

Supporting Information

Computational insights into [Ni]H-catalyzed remote C(sp³)-H hydroamidation of alkenes: mechanism and insertion selectivity

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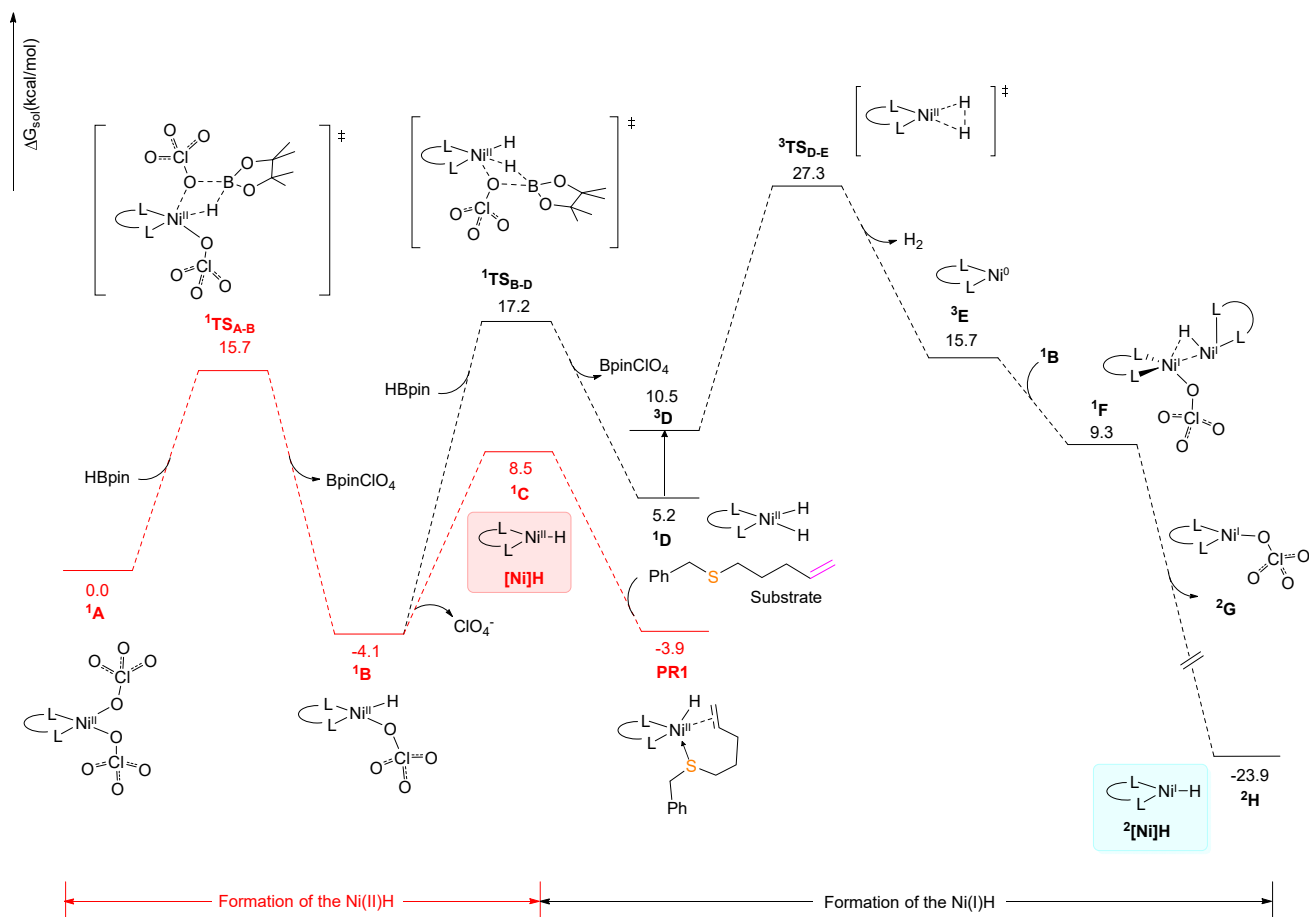
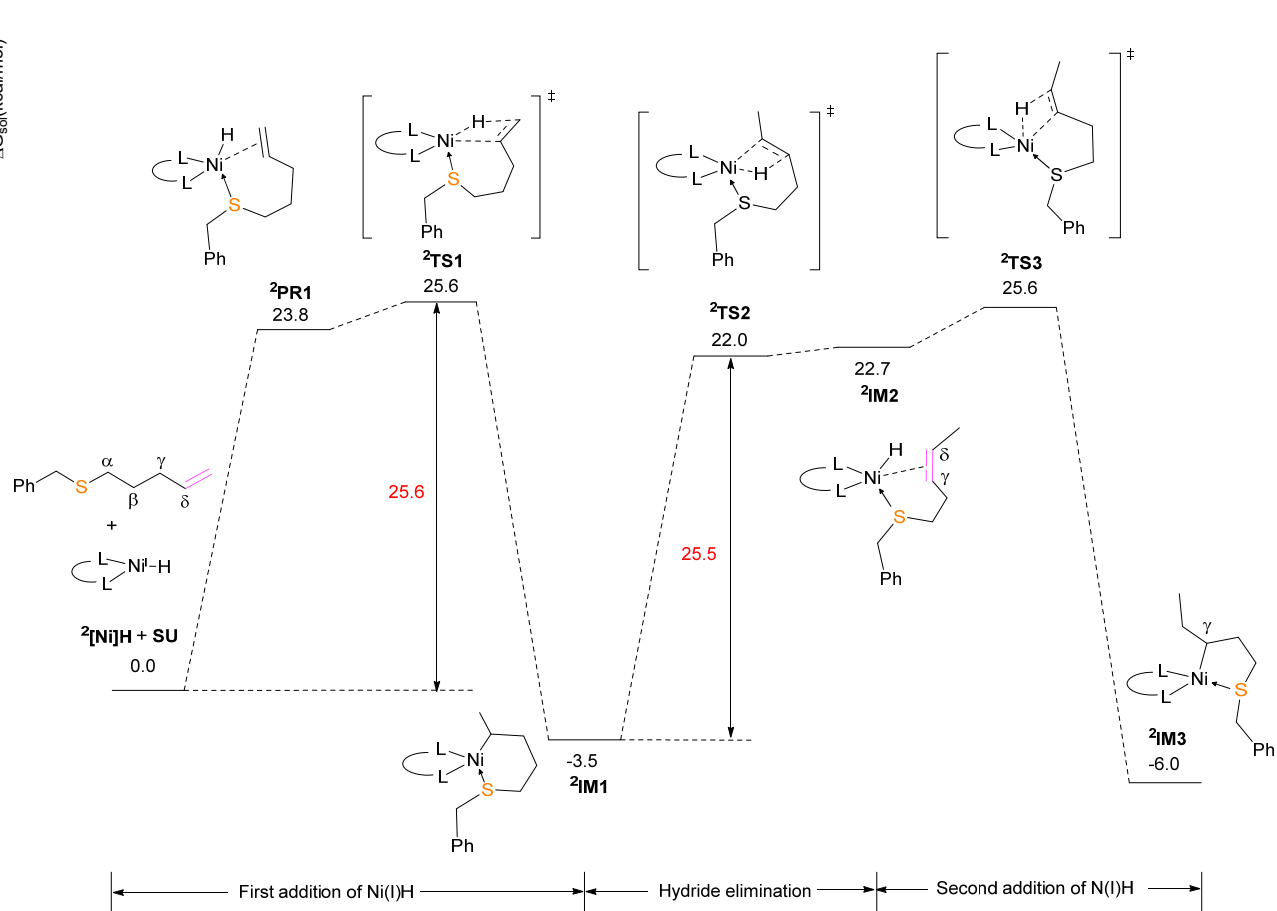
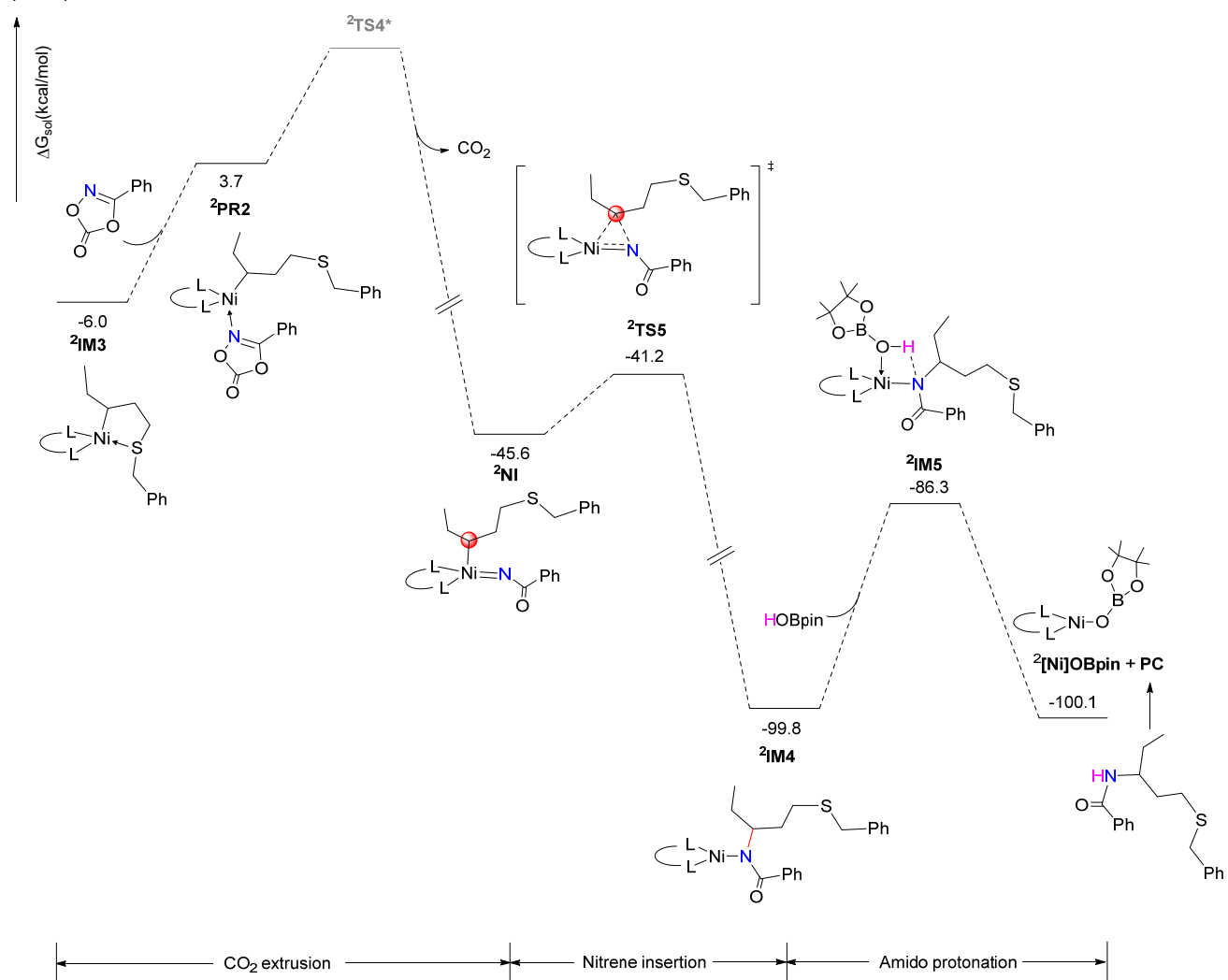


Fig. S1 Free energy profile of the formation of Ni(II)H/Ni(I)H catalytic species. The superscript (left) of the name of species represents the spin state of the species. For example, $^1\mathbf{A}$ and $^2\mathbf{H}$ are singlet and doublet state species, respectively. The formation mechanism of NiH is similar to that of CuH.¹ The transfer of hydride from HBpin to $^1\mathbf{A}$ proceeds through a transition state $^1\mathbf{TSA-B}$, affording the Ni(II) hydride species $^1\mathbf{B}$. Then, the cleavage of coordination bond Ni-O in $^1\mathbf{B}$ generates the nickel(II) catalytic species $[\text{Ni}]\text{H}$ that readily coordinates with the substrate accompanying by a decrease in energy by 12.4 kcal/mol, triggering the catalytic reaction. Alternatively, $^1\mathbf{B}$ can also accept hydride from HBpin via a transition state $^1\mathbf{TSB-D}$ to generate singlet $^1\mathbf{D}$, which converts into triplet $^3\mathbf{D}$, followed by a H_2 release transition state $^3\mathbf{TSD-E}$ with a barrier of 22.1 kcal/mol (relative to $^1\mathbf{D}$). In $^3\mathbf{E}$, the nickel center has been reduced to nickel(0). Subsequently, the comproportionation of the nickel(0) species $^3\mathbf{E}$ with nickel(II) hydride $^1\mathbf{B}$ results in the formation of dimeric nickel(I) species $^1\mathbf{F}$ that dissociates to give nickel(I) hydride $^2[\text{Ni}]\text{H}$. For Ni-catalyzed hydrofunctionalization reactions, both Ni(I)H and Ni(II)H are likely to be catalytic species.²⁻⁴ We also consider the situation of alkene hydroamidation using $^2[\text{Ni}]\text{H}$ as catalyst and the corresponding free energy profile is shown in Fig. S2.

(a) Free energy profile of chain walking catalyzed by Ni(I)H



(b) Free energy profile of CO₂ extrusion, nitrene group insertion and amido protonation by Ni(I)H. The transition state of CO₂ extrusion (²TS4*) was not located



(c) Free energy profile of regeneration Ni(I)H catalyst.

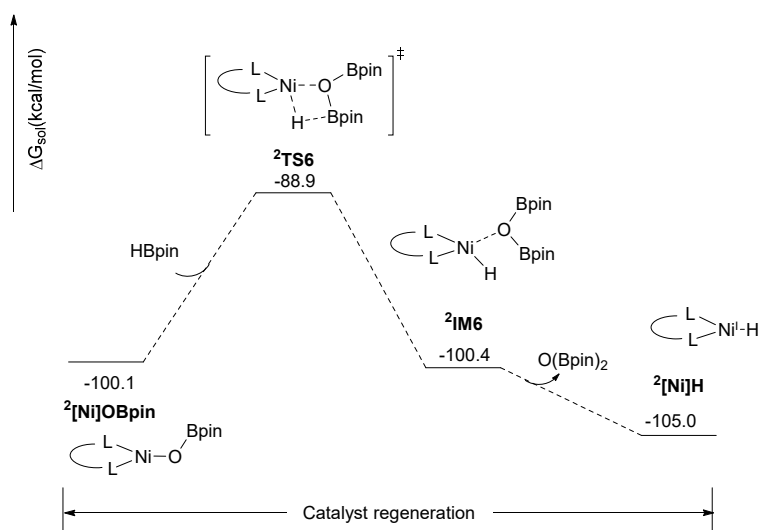


Fig. S2 Free energy profiles of the hydroamidation of alkenes by Ni(I)H catalysis. The hydride elimination transition state **TS2** by Ni(II)H (see Fig. 1) is greatly lower in energy than ${}^2\text{TS2}$ by Ni(I)H (18.5 vs. 25.6 kcal/mol), indicating that Ni(II)H catalysis might be more favorable and thus is discussed in the text.

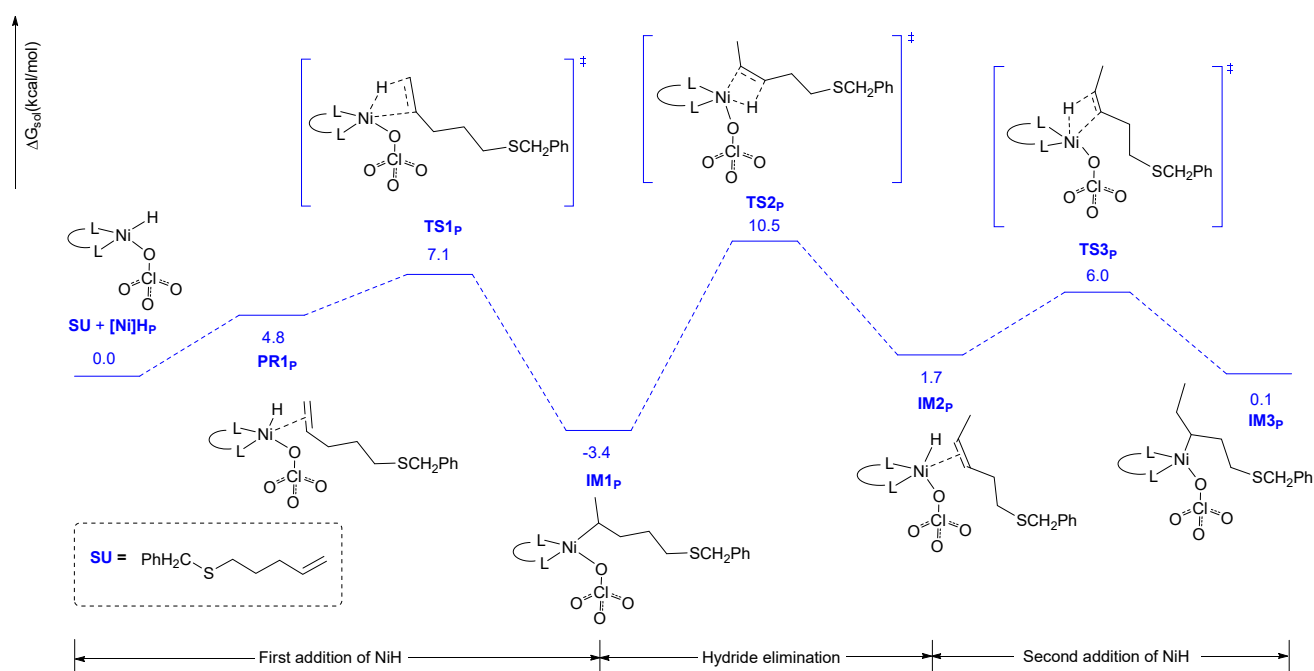
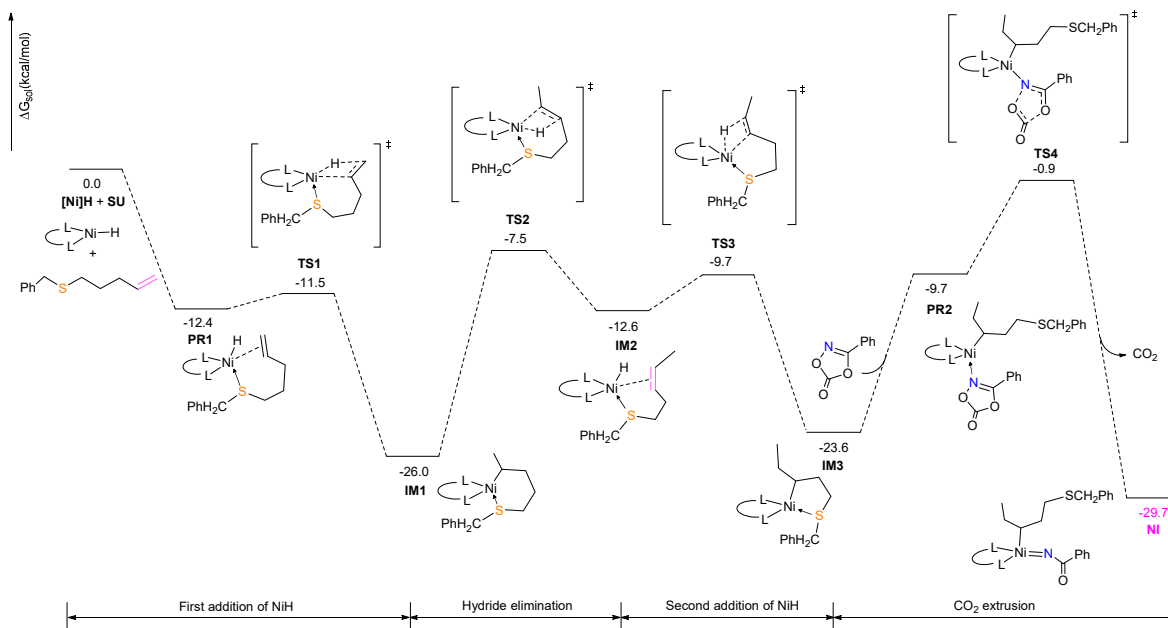


Fig. S3 Free energy profile of chain walking catalyzed by $[\text{Ni}]\text{H}_p$ (ClO_4^- anion coordinating to Ni center). The nickel hydride species $[\text{Ni}]\text{H}_p$ combines with the substrate SU to form a pentene-coordinated precursor PR1_p with an increase in energy by 4.8 kcal/mol. Then the addition of NiH to terminal C=C bond occurs via the transition state TS1_p , affording the intermediate IM1_p . Subsequently, IM1_p undergoes a hydride elimination transition state TS2_p to generate intermediate IM2_p , followed by a second addition transition state TS3_p , giving IM3_p . The coordinated S atom was substituted by O atom of ClO_4^- , leading to the disappearance of thioether-metallacycle (see Fig. 1 and Fig. S3 for the comparison of geometrics: TS1 vs. TS1_p , IM1 vs. IM1_p , TS2 vs. TS2_p , TS3 vs. TS3_p , IM3 vs. IM3_p). As for energy barriers, the addition of NiH with coordinated ClO_4^- (TS1_p and TS3_p) are higher than those (TS1 and TS3) without ClO_4^- , but for the hydride elimination the former (TS2_p) is lower than the latter (TS2). The coordination ability of ClO_4^- is extremely weak and it is hardly coordinated to metal center at the present of the ligands containing N, O or S atoms.⁵⁻⁶ For the system studied, ClO_4^- is readily dissociated in solvent at the presence of 1,10-phenanthroline ligand and alkene substrate that involves a sulfur atom owning higher coordination ability. Thus, the chain walking mechanism by $[\text{Ni}]\text{H}$ is considered to be favourable relative to by $[\text{Ni}]\text{H}_p$.

(a) Free energy profile of pathway a (Chain walking occurring prior to CO₂ extrusion)



(b) Free energy profile of pathway b (CO₂ extrusion occurring prior to Chain walking)

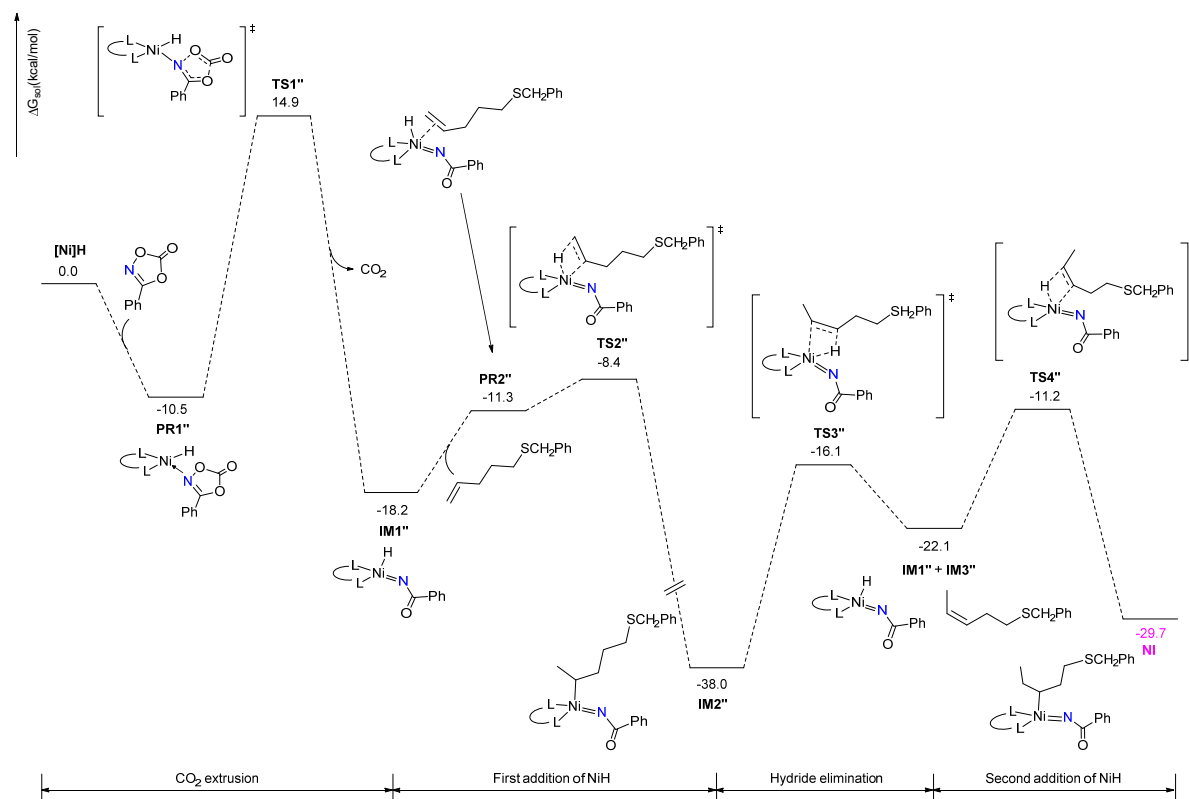


Fig. S4 Comparison of free energy profiles. For energy barriers, the second addition of NiH (**TS3**) and CO₂ extrusion (**TS4**) require 16.3 and 25.1 kcal/mol, respectively (both **TS3** and **TS4** relative to **IM1**), for pathway a, but these steps (**TS4''** and **TS1''**) require higher barriers: 25.4 and 26.8 kcal/mol, respectively (**TS4''** and **TS1''** relative to **IM2''** and **PR1''**, respectively), for pathway b. This indicates that pathway a is more favorable for the [Ni]H-catalyzed hydroamidation of alkenes.

Reference

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Cartesian coordinates of species

[Ni]H

Charge: 1, Spin: 1

C	-3.39655400	1.41559500	0.96253200
C	0.56039700	1.52069700	-0.30932200
C	1.26073500	2.73885300	-0.41017100
C	2.63688000	2.65678800	-0.72606600
C	3.21721500	1.42075500	-0.89008500
C	2.45566200	0.22706000	-0.79365000
N	1.13844500	0.29421800	-0.53799600
H	3.22566800	3.56444500	-0.82001200
H	4.27675600	1.33352400	-1.10280300
C	-0.81213900	1.52998000	0.09506000
C	-1.47414400	2.74901700	0.35352500
C	-2.81852300	2.65613400	0.78164800
C	-2.65934200	0.23515000	0.70800400
N	-1.40322000	0.31413400	0.25680300
H	-3.38260400	3.56192700	0.98402900
H	-4.41770100	1.33029700	1.31704500
H	0.63233000	-1.99610600	-1.24915600
Ni	-0.20506700	-1.06701500	-0.53817200
C	3.15533300	-1.09702400	-0.89668400
H	2.48480800	-1.82774900	-1.35363300
C	-3.22709100	-1.13188300	1.00777400
H	-2.59372100	-1.58395500	1.78357300
C	-3.32818100	-2.11372400	-0.17569700
H	-3.99716700	-1.71297800	-0.94561200
C	3.62235400	-1.61918700	0.48703800
H	4.21709400	-2.52240300	0.30702900
H	-3.80180900	-3.02551900	0.20406300
C	-1.98883000	-2.50591900	-0.82068300
H	-1.22836600	-2.65247700	-0.01262300
H	-1.68860100	-1.70335600	-1.53680500
H	4.30373800	-0.88695600	0.94002100
C	2.49020600	-1.94539300	1.46872900
H	1.79170500	-2.64601400	0.99055300
H	1.90962000	-1.03849400	1.68405600
C	0.56278100	3.97018400	-0.17061500
H	1.11130100	4.90128400	-0.27300300
C	-0.75398600	3.97813000	0.19032100
H	-1.27044500	4.91442500	0.37658500
H	-4.21924900	-1.00878600	1.44986900
H	4.02673200	-0.98277200	-1.54840700
C	-2.03114500	-3.80213100	-1.63878600

H	-1.06142600	-4.00101200	-2.10044000
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H	-2.78140000	-3.72689400	-2.43144300
C	3.01249900	-2.54011400	2.78041600
H	2.19269300	-2.76517700	3.46929000
H	3.56288100	-3.46964500	2.60049200
H	3.69163100	-1.84472700	3.28560200

PR1

Charge: 1, Spin: 1

C	3.07804600	1.13633400	-2.31489600
C	2.75433300	2.47117000	-2.29418500
C	1.53740800	2.87566100	-1.70243800
C	0.68791400	1.85745500	-1.20773800
C	2.19461300	0.16998100	-1.77329700
C	1.15282800	4.25024900	-1.58124200
C	-0.54443800	2.22346900	-0.56655700
C	-0.88152600	3.59242400	-0.42983400
C	-0.01182600	4.59668500	-0.96485400
C	-2.07610000	3.89828400	0.25745600
C	-2.83660900	2.87445200	0.77450100
C	-2.44139600	1.52748700	0.60199200
H	1.81588600	5.01054700	-1.98249000
H	4.01990400	0.79833800	-2.73337200
H	-0.29750200	5.63900400	-0.86189000
H	-3.74812300	3.08266600	1.32429400
N	1.00250000	0.52524100	-1.27416600
N	-1.32639200	1.21759300	-0.07423700
H	-2.37503300	4.93475100	0.38385300
H	3.42722100	3.21686700	-2.70753200
C	-0.87295400	-3.43522200	-1.84448900
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H	0.09081600	-3.95886500	-1.85148500
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H	0.06782900	-4.41859300	0.75068500
H	-1.23234900	-3.63380600	1.65840200
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C	0.16962400	-1.48762900	2.58059300
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H	0.58728500	-2.27638400	3.21253700
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C	2.30165500	-0.15338300	2.78079000
C	0.19705200	1.02800500	2.75347700
C	2.98468900	1.06207800	2.80947600
H	2.85577300	-1.08826600	2.78730800
C	0.87744600	2.24597500	2.78332500
H	-0.88726900	1.01480800	2.74398000
C	2.27345800	2.26550100	2.79993900
H	4.06981600	1.07025300	2.84406800
H	0.31673400	3.17585600	2.79537000

H	2.80527500	3.21180500	2.82304200
C	-3.29415400	0.42840100	1.17492000
C	-4.36192700	-0.06886600	0.17994300
H	-3.78433500	0.78849700	2.08641600
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H	-3.87714100	-0.28323100	-0.77854600
C	-6.12578500	-1.83838900	-0.32366500
H	-4.34772500	-2.10723500	0.88134600
H	-5.57476800	-1.10505300	1.63932800
H	-6.62931500	-2.73439200	0.05072500
H	-6.89310700	-1.08287700	-0.52328400
H	-5.65544800	-2.09379300	-1.28043900
C	2.67747800	-1.25113500	-1.66861200
C	3.70200900	-1.39319400	-0.52212300
H	3.13949000	-1.55652600	-2.61509400
H	1.84435700	-1.92197200	-1.47396300
C	4.09677300	-2.85142100	-0.27198100
H	4.59474400	-0.79537100	-0.74705200
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C	5.09653900	-2.99676400	0.87889100
H	3.18933900	-3.42867500	-0.04889600
H	4.52051500	-3.27972800	-1.18991000
H	5.36462500	-4.04429200	1.04487700
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H	4.67926500	-2.60755700	1.81512100
C	-1.60213400	-1.01332200	-2.45721800
C	-0.63359200	-1.98496500	-2.25344300
H	-1.39352200	-0.15877900	-3.09596500
H	-2.65268900	-1.21866800	-2.27569000
H	0.31425900	-1.81769600	-2.75653600
Ni	-0.62419100	-0.57463700	-0.65742100
H	-1.78926000	-1.16694900	-0.16176600

TS1

Charge: 1, Spin: 1

C	-3.13672300	1.36911200	2.07344500
C	-2.62795200	2.64334200	2.14488900
C	-1.30393400	2.88036600	1.71460800
C	-0.55619700	1.76204500	1.27649500
C	-2.33855600	0.29725200	1.60235000
C	-0.71295500	4.18522100	1.69959700
C	0.77492300	1.96277400	0.77889200
C	1.32729900	3.26599900	0.75639200
C	0.55720100	4.37120300	1.24220800
C	2.62633900	3.40857500	0.22351900
C	3.27295700	2.30310500	-0.28037700
C	2.65395500	1.03306500	-0.24694500
H	-1.30223700	5.02424700	2.05673700
H	-4.15920300	1.16153500	2.36971800
H	1.00266200	5.36115300	1.22642100
H	4.26169600	2.38814500	-0.71822300
N	-1.05672700	0.48641400	1.25996400

N	1.44126900	0.87040600	0.30091700
H	3.09329500	4.38883900	0.19734000
H	-3.23297200	3.46834400	2.50962700
Ni	0.44125600	-0.80903900	0.68548400
C	0.02574400	-2.47576900	1.81260000
C	1.36074800	-2.08450900	2.03872600
H	-0.70811100	-2.13727300	2.54007400
H	1.64975500	-1.52275200	0.47980300
H	1.60269800	-1.41452100	2.86076600
H	2.18023200	-2.74238000	1.75645000
C	-0.32027400	-3.77234000	1.08949000
H	-0.08845100	-4.59910800	1.77403400
H	-1.40325200	-3.82282600	0.92298000
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H	-1.17695900	-3.93358200	-1.73356400
H	0.41165700	-3.45108800	-2.34691000
S	-0.72142800	-1.62681400	-1.23012600
C	-0.21294800	-0.80902000	-2.81118400
H	0.83269300	-1.05177900	-3.01684100
H	-0.83588900	-1.22643000	-3.60829600
C	-0.40982600	0.68072300	-2.65973600
C	-1.67090000	1.20862100	-2.34513500
C	0.67298100	1.55628400	-2.79547700
C	-1.83664400	2.57775700	-2.13964600
H	-2.52418000	0.54265300	-2.25814800
C	0.50598300	2.92922100	-2.60690100
H	1.65322400	1.16142700	-3.04748600
C	-0.74632600	3.44247900	-2.26569800
H	-2.81759000	2.96988800	-1.88867200
H	1.35673300	3.59414000	-2.71683200
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C	4.27895700	-0.84402800	0.24629000
H	3.98239600	0.14518900	-1.66326300
H	2.63142900	-0.87742600	-1.17150800
C	4.73106700	-2.24173900	-0.18890100
H	5.15143400	-0.20821200	0.44081300
H	3.73650900	-0.91503800	1.19610300
C	5.61757700	-2.92871300	0.85321100
H	3.83921700	-2.85689700	-0.38034400
H	5.26307200	-2.17321000	-1.14669200
H	5.91664800	-3.92838700	0.52499800
H	6.52955000	-2.35122500	1.03800500
H	5.09340200	-3.03311500	1.81052400
C	-2.98490200	-1.04769900	1.41490800
C	-4.02684700	-1.03552800	0.27649600
H	-3.46899800	-1.36005400	2.34889000
H	-2.22319100	-1.78219100	1.17436200
C	-4.53684500	-2.44337900	-0.04760500
H	-4.86932000	-0.38401300	0.54034000
H	-3.56292400	-0.60493300	-0.61763400

C	-5.55287000	-2.45187700	-1.19291400
H	-3.67800900	-3.07665100	-0.31145000
H	-4.98298700	-2.88731600	0.85216500
H	-5.89911500	-3.46639200	-1.41120300
H	-6.43149300	-1.84586400	-0.94640900
H	-5.11405100	-2.04288900	-2.11020700

IM1

Charge: 1, Spin: 1

C	3.44760100	-1.50210700	-2.04585800
C	4.02726300	-0.25647800	-1.98860800
C	3.25287400	0.84973800	-1.57857300
C	1.89667500	0.60537000	-1.23392300
C	2.07939800	-1.65935900	-1.71890500
C	3.79442300	2.17321100	-1.50966500
C	1.09185000	1.70961900	-0.75921000
C	1.66043000	3.00918600	-0.71673900
C	3.02223700	3.21793600	-1.10645900
C	0.84741200	4.06639400	-0.25757500
C	-0.44489600	3.80742100	0.13326200
C	-0.94795800	2.48913400	0.07980800
H	4.83174000	2.32489200	-1.79271200
H	4.02044300	-2.37018100	-2.35383800
H	3.42519200	4.22502600	-1.06088900
H	-1.09253900	4.60272000	0.48619100
N	1.32755700	-0.62603800	-1.32955600
N	-0.19064200	1.46917700	-0.34987400
H	1.25257800	5.07325600	-0.21257500
H	5.07048100	-0.11212900	-2.25496600
Ni	-0.85713600	-0.46174900	-0.43724400
C	-1.86699100	-1.97356100	-1.04336400
C	-2.21032700	-1.07334700	-2.21954900
H	-1.19334200	-2.78001700	-1.32700800
H	-3.24633600	-0.72769200	-2.20970300
H	-1.58337100	-0.13252400	-2.23135500
H	-1.97145600	-1.52696200	-3.18576100
C	-3.03972100	-2.53171400	-0.23242200
H	-3.80850200	-2.90106900	-0.92431700
H	-2.70462900	-3.40644400	0.33872400
C	-3.67812700	-1.51372400	0.72806400
H	-3.80437500	-0.55902300	0.20552900
H	-4.67652600	-1.84561900	1.03315900
C	-2.85365000	-1.28999300	2.00257200
H	-2.96218500	-2.13048600	2.69327800
H	-3.15388300	-0.37406700	2.51961600
S	-1.04699800	-1.16559000	1.60953900
C	-0.45718700	0.07926000	2.84407500
H	-1.09872000	0.96245200	2.79111700
H	-0.59386100	-0.39005200	3.82426200
C	0.98680400	0.44023300	2.58415400
C	1.95125800	-0.53965800	2.30588600
C	1.37631000	1.78388500	2.61947600
C	3.27231400	-0.17637400	2.04589000
H	1.67030100	-1.58841500	2.28073700

C	2.70199500	2.14553300	2.37688100
H	0.63781200	2.55325800	2.82649900
C	3.65190400	1.16735200	2.07974900
H	4.00515800	-0.94442400	1.81817300
H	2.98832900	3.19223200	2.40718400
H	4.68006100	1.44980400	1.87674700
C	-2.38666000	2.24210200	0.44787400
C	-3.32271100	2.37922400	-0.77095200
H	-2.69029000	2.95926600	1.21893400
H	-2.49289800	1.23954700	0.86780500
C	-4.80439000	2.23942600	-0.40385100
H	-3.15422900	3.35117300	-1.25190900
H	-3.04727700	1.61814100	-1.51082200
C	-5.71748100	2.28125400	-1.63255400
H	-4.96082800	1.29821400	0.14005800
H	-5.07920200	3.04136100	0.29359800
H	-6.77009600	2.19194800	-1.34923800
H	-5.59734300	3.22141300	-2.18135000
H	-5.48627500	1.46222400	-2.32346300
C	1.45367900	-3.02825400	-1.75758100
C	1.25148500	-3.59641100	-0.33962800
H	2.08241200	-3.70560400	-2.34455800
H	0.49074700	-2.96476700	-2.27330000
C	0.52556600	-4.94503200	-0.31947700
H	2.22925100	-3.69470600	0.15087500
H	0.68311400	-2.86753400	0.24563900
C	0.22691200	-5.41768500	1.10650900
H	-0.41527600	-4.86127100	-0.88114300
H	1.12666200	-5.69626000	-0.84735500
H	-0.29563000	-6.37876600	1.10915600
H	1.14952200	-5.53828200	1.68504000
H	-0.40110900	-4.68964900	1.63429900

TS2

Charge: 1, Spin: 1

C	3.29015000	1.95244300	-1.86262500
C	2.59050100	3.13642000	-1.77828900
C	1.22952000	3.11113400	-1.40689000
C	0.65914900	1.84480800	-1.12475300
C	2.65378300	0.72650000	-1.56320900
C	0.43070200	4.29396400	-1.28994500
C	-0.72532500	1.75664100	-0.74784000
C	-1.48186700	2.94621100	-0.62821800
C	-0.87429500	4.21357500	-0.90781200
C	-2.82746200	2.81891800	-0.22424100
C	-3.33560700	1.56962100	0.03822000
C	-2.52872900	0.41550200	-0.10374300
H	0.88841400	5.25446200	-1.50642200
H	4.33342700	1.94424900	-2.15962900
H	-1.48063400	5.10904100	-0.81127700
H	-4.36307400	1.45012100	0.35837600
N	1.37134200	0.68590100	-1.18166600
N	-1.25148300	0.51280600	-0.50531200
H	-3.44517400	3.70600600	-0.11792800

H	3.07043000	4.08507400	-2.00082000
C	-3.11102400	-0.93498400	0.22740900
C	-4.49001000	-1.23168000	-0.41840500
H	-3.19644700	-1.00211700	1.32002000
H	-2.38236000	-1.69022800	-0.05513000
C	-5.68573900	-1.07878100	0.53300500
H	-4.63479100	-0.59535600	-1.30052400
H	-4.48312900	-2.26152200	-0.79492700
C	-7.02208900	-1.37372400	-0.15287300
H	-5.54599200	-1.75591900	1.38611900
H	-5.70814400	-0.06636700	0.95787300
H	-7.85847500	-1.27322400	0.54483600
H	-7.19750100	-0.68587500	-0.98752800
H	-7.04222500	-2.39316800	-0.55371900
C	3.42110200	-0.56764300	-1.64628100
C	3.87660700	-1.07835100	-0.26643000
H	4.29212300	-0.43569500	-2.29609800
H	2.78176000	-1.31882600	-2.12133400
C	4.48113100	-2.48488900	-0.31089000
H	4.60056400	-0.37296000	0.16213600
H	3.00677000	-1.07862500	0.39982800
C	4.87580400	-2.99665900	1.07751600
H	3.75469600	-3.17396400	-0.76518700
H	5.35651700	-2.48977800	-0.97233600
H	5.30647500	-4.00077200	1.02747700
H	5.61557700	-2.33877300	1.54587900
H	4.00649400	-3.04164300	1.74596000
Ni	0.16689100	-0.89056000	-0.56887800
C	-0.32920800	-2.13216100	-2.23701500
C	0.45850700	-2.87941100	-1.33911200
H	1.28820000	-1.77423000	-0.52563700
H	0.21844000	-1.69735000	-3.07381900
C	-1.80239000	-2.30322700	-2.50788900
H	-2.31302100	-1.33889800	-2.58145900
H	-1.93478100	-2.81384000	-3.46985000
H	-2.31342300	-2.89938300	-1.75103400
H	1.46690700	-3.12772100	-1.67472800
C	-0.06316600	-3.81338700	-0.25311300
C	0.48555200	-3.46429300	1.14678300
H	0.23052500	-4.84423600	-0.48584700
H	-1.15608600	-3.79338000	-0.22155700
H	0.12780400	-4.17011100	1.89945700
H	1.58031500	-3.46343500	1.14988700
S	-0.09577800	-1.75566600	1.56706300
C	1.16826600	-1.05929700	2.73854600
H	2.16205000	-1.38101000	2.41966400
H	0.95946900	-1.46631100	3.73154300
C	1.01952300	0.44154900	2.68456600
C	-0.16401700	1.05144900	3.12801900
C	2.01973600	1.23744400	2.11452700
C	-0.34957800	2.42586500	2.98275300
H	-0.94379600	0.44458400	3.58095800
C	1.84051800	2.61535900	1.98242800
H	2.94150200	0.77961000	1.77157900

C	0.65145700	3.21145000	2.40471100
H	-1.27183500	2.88454800	3.32624900
H	2.62686200	3.21919700	1.54029400
H	0.50704000	4.28101900	2.28963000

IM2

Charge: 1, Spin: 1

C	-2.74793200	1.88734000	2.17983000
C	-1.93376200	2.97908000	2.37086200
C	-0.61565500	2.95334100	1.86528100
C	-0.17753400	1.74709500	1.26782400
C	-2.26073100	0.73413500	1.51927100
C	0.25566900	4.09030600	1.90019200
C	1.12858000	1.69020500	0.67468100
C	1.93393000	2.85256000	0.65171400
C	1.48082900	4.04457800	1.30472100
C	3.15258500	2.77652200	-0.05756400
C	3.47879700	1.60974100	-0.70706400
C	2.63976400	0.47099000	-0.62077700
H	-0.09269100	4.99647200	2.38604800
H	-3.77875300	1.90370600	2.51450400
H	2.12933600	4.91531700	1.30280600
H	4.39095300	1.53446500	-1.28792700
N	-0.97780900	0.64281700	1.14041100
N	1.50443900	0.51392900	0.08915200
H	3.80515300	3.64346000	-0.10436900
H	-2.30307800	3.86996100	2.87047000
C	3.03864300	-0.79677200	-1.32783500
C	3.88669900	-1.75480000	-0.46072600
H	3.61136300	-0.52264000	-2.22087200
H	2.13603900	-1.30901000	-1.66588900
C	5.24077700	-1.19381400	-0.01300800
H	3.30338400	-2.04361000	0.42057000
H	4.04630700	-2.67254500	-1.04027200
C	6.04287600	-2.20676900	0.80982800
H	5.82034100	-0.89048900	-0.89575500
H	5.08667200	-0.28363500	0.58127400
H	7.00354100	-1.79153600	1.12810800
H	5.49278700	-2.50445700	1.71000600
H	6.24605300	-3.11396600	0.23044500
C	-3.21855800	-0.37516300	1.16410600
C	-4.46192400	0.09353100	0.38175500
H	-3.55098900	-0.89114700	2.07501200
H	-2.67665200	-1.09914300	0.55902200
C	-5.33456900	-1.08851600	-0.05919200
H	-5.06399600	0.77847600	0.98978300
H	-4.14776000	0.66694300	-0.50013200
C	-6.56564400	-0.64882300	-0.85624500
H	-4.73113600	-1.77955300	-0.66550900
H	-5.64608000	-1.65659500	0.82732200
H	-7.17231100	-1.50847200	-1.15484400
H	-7.20071100	0.01805100	-0.26336000
H	-6.27612400	-0.11097400	-1.76583500
Ni	0.23422500	-0.94484800	0.59227600

C	0.43150200	-1.97430500	2.46203500
C	-0.63995600	-2.44703100	1.70740100
H	1.25062300	-1.87330700	0.31203000
H	0.19081700	-1.20069600	3.19228200
C	1.74669200	-2.66775800	2.70863800
H	2.57378000	-1.95260200	2.72921500
H	1.71582000	-3.15914100	3.68956400
H	1.96965600	-3.42736700	1.95699500
H	-1.61381000	-2.05681100	1.98233000
C	-0.71554700	-3.69726700	0.85265600
C	-1.48281800	-3.42623300	-0.45919300
H	-1.24439900	-4.49164400	1.39668700
H	0.28258800	-4.08002600	0.62183700
H	-1.53579300	-4.31802200	-1.08766900
H	-2.50241800	-3.08834300	-0.24994300
S	-0.58515800	-2.08203800	-1.36244800
C	-1.82621600	-1.10558600	-2.34024600
H	-2.71612500	-0.92487700	-1.73431500
H	-2.10323200	-1.68824800	-3.22245400
C	-1.10678100	0.17370300	-2.69302600
C	-1.36829600	1.35853500	-1.99519900
C	-0.07446700	0.15997700	-3.64274800
C	-0.60319400	2.50276100	-2.22330600
H	-2.16471400	1.38331300	-1.26000100
C	0.69466900	1.30147900	-3.86935800
H	0.13445700	-0.75324900	-4.19362500
C	0.43804400	2.47367000	-3.15304100
H	-0.81809600	3.41399500	-1.67272400
H	1.49074400	1.27707900	-4.60736000
H	1.03745200	3.36172500	-3.32857700

TS3

Charge: 1, Spin: 1

C	1.59097600	4.21522000	0.65596600
C	2.86940400	4.14633400	0.15341200
C	3.35371400	2.90975300	-0.32861100
C	2.50146400	1.78920300	-0.19312000
C	0.78320500	3.05430300	0.74025600
C	4.62934400	2.75731700	-0.96432800
C	2.90393400	0.52835800	-0.74563900
C	4.13351300	0.42459200	-1.43606500
C	5.00355300	1.56149000	-1.50236000
C	4.41469100	-0.80973800	-2.06308000
C	3.48454000	-1.82263500	-2.00486200
C	2.28190200	-1.65972500	-1.27492500
H	5.28125000	3.62284900	-1.03179400
H	1.17370900	5.16074700	0.98520300
H	5.95775500	1.45577200	-2.00916800
H	3.65648600	-2.76371300	-2.51447300
N	1.25957700	1.85346400	0.38106700
N	2.02269500	-0.51211900	-0.63348500
H	5.34493300	-0.93817800	-2.60863300
H	3.49462600	5.03233200	0.09259400
Ni	0.63735100	-0.07183700	0.71906300

C	-0.10295200	0.19011900	2.62405600
C	0.80905900	-0.87589100	2.72167800
H	0.28478200	1.17528100	2.87131800
H	0.57400700	-1.45590000	1.07774800
H	1.85120300	-0.60239900	2.88922700
C	-1.61113200	0.00891300	2.77497500
H	-1.83662400	-0.52799700	3.70580800
H	-2.07857100	0.99316400	2.87191000
C	-2.28385500	-0.74429400	1.61771400
H	-2.00322400	-1.80091200	1.61301400
H	-3.37274200	-0.67771800	1.67562400
C	1.27458800	-2.77664200	-1.21515000
C	1.55296000	-3.81921600	-0.10928800
H	1.25658600	-3.28306300	-2.18733200
H	0.29015900	-2.33119200	-1.05457600
C	2.82116900	-4.65791100	-0.30432200
H	1.60703600	-3.30207600	0.85485800
H	0.68370900	-4.48664900	-0.05457500
C	2.99061100	-5.71157200	0.79463400
H	2.78527500	-5.14910700	-1.28633700
H	3.70110300	-4.00247100	-0.31754300
H	3.90018000	-6.30020300	0.64483700
H	3.05708700	-5.24255400	1.78322000
H	2.14258400	-6.40477300	0.81141200
C	-0.66445400	3.19675100	1.11258000
C	-1.51937300	3.53013900	-0.13172100
H	-0.78444500	3.98431900	1.86480100
H	-1.03294600	2.26888100	1.54091900
C	-3.01839700	3.54819800	0.18504900
H	-1.20702100	4.49732100	-0.54586500
H	-1.31920000	2.77606500	-0.90247700
C	-3.87617400	3.80712800	-1.05633200
H	-3.29756900	2.58157700	0.62342300
H	-3.22212000	4.31159600	0.94751400
H	-4.94163200	3.81178500	-0.80797000
H	-3.63465900	4.77223700	-1.51484500
H	-3.71284100	3.02944300	-1.81129600
C	0.46560300	-2.25701700	3.24521400
H	0.47858700	-2.21442600	4.34142100
H	1.20261900	-3.00279100	2.94038100
H	-0.52092500	-2.60455500	2.93564800
S	-1.71173500	-0.02757700	0.02237500
C	-2.38628200	-1.28772000	-1.15326200
H	-1.96475000	-1.00747300	-2.12310700
H	-1.98504000	-2.26716200	-0.87652400
C	-3.89144100	-1.28478800	-1.16840800
C	-4.61025600	-2.29532000	-0.51868200
C	-4.59210600	-0.24412800	-1.79534700
C	-6.00675600	-2.27087200	-0.49894300
H	-4.07620600	-3.10934200	-0.03421400
C	-5.98465900	-0.21797300	-1.77550400
H	-4.04045300	0.54812900	-2.29507800
C	-6.69559500	-1.23200600	-1.12588300
H	-6.55376500	-3.06338900	0.00270100

H	-6.51672200	0.59009200	-2.26835900
H	-7.78097700	-1.21252200	-1.11248600

IM3

Charge: 1, Spin: 1

Ni	0.51463600	0.23084400	0.11560900
C	1.49014300	-3.99269600	-0.96078700
C	3.20069600	-0.38069500	0.17668000
C	4.57654800	-0.30839700	0.48889800
C	5.13097800	0.98396600	0.62224400
C	4.34310000	2.08776300	0.37525500
C	2.96457000	1.94239700	0.09319600
N	2.40508700	0.72248300	0.08563800
H	6.18159300	1.09661800	0.87361900
H	4.76645200	3.08564700	0.40008100
C	2.60016200	-1.64376600	-0.14557900
C	3.38744300	-2.81463600	-0.07120600
C	2.77622200	-4.02300400	-0.47794900
C	0.76772500	-2.77272800	-1.02247200
N	1.30315000	-1.62559000	-0.59089800
H	3.33587000	-4.95288200	-0.43558800
H	1.01174600	-4.89768100	-1.31943000
C	-0.61878700	-2.78185400	-1.60232700
C	-1.63518300	-3.54285600	-0.72886800
H	-0.57497200	-3.25839500	-2.59033400
H	-0.94838100	-1.75386600	-1.76464400
C	-3.03864200	-3.55637700	-1.34807200
H	-1.29723000	-4.57466200	-0.57269200
H	-1.66058100	-3.08707800	0.26995000
C	-4.09650400	-4.14813800	-0.41281100
H	-3.32383300	-2.53308700	-1.62798700
H	-3.00780400	-4.12221700	-2.28765900
H	-5.08052400	-4.16806900	-0.88963900
H	-3.84192400	-5.17408100	-0.12636500
H	-4.18601700	-3.55981400	0.50796900
C	-1.73743300	2.17146400	0.10043600
H	-2.77620300	2.50427200	0.02710200
H	-1.13634700	2.72472700	-0.62469800
C	-1.14865000	2.25020500	1.50429800
H	-0.93567700	3.30036600	1.73925100
H	-1.91105600	1.93303300	2.22531600
C	0.02436500	0.38142800	2.82766800
H	-0.76850300	-0.35696400	2.64716500
H	-0.30158100	0.94626900	3.71591600
C	5.33225500	-1.51987200	0.61314800
H	6.37827900	-1.45418100	0.89592900
C	4.75443600	-2.72784400	0.35423500
H	5.33113200	-3.64440500	0.43114000
C	-2.88182600	-0.38769300	0.62993700
H	-2.51735200	-0.33070200	1.65491800
H	-2.87048000	-1.43013900	0.31760300
C	1.67027100	5.57585800	-2.29402600
H	1.05490900	6.38152400	-2.70460100
H	1.98737600	5.88837300	-1.29362500

H	2.56660400	5.49014600	-2.91838600
C	2.13639200	3.13389600	-0.31115200
H	2.71510400	4.04334000	-0.13163000
H	1.23260500	3.19800000	0.29735700
C	1.71817000	3.04655300	-1.79688100
H	1.13800800	2.12404400	-1.93137300
H	2.61369100	2.94691500	-2.42381700
C	0.89348500	4.25438100	-2.26650700
H	0.00921300	4.36495100	-1.62326800
H	0.51390900	4.03836000	-3.27219400
C	0.12141100	1.37291800	1.65717900
H	0.99100000	2.00687300	1.84862400
C	1.32666800	-0.35462100	3.16769700
H	1.23155200	-0.90443900	4.10844000
H	1.59833600	-1.07718200	2.39185000
H	2.15914400	0.35009800	3.27235000
S	-1.62632200	0.42987900	-0.48555600
C	-4.24422800	0.22845400	0.48210000
C	-4.98604900	0.04967100	-0.69485500
C	-4.78432600	1.00068700	1.51863600
C	-6.24676500	0.62767200	-0.82843200
H	-4.57070800	-0.53988600	-1.50764100
C	-6.04842700	1.57874400	1.38580400
H	-4.22153500	1.13658300	2.43863900
C	-6.78037800	1.39408700	0.21211600
H	-6.81532900	0.47879900	-1.74126700
H	-6.46009700	2.16901300	2.19865000
H	-7.76374300	1.84203400	0.10803100

Dioxazolone

Charge: 0, Spin: 1

O	3.75411700	-0.96131300	0.00004200
C	2.75500200	-0.31237400	0.00002700
O	1.46090200	-0.80988200	-0.00006800
C	0.64150400	0.27990200	-0.00000100
O	2.64621800	1.04398000	0.00007400
N	1.27264600	1.40693200	-0.00002400
H	-1.22500400	2.20699800	-0.00008600
C	-1.65356500	1.21027900	-0.00007000
C	-0.80484700	0.09064900	-0.00009200
C	-1.34337100	-1.20438100	-0.00006300
H	-0.68094300	-2.06308800	-0.00010100
C	-2.72657600	-1.37563000	0.00003600
H	-3.14374700	-2.37778000	0.00006600
C	-3.57108900	-0.26374600	0.00008500
H	-4.64829800	-0.40097000	0.00016400
C	-3.03226300	1.02738000	0.00002500
H	-3.68921600	1.89156100	0.00007200

PR2

Charge: 1, Spin: 1

C	2.60508100	-3.67750100	0.27433800
C	3.64750700	0.35521200	0.50316500
C	5.00417000	0.73670900	0.62472700

C	5.28419000	2.12133500	0.63350800
C	4.25300500	3.02045100	0.47879400
N	2.62527000	1.26275100	0.44770300
H	6.30982300	2.46322000	0.73789400
H	4.44778800	4.08646000	0.44081800
C	3.31446400	-1.04071400	0.40555600
C	4.33644500	-2.01325400	0.50705500
C	3.93830300	-3.36871500	0.42490500
C	1.64164800	-2.64421400	0.17277500
N	2.00510800	-1.35945100	0.20363300
H	4.68732700	-4.15269000	0.49105700
H	2.27372900	-4.70945100	0.22926100
C	0.17713300	-2.96846600	0.11230200
C	-0.33476100	-3.47304600	1.47944500
H	-0.01526700	-3.72140200	-0.66095400
H	-0.37201300	-2.06570800	-0.16611600
C	-1.86145900	-3.57316800	1.51572100
H	0.11897700	-4.44451300	1.71281200
H	0.00569300	-2.78313500	2.26274400
C	-2.40516600	-3.94405200	2.89729400
H	-2.28316000	-2.61082200	1.20600800
H	-2.19512700	-4.30713100	0.76990400
H	-3.49812100	-4.00549500	2.88942500
H	-2.02150700	-4.91277000	3.23494000
H	-2.11832800	-3.19498800	3.64470300
C	6.01874300	-0.27196300	0.72051700
H	7.05183700	0.04320300	0.82995600
C	5.69741000	-1.59658700	0.67354000
H	6.46887300	-2.35657000	0.75085500
C	-0.11026500	4.32759500	-3.26309800
H	-0.97468800	4.95631300	-3.49198400
H	0.71134400	4.62409400	-3.92394400
H	-0.37785800	3.29513700	-3.52141200
C	1.81201400	3.54797000	0.07157600
H	2.12336700	4.55750900	0.35719100
H	0.92111800	3.29918200	0.64796600
C	1.45532000	3.51596500	-1.43200400
H	1.19242800	2.48368300	-1.69870600
H	2.34045500	3.77583000	-2.02724600
C	0.29139000	4.44547500	-1.78950700
H	0.56853200	5.48278300	-1.56333700
H	-0.56846400	4.20979600	-1.15133500
C	-0.13581900	1.27526500	1.71917300
H	-0.63436000	2.18797500	1.38153200
C	-1.17778100	0.17933200	1.96414000
C	-2.12253300	0.46647300	3.15360500
H	-0.68406400	-0.77901900	2.16912900
H	-1.80564500	0.03264200	1.08322800
H	-2.75751400	-0.40681000	3.33193900
H	-1.55618200	0.64440500	4.07078800
C	1.46687600	0.35705800	3.54534800
H	2.07357600	-0.17863000	2.80866600
H	2.12595100	0.66898900	4.36060600
C	0.76617300	1.57010900	2.91885500

H	0.15191000	2.06030700	3.68993700
H	1.51427600	2.31734400	2.64154400
C	2.91533100	2.57232500	0.37338200
H	0.74845700	-0.35713000	3.95958300
S	-3.21474600	1.92447300	2.90399100
C	-4.78904500	1.08711000	2.41090200
H	-5.13081200	0.48160500	3.25522900
H	-5.49415000	1.91503500	2.29298000
C	-4.71944500	0.26056700	1.15229400
C	-4.72880100	0.87263100	-0.11047800
C	-4.66695700	-1.13763500	1.21855400
C	-4.70466400	0.10407700	-1.27457200
H	-4.76360800	1.95587900	-0.18219800
C	-4.62730600	-1.91040100	0.05395000
H	-4.67762200	-1.62950700	2.18802300
C	-4.64686500	-1.29210400	-1.19616700
H	-4.75052600	0.59627800	-2.24110700
H	-4.59866700	-2.99331500	0.12763400
H	-4.65306600	-1.89201300	-2.10205600
C	-1.01629300	0.10817200	-2.16328800
C	-2.26229800	1.91308700	-1.93850200
O	-3.04194200	2.78197900	-2.14947200
O	-1.98475900	0.83239400	-2.76828600
O	-1.44257000	1.78362000	-0.85905300
N	-0.65434600	0.60726700	-1.01743300
C	-0.49777800	-1.08673300	-2.81011300
C	-1.39456800	-1.97315900	-3.42872600
C	0.88008200	-1.34968700	-2.80598400
C	-0.90741400	-3.14012200	-4.01025500
H	-2.45629800	-1.75082600	-3.42895700
C	1.35650600	-2.51856700	-3.39366900
H	1.56253400	-0.64142500	-2.35029000
C	0.46447800	-3.41480000	-3.98938700
H	-1.59478200	-3.83469000	-4.48190200
H	2.42187200	-2.72512900	-3.39574400
H	0.83891500	-4.32378600	-4.44993800
Ni	0.83495100	0.44420100	0.25664800

TS4

Charge: 1, Spin: 1

C	2.20294200	3.91794400	0.12102000
C	3.81361800	0.11136700	-0.36762900
C	5.20035800	-0.07346900	-0.55358000
C	5.65287500	-1.40926600	-0.66809200
C	4.74964700	-2.44555700	-0.57870500
N	2.92599200	-0.92389900	-0.33179100
H	6.71051500	-1.60777700	-0.81559900
H	5.08032900	-3.47611300	-0.64473000
C	3.28600600	1.43348000	-0.19369800
C	4.15238100	2.54547000	-0.25278200
C	3.55992400	3.82027900	-0.08655000
C	1.39141800	2.75608800	0.17750400
N	1.94156800	1.54408400	0.02557100
H	4.18121400	4.71055800	-0.12200900

H	1.73097900	4.88528300	0.25191100
C	-0.08761700	2.87577900	0.40818500
C	-0.83948200	3.68229300	-0.67018500
H	-0.25462600	3.34192000	1.38613700
H	-0.51081400	1.87478600	0.47201100
C	-2.35757100	3.53257600	-0.50628800
H	-0.55918100	4.74182000	-0.61946800
H	-0.54163700	3.33976600	-1.66991400
C	-3.14975600	4.26639800	-1.59004600
H	-2.62019600	2.46725100	-0.52294600
H	-2.64858900	3.89706100	0.48764800
H	-4.22645600	4.13201800	-1.44951700
H	-2.94345400	5.34203000	-1.58018500
H	-2.89513000	3.88849000	-2.58710000
C	6.05909300	1.07335700	-0.60756900
H	7.12269400	0.91834400	-0.75955400
C	5.55398400	2.33422400	-0.46859800
H	6.20851800	3.19911800	-0.51203000
C	0.62923400	-4.91256500	2.86377200
H	0.00186200	-5.79984500	2.98541900
H	1.45232300	-4.98011600	3.58432400
H	0.02088400	-4.04034600	3.12967200
C	2.38379400	-3.31181500	-0.24867200
H	2.80019200	-4.22173700	-0.69224200
H	1.45528500	-3.08130200	-0.77790900
C	2.04350100	-3.56542200	1.23949000
H	1.52897400	-2.67823000	1.62802200
H	2.96999200	-3.68114700	1.81743900
C	1.14749600	-4.79460600	1.42792800
H	1.70952000	-5.69716700	1.15447600
H	0.29803700	-4.72342000	0.74133900
C	0.15921900	-0.75969400	-1.69851700
H	-0.20284100	-1.74393900	-1.40238000
C	-0.95996900	0.24643000	-1.82909500
C	-1.72193400	0.11456800	-3.17311100
H	-0.56049600	1.26281800	-1.78304600
H	-1.67132900	0.11890900	-1.01285900
H	-2.53626700	0.84430900	-3.17388400
H	-1.07161100	0.35188000	-4.01785200
C	1.76671400	0.49823900	-3.32275100
H	2.37352500	0.97848300	-2.55368000
H	2.40781400	0.31519100	-4.18902300
C	1.16638000	-0.81900000	-2.82406300
H	0.59890700	-1.28693700	-3.64783100
H	1.95387700	-1.53737500	-2.59411100
C	3.36679300	-2.18780300	-0.40834200
H	0.99648300	1.21162400	-3.62803700
S	-2.43025900	-1.55369100	-3.47780000
C	-4.21551600	-1.24569400	-3.10001700
H	-4.62219600	-0.60201600	-3.88485600
H	-4.67069100	-2.23395600	-3.21307100
C	-4.49838900	-0.67391800	-1.73552700
C	-4.91224300	0.65835000	-1.60112600
C	-4.38778000	-1.46884100	-0.58443800

C	-5.24352700	1.17923500	-0.34688700
H	-5.01104100	1.28271000	-2.48598900
C	-4.72568200	-0.95560200	0.66727300
H	-4.05561900	-2.49962600	-0.66691600
C	-5.16564300	0.36819100	0.78605400
H	-5.58715400	2.20622600	-0.26280500
H	-4.65279800	-1.59701000	1.53904200
H	-5.47058800	0.75577700	1.75448000
C	-1.15532500	0.61829900	2.72895900
C	-2.34376300	1.34029000	2.88969000
C	0.04769700	1.08680700	3.27476600
C	-2.31879800	2.54592500	3.58836600
H	-3.26062600	0.96402500	2.45271500
C	0.05873200	2.28263600	3.99133000
H	0.95637500	0.50613700	3.14876100
C	-1.12224600	3.01558300	4.14115200
H	-3.23495700	3.11499400	3.71126000
H	0.98290900	2.63912800	4.43533600
H	-1.11329400	3.94842300	4.69659700
Ni	1.07870800	-0.31057400	0.10352400
C	-1.16635500	-0.65157200	1.95324400
O	-2.01900500	-1.56727200	2.29478600
N	-0.31914800	-0.74889500	0.97829100
C	-2.01371400	-2.80515100	1.32419200
O	-1.05019000	-2.69113800	0.53215400
O	-2.90795100	-3.57133000	1.53988900

NI

Charge: 1, Spin: 1

C	-3.77248300	0.67116300	-0.14549200
C	-5.16769700	0.77875700	0.03383800
C	-5.85467100	-0.40403700	0.39474600
H	-6.92970200	-0.37735500	0.54757300
C	-5.15302100	-1.57851000	0.53999100
H	-5.66142500	-2.49851400	0.80552700
C	-3.74655000	-1.62012900	0.35632300
C	-3.01456000	1.81578400	-0.54272700
C	-3.66598800	3.04705500	-0.76173700
C	-2.85668100	4.11908100	-1.20769300
C	-0.92374400	2.64203400	-1.18179800
C	-1.51520000	3.91002400	-1.42515900
H	-3.30399600	5.09140900	-1.39274600
H	-0.88499500	4.71116300	-1.79136400
N	-1.67122400	1.63132700	-0.72211300
N	-3.08819800	-0.49868300	0.02596200
C	0.61515400	-2.52662100	0.04989100
O	0.19091900	-3.11226000	1.06057100
C	-0.45333200	-0.04256500	1.71853100
H	-0.15126900	-1.06657500	1.94096300
Ni	-1.14263500	-0.27600100	-0.24815800
N	-0.09972500	-1.53084700	-0.54518200
C	-3.00204000	-2.91317200	0.48621900
C	-2.73263100	-3.55712200	-0.89544000

H	-3.59166900	-3.60115300	1.10059600
H	-2.04397200	-2.75317100	0.98872200
C	-2.03332200	-4.91709800	-0.77005200
H	-3.67824600	-3.67097200	-1.44215000
H	-2.10551900	-2.87369700	-1.47968200
C	-1.57759100	-5.45772000	-2.12868200
H	-1.17082800	-4.81678300	-0.10288500
H	-2.71734000	-5.63083600	-0.29247400
H	-1.11074700	-6.44181500	-2.02632100
H	-2.41927400	-5.55701500	-2.82340400
H	-0.84215500	-4.78671700	-2.58789300
C	0.54518300	2.43975300	-1.43857300
C	1.45144700	3.37917800	-0.58942400
H	0.72871000	2.63115300	-2.50375500
H	0.79751000	1.39028700	-1.27431500
C	2.02656500	4.56998200	-1.36593500
H	0.88996400	3.74979400	0.27736300
H	2.28376600	2.79286400	-0.19015200
C	2.82557000	5.51541100	-0.46621300
H	2.66727500	4.18430100	-2.16858400
H	1.22325300	5.13085600	-1.86230000
H	3.26810900	6.33439900	-1.04064600
H	2.18706000	5.95607700	0.30786400
H	3.63553200	4.97851200	0.03725000
C	1.90422300	-2.86994200	-0.60411800
C	2.15311200	-2.55672100	-1.95091100
C	2.89374500	-3.49697300	0.16867100
C	3.39410100	-2.85293300	-2.51278800
H	1.37257800	-2.09273200	-2.54473500
C	4.13300800	-3.78361000	-0.39698900
H	2.67257600	-3.73553600	1.20298200
C	4.38590800	-3.45651800	-1.73455700
H	3.58796800	-2.61873600	-3.55496700
H	4.90346700	-4.26253000	0.19947800
H	5.35474600	-3.67930100	-2.17123200
C	-5.80313000	2.04745900	-0.16672000
C	-5.08000600	3.14072000	-0.54984600
H	-6.87596700	2.11909300	-0.01761100
H	-5.56751800	4.09688500	-0.71216300
C	0.69842200	0.93267000	1.61616600
C	1.77034300	0.76110400	2.72548000
H	0.31352000	1.95868900	1.64223400
H	1.23052000	0.80564600	0.67343500
H	2.49603300	1.57257300	2.61795200
H	1.33552600	0.83283500	3.72183600
C	-1.66980400	0.39175400	2.50813600
H	-2.43111300	-0.38874200	2.46294600
S	2.68148600	-0.83061200	2.61614100
C	4.35021400	-0.24446100	2.08046500
H	4.82562500	0.27155600	2.91903100
H	4.89732400	-1.17931400	1.91873200
C	4.39447900	0.60858300	0.83399600
C	3.87950500	0.13371800	-0.38127600
C	5.01701100	1.86275500	0.85666600

C	4.00766500	0.88123200	-1.55020400
H	3.39653400	-0.83371800	-0.40646600
C	5.15637600	2.61058800	-0.31738600
H	5.42486600	2.24409400	1.78940800
C	4.65600500	2.12092100	-1.52457800
H	3.62034200	0.48234200	-2.48354000
H	5.66718300	3.56828400	-0.28830100
H	4.77733200	2.69572000	-2.43782700
H	-2.10030600	1.30414500	2.08102600
C	-1.33517800	0.65104800	3.99576700
H	-0.83098100	-0.20853900	4.44711600
H	-0.70212200	1.53256300	4.12222100
H	-2.26394400	0.82598400	4.54667400

NI'

Charge: 1, Spin: 1

C	-3.91343400	1.05609100	0.21398900
C	-5.08967700	1.82989300	0.13704800
C	-4.92802300	3.19452900	-0.20054800
H	-5.79997500	3.83746200	-0.27777200
C	-3.66378400	3.69762500	-0.41389100
H	-3.51827000	4.74475800	-0.65483900
C	-2.52070700	2.86283400	-0.32479800
C	-3.98474200	-0.31928400	0.59816700
C	-5.23298100	-0.90119700	0.90215500
C	-5.21180800	-2.24998200	1.32768000
C	-2.78679500	-2.25182100	1.13685500
C	-4.00529700	-2.90282500	1.45615800
H	-6.14301200	-2.75464100	1.56805100
H	-3.96682900	-3.92864000	1.80462100
N	-2.80179900	-0.99258600	0.68408100
N	-2.67012000	1.56366700	-0.03163500
C	1.61601000	0.47503800	1.02552200
O	2.09098800	1.61631000	0.89741100
C	-1.11037100	0.02738600	-1.89430500
H	-1.23153900	1.08581700	-2.13599600
Ni	-1.24639100	0.20716800	0.17961600
N	0.32695400	0.25714900	0.69585600
C	-1.14246300	3.43520400	-0.48323800
C	-0.49314200	3.76477400	0.88200200
H	-1.20190500	4.34312300	-1.09216400
H	-0.49483500	2.72734800	-1.00690400
C	0.84282200	4.49603600	0.71035000
H	-1.18265700	4.37483200	1.48038600
H	-0.33039500	2.82601900	1.42346900
C	1.56959000	4.68874800	2.04296100
H	1.47955500	3.91105700	0.03861900
H	0.66334000	5.46730700	0.22995800
H	2.49943600	5.24865300	1.90563100
H	0.95140300	5.23812800	2.76232900
H	1.82448300	3.71611600	2.47469400
C	-1.46846400	-2.96213400	1.28752600
C	-0.90888400	-3.49875700	-0.04620500
H	-1.59743400	-3.79010000	1.99147000

H	-0.74207400	-2.26671600	1.72202500
C	-1.83610000	-4.45318400	-0.80518900
H	-0.66453300	-2.64333500	-0.68302100
H	0.04015700	-4.00324500	0.16762500
C	-1.22469000	-4.91428500	-2.13176200
H	-2.06166600	-5.32289700	-0.17417400
H	-2.79922300	-3.96108000	-0.99875500
H	-1.89263400	-5.59796000	-2.66318400
H	-1.02617800	-4.06097100	-2.79121900
H	-0.27402700	-5.43303100	-1.96951800
C	2.33149400	-0.66090700	1.66475400
C	2.17787500	-1.97397500	1.20057100
C	3.18518800	-0.38746600	2.74222500
C	2.88361700	-3.01022100	1.80748800
H	1.54728400	-2.16529700	0.34102400
C	3.88531000	-1.42762600	3.34849400
H	3.29598200	0.63758000	3.08082100
C	3.73454800	-2.73797900	2.88261900
H	2.78701000	-4.02516400	1.43375400
H	4.55100000	-1.21940500	4.18029200
H	4.28719200	-3.54564700	3.35289100
C	-6.35124800	1.20840700	0.41878500
C	-6.42044100	-0.10513200	0.78691700
H	-7.25249600	1.80905500	0.34630000
H	-7.37756100	-0.56486800	1.01238600
C	0.25396600	-0.49905500	-2.27696000
C	1.35143500	0.56866400	-2.27571600
H	0.17684000	-0.94210700	-3.28072600
H	0.52842900	-1.33046600	-1.62215400
H	1.31040800	1.15908100	-3.19776400
H	1.22349000	1.24816000	-1.42883000
C	-2.30334100	-0.78622500	-2.35219000
H	-3.21759000	-0.42538700	-1.87904200
S	2.97570400	-0.25195400	-2.08939400
C	4.04749000	1.21838700	-1.74967300
H	4.21233600	1.75710900	-2.68738600
H	3.49848300	1.85752800	-1.05215600
C	5.34076600	0.75019900	-1.13648100
C	5.47160400	0.70420800	0.25763200
C	6.40417100	0.31600300	-1.93751600
C	6.64569800	0.23050100	0.84112000
H	4.64604200	1.04529700	0.87390000
C	7.58079800	-0.15592300	-1.35382100
H	6.30825000	0.34736500	-3.01999300
C	7.70315900	-0.20151500	0.03681100
H	6.73522800	0.19886800	1.92333800
H	8.40160500	-0.48616600	-1.98368800
H	8.61949700	-0.56788200	0.49031400
H	-2.18388700	-1.83642100	-2.07291400
C	-2.49461200	-0.67065800	-3.88311600
H	-2.61028200	0.37411500	-4.18900600
H	-1.65289100	-1.09557800	-4.43519200
H	-3.39827400	-1.21155600	-4.17835800

T55

Charge: 1, Spin: 1

C	-3.81414300	0.61438300	-0.11277100
C	-5.21269500	0.67336200	0.05148600
C	-5.85080900	-0.52341800	0.45347400
H	-6.92648900	-0.53794100	0.60303400
C	-5.10107900	-1.66529000	0.63102000
H	-5.57481800	-2.59790000	0.91616200
C	-3.69469500	-1.65893400	0.44420800
C	-3.09523400	1.75976800	-0.56601800
C	-3.78510200	2.95140100	-0.86437700
C	-3.00836800	4.01361000	-1.38387300
C	-1.02050900	2.61583500	-1.21921100
C	-1.65585200	3.83616600	-1.56875800
H	-3.48527400	4.95297100	-1.64809400
H	-1.05047300	4.62931700	-1.98941200
N	-1.74584400	1.60315100	-0.72457800
N	-3.08036700	-0.51622800	0.10121500
C	-2.89894000	-2.92519700	0.55734500
C	-2.56792100	-3.51017000	-0.83774800
H	-3.47316200	-3.65638600	1.13503400
H	-1.95814500	-2.74752300	1.08702600
C	-1.85310500	-4.86473300	-0.74484100
H	-3.49018000	-3.61340800	-1.42472500
H	-1.93138700	-2.79232100	-1.36812500
C	-1.31553800	-5.32530600	-2.10326300
H	-1.02808200	-4.78784800	-0.02936300
H	-2.55005200	-5.61220900	-0.34380000
H	-0.84424400	-6.30971900	-2.02824100
H	-2.11503100	-5.39302400	-2.84985300
H	-0.56165700	-4.62459900	-2.48111300
C	0.46853600	2.46047500	-1.36161600
C	1.26533100	3.35621100	-0.36889900
H	0.75679700	2.71737300	-2.38799800
H	0.73177300	1.40923200	-1.22224700
C	1.71749400	4.70672800	-0.93486500
H	0.66638600	3.52505900	0.53444200
H	2.15369000	2.80259900	-0.05380800
C	2.47629800	5.53607000	0.10512200
H	2.35863000	4.52344200	-1.80615200
H	0.85758700	5.28356300	-1.29773300
H	2.82638900	6.48260300	-0.31691300
H	1.83904600	5.76926000	0.96570200
H	3.34828900	4.98792200	0.47581300
C	-5.88997900	1.90850800	-0.21706200
C	-5.20367100	3.00375000	-0.66038800
H	-6.96548900	1.95150800	-0.07645000
H	-5.72555600	3.93016200	-0.87884700
C	0.71151000	-2.47638100	0.19643600
O	0.36976900	-3.18684500	1.15516100
C	-0.12818200	-0.30448200	1.90386600
H	0.28208900	-1.28113600	2.13720900
Ni	-1.18865900	-0.21864700	-0.18014300

N	0.01430100	-1.36003000	-0.15638600
C	-1.40925800	-0.04264300	2.66199300
C	-1.09722300	0.11794500	4.17122900
H	-2.09044500	-0.88626500	2.54135400
H	-1.91640500	0.85903400	2.30315800
H	-2.03800800	0.17818900	4.72609300
H	-0.53082300	-0.73595200	4.55467700
H	-0.53096200	1.03081500	4.37132000
C	0.88080800	0.80645600	1.77690300
C	2.01829100	0.71971200	2.82637900
H	0.37454200	1.77404900	1.86741000
H	1.35928200	0.77291000	0.79886600
H	2.63452600	1.61897900	2.73535200
H	1.62403600	0.69240900	3.84317600
S	3.10894200	-0.74594100	2.61439800
C	4.61779000	0.04141100	1.89682000
H	5.28469600	-0.81178600	1.73197000
H	5.07994200	0.66870800	2.66422600
C	4.43233400	0.81677100	0.61242700
C	3.84534900	0.21706300	-0.51141500
C	4.91343000	2.12778000	0.50254200
C	3.75214700	0.90714100	-1.71860000
H	3.47547700	-0.79775700	-0.43683300
C	4.83578100	2.81626000	-0.71277800
H	5.37702800	2.60465400	1.36251100
C	4.25390700	2.20875800	-1.82632600
H	3.30719000	0.41492200	-2.57830300
H	5.23325100	3.82393800	-0.78717800
H	4.20002200	2.74048600	-2.77176200
C	1.88552000	-2.79273200	-0.66022800
C	1.96895900	-2.35286600	-1.99127800
C	2.93296800	-3.53691700	-0.09724600
C	3.10206600	-2.64683900	-2.74807000
H	1.14461400	-1.79257900	-2.41927100
C	4.06876300	-3.81388500	-0.85379700
H	2.84077800	-3.87028800	0.93058600
C	4.15524500	-3.36733100	-2.17714700
H	3.16544900	-2.31819300	-3.78096500
H	4.88687600	-4.37784800	-0.41651900
H	5.04158300	-3.58640000	-2.76487800

TS5'

Charge: 1, Spin: 1

C	-4.13371100	-0.10006800	-0.06457200
C	-5.50904900	-0.39403700	0.06251500
C	-5.84298300	-1.61948500	0.68853100
H	-6.88717200	-1.88744800	0.82183000
C	-4.84107300	-2.45468600	1.12085100
H	-5.07364700	-3.39649400	1.60526000
C	-3.47562800	-2.11372300	0.92354400
C	-3.72643200	1.14849000	-0.64586200
C	-4.70426000	2.02014300	-1.17713100
C	-4.23532800	3.18073800	-1.83352100
C	-1.95856900	2.53556700	-1.29852000

C	-2.88179800	3.41517800	-1.91633400
H	-4.94583100	3.86791100	-2.28380300
H	-2.50167300	4.27848700	-2.44842300
N	-2.38806600	1.43097700	-0.67189100
N	-3.15082700	-0.95796500	0.33525100
C	0.46828400	-2.04491400	-0.91067200
O	-0.32812200	-2.94575900	-1.20086900
C	-0.73902900	0.56057400	1.83894200
H	-0.77784000	-0.38773100	2.38690800
Ni	-1.26755600	-0.09745900	0.05157900
N	0.13670000	-1.14134300	0.06541400
C	-2.40070400	-3.07246300	1.34765300
C	-2.42292500	-4.37855400	0.52461100
H	-2.54423100	-3.31024800	2.41051300
H	-1.42603600	-2.59562500	1.23270400
C	-1.24418900	-5.29158400	0.87622300
H	-3.36914600	-4.91096200	0.69042700
H	-2.36943700	-4.12019800	-0.53654400
C	-1.22420500	-6.56595600	0.02800600
H	-0.31588400	-4.73100000	0.71458000
H	-1.28283400	-5.55011000	1.94353200
H	-0.37994500	-7.20891700	0.29575000
H	-2.14224900	-7.14900400	0.16255900
H	-1.13575700	-6.31966600	-1.03564200
C	-0.48178900	2.83468100	-1.33961700
C	-0.02093400	3.98325900	-0.40796500
H	-0.20931500	3.08900600	-2.37143300
H	0.06298600	1.92105100	-1.08370400
C	-0.46471300	5.39643700	-0.80641600
H	-0.35784600	3.78160700	0.61600700
H	1.07579400	3.95272400	-0.38316100
C	0.18395200	6.46984400	0.07398800
H	-0.20787300	5.57529800	-1.85939200
H	-1.55520300	5.48232900	-0.73013300
H	-0.14935400	7.47135100	-0.21239500
H	-0.07262900	6.32196300	1.12902100
H	1.27568200	6.44317900	-0.01024900
C	1.80644300	-1.93617900	-1.56606200
C	2.33349500	-0.69549100	-1.94726500
C	2.49907800	-3.11629200	-1.87252500
C	3.54995100	-0.63430400	-2.62871800
H	1.78610500	0.21455200	-1.72499500
C	3.72345200	-3.05106000	-2.53271000
H	2.05891400	-4.06902500	-1.59650300
C	4.24660400	-1.81042200	-2.91604400
H	3.95368200	0.32724300	-2.93006400
H	4.26498900	-3.96343600	-2.76232800
H	5.19340400	-1.76343900	-3.44614000
C	-6.48008300	0.53151400	-0.43991700
C	-6.09221600	1.68725900	-1.05314400
H	-7.53271400	0.28610300	-0.33778100
H	-6.82888300	2.37498900	-1.45658300
C	0.67203400	1.13401200	1.82761500
C	1.78459500	0.17430300	1.46180200

H	0.87729100	1.47470300	2.85490800
H	0.70943500	2.02852600	1.20194300
H	1.95708000	-0.61523600	2.20012700
H	1.20774100	-0.51639700	0.57567000
C	-1.81814400	1.51182900	2.33634900
H	-2.80072200	1.08409600	2.11499300
S	3.27200000	0.92191300	0.88804100
C	4.46312100	-0.49890400	0.98633900
H	4.31260800	-0.97209300	1.96139200
H	4.19677700	-1.20584300	0.19719600
C	5.87036600	0.01460200	0.83057600
C	6.53886000	-0.10560600	-0.39339300
C	6.51968400	0.63478500	1.90735700
C	7.83975200	0.37924800	-0.53720400
H	6.03957000	-0.58790700	-1.22767100
C	7.81829600	1.12038500	1.76375300
H	6.00443100	0.73393500	2.85958800
C	8.48095400	0.99348000	0.53982500
H	8.35292100	0.27484400	-1.48854800
H	8.31476600	1.59352900	2.60550100
H	9.49373000	1.36873200	0.42859000
H	-1.76223200	2.46351800	1.79896400
C	-1.73138400	1.75825600	3.85590900
H	-1.77532600	0.81533400	4.41093800
H	-0.80546300	2.27124400	4.13286800
H	-2.56740800	2.38200700	4.18561000

IM4

Charge: 1, Spin: 1

C	3.59142400	0.68414700	-0.32438300
C	4.96935300	0.59956000	-0.59767600
C	5.40188800	-0.54886600	-1.30311200
H	6.45306800	-0.67092600	-1.54713200
C	4.47900500	-1.49984600	-1.67332400
H	4.78744700	-2.38951600	-2.21118600
C	3.09975900	-1.35156800	-1.36782600
C	3.07453100	1.80754100	0.38223500
C	3.92875600	2.84362700	0.80676800
C	3.31531600	3.91821100	1.49275000
C	1.15426000	2.82211300	1.25668100
C	1.95268900	3.90158100	1.70871900
H	3.91932300	4.75021800	1.84278000
H	1.46664800	4.71963000	2.22807400
N	1.73128900	1.80172600	0.60627000
N	2.68009600	-0.26499900	-0.70531200
C	-1.05411900	-1.81394600	0.03040300
O	-1.97070400	-2.49854700	-0.41853700
C	-1.19332400	-0.47689700	-1.97890200
H	-1.39416700	-1.45267100	-2.43773000
Ni	0.89577700	0.24331400	-0.16901400
N	-0.53190600	-0.71596600	-0.67509000
C	2.14072500	-2.44333300	-1.73905800
C	2.19458600	-3.61754700	-0.73516300

H	2.39558200	-2.81241600	-2.73898000
H	1.12638500	-2.04785900	-1.77896700
C	1.19039800	-4.71858700	-1.09619600
H	3.21096800	-4.03168900	-0.71196100
H	1.98313500	-3.23975500	0.27242600
C	1.29759600	-5.93184900	-0.16807200
H	0.17530300	-4.30309300	-1.05965800
H	1.35566800	-5.03415300	-2.13481000
H	0.54744100	-6.68785200	-0.41801000
H	2.28413600	-6.40163200	-0.24575700
H	1.14984200	-5.64149400	0.87705500
C	-0.33760400	2.79969300	1.45629700
C	-1.12840700	2.98136900	0.14251700
H	-0.61297800	3.58516800	2.16654100
H	-0.63392600	1.84739400	1.91054000
C	-0.90537200	4.32364800	-0.55711500
H	-0.86525300	2.16718900	-0.54148500
H	-2.18969700	2.84114900	0.37125500
C	-1.68913000	4.41705000	-1.87052100
H	-1.20280800	5.13904800	0.11568400
H	0.16566900	4.46739400	-0.75775900
H	-1.54307800	5.38579800	-2.35676800
H	-1.36905300	3.63883400	-2.57340400
H	-2.76274400	4.28444400	-1.69898700
C	-0.44017600	-2.15002600	1.35460700
C	0.16488100	-1.20907600	2.20215900
C	-0.51170600	-3.48719600	1.77309900
C	0.74329100	-1.60321400	3.40867600
H	0.11965700	-0.15093200	1.96501100
C	0.06457200	-3.88355600	2.97786300
H	-1.01773000	-4.20232200	1.13462300
C	0.70494600	-2.94531300	3.79338500
H	1.19432400	-0.86046200	4.05983200
H	0.01231700	-4.92391400	3.28350200
H	1.14977200	-3.25467800	4.73415700
C	5.82866500	1.66118900	-0.15659500
C	5.32985500	2.74070100	0.51746700
H	6.89020400	1.59008800	-0.37180300
H	5.98907700	3.53846200	0.84479000
C	-2.55604600	0.23824100	-1.71942900
C	-3.75223500	-0.52424100	-2.29458600
H	-2.53248800	1.25082000	-2.13550100
H	-2.69161000	0.35581100	-0.64433100
H	-3.69449500	-0.57322100	-3.38677700
C	-0.28273800	0.32305800	-2.92338200
H	0.69398500	-0.17109300	-2.99106500
H	-0.09775000	1.32253600	-2.50490400
C	-0.87502200	0.46060600	-4.33022600
H	-1.82630400	1.00113500	-4.31826600
H	-0.19294800	1.00793000	-4.98690100
H	-1.05528400	-0.52277800	-4.77724300
H	-3.75966100	-1.55043800	-1.91699900
S	-5.36627600	0.26291300	-1.91972000
C	-5.68675200	-0.39488200	-0.22419700

H	-5.65362000	-1.48729200	-0.27020200
H	-6.72541100	-0.10791200	-0.03055200
C	-4.78644500	0.12149500	0.87454400
C	-4.78934700	1.48042500	1.22470900
C	-3.94640600	-0.75279000	1.57511800
C	-3.98131500	1.95066100	2.25896200
H	-5.42912800	2.16727700	0.67749000
C	-3.13624400	-0.28442100	2.61432000
H	-3.91437700	-1.80272100	1.29979800
C	-3.15149800	1.06759500	2.96015000
H	-4.01004100	3.00260500	2.53002300
H	-2.50340300	-0.97949000	3.15633600
H	-2.53968000	1.42890300	3.78238400

IM4'

Charge: 1, Spin: 1

C	-3.65720500	-0.70947100	0.05440500
C	-5.06443600	-0.75745400	-0.06850700
C	-5.67781100	0.26505100	-0.82811500
H	-6.75543300	0.26080100	-0.96384800
C	-4.90536600	1.27806500	-1.34956600
H	-5.35938400	2.10497200	-1.88437400
C	-3.49745000	1.25610000	-1.20700500
C	-2.97931300	-1.63978100	0.91631400
C	-3.73650100	-2.64335800	1.56828700
C	-3.03651900	-3.52196200	2.42445400
C	-0.99285400	-2.32380000	1.91564700
C	-1.68082300	-3.36037600	2.59251100
H	-3.57365100	-4.30930600	2.94527500
H	-1.11950800	-4.01843800	3.24627600
N	-1.63313500	-1.47662800	1.09944600
N	-2.89881900	0.23084400	-0.58147300
C	0.86781200	1.81463100	-0.17618600
O	0.98750400	2.56476300	-1.12733100
C	-0.68087000	-0.24789300	-2.43300500
H	-0.61733600	0.74270400	-2.89870200
Ni	-0.99905700	-0.13398800	-0.52039000
N	0.94647300	0.37373500	-0.37160400
C	-2.67837400	2.43775600	-1.63909300
C	-2.56182800	3.44586800	-0.46971000
H	-3.14962400	2.92438000	-2.49932000
H	-1.67647600	2.12656300	-1.93287500
C	-1.73425200	4.68137400	-0.83903200
H	-3.56712500	3.75026100	-0.14904400
H	-2.10059900	2.93720000	0.38717700
C	-1.67294400	5.69868300	0.30465400
H	-0.72204600	4.36068000	-1.11063700
H	-2.16619600	5.15365300	-1.73119300
H	-1.05875400	6.56243700	0.03208600
H	-2.67160400	6.06847600	0.56246200
H	-1.23948600	5.25070900	1.20522000
C	0.50042500	-2.20392600	2.06380500
C	1.25330100	-2.89143400	0.90417300
H	0.80859300	-2.65044200	3.01488900

H	0.77596700	-1.14661000	2.11502200
C	1.08646800	-4.41280700	0.84295300
H	0.90596700	-2.45423500	-0.03862000
H	2.31634100	-2.64101000	0.98211000
C	1.85591700	-5.02439600	-0.33216600
H	1.43454600	-4.85391800	1.78668400
H	0.02251100	-4.66924400	0.75693300
H	1.73715800	-6.11125700	-0.36335500
H	1.49894000	-4.62215200	-1.28738400
H	2.92631000	-4.80442800	-0.26092400
C	0.66919300	2.30667400	1.21336000
C	0.01796400	1.56886900	2.21516800
C	1.13782500	3.59955900	1.49765500
C	-0.15406700	2.11695900	3.48502400
H	-0.40231500	0.59321300	1.99822800
C	0.98085900	4.13453100	2.77339300
H	1.62049000	4.16647300	0.70930700
C	0.33434100	3.39498600	3.76836400
H	-0.67366700	1.54944000	4.25079300
H	1.35591300	5.12943900	2.99071900
H	0.20570900	3.81667300	4.76043100
C	-5.79601300	-1.80158500	0.58516000
C	-5.15363500	-2.71692200	1.36469600
H	-6.87303600	-1.84122000	0.45503100
H	-5.70792000	-3.50564600	1.86399700
C	0.70255700	-0.91008300	-2.45019500
C	1.65657000	-0.03580100	-1.64820200
H	1.08863700	-1.02347200	-3.47055300
H	0.64639200	-1.92066200	-2.02477800
H	1.83195300	0.89188300	-2.19404200
H	1.38859100	-0.07750300	0.42974800
C	-1.77170800	-1.09182400	-3.08883000
H	-2.72242000	-0.55264500	-3.04714800
S	3.25941200	-0.81837300	-1.29232900
C	4.24467200	0.69645600	-0.86392000
H	4.29637000	1.32903800	-1.75430500
H	3.71339600	1.24583900	-0.07999900
C	5.61234300	0.27948500	-0.39362800
C	5.85582300	0.05216800	0.96699700
C	6.64830100	0.07954400	-1.31502100
C	7.11597100	-0.35750900	1.40187900
H	5.05526800	0.20335400	1.68777000
C	7.90905300	-0.33110000	-0.88171800
H	6.46505700	0.24869000	-2.37294900
C	8.14508000	-0.55010900	0.47726500
H	7.29638000	-0.52276800	2.45989100
H	8.70680000	-0.47715900	-1.60361400
H	9.12740800	-0.86633400	0.81475700
H	-1.91591600	-2.01658300	-2.51113300
C	-1.47928500	-1.45297100	-4.55728600
H	-1.29482300	-0.55093700	-5.15107000
H	-0.60480100	-2.10311600	-4.65253400
H	-2.33057100	-1.97908300	-5.00003700

HOBpin

Charge: 0, Spin: 1

O	0.87888800	-1.03412500	0.41997300
O	0.79939600	1.10598000	-0.43971700
C	-0.50728000	-0.79750400	0.04997700
C	-0.55845800	0.77568500	-0.04767100
C	-0.80947800	1.44976000	1.30667900
H	-0.61962600	2.52150400	1.20695800
H	-1.84003500	1.30678500	1.64436500
H	-0.13329300	1.05496900	2.07025000
C	-1.51708200	1.32407700	-1.09984200
H	-2.54602700	1.02072300	-0.88028000
H	-1.47557200	2.41677800	-1.10045800
H	-1.25325100	0.97696800	-2.10009700
C	-1.40993000	-1.40834500	1.11674500
H	-2.45951200	-1.17053400	0.91521500
H	-1.30039200	-2.49653400	1.11401100
H	-1.15273100	-1.04585100	2.11329400
C	-0.73097800	-1.48799100	-1.30038300
H	-0.46828000	-2.54489900	-1.20462700
H	-1.77369100	-1.41631300	-1.62287200
H	-0.09547000	-1.04718200	-2.07359900
B	1.59091900	0.06628300	-0.01592100
O	2.94970200	0.13538600	-0.03115400
H	3.33863300	-0.69985100	0.25159400

IM5

Charge: 1, Spin: 1

C	-1.10982000	3.35173400	0.56654100
C	-1.36249400	4.52173600	1.31344500
C	-2.51033100	4.51532700	2.13679300
H	-2.75052500	5.38639800	2.73943600
C	-3.33012900	3.41264000	2.13152000
H	-4.24007800	3.39961200	2.72040400
C	-3.01217800	2.25502500	1.37368300
C	-0.03703100	3.34758400	-0.38016600
C	0.75328800	4.49969200	-0.56553500
C	1.68671800	4.45695900	-1.62570400
C	0.93988400	2.20634400	-2.17399000
C	1.74094100	3.34730600	-2.43824700
H	2.31655600	5.31934300	-1.82422300
H	2.38497600	3.33936800	-3.30750700
N	0.10514600	2.21454600	-1.12621400
N	-1.88765000	2.22169700	0.63648500
C	-2.21061700	-1.73708200	0.30369600
O	-2.46259200	-2.74979900	0.97957100
C	-0.99802400	-0.94599400	2.20824200
H	-1.82501400	-1.40231700	2.76517500
Ni	-0.78371100	0.73505700	-0.12410900
N	-1.51331100	-0.68965200	0.83542900
C	-3.96774400	1.10096800	1.37612400
C	-4.74214200	0.98355400	0.04620100
H	-4.67319900	1.22672000	2.20294300
H	-3.41014800	0.17995500	1.53969900

C	-5.67080400	-0.23575500	0.03324300
H	-5.32222600	1.89948400	-0.12811700
H	-4.02317400	0.90497400	-0.77531100
C	-6.34133600	-0.44027700	-1.32757500
H	-5.09216500	-1.12984800	0.29463200
H	-6.43203100	-0.11903500	0.81577400
H	-7.01339000	-1.30341700	-1.30987500
H	-6.93173300	0.43679300	-1.61601600
H	-5.59259800	-0.61690100	-2.10639000
C	0.93318900	1.03625800	-3.12990600
C	2.23963800	0.23134500	-3.32438100
H	0.64023900	1.44482200	-4.10727300
H	0.13997600	0.34920600	-2.83081500
C	3.43933100	0.96406000	-3.93704500
H	2.54230400	-0.22948400	-2.38039700
H	1.97789300	-0.59954900	-3.99025500
C	4.57006200	-0.00697300	-4.29337700
H	3.12205800	1.50781000	-4.83741200
H	3.82426300	1.71575800	-3.23745400
H	5.43652600	0.52211000	-4.70008200
H	4.90180500	-0.56266800	-3.40948500
H	4.24153000	-0.73716600	-5.04045300
C	-2.69998800	-1.71100600	-1.13119400
C	-2.43759200	-0.71329000	-2.07826800
C	-3.44004900	-2.82902600	-1.54896200
C	-2.86215400	-0.83317000	-3.40241600
H	-1.91474800	0.20113200	-1.80489100
C	-3.87476500	-2.95438500	-2.86674600
H	-3.65194200	-3.59791600	-0.81513700
C	-3.57802800	-1.96164300	-3.80481400
H	-2.64098400	-0.04175400	-4.11274700
H	-4.44374500	-3.83001900	-3.16390300
H	-3.91045600	-2.06077800	-4.83357400
C	-0.49114600	5.65206900	1.17221600
C	0.52982400	5.64394000	0.26687000
H	-0.68221900	6.52950300	1.78220700
H	1.16642900	6.51400300	0.14031800
C	0.17488600	-1.96446800	2.16973800
C	-0.01117400	-3.15823300	3.10730000
H	1.12692800	-1.47029600	2.39544400
H	0.26037200	-2.34665700	1.15718200
H	-0.05174500	-2.84464300	4.15502200
C	-0.61214200	0.34788500	2.94212900
H	-1.46293800	1.03348500	2.93584600
H	0.20531500	0.85304300	2.41112300
C	-0.19906500	0.10367600	4.39762100
H	0.69217800	-0.52605900	4.47485200
H	0.02497200	1.04964400	4.90025100
H	-1.00162100	-0.38945500	4.95653500
H	-0.95416100	-3.66036200	2.87199400
S	1.35732900	-4.37972400	3.02086300
C	0.90599900	-5.30434300	1.48763200
H	-0.10568500	-5.70074100	1.61193100
H	1.59400700	-6.15605300	1.48775700

C	1.02118200	-4.53708300	0.18999600
C	2.25700400	-4.02561400	-0.23277600
C	-0.11166100	-4.30948300	-0.60243700
C	2.36409200	-3.31814300	-1.42813100
H	3.13123600	-4.16273500	0.39620000
C	-0.01108700	-3.59903100	-1.80233800
H	-1.08359100	-4.65206200	-0.26305400
C	1.22771000	-3.10206300	-2.21966300
H	3.32569300	-2.92116600	-1.73620000
H	-0.89524600	-3.43654700	-2.40839700
H	1.31157300	-2.57530700	-3.16467100
O	3.14319500	-0.84784000	0.22712000
O	2.16269800	1.17585900	0.72929100
C	3.44509500	1.18446300	1.44340400
C	4.22771500	-0.01229900	0.75727400
B	2.04545700	-0.05822700	0.16009100
O	0.86352000	-0.41028200	-0.48021200
H	0.81246700	-1.32939300	-0.81073600
C	4.06983000	2.56126800	1.24684200
H	3.44729700	3.31562000	1.73596300
H	5.06715500	2.60063100	1.69411300
H	4.14705700	2.81993500	0.18941300
C	3.13358800	0.94381900	2.92107900
H	4.04134600	0.99261100	3.52746900
H	2.44114500	1.71307200	3.27205700
H	2.66431200	-0.02914700	3.07881800
C	5.05448200	-0.87099700	1.70583600
H	5.54122300	-1.67085600	1.14210100
H	5.83279600	-0.27289900	2.18915400
H	4.43187400	-1.33266700	2.47307100
C	5.06040700	0.42156200	-0.45009600
H	5.92447000	1.01781700	-0.14677700
H	5.42150200	-0.46873300	-0.97028200
H	4.46121300	1.00613200	-1.15268700

IM5'

Charge: 1, Spin: 1

C	-2.10897200	1.92462400	0.96027700
C	-2.20022500	3.32368100	0.80291100
C	-1.54182000	3.88579000	-0.31467100
H	-1.56901500	4.95986600	-0.47359300
C	-0.92747800	3.05406000	-1.22022500
H	-0.47008300	3.45502700	-2.11678200
C	-0.87707900	1.65240700	-1.00689600
C	-2.87274500	1.27645100	1.98665200
C	-3.70398700	2.04532500	2.83216100
C	-4.49555000	1.33621300	3.76302900
C	-3.57065700	-0.74431500	2.92196400
C	-4.43454100	-0.03894200	3.79409800
H	-5.15311400	1.87908900	4.43584100
H	-5.04814400	-0.60309300	4.48729500
N	-2.80141800	-0.08478300	2.04671800
N	-1.39687000	1.11806800	0.10907500
C	4.39534300	0.97222600	0.26946200

O	3.73592400	1.39504700	-0.68668700
C	0.41392200	-1.36240800	0.38380300
H	0.53816600	-1.65381900	-0.66194500
Ni	-1.29178200	-0.66927300	0.88047600
N	4.02220200	-0.16020400	0.93260900
C	-0.30209100	0.76355100	-2.07403300
C	1.10547400	1.15869800	-2.55666000
H	-1.01051300	0.77732900	-2.91490900
H	-0.29800600	-0.25468400	-1.69481300
C	1.75547300	0.05968400	-3.40579000
H	1.05514500	2.08301100	-3.14629300
H	1.75404000	1.36586400	-1.70171800
C	3.13833100	0.47235300	-3.92102900
H	1.84776500	-0.85077400	-2.79472400
H	1.09983100	-0.20386100	-4.24741900
H	3.61450300	-0.33992100	-4.48018100
H	3.06227100	1.33461600	-4.59270800
H	3.78662100	0.75575100	-3.08653100
C	-3.52500200	-2.25128500	2.94677000
C	-4.04524700	-2.90061300	1.64684500
H	-4.11438400	-2.60714100	3.79760100
H	-2.49194700	-2.56943400	3.13308200
C	-5.51296200	-2.57794500	1.34564600
H	-3.42761700	-2.57380800	0.80457500
H	-3.91330300	-3.98621300	1.73484700
C	-6.00064900	-3.25935700	0.06464200
H	-6.13930100	-2.88506300	2.19429200
H	-5.62599900	-1.49364800	1.23671900
H	-7.04317500	-3.00396500	-0.15058300
H	-5.39296800	-2.94369200	-0.78938600
H	-5.93408000	-4.35025300	0.14088400
C	5.61770300	1.68090700	0.76055900
C	6.60462600	1.06206200	1.54124800
C	5.77977700	3.02031600	0.38122900
C	7.72741600	1.77993500	1.94992600
H	6.53727300	0.00711700	1.78710800
C	6.89927900	3.73807900	0.79515500
H	5.01785300	3.47506000	-0.24257200
C	7.87359300	3.11998500	1.58379300
H	8.49325200	1.29044200	2.54393700
H	7.01531300	4.77713400	0.50197400
H	8.74831600	3.67788300	1.90472200
C	-2.99765200	4.08743200	1.71683400
C	-3.72620100	3.47168800	2.69207300
H	-3.03289100	5.16579100	1.59664800
H	-4.34953300	4.05039000	3.36674200
C	1.56908700	-0.52909200	0.90727400
C	2.95744200	-1.01384200	0.43112000
H	1.54907300	-0.49216800	2.00319600
H	1.49127800	0.50617000	0.55827000
H	2.97755000	-0.95403600	-0.66136400
H	4.54996100	-0.49081000	1.72538300
C	-0.13702600	-2.44902500	1.23367200
H	-1.18308000	-2.09675900	1.65643200

S	3.26523300	-2.76219500	0.91134200
C	4.35755200	-3.30815400	-0.49122000
H	4.61504600	-4.33767600	-0.22593100
H	3.74237200	-3.33859500	-1.39471700
C	5.58661900	-2.46589900	-0.70060600
C	5.61562600	-1.50133400	-1.71441000
C	6.71071200	-2.61852900	0.12361200
C	6.73845800	-0.69163700	-1.89540100
H	4.75476800	-1.37657800	-2.36501200
C	7.83858300	-1.82099400	-0.06509500
H	6.69795000	-3.36626000	0.91273500
C	7.85271200	-0.85028500	-1.07161500
H	6.73782800	0.06205000	-2.67675000
H	8.70708200	-1.95370400	0.57351100
H	8.72577600	-0.21980300	-1.20729200
H	0.40108400	-2.56598300	2.17899000
C	-0.44081400	-3.78960000	0.56475900
H	-1.04709400	-3.64347300	-0.33251700
H	0.50486200	-4.26163900	0.28687000
H	-0.98491400	-4.46191200	1.23401700
O	-3.59939000	-0.28480900	-2.91513400
O	-4.49125100	-0.33611500	-0.78838700
C	-5.28284000	0.64502600	-1.52813400
C	-4.93756700	0.29932700	-3.03145600
B	-3.51160400	-0.77129600	-1.63771100
O	-2.53084900	-1.63547900	-1.21944700
H	-1.94226100	-1.87289600	-1.94561400
C	-6.74588800	0.46050100	-1.14350700
H	-6.88273500	0.71800400	-0.08935000
H	-7.38783900	1.11581500	-1.73990000
H	-7.06806200	-0.57170000	-1.28328400
C	-4.78876700	2.02932000	-1.10545100
H	-5.37767400	2.82202300	-1.57399800
H	-4.88132200	2.12677100	-0.02115100
H	-3.74052200	2.17157700	-1.37654500
C	-4.85888400	1.49763500	-3.96907200
H	-4.60320600	1.15905900	-4.97643000
H	-5.82368200	2.01160800	-4.01840800
H	-4.09742700	2.21066100	-3.64840800
C	-5.83927700	-0.78925700	-3.62121900
H	-6.85253900	-0.41763400	-3.79489100
H	-5.42207500	-1.11687300	-4.57651000
H	-5.89801400	-1.65828500	-2.95938900

PC

Charge: 0, Spin: 1

C	-0.18306400	1.56025000	-0.28732900
O	0.18308700	1.47540200	-1.45968300
N	0.68518700	1.71896300	0.75678200
H	0.29575800	1.95247200	1.65620900
C	-1.63988400	1.48440800	0.07997400
C	-2.57278400	1.84345000	-0.90082700
C	-2.09341600	1.01258300	1.31829700
C	-3.93814500	1.75639700	-0.63943300

H	-2.20215900	2.17621400	-1.86457100
C	-3.46079500	0.91697000	1.57780300
H	-1.38441700	0.66359300	2.06335400
C	-4.38550400	1.29370200	0.60217700
H	-4.65504800	2.04408100	-1.40307700
H	-3.80317400	0.53407500	2.53480300
H	-5.45018400	1.21909800	0.80439200
C	2.14998300	1.77392200	0.61387100
H	2.53196600	1.87497300	1.63920200
C	2.69080900	0.45751700	0.02451700
C	2.30971500	-0.76267200	0.86658300
H	3.78104600	0.52778800	-0.05037300
H	2.29726200	0.34173500	-0.98774100
H	2.73476400	-0.69439700	1.87438500
H	1.22280600	-0.82164400	0.95922500
C	2.58323800	3.02024100	-0.18479000
C	4.09450800	3.27165000	-0.17175300
H	2.06613700	3.88585500	0.24786100
H	2.21564100	2.91390600	-1.20931300
H	4.33044200	4.22240300	-0.65985900
H	4.48359400	3.31972500	0.85277900
H	4.64604500	2.48854900	-0.70068800
S	2.88034600	-2.31975800	0.06471300
C	1.39989800	-3.40595100	0.27769700
H	1.63635100	-4.27616100	-0.34523400
H	1.35031300	-3.75590400	1.31334600
C	0.07528300	-2.79507300	-0.12792300
C	-1.03486900	-2.92462200	0.71713800
C	-0.07572900	-2.09269200	-1.33229700
C	-2.27249400	-2.38481300	0.35959200
H	-0.92848300	-3.45311500	1.66185700
C	-1.30644100	-1.54120700	-1.68342200
H	0.78687400	-1.94952900	-1.97562900
C	-2.41151100	-1.69186900	-0.84244200
H	-3.12110000	-2.48634600	1.03010000
H	-1.39256400	-0.96522300	-2.59900400
H	-3.36119900	-1.23510600	-1.10203500

PC'

Charge: 0, Spin: 1

C	1.39953900	0.80630700	0.78050700
O	0.98003400	0.72056900	1.93252700
C	2.65793000	-2.86915600	0.29120200
H	2.52373800	-3.02439500	1.37067300
N	1.27013200	-0.21619400	-0.13017200
C	2.08235800	2.04607000	0.27893000
C	2.97125300	2.05188800	-0.80568800
C	1.82025200	3.24269000	0.95948600
C	3.57204100	3.24245900	-1.21522600
H	3.22666000	1.12510400	-1.31184700
C	2.41406600	4.43222000	0.54420900
H	1.14929700	3.21219100	1.81131600
C	3.28913600	4.43490000	-0.54572800
H	4.26678700	3.23737400	-2.04996800

H	2.19838000	5.35717000	1.07096700
H	3.75558600	5.36170600	-0.86714800
C	1.28233200	-2.67207000	-0.36080400
C	0.55138300	-1.43540500	0.17693600
H	0.64780700	-3.54684600	-0.18526200
H	1.39441200	-2.58146400	-1.45059200
H	0.47533800	-1.47619400	1.26538500
H	1.40230100	-0.00729600	-1.11014500
C	3.46117400	-4.03912200	-0.29766700
H	4.46156700	-4.03595700	0.15300600
S	-1.17366600	-1.41689200	-0.50974800
C	-1.80602600	0.12682700	0.29629600
H	-1.54166500	0.08551700	1.35586300
H	-1.28836200	0.98307800	-0.14417300
C	-3.29331200	0.23278500	0.08713400
C	-3.81255800	0.95799700	-0.99259400
C	-4.18241800	-0.41255400	0.95741200
C	-5.19079000	1.04520200	-1.19494000
H	-3.13064600	1.45793200	-1.67600300
C	-5.55981400	-0.32608100	0.75874300
H	-3.78686400	-0.98466600	1.79258400
C	-6.06821600	0.40374300	-0.31885700
H	-5.57848000	1.61481600	-2.03486300
H	-6.23690300	-0.82695000	1.44494400
H	-7.14122600	0.47258700	-0.47332500
H	3.61107500	-3.86902000	-1.37297300
C	2.81857500	-5.41459300	-0.08184700
H	2.64038500	-5.60049200	0.98377800
H	1.85712500	-5.50132000	-0.59827900
H	3.46445300	-6.21522400	-0.45665200
H	3.23527900	-1.94321000	0.18463400

[Ni]OBpin

Charge: 1, Spin: 1

C	-2.78274400	-1.10371800	0.44191600
C	-3.73627000	-1.92006300	1.07078100
C	-3.26812000	-3.17280200	1.53677100
H	-3.95124200	-3.85850900	2.02931800
C	-1.94215300	-3.50924600	1.36336900
H	-1.56612900	-4.46255900	1.71709600
C	-1.02462900	-2.62900400	0.72929800
C	-3.14904700	0.17019900	-0.06101300
C	-4.46213800	0.65291600	0.06580900
C	-4.69766300	1.94543700	-0.46295700
C	-2.36289900	2.08835600	-1.15240300
C	-3.66268100	2.64424800	-1.05505200
H	-5.68940100	2.38342200	-0.39916500
H	-3.82855100	3.63636900	-1.45922300
N	-2.14269400	0.86481000	-0.65568500
N	-1.47054300	-1.44770100	0.27630400
Ni	-0.50816700	-0.09730400	-0.65147600
C	0.41276900	-3.00153600	0.52922600
C	0.71634100	-3.43192900	-0.92572000
H	0.66318200	-3.81848800	1.21296000

H	1.05139400	-2.15131000	0.78805900
C	2.21134900	-3.70153600	-1.12962100
H	0.12897200	-4.32444900	-1.17737500
H	0.40115000	-2.63372800	-1.60768600
C	2.54649900	-4.06327100	-2.57873100
H	2.76946400	-2.80860300	-0.82603700
H	2.52959000	-4.51045500	-0.45840600
H	3.61692900	-4.25417200	-2.70019300
H	2.00930200	-4.96253200	-2.89982400
H	2.27292600	-3.24870400	-3.25871500
C	-1.19672200	2.82220300	-1.75874900
C	-0.18306400	3.32155000	-0.69947500
H	-1.57178100	3.66984200	-2.33960700
H	-0.68306400	2.15175500	-2.45898600
C	-0.76560300	4.33292500	0.29229700
H	0.22828600	2.46207700	-0.15271800
H	0.66615900	3.76153200	-1.23341700
C	0.27386800	4.81326700	1.30936400
H	-1.16878800	5.19089600	-0.26218800
H	-1.61685900	3.88378500	0.82269900
H	-0.15607900	5.53938000	2.00510200
H	0.66571600	3.97575100	1.89702600
H	1.12240900	5.29141500	0.80836700
C	-5.08023500	-1.42494100	1.18900100
C	-5.42937300	-0.19081400	0.71002800
H	-5.82140300	-2.05306900	1.67298600
H	-6.44858900	0.16813800	0.81131700
O	2.69554900	-0.56171200	0.69190500
O	3.10299000	1.17575200	-0.77133400
C	4.03195900	1.35186100	0.34171700
C	4.04412000	-0.08037100	0.99670100
B	2.28615300	0.12905900	-0.43053400
O	1.15850600	-0.19227300	-1.12799200
C	5.37280800	1.81829600	-0.21142200
H	5.26522000	2.81502000	-0.64737600
H	6.11859700	1.87407800	0.58764400
H	5.74003400	1.14800900	-0.98965400
C	3.42099800	2.42218600	1.25255500
H	4.08374800	2.67152800	2.08529600
H	3.24521900	3.32733400	0.66601800
H	2.46153600	2.08887000	1.66032500
C	4.23562000	-0.09985700	2.50808400
H	4.21910500	-1.13181300	2.86898900
H	5.20216000	0.33768800	2.77634300
H	3.44707000	0.45269600	3.02151400
C	5.01962300	-1.04456300	0.31528600
H	6.05828300	-0.79177100	0.54366000
H	4.82434300	-2.05880300	0.67316700
H	4.88963000	-1.03407900	-0.77063200

HBpin

Charge: 0, Spin: 1

O	-1.07867300	1.19635500	-0.38911700
O	1.07856200	1.19656800	0.38892300

C	-0.78643400	-0.19121300	-0.04845600
C	0.78649200	-0.19113800	0.04849200
C	1.47631200	-0.46368300	-1.29305400
H	2.54294300	-0.24699300	-1.19257800
H	1.35923100	-1.50691400	-1.60023900
H	1.07268400	0.18033100	-2.07905200
C	1.36824600	-1.08986100	1.13540900
H	1.10526900	-2.13669700	0.95149400
H	2.45846900	-1.00630300	1.13544400
H	1.00878100	-0.80650800	2.12581300
C	-1.36805700	-1.09012700	-1.13529700
H	-1.10496500	-2.13690000	-0.95124500
H	-2.45828600	-1.00666200	-1.13532600
H	-1.00863200	-0.80686200	-2.12574900
C	-1.47635300	-0.46363200	1.29312900
H	-2.54292100	-0.24659800	1.19266400
H	-1.35959800	-1.50688900	1.60029300
H	-1.07254500	0.18026300	2.07914600
B	-0.00010900	1.94210700	-0.00007100
H	-0.00023000	3.13073600	-0.00009300

TS6

Charge: 1, Spin: 1

C	-3.45473800	-0.78171400	-0.51069800
C	-4.59113800	-1.56649700	-0.78989600
C	-4.35091100	-2.89743800	-1.20639400
H	-5.18818000	-3.55066300	-1.43439400
C	-3.05531000	-3.35000600	-1.32117300
H	-2.84991300	-4.36431200	-1.64439000
C	-1.95539800	-2.50526700	-1.02320800
C	-3.61899300	0.57321700	-0.08642900
C	-4.90670400	1.12505400	0.06657700
C	-4.96607400	2.46486800	0.51705100
C	-2.53888600	2.53252300	0.62112400
C	-3.80040200	3.14862900	0.79722200
H	-5.93135800	2.94404200	0.65239400
H	-3.83274500	4.16865100	1.16277400
N	-2.47998900	1.27308600	0.16844700
N	-2.17451100	-1.24670800	-0.61807200
C	-0.54338400	-2.96641500	-1.21682500
C	0.05642200	-2.38608000	-2.51826800
H	-0.51839400	-4.05989600	-1.24942000
H	0.04984900	-2.64435200	-0.35985900
C	1.54808100	-2.69480200	-2.67041500
H	-0.50101900	-2.78026400	-3.37826000
H	-0.07521500	-1.29860400	-2.52019700
C	2.10286800	-2.14445600	-3.98744100
H	2.08522300	-2.24561000	-1.82665800
H	1.71015300	-3.77970700	-2.61537900
H	3.17401300	-2.34792000	-4.08274000
H	1.60111300	-2.59827000	-4.84946500
H	1.95389700	-1.06109900	-4.03740000
C	-1.24790800	3.22927500	0.96768700
C	-0.38500000	2.43886100	1.97336100

H	-1.48148400	4.21782600	1.37299300
H	-0.65938900	3.38302300	0.05545200
C	-1.08783900	2.08441500	3.28613900
H	-0.01878800	1.51337400	1.50170600
H	0.52776400	3.01243200	2.16139300
C	-0.22051700	1.18295300	4.16930800
H	-1.35091700	3.00700800	3.81941400
H	-2.03580200	1.57213100	3.07211300
H	-0.72790000	0.93017500	5.10483400
H	0.01297200	0.24949000	3.64539200
H	0.72558600	1.67332000	4.42422700
C	-5.89467600	-0.98499300	-0.64012700
C	-6.04837300	0.30820900	-0.22740300
H	-6.76250200	-1.59859000	-0.86078500
H	-7.03873400	0.73740000	-0.11337100
O	0.91358500	-1.59297900	1.77523200
O	2.91232900	-0.90828000	0.85110600
C	3.23940000	-1.46446100	2.15899200
C	1.96474800	-2.33609400	2.47138100
B	1.54134300	-0.91011800	0.74467900
C	4.54122300	-2.24721200	2.03802000
H	5.36238700	-1.56154000	1.81274400
H	4.77203400	-2.75800500	2.97797600
H	4.49132400	-2.98726600	1.23792900
C	3.40711300	-0.28038200	3.11593600
H	3.71258200	-0.61090400	4.11230200
H	4.17728600	0.38804600	2.72290900
H	2.47741900	0.28731900	3.20601200
C	1.60315100	-2.44632000	3.94658200
H	0.69436700	-3.04367500	4.06096500
H	2.40720600	-2.94188200	4.49932800
H	1.42647600	-1.46793400	4.39411100
C	2.01972300	-3.72372100	1.82389600
H	2.74667300	-4.37053900	2.32168800
H	1.03385900	-4.19057400	1.89965300
H	2.28682500	-3.65277000	0.76532900
O	0.86815300	-0.34480800	-0.28493300
B	1.02110100	1.41977500	-1.31376400
O	1.65731000	2.26475100	-0.44440300
C	2.92340700	2.65260400	-1.07474100
O	1.67129800	1.16210300	-2.48129100
C	3.04537400	1.65573400	-2.31369600
H	-0.23077200	1.43105700	-1.34358000
C	4.02109700	2.49692200	-0.02620700
H	3.83591500	3.19189100	0.79799000
H	4.03541900	1.48292900	0.37563100
H	5.00186200	2.72948100	-0.45182600
C	3.93935100	0.44309700	-2.04662300
H	4.98296700	0.74978800	-1.93206900
H	3.63518600	-0.09955600	-1.15238900
H	3.87890400	-0.23532200	-2.89978000
C	3.44881600	2.31996700	-3.62725500
H	4.45125200	2.75163500	-3.54916200
H	3.46437300	1.56872900	-4.42115400

H	2.74958600	3.10450200	-3.91981000
C	2.75829500	4.12021300	-1.47391400
H	3.66718200	4.51659300	-1.93401100
H	1.92835800	4.24724100	-2.17392100
H	2.54053500	4.70926900	-0.57884300
Ni	-0.87594500	0.22494900	-0.18988100

IM6

Charge: 1, Spin: 1

C	-2.27436100	-2.68552900	-0.50473800
C	-2.80988900	-3.74523800	-1.26076200
C	-3.78752200	-3.39407400	-2.22077000
H	-4.22420000	-4.15816100	-2.85731800
C	-4.23161200	-2.09117700	-2.27773400
H	-5.04332400	-1.81603600	-2.94196100
C	-3.66014500	-1.07931000	-1.46265400
C	-1.42484600	-2.97528400	0.60420000
C	-1.12998200	-4.30117200	0.96367200
C	-0.43291200	-4.47266700	2.18415000
C	-0.46466500	-2.06109300	2.53293600
C	-0.14980100	-3.37411400	2.96920600
H	-0.16552500	-5.47158400	2.51648900
H	0.32312200	-3.49432800	3.93734600
N	-1.03694400	-1.89667500	1.33631300
N	-2.62344700	-1.36825000	-0.66501600
C	-1.64428600	2.42353400	-0.92115200
O	-2.32117300	2.73445100	-1.88513800
C	-0.18361100	1.11208400	-2.45581100
H	-0.35106500	2.05905900	-2.97897900
Ni	-1.02835400	-0.37355400	0.14068600
N	-0.68973600	1.33959200	-1.03711300
C	-4.26894100	0.29407200	-1.41793500
C	-4.50850900	0.78602800	0.02205800
H	-5.22095500	0.26231900	-1.95760700
H	-3.64333700	1.01554600	-1.94931400
C	-5.24725500	2.12558600	0.07007200
H	-5.07719900	0.02713100	0.57580900
H	-3.54696000	0.88097300	0.54226500
C	-5.44170900	2.62656400	1.50370600
H	-4.68382800	2.86194200	-0.51445100
H	-6.22237300	2.01973300	-0.42325900
H	-5.96127900	3.58929700	1.52027000
H	-6.03459900	1.91770400	2.09246400
H	-4.47825400	2.76072300	2.00655100
C	-0.23313600	-0.86182000	3.41082600
C	1.22286400	-0.63995800	3.86064700
H	-0.87080700	-0.98539700	4.29773800
H	-0.59139400	0.02048800	2.88063200
C	1.41566900	0.74607600	4.48580100
H	1.51701100	-1.41591000	4.57949000
H	1.89031100	-0.72700100	3.00243900
C	2.84789800	0.96814100	4.97964100
H	1.16722900	1.50111300	3.72719800
H	0.70812100	0.88695300	5.31443000

H	2.98190300	1.97804700	5.37840500
H	3.10611800	0.25839700	5.77310700
H	3.56850300	0.83026200	4.16574600
C	-1.74440300	3.12650600	0.38707200
C	-1.13773400	2.67306100	1.57045100
C	-2.50081600	4.31151200	0.40983200
C	-1.31937500	3.37582300	2.76042600
H	-0.49866300	1.79858300	1.57276100
C	-2.65925700	5.02134900	1.59586300
H	-2.95259000	4.65965900	-0.51207300
C	-2.07805100	4.54854600	2.77659300
H	-0.85355400	3.01268900	3.67141000
H	-3.23975100	5.93820100	1.60302600
H	-2.21008900	5.09710900	3.70418600
C	-2.39865900	-5.08830100	-0.96024800
C	-1.59492500	-5.35802500	0.11259600
H	-2.77832800	-5.89555100	-1.57887400
H	-1.32672800	-6.38121800	0.35640900
C	1.32785900	0.81044900	-2.40886300
C	2.11485600	1.47996300	-3.54543200
H	1.48543800	-0.26993600	-2.42974700
H	1.74942600	1.16060400	-1.46575600
H	1.84994100	1.06865700	-4.52126700
C	-0.99971800	0.02794300	-3.16479500
H	-2.05347100	0.30708100	-3.11540100
H	-0.88042300	-0.91274200	-2.61341100
C	-0.60768900	-0.18969400	-4.62868300
H	0.40052500	-0.60268600	-4.72322700
H	-1.29507800	-0.89649500	-5.10251500
H	-0.64907900	0.74513900	-5.19740100
H	1.89829000	2.55276600	-3.58127300
S	3.93494400	1.27512600	-3.38026500
C	4.35809300	2.81940300	-2.44458600
H	4.22917000	3.67059100	-3.11900700
H	5.42762900	2.71495400	-2.23977600
C	3.57295400	3.01399400	-1.17430800
C	2.54389500	3.96376100	-1.11210400
C	3.82172600	2.21272000	-0.05123300
C	1.78993100	4.12182800	0.05466900
H	2.34031000	4.59151500	-1.97622200
C	3.07606300	2.37071900	1.11390500
H	4.58363500	1.44163600	-0.10125900
C	2.06508600	3.33300400	1.17347900
H	0.99934000	4.86574700	0.09418700
H	3.26932500	1.72482700	1.96235800
H	1.49146600	3.46577000	2.08413500
O	1.43092200	-2.02342600	-0.29808900
O	2.94961700	-0.73119900	0.85231100
C	3.62368200	-1.99440800	0.60976500
C	2.71568400	-2.67840500	-0.49409500
B	1.64129900	-0.85322600	0.42477300
O	0.67081300	0.03781400	0.72458200
H	0.12397300	1.55774000	-0.45272200
C	5.05282800	-1.69357200	0.16713800

H	5.59258600	-1.20809200	0.98508400
H	5.58352500	-2.61560800	-0.08957100
H	5.07122900	-1.02620900	-0.69598000
C	3.63420500	-2.75665700	1.94013300
H	4.18217400	-3.69932500	1.85951200
H	4.11928200	-2.13801100	2.69951100
H	2.61790800	-2.97236700	2.27989600
C	2.50794600	-4.18041800	-0.31466700
H	1.85084200	-4.55404000	-1.10548600
H	3.45954600	-4.71617600	-0.38136400
H	2.04342400	-4.40843500	0.64596800
C	3.17662100	-2.38318800	-1.92330000
H	4.09109400	-2.93170700	-2.16544500
H	2.39440000	-2.69778300	-2.62078800
H	3.36950800	-1.31971000	-2.07463200

IM7

Charge: 1, Spin: 1

C	3.32721500	0.38460000	-0.26227800
C	4.72074500	0.31583100	-0.06075800
C	5.32030300	1.41091800	0.60201300
H	6.39125100	1.41219800	0.78291600
C	4.54098800	2.48069500	0.98600300
H	4.98845000	3.34470300	1.46407400
C	3.13963400	2.47558500	0.78135900
C	2.66816300	-0.62980900	-1.03158300
C	3.40619400	-1.70929500	-1.55753800
C	2.69623900	-2.60586600	-2.39059000
C	0.70281700	-1.23427200	-2.13775000
C	1.37615200	-2.35197900	-2.69718900
H	3.20957700	-3.46006300	-2.82291900
H	0.84356500	-2.98510300	-3.39626400
N	1.34392800	-0.43274000	-1.28113900
N	2.55462900	1.42017800	0.19429300
Ni	0.72493400	0.90782500	0.12857500
C	2.28943200	3.64713900	1.18575100
C	1.58426100	4.31622000	-0.01207700
H	2.90774200	4.37886900	1.71457500
H	1.52686600	3.28708600	1.88582100
C	0.57482800	5.38182900	0.42456000
H	2.33707100	4.75730300	-0.67857500
H	1.06074400	3.54572300	-0.59174100
C	-0.11838900	6.05068500	-0.76603900
H	-0.17591200	4.91037100	1.07317000
H	1.07844800	6.14199800	1.03595900
H	-0.85918600	6.78498700	-0.43532300
H	0.60394700	6.57037000	-1.40485300
H	-0.63338500	5.30921900	-1.38853400
C	-0.68741100	-0.84283100	-2.57950900
C	-1.86808600	-1.76277400	-2.19693600
H	-0.65764700	-0.76946400	-3.67528900
H	-0.88612900	0.16360700	-2.20499900
C	-1.88894400	-3.15583300	-2.83778200

H	-1.93268400	-1.87186900	-1.11041400
H	-2.77727900	-1.22903100	-2.50131000
C	-3.21639800	-3.87784400	-2.58402100
H	-1.71885500	-3.06743300	-3.91950100
H	-1.06691300	-3.76383600	-2.44111800
H	-3.20905300	-4.88865000	-3.00185900
H	-3.42196600	-3.95812400	-1.51084300
H	-4.05166800	-3.33342400	-3.03769500
C	5.44079000	-0.82286200	-0.55698000
C	4.80857600	-1.80128600	-1.26952900
H	6.50857800	-0.88030800	-0.36941200
H	5.36553800	-2.64886300	-1.65692000
O	-1.74456000	-2.14746300	1.43601900
O	0.49359200	-1.59946800	1.48207500
C	0.36266800	-2.79400900	2.32573700
C	-1.03508800	-3.36421200	1.86536000
B	-0.77784900	-1.24408200	1.14519600
O	-0.99048800	-0.04179400	0.46855900
C	1.55548400	-3.69953900	2.04913100
H	2.47165600	-3.21373300	2.39550400
H	1.45020200	-4.64785000	2.58438800
H	1.66285500	-3.90675000	0.98301700
C	0.37024500	-2.30352400	3.77473700
H	0.33491100	-3.13980200	4.47760000
H	1.28803400	-1.73774800	3.95342000
H	-0.48029200	-1.64549800	3.97380800
C	-1.85359900	-4.03223300	2.96073500
H	-2.80501600	-4.37828900	2.54909500
H	-1.31874800	-4.89890600	3.36096600
H	-2.06847500	-3.34270600	3.77785400
C	-0.93329400	-4.26369700	0.63174700
H	-0.46872100	-5.22183400	0.87795800
H	-1.93638700	-4.45515300	0.24478500
H	-0.34671400	-3.78531200	-0.15756500
O	-2.28363300	1.58000800	-0.69817800
O	-3.28347400	0.48685100	1.07013100
C	-3.52846200	2.31491400	-0.42556700
C	-4.35073600	1.26254800	0.41860000
B	-2.18918500	0.65481500	0.29444500
C	-5.13447800	0.27262600	-0.44560400
H	-5.50225200	-0.53804900	0.18777800
H	-5.98885000	0.75545500	-0.92682600
H	-4.49905300	-0.16385400	-1.22108700
C	-5.23740800	1.85993400	1.50212300
H	-5.99563600	2.51108600	1.05650800
H	-5.74986700	1.05893100	2.04085400
H	-4.65729500	2.43738000	2.22294000
C	-4.15592400	2.70674700	-1.75555900
H	-5.12765600	3.18222300	-1.59223300
H	-3.50964800	3.42174800	-2.27155100
H	-4.29414100	1.84133400	-2.40527200
C	-3.12626400	3.55465300	0.37709200
H	-2.39948600	4.13157500	-0.19961200
H	-3.98975700	4.19218600	0.58331300

H	-2.66273900	3.27716800	1.32816600
H	0.37608300	1.80789000	1.20207300

O(Bpin)2

Charge: 0, Spin: 1

O	-2.34894400	-1.48003200	0.03018900
O	-1.45195400	0.62050700	-0.26933300
C	-2.89349500	0.78735100	-0.33534100
C	-3.41288200	-0.54040900	0.33858000
B	-1.21718700	-0.73209400	-0.18088700
O	0.00814500	-1.31060900	-0.32611700
C	-3.26956900	2.07259200	0.39477700
H	-2.85871000	2.93312000	-0.14060700
H	-4.35764700	2.18590700	0.44107100
H	-2.87010200	2.08564400	1.40992200
C	-3.25831600	0.88909800	-1.82106100
H	-4.32479100	1.08674500	-1.96305400
H	-2.68937900	1.70871200	-2.26777800
H	-2.99955900	-0.03229700	-2.35025900
C	-4.72185700	-1.08171900	-0.22634800
H	-4.99140200	-2.00560000	0.29281900
H	-5.53217500	-0.35942200	-0.08295200
H	-4.63517300	-1.30659400	-1.29040700
C	-3.48804600	-0.44505800	1.86706100
H	-4.31222300	0.19698100	2.19098900
H	-3.64433900	-1.44686500	2.27541600
H	-2.55465600	-0.05153400	2.27945700
O	2.33615400	-1.15876600	-0.85920000
O	1.48479900	0.30844700	0.69836000
C	3.48155000	-0.49305100	-0.26185400
C	2.82236000	0.78182200	0.39005300
C	2.66089200	1.94547600	-0.59551700
H	2.00423000	2.69575600	-0.14793900
H	3.62154700	2.41301600	-0.83034700
H	2.19909400	1.60720300	-1.52735100
C	3.47967500	1.26321500	1.67930300
H	4.52113200	1.54848100	1.49840200
H	2.94616100	2.13923800	2.05853200
H	3.45501300	0.49314000	2.45186600
C	4.50299900	-0.20142000	-1.35610000
H	5.33953700	0.38065000	-0.95577200
H	4.89801200	-1.14125000	-1.75176400
H	4.05451800	0.35055700	-2.18338000
C	4.06616600	-1.46007000	0.77412200
H	4.30469500	-2.40530700	0.27980200
H	4.97870600	-1.06208200	1.22752100
H	3.34187800	-1.66473000	1.56755800
B	1.22981800	-0.72646500	-0.17091000

¹A

C	-1.12846900	-2.10873100	0.38062300
C	-1.50105000	-3.43964800	0.67062500
C	-0.48559700	-4.29247300	1.15377300
H	-0.71849200	-5.32443700	1.40047800

C	0.79274500	-3.80645000	1.28292000
H	1.59595200	-4.44994900	1.62294800
C	1.10674800	-2.45678800	0.97601000
C	-2.10109200	-1.20666700	-0.15372100
C	-3.43329400	-1.63550300	-0.33245400
C	-4.35075100	-0.67219100	-0.80420700
C	-2.57018000	0.99267300	-0.81538800
C	-3.92416300	0.61664800	-1.01476700
H	-5.38750100	-0.95027300	-0.97087300
H	-4.62127900	1.38106300	-1.33700700
N	-1.67744300	0.05939300	-0.44455300
N	0.13379900	-1.62066100	0.57387700
C	2.54083100	-2.01221000	1.03426200
C	3.10507700	-1.70642700	-0.37215200
H	3.13040100	-2.80525500	1.50482900
H	2.63447400	-1.12888100	1.66318600
C	4.45584500	-0.98771100	-0.31943500
H	3.19102100	-2.64233600	-0.94114300
H	2.39639900	-1.08439800	-0.92585800
C	4.95609400	-0.61581200	-1.71903600
H	4.33940000	-0.08070800	0.28483400
H	5.19442300	-1.61950500	0.19321900
H	5.91648900	-0.09260600	-1.67108800
H	5.09150400	-1.50780000	-2.34226900
H	4.23898700	0.03923400	-2.22588900
C	-2.19430600	2.44480700	-0.96275200
C	-1.61726200	3.08265100	0.31952400
H	-3.10286000	2.98307900	-1.25064400
H	-1.48026100	2.55380400	-1.77896900
C	-2.47889700	2.88295500	1.57063800
H	-0.61015400	2.70359300	0.51029800
H	-1.49456100	4.15373000	0.11849900
C	-1.92714900	3.64740700	2.77732100
H	-3.51152800	3.19909300	1.36241200
H	-2.52093200	1.81284200	1.81276100
H	-2.53590900	3.47403200	3.67070900
H	-0.90377100	3.33023100	2.99425900
H	-1.91276900	4.72628500	2.58435600
C	-2.85437000	-3.85854100	0.45832000
C	-3.78779800	-2.98761600	-0.02028600
H	-3.11985100	-4.88536900	0.69056200
H	-4.81562700	-3.30233100	-0.17270400
O	1.83915300	0.78413800	0.75747000
Ni	0.21831300	0.23910000	-0.08538100
Cl	1.50655500	1.36656100	2.20651500
O	2.51580000	0.78702300	3.11302100
O	1.58465300	2.83437100	2.12618500
O	0.12328900	0.90364800	2.52934200
O	0.63431100	-0.53890700	-2.60726400
Cl	0.70140600	0.93707600	-2.82139300
O	0.55519200	1.60653800	-1.37648600
O	2.00334700	1.36657800	-3.35079300
O	-0.43748700	1.41996700	-3.63116200

¹TS_{A-B}

C	-2.47893600	-0.89301300	-1.14254000
C	-3.68162600	-0.98626100	-1.86365700
C	-4.19824000	0.22582000	-2.38242600
H	-5.11101500	0.21450800	-2.97122400
C	-3.56502900	1.41009300	-2.08908500
H	-3.97303100	2.35766900	-2.42255400
C	-2.37052800	1.43685900	-1.32027800
C	-1.94497000	-2.02887300	-0.47364400
C	-2.62369200	-3.26114700	-0.53393100
C	-2.09406300	-4.30890900	0.25222200
C	-0.34639100	-2.80499000	1.04306400
C	-0.98892200	-4.07073400	1.03600600
H	-2.57569800	-5.28254800	0.25152600
H	-0.58276800	-4.84947200	1.67089200
N	-0.81962100	-1.81923400	0.27330500
N	-1.81781700	0.28131100	-0.94318700
C	-1.83104300	2.73841200	-0.81052300
C	-2.73148100	3.23930200	0.34897900
H	-1.79810800	3.47038400	-1.62401700
H	-0.81710400	2.60551600	-0.44347000
C	-2.01149000	4.26421800	1.23121200
H	-3.65674400	3.66727100	-0.06053700
H	-3.02583900	2.38637800	0.96617100
C	-2.88139700	4.71912100	2.40628200
H	-1.09939400	3.79518400	1.61790200
H	-1.70272100	5.12681400	0.62373300
H	-2.35913400	5.45925900	3.02155400
H	-3.81794100	5.17303700	2.05975500
H	-3.12630700	3.86360200	3.04327800
C	0.87815500	-2.59034800	1.88791800
C	2.19516200	-2.94069000	1.15728000
H	0.78362900	-3.21385100	2.78335700
H	0.88330100	-1.55645800	2.23701900
C	2.35454800	-4.41544100	0.77301000
H	2.30160000	-2.32409300	0.25918300
H	3.01990900	-2.65280400	1.82036500
C	3.70802900	-4.68711000	0.10809400
H	2.24501200	-5.04451700	1.66761100
H	1.54878400	-4.70998500	0.08826400
H	3.81458100	-5.73934100	-0.17413400
H	3.82406600	-4.08158600	-0.79774100
H	4.53448800	-4.43569100	0.78270700
C	-4.31750800	-2.26586600	-1.97614900
C	-3.80941200	-3.35983900	-1.33418900
H	-5.23091900	-2.34228600	-2.55818400
H	-4.31212900	-4.32009900	-1.39744700
O	0.90569200	1.29745400	-1.04463600
B	2.13179500	0.41771800	0.14687900
O	3.13686900	-0.12705200	-0.60990000
C	4.37548900	0.50072500	-0.14717400
O	2.51720300	1.36568400	1.04864800
C	3.85552700	1.77937400	0.62790800

H	1.25182300	-0.39336600	0.55487900
C	5.23896900	0.79800900	-1.36737200
H	5.54455800	-0.14148900	-1.83635300
H	4.68895300	1.38004200	-2.10633500
H	6.14150500	1.34430300	-1.07444300
C	3.69029800	3.01408800	-0.26396800
H	4.66286600	3.41792400	-0.56031600
H	3.11651600	2.78754500	-1.16276900
H	3.15253300	3.78006800	0.30077800
C	4.64865200	2.13310700	1.88113500
H	5.68752700	2.36428000	1.62448900
H	4.20741200	3.01418700	2.35417000
H	4.63658700	1.31968400	2.60772700
C	5.06060700	-0.52122300	0.76481900
H	6.03989000	-0.16670600	1.09841700
H	4.44829500	-0.73515300	1.64437500
H	5.19684300	-1.45348300	0.21039300
Ni	-0.14278400	-0.02264800	-0.09263600
Cl	0.99547200	0.99030400	-2.68360900
O	-0.14299200	1.72621700	-3.25759800
O	2.29709000	1.53403200	-3.09013100
O	0.87911300	-0.46953400	-2.85661500
O	-2.90355500	0.06238400	1.79195500
Cl	-1.75317200	0.46306000	2.66478700
O	-0.67782100	1.11207600	1.77818600
O	-2.17930000	1.46529200	3.66747000
O	-1.16281700	-0.74517800	3.30906600

BpinClO₄

O	-0.28552100	-0.66056100	0.35355900
O	-1.00360800	1.36982800	-0.47701700
C	-1.70699600	-0.83174200	0.04563800
C	-2.20847900	0.66201300	-0.03159300
C	-2.57746100	1.24779400	1.33391600
H	-2.70387700	2.32846800	1.23217800
H	-3.51057900	0.82137400	1.71237300
H	-1.78732400	1.06449000	2.06735800
C	-3.31494900	0.91723200	-1.04721900
H	-4.20558400	0.33327400	-0.79400000
H	-3.58601000	1.97621900	-1.03838800
H	-2.99894700	0.65667200	-2.05823800
C	-2.33864000	-1.66833700	1.15084000
H	-3.41998400	-1.74512000	0.99921700
H	-1.91762000	-2.67692900	1.13410100
H	-2.15000900	-1.23949100	2.13581400
C	-1.77488900	-1.56406800	-1.29731600
H	-1.21790800	-2.50071500	-1.21723200
H	-2.80791000	-1.79199700	-1.57401900
H	-1.32222700	-0.96829200	-2.09477200
B	0.03644400	0.57913000	-0.10079100
O	1.34045100	1.08854600	-0.19775500
Cl	2.63495200	-0.02662900	0.01801200
O	2.42571300	-1.06033200	-0.99802400

O	2.52205900	-0.49696200	1.39857900
O	3.77341200	0.84969700	-0.23337300
¹B			
C	-2.57008500	0.20124800	-0.19653900
C	-3.92755300	0.59285500	-0.25150900
C	-4.19537500	1.93506700	-0.59507300
H	-5.22321700	2.28236000	-0.65138800
C	-3.14534300	2.79029700	-0.83507200
H	-3.32530500	3.83205000	-1.07555400
C	-1.80517700	2.33675200	-0.78166800
C	-2.23313800	-1.13305300	0.21843700
C	-3.26822700	-2.04608600	0.52872400
C	-2.87601300	-3.33653900	0.94833100
C	-0.55294200	-2.66397400	0.72835500
C	-1.53752500	-3.63468900	1.04622100
H	-3.63343600	-4.07523800	1.19588700
H	-1.20911800	-4.61570400	1.37208400
N	-0.90816700	-1.43924300	0.31806100
N	-1.53558600	1.04851600	-0.49487900
Ni	0.18520700	0.21167900	-0.39309500
C	-0.68139500	3.31148600	-0.99843500
C	0.09422900	3.62395400	0.30142500
H	-1.08505700	4.23701000	-1.42266400
H	0.01471200	2.88426200	-1.72636700
C	1.38979000	4.39338200	0.02548600
H	-0.55419700	4.19142300	0.98332800
H	0.34950500	2.68423100	0.80284900
C	2.16108400	4.70949300	1.31000600
H	2.02105300	3.78062900	-0.62946200
H	1.16128200	5.32058000	-0.51937700
H	3.07568500	5.27068500	1.09251900
H	1.55671700	5.30887000	2.00188400
H	2.44708200	3.78254400	1.81576000
C	0.90246000	-3.02183800	0.79869800
C	1.47121500	-3.36201800	-0.59653600
H	1.03101900	-3.87881700	1.46910700
H	1.46312500	-2.17880100	1.20485900
C	2.98547300	-3.58713300	-0.56083100
H	0.96061000	-4.25060800	-0.99496400
H	1.24797200	-2.53028400	-1.27390700
C	3.56398800	-3.86784000	-1.95039600
H	3.45981700	-2.69480000	-0.13832000
H	3.21465800	-4.42310700	0.11502300
H	4.64607300	-4.02711700	-1.90510300
H	3.11221000	-4.75934600	-2.40240900
H	3.38059600	-3.02230800	-2.62291100
C	-4.95347900	-0.36033200	0.05384100
C	-4.63614000	-1.63295300	0.42437500
H	-5.98975600	-0.04193800	-0.00957800
H	-5.41440700	-2.35274500	0.66041800
Cl	3.04095700	0.51616600	0.38634600
O	1.92033200	-0.47655100	-0.17727700
O	2.45752300	1.23055600	1.55164700

O	4.13858800	-0.39053800	0.77809600
O	3.43485900	1.45303600	-0.68705100
H	0.79107700	1.28891700	-1.09556100

¹TS2_{B-D}

C	3.04323500	-0.81837100	0.17709200
C	4.28836100	-1.32415100	-0.25759600
C	4.28341700	-2.60307200	-0.85740300
H	5.21679600	-3.03846300	-1.20326000
C	3.08854500	-3.26423700	-1.03049200
H	3.05355000	-4.22682000	-1.52881100
C	1.87313000	-2.70338000	-0.56842400
C	2.95022000	0.51386800	0.70201500
C	4.12614200	1.28651100	0.82921500
C	3.97504500	2.59645100	1.33527100
C	1.57453000	2.22856700	1.46935000
C	2.71745800	3.05203800	1.64908700
H	4.84778900	3.23123600	1.46095000
H	2.57047600	4.05925300	2.02209100
N	1.70273500	0.97569600	1.01723900
N	1.88123500	-1.52625300	0.07499100
C	0.56635200	-3.40804700	-0.80356100
C	0.12862000	-4.30879900	0.37341100
H	0.65677800	-4.01409000	-1.71204500
H	-0.19675800	-2.64955800	-0.99303200
C	-1.36589300	-4.64158700	0.29787900
H	0.73057300	-5.22779900	0.38182900
H	0.32798900	-3.78826400	1.31714700
C	-1.82275700	-5.55891300	1.43519800
H	-1.92867200	-3.69992700	0.33010800
H	-1.58756400	-5.10988700	-0.67121300
H	-2.89416900	-5.77424600	1.36792500
H	-1.28751200	-6.51578000	1.41729400
H	-1.63781600	-5.09267900	2.40984200
C	0.21242000	2.80656900	1.74155800
C	-0.43772100	3.45299300	0.49453800
H	0.31496300	3.55957400	2.53217200
H	-0.45606400	2.02736700	2.11197600
C	0.39688000	4.52108500	-0.21498200
H	-0.68421500	2.67001300	-0.21815600
H	-1.39632900	3.87709500	0.81510800
C	-0.34854300	5.08459100	-1.42961100
H	0.65815200	5.33216500	0.48145600
H	1.34357800	4.08145200	-0.55282700
H	0.25305500	5.82779800	-1.96348800
H	-0.59807600	4.27810100	-2.12677400
H	-1.28658200	5.56522600	-1.12800300
C	5.46546300	-0.52307400	-0.09662800
C	5.38710800	0.73048000	0.43479800
H	6.41899700	-0.93163100	-0.41782400
H	6.27892100	1.33940600	0.55067700
O	-1.03964300	-0.37449000	-1.04571400
B	-1.83989100	-0.00309600	0.65308900

O	-2.45376700	1.22987500	0.56895900
C	-3.88780300	1.00596600	0.63109300
O	-2.72778800	-1.05282500	0.78073300
C	-4.01886200	-0.54288900	0.34116000
H	-0.86028900	0.04966500	1.48352000
C	-4.55365000	1.90968500	-0.40277600
H	-4.42169800	2.95589900	-0.11159100
H	-4.09982300	1.77670100	-1.38468700
H	-5.62762800	1.70420000	-0.46407500
C	-4.17999100	-0.87335700	-1.14819000
H	-5.18183100	-0.61051500	-1.50146600
H	-3.44296600	-0.35351800	-1.75875400
H	-4.03476500	-1.94869800	-1.28281900
C	-5.09761800	-1.25710100	1.15168200
H	-6.08662300	-0.84321600	0.92936400
H	-5.10577200	-2.31901600	0.88993100
H	-4.91384000	-1.17622000	2.22423300
C	-4.31831900	1.39617300	2.04955100
H	-5.40222600	1.32487300	2.17969500
H	-3.83182800	0.75938000	2.79361200
H	-4.01341600	2.42976300	2.23520300
Ni	0.39775700	-0.58638900	0.83193900
Cl	-0.62933800	0.61575700	-2.21269900
O	-0.39979800	-0.24983400	-3.38591100
O	-1.74264800	1.57251200	-2.41820100
O	0.61324600	1.31891000	-1.79823200
H	-0.29338300	-1.80959600	1.06272400

¹D

C	0.67956100	1.64576700	-0.22114000
C	1.34612300	2.87581500	-0.43100300
C	2.69022900	2.81021100	-0.85712100
H	3.24617300	3.72690800	-1.03410000
C	3.27633200	1.57749100	-1.04019200
H	4.30933000	1.49807600	-1.36213300
C	2.54462500	0.38658100	-0.81418200
C	-0.68706700	1.64459500	0.22060400
C	-1.35616500	2.87347300	0.42919500
C	-2.70060300	2.80549300	0.85391300
C	-2.55044800	0.38210400	0.81189500
C	-3.28470300	1.57172900	1.03639400
H	-3.25850700	3.72119600	1.02986300
H	-4.31805800	1.49051500	1.35671900
N	-1.26887200	0.42484100	0.41675000
N	1.26370700	0.42702100	-0.41671800
Ni	0.00051100	-1.07518500	0.00585800
C	3.21055600	-0.95164600	-0.96028000
C	3.61042400	-1.53389000	0.41033500
H	4.09631600	-0.85461900	-1.59891000
H	2.50581900	-1.63937300	-1.43578200
C	4.21279400	-2.93660300	0.29427800
H	4.32157500	-0.85721800	0.90535000
H	2.70816800	-1.57535200	1.03237400

C	4.60394000	-3.52094800	1.65490800
H	3.47922200	-3.59252600	-0.19179200
H	5.09207400	-2.90810900	-0.36474600
H	5.02449800	-4.52693300	1.55390800
H	5.35201300	-2.89438800	2.15497000
H	3.73143700	-3.58700800	2.31440600
C	-3.21401700	-0.95735900	0.95748700
C	-3.60096400	-1.54643300	-0.41388700
H	-4.10505700	-0.86038800	1.58870800
H	-2.51112500	-1.64127500	1.44125800
C	-4.20104100	-2.95001900	-0.29688100
H	-4.30939100	-0.87362300	-0.91797300
H	-2.69334100	-1.58841700	-1.02806600
C	-4.57826900	-3.54167500	-1.65827500
H	-3.47051700	-3.60199700	0.19901100
H	-5.08644400	-2.92059900	0.35386900
H	-4.99786400	-4.54796300	-1.55631100
H	-5.32280300	-2.91901000	-2.16839000
H	-3.69951800	-3.60927800	-2.30927900
C	0.64367200	4.10580200	-0.20733900
C	-0.65595400	4.10467200	0.20520700
H	1.17086900	5.04068000	-0.37528700
H	-1.18494700	5.03863000	0.37264100
H	-0.81935100	-2.22300300	0.33468000
H	0.82711000	-2.22376600	-0.30272100

³D

C	0.66866800	1.68644300	-0.19985100
C	1.35928200	2.91389000	-0.41779100
C	2.69361800	2.85330500	-0.82678800
H	3.24916400	3.76952900	-1.00414400
C	3.30334400	1.59698300	-1.00771000
H	4.33830600	1.52699400	-1.32562800
C	2.58575900	0.42959500	-0.77962500
C	-0.67892500	1.67734700	0.20817700
C	-1.37735100	2.90372700	0.41911800
C	-2.71076600	2.83423400	0.82634000
C	-2.57765200	0.41118100	0.78280100
C	-3.30847200	1.57797800	1.00785700
H	-3.27401500	3.74704700	0.99900600
H	-4.34404000	1.49902000	1.32150100
N	-1.28240400	0.44049500	0.39321400
N	1.28669200	0.45693400	-0.38234400
Ni	0.06945100	-0.98741800	0.00559200
C	3.20525500	-0.93631000	-0.92201800
C	3.50816300	-1.60249800	0.43446700
H	4.12636100	-0.86911300	-1.51131600
H	2.50964000	-1.57623700	-1.48649100
C	4.03653400	-3.03339300	0.29573500
H	4.23359800	-0.98635700	0.98175300
H	2.59233200	-1.60703600	1.04299000
C	4.32850400	-3.69165800	1.64752900
H	3.30203400	-3.63592400	-0.25706000
H	4.94795800	-3.02725800	-0.31774400

H	4.70333400	-4.71305700	1.52518300
H	5.08031700	-3.12398300	2.20746800
H	3.42395800	-3.73863500	2.26510700
C	-3.21468800	-0.94744700	0.91860800
C	-3.53183200	-1.58918500	-0.44574400
H	-4.13495100	-0.86891100	1.50790900
H	-2.53416000	-1.60191700	1.47881000
C	-4.02248400	-3.03508200	-0.32797500
H	-4.28579200	-0.97946200	-0.96086900
H	-2.63163100	-1.55382900	-1.07350700
C	-4.33994100	-3.66744300	-1.68628500
H	-3.25744000	-3.63352200	0.18726800
H	-4.91370900	-3.06700500	0.31366300
H	-4.68600400	-4.70059200	-1.57858000
H	-5.12215300	-3.10516100	-2.20873500
H	-3.45414800	-3.67651300	-2.33209600
C	0.63609000	4.13983800	-0.20184200
C	-0.66643700	4.13472400	0.19774800
H	1.15770500	5.07919200	-0.36624500
H	-1.19698100	5.06996200	0.35723500
H	-0.50154000	-2.37843300	0.63248100
H	-0.68279800	-2.42046700	-0.16712900

³TS_{D-E}

C	2.54888200	-0.37506700	-1.03023000
C	1.07882400	1.31335400	-0.30935900
N	1.33866900	-0.02417000	-0.53342000
C	-0.20821700	1.64024900	0.18266700
C	-0.53926400	2.99181400	0.47282400
C	-1.82512000	3.24987000	0.96792000
C	-2.33004100	0.87753200	0.83300400
C	-2.71096900	2.18779000	1.14770200
H	-2.12145400	4.26796400	1.20421500
H	-3.71326100	2.36370300	1.52411400
N	-1.09448900	0.59898700	0.35939800
Ni	-0.20541100	-1.17064600	-0.07142500
H	-0.99064300	-2.05912400	-0.95391400
H	-1.06889400	-2.23647200	0.49904700
C	3.53238200	0.58178100	-1.29265400
C	2.04285700	2.32945600	-0.54452500
C	3.29253700	1.93607800	-1.04476500
C	0.45152500	4.00590100	0.23717000
C	1.68380100	3.69060700	-0.25371600
H	0.19379100	5.03836100	0.45759400
H	2.42198300	4.46772500	-0.43243300
H	4.05775700	2.68149200	-1.24081100
H	4.48868700	0.25404100	-1.68737400
C	2.81225000	-1.84334800	-1.24928600
C	3.48950100	-2.53400400	-0.04482900
H	3.45157200	-1.96039000	-2.13160400
H	1.86206100	-2.34519400	-1.47507600
C	2.63742300	-2.56033600	1.22896800
H	3.73885200	-3.56326500	-0.33528100

H	4.44268900	-2.02996900	0.16488100
C	3.32570100	-3.29141800	2.38527000
H	2.39746000	-1.53389000	1.53101300
H	1.67312200	-3.04115800	1.00905200
H	2.69763500	-3.29866300	3.28169500
H	3.54464500	-4.33242900	2.12100800
H	4.27518400	-2.80930400	2.64548000
C	-3.29460000	-0.26918800	0.95646200
C	-3.85030600	-0.71466800	-0.41026300
H	-4.12125700	0.01206400	1.61881000
H	-2.76913100	-1.11577600	1.41491200
C	-4.71783000	-1.97263900	-0.31215600
H	-4.43081100	0.10728800	-0.85118900
H	-3.00580300	-0.90477300	-1.08231900
C	-5.26778900	-2.41756800	-1.67064900
H	-4.11918200	-2.78233900	0.12607100
H	-5.54941900	-1.79245900	0.38358300
H	-5.88121200	-3.32012300	-1.58013200
H	-5.88910900	-1.63470400	-2.12105400
H	-4.45228100	-2.63540000	-2.36958000

³E

C	2.49911900	-0.39934000	-1.05126900
C	1.01808000	1.29621400	-0.35092000
N	1.28478900	-0.04384100	-0.59579600
C	-0.27297500	1.63665300	0.11621200
C	-0.59716300	2.99295300	0.41122200
C	-1.89086200	3.27420000	0.86312500
C	-2.43382000	0.91389800	0.74098100
C	-2.81136700	2.22386300	1.02036300
H	-2.17512200	4.29813800	1.08762600
H	-3.82354500	2.42202800	1.35701200
N	-1.18838300	0.61310000	0.30161000
Ni	-0.22018000	-1.06883500	0.12248200
C	3.50796700	0.54578900	-1.26996400
C	2.01515600	2.30091100	-0.53224000
C	3.26928700	1.89952000	-1.00206700
C	0.42362900	3.99043400	0.22147100
C	1.66792200	3.66174300	-0.22729000
H	0.17752900	5.02447000	0.44894600
H	2.42483600	4.42971000	-0.36413400
H	4.04739800	2.64071000	-1.16252500
H	4.46784800	0.21448900	-1.65204400
C	2.74540000	-1.87072400	-1.28097300
C	3.46497500	-2.55716900	-0.10113500
H	3.34450500	-1.99605800	-2.19016800
H	1.78064700	-2.36317700	-1.46133000
C	2.65283800	-2.57398400	1.19851200
H	3.70882500	-3.58767600	-0.39178200
H	4.42190400	-2.04788300	0.07641000
C	3.36929500	-3.30030500	2.34017200
H	2.41946300	-1.54578300	1.49904700
H	1.67972300	-3.05485300	1.00698600

H	2.76600300	-3.30071900	3.25357700
H	3.58069000	-4.34302600	2.07648700
H	4.32545500	-2.81713600	2.57174400
C	-3.37636100	-0.25091200	0.88157400
C	-3.72951600	-0.90523200	-0.46723100
H	-4.29163900	0.06725200	1.39256000
H	-2.89320800	-1.00794700	1.52123900
C	-4.64332900	-2.12560500	-0.32054700
H	-4.20470900	-0.15768300	-1.11641600
H	-2.79703500	-1.19920000	-0.97036800
C	-4.97291400	-2.78479400	-1.66332600
H	-4.16169300	-2.85832400	0.34198000
H	-5.57309900	-1.82575500	0.18232500
H	-5.62499200	-3.65496200	-1.53499000
H	-5.48103200	-2.08153400	-2.33292900
H	-4.06070300	-3.12118100	-2.16946000

¹F

C	3.48018800	1.78837900	3.40918400
C	3.86763400	-0.84030400	0.21477100
C	5.14031200	-1.18750900	-0.29272300
C	5.17147900	-2.11777800	-1.35629400
C	3.98762900	-2.64783500	-1.82166600
C	2.74601200	-2.24002600	-1.27527000
N	2.69712100	-1.31608900	-0.30333600
H	6.12457600	-2.41292300	-1.78668400
H	3.98271700	-3.38280600	-2.61983400
C	3.76086900	0.05678500	1.32728200
C	4.92804800	0.64283800	1.86803600
C	4.75373900	1.53916200	2.94549500
C	2.35570000	1.15454600	2.82801200
N	2.49890500	0.29817100	1.80319700
H	5.61868900	2.01620800	3.39795400
H	3.31568900	2.47005000	4.23769000
Ni	1.12467600	-0.44498200	0.55914900
C	1.46226100	-2.86723600	-1.72401600
H	0.64111700	-2.17159600	-1.54048300
C	0.97618000	1.47064800	3.34374800
H	0.29273900	0.70371200	2.97698800
C	0.47102700	2.86566600	2.89874500
H	1.03517300	3.64944300	3.42436600
C	1.15087600	-4.18030000	-0.96457100
H	0.17261800	-4.51628400	-1.32216800
H	-0.57037100	2.96138400	3.23284900
C	0.55036400	3.10601900	1.38586400
H	0.14026600	2.23810400	0.86110100
H	1.60445100	3.16172100	1.08714000
H	1.87884600	-4.95518000	-1.24399800
C	1.11482100	-4.02916700	0.56210100
H	0.56338900	-3.11721800	0.81538800
H	2.13458300	-3.89743900	0.94901900
C	6.30866100	-0.58609200	0.28104500
H	7.28053200	-0.84914900	-0.12683700

C	6.20535600	0.30136400	1.31299000
H	7.09339400	0.75990600	1.73857800
H	0.99074700	1.42966500	4.44003800
H	1.50132000	-3.07223800	-2.79935600
C	-0.17375200	4.38060000	0.94700100
H	-0.06010500	4.54798300	-0.12875100
H	-1.24822900	4.31445000	1.15513500
H	0.21248900	5.26509100	1.46828000
C	0.44108100	-5.22595100	1.23894200
H	0.45460400	-5.12617600	2.32977000
H	-0.60340400	-5.29825000	0.91827700
H	0.94218900	-6.16789600	0.98279800
C	-0.04261800	2.85827700	-3.24537800
C	-2.94379400	1.98597800	-0.37512700
C	-3.96366400	2.93049100	-0.09451100
C	-4.90332500	2.57842400	0.89874100
C	-4.77773600	1.37492400	1.55471100
C	-3.73503900	0.47732700	1.21065500
N	-2.87412200	0.77511000	0.23426400
H	-5.70980500	3.26558400	1.14095700
H	-5.48017000	1.09671000	2.33191100
C	-1.92069700	2.30754000	-1.33705300
C	-2.01843200	3.52366400	-2.05787500
C	-1.03772000	3.78388000	-3.03734100
C	0.03076500	1.68433700	-2.46355400
N	-0.87869600	1.42157700	-1.50512500
H	-1.08356600	4.70141400	-3.61727900
H	0.71585900	3.02133100	-4.00343000
H	-0.11641500	0.12091100	1.13695300
Ni	-1.01637100	-0.19126600	-0.41193300
C	-3.51537400	-0.79717600	1.99097000
H	-2.84824500	-1.43912600	1.41853900
C	1.14545900	0.70579600	-2.72149300
H	1.05264400	-0.08994800	-1.98255600
C	2.56121400	1.31344500	-2.65563500
H	2.76598700	1.92708700	-3.54381400
C	-4.77832100	-1.56977600	2.40638500
H	-4.45806900	-2.41565400	3.02800400
H	3.27607900	0.48127600	-2.69187600
C	2.80331100	2.14464200	-1.39071700
H	2.44071100	1.57901800	-0.52690300
H	2.18680700	3.05137800	-1.42851000
H	-5.41511500	-0.95312900	3.05750900
C	-5.60227200	-2.09783300	1.22638200
H	-4.97217800	-2.74806600	0.61220000
H	-5.88845900	-1.26137200	0.57515000
C	-4.00852500	4.16653200	-0.81469400
H	-4.80371400	4.87193000	-0.58997400
C	-3.07990100	4.44321600	-1.77226900
H	-3.11938400	5.37251500	-2.33327500
H	0.98142000	0.25036600	-3.70738000
H	-2.95549300	-0.51200800	2.89488600
C	4.27039800	2.52782900	-1.19084600
H	4.40483600	3.12259700	-0.28115100

H	4.90150300	1.63760500	-1.09849200
H	4.64758000	3.11657700	-2.03557600
C	-6.85554700	-2.85124500	1.68014700
H	-7.42784700	-3.22398500	0.82447200
H	-6.59297700	-3.71360100	2.30431700
H	-7.51867600	-2.20698800	2.27114900
O	-1.38044600	-2.06809000	-0.04668000
Cl	-2.34388300	-2.77396900	-1.08363700
O	-3.53588900	-1.91281100	-1.29438000
O	-1.59832600	-2.97171800	-2.35377000
O	-2.70162800	-4.06318400	-0.44858900

²G

C	2.51506000	0.61228600	0.16177000
C	3.77317300	1.25231400	0.16881000
C	3.78923500	2.61130900	0.55860600
H	4.73029900	3.15392700	0.57973800
C	2.60785700	3.23494200	0.90859500
H	2.59849200	4.27731000	1.20884700
C	1.38691500	2.52180200	0.88490300
C	2.40897600	-0.76477600	-0.23560400
C	3.56744500	-1.48057300	-0.60672600
C	3.38054000	-2.82964700	-0.98619800
C	0.99456200	-2.58038900	-0.60626400
C	2.10979100	-3.36789100	-0.98266600
H	4.23707200	-3.43004200	-1.28033600
H	1.94478700	-4.39989200	-1.27327200
N	1.16187600	-1.30536100	-0.23766400
N	1.35998200	1.23567900	0.51542500
Ni	-0.22029500	0.04856400	0.32790400
C	0.06394600	3.15260600	1.22196600
C	-0.77065200	3.47137200	-0.03970700
H	0.21747900	4.06132200	1.81386500
H	-0.49956200	2.44649600	1.84539300
C	-2.22540200	3.82054000	0.29365100
H	-0.29464400	4.29470600	-0.58941400
H	-0.76595400	2.60058200	-0.70522300
C	-3.04572400	4.14589200	-0.95762400
H	-2.68322700	2.96568600	0.80681900
H	-2.25077000	4.66576400	0.99611100
H	-4.08138400	4.38487400	-0.69708500
H	-2.62554200	5.00409900	-1.49597000
H	-3.06086900	3.28635200	-1.63344300
C	-0.40402800	-3.13152200	-0.56526500
C	-0.90030000	-3.35366300	0.87997800
H	-0.44618600	-4.07348800	-1.12266000
H	-1.08199800	-2.42635300	-1.06000100
C	-2.35998100	-3.81527800	0.93005600
H	-0.25031700	-4.08260700	1.38437100
H	-0.80536800	-2.40877000	1.42937600
C	-2.86935300	-3.96896400	2.36589100
H	-2.97587400	-3.08521600	0.39414800
H	-2.45968000	-4.76937900	0.39387700

H	-3.91153800	-4.30330000	2.38442500
H	-2.27308000	-4.69809200	2.92785900
H	-2.81700300	-3.01240200	2.89802700
C	4.93551700	0.50112000	-0.21361400
C	4.83680000	-0.80991900	-0.58301600
H	5.90063700	0.99928600	-0.20370500
H	5.72269900	-1.36856800	-0.87098100
Cl	-3.01602000	0.08345300	-0.74714500
O	-2.12508200	-0.14868400	0.54391200
O	-2.18381500	0.82731900	-1.73681800
O	-3.38358000	-1.25818800	-1.26119500
O	-4.18841300	0.86675700	-0.31342500

²H

C	3.10762100	1.31958100	-1.39692500
C	-0.69495600	1.34379500	0.29867200
C	-1.35553800	2.56308500	0.57874900
C	-2.64541400	2.47201600	1.14865300
C	-3.18867200	1.22984400	1.39469100
C	-2.46209400	0.05291900	1.08536600
N	-1.23737700	0.12132900	0.55341000
H	-3.19449400	3.37933400	1.38610900
H	-4.17925300	1.13144200	1.82704100
C	0.61549000	1.36175000	-0.28836200
C	1.24109800	2.59797500	-0.57227100
C	2.53112500	2.54749500	-1.14594600
C	2.41902600	0.12478400	-1.08820400
N	1.19330100	0.15057600	-0.54302800
H	3.05262300	3.47011500	-1.38506000
H	4.09760800	1.25039800	-1.83642900
H	-0.28769400	-2.92200800	0.33303200
Ni	0.07751700	-1.42613700	0.03951800
C	-3.07446400	-1.30456100	1.29493100
H	-2.26711000	-2.03813900	1.37559800
C	3.07028000	-1.21349800	-1.31914600
H	2.29010900	-1.97788000	-1.40326600
C	4.05237500	-1.60229400	-0.18958900
H	4.86737100	-0.86546700	-0.14838600
C	-4.01256400	-1.70902600	0.13274800
H	-4.42827200	-2.69672700	0.37060500
H	4.51533400	-2.55974900	-0.46138300
C	3.39877400	-1.72523900	1.19155700
H	2.54779900	-2.41567500	1.13051100
H	2.97002400	-0.75769000	1.48170500
H	-4.86593700	-1.01658300	0.08704700
C	-3.31700400	-1.76573300	-1.23278300
H	-2.41337700	-2.38171600	-1.14721800
H	-2.96682900	-0.76211800	-1.50690200
C	-0.69879300	3.80195600	0.27890200
H	-1.21668600	4.73067300	0.50172000
C	0.54904800	3.81846200	-0.27340600
H	1.04107500	4.76048900	-0.49866200
H	3.61140800	-1.18694100	-2.27248200

H	-3.64296800	-1.30092400	2.23271200
C	4.38440800	-2.19457200	2.26520100
H	3.89857800	-2.27006100	3.24317900
H	4.79521300	-3.18095300	2.02041900
H	5.22801100	-1.50040700	2.36287500
C	-4.23504000	-2.30543200	-2.33299300
H	-3.72559500	-2.32603000	-3.30196300
H	-4.56212900	-3.32714700	-2.10752700
H	-5.13499200	-1.68755800	-2.44152100

²PR1

C	2.74744700	1.66011000	-2.36758500
C	2.39567700	2.99547600	-2.12606200
C	1.25426600	3.27175500	-1.37934300
C	0.45084700	2.16922800	-0.93801700
C	1.93863400	0.61946100	-1.89621500
C	0.85112000	4.59834900	-1.00140600
C	-0.67302100	2.38941600	-0.12883300
C	-1.02659700	3.71293900	0.28739400
C	-0.23251700	4.80864900	-0.20466700
C	-2.09909700	3.86753700	1.16102200
C	-2.78247700	2.72193400	1.61711500
C	-2.42139300	1.45784600	1.16313100
H	1.44729100	5.43619500	-1.35455700
H	3.66599100	1.41252100	-2.88894500
H	-0.51312000	5.81673600	0.09011900
H	-3.60374500	2.81199000	2.32025900
N	0.77451100	0.84741200	-1.25144600
N	-1.39919900	1.27229200	0.28598200
H	-2.38565800	4.85866000	1.50063400
H	3.01939200	3.80964400	-2.48551800
C	-1.18145100	-2.94668900	-2.34470700
H	-1.76327700	-3.28941900	-3.21113500
H	-0.22575600	-3.48385700	-2.39643600
C	-1.92725600	-3.37534400	-1.06438100
H	-2.75725500	-2.68612400	-0.88915500
H	-2.36898100	-4.36694500	-1.22166000
C	-1.06138500	-3.47383600	0.20890300
H	-0.54398500	-4.43731000	0.24472600
H	-1.69516900	-3.39440000	1.09758400
S	0.24956200	-2.16939600	0.34923300
C	0.29795000	-1.87235000	2.17770400
H	-0.66717100	-1.45187600	2.47323300
H	0.44150400	-2.83478500	2.67682500
C	1.43714500	-0.92547200	2.45084200
C	2.66924700	-1.40044300	2.91599500
C	1.30012600	0.43632100	2.14772100
C	3.74876200	-0.52911900	3.07317400
H	2.78729300	-2.45696500	3.14403100
C	2.38196300	1.30406800	2.28967900
H	0.35379200	0.80252400	1.76719800
C	3.60945200	0.82296300	2.75154900
H	4.70025800	-0.90914000	3.43368800

H	2.26272700	2.35091700	2.02679000
H	4.45423900	1.49717400	2.85898900
C	-3.19665400	0.24887400	1.62318200
C	-4.34216700	-0.13334100	0.66782500
H	-3.60506300	0.43599700	2.62317100
H	-2.50859300	-0.59962300	1.70267500
C	-4.97650700	-1.48390500	1.01387300
H	-5.10385500	0.65689900	0.68211600
H	-3.94765500	-0.16703700	-0.35361500
C	-6.07399100	-1.89679100	0.02902400
H	-4.18966300	-2.25196600	1.02744000
H	-5.38381700	-1.44884800	2.03361900
H	-6.51266000	-2.86439700	0.29428900
H	-6.88233200	-1.15726800	0.00660800
H	-5.67468000	-1.97797100	-0.98900300
C	2.46041200	-0.79329600	-1.99929300
C	3.47473500	-1.09031500	-0.87638500
H	2.94492800	-0.94047000	-2.97275500
H	1.64452800	-1.51037700	-1.92691600
C	3.95244600	-2.54536100	-0.88729200
H	4.33216100	-0.41209300	-0.97614800
H	3.01340800	-0.86060200	0.09036500
C	5.00763900	-2.83029700	0.18576800
H	3.08501300	-3.20116000	-0.73479900
H	4.35739000	-2.79075500	-1.87927800
H	5.32438600	-3.87880000	0.17247400
H	5.89873900	-2.20950200	0.03627200
H	4.61524600	-2.60497100	1.18250600
C	-1.85657100	-0.43731600	-2.50387300
C	-0.90643400	-1.45489500	-2.51242900
H	-1.64324700	0.50867100	-2.99522400
H	-2.90723000	-0.64060800	-2.31531600
H	0.02097400	-1.23191300	-3.03104300
Ni	-0.80256200	-0.31725100	-0.73693400
H	-1.95688200	-0.96027500	-0.25991100

²Ts1

C	2.94607200	0.65394700	-2.56520800
C	2.81310900	2.04426000	-2.51124900
C	1.71868500	2.59758700	-1.85029900
C	0.72775800	1.70687500	-1.32166100
C	1.97056500	-0.17139200	-1.98406800
C	1.54963600	4.00555800	-1.63384000
C	-0.36217400	2.20630300	-0.59436800
C	-0.47574800	3.60590000	-0.32289600
C	0.50801700	4.48642100	-0.89905400
C	-1.50374300	4.03872300	0.51276900
C	-2.39011300	3.08252100	1.05815500
C	-2.26487300	1.73901200	0.73228300
H	2.28978800	4.68354700	-2.05180200
H	3.82275600	0.19404200	-3.00867800
H	0.40647400	5.55378000	-0.71896600
H	-3.18760100	3.38826500	1.72742300

N	0.84203000	0.32099800	-1.44098400
N	-1.27897400	1.28489300	-0.09249300
H	-1.60517900	5.09312100	0.75187600
H	3.57242300	2.69373300	-2.93924900
Ni	-0.88904900	-0.51174800	-0.76755000
C	-1.05167400	-2.17395400	-1.93632200
C	-2.23059000	-1.39595600	-2.03486000
H	-0.31942500	-2.05402300	-2.73058200
H	-2.24279100	-0.84788700	-0.46839000
H	-2.32142300	-0.64812900	-2.82050400
H	-3.19042700	-1.80446800	-1.72209400
C	-1.06543500	-3.54648300	-1.26738100
H	-1.54724400	-4.25677000	-1.95461600
H	-0.03524400	-3.90604800	-1.14755400
C	-1.79451900	-3.62461400	0.09540500
H	-2.68223900	-2.98540900	0.07337300
H	-2.15867900	-4.64741200	0.24855500
C	-0.94891400	-3.26035700	1.33005400
H	-0.31155600	-4.10271500	1.61766900
H	-1.60222400	-3.02733800	2.17666600
S	0.15468600	-1.81362900	1.03121500
C	0.15584700	-0.92738600	2.65625000
H	-0.82520300	-0.47272300	2.81529400
H	0.34258700	-1.66785500	3.44022300
C	1.24987400	0.10859500	2.59181000
C	2.59168100	-0.28043500	2.72079400
C	0.95495600	1.44696700	2.31137200
C	3.61792000	0.64770900	2.55572800
H	2.82700400	-1.32099400	2.93050000
C	1.98216800	2.37592500	2.13543000
H	-0.07704800	1.76136100	2.20485400
C	3.31436200	1.97833200	2.25198200
H	4.65265300	0.33127700	2.65191200
H	1.73356100	3.40230900	1.88442200
H	4.11352900	2.69900900	2.10465300
C	-3.25956800	0.73769000	1.26225900
C	-4.42578300	0.48639400	0.28483700
H	-3.66077100	1.08727500	2.22071700
H	-2.74045900	-0.20946200	1.45155800
C	-5.25765000	-0.74483400	0.65464900
H	-5.06436200	1.37840700	0.25269500
H	-4.02245500	0.36346200	-0.72681100
C	-6.40965900	-1.00310600	-0.32081300
H	-4.59606100	-1.62297400	0.68283500
H	-5.65091400	-0.62998000	1.67406400
H	-6.98521900	-1.89190000	-0.04178800
H	-7.09976300	-0.15235400	-0.34873100
H	-6.03347300	-1.15371100	-1.33973900
C	2.27266600	-1.64180300	-1.83488600
C	3.32551300	-1.86880400	-0.73081500
H	2.63628300	-2.05883300	-2.78292900
H	1.36681800	-2.17533200	-1.56040400
C	3.49408300	-3.34684400	-0.36984100
H	4.28825700	-1.44626500	-1.04649800

H	3.02093600	-1.31134700	0.16166500
C	4.52728500	-3.56609300	0.73928000
H	2.52154200	-3.74213900	-0.04643200
H	3.78022600	-3.91729500	-1.26460300
H	4.63143800	-4.62622700	0.99366500
H	5.51407500	-3.19516000	0.43907700
H	4.23791100	-3.02902700	1.64998800

²IM1

C	-3.07192800	-0.38059800	-2.57247000
C	-3.13370300	-1.76284900	-2.44704800
C	-2.11336200	-2.43394500	-1.75720100
C	-1.04054100	-1.65041600	-1.24997900
C	-1.99985600	0.33745300	-2.01439800
C	-2.10609800	-3.84758700	-1.51292000
C	0.01460300	-2.26167600	-0.52748000
C	-0.02433400	-3.65392100	-0.24941200
C	-1.11016700	-4.42963900	-0.78458900
C	0.98311900	-4.18620600	0.57079700
C	1.96549700	-3.32605500	1.07106800
C	1.96702400	-1.97149000	0.73528600
H	-2.92277600	-4.44555700	-1.90877200
H	-3.85829200	0.16723500	-3.08162800
H	-1.12443100	-5.49829700	-0.58682800
H	2.74926200	-3.70377900	1.72061400
N	-0.98621500	-0.28396800	-1.38653100
N	1.01621900	-1.42960200	-0.06992900
H	0.98303900	-5.24280500	0.82091700
H	-3.96718800	-2.32393100	-2.86118500
Ni	0.76736800	0.48320000	-0.61432000
C	1.68401300	1.95839100	-1.69729200
C	3.01875100	1.48034100	-2.29187500
H	1.01960900	2.16711800	-2.55000500
H	3.77580100	1.30947600	-1.51649600
H	2.90025300	0.53504700	-2.83377200
H	3.45855000	2.21379400	-2.99156700
C	1.88895800	3.28276300	-0.93307500
H	2.56690800	3.95525700	-1.48695500
H	0.93688600	3.82911200	-0.85260100
C	2.46687400	3.07741400	0.48946200
H	3.07292900	2.16473800	0.48726400
H	3.13849800	3.89984200	0.76901300
C	1.41687600	2.97614200	1.60333800
H	0.98825100	3.96007200	1.81778800
H	1.85869500	2.59084600	2.52809800
S	-0.00710300	1.87213200	1.16513300
C	-0.25035700	0.89921500	2.72396300
H	0.64858200	0.30575700	2.91101700
H	-0.38805500	1.61071800	3.54446800
C	-1.46201800	0.02489200	2.52722100
C	-2.74548800	0.59135200	2.52766100
C	-1.32386800	-1.34008700	2.25576800
C	-3.86466500	-0.18773700	2.23972000

H	-2.85994700	1.65291500	2.73180500
C	-2.44307100	-2.12118100	1.96228300
H	-0.33698900	-1.79083200	2.24925700
C	-3.71396800	-1.54611800	1.94633500
H	-4.85144600	0.26622500	2.23460600
H	-2.31363900	-3.17172200	1.72197400
H	-4.58304200	-2.15147100	1.70559500
C	3.07274700	-1.05842300	1.19533900
C	4.23632400	-1.02948600	0.18589800
H	3.44363700	-1.38418100	2.17489300
H	2.67158400	-0.04429200	1.31982600
C	5.35292500	-0.05587700	0.57456000
H	4.64723500	-2.04347900	0.09109000
H	3.83546100	-0.76189600	-0.79744800
C	6.48594600	-0.01979900	-0.45532100
H	4.93081200	0.95136900	0.68759400
H	5.75214100	-0.33267100	1.56035100
H	7.27535000	0.67917800	-0.16022200
H	6.94171700	-1.00953300	-0.57448900
H	6.10961700	0.29260700	-1.43558700
C	-2.00844900	1.84255900	-2.00988200
C	-2.90380500	2.38593200	-0.87701500
H	-2.36253900	2.22420000	-2.97597800
H	-0.98647800	2.19938200	-1.86750900
C	-2.70880900	3.88488600	-0.63627700
H	-3.95727500	2.17407900	-1.10550200
H	-2.67340100	1.84196300	0.04453300
C	-3.55855300	4.40626900	0.52596400
H	-1.64756000	4.06957600	-0.42389800
H	-2.94396700	4.44231300	-1.55337800
H	-3.40935200	5.47903500	0.68751000
H	-4.62665300	4.24060300	0.34273600
H	-3.29817200	3.88794500	1.45634800

²TS2

C	3.49927900	2.73677100	0.94223300
C	2.66032900	3.83027300	1.10789900
C	1.33891900	3.75107800	0.63823100
C	0.93803300	2.53952600	0.01354300
C	3.03452600	1.56588800	0.32275400
C	0.38697100	4.81932900	0.75576800
C	-0.38742500	2.40223900	-0.49184000
C	-1.31412300	3.46798900	-0.34886500
C	-0.88429700	4.68321500	0.28331100
C	-2.61858500	3.25472700	-0.82281400
C	-2.94212700	2.02176300	-1.37015700
C	-1.98075000	1.00278300	-1.47403100
H	0.70345100	5.74231000	1.23401700
H	4.52608600	2.77005100	1.29259800
H	-1.60064600	5.49439200	0.38168000
H	-3.95240500	1.82518900	-1.70989300
N	1.77005900	1.45989300	-0.13630100
N	-0.70577400	1.20032900	-1.07573200

H	-3.36280800	4.04172500	-0.73961300
H	3.01171900	4.73747800	1.59118600
C	-2.33402500	-0.35450900	-2.03480700
C	-3.71953000	-0.89630400	-1.63908400
H	-1.56795600	-1.05954000	-1.69977600
H	-2.26343500	-0.30303800	-3.12846500
C	-3.91703900	-1.03230500	-0.12618100
H	-4.51587600	-0.26986400	-2.06523400
H	-3.83573600	-1.88072600	-2.11099500
C	-5.27057300	-1.63665700	0.25096000
H	-3.11097200	-1.64868200	0.28338400
H	-3.80896000	-0.05183300	0.35004700
H	-5.37098400	-1.71763300	1.33809100
H	-6.10083600	-1.02231000	-0.11874900
H	-5.38972700	-2.64120100	-0.17221600
C	3.91958300	0.35534600	0.19829000
C	3.68163000	-0.64101400	1.35021300
H	4.97197400	0.66144700	0.18322700
H	3.70778100	-0.13397500	-0.75659000
C	4.33901000	-2.00310200	1.11159800
H	4.04918300	-0.20662600	2.28943700
H	2.60107700	-0.77531100	1.46347600
C	4.06447300	-2.99947000	2.24205800
H	3.96692900	-2.41261500	0.16296900
H	5.42237100	-1.87313100	0.98393900
H	4.54182500	-3.96623100	2.05149200
H	4.44064100	-2.62298500	3.20001400
H	2.98874100	-3.17434300	2.35799500
Ni	0.85469100	-0.03467700	-1.18527200
C	1.41252900	-0.68214700	-3.06063400
C	1.78236700	-1.67567600	-2.08699700
H	1.49745400	-1.27327300	-0.55073300
H	2.21213300	0.00194500	-3.35016700
C	0.37946100	-0.88649000	-4.14855800
H	-0.04869200	0.07227600	-4.46134500
H	0.81203900	-1.35540900	-5.04734500
H	-0.45238200	-1.51669900	-3.82778400
H	2.84919600	-1.72675600	-1.85670400
C	1.15502200	-3.06922000	-2.09387800
C	0.97543300	-3.74692700	-0.72512300
H	1.80374000	-3.70548000	-2.71311900
H	0.18553400	-3.04839100	-2.59829900
H	0.94120000	-4.83378700	-0.84448600
H	1.80864800	-3.51632000	-0.05447000
S	-0.59910800	-3.23320400	0.09926400
C	-0.00455600	-2.51641800	1.70218900
H	0.92689200	-1.99527300	1.47874900
H	0.19104700	-3.32965800	2.40767200
C	-1.02631800	-1.55210800	2.24565500
C	-2.12665300	-2.00792900	2.98279000
C	-0.90962700	-0.18072500	1.97946300
C	-3.09400000	-1.11143700	3.44165000
H	-2.22787500	-3.07027200	3.19088600
C	-1.87360500	0.71662900	2.43771500

H	-0.07040500	0.17102800	1.38856900
C	-2.97040300	0.25297000	3.16893700
H	-3.94287500	-1.47829700	4.01196600
H	-1.77118500	1.77433500	2.21142400
H	-3.72508500	0.94961200	3.52309600

²IM2

C	2.12833400	2.50412400	-2.26905100
C	1.29261300	3.61402800	-2.03036200
C	0.14247400	3.43411600	-1.26532000
C	-0.18852600	2.10843300	-0.84412200
C	1.78481100	1.24240100	-1.79540200
C	-0.71650300	4.51092900	-0.84648100
C	-1.31198500	1.88066800	-0.03698400
C	-2.10659100	2.97250000	0.43712400
C	-1.77942000	4.29363000	-0.02294700
C	-3.13192300	2.69058400	1.33694700
C	-3.33867700	1.36702400	1.74739600
C	-2.57632800	0.32518400	1.20236200
H	-0.47712100	5.51654600	-1.18301200
H	3.07824400	2.63266700	-2.77792800
H	-2.39834000	5.12281000	0.31072500
H	-4.10633800	1.12596600	2.47402500
N	0.60122600	1.00012800	-1.16715200
N	-1.60199200	0.56115800	0.29947800
H	-3.74624300	3.49650300	1.72941400
H	1.56446600	4.60384800	-2.38503600
C	-2.86133000	-1.09941000	1.61494600
C	-3.87721000	-1.82476500	0.70676500
H	-3.24461300	-1.09318700	2.64236300
H	-1.92146200	-1.65730600	1.61892200
C	-5.28619600	-1.22343700	0.70945100
H	-3.48677700	-1.82961100	-0.31669300
H	-3.93002200	-2.87551100	1.02327100
C	-6.24382300	-1.97998000	-0.21631100
H	-5.68270800	-1.22382300	1.73467300
H	-5.23271400	-0.17142500	0.40487700
H	-7.24681900	-1.54063600	-0.20602700
H	-5.88208500	-1.96187000	-1.25124900
H	-6.33591700	-3.03114200	0.08143400
C	2.80794800	0.12933600	-1.86186400
C	4.05134100	0.42294700	-0.99905000
H	3.12454600	-0.03929600	-2.90039500
H	2.35024700	-0.79362200	-1.50630200
C	5.11960100	-0.67249100	-1.10158400
H	4.48959100	1.38368700	-1.29335500
H	3.73644000	0.54387000	0.04598300
C	6.29768700	-0.44026600	-0.15116400
H	4.66832800	-1.65231500	-0.88944600
H	5.47904300	-0.72843900	-2.13815400
H	7.05734200	-1.22240900	-0.25132100
H	6.78023000	0.52300700	-0.35156100
H	5.96169500	-0.42926700	0.89201000

Ni	-0.53744200	-0.64512900	-0.84960400
C	-1.10375900	-1.03424000	-2.80860700
C	0.04321400	-1.75736400	-2.47380500
H	-1.48024100	-1.67622500	-0.58170900
H	-0.93125000	-0.07529000	-3.29872500
C	-2.50219200	-1.57006600	-2.98040600
H	-3.23718300	-0.87110900	-2.57066100
H	-2.72227400	-1.69366700	-4.04970000
H	-2.64353600	-2.53470700	-2.48900700
H	0.98443400	-1.32922600	-2.80420800
C	0.14464400	-3.21491300	-2.07862200
C	1.17921400	-3.41132500	-0.95435100
H	0.46701000	-3.82253500	-2.93744000
H	-0.82613400	-3.60289200	-1.75811700
H	1.27772000	-4.46561700	-0.68116800
H	2.16062200	-3.05085300	-1.28206800
S	0.68873200	-2.42699400	0.53456900
C	2.32106200	-1.99356700	1.28791400
H	2.95814800	-1.59872400	0.49464300
H	2.78581300	-2.89802800	1.69020300
C	2.09489000	-0.96647200	2.37121800
C	1.58908100	0.30224200	2.04568200
C	2.36049700	-1.26883100	3.71132800
C	1.35969100	1.24794700	3.04352700
H	1.34762900	0.53619400	1.01418300
C	2.13723300	-0.31844700	4.71034700
H	2.74285900	-2.25203300	3.97490300
C	1.63498900	0.94118100	4.37890900
H	0.95696400	2.21973000	2.77292900
H	2.35021700	-0.56556700	5.74660300
H	1.45506000	1.67781700	5.15676800

²Ts3

C	-1.76957000	-4.15084600	0.70893100
C	-3.07445600	-4.03294100	0.19903400
C	-3.49446800	-2.80351800	-0.30035700
C	-2.59818700	-1.69219600	-0.19691700
C	-0.93077900	-3.03620900	0.77283000
C	-4.76053400	-2.58798000	-0.94939000
C	-2.93270900	-0.45404400	-0.75778500
C	-4.15623100	-0.28012200	-1.47722000
C	-5.07317500	-1.38946100	-1.51560600
C	-4.36767100	0.93273500	-2.12714300
C	-3.36901000	1.92477400	-2.06861300
C	-2.21936500	1.72887300	-1.30393500
H	-5.45739800	-3.42080300	-1.00326900
H	-1.38274500	-5.11447800	1.02354600
H	-6.02111100	-1.25358600	-2.03030600
H	-3.48393600	2.85698700	-2.61052500
N	-1.34669200	-1.79803800	0.41384500
N	-2.00469500	0.57747800	-0.62190700
H	-5.27822500	1.09402200	-2.69722300
H	-3.73294300	-4.89571100	0.14818200

Ni	-0.70874800	0.08029000	0.75787400
C	0.13344400	-0.22363200	2.60117100
C	-0.75108100	0.86958500	2.70689100
H	-0.26419200	-1.19597700	2.87731700
H	-0.55455900	1.47382600	1.07523900
H	-1.79385400	0.62099000	2.91009500
C	1.64643200	-0.06375700	2.71605200
H	1.90952300	0.45994500	3.64639000
H	2.10435000	-1.05551700	2.78658800
C	2.30552100	0.69368400	1.55303600
H	1.99731800	1.74324400	1.54101400
H	3.39623300	0.65556500	1.62288200
C	-1.17568100	2.81580900	-1.20631100
C	-1.43352600	3.83599500	-0.07745200
H	-1.12344300	3.34922100	-2.16346900
H	-0.20604300	2.33766000	-1.04137000
C	-2.63845200	4.75525500	-0.30281800
H	-1.57274700	3.28741800	0.86037400
H	-0.53087600	4.44964500	0.05222600
C	-2.84075900	5.74399900	0.84952100
H	-2.50469100	5.30590900	-1.24459300
H	-3.53996100	4.14483900	-0.42948300
H	-3.70367600	6.39493900	0.67505900
H	-3.00977400	5.21476000	1.79493200
H	-1.96055500	6.38403200	0.98282600
C	0.52609000	-3.23473100	1.10656700
C	1.34135900	-3.57989200	-0.15627300
H	0.63996800	-4.03604400	1.84680900
H	0.93779700	-2.32597200	1.53921800
C	2.84818000	-3.64862900	0.11018700
H	0.98498500	-4.53218100	-0.57006000
H	1.14144800	-2.81457300	-0.91565400
C	3.65896700	-3.93101600	-1.15790400
H	3.17374200	-2.69335400	0.54116400
H	3.05397900	-4.42151700	0.86384400
H	4.73399200	-3.96281700	-0.95122300
H	3.37440700	-4.88920600	-1.60765800
H	3.48556000	-3.15149200	-1.90926000
C	-0.36676100	2.23675900	3.24404000
H	-0.36912900	2.18895000	4.34088400
H	-1.08366300	3.00537100	2.94631400
H	0.62587500	2.56006900	2.92658100
S	1.76224200	-0.04626900	-0.03766600
C	2.50969900	1.16644600	-1.20907800
H	2.13563200	0.85924400	-2.19037400
H	2.10339600	2.15953600	-0.99324000
C	4.01564500	1.16378900	-1.16249500
C	4.71425700	2.22196000	-0.56951200
C	4.74053000	0.07773900	-1.67532900
C	6.10941200	2.20134900	-0.49443000
H	4.16239200	3.06857700	-0.16802600
C	6.13119100	0.05520100	-1.60262600
H	4.20426400	-0.75613900	-2.12038600
C	6.82102000	1.11846400	-1.01092700

H	6.63735600	3.03120400	-0.03320100
H	6.67861300	-0.79166300	-2.00650800
H	7.90547400	1.10053300	-0.95388800

³IM3

Ni	0.48067700	-0.04393500	0.15229700
C	2.26635700	-3.65902600	-1.41954900
C	3.23579000	0.23851500	-0.35756800
C	4.58963400	0.67487200	-0.29843300
C	4.82634400	2.00793100	0.06295100
C	3.74573900	2.83753500	0.34386600
C	2.43472100	2.34329100	0.27468500
N	2.17652500	1.06484200	-0.06049200
H	5.84538500	2.38055100	0.12081900
H	3.90038700	3.87628200	0.61751300
C	2.92761800	-1.09985200	-0.71122500
C	3.97456000	-2.01192200	-1.01625900
C	3.62096200	-3.32110700	-1.37091200
C	1.28107400	-2.72566100	-1.09891800
N	1.58927300	-1.45355000	-0.72296800
H	4.38958800	-4.04813500	-1.61503500
H	1.96168000	-4.65772400	-1.71648200
C	-0.17647900	-3.10489500	-1.15175400
C	-0.81062100	-3.31711900	0.23597100
H	-0.28563700	-4.02247700	-1.74108700
H	-0.72500900	-2.31815300	-1.68529800
C	-2.23872400	-3.86999800	0.16974400
H	-0.18062300	-4.00204000	0.81787900
H	-0.79982700	-2.36737900	0.78217000
C	-2.89013800	-3.98592800	1.55148400
H	-2.85742700	-3.22984800	-0.47373900
H	-2.22354000	-4.85418300	-0.31767400
H	-3.90776200	-4.38479600	1.48541000
H	-2.31100800	-4.64814100	2.20464500
H	-2.94139800	-3.00917600	2.04624600
C	-2.19389800	1.32085400	1.23522800
H	-3.28492600	1.39307800	1.21442900
H	-1.79772900	2.28914200	1.55778600
C	-1.67733000	0.19946000	2.13900300
H	-2.04889700	0.41482000	3.15771300
H	-2.16313200	-0.74419300	1.84987400
C	0.34948500	-1.04930900	3.02639400
H	-0.10989000	-2.01183200	2.76016200
H	0.02860000	-0.85288500	4.06639600
C	5.62999200	-0.26442400	-0.60590200
H	6.66206000	0.07257200	-0.55784500
C	5.33393300	-1.54918600	-0.94962000
H	6.12731100	-2.25485300	-1.18152700
C	-2.64123500	-0.25744200	-1.09111700
H	-2.32174400	-1.14461900	-0.54710900
H	-2.35089800	-0.38145000	-2.13829100
C	-0.28443000	5.99309200	0.23623600
H	-1.18447900	6.61564600	0.27114000
H	-0.02847700	5.73171500	1.26847500

H	0.53155300	6.60843500	-0.16126800
C	1.26175000	3.25637300	0.51014100
H	1.55576900	4.04926000	1.20528500
H	0.46177900	2.68353900	0.98666800
C	0.74305900	3.87232600	-0.80595400
H	0.52050100	3.05546100	-1.50143100
H	1.54735300	4.46552400	-1.26216900
C	-0.50638300	4.74759400	-0.62986200
H	-1.31450200	4.13932900	-0.20375500
H	-0.85597200	5.05647200	-1.62307900
C	-0.15285500	0.05155400	2.08717500
H	0.27778100	1.00168600	2.45221400
C	1.87363600	-1.20787500	3.00019700
H	2.22177100	-1.94636800	3.73170500
H	2.20965600	-1.52203200	2.00683900
H	2.36673000	-0.25396900	3.22367900
S	-1.60885000	1.16817000	-0.51212600
C	-4.12166100	-0.03924100	-0.94148400
C	-4.80313700	0.86485600	-1.76842400
C	-4.83799700	-0.72716800	0.04628100
C	-6.17283000	1.07000300	-1.61560900
H	-4.25017500	1.41172900	-2.52776900
C	-6.21104200	-0.52210200	0.20121500
H	-4.31807200	-1.42751500	0.69419900
C	-6.88129700	0.37628300	-0.62931400
H	-6.68985300	1.77018100	-2.26554700
H	-6.75349700	-1.06383800	0.97072700
H	-7.94893500	0.53688300	-0.51093800

²PR2

C	2.23877600	3.58973400	-0.74020800
C	3.78717100	-0.26039800	-0.49928100
C	5.16783700	-0.51585000	-0.70587700
C	5.59475400	-1.85286700	-0.61785200
C	4.66508500	-2.84711900	-0.33512500
N	2.88625200	-1.24727300	-0.20632600
H	6.64198900	-2.09743900	-0.77109800
H	4.97208700	-3.88512800	-0.25929700
C	3.27754700	1.06634500	-0.59788600
C	4.16194100	2.14384100	-0.85513900
C	3.60645600	3.43643000	-0.90517800
C	1.40859100	2.47094000	-0.54084700
N	1.91890300	1.22861900	-0.45052000
H	4.24856600	4.29580600	-1.07653300
H	1.78310500	4.57364300	-0.77835100
C	-0.08583800	2.64115700	-0.47675800
C	-0.68794100	3.11717700	-1.81254100
H	-0.33692200	3.35858500	0.31378100
H	-0.53920600	1.68682600	-0.20055300
C	-2.21806300	3.15355000	-1.76063600
H	-0.29535300	4.10987300	-2.07043800
H	-0.36011700	2.44150100	-2.61215200
C	-2.85793300	3.48412600	-3.11057000

H	-2.58659300	2.18176300	-1.41657700
H	-2.53755500	3.88350900	-1.00393500
H	-3.95078700	3.49888900	-3.03929800
H	-2.53350300	4.46310800	-3.48214400
H	-2.58424100	2.73604700	-3.86360300
C	6.03923300	0.59082500	-0.98200300
H	7.09617900	0.39152500	-1.13612300
C	5.55824300	1.86588400	-1.04363700
H	6.22660700	2.69852400	-1.24516200
C	0.22920800	-4.26569800	3.49948600
H	-0.62603800	-4.91351100	3.71401900
H	1.03524000	-4.52454800	4.19604000
H	-0.07591400	-3.23569600	3.71602700
C	2.28107600	-3.55566700	0.22873900
H	2.66120500	-4.55884100	0.00729100
H	1.39836200	-3.39274600	-0.40193700
C	1.85343900	-3.46906600	1.70811600
H	1.56377800	-2.43454600	1.92787800
H	2.71583400	-3.69579700	2.34977900
C	0.68568300	-4.40172800	2.04422200
H	0.97568300	-5.44178200	1.84114000
H	-0.15399900	-4.17358800	1.37754000
C	-0.15357700	-1.32051200	-1.67320300
H	-0.50910800	-2.27063300	-1.23428600
C	-1.39236200	-0.47252700	-1.97548100
C	-2.38617400	-1.06677900	-2.99111000
H	-1.08437000	0.50073700	-2.37421000
H	-1.93630100	-0.26436500	-1.04639900
H	-3.14974100	-0.33120700	-3.26612300
H	-1.87328000	-1.35570300	-3.91267700
C	1.28462700	-0.42678400	-3.62294400
H	1.86842600	0.18290200	-2.92569800
H	1.93440600	-0.71773800	-4.45602500
C	0.70344800	-1.65268400	-2.90520100
H	0.14375000	-2.25278800	-3.64384000
H	1.53765000	-2.29241000	-2.58727800
C	3.31485400	-2.52187900	-0.13092300
H	0.49369200	0.21196300	-4.03244200
S	-3.26973800	-2.57100700	-2.38733900
C	-4.93139500	-1.84657100	-2.01977900
H	-5.38674300	-1.52238000	-2.96078300
H	-5.51261700	-2.69512400	-1.64575400
C	-4.92582300	-0.71995500	-1.01827000
C	-4.70983500	-0.97479700	0.34403100
C	-5.13201500	0.60267900	-1.42887500
C	-4.70963600	0.06623900	1.27104400
H	-4.53201200	-1.99226000	0.67877700
C	-5.12005700	1.65043500	-0.50334200
H	-5.30754600	0.81569300	-2.48056800
C	-4.90663600	1.38565200	0.84895600
H	-4.55682700	-0.15752200	2.32152100
H	-5.27667200	2.67041100	-0.84282900
H	-4.90185800	2.19741400	1.57111100
C	-0.83637600	0.28586300	2.32179300

C	-2.07624500	-1.54065700	2.37122200
O	-2.91627700	-2.33799900	2.66149200
O	-1.96494600	-0.26564500	2.87319500
O	-1.04886900	-1.72065700	1.50477400
N	-0.26417700	-0.52105800	1.45458700
C	-0.39776600	1.58632200	2.75302400
C	-1.30676100	2.46849500	3.37603900
C	0.93929600	1.98852600	2.55323000
C	-0.88488900	3.73679100	3.75759800
H	-2.33220900	2.15399500	3.53756700
C	1.34671700	3.25765800	2.94515300
H	1.63513200	1.30249600	2.08465100
C	0.43812200	4.14127900	3.53979800
H	-1.59036800	4.41685100	4.22574700
H	2.37624400	3.56058400	2.78031200
H	0.75843500	5.13575500	3.83499900
Ni	0.97344800	-0.56659300	-0.18833100

²Ni

C	3.73414100	0.16890800	-0.28493000
C	5.11924500	0.41694600	-0.14632200
C	5.49326700	1.72682900	0.22999200
H	6.54514300	1.97231100	0.34948600
C	4.51789400	2.67524300	0.44245400
H	4.78161900	3.68637000	0.73334700
C	3.14473800	2.34983400	0.29262800
C	3.28432400	-1.14272700	-0.66663900
C	4.22913700	-2.16268400	-0.92081300
C	3.71763900	-3.41480300	-1.33178200
C	1.47182300	-2.50422400	-1.21564700
C	2.35936300	-3.57457000	-1.49062800
H	4.40189400	-4.23396100	-1.53579100
H	1.94789600	-4.51849200	-1.82944500
N	1.93913400	-1.32951500	-0.78016700
N	2.78210300	1.11458800	-0.07250600
C	-1.23648500	2.22350100	0.33695300
O	-0.93144700	2.71174500	1.45526200
C	0.45413100	-0.15128200	1.79275700
H	-0.09725800	0.71004200	2.17294000
Ni	0.84129300	0.30350400	-0.12557900
N	-0.60657500	1.23671300	-0.29796300
C	2.07814100	3.37869600	0.51892800
C	1.49200100	3.92635000	-0.80270100
H	2.50129200	4.20595800	1.10072700
H	1.25309100	2.94397200	1.09780400
C	0.49549800	5.06584500	-0.55028400
H	2.30256300	4.27561800	-1.45865800
H	0.98535600	3.10180400	-1.31545800
C	-0.25619300	5.48030800	-1.81834800
H	-0.21885400	4.74261700	0.21315100
H	1.03433400	5.92949900	-0.13476500
H	-0.94592100	6.30647400	-1.61720300
H	0.43458200	5.80244300	-2.60752400

H	-0.84988600	4.64550800	-2.20475800
C	-0.00998700	-2.65974800	-1.43321400
C	-0.66031600	-3.83104800	-0.64902700
H	-0.17434400	-2.81266100	-2.50871900
H	-0.50032400	-1.71578900	-1.19062300
C	-1.00855700	-5.04881000	-1.51218100
H	-0.00319900	-4.13909700	0.17388600
H	-1.57961000	-3.46497900	-0.18461900
C	-1.67596000	-6.16230200	-0.70153600
H	-1.68307900	-4.72276500	-2.31414200
H	-0.10812200	-5.43915800	-2.00723100
H	-1.93673100	-7.01941600	-1.33090800
H	-1.01610400	-6.52103600	0.09704500
H	-2.59469900	-5.79451500	-0.23228500
C	-2.41226100	2.82229800	-0.41473500
C	-2.73488000	2.44398500	-1.72585900
C	-3.18437200	3.80100500	0.22249000
C	-3.81189600	3.03410700	-2.38740800
H	-2.12416300	1.69239400	-2.21512700
C	-4.26267200	4.39010500	-0.43735600
H	-2.91200600	4.08091900	1.23451200
C	-4.57938700	4.00903000	-1.74410900
H	-4.05213800	2.73621600	-3.40478400
H	-4.85727000	5.14786700	0.06634100
H	-5.41827700	4.46984700	-2.25896900
C	6.05367600	-0.64282700	-0.38877700
C	5.62656700	-1.88360900	-0.76334400
H	7.11361700	-0.43522700	-0.27281100
H	6.33933700	-2.68080700	-0.95343900
C	-0.41206400	-1.41158600	1.77627000
C	-1.41092100	-1.53714200	2.94505500
H	0.23369700	-2.30229000	1.76994800
H	-1.00779500	-1.45277100	0.86399600
H	-1.87023700	-2.53248600	2.94374500
H	-0.91756100	-1.40800100	3.90997800
C	1.79921800	-0.29045300	2.50257400
H	2.33793400	0.65913100	2.42841100
S	-2.77508700	-0.29722200	2.90771500
C	-4.11627300	-1.27873700	2.12171800
H	-4.35557400	-2.13408000	2.76308500
H	-4.97823500	-0.60209500	2.16330100
C	-3.90952000	-1.74331400	0.69284000
C	-3.35439400	-0.90299200	-0.28246200
C	-4.34811100	-3.01888600	0.31068200
C	-3.25965700	-1.32441300	-1.60840400
H	-2.96957700	0.07013600	-0.00177100
C	-4.25902000	-3.44006800	-1.01915400
H	-4.77487000	-3.68431500	1.05785100
C	-3.71601100	-2.59082400	-1.98514700
H	-2.82571400	-0.65409100	-2.34416400
H	-4.61008100	-4.43012000	-1.29686500
H	-3.64589100	-2.91422000	-3.02007300
H	2.42023400	-1.04393800	1.99840000
C	1.69391400	-0.66702700	3.99279700

H	1.05238100	0.03922000	4.53051200
H	1.27926000	-1.67113300	4.12716900
H	2.68274000	-0.65339900	4.46564900

²TSS

C	-3.66737200	0.83344900	-0.18856100
C	-5.06811900	0.96506000	-0.04752400
C	-5.77312100	-0.18575400	0.36940400
H	-6.85105600	-0.13968000	0.49913800
C	-5.08331200	-1.35782500	0.59417200
H	-5.60616100	-2.25719800	0.90155600
C	-3.67665000	-1.41455400	0.42996800
C	-2.88881700	1.95171600	-0.64214000
C	-3.52947200	3.17125800	-0.95742200
C	-2.71113100	4.20763400	-1.45950200
C	-0.78775200	2.73456400	-1.28440000
C	-1.36297500	3.98073000	-1.63372400
H	-3.15337400	5.16511500	-1.72088300
H	-0.72208700	4.75222300	-2.04426400
N	-1.54561500	1.75138600	-0.77912600
N	-2.99532500	-0.32220800	0.05942800
C	-2.92458900	-2.69934400	0.61833700
C	-2.49147500	-3.32534400	-0.72777600
H	-3.55885400	-3.40811700	1.16291200
H	-2.01845500	-2.53458700	1.21451900
C	-1.87362600	-4.71676600	-0.53983900
H	-3.35372700	-3.38745000	-1.40717500
H	-1.76096300	-2.65542900	-1.19608600
C	-1.30029700	-5.28493600	-1.84114300
H	-1.08475500	-4.64854800	0.21565100
H	-2.63969400	-5.39702700	-0.14052700
H	-0.87560600	-6.28167300	-1.68387000
H	-2.07159600	-5.36634100	-2.61722600
H	-0.49901900	-4.64458000	-2.22330900
C	0.68558500	2.48255000	-1.47249200
C	1.60387700	3.40335100	-0.62415600
H	0.92880400	2.61603300	-2.53504800
H	0.88844100	1.43459300	-1.24354500
C	2.19289300	4.59693200	-1.38383400
H	1.05793700	3.75981400	0.25790400
H	2.43304800	2.80030200	-0.24668800
C	3.11367200	5.44332700	-0.50053100
H	2.75742000	4.21568000	-2.24447400
H	1.39373100	5.22986200	-1.79282800
H	3.54869100	6.28073100	-1.05580200
H	2.56866400	5.85600900	0.35641000
H	3.93416100	4.83255600	-0.10924600
C	-5.68705600	2.22513400	-0.33972800
C	-4.94808600	3.28543800	-0.77851200
H	-6.76241100	2.31540700	-0.21495000
H	-5.42471000	4.23349900	-1.01072200
C	0.58271300	-2.42281900	0.48824800
O	0.14835600	-2.98492400	1.52154800
C	-0.05958400	-0.06172100	1.90964200

H	0.41844200	-0.94295000	2.32567400
Ni	-0.95852400	-0.06282900	-0.05933000
N	0.41258200	-1.15351600	0.10819500
C	-1.36931300	0.16851400	2.67479200
C	-1.13956700	0.39050600	4.18299400
H	-2.00722500	-0.70998200	2.55416200
H	-1.92378300	1.02584800	2.27166700
H	-2.09661700	0.41322700	4.71650500
H	-0.53346800	-0.41589600	4.60948600
H	-0.63159600	1.33978500	4.38014000
C	0.89823300	1.12039800	1.82674000
C	1.96286300	1.17100000	2.94082800
H	0.33059500	2.06202100	1.84247300
H	1.43248900	1.08437200	0.87864300
H	2.56084000	2.08478400	2.84810400
H	1.50325300	1.18317100	3.93111300
S	3.12587400	-0.26000100	2.95242500
C	4.56501900	0.43203300	2.04437600
H	5.31448100	-0.36479400	2.12309600
H	4.95713000	1.28701400	2.60590400
C	4.38159900	0.81099100	0.58716700
C	3.62321700	0.03158400	-0.29744100
C	5.05298400	1.93635200	0.08743700
C	3.55310100	0.36729000	-1.64986000
H	3.06105100	-0.81894300	0.07208800
C	4.98637600	2.27011300	-1.26755700
H	5.64164900	2.55226400	0.76376500
C	4.23498200	1.48321500	-2.14232000
H	2.96351400	-0.25443100	-2.31562100
H	5.51516900	3.14539200	-1.63462700
H	4.17918100	1.73858300	-3.19693500
C	1.42037800	-3.23917900	-0.48225300
C	1.67639700	-2.81572600	-1.79405000
C	1.91378900	-4.47843500	-0.05701700
C	2.42003800	-3.61507800	-2.66276700
H	1.26872200	-1.86477000	-2.11960200
C	2.66134900	-5.27591400	-0.92341700
H	1.68824100	-4.79524900	0.95560900
C	2.91686400	-4.84716200	-2.22861600
H	2.60710300	-3.28087800	-3.68004900
H	3.04267100	-6.23485600	-0.58245600
H	3.49438700	-5.47139200	-2.90515900

²IM4

C	-3.79819100	-0.82780100	-0.16853100
C	-5.17455800	-0.99172400	-0.44190000
C	-5.79843500	0.03602800	-1.18430600
H	-6.85472900	-0.03954600	-1.42755600
C	-5.05737600	1.13011500	-1.58515900
H	-5.51869400	1.93582000	-2.14659200
C	-3.68151600	1.22138200	-1.26897700
C	-3.09506900	-1.81927800	0.59627100
C	-3.78238100	-2.95536500	1.07886300

C	-3.03005700	-3.87357500	1.84469500
C	-1.07617400	-2.45927100	1.56851500
C	-1.69486800	-3.61971600	2.08873800
H	-3.50777900	-4.76645400	2.23849900
H	-1.09801200	-4.30677300	2.67880400
N	-1.77332300	-1.58818100	0.82543800
N	-3.07388700	0.24500600	-0.58307100
C	1.17770500	1.92255400	-0.38002400
O	2.18346500	2.40711500	-0.94605800
C	0.91892900	0.48771000	-2.23153100
H	1.18341800	1.37511100	-2.82368900
Ni	-1.10348000	0.03614800	-0.15980000
N	0.40001400	0.95708400	-0.92518400
C	-2.85353600	2.42535400	-1.62244000
C	-2.62732800	3.33621300	-0.39721500
H	-3.33349200	2.98918200	-2.42991100
H	-1.87358600	2.08570200	-1.97395900
C	-1.64126700	4.47202900	-0.68230400
H	-3.58994400	3.74477600	-0.05922300
H	-2.23552100	2.72245000	0.42202400
C	-1.43391400	5.37697000	0.53545000
H	-0.68096900	4.03698000	-0.98425800
H	-1.99936800	5.06581900	-1.53499600
H	-0.70522300	6.16600000	0.32421000
H	-2.37305200	5.85793600	0.83465800
H	-1.06040200	4.80137700	1.38758700
C	0.38493700	-2.16689600	1.77228500
C	1.22343300	-2.50759800	0.52241500
H	0.76275600	-2.71979100	2.63923300
H	0.50101000	-1.10010900	1.98909500
C	1.43968600	-4.00446900	0.29326700
H	0.73445800	-2.06137100	-0.35007100
H	2.19217100	-2.01313300	0.61741100
C	2.23941100	-4.27123500	-0.98627400
H	1.97241400	-4.42483100	1.15804000
H	0.47239800	-4.52446500	0.24359500
H	2.44186500	-5.33881300	-1.12218600
H	1.69270100	-3.91839600	-1.86817200
H	3.19693800	-3.73986500	-0.96543900
C	0.86050600	2.45467900	1.00994700
C	-0.05796200	1.89256100	1.90624000
C	1.59624000	3.57045800	1.43913400
C	-0.24609800	2.42500900	3.18255400
H	-0.64203600	1.01980300	1.61120300
C	1.41569900	4.10718900	2.71296200
H	2.31410100	3.99497000	0.74664200
C	0.49263000	3.53672600	3.59321000
H	-0.96543800	1.96596200	3.85571800
H	1.99611100	4.97293500	3.01978300
H	0.35170600	3.95193200	4.58729300
C	-5.84543000	-2.16366500	0.04563100
C	-5.17795300	-3.10464400	0.77576300
H	-6.90204800	-2.28523000	-0.17532600
H	-5.69615400	-3.98508900	1.14496300

C	2.20879800	-0.36200200	-2.03138200
C	3.41909400	0.14877500	-2.81084900
H	2.02768900	-1.41117900	-2.29286800
H	2.45288300	-0.35078200	-0.97127700
H	3.29199000	0.01357700	-3.89045500
C	-0.15533500	-0.28435100	-3.01233600
H	-1.07699100	0.30917400	-3.03760900
H	-0.40317300	-1.21216200	-2.47675200
C	0.27248400	-0.61658800	-4.44609000
H	1.16367900	-1.25250000	-4.46499000
H	-0.52133400	-1.14588700	-4.98350300
H	0.50644600	0.29609700	-5.00615900
H	3.55318900	1.21589300	-2.61530400
S	4.99041400	-0.72025800	-2.39893300
C	5.46030100	0.12990600	-0.82434400
H	5.30692200	1.20243800	-0.97216900
H	6.53891300	-0.04219300	-0.74731400
C	4.77389300	-0.33157200	0.44126100
C	5.03295200	-1.60103600	0.97845600
C	3.89544000	0.52181200	1.12145300
C	4.44177200	-2.00107700	2.17709600
H	5.70217000	-2.27531000	0.44979300
C	3.29361800	0.12035300	2.31736900
H	3.66023300	1.49176700	0.69561100
C	3.57282000	-1.13815800	2.85376400
H	4.65866300	-2.98520600	2.58401400
H	2.60652600	0.79540000	2.81925700
H	3.11265300	-1.44915500	3.78779200

²IM5

C	2.69263000	2.33359000	0.53692800
C	3.73685500	2.76951400	1.38626900
C	3.37343100	3.61796000	2.45573400
H	4.13674300	3.97978000	3.13930000
C	2.05454300	3.99647900	2.60311700
H	1.75735300	4.66787400	3.40196800
C	1.06354100	3.50401300	1.72128600
C	2.99675900	1.53098000	-0.62033200
C	4.34274100	1.20772900	-0.90541600
C	4.59143600	0.51825300	-2.11184900
C	2.21677700	0.61089800	-2.60686700
C	3.54219600	0.26152300	-2.96427100
H	5.60753700	0.23605900	-2.37413000
H	3.71116600	-0.21562100	-3.92326300
N	1.95112700	1.17647300	-1.42369200
N	1.38903800	2.66639700	0.72908900
C	-2.62081900	1.09685900	0.57161300
O	-3.58125100	0.85790800	1.34331600
C	-1.17519800	0.16113700	2.16745200
H	-1.79425600	0.69726500	2.90198400
Ni	0.26700100	1.24941100	-0.25307600
N	-1.32681600	0.84706200	0.86058400
C	-0.38641000	3.87676800	1.86969100

C	-0.98329000	4.51890200	0.60505600
H	-0.50484500	4.54710700	2.72826100
H	-0.95093600	2.96059700	2.07580400
C	-2.47165100	4.84344600	0.76217200
H	-0.42456100	5.43151200	0.35394500
H	-0.85235300	3.82434200	-0.23241700
C	-3.06788200	5.44533900	-0.51310700
H	-3.01138400	3.92495500	1.02211500
H	-2.61014600	5.53637100	1.60417300
H	-4.13568600	5.65564900	-0.39436100
H	-2.56701300	6.38454700	-0.77749000
H	-2.95953000	4.75345400	-1.35396400
C	1.10093800	0.41128600	-3.60554300
C	0.43356200	-0.98198100	-3.63535200
H	1.52030200	0.62350200	-4.59731900
H	0.33640700	1.16915500	-3.41354300
C	1.41082200	-2.16095800	-3.70977100
H	-0.18450900	-1.09034300	-2.74561300
H	-0.24125500	-1.00625200	-4.50123400
C	0.69416800	-3.51383300	-3.65792600
H	2.01256400	-2.09196300	-4.62762700
H	2.11134500	-2.10076300	-2.86971100
H	1.40226200	-4.34685200	-3.72708500
H	0.14120100	-3.61766500	-2.71883400
H	-0.02570700	-3.62033400	-4.47798800
C	-2.97246000	1.67543700	-0.78822200
C	-2.10295600	1.72291500	-1.88441200
C	-4.28907100	2.12230700	-0.97486500
C	-2.51829700	2.21605600	-3.12162900
H	-1.08527500	1.34656400	-1.78237600
C	-4.71427100	2.61431900	-2.20819300
H	-4.96397200	2.06149800	-0.12847000
C	-3.83015600	2.66518800	-3.28943100
H	-1.82211300	2.23700700	-3.95628500
H	-5.73780300	2.95904000	-2.32724000
H	-4.16033900	3.04559600	-4.25208500
C	5.08367300	2.36163400	1.10905600
C	5.37448200	1.61338600	0.00545300
H	5.87223500	2.67985600	1.78522000
H	6.39929500	1.32699400	-0.21399900
C	-1.70893900	-1.30023100	2.09071500
C	-2.75579500	-1.61284500	3.16082000
H	-0.89433200	-2.02967300	2.14158800
H	-2.18829200	-1.42607900	1.12152500
H	-2.31465800	-1.60837300	4.16343100
C	0.27443400	0.20637400	2.67071900
H	0.59669100	1.24662500	2.74533800
H	0.92942400	-0.25908200	1.92559500
C	0.47994000	-0.47216600	4.02911300
H	0.26084100	-1.54383800	3.98903400
H	1.51592800	-0.35956600	4.36800600
H	-0.16900500	-0.02884800	4.79324000
H	-3.53684000	-0.84870800	3.12524300
S	-3.54738600	-3.26644500	3.00012600

C	-4.64996400	-2.97691600	1.54664000
H	-5.24219500	-2.07885600	1.74410800
H	-5.33236700	-3.83380400	1.56027900
C	-3.96444900	-2.86995800	0.20199500
C	-3.16284300	-3.91341700	-0.28241100
C	-4.10447800	-1.70967900	-0.57019500
C	-2.51843600	-3.80092600	-1.51327800
H	-3.02484700	-4.80210600	0.32712100
C	-3.45842100	-1.59392400	-1.80443700
H	-4.66254500	-0.86722600	-0.17418400
C	-2.66609400	-2.64005100	-2.28054000
H	-1.90058800	-4.61789100	-1.87630600
H	-3.56241100	-0.67946200	-2.37914200
H	-2.16140200	-2.55200500	-3.23724000
O	1.01789500	-2.98701400	0.84164300
O	2.47746900	-1.71391300	-0.40774100
C	3.30356600	-2.50588200	0.48781900
C	2.31025100	-3.64800500	0.93575000
B	1.16853600	-1.96132000	-0.05709000
O	0.15919500	-1.21533100	-0.57885400
H	-0.72620400	-1.42832300	-0.25194600
C	4.52776500	-2.97950000	-0.28875100
H	5.13367200	-2.11409900	-0.57186300
H	5.14254400	-3.64534000	0.32522500
H	4.24367200	-3.50429700	-1.20252800
C	3.72643500	-1.59108800	1.64327400
H	4.40342800	-2.10657900	2.33059900
H	4.24103100	-0.71646800	1.23862800
H	2.85874300	-1.24136000	2.20723900
C	2.49349300	-4.14094600	2.36626700
H	1.75038700	-4.91227400	2.58550500
H	3.48982700	-4.57426300	2.50119500
H	2.35954300	-3.33115800	3.08513300
C	2.26986900	-4.82524300	-0.04420600
H	3.18592200	-5.42113800	0.00126900
H	1.42234900	-5.46608700	0.21173500
H	2.12999000	-4.47362500	-1.07040800

²[Ni]OBpin

C	-2.81158100	-1.08073000	0.42363000
C	-3.81392600	-1.84709000	1.05744600
C	-3.42392800	-3.11352000	1.54690900
H	-4.15364100	-3.75029100	2.03964200
C	-2.11197400	-3.52246200	1.40149100
H	-1.78886800	-4.48662700	1.77998100
C	-1.16152400	-2.69047200	0.76423400
C	-3.12015400	0.22378500	-0.08561400
C	-4.42382700	0.74906100	0.04994000
C	-4.63625200	2.04919400	-0.45958400
C	-2.30753900	2.13263200	-1.14740200
C	-3.58516900	2.72921600	-1.04616500
H	-5.61939200	2.50544400	-0.38314400
H	-3.72487900	3.73206100	-1.43566400

N	-2.09604100	0.89647700	-0.67596500
N	-1.52540100	-1.49735800	0.27371500
Ni	-0.40726600	-0.16832100	-0.73594900
C	0.27754600	-3.09334800	0.59423500
C	0.62260300	-3.49645300	-0.85538900
H	0.50920000	-3.92064800	1.27509800
H	0.91552100	-2.24421100	0.86795600
C	2.12126300	-3.76224700	-1.03133000
H	0.03662200	-4.37979900	-1.14631600
H	0.33012000	-2.67790600	-1.52360900
C	2.49319900	-4.06483800	-2.48531900
H	2.66532600	-2.87668800	-0.68548800
H	2.42463800	-4.59844600	-0.38478000
H	3.56612100	-4.25778400	-2.59119000
H	1.95684100	-4.94391200	-2.86295000
H	2.24111000	-3.21563600	-3.13009400
C	-1.12195100	2.84922700	-1.74109400
C	-0.11132400	3.32057700	-0.67049000
H	-1.47093200	3.70678000	-2.32749400
H	-0.60545000	2.16037200	-2.41905000
C	-0.68353800	4.34231400	0.31641700
H	0.26198600	2.44224400	-0.13157000
H	0.75982500	3.74133400	-1.18567800
C	0.34613000	4.78835500	1.35900000
H	-1.05558400	5.21698300	-0.23629300
H	-1.55599400	3.91213400	0.82682700
H	-0.07454400	5.52343200	2.05326400
H	0.70222900	3.93473700	1.94559700
H	1.22050300	5.24223500	0.87866800
C	-5.13657700	-1.29835300	1.17003700
C	-5.42881500	-0.05391000	0.68879200
H	-5.90464300	-1.89490500	1.65428100
H	-6.43197100	0.35183900	0.78495600
O	2.75570500	-0.64297600	0.40320300
O	3.16127200	1.36291300	-0.66262000
C	3.98584500	1.34731700	0.51523300
C	4.03773100	-0.18551200	0.86912400
B	2.32741100	0.23585700	-0.61982400
O	1.29296600	0.01581900	-1.41652300
C	5.33636600	1.97981200	0.18847100
H	5.20061900	3.04123200	-0.03970700
H	6.02253500	1.89759800	1.03848300
H	5.79501600	1.50681400	-0.68159900
C	3.25956500	2.17533600	1.58609200
H	3.84719700	2.27223000	2.50435600
H	3.06822600	3.17458400	1.18653000
H	2.29548000	1.71994200	1.83238700
C	4.16758900	-0.50294300	2.35682600
H	4.19061600	-1.58749900	2.50110400
H	5.09320500	-0.08483600	2.76704000
H	3.32193300	-0.10649100	2.92181400
C	5.11158100	-0.93951000	0.07147300
H	6.12300100	-0.68679700	0.40466700
H	4.96049700	-2.01464600	0.20425400

H 5.02646300 -0.71369900 -0.99509200

²TS6

C -3.64276600 -0.79245100 -0.43196500
C -4.79315700 -1.56229000 -0.71436000
C -4.57792700 -2.90599400 -1.09521400
H -5.42746300 -3.54282300 -1.32657500
C -3.28852900 -3.39409000 -1.16666900
H -3.10063500 -4.42265900 -1.45648200
C -2.18610100 -2.56201400 -0.85858000
C -3.77563500 0.58552200 -0.04682600
C -5.05966200 1.16328000 0.05845500
C -5.11388700 2.51971200 0.44768800
C -2.68467100 2.55991900 0.55549900
C -3.93871200 3.20050300 0.69394600
H -6.07582500 3.01427900 0.55053100
H -3.95972500 4.24228700 0.99561100
N -2.62058400 1.26953900 0.19563400
N -2.37793500 -1.28601500 -0.50236600
C -0.76516600 -3.04686300 -0.94263000
C -0.04867800 -2.55269700 -2.21896000
H -0.74704300 -4.14232400 -0.90489600
H -0.22839200 -2.67414500 -0.06471600
C 1.42903700 -2.95760300 -2.26182900
H -0.56941100 -2.94777900 -3.10258000
H -0.12071400 -1.46168200 -2.26097100
C 2.14083600 -2.45586800 -3.52231900
H 1.94133700 -2.53948500 -1.38832900
H 1.50975900 -4.05221500 -2.18783400
H 3.17262000 -2.82197900 -3.55975000
H 1.63113900 -2.79901900 -4.43110200
H 2.17827200 -1.36288400 -3.52679400
C -1.39850200 3.31666400 0.79023900
C -0.39407900 2.66190000 1.76516000
H -1.66033100 4.32004000 1.14276000
H -0.88123900 3.43182100 -0.17198600
C -0.98522900 2.10103100 3.06152500
H 0.15421200 1.87297000 1.24240900
H 0.36281900 3.41877600 2.00480000
C 0.07660900 1.36572200 3.88797200
H -1.44000200 2.91030600 3.64984400
H -1.79172200 1.39771200 2.81938100
H -0.33420800 0.99349700 4.83262700
H 0.46315200 0.50803900 3.32651800
H 0.91976100 2.02551000 4.12617500
C -6.08564200 -0.94877500 -0.60180400
C -6.21313800 0.35821200 -0.22890200
H -6.96486000 -1.54826700 -0.82030400
H -7.19544800 0.81451700 -0.14551800
O 1.08592400 -1.47501500 1.72772700
O 2.99514900 -0.96034200 0.54702900
C 3.43548200 -1.57868900 1.77479000
C 2.13058700 -2.30693700 2.27742800

B	1.61534000	-0.78066600	0.62867400
C	4.60819200	-2.50253200	1.45864400
H	5.45911900	-1.90942100	1.11154000
H	4.91823000	-3.05842600	2.34981900
H	4.35137500	-3.21229800	0.67056800
C	3.88637400	-0.45230100	2.71477800
H	4.29717600	-0.84399100	3.65006800
H	4.65957800	0.13629800	2.21412300
H	3.05425200	0.21684100	2.95115900
C	1.96826200	-2.36095400	3.79456200
H	1.03039700	-2.86552100	4.04489400
H	2.79077100	-2.92013700	4.25306500
H	1.93701100	-1.36125500	4.23071100
C	1.96059500	-3.71122800	1.68318200
H	2.68071400	-4.41893800	2.10457900
H	0.95122200	-4.06764600	1.90753700
H	2.08062200	-3.69604600	0.59744000
O	0.87128100	-0.05732800	-0.20753000
B	1.25673700	1.11744600	-1.74901100
O	1.34003600	2.40862200	-1.20310300
C	2.73669500	2.73368000	-1.03708600
O	2.49667500	0.68373000	-2.21733800
C	3.44879800	1.75228800	-2.05850400
H	0.24192000	0.80661600	-2.30919900
C	3.13055600	2.47817900	0.42366700
H	2.48354200	3.07182700	1.07463800
H	3.01257200	1.42881900	0.68272400
H	4.16858900	2.76913800	0.61393400
C	4.76289800	1.15186100	-1.55765000
H	5.49332500	1.93426800	-1.32343800
H	4.58742600	0.53367800	-0.67685700
H	5.18792000	0.51135000	-2.33668700
C	3.64553200	2.37324800	-3.44898700
H	4.40258600	3.16404900	-3.44405000
H	3.96673400	1.58795500	-4.13889300
H	2.70534500	2.78598900	-3.82485200
C	2.90957900	4.22093100	-1.35063300
H	3.96516300	4.51105700	-1.31540300
H	2.50774800	4.47200300	-2.33348100
H	2.36924200	4.81325500	-0.60540900
Ni	-1.02618600	0.13935500	-0.07087600

²IM6

C	-0.52178400	2.48985200	0.38815300
C	-0.25253600	3.39303500	1.44294900
C	-1.19372100	3.43902100	2.49475900
H	-1.03210100	4.11117600	3.33350600
C	-2.30832000	2.62876900	2.44137100
H	-3.04563100	2.64415600	3.23735200
C	-2.51283600	1.76349700	1.33944900
C	0.40748100	2.36660300	-0.70003600
C	1.57031100	3.16927600	-0.72600400
C	2.45116400	2.98412300	-1.81224100

C	0.96311400	1.27873500	-2.67811400
C	2.14952200	2.03764000	-2.77086700
H	3.35884100	3.57804700	-1.87964400
H	2.81654700	1.86283300	-3.60846800
N	0.10353900	1.45611400	-1.66487500
N	-1.62934900	1.70702400	0.33891600
Ni	-1.69065900	0.55894700	-1.40617800
C	-3.74217100	0.91060000	1.21791900
C	-4.77133200	1.51595200	0.24449600
H	-4.19372100	0.76623300	2.20675200
H	-3.42719300	-0.06334500	0.83975600
C	-5.95840400	0.57828900	0.00858300
H	-5.12248200	2.48615300	0.62445600
H	-4.26457600	1.69540500	-0.71110000
C	-6.98865500	1.16498600	-0.96033300
H	-5.57384900	-0.36791500	-0.39241600
H	-6.44107100	0.34228400	0.96796100
H	-7.82422300	0.47611900	-1.12439300
H	-7.40160300	2.10643900	-0.57851900
H	-6.52954000	1.37312500	-1.93310800
C	0.61161900	0.22420000	-3.69427300
C	0.79143100	-1.21021400	-3.15568800
H	1.22129200	0.36296300	-4.59460500
H	-0.43978900	0.36201900	-3.97587100
C	2.24064700	-1.58684000	-2.83382000
H	0.17917300	-1.32490300	-2.25472000
H	0.38288200	-1.90716500	-3.89885100
C	2.36587000	-3.04876100	-2.38964700
H	2.87247200	-1.40767100	-3.71598800
H	2.61183900	-0.92654000	-2.04076600
H	3.40906000	-3.32726300	-2.20382500
H	1.79423500	-3.22072700	-1.47208200
H	1.97850300	-3.72674800	-3.15984600
C	0.93196400	4.20029400	1.38846200
C	1.80092600	4.10040900	0.34085700
H	1.12203600	4.89817200	2.19927400
H	2.69306700	4.71968600	0.30332700
O	2.62243700	-1.19408200	2.00741500
O	2.61380300	0.30096300	0.25851800
C	3.97058500	0.30374500	0.78005000
C	4.01169900	-1.03507000	1.61449600
B	1.86804200	-0.49219400	1.09903300
O	0.50989600	-0.52305400	1.06528700
C	4.94190200	0.36604500	-0.39361000
H	4.80174400	1.30819400	-0.93028400
H	5.97704800	0.31871100	-0.04048300
H	4.77353600	-0.44851000	-1.09910500
C	4.10559300	1.55725900	1.65136500
H	5.11761700	1.66195500	2.05276800
H	3.87365100	2.43547300	1.04593600
H	3.39765800	1.53146300	2.48448000
C	4.87017900	-0.98236900	2.87400600
H	4.82537600	-1.94645500	3.38792100
H	5.91557100	-0.77815400	2.62034500

H	4.51918000	-0.21505400	3.56568300
C	4.37223600	-2.26011900	0.76910300
H	5.42625900	-2.25366300	0.47643100
H	4.17739900	-3.16232300	1.35452200
H	3.75590600	-2.30502800	-0.13052400
O	0.06402200	-2.74989100	0.26702600
O	-1.60600200	-1.60509700	1.36495500
C	-1.13195700	-3.56869700	0.10736600
C	-2.11262200	-2.95740400	1.19079000
B	-0.31817100	-1.59231800	0.90251400
C	-2.00318800	-3.63458800	2.56134900
H	-2.57035800	-3.04883400	3.28962600
H	-2.40616300	-4.65120800	2.54185200
H	-0.96319000	-3.67558900	2.89756500
C	-3.56967300	-2.87221400	0.74598500
H	-3.96376500	-3.86958700	0.52551800
H	-4.17317600	-2.43795800	1.54839800
H	-3.67264300	-2.24147700	-0.13896400
C	-0.73837900	-5.02394200	0.34472900
H	-1.61936000	-5.67276500	0.31061900
H	-0.04868100	-5.34534900	-0.44090200
H	-0.24000900	-5.15597900	1.30660900
C	-1.62395000	-3.37453500	-1.32851700
H	-0.81933700	-3.64701800	-2.01668100
H	-2.48791500	-4.01226300	-1.53835500
H	-1.90474800	-2.33334200	-1.51634600
H	-2.95954000	-0.27385700	-1.80196300

PR1p

C	4.89273300	-0.65695700	-2.37351000
C	5.36066400	0.63598000	-2.40571300
C	4.64964400	1.64905600	-1.72211300
C	3.43454300	1.27200000	-1.10572200
C	3.67774900	-0.96433000	-1.70994300
C	5.11563900	2.99852000	-1.59822500
C	2.71735700	2.22481900	-0.30244800
C	3.23409400	3.53277300	-0.15033900
C	4.43416100	3.90473000	-0.84024500
C	2.53331300	4.40020000	0.71702000
C	1.41636900	3.93955500	1.37466200
C	0.95152100	2.61638600	1.16784600
H	6.03761400	3.27730900	-2.10017800
H	5.45117000	-1.46490900	-2.83422300
H	4.80222400	4.92038300	-0.72725100
H	0.87368900	4.57827900	2.06341100
N	2.93734200	0.00508300	-1.16746400
N	1.58900500	1.79472700	0.32981400
H	2.89361500	5.41379800	0.87023900
H	6.28924800	0.88130100	-2.91394400
C	-1.01262200	-1.99473900	-1.40079900
H	-1.26944200	-2.67028400	-2.23104300
H	-0.61091100	-2.63652600	-0.60553700
C	-2.28735200	-1.30590400	-0.90272500
H	-2.03159600	-0.57723300	-0.12776500

H	-2.75102800	-0.74665800	-1.72418000
C	-3.28470100	-2.31223300	-0.32311600
H	-2.82153200	-2.86346800	0.50250700
H	-3.58423900	-3.05123600	-1.07674200
S	-4.79453100	-1.56792300	0.40794400
C	-5.63437800	-0.96874900	-1.12564400
H	-5.01327000	-0.20747200	-1.60489200
H	-5.72532700	-1.81924300	-1.81084900
C	-6.98989100	-0.40432600	-0.78301100
C	-8.04878000	-1.25861200	-0.44405700
C	-7.21032000	0.97835700	-0.77776700
C	-9.30068000	-0.74180300	-0.11356000
H	-7.88140700	-2.33237600	-0.43348800
C	-8.46318900	1.49841000	-0.44695200
H	-6.39636600	1.64984800	-1.03562300
C	-9.51159100	0.63969500	-0.11394200
H	-10.11207100	-1.41634700	0.14477700
H	-8.61850300	2.57360500	-0.44949900
H	-10.48687400	1.04268100	0.14357900
C	-0.30277600	2.14232100	1.84641200
C	-1.54839000	2.41808400	0.98071300
H	-0.40522400	2.65252300	2.81090200
H	-0.20506200	1.07444600	2.05242700
C	-2.83383100	1.84559600	1.58518800
H	-1.65730400	3.50093800	0.82702000
H	-1.38748600	1.97868800	-0.01078100
C	-4.05861800	2.10352900	0.70508400
H	-2.71648100	0.76473100	1.73192600
H	-2.99283100	2.27592300	2.58303100
H	-4.95829500	1.65092500	1.12924500
H	-4.23845600	3.17783000	0.57659200
H	-3.91529500	1.66675300	-0.29025200
C	3.28971000	-2.39817900	-1.47777800
C	4.19006600	-3.01545000	-0.37871000
H	3.37331000	-2.97856800	-2.40492400
H	2.26112200	-2.44264200	-1.12655100
C	3.59670200	-4.30835300	0.18921900
H	5.19495100	-3.20012800	-0.78272400
H	4.30359200	-2.28967500	0.43151400
C	4.45843300	-4.89404100	1.31102800
H	2.60002500	-4.07978400	0.58443400
H	3.46649700	-5.04428900	-0.61736700
H	4.02685200	-5.82241700	1.69953400
H	5.47364200	-5.11743100	0.96100900
H	4.52730900	-4.18271100	2.13967100
C	0.03043400	0.30031600	-2.07938300
C	0.10343700	-1.08369000	-1.87267100
H	0.72379700	0.78329600	-2.76494700
H	-0.88566300	0.85027700	-1.88531200
H	0.89506400	-1.61123500	-2.40117000
Ni	1.04480500	-0.05438000	-0.37725800
H	-0.21103000	0.01108400	0.24479300
Cl	2.42269000	-1.02675200	2.22909200
O	1.55647200	-1.46242100	1.00489400

O	1.59557100	-0.15149100	3.09784500
O	2.81629500	-2.27916400	2.91242000
O	3.61579500	-0.28970100	1.72170700

TS1p

C	-5.10035000	1.21123400	-1.59249000
C	-5.81176000	0.05050400	-1.39503100
C	-5.14576700	-1.08969900	-0.88787400
C	-3.74905500	-0.98217200	-0.70879400
C	-3.70269600	1.25031700	-1.35113000
C	-5.81149400	-2.30123000	-0.50715800
C	-3.03269800	-2.05276900	-0.07681700
C	-3.72566600	-3.19943300	0.36849500
C	-5.12953100	-3.31496500	0.10128100
C	-2.97812900	-4.15113200	1.09920500
C	-1.65275800	-3.90247800	1.37731100
C	-1.01978500	-2.72981300	0.89601600
H	-6.88055000	-2.38150100	-0.68170900
H	-5.59651000	2.12280100	-1.90864600
H	-5.64571400	-4.21576800	0.42025900
H	-1.07100900	-4.59465200	1.97661400
N	-3.03918400	0.14419500	-1.00749800
N	-1.70177700	-1.85906200	0.14542500
H	-3.46444900	-5.05184800	1.46352700
H	-6.88254200	0.01317400	-1.57589000
Ni	-1.04414900	-0.32312400	-0.89121000
C	-0.27170100	0.83502600	-2.35849000
C	0.08189100	-0.50931200	-2.59577800
H	-1.12995800	1.22260200	-2.90401300
H	0.19964900	-0.99988600	-0.98568600
H	-0.53944900	-1.12991800	-3.23901600
H	1.12199900	-0.82441100	-2.56464400
C	0.71185800	1.87483900	-1.84971300
H	1.05874600	2.48691300	-2.69647200
H	0.17585100	2.55461000	-1.17911600
C	1.91846400	1.29430000	-1.09520200
H	1.57991700	0.51042000	-0.41387300
H	2.61548600	0.82939300	-1.80397500
C	2.64892900	2.33459900	-0.24600900
H	1.98105900	2.69213500	0.54387700
H	2.96521400	3.20402800	-0.83481200
S	4.11194600	1.63332000	0.61801900
C	5.32335700	1.63333600	-0.78261700
H	4.79456400	1.33209700	-1.69162800
H	5.69441200	2.65304200	-0.92593800
C	6.45285900	0.68059500	-0.49307000
C	7.57861300	1.10082400	0.22579800
C	6.37697300	-0.65556500	-0.90781000
C	8.60994200	0.20664200	0.51898500
H	7.64340500	2.13368900	0.55839300
C	7.40700800	-1.55033800	-0.62022600
H	5.50124900	-0.99419400	-1.45506000
C	8.52750600	-1.12117800	0.09606400
H	9.47750000	0.54779700	1.07672200

H	7.33587700	-2.58127700	-0.95594500
H	9.33074100	-1.81684600	0.32126200
C	0.42269200	-2.44772200	1.21553400
C	1.41061800	-3.11168000	0.23653500
H	0.62814300	-2.80316800	2.23152100
H	0.56583900	-1.36563200	1.23359900
C	2.85953400	-2.69805000	0.52094100
H	1.31288900	-4.20470800	0.29414200
H	1.14566000	-2.83487200	-0.79288400
C	3.86421300	-3.35943500	-0.42601300
H	2.94869500	-1.60596300	0.45065000
H	3.10935300	-2.95378100	1.55911200
H	4.88734600	-3.05722400	-0.18530500
H	3.81081000	-4.45277400	-0.36451100
H	3.66787000	-3.07902100	-1.46855800
C	-2.97567700	2.56351500	-1.31653100
C	-3.38334400	3.36310900	-0.05468000
H	-3.17474100	3.15218900	-2.22076400
H	-1.90993200	2.36723000	-1.25119100
C	-2.39170300	4.49066300	0.25184300
H	-4.39692500	3.76778500	-0.18088700
H	-3.41539100	2.67939900	0.79857600
C	-2.76927200	5.26142800	1.51913300
H	-1.40031600	4.04289000	0.39047200
H	-2.32543500	5.17356300	-0.60756900
H	-2.05788900	6.06967700	1.71845000
H	-3.76786800	5.70705700	1.43373000
H	-2.76255100	4.58722700	2.38066700
Cl	-1.31048900	1.06217300	2.06882400
O	-0.54433500	0.06504500	2.86334800
O	-2.72279100	0.60652100	1.89117400
O	-1.26735700	2.40982200	2.68942700
O	-0.65043900	1.18304200	0.68059700

IM1p

C	-5.54953700	1.03792500	-1.91840300
C	-6.11050500	-0.19759600	-1.69055500
C	-5.32016600	-1.22899600	-1.14023200
C	-3.95397000	-0.93347200	-0.87956100
C	-4.17914800	1.24836800	-1.63389400
C	-5.85709800	-2.51925100	-0.82922600
C	-3.12930400	-1.94295500	-0.24465800
C	-3.70868000	-3.19723300	0.07682300
C	-5.07845900	-3.46876700	-0.24419700
C	-2.89707600	-4.14469000	0.73584600
C	-1.60241900	-3.81917300	1.05835200
C	-1.08575600	-2.54830400	0.71987100
H	-6.90085300	-2.71640900	-1.05688400
H	-6.14312700	1.85751600	-2.30982800
H	-5.48301000	-4.44497800	0.00699500
H	-0.96319500	-4.51995700	1.58405000
N	-3.40490500	0.27182500	-1.16159500
N	-1.83177700	-1.64901100	0.06523000
H	-3.31146600	-5.11496900	0.99596300

H	-7.15876300	-0.38504200	-1.90769900
Ni	-1.09847500	0.15738400	-0.47333100
C	-0.19884700	1.55357200	-1.37596600
C	-0.08825400	0.45152600	-2.37965300
H	-0.90347300	2.32927600	-1.66950600
H	0.91733000	0.06168100	-2.54635800
H	-0.67436700	-0.48346900	-2.00637400
H	-0.59539400	0.64206000	-3.32889300
C	1.01521400	2.17398800	-0.71016900
H	1.46697900	2.92158900	-1.38343800
H	0.64374600	2.73116100	0.15870300
C	2.10607400	1.20401900	-0.24297000
H	1.65751700	0.43008700	0.38477800
H	2.55624100	0.69402100	-1.10374500
C	3.19027800	1.93597700	0.55451400
H	2.78528800	2.26863400	1.51569000
H	3.52572000	2.83433900	0.02140200
S	4.67619100	0.93725500	0.96530300
C	5.51105800	0.96027800	-0.68442000
H	4.87870700	0.45342400	-1.41839100
H	5.60950900	2.00970300	-0.98637900
C	6.86387800	0.29663700	-0.60888500
C	7.88924600	0.85770700	0.16659300
C	7.12190700	-0.88649700	-1.31162600
C	9.14136100	0.24907800	0.23620500
H	7.69437500	1.77031200	0.72313300
C	8.37597700	-1.49755500	-1.24424000
H	6.33737600	-1.32836500	-1.91935000
C	9.38872600	-0.93212400	-0.46886600
H	9.92514500	0.69589700	0.84134200
H	8.55928500	-2.41453200	-1.79722800
H	10.36437200	-1.40645400	-0.41389800
C	0.33926200	-2.21646800	1.06686300
C	1.31092500	-2.49166500	-0.09771300
H	0.63236400	-2.81979200	1.93288200
H	0.39770000	-1.17120600	1.37771900
C	2.77695800	-2.40986200	0.33750100
H	1.10746000	-3.48291700	-0.52640800
H	1.11805500	-1.76346000	-0.89534700
C	3.75419200	-2.54463300	-0.83154100
H	2.96181300	-1.45798300	0.84616400
H	2.97453100	-3.19719900	1.07739900
H	4.78988200	-2.47668300	-0.48717900
H	3.62913900	-3.50060300	-1.35394600
H	3.59568100	-1.74404600	-1.56505100
C	-3.56854900	2.61941400	-1.78001700
C	-3.19361700	3.20036000	-0.40185400
H	-4.26689300	3.28518900	-2.29950600
H	-2.67361400	2.54879600	-2.40827600
C	-2.43302700	4.52707300	-0.46911900
H	-4.10641100	3.32345800	0.19493000
H	-2.58451500	2.46604400	0.12912400
C	-1.99716800	4.99143100	0.92521900
H	-1.54621200	4.40581100	-1.10677800

H	-3.05202500	5.29657200	-0.95126200
H	-1.41302800	5.91649700	0.87847200
H	-2.86664000	5.17418400	1.56634200
H	-1.39102000	4.22252100	1.41650200
Cl	-1.91946100	0.68877000	2.42331500
O	-0.91984600	1.02539700	1.23951900
O	-1.48013700	-0.59069600	3.03533500
O	-1.79438800	1.82643300	3.35397400
O	-3.28927800	0.56998800	1.86324900

TS2p

C	5.47211600	-0.43524000	-1.52172700
C	5.75197500	0.89323000	-1.27985700
C	4.73443500	1.74631300	-0.79863000
C	3.45000600	1.17362900	-0.61696900
C	4.16719400	-0.93082400	-1.29516400
C	4.95262100	3.12220600	-0.46299300
C	2.37339300	1.98080200	-0.09213100
C	2.64708100	3.31337400	0.29504800
C	3.94971500	3.87166000	0.07483300
C	1.60574900	4.02279100	0.93146200
C	0.40056500	3.40076100	1.15160300
C	0.17375400	2.08125900	0.68650300
H	5.94047700	3.54608200	-0.61949600
H	6.24372000	-1.11328500	-1.87129500
H	4.12231000	4.90499600	0.36182000
H	-0.38859800	3.90339200	1.69608900
N	3.19329900	-0.12907900	-0.86680800
N	1.14381800	1.40690900	0.05630200
H	1.77858100	5.04011600	1.27210500
H	6.75160000	1.28929500	-1.43789500
C	-1.15304900	1.41353200	0.94585400
C	-2.38007400	1.97922700	0.19587800
H	-1.33692800	1.47251300	2.02450600
H	-1.04756400	0.34966900	0.73256600
C	-2.88169000	3.35963200	0.63808800
H	-2.18526500	2.00791900	-0.88431100
H	-3.18412600	1.24821200	0.33890800
C	-4.24362200	3.69828900	0.02108600
H	-2.96031300	3.38288400	1.73362700
H	-2.15819300	4.13550400	0.35972000
H	-4.58582400	4.69382900	0.32197000
H	-4.19387100	3.68102600	-1.07455100
H	-5.00276200	2.97188200	0.32994700
C	3.82003400	-2.38781000	-1.44934300
C	3.62305600	-3.05550500	-0.06967000
H	4.58832200	-2.90806800	-2.03179200
H	2.87976800	-2.45258400	-2.00925100
C	2.82920600	-4.36239700	-0.13084500
H	4.60366600	-3.22652100	0.39336900
H	3.09156900	-2.35612200	0.57838400
C	2.59711800	-4.95104500	1.26465100
H	1.85823500	-4.15608300	-0.60345500

H	3.34140800	-5.09126900	-0.77498100
H	1.99484300	-5.86459200	1.21922100
H	3.54872500	-5.20178800	1.74775900
H	2.08057800	-4.22850600	1.90515300
Ni	1.06757000	-0.53617300	-0.62548800
C	0.65499700	-0.16112200	-2.53753300
C	-0.16517900	-1.24804600	-2.12380200
H	0.95977400	-1.90283400	-1.00958900
H	1.53178700	-0.44348200	-3.12323500
C	0.16789100	1.23847400	-2.82403600
H	0.98389300	1.95827500	-2.71311200
H	-0.20370100	1.31243000	-3.85513000
H	-0.63441900	1.54654300	-2.15412900
H	0.06675600	-2.22085500	-2.55992600
C	-1.61274500	-1.12715800	-1.69958700
C	-1.99007700	-2.11838100	-0.58554000
H	-2.23979700	-1.30720200	-2.58459900
H	-1.82523800	-0.11317500	-1.36392300
H	-2.02459200	-3.14443100	-0.96882000
H	-1.23374700	-2.08707400	0.20546900
S	-3.54833600	-1.71128600	0.29161600
C	-4.78679600	-1.72920500	-1.08394300
H	-5.01764700	-2.76500400	-1.35097600
H	-4.34508900	-1.23905700	-1.95530600
C	-6.02231800	-0.98805900	-0.64282200
C	-6.10819600	0.40162500	-0.80755100
C	-7.08326400	-1.66174000	-0.02657700
C	-7.23480700	1.10097000	-0.37709500
H	-5.28321500	0.93542200	-1.27208200
C	-8.21176900	-0.96357900	0.40820400
H	-7.02212800	-2.73785100	0.11412800
C	-8.29105700	0.41891700	0.23318000
H	-7.28880200	2.17669500	-0.51901400
H	-9.02815200	-1.50022200	0.88309300
H	-9.16967800	0.96207500	0.56893900
Cl	1.55587500	-0.81291800	2.47995600
O	2.91629700	-0.35428100	2.09297000
O	1.60617500	-1.96601000	3.40202400
O	0.75886200	0.30968900	3.03667000
O	0.82213500	-1.33565000	1.19192700

IM2_p

C	-3.94652700	1.83699800	-2.41685100
C	-4.72114500	0.73365000	-2.68912900
C	-4.41321500	-0.50169100	-2.07291500
C	-3.26335200	-0.53594600	-1.25173800
C	-2.81378200	1.72895800	-1.56955300
C	-5.21194800	-1.68223000	-2.21875600
C	-2.94916800	-1.72818200	-0.51125200
C	-3.78950200	-2.85929900	-0.63328000
C	-4.90941100	-2.81822400	-1.52707600
C	-3.48311600	-3.97268500	0.18037200
C	-2.43368900	-3.89139600	1.06550000

C	-1.63510300	-2.72077600	1.13992800
H	-6.07637900	-1.64614200	-2.87534500
H	-4.19341600	2.80875600	-2.83118000
H	-5.52840200	-3.70568600	-1.62200600
H	-2.20108800	-4.71829300	1.72726000
N	-2.45703300	0.54565400	-1.06714800
N	-1.87919500	-1.68302000	0.33478300
H	-4.09510600	-4.86847400	0.12014400
H	-5.58583700	0.80618400	-3.34321300
C	-0.51907800	-2.63611200	2.14945800
C	0.86032700	-3.09148900	1.63036000
H	-0.79967200	-3.25715400	3.00833200
H	-0.46069300	-1.60479200	2.50210700
C	0.90984200	-4.51288500	1.06153500
H	1.19680100	-2.38229100	0.86911900
H	1.57008500	-3.00704600	2.46310800
C	2.31318600	-4.90025300	0.58524700
H	0.56516200	-5.22697000	1.82274900
H	0.20559500	-4.59970800	0.22324900
H	2.33478800	-5.91576500	0.17686400
H	2.66117600	-4.21716500	-0.19832200
H	3.03597300	-4.85414300	1.40753200
C	-2.08457600	2.96605600	-1.12430400
C	-2.94167000	3.74676300	-0.09793800
H	-1.85400200	3.60692200	-1.98456100
H	-1.15253700	2.68356200	-0.63790800
C	-2.11944800	4.79656800	0.65575600
H	-3.79031000	4.22090100	-0.61020500
H	-3.36234600	3.03929800	0.62223100
C	-2.95532800	5.54084100	1.70013900
H	-1.29093200	4.28432200	1.15832100
H	-1.67862600	5.50713000	-0.05826700
H	-2.35596400	6.29127600	2.22601300
H	-3.80723900	6.05554400	1.23914000
H	-3.33930200	4.83551700	2.44333100
Ni	-0.74432900	-0.02448300	-0.10311800
C	0.19118000	-0.55508400	-1.82388800
C	0.58724500	0.73752300	-1.43226300
H	0.38332700	-0.51100900	0.58785200
H	-0.62552100	-0.62035900	-2.54413800
C	1.05795700	-1.78919800	-1.78298500
H	0.48274800	-2.66482300	-1.46708300
H	1.45526000	-2.00018900	-2.78463100
H	1.90436300	-1.67929600	-1.10299000
H	0.07030000	1.56685700	-1.91234500
C	1.94708100	1.09747900	-0.87742600
C	2.95454200	1.35292800	-2.01124100
H	2.30953200	0.29703100	-0.22901200
H	1.86712400	1.98819200	-0.24704400
H	3.00537000	0.48391200	-2.67819100
H	2.64060400	2.20773000	-2.62008200
S	4.65168000	1.76185100	-1.44484600
C	5.15311000	0.11698000	-0.76231100
H	5.05336100	-0.62743900	-1.55971500

H	4.47245300	-0.15379000	0.04966400
C	6.57134900	0.18526800	-0.25889200
C	7.64722200	-0.08043000	-1.11578500
C	6.83622500	0.54655400	1.06841200
C	8.96077100	0.00067300	-0.65294400
H	7.45036500	-0.35050400	-2.15020800
C	8.14888300	0.62923500	1.53359100
H	6.00734600	0.76502000	1.73688900
C	9.21477200	0.35517800	0.67388200
H	9.78530900	-0.21283400	-1.32726000
H	8.33908200	0.90687000	2.56641400
H	10.23711100	0.41726400	1.03564700
Cl	-2.12698900	1.17519900	2.43682400
O	-0.98784100	1.35516000	1.38650300
O	-3.37797500	0.79176400	1.72112400
O	-1.72086700	0.11010900	3.38891800
O	-2.27468300	2.48747100	3.10610600

TS3p

C	2.84379700	-3.44202600	-1.80159000
C	4.16796000	-3.07610300	-1.74967200
C	4.51324000	-1.81830200	-1.20417400
C	3.44696800	-0.96350900	-0.84462800
C	1.83077100	-2.54514000	-1.37562900
C	5.86263600	-1.40816800	-0.95058400
C	3.72461300	0.26887800	-0.16516300
C	5.05875100	0.59893400	0.16327200
C	6.12525900	-0.24769600	-0.28387100
C	5.25420300	1.74027400	0.97135100
C	4.16041500	2.44892000	1.41103300
C	2.85027200	2.08321000	1.01260700
H	6.67103500	-2.06214500	-1.26444200
H	2.54990700	-4.43056800	-2.13830700
H	7.14668300	0.04083600	-0.05364600
H	4.27954500	3.30198700	2.06912000
N	2.13390500	-1.29747700	-1.00456300
N	2.65444100	1.02756200	0.21475700
H	6.26037700	2.02817900	1.26305800
H	4.95084000	-3.75825900	-2.06964100
Ni	0.99413600	0.36632900	-0.65004900
C	-0.48241900	0.05800400	-1.98636500
C	0.00011200	1.36805300	-2.20920000
H	-0.08878100	-0.72439200	-2.63392700
H	0.44345800	1.67679500	-0.57350600
H	0.83250700	1.46791000	-2.90772700
C	-1.84110900	-0.20033900	-1.37131100
H	-1.86248800	-1.17916400	-0.88788000
H	-2.01168100	0.51936100	-0.56632900
C	-2.97048800	-0.13105200	-2.41225900
H	-3.01519200	0.85905100	-2.87933200
H	-2.79101300	-0.85655500	-3.21335300
C	1.66916300	2.90027800	1.46028400
C	1.37289500	4.09127300	0.52281900

H	1.86531800	3.27179000	2.47224300
H	0.80417600	2.24009300	1.53224600
C	2.40743700	5.22211600	0.55736100
H	1.28558400	3.71839400	-0.50452500
H	0.38830900	4.49515300	0.79050100
C	2.02438800	6.38943300	-0.35777100
H	2.51779700	5.58157800	1.58977100
H	3.39002000	4.83470200	0.25949700
H	2.77134500	7.18894800	-0.32431200
H	1.93597900	6.05891800	-1.39940300
H	1.06007800	6.81974200	-0.06474900
C	0.42935100	-3.03830000	-1.17348600
C	0.36227700	-3.93617700	0.08790200
H	0.06865800	-3.58689400	-2.05220100
H	-0.21619000	-2.18556300	-0.99979700
C	-1.07559200	-4.10570600	0.59000700
H	0.81285000	-4.91488100	-0.12682800
H	0.96128400	-3.47459600	0.87841400
C	-1.14483300	-4.95536100	1.86149900
H	-1.48109300	-3.11022100	0.80539800
H	-1.69865900	-4.54680700	-0.20115300
H	-2.17917800	-5.07867400	2.19902100
H	-0.72375400	-5.95510900	1.69852900
H	-0.58418900	-4.46900600	2.66540000
C	-0.86484700	2.61735200	-2.14525100
H	-1.38737300	2.72858700	-3.10311800
H	-0.26661800	3.51788500	-1.98933100
H	-1.61564600	2.56537700	-1.35411100
S	-4.63147300	-0.55701100	-1.75910500
C	-4.88667200	0.85018400	-0.58565100
H	-4.11674000	0.81160600	0.18947800
H	-4.77237400	1.78556400	-1.14451100
C	-6.25842800	0.75050100	0.02928600
C	-7.36691000	1.33415900	-0.59773400
C	-6.44965000	0.04399700	1.22369400
C	-8.63924900	1.22547500	-0.03633800
H	-7.22801800	1.87417700	-1.53097200
C	-7.72153200	-0.06708400	1.78646500
H	-5.59599100	-0.41962300	1.71137600
C	-8.81953300	0.52459800	1.15833200
H	-9.48920300	1.68763100	-0.53060700
H	-7.85415600	-0.61420000	2.71544500
H	-9.80966000	0.44074200	1.59720900
Cl	0.68466200	-0.92489700	2.31660300
O	-0.08815800	-0.58152500	1.02934200
O	1.99766600	-1.53474700	1.94108300
O	0.90650600	0.33579000	3.07823200
O	-0.14065300	-1.89011600	3.08372300

IM3p

Ni	1.13035800	-0.22945000	-0.11706200
C	2.59408300	3.86966400	0.72074600
C	3.80947200	0.22373000	-0.91121200

C	5.14103500	0.08140800	-1.37650000
C	5.54122400	-1.19624400	-1.81579000
C	4.65022600	-2.23791600	-1.73432300
C	3.32345900	-2.02767000	-1.28831600
N	2.89497100	-0.79931700	-0.94258500
H	6.55156000	-1.34868600	-2.18488000
H	4.94408800	-3.24105700	-2.02193000
C	3.40913400	1.48851800	-0.34601500
C	4.31726200	2.57561200	-0.34930400
C	3.86763500	3.79156700	0.21139500
C	1.74387900	2.73537300	0.70636600
N	2.16579900	1.57142600	0.19998800
H	4.53369900	4.64969300	0.23472600
H	2.22140400	4.79278600	1.15152600
C	0.32635600	2.87294300	1.18657300
C	-0.61395400	3.25396900	0.02223500
H	0.28536500	3.64899700	1.95859000
H	-0.00403100	1.94107200	1.64149700
C	-2.04858900	3.52174300	0.49250700
H	-0.22468100	4.14075200	-0.49758400
H	-0.60519800	2.43786100	-0.71094700
C	-3.01841500	3.76935200	-0.66592600
H	-2.40818200	2.67250600	1.08403700
H	-2.04609300	4.38761600	1.16816100
H	-4.03070300	3.96288900	-0.29801300
H	-2.70767900	4.62754500	-1.27363700
H	-3.07024900	2.89533900	-1.32448000
C	-2.24358200	0.08555300	-0.17086800
H	-1.67054400	0.60867300	0.59283500
H	-2.26790200	0.72399800	-1.05962500
C	-1.58970500	-1.26558700	-0.46878400
H	-1.50128500	-1.82601400	0.46527300
H	-2.25606700	-1.84572500	-1.12787000
C	-0.27187500	-0.38484200	-2.48096200
H	-0.21180200	0.69890400	-2.29588800
H	-1.26902700	-0.53422900	-2.92795900
C	6.03337200	1.20220700	-1.37079900
H	7.03918100	1.06105400	-1.75525300
C	5.63315700	2.40994500	-0.88700500
H	6.30863400	3.26036800	-0.88150700
C	-4.86846300	-0.26836000	-1.09610500
H	-4.57622800	-1.23528200	-1.51667500
H	-4.56713700	0.51617600	-1.79946600
C	0.51500500	-4.87821000	1.83070200
H	-0.27653200	-5.63225300	1.89078900
H	1.36735700	-5.23871700	2.41787300
H	0.15550000	-3.96075000	2.30781400
C	2.41632900	-3.22403800	-1.17318400
H	2.93683300	-4.09575400	-1.58329400
H	1.53662900	-3.07031900	-1.79934000
C	1.98568500	-3.51520200	0.27809300
H	1.59443100	-2.60104000	0.72859100
H	2.87032700	-3.78771700	0.86779100
C	0.92467700	-4.61397700	0.37791300

H	1.29549800	-5.53885700	-0.08631400
H	0.04283800	-4.30939200	-0.20230700
C	-0.21670000	-1.17370000	-1.15532800
H	0.08235300	-2.20128200	-1.36546400
C	0.78060700	-0.76665300	-3.52776400
H	0.62795100	-0.21158900	-4.45946000
H	1.79335200	-0.55582000	-3.17618800
H	0.72465500	-1.83520100	-3.76637400
S	-3.95313200	0.00704500	0.48635300
C	-6.35267100	-0.21781000	-0.84684800
C	-7.02958200	1.00928900	-0.84846200
C	-7.07433200	-1.38672000	-0.57509700
C	-8.40020300	1.06585600	-0.59749700
H	-6.47250000	1.92218200	-1.04427400
C	-8.44582600	-1.33331400	-0.32221300
H	-6.55502800	-2.34157700	-0.56012000
C	-9.11272000	-0.10668900	-0.33430500
H	-8.91241300	2.02394700	-0.60655500
H	-8.99288000	-2.24892300	-0.11574300
H	-10.18053100	-0.06409900	-0.13934000
Cl	1.04138500	-0.50615000	2.81201400
O	0.10257200	-0.28815400	1.55473500
O	2.41754500	-0.77318000	2.30538400
O	0.99108100	0.73990400	3.60813400
O	0.49009000	-1.66546600	3.53893400

PR1''

C	-3.87530000	-2.32757200	1.03970300
C	-2.57113700	1.50260500	0.05693600
C	-3.48900400	2.57827500	0.02623900
C	-2.95744200	3.86552700	-0.20563100
C	-1.59832400	4.01554500	-0.35333300
N	-1.22702900	1.65588900	-0.13956000
H	-3.62101900	4.72432500	-0.24701100
H	-1.16466100	4.99755900	-0.50481500
C	-3.04688500	0.18116200	0.35023400
C	-4.42105800	-0.02618800	0.60292300
C	-4.82257300	-1.33681700	0.94449600
C	-2.51034200	-2.06144900	0.77103500
N	-2.11667500	-0.82741300	0.40892600
H	-5.86959000	-1.54535800	1.14391400
H	-4.15553600	-3.33678600	1.31977500
C	-1.52859700	-3.19631800	0.85262900
C	-1.41343700	-3.95254000	-0.48882600
H	-1.85927500	-3.89125600	1.63236600
H	-0.54830900	-2.81277000	1.14497500
C	-0.35989600	-5.06436900	-0.44117800
H	-2.39256300	-4.37360700	-0.75181200
H	-1.15750400	-3.23466500	-1.27815900
C	-0.24201200	-5.81612400	-1.77012800
H	0.61107000	-4.62357200	-0.17605800
H	-0.60886800	-5.76780400	0.36429600
H	0.52048600	-6.59865700	-1.71654000

H	-1.19068700	-6.29252900	-2.04021600
H	0.03217200	-5.13611600	-2.58453400
C	-4.88317200	2.33276200	0.24564600
H	-5.57157800	3.17065600	0.19742000
C	-5.33240800	1.07670900	0.52459900
H	-6.38654300	0.89077200	0.70465100
C	3.75075900	2.62895600	2.08230100
H	4.82701100	2.78930700	1.97106500
H	3.40440800	3.25437300	2.91201000
H	3.59475500	1.58305800	2.36425700
C	0.75126900	3.10225500	-0.40325600
H	0.94249800	4.15003600	-0.65338100
H	1.14814000	2.51402100	-1.23203800
C	1.49148500	2.74862200	0.90108700
H	1.28364400	1.70454200	1.16457500
H	1.08984800	3.35776800	1.72082000
C	3.00409000	2.97098400	0.79019500
H	3.19535500	4.01620800	0.51554900
H	3.40258800	2.36784600	-0.03752600
C	-0.73654500	2.89216900	-0.31051700
C	2.52269100	-0.12951000	-0.83699400
C	2.43819100	0.54560300	-2.94650000
O	2.75245500	0.86637400	-4.04160700
O	3.28607500	0.15398500	-1.92017000
O	1.16927200	0.49398100	-2.43031500
N	1.25854600	0.07010200	-1.07733900
C	3.16679000	-0.57323600	0.38480100
C	4.57211600	-0.64757600	0.41458000
C	2.41923900	-0.90427900	1.53087900
C	5.21660600	-1.04856200	1.58048900
H	5.14738000	-0.38929400	-0.46712500
C	3.07565700	-1.30886700	2.68770300
H	1.33664100	-0.84469900	1.51339100
C	4.47233200	-1.38002600	2.71590500
H	6.29989100	-1.10194800	1.60315600
H	2.49909300	-1.56369700	3.57088100
H	4.97973400	-1.69100100	3.62367800
Ni	-0.40850400	-0.25420200	-0.25416900
H	0.02468200	-1.61027000	-0.34436400

TS1''

C	-1.98264700	-3.86603200	0.41642300
C	-3.09125800	0.12250400	-0.02671200
C	-4.45342500	0.49340300	-0.01358400
C	-4.73172600	1.87995200	-0.00310900
C	-3.69024100	2.77921200	0.03165900
N	-2.06674600	1.02385300	-0.05440300
H	-5.76228900	2.22296600	-0.00009300
H	-3.88176700	3.84548400	0.07356800
C	-2.73776300	-1.26342200	0.05479700
C	-3.74754400	-2.24569900	0.13479300
C	-3.32492800	-3.58563300	0.29547800
C	-1.01481500	-2.83656300	0.33848000
N	-1.40092000	-1.56847300	0.11457100

H	-4.06412200	-4.37944600	0.35106100
H	-1.64075900	-4.88190100	0.58010400
C	0.44216100	-3.16310000	0.51051500
C	1.13309500	-3.59712100	-0.80022300
H	0.52841600	-3.97313500	1.24344000
H	0.96043400	-2.29463300	0.92863000
C	2.63484200	-3.83116000	-0.60094200
H	0.65384400	-4.50601500	-1.18575700
H	0.97988100	-2.82126100	-1.56282900
C	3.35030400	-4.19996800	-1.90309600
H	3.08396600	-2.92446200	-0.17609900
H	2.78076500	-4.62482100	0.14370400
H	4.41855500	-4.36402800	-1.73362700
H	2.93786800	-5.11630000	-2.33884600
H	3.24874400	-3.40232700	-2.64776900
C	-5.46225900	-0.52449900	0.01594000
H	-6.50474700	-0.22244200	-0.00164000
C	-5.12287700	-1.84437300	0.08504900
H	-5.88877300	-2.61240500	0.12401400
C	1.72820800	3.83371400	2.65420300
H	2.63385300	4.44530800	2.60950400
H	1.16464200	4.13487000	3.54386400
H	2.03970600	2.79189400	2.79292000
C	-1.20799000	3.30979000	0.10553900
H	-1.59810300	4.32842300	0.02130300
H	-0.54188100	3.15016000	-0.74313800
C	-0.40067600	3.16783100	1.41433100
H	-0.15256100	2.11029200	1.56367400
H	-1.02198500	3.46687100	2.26807800
C	0.88843300	3.99517800	1.38394300
H	0.63704500	5.05325000	1.23679900
H	1.48242000	3.69912300	0.50906600
C	-2.34424300	2.33332800	0.01081700
C	3.02810600	0.30854500	0.45445500
C	4.27314700	-0.23288900	0.10496300
C	2.45223300	0.03381600	1.70390100
C	4.93793900	-1.05414000	1.01383100
H	4.70779400	0.00515900	-0.85932700
C	3.12909100	-0.78658500	2.60566700
H	1.49896700	0.47480500	1.97223300
C	4.36650400	-1.33515000	2.25926000
H	5.90637200	-1.46841400	0.75224500
H	2.69568300	-0.98832600	3.58009900
H	4.89182400	-1.97316400	2.96303400
Ni	-0.30215100	-0.05932100	-0.37126700
C	2.35180900	1.16097100	-0.58218800
O	3.01919800	1.90257000	-1.33999200
N	1.03430300	1.01503400	-0.57981500
C	1.78813500	2.68853000	-2.63178000
O	0.73715900	2.23674500	-2.20576800
O	2.42668000	3.32529200	-3.37634300
H	0.68598400	-0.96691700	-0.79286300

IM1''

C	2.93137700	-0.01595800	-0.23736800
C	4.27745600	-0.24330200	-0.58089800
C	4.59335400	-1.54043600	-1.05298900
H	5.61526600	-1.77727500	-1.33455300
C	3.60113700	-2.49231600	-1.15292100
H	3.82679400	-3.49046800	-1.51114900
C	2.26070000	-2.19401200	-0.79609300
C	2.51920600	1.25961700	0.24940400
C	3.45464600	2.30363300	0.38841100
C	2.95381700	3.53169200	0.88227900
C	0.73087400	2.55418500	1.03082000
C	1.61565800	3.64824400	1.19762000
H	3.62585200	4.37503300	1.01165700
H	1.21648600	4.58157100	1.57787200
N	1.19887900	1.39005500	0.56439800
N	1.96130300	-0.96846700	-0.34436600
C	-2.40600700	-1.42553300	-0.36249400
O	-2.23715400	-2.41264300	-1.07749400
Ni	0.16043700	-0.28787400	0.18208100
N	-1.30945500	-0.97813500	0.37170900
C	1.17790300	-3.23060000	-0.84953600
C	0.88077300	-3.81419200	0.55214000
H	1.48154800	-4.03451800	-1.52681000
H	0.25685700	-2.79038800	-1.24613300
C	-0.24795900	-4.85028100	0.51581100
H	1.79431000	-4.25940500	0.96772700
H	0.59638800	-2.99195400	1.22274900
C	-0.58485700	-5.38968900	1.90879200
H	-1.13389500	-4.38909400	0.06482200
H	0.04453600	-5.67848300	-0.14303700
H	-1.38765100	-6.13111700	1.86002200
H	0.28433900	-5.86897000	2.37300200
H	-0.91626700	-4.58374800	2.57384200
C	-0.73968000	2.66741900	1.32914700
C	-1.59170300	2.91682100	0.06192800
H	-0.89786400	3.48132300	2.04378000
H	-1.06871200	1.73998400	1.81034500
C	-1.30459200	4.24869700	-0.63817200
H	-1.43523100	2.08656600	-0.63850300
H	-2.64670400	2.86913800	0.35418200
C	-2.20354800	4.46633500	-1.85905900
H	-1.44434000	5.07081100	0.07690700
H	-0.25141300	4.28669800	-0.94768900
H	-1.98757700	5.42124000	-2.34655800
H	-2.06024600	3.67211900	-2.60038200
H	-3.26112600	4.46753900	-1.57401600
C	-3.68406900	-0.70634800	-0.18195400
C	-3.86636300	0.22158700	0.85668800
C	-4.72141600	-0.96147300	-1.09164000
C	-5.07780100	0.89822500	0.97514500
H	-3.07223100	0.38910300	1.57725500
C	-5.92860800	-0.27946400	-0.96975500
H	-4.56099200	-1.68958600	-1.87991400
C	-6.10611700	0.65096600	0.06009000

H	-5.22751600	1.60659400	1.78400100
H	-6.73251000	-0.47188100	-1.67304400
H	-7.05056000	1.17833300	0.15425700
C	5.21707600	0.83161400	-0.43335900
C	4.82235800	2.05511000	0.03165900
H	6.25412000	0.65363900	-0.69996900
H	5.54170100	2.86067700	0.13979800
H	-0.39514100	0.01069900	-1.09313300

PR2''

C	-5.64179300	0.93990500	-1.65497300
C	-6.25055500	-0.28833100	-1.53116100
C	-5.54106600	-1.36472600	-0.94700800
C	-4.21856600	-1.09821200	-0.52751000
C	-4.30748800	1.13355200	-1.21276800
C	-6.09017100	-2.67475000	-0.75744200
C	-3.44901900	-2.13447200	0.09782000
C	-4.02535600	-3.40793700	0.30315800
C	-5.36087200	-3.65801700	-0.15410100
C	-3.23575500	-4.36617000	0.97953300
C	-1.98733000	-4.01486900	1.44053800
C	-1.46494900	-2.71814500	1.21225400
H	-7.10402500	-2.86716400	-1.09449700
H	-6.17035800	1.78019500	-2.09197000
H	-5.78404400	-4.64555300	0.00049700
H	-1.38162600	-4.72288800	1.99531000
N	-3.62535800	0.12106600	-0.66793400
N	-2.17865900	-1.82580300	0.50904200
H	-3.63088800	-5.36290700	1.15292600
H	-7.27053100	-0.43968500	-1.87251100
C	0.21415300	1.11254900	-2.56837000
H	0.40658200	1.35495000	-3.62513500
H	-0.05405600	2.06531200	-2.09558100
C	1.48157100	0.56135400	-1.90680700
H	1.23640500	0.20240200	-0.90043600
H	1.86549800	-0.30282500	-2.46200900
C	2.56502200	1.63688800	-1.77183200
H	2.15087400	2.50096900	-1.24469000
H	2.90758000	1.98533300	-2.75295700
S	4.01960200	1.10447300	-0.79090000
C	4.98053900	0.19468100	-2.08559700
H	4.39018500	-0.65271800	-2.44589400
H	5.13843600	0.88466400	-2.92153100
C	6.29525400	-0.27604200	-1.51623300
C	7.29580800	0.65016000	-1.18813900
C	6.53641500	-1.63801200	-1.29925300
C	8.51114500	0.22177500	-0.65634900
H	7.11388300	1.70947500	-1.34842100
C	7.75357500	-2.06918000	-0.76799800
H	5.77028600	-2.36501300	-1.55442500
C	8.74305400	-1.13996900	-0.44397400
H	9.27896500	0.94935200	-0.41037600
H	7.92850500	-3.12947600	-0.61055600
H	9.69088100	-1.47358600	-0.03224700

C	-0.11999400	-2.33999300	1.76794200
C	1.05974000	-2.61910400	0.81426400
H	0.03788400	-2.89545500	2.69880100
H	-0.13004800	-1.27906000	2.03095000
C	2.37679300	-2.03723600	1.34215000
H	1.15458700	-3.70126000	0.65760500
H	0.84620200	-2.18151500	-0.16744800
C	3.56387100	-2.38673200	0.44411300
H	2.28485000	-0.94603700	1.41762800
H	2.55461100	-2.40478100	2.36131700
H	4.48516400	-1.92063300	0.80061900
H	3.72351900	-3.47014100	0.39767400
H	3.39731600	-2.02223700	-0.57469000
C	-3.66394800	2.48754000	-1.29674400
C	-3.94560700	3.33375000	-0.03339100
H	-4.03699600	3.01439600	-2.18211900
H	-2.58274200	2.37681500	-1.40083100
C	-3.14914500	4.64326300	-0.04110600
H	-5.02172400	3.54005500	0.03768100
H	-3.66863500	2.74429700	0.84730800
C	-3.39334900	5.48100300	1.21717200
H	-2.08189700	4.40407700	-0.12645300
H	-3.41425300	5.22617700	-0.93352300
H	-2.81530900	6.40950200	1.19201200
H	-4.45098000	5.74836700	1.32037700
H	-3.09965000	4.93006300	2.11805500
C	-1.06411400	-1.07386500	-2.16976400
C	-0.99723400	0.23009900	-2.53771800
H	-1.97873300	-1.64060200	-2.30542300
H	-0.17898700	-1.63114500	-1.88621200
H	-1.91484300	0.69544300	-2.89438900
Ni	-1.63645700	-0.02673600	-0.07331500
H	-0.29075200	-0.23385000	0.25396700
C	-0.17848000	2.13415800	0.90424600
O	0.11382000	2.98256700	0.04236400
N	-1.35464200	1.49450400	0.65682700
C	0.64465300	1.80061000	2.08545100
C	0.10873600	1.08390400	3.16676000
C	2.00104200	2.15167600	2.07136100
C	0.93519000	0.70872700	4.22330400
H	-0.94935200	0.83689700	3.17910400
C	2.82603100	1.75986900	3.12385500
H	2.39665400	2.71525200	1.23390800
C	2.29475900	1.03813200	4.19644700
H	0.52347700	0.16493100	5.06787200
H	3.88071700	2.01406600	3.10406300
H	2.93922300	0.73670200	5.01663900

TS2''

C	-3.33257300	3.55701500	0.03099300
C	-4.55714500	3.04262300	-0.32532600
C	-4.70029800	1.64658300	-0.51118600
C	-3.54323600	0.85862100	-0.32465100
C	-2.20563500	2.70872600	0.19465000

C	-5.93672200	1.01058800	-0.85828600
C	-3.62783900	-0.56724600	-0.45287900
C	-4.86808700	-1.17285500	-0.75694500
C	-6.01823000	-0.34687300	-0.97763800
C	-4.89662600	-2.58674700	-0.79310900
C	-3.75766700	-3.29805500	-0.49011500
C	-2.54725700	-2.62863600	-0.18305700
H	-6.81375100	1.63168000	-1.01193200
H	-3.20211200	4.62166400	0.19165900
H	-6.96084100	-0.82489300	-1.22514700
H	-3.76891500	-4.38234300	-0.46853100
N	-2.32969200	1.39018900	0.00672100
N	-2.49055100	-1.29082800	-0.21658700
H	-5.82437700	-3.09954000	-1.02974000
H	-5.41625900	3.69360100	-0.45893600
Ni	-0.90896500	-0.06339400	0.05199200
C	-0.63478200	0.35208900	-2.18175800
C	0.09264200	-0.78270600	-1.85338800
H	-1.66499100	0.21812700	-2.50689700
H	0.12697900	-1.03568600	-0.18121800
H	-0.35450000	-1.75567700	-2.01595500
H	1.17672700	-0.76173300	-1.79560200
C	-0.01695400	1.70384200	-2.43449500
H	-0.06885600	1.86756400	-3.52288800
H	-0.64983000	2.48701400	-2.00124000
C	1.43031700	1.80936500	-1.95145100
H	1.49169000	1.61494100	-0.87561300
H	2.00784200	1.02243400	-2.43617300
C	2.11170500	3.14220200	-2.25810500
H	1.55136000	3.98147300	-1.83013800
H	2.17971900	3.31389400	-3.33906600
S	3.78126300	3.29577800	-1.50310200
C	4.74125500	1.96642200	-2.35076500
H	4.72744200	2.15168900	-3.42962500
H	5.76530000	2.15814900	-2.01095100
C	4.35131500	0.52892000	-2.05679100
C	4.11631500	0.08287800	-0.74869900
C	4.19890600	-0.37935900	-3.11406100
C	3.73189800	-1.23685000	-0.50674300
H	4.17927400	0.78373200	0.07608800
C	3.81617800	-1.70249100	-2.87514600
H	4.37458500	-0.04783700	-4.13457200
C	3.58211300	-2.13668400	-1.56820800
H	3.54894800	-1.56127900	0.51355300
H	3.70815500	-2.39158700	-3.70805500
H	3.29708100	-3.16786100	-1.37839400
C	-1.33127200	-3.42033600	0.22036000
C	-0.70275400	-4.27268800	-0.90225800
H	-1.62129400	-4.08572300	1.04352000
H	-0.58326700	-2.73720400	0.62846100
C	0.67221600	-4.81563800	-0.49267100
H	-1.37344800	-5.10019600	-1.16468600
H	-0.59669800	-3.67633400	-1.81680200
C	1.36211800	-5.59186600	-1.61696500

H	1.30640500	-3.97363800	-0.18266900
H	0.55997800	-5.45402100	0.39302500
H	2.33481100	-5.97452000	-1.29414400
H	0.75870500	-6.44689700	-1.93993300
H	1.52805500	-4.95203500	-2.49153200
C	-0.88935800	3.28863600	0.62616600
C	-0.82275700	3.49731800	2.15592000
H	-0.73996400	4.25067800	0.12162000
H	-0.07489700	2.62469500	0.33692800
C	0.55770900	4.00500100	2.59072200
H	-1.60491900	4.20155400	2.46989100
H	-1.03276600	2.53885100	2.64286200
C	0.66370400	4.17137900	4.10909600
H	1.31893100	3.29885000	2.23875600
H	0.76416600	4.96396300	2.09623300
H	1.65358800	4.53756400	4.39719900
H	-0.07894400	4.88311000	4.48718700
H	0.49988600	3.21602300	4.62069300
C	1.25916200	0.21227500	1.84180200
O	2.07879500	1.04082300	1.39925700
N	-0.01735200	0.40369900	1.44640700
C	1.60773200	-0.89097900	2.77134500
C	0.65723400	-1.84060700	3.17401700
C	2.93204300	-0.98568600	3.21934500
C	1.03556300	-2.88769600	4.01179900
H	-0.37126000	-1.74889300	2.83739200
C	3.30684400	-2.03749700	4.05282000
H	3.64604300	-0.23178100	2.90384800
C	2.36063400	-2.98860000	4.44715700
H	0.30172600	-3.62236300	4.32910800
H	4.33280900	-2.11501100	4.39877200
H	2.65481900	-3.80594300	5.09867600

IM2''

C	-5.41809000	1.98061300	-1.46018300
C	-6.22637600	0.86612500	-1.52068800
C	-5.76059600	-0.36696100	-1.00415900
C	-4.46336700	-0.36578600	-0.45453000
C	-4.11498400	1.90989700	-0.90339000
C	-6.51324800	-1.58828800	-1.00055300
C	-3.92198600	-1.56135900	0.10987200
C	-4.68593100	-2.74548500	0.12269800
C	-5.99653500	-2.73251400	-0.46029500
C	-4.08947800	-3.87040500	0.74192600
C	-2.84091800	-3.75254400	1.31277200
C	-2.13222800	-2.52478600	1.26666900
H	-7.50971000	-1.58459400	-1.43115600
H	-5.76162200	2.93434600	-1.84487600
H	-6.57674400	-3.64986400	-0.45447200
H	-2.38467600	-4.59685200	1.81666100
N	-3.67016600	0.74284500	-0.41839900
N	-2.66875900	-1.46858600	0.64315900
H	-4.62811900	-4.81279600	0.78067600
H	-7.21873400	0.92641300	-1.95810400

Ni	-1.88444900	0.37589600	0.33607000
C	-0.83731000	0.04566600	-1.44910900
C	-1.83403600	-0.33994600	-2.51256100
H	-0.41947500	1.04012600	-1.60696100
H	-2.40669000	-1.23224500	-2.24591200
H	-2.51684800	0.46980000	-2.76902800
H	-1.26021700	-0.58644600	-3.41855800
C	0.18681900	-1.00974800	-1.11648800
C	1.42212800	-0.93349000	-2.04663000
H	1.13205000	-0.89897200	-3.10176800
H	1.94790900	0.00314200	-1.83525000
C	2.34487500	-2.14135900	-1.79791800
H	2.03208000	-2.99755800	-2.40264000
H	2.28682800	-2.45394300	-0.74966000
S	4.10752900	-1.82984600	-2.17926600
C	4.50867700	-0.90600800	-0.62785700
H	3.71447000	-0.17181400	-0.46154400
H	4.48957200	-1.61244400	0.20789000
C	5.84064500	-0.20953600	-0.70977600
C	6.91805300	-0.63408200	0.07532600
C	6.00891900	0.90115900	-1.54949800
C	8.13834700	0.04503100	0.03556100
H	6.80023800	-1.49890000	0.72355200
C	7.22591500	1.57900000	-1.59314900
H	5.17842100	1.22923800	-2.16894700
C	8.29405100	1.15395300	-0.79684600
H	8.96556400	-0.29429600	0.65194100
H	7.34341500	2.43792200	-2.24739600
H	9.24191200	1.68261600	-0.82950000
C	-0.79922000	-2.37406900	1.95139700
C	0.27327600	-3.40292200	1.53996200
H	-0.97015500	-2.45365400	3.03385800
H	-0.43178500	-1.36038100	1.77662900
C	1.65336600	-3.03624200	2.10232700
H	-0.01058000	-4.40285800	1.89008900
H	0.32902200	-3.46463600	0.44729000
C	2.73260000	-4.06508000	1.75376400
H	1.94650500	-2.04900100	1.72095400
H	1.58165300	-2.92997800	3.19315600
H	3.70498400	-3.76738700	2.15755000
H	2.48897800	-5.05038100	2.16520200
H	2.84446100	-4.17815800	0.66981500
C	-3.23973400	3.12321500	-0.79913600
C	-3.28047600	3.72834100	0.62443600
H	-3.57151600	3.87000200	-1.52722600
H	-2.20165000	2.86443100	-1.03179100
C	-2.38520300	4.96658400	0.74586800
H	-4.31621100	3.97985300	0.88876600
H	-2.94327200	2.96450500	1.33628200
C	-2.35520600	5.52076500	2.17303700
H	-1.37235100	4.70017500	0.42393200
H	-2.74308700	5.74020500	0.05348300
H	-1.71696800	6.40692600	2.23828900
H	-3.35725300	5.80547000	2.51333900

H	-1.96347100	4.77565800	2.87507800
C	0.37706000	2.10247300	0.43928900
O	0.20882200	2.96804700	-0.43669700
N	-0.70093900	1.39659500	0.88745000
C	1.70761600	1.78319700	1.02450400
C	1.86188000	0.84532500	2.05799500
C	2.83285000	2.44302800	0.50499000
C	3.13290300	0.56601400	2.55932500
H	0.98893800	0.35774900	2.47968800
C	4.09801600	2.16957300	1.01762200
H	2.68985600	3.16494700	-0.29209100
C	4.24955700	1.22807000	2.04156300
H	3.25131800	-0.15971800	3.35810000
H	4.97076400	2.66444500	0.60617000
H	5.24100700	1.00433300	2.42197600
H	-0.27748700	-2.00058200	-1.17628500
H	0.56546100	-0.88726400	-0.09961100

TS3''

C	5.04426200	-1.59067100	1.95903300
C	5.10945100	-2.89785700	1.53990100
C	4.08889800	-3.41416700	0.70798400
C	3.04954000	-2.52679600	0.34365600
C	3.96541200	-0.75472700	1.57024800
C	4.06978700	-4.76453900	0.23201400
C	1.99079600	-2.98599600	-0.51140500
C	2.01397900	-4.31804100	-0.98523900
C	3.06836000	-5.20073400	-0.58412400
C	0.98003300	-4.70113000	-1.86795300
C	0.03973800	-3.77577300	-2.25334000
C	0.07110300	-2.45271700	-1.74563200
H	4.87385400	-5.43101700	0.52826100
H	5.81319100	-1.17324200	2.60000500
H	3.05864400	-6.22115900	-0.95421300
H	-0.73078900	-4.04458500	-2.96499800
N	3.00449200	-1.23007300	0.76754300
N	1.01018600	-2.09227700	-0.85711300
H	0.95247200	-5.71506600	-2.25643900
H	5.93142100	-3.53989300	1.84295800
Ni	1.29883100	-0.31337000	0.08264200
C	0.40553700	-0.86290900	1.99792200
C	0.09200000	-2.32138600	2.17186900
H	1.22216300	-0.47401100	2.60183400
H	-0.53878800	-2.71317000	1.37164000
H	1.00497500	-2.91865100	2.22188900
H	-0.44206400	-2.46320200	3.12075400
C	-0.48635000	0.08275100	1.49063800
H	-0.24544900	1.12820000	1.69015500
H	0.06220100	0.32011800	-0.24797000
C	-1.90480000	-0.22509400	1.08567100
H	-1.96935800	-1.15718000	0.51834100
H	-2.45291600	-0.40516100	2.02166400
C	-2.57587900	0.91803600	0.31586700
H	-2.06815100	1.08479700	-0.64069000

H	-2.50078400	1.85578300	0.87780700
S	-4.32743800	0.59574800	-0.09999200
C	-5.12848900	0.93458900	1.53573000
H	-4.71567300	0.25401000	2.28637800
H	-4.88438300	1.96205100	1.82335400
C	-6.61679300	0.74137500	1.40195800
C	-7.42854200	1.78791200	0.94498100
C	-7.20328900	-0.49517900	1.69937700
C	-8.80350400	1.60482300	0.79980300
H	-6.97916800	2.74785300	0.70405000
C	-8.57852200	-0.67995700	1.55507000
H	-6.57956400	-1.31428100	2.04921900
C	-9.38135300	0.37036500	1.10526600
H	-9.42363500	2.42520400	0.45119300
H	-9.02319300	-1.64101100	1.79590400
H	-10.45228400	0.22853900	0.99555200
C	-0.88889900	-1.42527800	-2.29370900
C	-2.36354600	-1.84935600	-2.41565100
H	-0.51497000	-1.16391500	-3.29505800
H	-0.80976700	-0.50894400	-1.70479900
C	-3.19562100	-0.81711800	-3.18815800
H	-2.44468000	-2.81361000	-2.93104800
H	-2.79489000	-1.99665200	-1.41781300
C	-4.66524400	-1.22611000	-3.31303400
H	-3.12594900	0.15900500	-2.69175300
H	-2.75878200	-0.68224600	-4.18687300
H	-5.23554800	-0.47602700	-3.86811100
H	-4.76430600	-2.18099300	-3.84157800
H	-5.12583300	-1.33281400	-2.32620800
C	3.93858400	0.67054800	2.04728300
C	4.80853700	1.59504700	1.16310100
H	4.31571900	0.69997300	3.07647500
H	2.91637000	1.05354000	2.05969400
C	4.73530300	3.05889500	1.61764500
H	5.85030400	1.24811400	1.18029800
H	4.45860400	1.51177000	0.12931700
C	5.46153000	4.00325400	0.65525000
H	3.68410000	3.35758100	1.70240000
H	5.16284900	3.14651900	2.62539800
H	5.40966700	5.03838400	1.00560700
H	6.51970500	3.73630300	0.55594900
H	5.00848800	3.96693300	-0.34145300
C	1.59511100	2.53146100	0.14065700
O	1.11166500	2.75967900	1.27727600
N	1.93048400	1.26621800	-0.14548100
C	1.95031800	3.60159500	-0.82656600
C	2.62558800	3.31512700	-2.02276000
C	1.62376000	4.92390200	-0.50040800
C	2.97013500	4.35111600	-2.88811200
H	2.89098100	2.28878800	-2.26045100
C	1.97181700	5.95638800	-1.36861800
H	1.11034300	5.11939100	0.43516800
C	2.64437600	5.67121500	-2.56059000
H	3.49719700	4.13402300	-3.81204300

H	1.72325000	6.98263400	-1.11657700
H	2.91795600	6.47804000	-3.23388600

IM3''

C	5.16443800	0.04115000	-0.42462000
C	5.47390800	1.01879800	0.67435600
H	6.03709600	-0.42690500	-0.88089000
H	4.57900400	1.46212200	1.11732100
H	6.03821400	0.52981800	1.47858300
H	6.10553200	1.83563900	0.30249100
C	3.96120700	-0.30733500	-0.89608000
H	3.92609300	-1.04701900	-1.69673900
C	2.61661100	0.17863200	-0.42184600
H	2.70709100	1.03887000	0.24666300
H	2.03033300	0.51537700	-1.28669000
C	1.84650100	-0.93864200	0.30580500
H	2.40418200	-1.25591500	1.19262600
H	1.73967400	-1.82039700	-0.33755200
S	0.18775700	-0.45847500	0.92931500
C	-0.73251700	-0.31899700	-0.66905100
H	-0.29579100	0.48559000	-1.26729500
H	-0.60862800	-1.26048300	-1.21488100
C	-2.18780100	-0.04323500	-0.39229000
C	-3.08113900	-1.09815300	-0.16335900
C	-2.66448700	1.27213700	-0.32692400
C	-4.42455800	-0.84474800	0.11259900
H	-2.71666400	-2.12155600	-0.20011800
C	-4.00784800	1.52877500	-0.04975600
H	-1.97677500	2.09731400	-0.49388200
C	-4.89181100	0.47046500	0.16965700
H	-5.10650300	-1.67300200	0.28309200
H	-4.36383900	2.55419600	-0.00609200
H	-5.93815900	0.66887000	0.38338800

TS4''

C	0.36000000	-4.00998700	1.22479700
C	1.64159600	-4.46163100	1.42608300
C	2.72581800	-3.56612300	1.27021100
C	2.41367400	-2.24280600	0.88170900
C	0.11433100	-2.66505300	0.84178300
C	4.09003200	-3.93596500	1.50191100
C	3.47169100	-1.28212400	0.74656400
C	4.80462900	-1.66324100	1.02751900
C	5.09312800	-3.01849100	1.38884800
C	5.78897400	-0.65064800	0.95916900
C	5.41617500	0.63879200	0.66015600
C	4.06339600	0.95276500	0.37841600
H	4.30749900	-4.96083000	1.78645800
H	-0.49104000	-4.66960000	1.35370700
H	6.12411600	-3.29594500	1.58460700
H	6.14923900	1.43754500	0.64009400
N	1.13436800	-1.81651400	0.65859900
N	3.12788400	-0.00635200	0.39045400
H	6.82650100	-0.89496200	1.16789000

H	1.83186700	-5.49165400	1.71344000
Ni	1.14047500	0.12613500	-0.07701000
C	1.38102300	-0.73243800	-2.07261000
C	1.56324200	0.64230000	-2.26527700
H	2.29329600	-1.29312000	-1.87234600
H	1.21808800	1.38883200	-0.74023100
H	2.59834100	0.96193200	-2.17562500
C	0.23956900	-1.61413700	-2.51302000
H	0.55557700	-2.06681400	-3.46597700
H	0.19171900	-2.45365800	-1.81106300
C	-1.15993700	-1.01059900	-2.68208800
H	-1.43476700	-0.38696900	-1.82811100
H	-1.21135700	-0.38759600	-3.57878600
C	3.68950800	2.38235900	0.08365500
C	4.32096700	2.94557700	-1.20679800
H	4.01702500	2.99804100	0.93123100
H	2.60128500	2.47368300	0.04389000
C	3.77969600	4.33697400	-1.55636400
H	5.41151900	2.99030100	-1.09591500
H	4.13757800	2.26222600	-2.04672500
C	4.40245200	4.90753600	-2.83327300
H	2.68781400	4.27888300	-1.66833600
H	3.96298500	5.01713500	-0.71455600
H	3.99747600	5.89730900	-3.06194600
H	5.48865800	5.00622300	-2.73311400
H	4.20539100	4.25877700	-3.69434700
C	-1.29737700	-2.18440700	0.70971700
C	-1.85586500	-1.71374200	2.07087400
H	-1.92390700	-2.98363900	0.30282500
H	-1.34185600	-1.34943400	0.01413700
C	-3.24526600	-1.09453300	1.90885900
H	-1.89011500	-2.55852000	2.77205000
H	-1.16648100	-0.97404100	2.49410500
C	-3.83226100	-0.58569500	3.22621600
H	-3.18462300	-0.26866400	1.19204700
H	-3.92209800	-1.82763800	1.45456700
H	-4.82704600	-0.15946600	3.06555400
H	-3.92665400	-1.39212400	3.96221400
H	-3.20297000	0.19809900	3.66164500
C	-1.19806300	1.72220700	0.29484700
O	-1.62650200	1.86526200	-0.86957700
N	-0.33314000	0.72359900	0.56712200
C	-1.67759900	2.54623900	1.43672100
C	-1.35274700	2.23180000	2.76509800
C	-2.48216600	3.65875400	1.15435900
C	-1.83514700	3.02608300	3.80348000
H	-0.74112600	1.36092500	2.97865500
C	-2.96621000	4.44650100	2.19601100
H	-2.71687900	3.88392500	0.11915100
C	-2.64378400	4.13075700	3.51983300
H	-1.59112900	2.78010100	4.83234200
H	-3.59382300	5.30537600	1.97916600
H	-3.02453400	4.74462600	4.33057200
S	-2.34307000	-2.40206800	-2.87217600

C	-3.90869100	-1.47429300	-3.21446800
H	-4.56432300	-2.22749600	-3.65996700
H	-3.68673900	-0.73463700	-3.99005400
C	-4.55870700	-0.83401700	-2.01527100
C	-4.24884300	0.48286800	-1.65414800
C	-5.50144900	-1.53937200	-1.25357900
C	-4.86981500	1.08600200	-0.55864300
H	-3.51779700	1.04498000	-2.22454800
C	-6.13499800	-0.93391400	-0.16855900
H	-5.75032600	-2.56284100	-1.52323000
C	-5.82292000	0.38340300	0.17986900
H	-4.60448000	2.10229400	-0.28583900
H	-6.87608300	-1.48670700	0.40144200
H	-6.31852900	0.85616900	1.02263500
C	0.66581100	1.58721300	-3.02743900
H	0.66876700	1.29331300	-4.08363300
H	-0.35524700	1.58257400	-2.64903200
H	1.05004800	2.60765200	-2.95758200