.04475500	3.25544200
H	1.26598400	-0.09441300	5.17231700
C	-2.28826700	-1.61435300	-0.08087400
C	-3.48359200	-1.05563600	-0.53783400
C	-2.26864500	-2.93877800	0.38297400
C	-4.65202900	-1.81580000	-0.52096000
H	-3.51182200	-0.03255800	-0.89683000
C	-3.43779000	-3.68840800	0.39803900

H	-1.33575000	-3.38492400	0.72040000
C	-4.63148300	-3.12465600	-0.05274200
H	-5.57878200	-1.37719700	-0.87603200
H	-3.41706100	-4.71230900	0.75683700
H	-5.54455600	-3.71155200	-0.04136000
C	6.72628900	-0.38208500	1.62367900
C	6.09193300	0.27980200	0.40264200
H	7.77632600	-0.63664200	1.44949200
H	6.68152700	0.28288000	2.49294600
H	6.19523600	-1.30371000	1.88620500
C	4.62506200	0.64161500	0.61822800
H	6.65295100	1.18621200	0.14074300
H	6.17625300	-0.39094600	-0.46382300
C	3.96951100	1.31369800	-0.59002100
H	4.05536800	-0.26619900	0.87374200
H	4.52593800	1.31850600	1.47839700
H	4.54955900	2.22721200	-0.83174000
H	4.11600000	0.64141100	-1.46973300
O	2.63689200	1.59223400	-0.35640300
H	0.61335100	0.60974200	-2.14397300
IM2			
C	0.78066300	0.93282100	0.45404000
C	0.52784400	2.25982100	0.61709900
C	2.12846600	0.30058000	0.53339800
C	3.22788900	0.99037200	-0.00409500
C	2.32265700	-0.98921200	1.03981800
C	4.48499500	0.39877700	-0.00423800
H	3.07425000	1.98158900	-0.42682500
C	3.58478600	-1.57760200	1.03162100
H	1.48486000	-1.55265500	1.44595400
C	4.67130700	-0.88315900	0.51224300
H	5.32756400	0.94463600	-0.41822800
H	3.71399200	-2.57802500	1.43366000
H	5.65709000	-1.33868900	0.50421600
C	1.57023300	3.32917900	0.81015000
O	1.75560000	3.81692500	-0.35559100
C	2.09959800	3.56856800	2.03417100
H	1.80155100	2.96889700	2.88738600
H	2.82975700	4.35682300	2.17857400
P	-0.57639100	-0.10525100	-0.04644600
C	-1.92213500	0.85548300	-0.78991800
C	-2.90162300	1.41995300	0.03507400
C	-1.94382200	1.09245700	-2.16683600
C	-3.89444000	2.22050600	-0.51914400

H	-2.88582900	1.23826100	1.10623200
C	-2.94336700	1.89032600	-2.71362400
H	-1.18701600	0.65657700	-2.81178600
C	-3.91578300	2.45421800	-1.89202100
H	-4.64853600	2.66346100	0.12314100
H	-2.95846400	2.07417300	-3.78278500
H	-4.69066800	3.08086700	-2.32228500
C	0.00844300	-1.30977700	-1.26864300
C	-0.40898300	-2.64155800	-1.28493800
C	0.92936500	-0.84806900	-2.21845600
C	0.07581200	-3.50380000	-2.26497100
H	-1.09233000	-3.01572500	-0.52934700
C	1.40485600	-1.71494200	-3.19529400
H	1.29087100	0.17716500	-2.17363500
C	0.97609500	-3.04078500	-3.22010200
H	-0.24480000	-4.54060600	-2.27475900
H	2.12247200	-1.35697100	-3.92602400
H	1.35595600	-3.71855800	-3.97816500
C	-1.33856200	-0.95894900	1.36236900
C	-0.78735800	-0.80099200	2.63652900
C	-2.51699900	-1.69878200	1.19499000
C	-1.39269200	-1.41209000	3.73280700
H	0.10336700	-0.19148900	2.76923400
C	-3.11310000	-2.30804600	2.29246200
H	-2.97752400	-1.78084000	0.21304300
C	-2.54741300	-2.16824900	3.56012500
H	-0.96259000	-1.28730600	4.72107200
H	-4.02537800	-2.88141400	2.16227600
H	-3.01890300	-2.64083900	4.41612200
H	-0.46900900	2.64173000	0.39665600

IM2a

C	0.79452400	0.65603100	-0.90339800
C	0.61479000	1.85206600	-1.52211800
C	2.12281400	0.04709400	-0.62050800
C	3.08961000	0.78925500	0.06919800
C	2.40590500	-1.26717200	-0.99901400
C	4.31524200	0.20958800	0.37671200
H	2.86094000	1.81744800	0.34127700
C	3.63308300	-1.84636000	-0.68316000
H	1.66376000	-1.83424000	-1.55947100
C	4.58802300	-1.10785500	0.00867300
H	5.06397400	0.79027600	0.90680100
H	3.84493300	-2.86743600	-0.98645300
H	5.54696900	-1.55409700	0.25452900

C	1.67889600	2.90595100	-1.66535900
O	1.45376300	3.62759600	-0.62575400
C	2.58410800	2.94355300	-2.66494300
H	2.58498400	2.17561900	-3.42929700
H	3.32474500	3.73338600	-2.71146300
P	-0.60228900	-0.06474100	-0.07293000
C	-0.08360400	-0.85217400	1.47766500
C	0.42265700	-2.15730200	1.47122700
C	-0.10466600	-0.11820400	2.66685800
C	0.90072200	-2.72033900	2.64862800
H	0.44763800	-2.73068300	0.54962500
C	0.37617500	-0.68881500	3.84152100
H	-0.49529500	0.89467000	2.67843000
C	0.87809900	-1.98695100	3.83293700
H	1.29624900	-3.73068100	2.63904500
H	0.35815600	-0.11561300	4.76255500
H	1.25443700	-2.42855400	4.75031600
C	-1.80793500	1.21953000	0.35904900
C	-3.17182900	0.91585800	0.40669700
C	-1.34656200	2.49248900	0.73279600
C	-4.07955900	1.87924500	0.83518500
H	-3.52898200	-0.06276300	0.09994800
C	-2.26856500	3.44430600	1.15992500
H	-0.29382100	2.76655600	0.63774600
C	-3.62715200	3.14051700	1.21452600
H	-5.13887100	1.64557100	0.86487100
H	-1.91596500	4.43311300	1.43374600
H	-4.33756200	3.89299900	1.54285300
C	-1.42710300	-1.34613600	-1.05835500
C	-1.26225900	-1.32291100	-2.44579400
C	-2.23865900	-2.31987500	-0.46302500
C	-1.91423100	-2.26625600	-3.23577100
H	-0.61580200	-0.57391000	-2.89639400
C	-2.88741100	-3.25811600	-1.25842300
H	-2.35161200	-2.34970800	0.61792000
C	-2.72554100	-3.22995800	-2.64324900
H	-1.78305600	-2.24969800	-4.31271500
H	-3.51426000	-4.01491800	-0.79801500
H	-3.22991400	-3.96674800	-3.26050800
H	-0.39483400	2.23738400	-1.65625200
TS3			
C	1.37070900	-0.26596200	-0.48645600
C	0.78512300	0.75461600	-1.15562400
C	0.69217500	-1.41124700	0.18083800

C	0.14410400	-1.21544400	1.45375200
C	0.66113200	-2.68253100	-0.39816200
C	-0.43993300	-2.28351600	2.12933100
H	0.16170200	-0.21330600	1.88016000
C	0.07441900	-3.74844200	0.28156400
H	1.08517500	-2.83047300	-1.38881000
C	-0.47435100	-3.55006400	1.54631500
H	-0.86773500	-2.12697900	3.11527700
H	0.04179400	-4.73133600	-0.17893900
H	-0.93079800	-4.38092300	2.07600900
C	-0.64094700	0.99660900	-1.55314100
O	-0.90162000	2.17595000	-1.88946900
C	-1.60271700	-0.01859500	-1.44636900
H	-2.52234300	0.14167500	-1.99892800
H	-1.33803700	-1.04600800	-1.22560000
P	3.14212000	-0.22748600	-0.22930300
C	3.78840900	1.44617500	-0.35589000
C	4.95568700	1.72399400	-1.07542800
C	3.09586700	2.46420000	0.31039500
C	5.42997200	3.03085000	-1.11799800
H	5.48142200	0.93366700	-1.60334400
C	3.57388600	3.76909600	0.25055700
H	2.17455700	2.28520900	0.86398400
C	4.73998000	4.04850900	-0.45895200
H	6.33219400	3.25706200	-1.67725600
H	2.99530200	4.54021800	0.74845400
H	5.11155200	5.06763900	-0.51025500
C	3.54134800	-0.90802800	1.40266700
C	3.45043300	-2.29019900	1.61514200
C	3.85210200	-0.05506000	2.46445400
C	3.66768000	-2.80921700	2.88494000
H	3.19697200	-2.95585800	0.79478700
C	4.06886300	-0.58486000	3.73413600
H	3.92209600	1.01657700	2.30689000
C	3.97577900	-1.95676200	3.94425300
H	3.58969200	-3.87918100	3.04834500
H	4.30738200	0.08000400	4.55772400
H	4.14091300	-2.36562700	4.93631300
C	3.97531100	-1.26915800	-1.45835400
C	3.39475300	-1.40863300	-2.72273000
C	5.21056200	-1.86462300	-1.18100200
C	4.04977300	-2.14431100	-3.70576100
H	2.43218900	-0.94715000	-2.92914600
C	5.85935700	-2.59801100	-2.16942800

H	5.65833200	-1.75861300	-0.19641300
C	5.27898600	-2.73758500	-3.42907100
H	3.59788800	-2.25549300	-4.68601100
H	6.81652200	-3.06288300	-1.95593800
H	5.78694800	-3.31243100	-4.19715800
H	1.41077200	1.57914000	-1.49829500
Br	-8.28792200	-1.06115300	-0.48495900
O	0.80285400	3.77379600	1.48731400
N	-1.98471400	2.00879500	0.66793000
N	-0.72259500	2.07909200	1.22107000
C	-4.91924500	1.35136400	-0.19447600
H	-4.71689900	2.39962900	-0.36293000
C	-6.21915000	0.89820000	-0.40385400
H	-6.99382800	1.58667800	-0.72308100
C	-6.52158400	-0.44098800	-0.20508300
C	-5.53860300	-1.33891700	0.19924000
H	-5.78509600	-2.38403600	0.35075700
C	-4.24938500	-0.87562500	0.40545000
H	-3.47296200	-1.57384600	0.71077200
C	-3.90846500	0.47458200	0.21831800
C	-2.49765500	0.80843300	0.48503100
H	-1.95267500	0.04474100	1.02462200
C	-0.27833100	3.34107200	1.07165000
C	-1.26854000	4.19207700	0.27051000
H	-0.83355900	4.34707100	-0.71981500
H	-1.43871700	5.15316000	0.75824100
C	-2.50022900	3.30899500	0.18219300
H	-3.30736900	3.63876300	0.84760500
H	-2.86026200	3.18640300	-0.83838400
TS3a			
C	-1.17867100	-0.72502200	-0.60306400
C	-0.53201400	-0.16612800	-1.64145400
C	-0.61330300	-1.70192600	0.37734200
C	-0.26035200	-1.26953700	1.66155200
C	-0.45146100	-3.04827500	0.03875200
C	0.24622200	-2.17514600	2.59095400
H	-0.36446500	-0.21541200	1.91391300
C	0.04929600	-3.94960200	0.97070800
H	-0.67516200	-3.37073000	-0.97246900
C	0.39502400	-3.51627000	2.24982300
H	0.52597600	-1.82738400	3.58073800
H	0.18481000	-4.99042500	0.69341600
H	0.78987400	-4.22230000	2.97432200
C	0.91805200	-0.42934800	-1.97835500

O	1.40169000	-1.55884700	-1.76312200
C	1.60030900	0.75109200	-2.30102700
H	1.04532100	1.65121500	-2.54830600
H	2.63961500	0.69652600	-2.60408400
P	-2.87987200	-0.22656400	-0.27132200
C	-3.09822300	0.09291000	1.49210000
C	-3.37115400	-0.96852500	2.36509200
C	-2.81171500	1.36739300	1.99079700
C	-3.37776600	-0.74498000	3.73645100
H	-3.55304200	-1.96771000	1.97877000
C	-2.80522500	1.57305800	3.36772900
H	-2.54515300	2.20590200	1.35205900
C	-3.09183400	0.52491100	4.23718600
H	-3.58911600	-1.56616600	4.41382300
H	-2.55992200	2.56220000	3.74078100
H	-3.08501500	0.69182400	5.31025400
C	-3.36063800	1.23175600	-1.22371700
C	-4.55882800	1.24502600	-1.94617800
C	-2.54982600	2.37272100	-1.16675800
C	-4.94790300	2.40738800	-2.60360400
H	-5.18290500	0.35831300	-1.99953900
C	-2.96137900	3.53324500	-1.81295600
H	-1.60456700	2.35202300	-0.62671900
C	-4.15487200	3.55069100	-2.53043100
H	-5.87325000	2.41963300	-3.17039100
H	-2.34436000	4.42249000	-1.73942100
H	-4.46983500	4.45833900	-3.03644300
C	-3.98014800	-1.58702800	-0.74353100
C	-3.56989100	-2.46701800	-1.74820900
C	-5.25612600	-1.70943700	-0.18039900
C	-4.42984600	-3.47220100	-2.18143700
H	-2.58268500	-2.36140900	-2.18984100
C	-6.11008700	-2.71595700	-0.61887900
H	-5.57632100	-1.02324400	0.59944400
C	-5.69609700	-3.59699000	-1.61669800
H	-4.10744500	-4.15735200	-2.95867000
H	-7.09784200	-2.81391100	-0.18014100
H	-6.36425600	-4.38323200	-1.95417300
H	-1.04286500	0.58209600	-2.24419900
Br	7.84398400	-0.99554800	-0.40746400
O	-1.22012600	3.92256600	1.26315500
N	1.54710700	2.08908300	0.48379300
N	0.17049500	2.20532300	0.64468000
C	3.74014700	-0.77836200	0.12108600

H	2.92861500	-1.47054100	0.32388500
C	5.04300300	-1.25088100	0.02068600
H	5.26209500	-2.30184800	0.17074400
C	6.06507700	-0.36191000	-0.28315800
C	5.80149800	0.98509500	-0.51153600
H	6.60936700	1.65763900	-0.77752000
C	4.49670900	1.44894900	-0.41268400
H	4.30175300	2.48831400	-0.64844500
C	3.44924300	0.58088000	-0.07070400
C	2.03155000	0.94870800	0.04607100
H	1.36066300	0.11587700	0.21211300
C	-0.09343500	3.45664200	1.04744000
C	1.20068000	4.27330200	1.20939500
H	1.40522400	4.40834700	2.27570100
H	1.09084500	5.25839600	0.75476100
C	2.23224300	3.39161300	0.52465300
H	2.42655700	3.71549100	-0.50678600
H	3.18086000	3.29407500	1.05568400
IM3			
C	1.52981100	-0.23629600	-0.96914700
C	1.19781200	0.98424300	-1.46217500
C	0.76762400	-1.47823300	-1.28986900
C	0.69491700	-1.87464300	-2.63435200
C	0.09984000	-2.24410200	-0.32706100
C	-0.04435300	-2.99098000	-3.00934800
H	1.21137600	-1.28012900	-3.38449600
C	-0.63954500	-3.36300000	-0.70578000
H	0.12366900	-1.94698900	0.71733000
C	-0.71655000	-3.73879200	-2.04359500
H	-0.09830200	-3.27431300	-4.05607100
H	-1.16895500	-3.93315600	0.05116100
H	-1.29858500	-4.60800200	-2.33317600
C	-0.00032000	1.27821700	-2.33109600
O	0.16140000	1.96553500	-3.31916600
C	-1.36486500	0.70011200	-1.98575200
H	-1.35067800	-0.36420000	-2.24296000
H	-2.07790800	1.18222600	-2.66092200
P	2.82513000	-0.30858200	0.26499600
C	3.99194200	-1.67443800	0.02230800
C	3.86071800	-2.58696100	-1.02544100
C	5.07257400	-1.78325600	0.91089200
C	4.79673600	-3.60963600	-1.17300000
H	3.03520200	-2.50665500	-1.72372400
C	5.99983700	-2.80570500	0.75856600

H	5.19464500	-1.05747000	1.71182700
C	5.85941500	-3.72221200	-0.28356300
H	4.69022800	-4.31779200	-1.98813600
H	6.83414900	-2.88393200	1.44801600
H	6.58572800	-4.51990300	-0.40347800
C	3.80262900	1.21112700	0.26204500
C	3.21251600	2.40329600	0.69020200
C	5.10720900	1.21257600	-0.25467600
C	3.92942600	3.59401200	0.60848300
H	2.17796700	2.44356400	1.01709500
C	5.82253800	2.40147500	-0.30180700
H	5.55969700	0.29844900	-0.62384900
C	5.23513200	3.58999100	0.13302700
H	3.42454800	4.51445600	0.87679200
H	6.83399700	2.40284400	-0.69543500
H	5.79284500	4.51970000	0.07405700
C	2.01822100	-0.55414500	1.87786800
C	0.93221000	0.27808000	2.18880900
C	2.38583300	-1.58932000	2.74249200
C	0.24062000	0.07535700	3.37959800
H	0.60081800	1.05871500	1.49521100
C	1.68424600	-1.77867300	3.92948800
H	3.19658200	-2.26383600	2.48995700
C	0.61510700	-0.94661900	4.24995900
H	-0.60350500	0.71619400	3.61432700
H	1.96891000	-2.58600700	4.59673300
H	0.06587000	-1.10349400	5.17336400
H	1.84025400	1.85296300	-1.33931000
Br	-7.63668300	-0.94591800	0.64115900
O	1.17460100	4.24133700	-0.24600500
N	-1.56144600	2.14819700	0.06803400
N	-0.15069900	2.38618700	0.03363800
C	-3.90353500	-0.49060500	-1.11883800
H	-3.41392600	-0.87580600	-2.00753000
C	-5.20893000	-0.89971900	-0.85352100
H	-5.72241200	-1.58363400	-1.52060000
C	-5.85375500	-0.41381600	0.27459700
C	-5.21344700	0.46486400	1.14074500
H	-5.73317900	0.83634200	2.01735200
C	-3.91039300	0.85918400	0.86417500
H	-3.39229100	1.54899900	1.52278000
C	-3.23530500	0.39428100	-0.27018600
C	-1.79656900	0.82935200	-0.50590000
H	-1.15154400	0.15441600	0.07583100

C	0.06535700	3.69308100	-0.18536000
C	-1.27625800	4.42684000	-0.32504400
H	-1.22578700	5.19709200	-1.09574100
H	-1.52071100	4.90159000	0.63238300
C	-2.21032600	3.27102200	-0.64625600
H	-3.23985500	3.39401300	-0.29902600
H	-2.22361600	3.10821000	-1.73455400

IM3a

C	-1.67055000	-0.52210400	-0.63989900
C	-0.45289500	-0.04477000	-0.95085400
C	-2.08720600	-1.95586600	-0.60410300
C	-1.84659700	-2.69036300	0.56176500
C	-2.80108500	-2.53464300	-1.65707400
C	-2.31929000	-3.99577200	0.66126400
H	-1.31328500	-2.20827900	1.37588500
C	-3.27425000	-3.83905900	-1.54694800
H	-2.97672000	-1.96984000	-2.56785600
C	-3.03790900	-4.56963400	-0.38466800
H	-2.12821500	-4.56427200	1.56648600
H	-3.82076500	-4.28635900	-2.37187300
H	-3.40856600	-5.58694200	-0.29866700
C	0.65933100	-0.90104100	-1.47348900
O	0.45636100	-1.99374000	-1.96179400
C	2.05675700	-0.31278200	-1.43560300
H	2.03421900	0.77868400	-1.34017000
H	2.53124200	-0.57072800	-2.38720100
P	-2.95288200	0.59626100	-0.06112500
C	-3.83537700	-0.03446100	1.38696600
C	-4.62727000	-1.18118100	1.23791800
C	-3.71742200	0.57927300	2.63462200
C	-5.29591600	-1.70352900	2.33844700
H	-4.71317700	-1.67246300	0.27163500
C	-4.39774200	0.05361600	3.72770800
H	-3.08880200	1.45247700	2.76125300
C	-5.18317200	-1.08559800	3.58178600
H	-5.89821700	-2.59884500	2.22282000
H	-4.30069900	0.53034300	4.69748600
H	-5.70518200	-1.49747000	4.44018700
C	-2.38000400	2.30608300	0.16894900
C	-2.85276700	3.31554100	-0.67913600
C	-1.45475000	2.61450800	1.17639800
C	-2.39962500	4.62207500	-0.52069500
H	-3.57081700	3.09246600	-1.46096600
C	-1.01310200	3.92520800	1.32446500

H	-1.10513800	1.81523800	1.82890200
C	-1.48016800	4.92818800	0.47813400
H	-2.76855800	5.39951500	-1.18194900
H	-0.29845700	4.16055400	2.10755500
H	-1.12820100	5.94838500	0.59743900
C	-4.20002800	0.68719200	-1.38652400
C	-3.77797300	0.62953300	-2.71876000
C	-5.54721800	0.91556900	-1.09186100
C	-4.70006900	0.78917200	-3.74835000
H	-2.72861200	0.45413800	-2.94359800
C	-6.46559000	1.07421800	-2.12586300
H	-5.87817400	0.96298800	-0.05846000
C	-6.04354500	1.00936900	-3.45144500
H	-4.36963000	0.73807600	-4.78083400
H	-7.51185900	1.24673000	-1.89471600
H	-6.76352100	1.13045800	-4.25482100
H	-0.23491400	1.01548100	-0.82704200
Br	8.96303200	0.30218300	-0.26731100
O	-0.85079500	-0.12892500	2.17351900
N	2.36800000	-0.63840600	1.03168000
N	0.98671200	-0.95781400	1.05873600
C	5.19722200	-1.17171700	0.64782400
H	4.74983600	-1.80942700	1.40502800
C	6.55938800	-0.90541200	0.67637400
H	7.19750400	-1.33915500	1.43864500
C	7.10437000	-0.06808900	-0.29316000
C	6.30869300	0.50101400	-1.27507200
H	6.74848100	1.15572700	-2.01940100
C	4.94174300	0.22442000	-1.28672900
H	4.32908000	0.68192500	-2.05707200
C	4.36856100	-0.61659000	-0.33507600
C	2.88848300	-0.94910300	-0.29155300
H	2.76700500	-2.03424000	-0.41373000
C	0.37957000	-0.12992600	1.89444600
C	1.39472400	0.85577900	2.49930000
H	1.70711000	0.48452200	3.48251200
H	0.98736600	1.86193000	2.62554500
C	2.51501500	0.75718700	1.47744800
H	2.32453100	1.47163700	0.65529400
H	3.52070300	0.93343900	1.86602700
TS4			
C	1.48234700	-0.24234700	-0.94168600
C	1.10176700	0.98929200	-1.43882700
C	0.78611200	-1.51678400	-1.27516600

C	0.68782700	-1.88888100	-2.62730600
C	0.25677600	-2.38491100	-0.31105500
C	0.06368800	-3.07302200	-3.00178000
H	1.10789800	-1.22713400	-3.38156200
C	-0.35523900	-3.57917300	-0.68720200
H	0.30217900	-2.11760900	0.74087400
C	-0.45725000	-3.92710100	-2.03008000
H	-0.00701500	-3.33438300	-4.05345500
H	-0.76483300	-4.23345800	0.07630600
H	-0.93908800	-4.85569200	-2.31977900
C	-0.03020300	1.16228400	-2.41824300
O	0.16250500	1.75777900	-3.45789900
C	-1.40724700	0.60122600	-2.07950300
H	-1.42080400	-0.45304000	-2.37773500
H	-2.11573700	1.12404100	-2.72907300
P	2.74731700	-0.26186600	0.28929800
C	3.99325600	-1.56481800	0.04871800
C	3.86385900	-2.52826500	-0.95319800
C	5.12737400	-1.56866300	0.87477300
C	4.85153800	-3.49875800	-1.11335200
H	3.00158000	-2.52479300	-1.60994400
C	6.10655600	-2.54077200	0.71107500
H	5.25049500	-0.79892100	1.63325400
C	5.96603900	-3.50992600	-0.28213000
H	4.74455600	-4.24513300	-1.89365900
H	6.98254500	-2.53730600	1.35164700
H	6.73252700	-4.26769400	-0.41121200
C	3.66831800	1.29427900	0.29087000
C	3.15323700	2.42035300	0.93312800
C	4.86465700	1.38172100	-0.43695200
C	3.84587900	3.62641200	0.86848700
H	2.19676300	2.37877100	1.44409300
C	5.55127300	2.58648300	-0.48723600
H	5.25555000	0.51454500	-0.96025000
C	5.04364000	3.70709600	0.17096000
H	3.41654600	4.50670900	1.33262200
H	6.47808100	2.65398400	-1.04790600
H	5.57676400	4.65136600	0.11847700
C	2.00315900	-0.52776600	1.93514200
C	0.84513100	0.20397000	2.23938000
C	2.48666000	-1.48117300	2.83584200
C	0.19837700	-0.01041000	3.45260000
H	0.44737800	0.92710900	1.52348300
C	1.82741100	-1.68857000	4.04460800

H	3.35838500	-2.07967100	2.59368300
C	0.68637700	-0.95395000	4.35472400
H	-0.69723600	0.55738000	3.68433300
H	2.20318800	-2.43307500	4.73935200
H	0.17212600	-1.12405200	5.29570300
H	1.77711900	1.84289100	-1.41544700
Br	-7.68672500	-0.81196500	0.69282500
O	1.24585700	4.02489700	-0.52523600
N	-1.49505500	1.98347000	0.01304800
N	-0.08418100	2.19820600	-0.11195300
C	-4.04772000	-0.35340000	-1.25001200
H	-3.65002800	-0.62444600	-2.22259100
C	-5.36524400	-0.69897300	-0.95344000
H	-5.97674200	-1.22403200	-1.67904600
C	-5.89285400	-0.35700700	0.28254200
C	-5.12621900	0.32016100	1.22504100
H	-5.55601900	0.58262900	2.18578700
C	-3.81419700	0.65386600	0.91476500
H	-3.20175100	1.19407000	1.63029100
C	-3.25403600	0.32518000	-0.32502000
C	-1.80274500	0.68883000	-0.59174200
H	-1.17697800	-0.03341100	-0.04710900
C	0.14051100	3.51383000	-0.34546100
C	-1.19375700	4.26938200	-0.33557900
H	-1.19556100	5.06917400	-1.07700100
H	-1.34746100	4.70648000	0.65758900
C	-2.17160400	3.14008000	-0.61789000
H	-3.16684400	3.26919000	-0.18560800
H	-2.27493200	3.01048500	-1.70583700
TS4a			
C	-1.43077500	-0.24739300	-0.48472900
C	-0.46448700	0.63741200	-0.85545800
C	-1.16132100	-1.68625400	-0.18834700
C	-1.03815400	-2.07443100	1.15504200
C	-1.01657600	-2.65384800	-1.18943400
C	-0.77086300	-3.40016800	1.48493200
H	-1.17260700	-1.32175600	1.92887700
C	-0.74561000	-3.97798500	-0.85388100
H	-1.09235300	-2.35817200	-2.22981300
C	-0.62259900	-4.35439900	0.48108900
H	-0.67740900	-3.68583300	2.52866300
H	-0.62809200	-4.71746000	-1.64032900
H	-0.41022000	-5.38824500	0.73733500
C	0.71298200	0.23754100	-1.71136100

O	0.52310100	-0.49651500	-2.65979800
C	2.08968600	0.77804100	-1.40082700
H	2.71972500	0.56285300	-2.26705500
H	2.06762800	1.85575300	-1.20796000
P	-3.07024500	0.32758200	-0.15370900
C	-3.24766900	2.12956100	-0.33756000
C	-2.46807200	3.00874100	0.42901000
C	-4.17341600	2.63543200	-1.25953300
C	-2.62879500	4.38177100	0.26676200
H	-1.75432100	2.59609800	1.14217700
C	-4.32380800	4.01076400	-1.40748500
H	-4.77417900	1.96660200	-1.86623300
C	-3.55310600	4.88427500	-0.64599900
H	-2.02245900	5.05958000	0.85925900
H	-5.04208100	4.39704900	-2.12354500
H	-3.67091300	5.95708100	-0.76671300
C	-4.11305500	-0.39951200	-1.46422800
C	-5.48382600	-0.61254000	-1.28183800
C	-3.52700000	-0.65859800	-2.70731500
C	-6.25870600	-1.08876600	-2.33472500
H	-5.94283200	-0.40976900	-0.31806600
C	-4.30773700	-1.13708900	-3.75589200
H	-2.46247700	-0.48401100	-2.84802600
C	-5.67046700	-1.35329800	-3.57025500
H	-7.32131300	-1.25580100	-2.18914400
H	-3.84826900	-1.34031300	-4.71797000
H	-6.27703400	-1.72756500	-4.38933000
C	-3.81129000	-0.24373600	1.39965500
C	-4.20478100	-1.58335700	1.50586200
C	-3.94610400	0.61549600	2.49156100
C	-4.73923000	-2.05489100	2.69971900
H	-4.08665400	-2.25904600	0.66249200
C	-4.49133600	0.13809800	3.67875800
H	-3.60386000	1.64174300	2.42325100
C	-4.88676100	-1.19266600	3.78380200
H	-5.03769500	-3.09511400	2.78138100
H	-4.59469900	0.80728800	4.52665600
H	-5.30621900	-1.56148400	4.71498900
H	-0.70786300	1.69523300	-0.93586900
Br	8.84062700	0.12638100	-0.34231700
O	-1.11137900	1.05888400	2.19228200
N	2.14863900	0.71206100	1.05168300
N	0.77786800	1.10566700	0.88442100
C	4.86403900	-0.94766700	-0.81156000

H	4.31342300	-1.76240400	-1.27657100
C	6.25352500	-0.93815200	-0.87525800
H	6.79475600	-1.73099800	-1.37979900
C	6.94631900	0.10508100	-0.27213100
C	6.27581200	1.12847500	0.38721200
H	6.83694100	1.92952000	0.85626100
C	4.88529600	1.10613400	0.43826200
H	4.33652100	1.88552000	0.95756300
C	4.16658200	0.07025900	-0.15977300
C	2.65003000	0.06841600	-0.15041400
H	2.31150800	-0.98841500	-0.19705500
C	0.11557500	0.86551400	2.00435600
C	1.05610200	0.31097600	3.07839100
H	0.56890100	-0.46076600	3.67811700
H	1.36086100	1.12758100	3.74297100
C	2.20115200	-0.19232400	2.21740700
H	3.18995300	-0.15278800	2.68213000
H	1.99638000	-1.23151800	1.90258000
IM4			
C	-1.34558200	0.42119800	-0.75915700
C	-0.69770300	-0.76717800	-1.42866800
C	-0.60928700	1.68893900	-0.54118700
C	-0.32612700	2.20290400	0.73656800
C	-0.15929400	2.44449000	-1.64364900
C	0.38163600	3.38948800	0.90816200
H	-0.66334000	1.65608000	1.61380600
C	0.57951100	3.61076500	-1.47327300
H	-0.40956500	2.10855300	-2.64507300
C	0.85776400	4.09204800	-0.19550100
H	0.57415900	3.75730000	1.91237000
H	0.91882700	4.16019900	-2.34713900
H	1.42411700	5.00874000	-0.06293300
C	0.18578500	-0.43530200	-2.64667700
O	-0.27462200	-0.10422700	-3.71024500
C	1.68677400	-0.59789900	-2.40914300
H	1.94230200	-1.65023000	-2.59557900
H	2.22241900	0.01647000	-3.13751200
P	-2.77947400	0.10381400	0.10758100
C	-4.00456300	-0.83861700	-0.87073400
C	-4.91341900	-0.14853500	-1.68009900
C	-3.99764200	-2.23742600	-0.87115000
C	-5.81075600	-0.84967400	-2.47718200
H	-4.92611200	0.93718800	-1.68374900
C	-4.89253500	-2.93268100	-1.68211700

H	-3.27971000	-2.78400400	-0.26691400
C	-5.80014700	-2.24314200	-2.47970000
H	-6.51831400	-0.30708600	-3.09635300
H	-4.87285900	-4.01793100	-1.68800000
H	-6.49894300	-2.79016400	-3.10559100
C	-2.65580000	-0.86369300	1.66913700
C	-1.39680000	-0.98055500	2.26384100
C	-3.76540100	-1.46438400	2.27583900
C	-1.25524800	-1.67015400	3.46717700
H	-0.52516500	-0.54763400	1.77184700
C	-3.61931400	-2.15478600	3.47445200
H	-4.74350600	-1.39563500	1.80486000
C	-2.36368200	-2.25480100	4.07233800
H	-0.27551300	-1.75403000	3.92928700
H	-4.48277600	-2.61951900	3.94044300
H	-2.25078600	-2.79435900	5.00785900
C	-3.56004500	1.68437100	0.57571500
C	-3.56036700	2.73279200	-0.35365600
C	-4.16716800	1.86709400	1.81967000
C	-4.17379700	3.94036900	-0.04230700
H	-3.06236000	2.60114700	-1.31022200
C	-4.78029800	3.07989700	2.12654600
H	-4.15488100	1.07110800	2.55721000
C	-4.78691800	4.11463000	1.19745800
H	-4.16519400	4.74958700	-0.76570600
H	-5.24733600	3.21467100	3.09719000
H	-5.26307600	5.05997000	1.43956600
H	-1.46315100	-1.46686400	-1.79017100
Br	7.99793600	0.19977900	0.60844900
O	-1.19559000	-3.45202800	-0.31569200
N	1.34594600	-1.06818000	0.02384400
N	0.15118400	-1.60893700	-0.56831800
C	4.48438800	-0.79056300	-1.35525500
H	4.21126700	-1.40899600	-2.20572900
C	5.82510800	-0.70110900	-0.98998600
H	6.58912800	-1.23969200	-1.53949900
C	6.17876400	0.09013100	0.09548200
C	5.22104000	0.80099600	0.81177500
H	5.51911800	1.42108300	1.64991800
C	3.88815800	0.70498800	0.43026400
H	3.12483100	1.26025800	0.97095200
C	3.50334100	-0.09527900	-0.64921200
C	2.03017300	-0.19075900	-0.97234300
H	1.61754500	0.80868100	-0.81253400

C	-0.17410500	-2.82745300	-0.07419000
C	0.97541800	-3.23510300	0.83563000
H	1.20371200	-4.29586600	0.72901000
H	0.67403900	-3.03872100	1.87091900
C	2.08530100	-2.29916500	0.37537600
H	2.83723700	-2.07026700	1.13133600
H	2.58704500	-2.73067400	-0.50597000
IM4a			
C	-1.27065700	0.04868500	-0.05106200
C	-0.53754400	1.24184300	-0.60477800
C	-0.49568200	-1.20142800	0.21522300
C	0.10771500	-1.40569800	1.46481400
C	-0.32287700	-2.18916900	-0.76789900
C	0.86452800	-2.54507200	1.72065200
H	-0.02568900	-0.64485600	2.22794800
C	0.43299400	-3.33405900	-0.51617100
H	-0.78270300	-2.04127600	-1.74272900
C	1.03189100	-3.51189000	0.72837400
H	1.32035400	-2.68455000	2.69723800
H	0.55666400	-4.08399400	-1.29208600
H	1.62133200	-4.40202700	0.92846900
C	0.18163800	0.97319500	-1.94669200
O	-0.42012800	0.64110100	-2.94075400
C	1.69655700	1.11286500	-1.92095800
H	1.95729800	2.17995500	-1.93601700
H	2.10846000	0.63703900	-2.81416500
P	-2.95924200	-0.10773100	-0.01622800
C	-3.46583100	-1.08424800	1.44809500
C	-3.19023000	-2.45708700	1.48945100
C	-4.05897900	-0.47041500	2.55349100
C	-3.49354700	-3.19751600	2.62686900
H	-2.73443000	-2.94776400	0.63311000
C	-4.36890100	-1.21783200	3.68755200
H	-4.28518600	0.59143300	2.53059700
C	-4.08419100	-2.57936500	3.72716600
H	-3.26896700	-4.25933500	2.65191400
H	-4.83660900	-0.73313800	4.53901200
H	-4.32554900	-3.15982100	4.61246100
C	-3.77663000	1.51265000	0.06450400
C	-4.89131500	1.82494400	-0.72198700
C	-3.26891000	2.46174000	0.95686600
C	-5.48896300	3.07619200	-0.60811500
H	-5.28594400	1.09827800	-1.42495600
C	-3.86013100	3.71681700	1.05447900

H	-2.38971400	2.23122300	1.54836400
C	-4.97401500	4.02139000	0.27755100
H	-6.35264000	3.31718600	-1.21996800
H	-3.42946900	4.45401500	1.72369900
H	-5.43716000	5.00073000	0.35369400
C	-3.83545200	-0.98672300	-1.38015000
C	-3.30910500	-0.88316500	-2.67052500
C	-5.02530800	-1.69311700	-1.17112200
C	-3.96798300	-1.48303500	-3.74179400
H	-2.38455500	-0.33065500	-2.83025400
C	-5.67974400	-2.29093600	-2.24447000
H	-5.44151000	-1.77538700	-0.17048200
C	-5.15002700	-2.18773600	-3.52956200
H	-3.55415000	-1.39985000	-4.74213900
H	-6.60197900	-2.83928500	-2.07720600
H	-5.65974800	-2.65926800	-4.36459200
H	-1.24246600	2.06307400	-0.79236300
Br	8.26325300	-0.53024600	0.03990400
O	-0.64698300	3.74108700	0.93058600
N	1.72189900	1.17854800	0.57107400
N	0.46970000	1.83970600	0.28072100
C	4.14130300	-0.71019400	0.40799400
H	3.41346400	-1.25624700	1.00456600
C	5.50029300	-0.93585700	0.58517500
H	5.85771500	-1.65336700	1.31550800
C	6.40931400	-0.22968000	-0.19711500
C	5.98048600	0.68837700	-1.14639200
H	6.70481100	1.22463400	-1.74951900
C	4.61385700	0.90853200	-1.30659500
H	4.27955300	1.62896000	-2.04829000
C	3.68372400	0.21608000	-0.53402800
C	2.19313800	0.44437100	-0.63380300
H	1.72575600	-0.54629800	-0.58011100
C	0.32895300	3.00816600	0.95484000
C	1.61952900	3.20471000	1.73639300
H	1.46602100	2.84109000	2.75852600
H	1.90114500	4.25714300	1.76896100
C	2.58111400	2.31367200	0.96514100
H	2.96203300	2.85757100	0.08429700
H	3.42827200	1.94404000	1.54362300
TS5₁			
C	-1.01830300	-0.19009500	0.02439400
C	-0.43297700	-0.53558600	-1.38364400
C	-0.30345500	-0.83426100	1.20197100

C	0.35538700	-0.02372300	2.13495800
C	-0.24728600	-2.22637300	1.36513800
C	1.04154000	-0.59133400	3.20685100
H	0.36130600	1.05270400	1.97346500
C	0.44117700	-2.79037000	2.43392500
H	-0.72710200	-2.87809300	0.63854100
C	1.08458100	-1.97429400	3.36152700
H	1.55011300	0.05297000	3.91852700
H	0.47630400	-3.87087100	2.54004600
H	1.61970600	-2.41595500	4.19730000
C	0.16826300	0.68980900	-2.12732300
O	-0.50804800	1.36360200	-2.86613400
C	1.67750600	0.85019200	-2.03323900
H	2.10852200	0.45260100	-2.96280300
H	1.89254200	1.92113300	-1.98853700
P	-2.78490100	-0.46168900	0.15773600
C	-3.62705800	0.25382500	-1.27227900
C	-4.76261700	-0.33130200	-1.84191800
C	-3.16389700	1.49094100	-1.72833700
C	-5.41791400	0.31719600	-2.88306300
H	-5.12962800	-1.28655000	-1.47794100
C	-3.82316900	2.12979000	-2.77296100
H	-2.28372700	1.94718800	-1.28485200
C	-4.94600800	1.54356700	-3.34956100
H	-6.29516800	-0.13687100	-3.33260300
H	-3.44471900	3.07932000	-3.13720000
H	-5.45725100	2.04201200	-4.16741900
C	-3.24898300	-2.20699700	0.29012600
C	-3.13576100	-3.00778700	-0.85330100
C	-3.46660400	-2.80210400	1.53851000
C	-3.25392900	-4.38967800	-0.74749100
H	-2.91398200	-2.56967700	-1.82137000
C	-3.60405800	-4.18256700	1.63306000
H	-3.50128100	-2.19295700	2.43649800
C	-3.49673300	-4.97552800	0.49222700
H	-3.13607800	-5.00136900	-1.63562700
H	-3.77481900	-4.64004500	2.60231700
H	-3.58812200	-6.05447000	0.57293800
C	-3.42030200	0.42687300	1.60178900
C	-2.69580300	1.49848100	2.13256100
C	-4.70584500	0.13882500	2.07765600
C	-3.25494800	2.25605000	3.16011800
H	-1.72238600	1.77281300	1.72839700
C	-5.24888200	0.89631900	3.10753500

H	-5.28233000	-0.67344300	1.64142100
C	-4.51977800	1.95275100	3.65252300
H	-2.69540600	3.09322500	3.56576400
H	-6.24286300	0.66829900	3.47905800
H	-4.94758400	2.54708700	4.45423700
H	-1.19919300	-0.92236700	-2.06452800
Br	8.21803200	0.55047900	0.57978400
O	-0.53540700	-3.26219000	-2.39817700
N	1.88607900	-1.31085800	-0.78943300
N	0.59784300	-1.54220100	-1.38969200
C	4.58309400	0.82724400	-1.40044100
H	4.24371900	1.18628200	-2.36752600
C	5.93832100	0.91672600	-1.08524200
H	6.64712000	1.33462200	-1.79148800
C	6.37554900	0.45660100	0.14849600
C	5.48593300	-0.08117700	1.07490300
H	5.84980600	-0.43185700	2.03429000
C	4.13846100	-0.15735500	0.74889200
H	3.42607700	-0.57941800	1.45472100
C	3.67297400	0.29233200	-0.49205300
C	2.20063000	0.13812500	-0.79261000
H	1.64805900	0.57869500	0.04578600
C	0.48448900	-2.78139600	-1.92789700
C	1.86606000	-3.40885200	-1.80173500
H	2.10616000	-4.01130000	-2.67788900
H	1.87348100	-4.04699500	-0.91052900
C	2.75207300	-2.18020500	-1.60532000
H	3.67989700	-2.37731200	-1.06801700
H	2.98831300	-1.72514700	-2.58208000
C	-0.35616700	3.43159100	-0.42882800
C	-1.46825300	4.20306800	0.29280400
H	-0.64351900	3.35120400	-1.50061100
H	0.54691000	4.07485600	-0.42100300
C	-1.74848900	5.57594500	-0.31138800
H	-2.39442900	3.60748600	0.28077600
H	-1.18483800	4.30733500	1.35081000
C	-2.84692400	6.33559200	0.42867300
H	-0.82447100	6.16878400	-0.31101800
H	-2.03149900	5.45398600	-1.36607400
H	-3.03953100	7.31443600	-0.02145600
H	-3.78503400	5.76970200	0.41981400
H	-2.56917200	6.49672900	1.47614000
O	-0.07493900	2.20161200	0.13584800
H	-0.81318800	1.04184700	0.08276800

TS5a₁

C	1.23523600	-0.29871300	-0.47057200
C	0.78760800	-1.72533000	-0.04240400
C	1.05609400	0.18374000	-1.90111700
C	0.52854400	1.47400500	-2.07441300
C	1.45332200	-0.53179000	-3.03934000
C	0.38272400	2.01782900	-3.34651700
H	0.28322000	2.04421300	-1.18000100
C	1.30004600	0.01502000	-4.31197300
H	1.88095700	-1.52272800	-2.94415200
C	0.76355400	1.28944200	-4.47075000
H	-0.02616600	3.01772900	-3.45726300
H	1.60783000	-0.56002200	-5.18026500
H	0.64754400	1.71321300	-5.46395200
C	0.11064900	-2.54846800	-1.14108400
O	0.73361200	-3.28703700	-1.86802700
C	-1.40644800	-2.44543200	-1.17627100
H	-1.80282600	-3.36070300	-0.71557300
H	-1.71987900	-2.44772900	-2.22455200
P	2.90272300	0.06799200	0.11671200
C	3.26767400	1.81073100	-0.21130800
C	3.70745700	2.17387100	-1.49066800
C	3.01799700	2.79009900	0.75185300
C	3.91982600	3.51333300	-1.79389900
H	3.86579000	1.41496700	-2.25301600
C	3.24082800	4.12789700	0.44083500
H	2.62379400	2.51598200	1.72287900
C	3.69166800	4.48885000	-0.82541200
H	4.25440700	3.79387700	-2.78733000
H	3.04767400	4.88933900	1.18938300
H	3.85875200	5.53538700	-1.06232300
C	2.99996100	-0.34410300	1.88032200
C	3.99260800	-1.21412700	2.34390100
C	2.03279800	0.16658200	2.76068600
C	4.02878600	-1.56535000	3.68917500
H	4.72938300	-1.62813000	1.66299200
C	2.09225900	-0.18959100	4.10411800
H	1.24034800	0.81941000	2.37308000
C	3.08156300	-1.05212200	4.56884500
H	4.79270500	-2.24897400	4.04513600
H	1.35037200	0.20633800	4.79158200
H	3.10917900	-1.33330800	5.61741600
C	4.22391300	-0.87282800	-0.71056500
C	3.96859400	-2.11544200	-1.29876100

C	5.53370000	-0.37680600	-0.67796200
C	5.01492100	-2.84638300	-1.85670700
H	2.96367600	-2.52714100	-1.33880200
C	6.57346400	-1.11354800	-1.23382500
H	5.73687000	0.58814700	-0.22128700
C	6.31368100	-2.34813800	-1.82570500
H	4.80802800	-3.80719800	-2.31672300
H	7.58531100	-0.72189900	-1.20672000
H	7.12562800	-2.92086200	-2.26329800
H	1.61496500	-2.33889600	0.33399600
Br	-8.01849200	-0.20813700	-0.51021400
O	1.09315000	-2.93239100	2.57609100
N	-1.43806400	-1.11958400	0.95482300
N	-0.13792200	-1.72028200	1.06566100
C	-3.93214100	0.19635800	0.04580000
H	-3.25680000	0.93062900	0.47555100
C	-5.30057100	0.43056500	0.04728700
H	-5.70566200	1.34529300	0.46579900
C	-6.15249700	-0.52305700	-0.50253100
C	-5.65453700	-1.69873700	-1.04433700
H	-6.33253100	-2.43140800	-1.46760200
C	-4.27855800	-1.92323900	-1.03262400
H	-3.90323800	-2.84908600	-1.45711500
C	-3.40275100	-0.98156000	-0.49465400
C	-1.90073500	-1.18696200	-0.45397100
H	-1.44012000	-0.32025200	-0.95063600
C	0.07249400	-2.35414600	2.25383000
C	-1.21251700	-2.15820100	3.04279700
H	-1.09084000	-1.27371400	3.67913900
H	-1.43241400	-3.02541100	3.66507300
C	-2.22428300	-1.90244400	1.92988800
H	-2.56254100	-2.86207300	1.50452700
H	-3.09582100	-1.32554700	2.23903900
C	-2.63120400	5.59904500	1.96653500
C	-2.53382700	4.13282800	1.55176400
H	-3.66944700	5.94238000	2.01448300
H	-2.17967600	5.75449400	2.95240500
H	-2.09774800	6.23933300	1.25556800
C	-1.09657900	3.62685600	1.46722600
H	-3.09432000	3.51225100	2.26519000
H	-3.02292900	3.99487700	0.57712000
C	-0.99607500	2.15208800	1.06351200
H	-0.52694400	4.22350900	0.74059600
H	-0.59352700	3.75534800	2.43611800

H	-1.59784200	1.55971400	1.78936500
H	-1.53814400	2.05013300	0.08976400
O	0.30350400	1.72524100	0.97448600
H	0.64365200	0.52025600	0.22139000
IM5₁			
C	-1.45833600	-0.45875300	0.25357400
C	-1.05588200	-1.28972800	-0.99732200
C	-1.84774500	-1.35014000	1.41608100
C	-1.28873700	-1.07635900	2.66830100
C	-2.70521800	-2.44403000	1.26182500
C	-1.62055700	-1.86884100	3.76353600
H	-0.57874000	-0.25269900	2.74320300
C	-3.02967200	-3.23369500	2.36189600
H	-3.08990200	-2.71331200	0.28095800
C	-2.49828400	-2.94030300	3.61524600
H	-1.18404300	-1.65407400	4.73442900
H	-3.68990700	-4.08611500	2.23338100
H	-2.75444600	-3.55730200	4.47154400
C	-0.37638200	-0.50738000	-2.12850000
O	-1.00165200	-0.08259200	-3.07217400
C	1.13796800	-0.39449900	-2.03147800
H	1.56841000	-1.00993500	-2.83360700
H	1.39302900	0.64726500	-2.25725500
P	-2.81020600	0.73392700	-0.12726000
C	-2.23013800	1.99075900	-1.29171000
C	-3.05320300	2.48088900	-2.30785000
C	-0.94021500	2.50083000	-1.09487700
C	-2.56578800	3.46002900	-3.16705900
H	-4.06175100	2.09974600	-2.43779100
C	-0.46906400	3.47793700	-1.96769800
H	-0.32132500	2.15625300	-0.24964000
C	-1.27094700	3.94768500	-3.00524900
H	-3.19714900	3.83746700	-3.96509900
H	0.53396800	3.87140300	-1.82655700
H	-0.89126700	4.70390800	-3.68578600
C	-4.18542600	-0.20683800	-0.83474600
C	-4.15879400	-0.54306800	-2.19621400
C	-5.16696800	-0.75677300	0.00002200
C	-5.13455800	-1.38773600	-2.71714000
H	-3.36108700	-0.17413100	-2.83705800
C	-6.13939000	-1.59627800	-0.53288300
H	-5.15990600	-0.54835300	1.06537900
C	-6.12814600	-1.90557900	-1.89064300
H	-5.10814400	-1.64891000	-3.76990500

H	-6.89806000	-2.01759400	0.11856400
H	-6.88476000	-2.56650800	-2.30186100
C	-3.34353000	1.61418600	1.36059900
C	-2.36670900	2.02985400	2.27451800
C	-4.67729200	2.01581000	1.50240000
C	-2.76196400	2.80172300	3.36504200
H	-1.30172800	1.80182900	2.11272600
C	-5.05001000	2.78774700	2.59720400
H	-5.42260400	1.73835000	0.76283200
C	-4.09366400	3.16876300	3.53543800
H	-2.01233400	3.12574700	4.08020900
H	-6.08480400	3.09424500	2.71208100
H	-4.38652700	3.76896100	4.39172400
H	-1.92708700	-1.79423300	-1.43108300
Br	7.71064000	-0.14657600	0.43557500
O	-1.48997100	-4.12750300	-1.26985300
N	1.19317900	-2.12885100	-0.21578000
N	-0.15472100	-2.36279900	-0.66634400
C	4.00238300	-0.16487800	-1.41680800
H	3.61788100	0.15059400	-2.38193300
C	5.36576200	-0.01315100	-1.16394300
H	6.02451700	0.41191400	-1.91324700
C	5.87259800	-0.40084300	0.06681800
C	5.04421600	-0.94327700	1.04610200
H	5.45717100	-1.23640200	2.00498600
C	3.68730700	-1.07407000	0.78441800
H	3.02036700	-1.47063300	1.54538800
C	3.14635900	-0.68333900	-0.44744100
C	1.64754300	-0.78281200	-0.64051600
H	1.20679400	-0.07237600	0.07887700
C	-0.41666000	-3.67783900	-0.91351700
C	0.89448300	-4.40673000	-0.66102000
H	1.02299900	-5.22835900	-1.36555600
H	0.88377600	-4.80370300	0.35982700
C	1.91021400	-3.27644200	-0.80807100
H	2.84367500	-3.44120400	-0.27020500
H	2.13556300	-3.10764100	-1.87428600
C	1.66838900	1.81332000	1.68707500
C	2.35534300	2.55092300	0.52339000
H	2.35244300	0.98625200	1.98576700
H	1.67577300	2.50744800	2.55637200
C	3.84941200	2.77670900	0.73086300
H	2.21004300	1.95924800	-0.39561300
H	1.84153000	3.50999400	0.35340700

C	4.52102200	3.47156200	-0.45038300
H	4.00853400	3.36208400	1.64662500
H	4.33140200	1.80453700	0.90037200
H	5.60116800	3.57249200	-0.30143600
H	4.36354100	2.89744500	-1.37146900
H	4.10491300	4.47299500	-0.60891100
O	0.40748200	1.36621700	1.37845300
H	-0.61561600	0.18508200	0.59121000
IM5a₁			
C	-1.55786700	-1.05842100	0.00824900
C	-0.18509200	-0.88008800	-0.66830600
C	-2.51031300	-2.05645800	-0.61885900
C	-2.65437900	-3.29499500	0.01379100
C	-3.27351800	-1.78506600	-1.76108400
C	-3.54617000	-4.24592700	-0.47415600
H	-2.06764900	-3.50720600	0.90505200
C	-4.17027200	-2.73577600	-2.24232500
H	-3.16021800	-0.83478900	-2.26902600
C	-4.31259400	-3.96459900	-1.60161400
H	-3.64713500	-5.20150000	0.03136400
H	-4.75968700	-2.51121200	-3.12608000
H	-5.01443500	-4.70041700	-1.98237100
C	-0.16759700	-0.43573400	-2.12530900
O	-1.16089700	-0.04372600	-2.69177800
C	1.18531400	-0.47371100	-2.81133300
H	1.62977900	0.50628800	-2.60786900
H	0.98611600	-0.55192000	-3.88207900
P	-2.37884100	0.51166100	0.54996300
C	-3.70708200	-0.05709300	1.67129100
C	-4.75676800	-0.86818500	1.21185300
C	-3.65652000	0.29491000	3.02498900
C	-5.73156700	-1.31449200	2.09675600
H	-4.81944400	-1.15561800	0.16745900
C	-4.63666600	-0.15893700	3.90437000
H	-2.85181600	0.91955500	3.39783500
C	-5.67226600	-0.96386100	3.44367300
H	-6.53578000	-1.94388900	1.72947400
H	-4.58419000	0.11934100	4.95202800
H	-6.43300400	-1.31917700	4.13193100
C	-1.25730700	1.48288000	1.58005300
C	-1.52549000	2.84268600	1.75200900
C	-0.22765400	0.86516400	2.29918800
C	-0.76180200	3.58724000	2.64701600
H	-2.31623900	3.32322600	1.18305300

C	0.53388300	1.62333800	3.18063900
H	0.00328200	-0.19052800	2.17346500
C	0.26620700	2.98000100	3.35999200
H	-0.96466000	4.64596800	2.77256900
H	1.34251200	1.14722400	3.72606600
H	0.86675500	3.56540800	4.04945100
C	-3.09581300	1.58575400	-0.71260500
C	-2.21593000	2.29048700	-1.54707200
C	-4.48130700	1.75863400	-0.81192000
C	-2.75099800	3.15647300	-2.49583500
H	-1.13029000	2.13050600	-1.44100600
C	-4.99423300	2.62538000	-1.77159800
H	-5.15818100	1.23737200	-0.14338000
C	-4.12925900	3.32062900	-2.61331300
H	-2.07863300	3.70573500	-3.14753900
H	-6.06790600	2.76120500	-1.85406500
H	-4.53330000	3.99981700	-3.35844900
H	0.34262500	-0.05818700	-0.15788300
Br	6.67959300	-0.39290900	1.62152800
O	0.75237800	-2.23370600	1.72228300
N	1.15225500	-2.64318700	-1.74197200
N	0.58141900	-2.10845600	-0.55773700
C	4.42170600	-1.97078900	-1.47069900
H	4.55026100	-2.74954000	-2.21991700
C	5.45581600	-1.72377900	-0.57423900
H	6.37637700	-2.29586100	-0.60882500
C	5.29230200	-0.71899900	0.37329500
C	4.13798000	0.05330000	0.40977600
H	4.03864800	0.85224900	1.13679800
C	3.11052800	-0.19916600	-0.49707300
H	2.23233300	0.45791800	-0.48968100
C	3.23094100	-1.23804700	-1.42881700
C	2.08327100	-1.63614200	-2.33842600
H	2.49817300	-2.14279400	-3.21634500
C	1.07992400	-2.60564800	0.60364200
C	2.04102500	-3.72322700	0.23172100
H	1.83014900	-4.61630800	0.82235400
H	3.05846200	-3.38773300	0.45663100
C	1.76535700	-3.90224700	-1.26653500
H	2.65386400	-4.12431000	-1.85962800
H	1.03223900	-4.69904900	-1.42427300
C	3.27519300	5.54253400	-2.29093900
C	2.31137900	4.99989100	-1.23770400
H	3.55782200	6.58131000	-2.09143100

H	4.19227700	4.94430400	-2.32253800
H	2.82270600	5.50255100	-3.28802100
C	1.89816800	3.55420000	-1.49637000
H	2.77394200	5.07293900	-0.24411600
H	1.41281700	5.63101100	-1.20226900
C	0.92211700	2.97930500	-0.45864000
H	1.42426500	3.47114900	-2.48603900
H	2.79019900	2.91008300	-1.52685100
H	1.39658800	3.08186200	0.54626400
H	0.04818300	3.68275100	-0.42075500
O	0.54920000	1.69615700	-0.74307900
H	-1.29800000	-1.45965700	0.99908400
TS5₂			
C	1.76171900	-0.99643000	-0.73370800
C	0.31593900	-0.49097700	-1.02906200
C	1.78219600	-2.35839500	-0.07267800
C	1.92845200	-3.48594200	-0.88562000
C	1.56423700	-2.53755800	1.29566200
C	1.89076100	-4.76555800	-0.33973300
H	2.05138300	-3.35225900	-1.95843100
C	1.53305600	-3.81814700	1.84382200
H	1.36372700	-1.67771100	1.92839800
C	1.70276800	-4.93528200	1.03058500
H	2.00343300	-5.63024300	-0.98681700
H	1.36227300	-3.93992500	2.90939500
H	1.67598200	-5.93280200	1.45854500
C	0.05769100	-0.57771300	-2.50671900
O	0.94725600	-0.48964200	-3.33288000
C	-1.40357100	-0.69014800	-2.90762000
H	-1.81450800	0.30819700	-2.72066300
H	-1.44117500	-0.88116000	-3.98130100
P	2.83946800	0.26137200	0.07275900
C	3.20550000	1.54604500	-1.16377400
C	4.54390300	1.82840900	-1.47307700
C	2.17363300	2.21948800	-1.83376000
C	4.84861600	2.78504600	-2.43464100
H	5.35259300	1.30480300	-0.97538800
C	2.49897700	3.17704700	-2.79048200
H	1.11551400	2.05023000	-1.61993300
C	3.82641400	3.46152800	-3.09440400
H	5.88731600	2.99691900	-2.66763100
H	1.69355700	3.69656600	-3.29956700
H	4.06565300	4.20758100	-3.84641500
C	2.15797600	0.98108000	1.58089000

C	1.26570900	2.04579800	1.46395600
C	2.46586500	0.45146900	2.84141000
C	0.70116200	2.59946900	2.60851000
H	0.97638000	2.41473100	0.48538200
C	1.88758200	1.00365600	3.97626600
H	3.14817400	-0.38847000	2.93660600
C	1.01089600	2.08171800	3.86024900
H	0.00516500	3.42715700	2.50875500
H	2.12164300	0.59235800	4.95302500
H	0.56276900	2.51053000	4.75125100
C	4.43940600	-0.48248900	0.49740800
C	4.89746000	-1.61700800	-0.17841400
C	5.28071000	0.16669400	1.41033900
C	6.17497900	-2.10840400	0.07380100
H	4.26235100	-2.12560300	-0.89557700
C	6.55704100	-0.32785400	1.65579900
H	4.93975900	1.06137900	1.92397500
C	7.00308600	-1.46785500	0.99050600
H	6.51995000	-2.99432200	-0.44929300
H	7.20273000	0.17919800	2.36555000
H	7.99871500	-1.85471400	1.18444600
H	-0.07257600	0.70382300	-0.80439200
Br	-7.30346300	0.06556700	0.84913600
O	-0.75005400	-0.32982000	1.70968400
N	-1.24249200	-2.34684100	-1.12051300
N	-0.69348000	-1.27331000	-0.37650200
C	-3.50715700	-0.02372600	-0.82781500
H	-2.63018600	0.62163000	-0.84127200
C	-4.64370400	0.37320500	-0.13033300
H	-4.65988900	1.31924100	0.40024600
C	-5.75838000	-0.45904300	-0.11501400
C	-5.76228600	-1.67100900	-0.79474900
H	-6.64732300	-2.29743200	-0.78513700
C	-4.61425300	-2.05890400	-1.47968400
H	-4.60957400	-3.00880800	-2.01052200
C	-3.47310000	-1.25416000	-1.49417200
C	-2.18980800	-1.76891700	-2.11614500
H	-2.43425400	-2.60254700	-2.78408300
C	-1.13107200	-1.16387300	0.90521100
C	-2.08877000	-2.33209400	1.13670200
H	-3.11594100	-1.95798700	1.19408400
H	-1.84114500	-2.81730400	2.08318500
C	-1.82100400	-3.22558900	-0.08284700
H	-1.06275000	-3.98027500	0.15540800

H	-2.71121800	-3.72593400	-0.46965100
C	-1.46850900	2.64113000	-0.15743000
C	-1.04452400	4.11521800	-0.17306100
H	-1.39464000	2.25425200	0.87979400
H	-2.55727800	2.63558900	-0.38768800
C	-1.90605100	5.00458400	0.72058700
H	0.01159800	4.20890000	0.12574500
H	-1.09361000	4.46648400	-1.21245400
C	-1.43549800	6.45678300	0.74599000
H	-2.94735000	4.95906300	0.37621000
H	-1.91229100	4.60171300	1.74385200
H	-2.07181100	7.08116800	1.38071600
H	-0.40957700	6.52760800	1.12466200
H	-1.44346100	6.88407700	-0.26253500
O	-0.75659600	1.87239400	-1.05873100
H	2.23774200	-1.07126700	-1.72360100
TS5a₂			
C	-1.65059600	-0.92892500	0.27080000
C	-0.27158000	-0.93062900	-0.41439200
C	-2.53137200	-2.13658400	0.01768400
C	-2.69238800	-3.05992400	1.05483800
C	-3.20153400	-2.35578900	-1.19356200
C	-3.50971300	-4.17580100	0.89764000
H	-2.18065100	-2.89271100	2.00019500
C	-4.02244100	-3.46970200	-1.34554800
H	-3.07582800	-1.65310800	-2.00923500
C	-4.18351500	-4.38014700	-0.30279300
H	-3.62509600	-4.88031000	1.71574000
H	-4.53827200	-3.62590500	-2.28830000
H	-4.82689700	-5.24597900	-0.42759300
C	-0.23163200	-1.12579100	-1.88987400
O	-1.16671600	-0.84032100	-2.61448600
C	1.11030800	-1.51845200	-2.49423000
H	1.62123300	-0.56887600	-2.69091800
H	0.88913300	-1.98177800	-3.45774700
P	-2.58316600	0.66837000	0.18068500
C	-4.04936000	0.45041100	1.25877900
C	-5.02501500	-0.52970100	1.01126500
C	-4.18862500	1.27837500	2.38002200
C	-6.11098300	-0.66624500	1.86918100
H	-4.94467000	-1.19259400	0.15646200
C	-5.27754400	1.13148900	3.23454700
H	-3.44813700	2.03956000	2.59827300
C	-6.24007800	0.16110100	2.98190500

H	-6.85524900	-1.42959100	1.66596000
H	-5.36617600	1.78021200	4.10002700
H	-7.08807900	0.04716900	3.65023700
C	-1.65104300	2.00785400	0.95650400
C	-2.02260500	3.32525100	0.66488000
C	-0.73017200	1.74215400	1.97267900
C	-1.48945900	4.37323900	1.40825800
H	-2.73064400	3.53191500	-0.13229900
C	-0.20057500	2.80096800	2.70561200
H	-0.38549200	0.73210000	2.17992800
C	-0.58697300	4.11085200	2.43670000
H	-1.77797400	5.39434000	1.17980400
H	0.52795500	2.59276400	3.48259000
H	-0.17133300	4.93019700	3.01536900
C	-3.10711900	1.23826300	-1.44883600
C	-2.12505400	1.78108200	-2.29177300
C	-4.44585700	1.17775600	-1.84463900
C	-2.51046300	2.25144700	-3.54198400
H	-1.07587800	1.81685600	-1.96849100
C	-4.80917400	1.64712400	-3.10360400
H	-5.20474400	0.78325200	-1.17699200
C	-3.84147000	2.18080200	-3.94977200
H	-1.75982600	2.66878700	-4.20540000
H	-5.84748200	1.60168700	-3.41623800
H	-4.12783700	2.54788000	-4.93103800
H	0.21989300	0.20474000	-0.42955400
Br	7.04108400	0.00742700	0.95079900
O	0.79552100	-0.99992900	2.31831500
N	1.05966100	-2.98548600	-0.56423900
N	0.59137600	-1.90078800	0.22185500
C	4.40312200	-2.56628800	-0.94179800
H	4.43595800	-3.58335600	-1.32767300
C	5.54055300	-2.03481100	-0.34145300
H	6.45154300	-2.61676100	-0.25371900
C	5.49776300	-0.73034800	0.13823200
C	4.35317400	0.04786800	0.00921200
H	4.34209600	1.07244700	0.36866000
C	3.22410000	-0.49539600	-0.59760700
H	2.33858900	0.12917700	-0.73193000
C	3.23161600	-1.81448400	-1.06452700
C	1.97191800	-2.45285900	-1.61606500
H	2.25631900	-3.33379900	-2.20158100
C	1.10356300	-1.83122900	1.47353300
C	2.05543700	-3.00832000	1.63261500

H	1.89793900	-3.49709300	2.59526100
H	3.08251000	-2.62986800	1.59469600
C	1.68384700	-3.88331300	0.43046900
H	2.53207800	-4.40041100	-0.02209500
H	0.93121100	-4.62490200	0.71676300
C	4.35912600	4.71406400	-1.26163400
C	3.27563800	4.05284000	-0.41330600
H	4.92894000	5.45473200	-0.69149400
H	5.06478800	3.96722600	-1.64151200
H	3.91859100	5.22118500	-2.12701300
C	2.45902200	3.01877200	-1.18307300
H	3.73802200	3.57369400	0.46170700
H	2.59892200	4.81997000	-0.01223100
C	1.36296100	2.36702500	-0.33339800
H	1.98546100	3.48598000	-2.05746300
H	3.12320100	2.23557400	-1.57767200
H	1.85261600	1.93552900	0.57237100
H	0.71878500	3.18375900	0.05474600
O	0.64449700	1.42410100	-1.03590000
H	-1.41451000	-0.93009700	1.34551200
IM5			
C	-1.60161400	0.43106400	-1.10487300
C	-0.27896100	-0.19470100	-0.88156200
C	-1.71611000	1.94989500	-1.04669800
C	-2.82326500	2.60305900	-1.60141700
C	-0.71775700	2.71707600	-0.43790500
C	-2.95477500	3.98595800	-1.51244900
H	-3.58860900	2.02974000	-2.11745200
C	-0.85162000	4.10122300	-0.35235800
H	0.17272700	2.23284400	-0.04680100
C	-1.97322100	4.74004200	-0.87472000
H	-3.82031800	4.47217700	-1.95252000
H	-0.06822800	4.68297000	0.12486500
H	-2.07329500	5.81905300	-0.80312900
C	0.36421000	-0.90318100	-1.90085200
O	-0.12481500	-1.25390200	-2.99454300
C	1.84197400	-1.16852200	-1.56486800
H	1.92591600	-2.00734900	-0.85988700
H	2.35721300	-1.45208200	-2.48627700
P	-2.89166600	-0.32054400	0.03675600
C	-2.99495700	-2.11206000	-0.16898500
C	-3.90356400	-2.81451300	0.63175000
C	-2.29074400	-2.76299500	-1.18554600
C	-4.07982400	-4.17987300	0.44446100

H	-4.47684100	-2.29544800	1.39679800
C	-2.48913700	-4.13012600	-1.37003100
H	-1.60771200	-2.23126000	-1.84683200
C	-3.36697300	-4.83847700	-0.55568200
H	-4.77699900	-4.72610200	1.07187600
H	-1.94568100	-4.63810600	-2.16010300
H	-3.50700400	-5.90480100	-0.70596800
C	-2.57732800	0.15779000	1.75609600
C	-2.34504600	-0.80235100	2.74581100
C	-2.55041000	1.52204500	2.08591700
C	-2.09277300	-0.39867800	4.05381600
H	-2.31644200	-1.85447900	2.48972300
C	-2.29493300	1.91306500	3.39570100
H	-2.72059800	2.27967500	1.32688900
C	-2.06646400	0.95395500	4.37988900
H	-1.90821500	-1.14856900	4.81631800
H	-2.26962100	2.96961400	3.64231700
H	-1.86484600	1.26238400	5.40136900
C	-4.57459200	0.23606300	-0.39800200
C	-5.08702000	-0.22567100	-1.61849900
C	-5.32427000	1.12420100	0.37424200
C	-6.32366300	0.21808900	-2.06902900
H	-4.51665900	-0.93451800	-2.21512400
C	-6.56760300	1.56055500	-0.07983600
H	-4.94907000	1.47339400	1.33029700
C	-7.06358900	1.11704900	-1.30119700
H	-6.71186200	-0.14067500	-3.01685800
H	-7.14762800	2.24935100	0.52621600
H	-8.02982200	1.46416500	-1.65363200
Br	8.57122600	0.07272400	0.05774400
O	-0.26736300	-2.02999200	1.30090200
N	1.73580400	0.62750400	0.23041000
N	0.46640900	-0.07353300	0.32493800
C	4.63694000	-1.12271800	-0.48416800
H	4.09537000	-2.06404500	-0.46024400
C	6.00803000	-1.12919200	-0.24056900
H	6.53004900	-2.05514200	-0.02558700
C	6.70812400	0.06980700	-0.27938400
C	6.06381000	1.26812300	-0.56671200
H	6.62899200	2.19299200	-0.60170100
C	4.69549600	1.25384700	-0.81169600
H	4.18069800	2.18474500	-1.03605400
C	3.96068800	0.06515600	-0.76837700
C	2.46595700	0.11927200	-0.99433500

H	2.29002700	0.89318400	-1.75145600
C	0.56541200	-1.15039300	1.18818200
C	1.86705000	-1.02243600	1.95810800
H	2.54857500	-1.80689400	1.60575200
H	1.70659100	-1.16295700	3.02877200
C	2.32805300	0.37576400	1.55590100
H	1.89847400	1.11867700	2.23661700
H	3.40813500	0.51012900	1.53268800
H	-1.91249100	0.08026900	-2.10230500

IM5a

C	1.32861200	0.87180400	0.59734900
C	0.20030900	1.34369400	-0.26231700
C	2.37261700	1.95135700	0.81120500
C	2.49873500	2.55170900	2.06552000
C	3.14774700	2.42470800	-0.25219000
C	3.41194700	3.58391200	2.26646500
H	1.85766500	2.21849000	2.87959200
C	4.06526300	3.44981200	-0.04830900
H	3.02037400	1.98981000	-1.24082600
C	4.20465000	4.02815600	1.21227200
H	3.49999800	4.04290500	3.24667800
H	4.67003100	3.80146700	-0.87877600
H	4.92201200	4.82799000	1.36858700
C	0.22586700	0.93253100	-1.53791400
O	1.24747900	0.15641700	-1.89853900
C	-0.84633800	1.28800300	-2.52528000
H	-1.20189300	0.37098000	-3.01131000
H	-0.41661000	1.92462600	-3.30699300
P	1.93636300	-0.67276800	-0.29496600
C	2.70796100	-1.55899100	1.20644300
C	2.94112500	-0.99096600	2.46001000
C	3.10150500	-2.89162400	1.01101400
C	3.53724100	-1.72864600	3.48659300
H	2.68107400	0.04279400	2.65820300
C	3.68963500	-3.63224300	2.02738400
H	2.94133000	-3.35950300	0.04047300
C	3.90911500	-3.04916900	3.27606600
H	3.70736800	-1.26069500	4.45173400
H	3.97832900	-4.66375200	1.84794600
H	4.36995400	-3.62276500	4.07464600
C	0.54105400	-1.87711800	-0.44691700
C	0.05231100	-2.31230000	-1.68269700
C	-0.09686300	-2.30327700	0.72354300
C	-1.04129000	-3.17199500	-1.74442400

H	0.50852700	-1.95292200	-2.59664300
C	-1.20910600	-3.13807800	0.65708500
H	0.26819800	-1.97940600	1.69356300
C	-1.67925600	-3.58079700	-0.57684900
H	-1.40288100	-3.51118400	-2.71020700
H	-1.70391000	-3.44460100	1.57395600
H	-2.54361800	-4.23620300	-0.62745000
C	3.49629500	-0.79702400	-1.27487000
C	3.49292600	-1.15003400	-2.62800500
C	4.71462300	-0.52001200	-0.64552000
C	4.69126800	-1.25474300	-3.32779400
H	2.55456900	-1.32550800	-3.13807400
C	5.90620300	-0.58051700	-1.36125400
H	4.73522700	-0.24719200	0.40514600
C	5.89866600	-0.96208200	-2.69961200
H	4.67734900	-1.54976800	-4.37256600
H	6.84133600	-0.34069100	-0.86503700
H	6.83086200	-1.02779400	-3.25268000
Br	-6.56678400	-1.32725500	0.72048000
O	-1.10580800	1.51577900	2.34511900
N	-1.45717200	2.95241600	-0.84279900
N	-0.79452200	2.22411600	0.18043100
C	-4.45218700	1.46607800	-1.48911300
H	-4.69546500	2.32690200	-2.10841000
C	-5.48723500	0.74402100	-0.90519700
H	-6.52283500	1.02720600	-1.05780200
C	-5.17228000	-0.35461600	-0.11414200
C	-3.85312700	-0.74662200	0.07606500
H	-3.62213900	-1.61094500	0.68846700
C	-2.82835800	-0.01753900	-0.52074500
H	-1.80028500	-0.33755800	-0.36511600
C	-3.11252700	1.11275800	-1.29697700
C	-2.02898700	2.01700300	-1.85204100
H	-2.49330600	2.67415300	-2.59508000
C	-1.46324400	2.15963500	1.37528600
C	-2.68492400	3.05733000	1.23788600
H	-2.75968800	3.73577300	2.08957600
H	-3.57290100	2.41597100	1.22755000
C	-2.43570900	3.77193300	-0.09589800
H	-3.33817100	3.90411000	-0.69644600
H	-1.98240800	4.75299900	0.07267300
H	0.94693800	0.53014300	1.56353500
TS6			
C	1.31942800	0.46276600	0.98501100

C	0.05818900	0.11778500	0.45789500
C	1.89156900	1.82271200	1.18152500
C	2.58298100	2.05346100	2.38017700
C	1.83911000	2.84637500	0.22901300
C	3.19056400	3.27848100	2.63249800
H	2.64782500	1.25601800	3.11703600
C	2.44312200	4.07426400	0.48771200
H	1.39296600	2.66129300	-0.74030700
C	3.11806700	4.29753000	1.68459100
H	3.71796300	3.43665900	3.56835300
H	2.40017900	4.85586900	-0.26514600
H	3.59032700	5.25652400	1.87585500
C	-0.47625000	-1.16058600	0.81103900
O	0.11644200	-2.00586500	1.49154800
C	-1.92305800	-1.34360900	0.36469700
H	-1.95821100	-1.56921100	-0.71069100
H	-2.35880000	-2.18300300	0.91202900
P	2.96929400	-0.56821100	-0.10231700
C	2.32873000	-2.01870800	-0.97856100
C	2.71743200	-3.31907800	-0.63530300
C	1.34238600	-1.82440000	-1.95586500
C	2.12662000	-4.41029700	-1.26034900
H	3.47791200	-3.48009400	0.12163000
C	0.75823100	-2.92638700	-2.57728300
H	1.05486600	-0.81545200	-2.23789300
C	1.14191700	-4.21697100	-2.22735900
H	2.43559800	-5.41523500	-0.99019400
H	-0.00025700	-2.77084500	-3.33878400
H	0.67933800	-5.07270900	-2.70988500
C	3.97394900	0.43155800	-1.23146300
C	4.04730800	0.15433400	-2.59990200
C	4.61729000	1.56939300	-0.72138200
C	4.76677900	0.99471500	-3.44330000
H	3.54239400	-0.71659600	-3.00572900
C	5.33968800	2.40027800	-1.57012100
H	4.55003300	1.81127400	0.33744500
C	5.41496300	2.11556100	-2.93158800
H	4.81932200	0.77135500	-4.50427300
H	5.83190700	3.27895400	-1.16473700
H	5.97510700	2.76928900	-3.59325500
C	4.04805600	-1.18573600	1.22055000
C	3.42592500	-1.89507700	2.26223400
C	5.42419500	-0.94373200	1.27182900
C	4.18453500	-2.35344700	3.33512300

H	2.35634700	-2.10487700	2.21449700
C	6.17151600	-1.40091500	2.35334400
H	5.91305300	-0.40612100	0.46520700
C	5.55426300	-2.10275900	3.38576100
H	3.70054400	-2.90586500	4.13456200
H	7.24013700	-1.21186100	2.38547800
H	6.14099200	-2.45605200	4.22834100
Br	-8.83160800	0.01789100	0.25198900
O	0.72520800	1.24316800	-2.18496800
N	-2.13409100	1.10145200	-0.14707500
N	-0.72647600	0.87766300	-0.44458800
C	-4.84800500	-1.08603300	-0.08231900
H	-4.29998300	-1.91735600	-0.51596000
C	-6.23817600	-1.07166600	-0.17802700
H	-6.76857000	-1.87611900	-0.67556300
C	-6.94271500	-0.01054100	0.37300100
C	-6.28415300	1.03234300	1.01821700
H	-6.85248200	1.85118700	1.44561700
C	-4.89857900	0.99881900	1.10950400
H	-4.37054500	1.80801200	1.60743800
C	-4.16329900	-0.05754300	0.56265300
C	-2.65352200	-0.02654400	0.67294400
H	-2.41211400	0.23214000	1.71130600
C	-0.39326300	1.31480600	-1.67559500
C	-1.64372400	1.93400000	-2.27339700
H	-1.67693300	1.78110900	-3.35207500
H	-1.65022800	3.00904700	-2.06068000
C	-2.72841100	1.20474500	-1.49286100
H	-3.67982100	1.73383400	-1.43227200
H	-2.90143300	0.21053900	-1.93827200
H	1.51826100	-0.17634000	1.84722200
TS6a			
C	-1.52320300	1.37975500	0.69645300
C	-0.29790800	1.84434100	0.17331300
C	-2.88164800	1.96579900	0.50395400
C	-3.35643100	2.53981500	-0.68134700
C	-3.73800300	1.91278300	1.61527900
C	-4.65130100	3.04815400	-0.73876400
H	-2.71526300	2.55773900	-1.55408200
C	-5.03223900	2.41676700	1.55138300
H	-3.38175800	1.46211400	2.53934100
C	-5.49541300	2.98643700	0.36717700
H	-5.00777100	3.48353500	-1.66761300
H	-5.67492600	2.36719700	2.42527200

H	-6.50539900	3.38115300	0.30858600
C	-0.01800400	2.25693500	-1.15963100
O	-0.79219600	2.10225100	-2.11605600
C	1.30600800	2.98647600	-1.42550400
H	1.00868000	4.02197700	-1.62724400
H	1.72218700	2.59231700	-2.35727400
P	-2.00430200	-0.77715700	-0.00709500
C	-3.35160500	-0.91114000	-1.23517400
C	-4.60859800	-0.39751800	-0.88308000
C	-3.18597400	-1.49175700	-2.49742300
C	-5.66933900	-0.45412500	-1.77904300
H	-4.76341600	0.04944600	0.09563600
C	-4.25148900	-1.54180600	-3.39256200
H	-2.22860000	-1.91292700	-2.78474100
C	-5.49245300	-1.02123300	-3.03896400
H	-6.63212700	-0.04342400	-1.49050700
H	-4.10791000	-1.99439600	-4.36887400
H	-6.31965200	-1.05937200	-3.74127700
C	-0.55195300	-1.55462800	-0.76183000
C	0.07100800	-2.66490100	-0.18492600
C	-0.03285200	-0.99644300	-1.93848500
C	1.17246700	-3.24416500	-0.80577700
H	-0.30939600	-3.07959800	0.74310800
C	1.06481900	-1.58956300	-2.55931000
H	-0.48606800	-0.10329600	-2.36582200
C	1.66131800	-2.71761500	-2.00042000
H	1.64625600	-4.11245800	-0.35832700
H	1.45935800	-1.16001900	-3.47523100
H	2.51617800	-3.17814000	-2.48763800
C	-2.54548100	-1.85781200	1.36583500
C	-1.88146000	-1.75919100	2.59642400
C	-3.60178800	-2.76582700	1.22332600
C	-2.27259900	-2.56414300	3.66312000
H	-1.03763100	-1.08205900	2.70377500
C	-3.99005600	-3.56084500	2.29746100
H	-4.11925200	-2.85417900	0.27320300
C	-3.32819100	-3.46046500	3.51866800
H	-1.74826600	-2.48750900	4.61072400
H	-4.80801100	-4.26442500	2.17630500
H	-3.63282200	-4.08216300	4.35519200
Br	6.54217600	-1.58751200	-0.21862300
O	0.75210800	-0.20907400	2.00305100
N	1.64752000	3.02909600	0.98640700
N	0.81529900	1.88236200	1.06805100

C	2.99565500	0.53164900	-0.59416100
H	1.95116700	0.27728100	-0.76144500
C	3.93229900	-0.49614500	-0.53795700
H	3.62139400	-1.52735900	-0.65863500
C	5.26903000	-0.18806200	-0.31433300
C	5.68851300	1.12729700	-0.15762000
H	6.73766400	1.35006400	0.00287600
C	4.73715700	2.14126400	-0.20401700
H	5.05809500	3.17283200	-0.07488400
C	3.38266400	1.86296400	-0.40680900
C	2.36953100	2.98627400	-0.31243900
H	2.92011900	3.93314700	-0.35728100
C	1.27570100	0.89281900	1.86758000
C	2.51087100	1.43011100	2.57970200
H	3.38955500	0.88524100	2.21910400
H	2.42466200	1.26707900	3.65600300
C	2.49873400	2.91499100	2.19084200
H	2.03316100	3.51416800	2.97886300
H	3.48974800	3.32338600	1.98167100
H	-1.39733600	1.07383200	1.73662400
TS7			
C	-0.58740700	-1.13761700	-0.82687200
C	0.13235100	-2.00310600	-1.62056600
C	-2.07414500	-1.19001800	-0.77053200
C	-2.79656800	-1.23860000	-1.97089400
C	-2.79113800	-1.25163600	0.43171400
C	-4.18378100	-1.33312500	-1.97023700
H	-2.24493300	-1.20739900	-2.90610500
C	-4.18062700	-1.33178800	0.43502400
H	-2.25343100	-1.24273500	1.37668400
C	-4.88353400	-1.37118600	-0.76588300
H	-4.72139600	-1.37038900	-2.91337400
H	-4.71329600	-1.37726200	1.38055400
H	-5.96727400	-1.43857500	-0.76385900
C	1.57192700	-2.11423900	-1.70931200
O	2.46246800	-1.27415300	-1.83227000
C	1.57880500	-3.54496700	-1.35139600
H	0.14101000	-3.30368200	-1.35754000
H	1.39760700	-4.25925400	-2.15415800
H	2.27448300	-3.89045400	-0.58356500
P	0.30604500	0.13493600	0.02888100
C	0.90477100	1.47565800	-1.04630700
C	1.01644600	1.27323600	-2.42235100
C	1.23430400	2.71677900	-0.48900800

C	1.46536600	2.30996500	-3.23495900
H	0.76298100	0.30781900	-2.84669400
C	1.69284500	3.74469200	-1.30593500
H	1.12311500	2.88326300	0.57985700
C	1.80672000	3.53996700	-2.67941700
H	1.55264200	2.15227300	-4.30508600
H	1.95125500	4.70553800	-0.87200700
H	2.15779900	4.34447100	-3.31864200
C	-0.74201800	1.00870600	1.23157900
C	-0.56000800	0.86289500	2.60790300
C	-1.78571700	1.80470700	0.74468600
C	-1.42565000	1.50347200	3.49244100
H	0.25135800	0.24953000	2.98905100
C	-2.64759000	2.43690400	1.63135400
H	-1.93018200	1.91564900	-0.32735000
C	-2.46875000	2.28500300	3.00597700
H	-1.28153200	1.39000000	4.56234100
H	-3.46179700	3.04519200	1.25076500
H	-3.14426100	2.77895300	3.69776400
C	1.68407800	-0.57380500	0.96516000
C	1.48204900	-1.82591600	1.55266600
C	2.89663700	0.09630400	1.13074200
C	2.49055200	-2.39533800	2.32528300
H	0.54714400	-2.35604900	1.38401500
C	3.89807800	-0.47778800	1.90584500
H	3.06573200	1.04840300	0.63705800
C	3.69483400	-1.72008800	2.50408300
H	2.33802900	-3.37038800	2.77730700
H	4.84464400	0.03797400	2.03156600
H	4.48291500	-2.16814000	3.10163000
TS7a			
C	-0.87408800	0.99912300	-0.03223800
C	-0.55448500	2.35485100	0.00830500
C	-2.23725400	0.40883600	-0.00400600
C	-3.25040500	0.93940800	-0.81710400
C	-2.55665200	-0.67092800	0.83012300
C	-4.52877400	0.39482500	-0.79894500
H	-3.02700300	1.80099400	-1.43717200
C	-3.83198300	-1.22958500	0.83118100
H	-1.80556900	-1.05969800	1.51536300
C	-4.82412700	-0.69907800	0.01344300
H	-5.30002400	0.82537900	-1.43089500
H	-4.05310000	-2.06851300	1.48517400
H	-5.82240900	-1.12641500	0.01612800

C	-1.46035100	3.47262400	0.13458800
O	-2.44129800	3.87243500	-0.47207200
C	-0.84107700	3.85135700	1.42959900
H	-1.48841300	3.93675800	2.30335400
H	0.10397600	2.80246000	1.01743300
H	0.00146300	4.54155600	1.40737700
P	0.51003900	-0.07397200	-0.03443500
C	0.22831800	-1.60724500	-0.98163400
C	-0.27563900	-2.76155200	-0.37338300
C	0.44953000	-1.59668200	-2.36222900
C	-0.55432000	-3.88886800	-1.13942600
H	-0.44844200	-2.78446700	0.69805400
C	0.16985300	-2.72620500	-3.12403400
H	0.84695200	-0.70793500	-2.84347000
C	-0.33332900	-3.87205500	-2.51378000
H	-0.94918200	-4.77942800	-0.66100000
H	0.34645400	-2.70978600	-4.19467700
H	-0.55447700	-4.75245600	-3.10919500
C	1.95208200	0.74699700	-0.78406400
C	3.24581400	0.48749600	-0.32875000
C	1.75851600	1.59772100	-1.87979700
C	4.34001300	1.06426900	-0.97000200
H	3.40779800	-0.15027000	0.53438400
C	2.85474600	2.16645000	-2.51736600
H	0.75053400	1.82609300	-2.21085000
C	4.14582800	1.89984500	-2.06447700
H	5.34275500	0.86353200	-0.60621800
H	2.69834200	2.82991400	-3.36194700
H	4.99889600	2.35207900	-2.56099700
C	1.02512000	-0.61105700	1.63230900
C	0.58083900	0.15119700	2.71689100
C	1.85644600	-1.71635500	1.85043000
C	0.97628800	-0.18464400	4.00941000
H	-0.07982700	0.99855900	2.54376100
C	2.24651800	-2.04786600	3.14383000
H	2.18868600	-2.32217100	1.01050200
C	1.80798600	-1.28029500	4.22203100
H	0.63010300	0.40824900	4.84991800
H	2.88817900	-2.90726700	3.31178100
H	2.11161200	-1.54255800	5.23085500
TS8			
C	-1.46979700	0.51698900	-0.84615700
C	-0.50593100	-0.53677300	-1.45391700
C	-0.94635400	1.90499400	-0.62605400

C	-0.36244800	2.29912500	0.58586000
C	-0.98054300	2.83320800	-1.67510400
C	0.16255300	3.57835900	0.74965300
H	-0.33304200	1.60098300	1.41856300
C	-0.44653400	4.10938400	-1.51597500
H	-1.41090300	2.52766500	-2.62286300
C	0.12432100	4.48796800	-0.30390200
H	0.59834100	3.86482500	1.70270200
H	-0.47861600	4.81039100	-2.34486300
H	0.53690200	5.48473700	-0.17990400
C	0.29923700	-0.06283700	-2.57418400
O	-0.08758200	0.67542400	-3.46891000
C	1.77676000	-0.44265700	-2.43223500
H	1.94068300	-1.51002800	-2.62590400
H	2.34992100	0.14410900	-3.15357200
P	-2.82400100	-0.04757500	0.10121300
C	-4.10666800	-0.90526900	-0.87167800
C	-5.39788000	-0.37309700	-0.96933300
C	-3.77902200	-2.08088600	-1.56236300
C	-6.35136300	-1.00405200	-1.76265600
H	-5.66552200	0.52827100	-0.42771100
C	-4.74091800	-2.69527500	-2.35963800
H	-2.78926400	-2.52115800	-1.46269700
C	-6.02262700	-2.16120700	-2.46306300
H	-7.35141100	-0.58755900	-1.83298300
H	-4.48294300	-3.60212500	-2.89734800
H	-6.76740600	-2.64863800	-3.08507500
C	-2.44715200	-1.15587200	1.49934500
C	-1.19796400	-1.07243100	2.12054900
C	-3.41786500	-2.02931200	1.99854800
C	-0.93552800	-1.83986700	3.25227600
H	-0.41434500	-0.44627100	1.69911600
C	-3.14600300	-2.80023300	3.12488400
H	-4.38251500	-2.11001100	1.50446900
C	-1.90777000	-2.70168900	3.75499800
H	0.03598000	-1.77083700	3.73324400
H	-3.89888800	-3.48243500	3.50672300
H	-1.69641300	-3.30364200	4.63355900
C	-3.60321900	1.41664900	0.84124300
C	-3.94172700	2.48853200	0.00496900
C	-3.85982400	1.49427900	2.21036100
C	-4.53158600	3.62595900	0.54027800
H	-3.72882400	2.43125900	-1.05908800
C	-4.45124200	2.63921800	2.74141700

H	-3.59385700	0.66967100	2.86432900
C	-4.78549200	3.70210500	1.90971000
H	-4.78659900	4.45708600	-0.10919200
H	-4.64526700	2.69801200	3.80767100
H	-5.24131200	4.59481400	2.32691000
H	-1.67540800	-0.25473900	-1.90074600
Br	8.11662100	0.19195100	0.61264300
O	-1.11763100	-3.31497000	-0.58333300
N	1.47337700	-1.00192600	-0.01936300
N	0.21491400	-1.43739200	-0.61891300
C	4.60226800	-0.57424800	-1.45112700
H	4.32860700	-1.07478600	-2.37568000
C	5.94527000	-0.51270300	-1.08551500
H	6.71259700	-0.95476100	-1.71134300
C	6.29478800	0.12160300	0.09882900
C	5.33064100	0.70323600	0.91645100
H	5.62536900	1.20060900	1.83406800
C	3.99706300	0.63815500	0.53290100
H	3.22999200	1.08907900	1.15799000
C	3.61579000	-0.00293200	-0.64959400
C	2.14345300	-0.08078800	-0.98222600
H	1.71701700	0.91230700	-0.78362700
C	-0.09232500	-2.71673500	-0.29458100
C	1.06530800	-3.24624300	0.53590100
H	1.26957900	-4.28952500	0.29339600
H	0.78883300	-3.17657700	1.59372400
C	2.18538200	-2.28350700	0.16990800
H	2.95534100	-2.16525200	0.93358600
H	2.66502500	-2.61545900	-0.76494700
TS8a			
C	1.17347400	0.52554400	0.44552500
C	-0.16031600	-0.19044600	0.07883500
C	1.25959800	2.00993800	0.27881600
C	1.27586300	2.84944700	1.39651000
C	1.36664900	2.59527900	-0.98881200
C	1.39896200	4.22871600	1.25855200
H	1.18929600	2.40167200	2.38326500
C	1.49638900	3.97223600	-1.13437400
H	1.36327400	1.95294300	-1.86678400
C	1.51378500	4.79288900	-0.00869200
H	1.40511100	4.86267200	2.14022600
H	1.58909600	4.40626700	-2.12573600
H	1.61477300	5.86851500	-0.12026200
C	-0.25556000	-1.58592800	0.32672100

O	0.55221300	-2.19142100	1.05449300
C	-1.29893400	-2.38785800	-0.44397600
H	-1.85307100	-3.01842100	0.25863800
H	-0.70013200	-3.05945000	-1.07147800
P	2.64673700	-0.40670200	0.25875700
C	3.94471200	0.72677700	-0.33494900
C	4.43920600	1.69915800	0.54327700
C	4.36590700	0.72002900	-1.66607300
C	5.32845900	2.66363000	0.08598200
H	4.11518200	1.70878900	1.58071600
C	5.26718800	1.68173900	-2.11605400
H	3.98924400	-0.03123200	-2.35371500
C	5.74334500	2.65645800	-1.24480800
H	5.69760900	3.42196200	0.76907600
H	5.59453600	1.66804500	-3.15107200
H	6.43966100	3.40958700	-1.60072000
C	3.37678900	-1.10452300	1.77595600
C	4.74392300	-1.40461500	1.78887700
C	2.61024800	-1.29550300	2.92549000
C	5.33481000	-1.91338200	2.94143700
H	5.34902900	-1.23046100	0.90205700
C	3.20931400	-1.79268400	4.07870900
H	1.54881600	-1.07803300	2.89418200
C	4.56689500	-2.10431400	4.08735600
H	6.39434900	-2.14928200	2.94638700
H	2.61162400	-1.94271800	4.97238900
H	5.02808800	-2.49387100	4.99000000
C	2.48704000	-1.70411200	-0.99688700
C	3.07862800	-2.96189300	-0.86522800
C	1.68462700	-1.41680300	-2.10488100
C	2.89449900	-3.91669300	-1.85925900
H	3.66271200	-3.19992900	0.01878400
C	1.49253400	-2.38307200	-3.09007100
H	1.18573100	-0.45345700	-2.18552700
C	2.10178500	-3.62887300	-2.97029000
H	3.35784100	-4.89323000	-1.75948400
H	0.85250500	-2.15958800	-3.93797400
H	1.95132100	-4.38304300	-3.73687100
Br	-7.51576600	0.38695600	1.28253800
O	-1.77926200	2.17859600	0.33809600
N	-1.49000200	-0.46409000	-1.93735200
N	-1.02290400	0.38583400	-0.88837300
C	-4.76390400	-1.30135500	-1.31019500
H	-4.79055800	-1.76253700	-2.29532300

C	-5.95060400	-0.84774500	-0.74421700
H	-6.89524800	-0.94730100	-1.26746900
C	-5.91013800	-0.25732200	0.51333300
C	-4.71474300	-0.13533200	1.21272800
H	-4.70268000	0.32768000	2.19303200
C	-3.53914800	-0.60566800	0.63601200
H	-2.60377900	-0.49611500	1.18067700
C	-3.54346700	-1.17471500	-0.64172700
C	-2.26228200	-1.59122500	-1.33871400
H	-2.53939100	-2.21876300	-2.19418900
C	-1.84461300	1.46715700	-0.64073300
C	-2.78324300	1.58222600	-1.83433000
H	-2.70013900	2.57692900	-2.27716400
H	-3.81021100	1.44720700	-1.48193500
C	-2.29082400	0.46472500	-2.76583800
H	-3.09491600	-0.08521700	-3.26006700
H	-1.62542800	0.87224800	-3.53297600
H	0.11209800	0.29427600	1.21445600