

Supporting Information

Theoretical Studies on Iron-Catalyzed Azaindoline Formation: Mechanism and Site-selectivity

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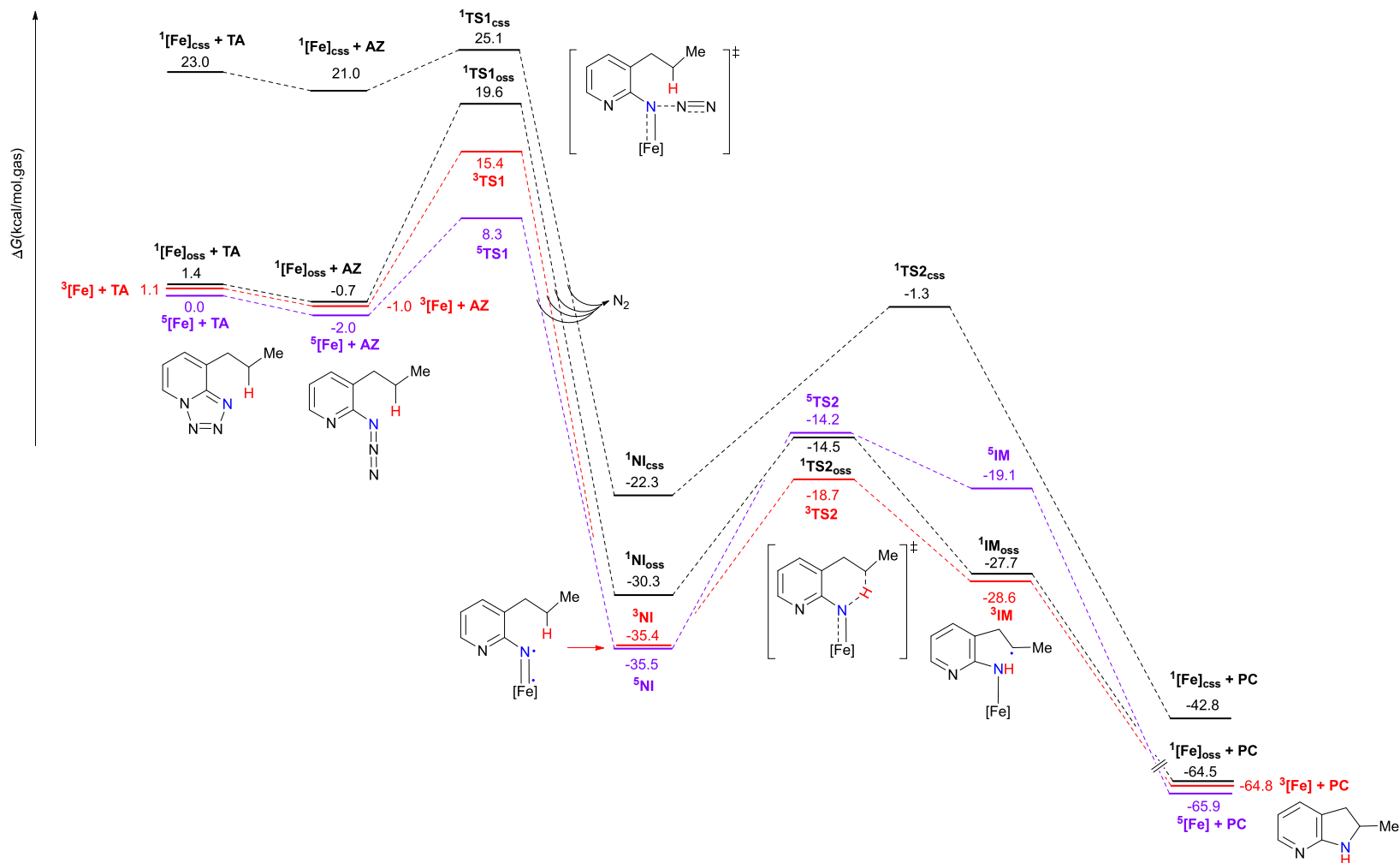


Fig. S1 Gibbs free energy profile of close- and open-shell singlet, triplet and quintet pathways for Fe-catalyzed C(sp³)-H amination. Based on comparison of energy, the most favorable transition state is quintet **⁵TS1** for N₂ release and triplet **³TS2** for H-atom abstraction. For overall C(sp³)-H amination, the most favorable pathway is **⁵[Fe] + TA → ⁵[Fe] + AZ → ⁵TS1 → ³NI + N₂ → ³TS2 → ³IM → ⁵[Fe] + PC**.

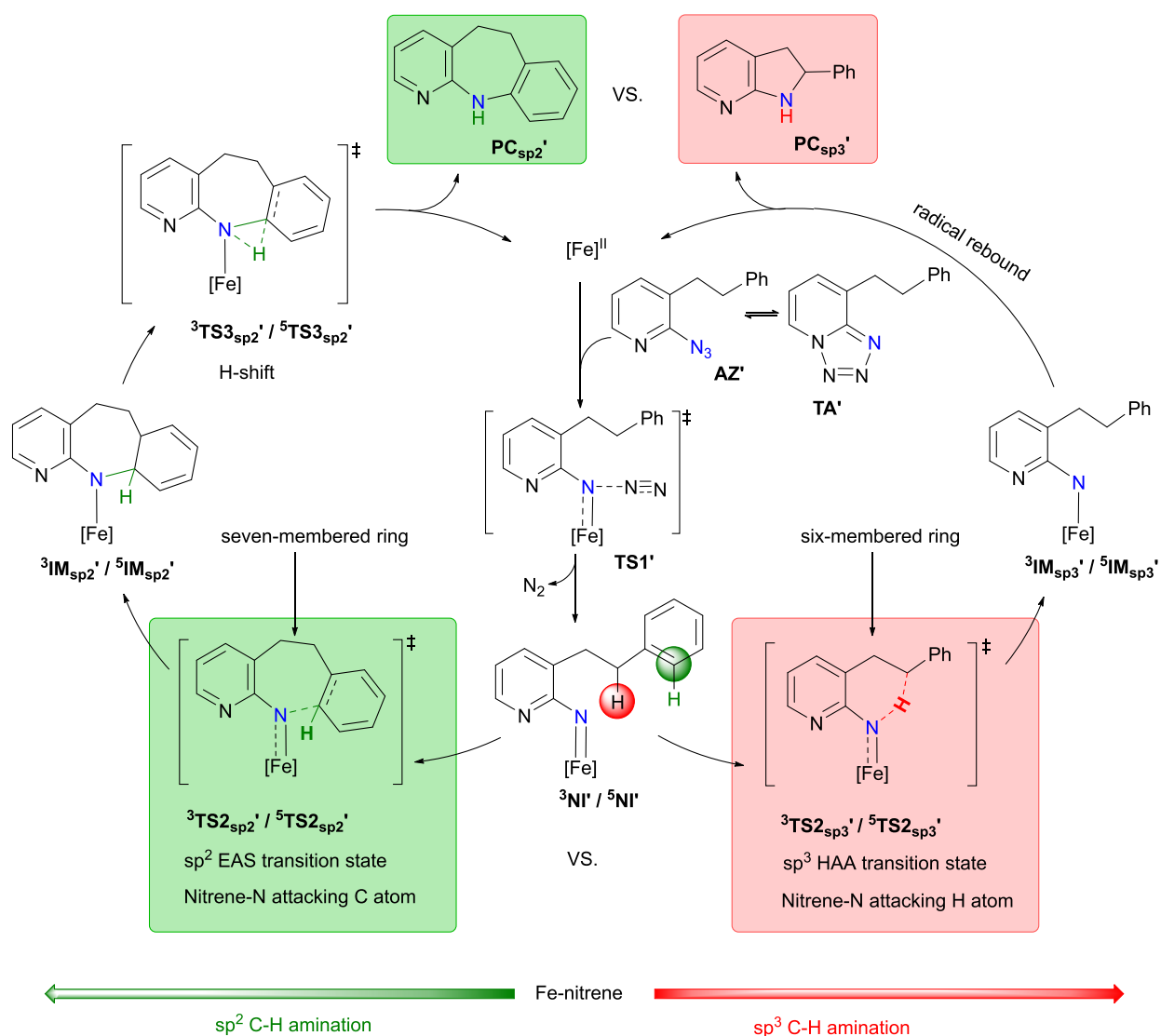


Fig. S2 Catalytic cycles of sp^3 - and sp^2 C-H bond aminations for the substrate TA' . Obviously, sp^3 -to- sp^2 C-H bond site-selectivity occurs after metal-nitrene is formed. Thus our investigations on site-selectivity start from Fe-nitrene. In addition, for sp^3 C-H amination mechanism, H-atom abstraction (HAA) for N-H bond formation preceding radical rebound (for C-N bond formation). Conversely, electrophilic aromatic substitution (EAS) for C-N bond formation preceding H-shift step (for N-H bond formation) in sp^2 C-H amination mechanism. Based on previous literature report (ACS Catal., 2018, 8, 8369–8375.), sp^3 -to- sp^2 C-H bond site-selectivity depends on barriers of HAA vs. EAS steps, thus Fe-nitrene and transition states of HAA and EAS are calculated for competition. In terms of spin states, the triplet and quintet are calculated because they are involved the most favorable pathway on the basis of the mechanism established in this work.

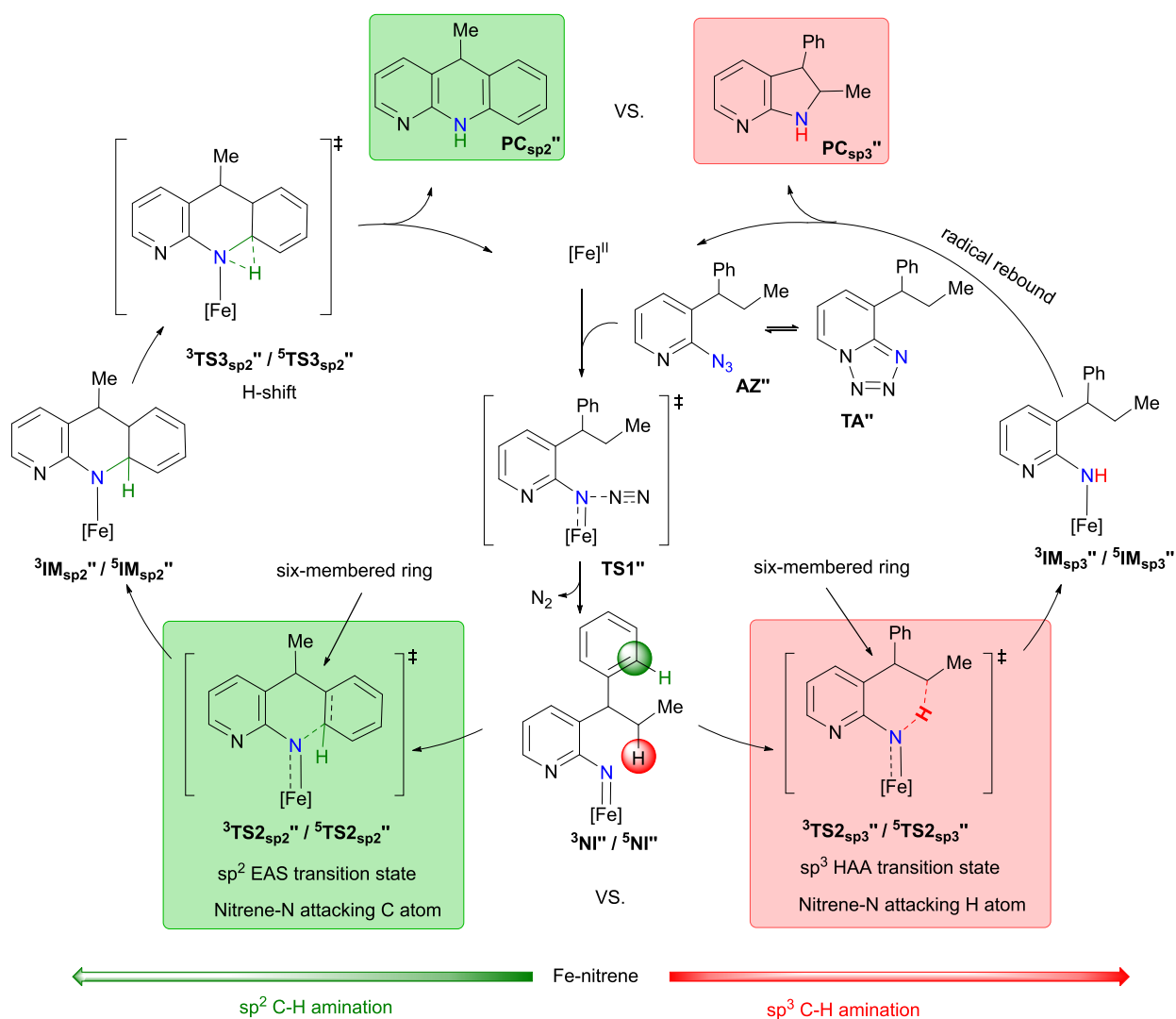


Fig. S3 Catalytic cycles for sp³- and sp² C-H bond aminations of the substrate **TA**. HAA: H-atom abstraction. EAS: electrophilic aromatic substitution. The sp³-to-sp² C-H bond site-selectivity depends on barriers of HAA vs. EAS steps. The triplet and quintet Fe-nitrene and transition states are calculated because they are involved the most favorable pathway on the basis of the mechanism established in this report.

Table S1 Calculation energies of sp³ C-H amination species for alkyl chain substrate **TA** at 393K (unit: a.u.).

Species	Thermal Correction of Gibbs Energies (BS1, gas)	Gibbs Free Energies (BS1, gas)	Singlet Point Energies (BS2, gas)	Singlet Point Energies (BS2, sol)
¹[Fe]_{css}	0.211141	-1111.665381	-1112.21938385	-1112.25078453
¹[Fe]_{oss}	0.210573	-1111.698667	-1112.25333521	-1112.27941015
³[Fe]	0.209134	-1111.699139	-1112.25240453	-1112.27924866
⁵[Fe]	0.205837	-1111.698333	-1112.25078638	-1112.28267567
TA	0.127569	-529.710665	-530.00942104	-530.02195655
AZ	0.123300	-529.710274	-530.00839375	-530.01537444
¹TS1_{css}	0.361961	-1641.366822	-1642.24870085	-1642.27656099
¹TS1_{oss}	0.359317	-1641.371646	-1642.25489540	-1642.28487342
³TS1	0.358981	-1641.379459	-1642.26120274	-1642.29067517
⁵TS1	0.354611	-1641.384765	-1642.26819889	-1642.29827342
N₂	-0.019923	-109.540641	-109.56018454	-109.55470218
¹Ni_{css}	0.359936	-1531.895781	-1532.74216055	-1532.77539918
¹Ni_{oss}	0.356384	-1531.90772	-1532.75130819	-1532.78493978
³Ni	0.354974	-1531.914984	-1532.75803596	-1532.79232418
⁵Ni	0.350706	-1531.90881	-1532.75402428	-1532.78779525
¹TS2_{css}	0.355875	-1531.858483	-1532.70456794	-1532.73869628
¹TS2_{oss}	0.354005	-1531.8778	-1532.72381902	-1532.75782734
³TS2	0.352042	-1531.884214	-1532.72847160	-1532.76280997
⁵TS2	0.348019	-1531.876264	-1532.71742073	-1532.75232881
¹IM_{oss}	0.354893	-1531.897633	-1532.74578347	-1532.78004898
³IM	0.353642	-1531.89909	-1532.74591219	-1532.78020884
⁵IM	0.348519	-1531.88108	-1532.72562194	-1532.75962086
PC	0.123738	-420.263804	-420.53043049	-420.54330749

Table S2 Calculation energies of sp³ H-abstraction vs. sp² electrocyclization species for aryl chain substrate **TA'** at 393K (unit: a.u.).

	Thermal Correction of Gibbs Energies (BS1, gas)	Gibbs Free Energies (BS1, gas)	Singlet Point Energies (BS2, gas)	Singlet Point Energies (BS2, sol)
³ NI'	0.401375	-1723.612851	-1724.56550581	-1724.60381062
⁵ NI'	0.395157	-1723.608807	-1724.56182014	-1724.59996503
³ TS _{sp3} '	0.396574	-1723.588137	-1724.54013389	-1724.57828936
⁵ TS _{sp3} '	0.392451	-1723.580758	-1724.52805481	-1724.56732562
³ TS _{sp2} '	0.406762	-1723.575374	-1724.53281747	-1724.56795342
⁵ TS _{sp2} '	0.401785	-1723.570773	-1724.52408240	-1724.56003107

Table S3 Calculation energies of sp³ H-abstraction vs. sp² electrocyclization species for aryl chain substrate **TA''** at 393K (unit: a.u.).

	Thermal Correction of Gibbs Energies (BS1, gas)	Gibbs Free Energies (BS1, gas)	Singlet Point Energies (BS2, gas)	Singlet Point Energies (BS2, sol)
³ NI''	0.428082	-1762.901617	-1763.89403716	-1763.93172840
⁵ NI''	0.422516	-1762.896474	-1763.88917003	-1763.92725036
³ TS _{sp3} ''	0.423166	-1762.875896	-1763.86693491	-1763.90488627
⁵ TS _{sp3} ''	0.418565	-1762.868544	-1763.85565751	-1763.89450875
³ TS _{sp2} ''	0.431705	-1762.861832	-1763.85833151	-1763.89446645
⁵ TS _{sp2} ''	0.427317	-1762.861464	-1763.85234361	-1763.88920504

Cartesian coordinates of species

¹[Fe]

C	-3.41158500	0.29033200	-0.00023100
C	0.29033500	3.41158600	0.00016600
C	3.41158500	-0.29033800	-0.00013000
C	-0.29033500	-3.41158100	0.00016300
C	-2.66978200	1.46373800	-0.00013400
C	-3.24130300	2.78842800	-0.00015900
C	-2.20061100	3.66587900	-0.00000300
C	-0.99154800	2.87873200	0.00009200
C	1.46374200	2.66977900	0.00013000
C	2.78843600	3.24129200	0.00006600
C	3.66588800	2.20060100	-0.00005900
C	2.87873400	0.99154400	-0.00004800
C	2.66977900	-1.46374500	-0.00005300
C	3.24128800	-2.78843200	-0.00006900
C	2.20059700	-3.66588200	0.00005500
C	0.99154700	-2.87873100	0.00012400
C	-1.46374100	-2.66977900	0.00009500
C	-2.78842300	-3.24129800	0.00000400
C	-3.66587400	-2.20060700	-0.00014500
C	-2.87873200	-0.99155100	-0.00013100
N	-1.29398600	1.53471900	-0.00000500
N	1.53471900	1.29398500	0.00004300
N	1.29397800	-1.53470800	0.00004100
N	-1.53470900	-1.29397700	-0.00000600
H	-4.49348800	0.38240400	-0.00041800
H	0.38241000	4.49348900	0.00015600
H	4.49348800	-0.38241600	-0.00029200
H	-0.38240900	-4.49348400	0.00015300
Fe	0.00000100	0.00000400	0.00005100
H	-4.30312800	2.99995700	-0.00018200
H	-2.22966300	4.74818000	0.00012400
H	-4.74817600	-2.22966400	-0.00016200
H	-2.99995600	-4.30312400	0.00013300
H	2.22965000	-4.74818500	0.00017500
H	4.30311200	-2.99996700	-0.00006800
H	4.74819000	2.22965100	-0.00005600
H	2.99996700	4.30311700	0.00019100

¹[Fe]_{oss}

C	-0.32963500	3.40869200	-0.00007500
C	3.40941900	0.32969600	0.00012000
C	0.32967400	-3.40874500	0.00009000

C	-3.40946300	-0.32964600	-0.00012900
C	0.95742200	2.88864500	-0.00001800
C	2.15547100	3.68876900	0.00002000
C	3.20745700	2.82257500	0.00005300
C	2.65237200	1.49320400	0.00007000
C	2.88931400	-0.95730700	0.00012900
C	3.68889200	-2.15562600	0.00017300
C	2.82240100	-3.20738000	0.00018700
C	1.49324400	-2.65175400	0.00011600
C	-0.95740400	-2.88873600	0.00002600
C	-2.15544600	-3.68878100	0.00000200
C	-3.20741500	-2.82253200	-0.00007700
C	-2.65233200	-1.49315500	-0.00007300
C	-2.88940400	0.95741400	-0.00013300
C	-3.68889600	2.15578800	-0.00019400
C	-2.82233200	3.20749100	-0.00016300
C	-1.49321700	2.65170000	-0.00010800
N	1.27490800	1.54742900	0.00001700
N	1.54778000	-1.27447900	0.00008500
N	-1.27485000	-1.54745000	-0.00001800
N	-1.54787500	1.27447600	-0.00008600
H	-0.43413800	4.48932200	-0.00009400
H	4.49007200	0.43417100	0.00015200
H	0.43417600	-4.48938400	0.00012300
H	-4.49011900	-0.43410000	-0.00017400
Fe	-0.00002600	-0.00008000	-0.00000300
H	-4.26645200	-3.04754500	-0.00012300
H	-2.17311100	-4.77132300	0.00003100
H	3.04719600	-4.26646600	0.00022800
H	4.77142700	-2.17357100	0.00020300
H	4.26650300	3.04757100	0.00007800
H	2.17304100	4.77130600	0.00000800
H	-3.04697500	4.26660900	-0.00018500
H	-4.77142700	2.17379100	-0.00024400

³[Fe]

C	0.00082300	-3.42365300	-0.00007500
C	-3.42385600	-0.00081500	0.00007100
C	-0.00080800	3.42365300	0.00008800
C	3.42387900	0.00081500	-0.00016900
C	-1.22938800	-2.78368000	-0.00001300
C	-2.50089200	-3.46431600	0.00004800
C	-3.46317200	-2.50257200	0.00008800
C	-2.78324100	-1.23069300	0.00004400
C	-2.78382700	1.22936700	0.00010400
C	-3.46436400	2.50092200	0.00021200
C	-2.50254200	3.46312500	0.00021600

C	-1.23071300	2.78309400	0.00012000
C	1.22938300	2.78365100	0.00002900
C	2.50088800	3.46430900	0.00003100
C	3.46317600	2.50257800	-0.00004400
C	2.78325300	1.23068700	-0.00009400
C	2.78383900	-1.22936100	-0.00015200
C	3.46436700	-2.50092900	-0.00016200
C	2.50253800	-3.46311800	-0.00013400
C	1.23070800	-2.78306600	-0.00010200
N	-1.41774800	-1.41829100	-0.00000600
N	-1.41842300	1.41761600	0.00006100
N	1.41776900	1.41826700	-0.00003600
N	1.41844400	-1.41759200	-0.00010300
H	0.00109900	-4.50917000	-0.00010200
H	-4.50937300	-0.00107400	0.00008800
H	-0.00104800	4.50917000	0.00011300
H	4.50939500	0.00107400	-0.00023100
Fe	-0.00002500	0.00000000	-0.00000500
H	4.53909500	2.62224400	-0.00009200
H	2.61994100	4.54029800	0.00005300
H	-2.62212600	4.53905400	0.00025000
H	-4.54034100	2.62007400	0.00024500
H	-4.53909200	-2.62223700	0.00011300
H	-2.61996300	-4.54030200	0.00002900
H	2.62210400	-4.53905000	-0.00016400
H	4.54034400	-2.62008200	-0.00021600

⁵[Fe]

C	-3.43968200	-0.09166100	-0.00008300
C	-0.09166100	3.43968000	-0.00006900
C	3.43968200	0.09166100	-0.00004400
C	0.09166100	-3.43968000	-0.00006300
C	-2.84954000	1.17728500	-0.00004200
C	-3.56188700	2.43539600	-0.00031900
C	-2.62164700	3.42712500	-0.00034500
C	-1.32738100	2.78279500	-0.00036000
C	1.17728500	2.84953800	-0.00002000
C	2.43539500	3.56188600	-0.00033300
C	3.42712500	2.62164700	-0.00029600
C	2.78279700	1.32738100	-0.00000900
C	2.84954000	-1.17728500	-0.00001000
C	3.56188700	-2.43539600	-0.00029900
C	2.62164700	-3.42712500	-0.00030100
C	1.32738100	-2.78279500	-0.00001800
C	-1.17728500	-2.84953700	-0.00003200
C	-2.43539600	-3.56188600	-0.00034900
C	-3.42712500	-2.62164700	-0.00032300

C	-2.78279700	-1.32738100	-0.00004300
N	-1.49706700	1.41934900	0.00022600
N	1.41935100	1.49706500	0.00025400
N	1.49706700	-1.41934900	0.00024700
N	-1.41935100	-1.49706500	0.00023400
H	-4.52589100	-0.12060300	-0.00027600
H	-0.12060300	4.52588900	-0.00027700
H	4.52589100	0.12060300	-0.00023500
H	0.12060300	-4.52588900	-0.00026100
Fe	0.00000000	0.00000000	0.00065000
H	-2.78302900	4.49805600	-0.00057900
H	-4.63989500	2.53950900	-0.00053300
H	-4.49805700	-2.78303100	-0.00054200
H	-2.53950700	-4.63989400	-0.00058700
H	2.78302900	-4.49805600	-0.00052100
H	4.63989500	-2.53950900	-0.00051700
H	4.49805700	2.78303000	-0.00051100
H	2.53950700	4.63989400	-0.00057900

TA

C	0.50109300	-0.38953500	0.19043800
C	-0.38215900	0.71812600	0.32976300
C	0.17553000	1.96566600	0.15339600
C	1.55921900	2.13986000	-0.15071700
C	2.38649200	1.05977000	-0.27741800
N	1.82766800	-0.17777500	-0.10082500
H	-0.45391100	2.84584600	0.25000400
H	1.96690900	3.13581200	-0.28276700
H	3.44433400	1.08415500	-0.50348000
N	0.31731900	-1.71006900	0.29099400
N	1.51926900	-2.26832500	0.06323900
N	2.44936700	-1.38714600	-0.17527200
C	-1.83712100	0.47019000	0.62521100
H	-2.31403200	1.41477900	0.91513100
H	-1.91664000	-0.21105600	1.48230000
C	-2.59361600	-0.15068200	-0.56829800
H	-2.50440200	0.51760000	-1.43510600
H	-2.10633700	-1.09380700	-0.83995600
C	-4.06958300	-0.39736200	-0.24451500
H	-4.58179200	0.53679100	0.01839100
H	-4.59287400	-0.83685600	-1.10079700
H	-4.17575300	-1.08626500	0.60216100

AZ

C	0.74342300	0.09182500	-0.12460700
C	-0.31730900	-0.81310800	-0.34184800
C	0.00164700	-2.16377900	-0.20224800

C	1.30038800	-2.55685300	0.13062300
C	2.25815900	-1.56264100	0.31590200
N	1.99172200	-0.25716200	0.19081600
H	-0.77459700	-2.90929900	-0.35868400
H	1.56188500	-3.60448200	0.24003800
H	3.28477500	-1.81502000	0.57383200
N	0.44130400	1.47051000	-0.25988100
C	-1.71437100	-0.34245200	-0.66279100
H	-2.27197000	-1.16269400	-1.13356300
H	-1.67137000	0.47513500	-1.39253700
C	-2.48174900	0.14309700	0.58383300
H	-2.52946100	-0.67497700	1.31503900
H	-1.91217800	0.95290100	1.05533900
C	-3.89411100	0.62682100	0.24376100
H	-4.48785400	-0.17332000	-0.21591200
H	-4.42533600	0.96478800	1.14061400
H	-3.86250000	1.46500400	-0.46306500
N	1.38076100	2.26126200	-0.06960400
N	2.14509100	3.08889100	0.07912000

¹TS1_{css}

H	-5.71277700	-0.59876100	0.61897400
C	-4.71559100	-0.86218900	0.28964000
C	-4.22077500	-2.09122200	-0.02410000
C	-3.64073400	0.07978400	0.10289000
C	-2.84467900	-1.90176400	-0.40814200
H	-4.72842000	-3.04742900	-0.01001400
N	-2.49995800	-0.56746600	-0.32602600
C	-3.74706600	1.43979800	0.35981000
C	-2.00794200	-2.92502900	-0.82523500
C	-2.72216700	2.36213300	0.20064200
H	-4.70632300	1.80892300	0.70951000
C	-0.69908000	-2.75910700	-1.25034600
H	-2.41580400	-3.93129800	-0.83450500
N	-1.45494500	2.05785500	-0.23691200
C	-2.84766900	3.77891700	0.45085700
N	-0.03136800	-1.55946200	-1.29726300
C	0.14936900	-3.83240100	-1.71260700
C	-0.78682600	3.25814100	-0.29082100
C	-1.64316600	4.33551300	0.14899000
H	-3.74952800	4.26567700	0.80007200
C	1.21983100	-1.85433000	-1.78535600
C	1.34423000	-3.27102800	-2.04120700
H	-0.15015900	-4.87096500	-1.77595600
C	0.50344300	3.43078900	-0.77080000
H	-1.34978100	5.37685300	0.19364700
C	2.21760400	-0.92304800	-2.02957900

H	2.23214100	-3.75030400	-2.43392700
C	1.30833000	2.42177100	-1.28027400
H	0.90489300	4.43982300	-0.77793900
C	2.09153100	0.44626600	-1.83956700
H	3.16187600	-1.28840300	-2.42189200
N	0.98231300	1.08164500	-1.32230700
C	2.63497400	2.63160600	-1.80570200
C	3.12288000	1.40583300	-2.14684500
H	3.11576500	3.59770100	-1.89429100
H	4.08542400	1.15834300	-2.57634800
Fe	-0.68372500	0.22094000	-0.59082400
C	0.79022200	-1.03455800	1.46108600
C	2.17100400	-0.74424900	1.56893300
C	1.08895600	-3.26841900	1.87040900
C	3.00909600	-1.84861100	1.74805000
H	0.61880600	-4.23653800	2.03066500
C	2.47500200	-3.12944000	1.88662300
H	4.08308400	-1.70561400	1.80574800
H	3.11645600	-3.99303000	2.03293300
N	0.25941500	-2.24649000	1.64665000
C	4.57634000	2.35129700	1.40647300
H	4.09298800	2.86792700	0.57015400
H	4.26699000	2.84955000	2.33370000
N	-0.05998300	0.06054800	1.13375500
N	-1.26927300	-0.04461800	2.19658500
N	-2.01220100	0.55523400	2.78293100
C	2.67187100	0.68602800	1.56634800
H	2.16928900	1.24451200	0.77638700
H	2.33846900	1.15666900	2.50429400
C	4.18640300	0.87010800	1.42171600
H	4.51857900	0.39178700	0.49051400
H	4.71433300	0.36660800	2.24303900
H	5.66020800	2.47727600	1.30346400

¹TS_{1oss}

H	0.04319700	5.46847700	0.88049600
C	-0.24587400	4.56330100	0.36174400
C	-1.37874200	4.31623800	-0.35158800
C	0.56013200	3.37158100	0.28678700
C	-1.28189500	2.96247200	-0.83219900
H	-2.21959700	4.97340900	-0.53363000
N	-0.08384800	2.39958700	-0.44859900
C	1.83699100	3.26349400	0.81436900
C	-2.28767400	2.31600300	-1.52920000
C	2.67785500	2.17992800	0.61430500
H	2.23095700	4.11476200	1.36062600
C	-2.26615100	0.97213300	-1.86398300

H	-3.17776400	2.88560500	-1.77760400
N	2.32562400	1.01785400	-0.03588200
C	4.06690600	2.14571400	0.99526300
N	-1.22011200	0.11172100	-1.62118100
C	-3.35830300	0.27547600	-2.49636000
C	3.47690300	0.25648500	-0.07381500
C	4.56614900	0.95926300	0.55359200
H	4.58070400	2.94338300	1.51642300
C	-1.62872500	-1.10947000	-2.10870600
C	-2.97033800	-1.02216100	-2.63138600
H	-4.29225600	0.73645000	-2.79177200
C	3.57301300	-1.02022400	-0.60028100
H	5.57363900	0.57396800	0.64419100
C	-0.83311700	-2.24041900	-2.19344100
H	-3.51438400	-1.84912900	-3.06981600
C	2.51461100	-1.72490800	-1.15273400
H	4.53622200	-1.51753500	-0.54542200
C	0.51156100	-2.28281700	-1.85841600
H	-1.27646300	-3.14044800	-2.60782000
N	1.23236900	-1.24122100	-1.31142800
C	2.60179400	-3.08277600	-1.62105600
C	1.35603200	-3.43223700	-2.05046800
H	3.50514900	-3.67921900	-1.61185600
H	1.02534100	-4.37442600	-2.46872300
Fe	0.48397000	0.49644000	-0.60856500
C	-1.45449800	-0.24426300	1.46330300
C	-1.93473100	-1.40988200	2.12331800
C	-3.52692900	0.76198700	1.52437100
C	-3.28710000	-1.41172900	2.47343600
H	-4.11549900	1.63972000	1.26078700
C	-4.10820900	-0.32611500	2.16962700
H	-3.70055500	-2.28303900	2.97659200
H	-5.16286000	-0.32469400	2.42837100
N	-2.23418600	0.81012200	1.20051800
C	0.36641300	-4.53646600	1.58637100
H	1.19747700	-4.24715700	2.24186800
H	-0.22570300	-5.29539400	2.11400100
N	-0.11419400	-0.16294200	1.01521000
N	0.81609300	-0.29555200	2.29552000
N	1.95709400	-0.36586200	2.37157300
C	-1.07395900	-2.61298600	2.44242700
H	-0.25183300	-2.31575300	3.10551500
H	-1.67824800	-3.33076800	3.01326800
C	-0.47982900	-3.31810200	1.21115400
H	0.13152600	-2.60300800	0.65912500
H	-1.29442800	-3.61467500	0.53741700
H	0.79658700	-5.00101700	0.69192900

³TS1

H	0.34478600	5.48934500	0.93265400
C	-0.01578000	4.60316600	0.42593200
C	-1.20407600	4.41161500	-0.21059500
C	0.72939000	3.37677900	0.29249800
C	-1.19498000	3.06105900	-0.71158100
H	-2.02654000	5.10550400	-0.32946400
N	-0.00201800	2.44505000	-0.41033100
C	2.02347400	3.19847100	0.75639500
C	-2.26321100	2.46775500	-1.36395600
C	2.79158700	2.06406100	0.54036700
H	2.48914600	4.02915200	1.27763900
C	-2.30928400	1.13703000	-1.74635900
H	-3.14260700	3.07664500	-1.54928800
N	2.34871200	0.91518600	-0.07707700
C	4.18948600	1.95287600	0.87404600
N	-1.29072600	0.22575100	-1.58208100
C	-3.45157700	0.50994200	-2.36245400
C	3.45146300	0.08777500	-0.14443000
C	4.60144600	0.73141000	0.43811400
H	4.76751400	2.72600700	1.36402500
C	-1.76544000	-0.95736800	-2.10419400
C	-3.12010000	-0.79369900	-2.57118600
H	-4.37761600	1.01820000	-2.59947600
C	3.45734500	-1.19112300	-0.67612000
H	5.58687200	0.28787700	0.50158400
C	-1.02602200	-2.11957100	-2.25194600
H	-3.71349700	-1.57873600	-3.02248900
C	2.35419500	-1.82243200	-1.23182700
H	4.39015500	-1.74543700	-0.64347700
C	0.32051000	-2.24390000	-1.94125600
H	-1.52226700	-2.98074100	-2.68844700
N	1.10199700	-1.26233300	-1.37118700
C	2.36131800	-3.17065800	-1.73684400
C	1.09644800	-3.43459200	-2.17149200
H	3.22844100	-3.81868400	-1.74817600
H	0.71015200	-4.34439900	-2.61311600
Fe	0.45097600	0.50558100	-0.62477000
C	-1.43148000	-0.25528800	1.52630200
C	-1.88230200	-1.46237100	2.13302700
C	-3.54037200	0.67810200	1.59686700
C	-3.23645200	-1.51765400	2.47163300
H	-4.15639900	1.54344200	1.35582700
C	-4.09205800	-0.45167900	2.19523400
H	-3.62549700	-2.41959000	2.93908900
H	-5.14878300	-0.49547500	2.44122200

N	-2.24528400	0.78694000	1.30070800
C	0.50800800	-4.50387800	1.51148600
H	1.33381900	-4.20768000	2.17078800
H	-0.06080300	-5.29066700	2.02377500
N	-0.10503100	-0.06937000	1.08200300
N	0.89575900	-0.36531100	2.32745000
N	2.02083800	-0.26167500	2.43061500
C	-0.99301100	-2.65251900	2.41789900
H	-0.18349700	-2.35883300	3.09851200
H	-1.58235200	-3.40443500	2.95957400
C	-0.37364400	-3.30103500	1.16879700
H	0.21630600	-2.55309800	0.63742000
H	-1.17741900	-3.60249800	0.48483600
H	0.94568600	-4.93429800	0.60415500

⁵TS1

H	-4.82106100	2.90565300	-1.11122600
C	-3.86589900	2.72908700	-0.63277900
C	-2.98090300	3.64717400	-0.14901800
C	-3.29537000	1.42399100	-0.38330600
C	-1.86460400	2.90838900	0.39676200
H	-3.06655200	4.72656600	-0.15182900
N	-2.08297000	1.56263700	0.24413400
C	-3.89714600	0.20856700	-0.71200200
C	-0.74124300	3.47557400	0.99484100
C	-3.39054400	-1.06467700	-0.45417100
H	-4.87016500	0.25866100	-1.19206300
C	0.34193200	2.78747500	1.54031500
H	-0.70700600	4.56003800	1.04466400
N	-2.16967200	-1.32968600	0.12582700
C	-4.08161300	-2.30379900	-0.71753800
N	0.48201900	1.42150400	1.57715300
C	1.48529800	3.40935200	2.16487300
C	-2.08296900	-2.69814300	0.25541500
C	-3.27406800	-3.31264600	-0.27917000
H	-5.06202900	-2.38021800	-1.17049600
C	1.67005400	1.16069800	2.21683300
C	2.30942500	2.40347800	2.57993200
H	1.62525000	4.47758400	2.27383600
C	-1.02333800	-3.38043300	0.85085700
H	-3.46259100	-4.37857400	-0.30195300
C	2.16500000	-0.11060800	2.50620400
H	3.25727200	2.48358700	3.09724000
C	0.09438100	-2.80788200	1.45924000
H	-1.08644400	-4.46462200	0.86611600
C	1.54064300	-1.32359000	2.21737000

H	3.11744600	-0.16023300	3.02576800
N	0.34444700	-1.46002400	1.55424800
C	1.16372600	-3.54603400	2.09128900
C	2.05913700	-2.62783400	2.55867500
H	1.21097800	-4.62529200	2.16450600
H	2.98549300	-2.80587900	3.09017400
Fe	-0.65484800	0.05562500	0.48121500
C	1.29640800	0.77128300	-1.64887700
C	2.49967300	0.23081600	-2.17385800
C	2.11902800	2.92172300	-1.70074900
C	3.51248900	1.14312400	-2.47830600
H	1.93298100	3.97197800	-1.48246000
C	3.33765800	2.50532600	-2.23548200
H	4.45201800	0.77629100	-2.88591600
H	4.12277600	3.22291100	-2.45429700
N	1.11318900	2.08536900	-1.44111000
C	3.00525700	-3.51607700	-1.20100100
H	2.13697800	-3.93821000	-1.72252600
H	3.89868000	-3.75523200	-1.79217700
N	0.22875800	-0.04492000	-1.22960200
N	-0.32170100	-0.90251200	-2.46045500
N	-1.15012800	-1.67962700	-2.52713800
C	2.72043900	-1.25334800	-2.34834400
H	1.89978400	-1.69383000	-2.92705400
H	3.63156700	-1.41177200	-2.94043700
C	2.84213700	-2.00676700	-1.00965400
H	1.94982400	-1.80685600	-0.41289300
H	3.69337100	-1.60145600	-0.44681400
H	3.08994600	-4.02186300	-0.23324400

¹Nl_{css}

N	0.01655300	0.09620600	1.03166000
H	-4.23213600	3.55567800	1.17523400
C	-3.82546600	2.57387900	0.96777400
C	-4.33624400	1.35559600	1.29380500
C	-2.59224000	2.32850800	0.25627800
C	-3.42042000	0.37101600	0.76630500
H	-5.25255400	1.12511100	1.82248700
N	-2.36228100	0.98094900	0.14221200
C	-1.75813000	3.31903700	-0.23621500
C	-3.61803400	-0.99999300	0.81509700
C	-0.55139000	3.09001000	-0.87987500
H	-2.05671200	4.35208100	-0.08628000
C	-2.80495300	-1.93361100	0.19192400
H	-4.50267100	-1.36734600	1.32607800
N	0.00430500	1.85380700	-1.13833600
C	0.33920100	4.13951600	-1.30483900

N	-1.63407700	-1.66239000	-0.48925300
C	-3.10582800	-3.34077800	0.13129400
C	1.25062700	2.11579300	-1.67186300
C	1.45989700	3.53556900	-1.78840100
H	0.12251300	5.19720400	-1.22432500
C	-1.19106300	-2.88378300	-0.95804600
C	-2.11615600	-3.92556600	-0.59708900
H	-3.97570300	-3.80072600	0.58287000
C	2.19094300	1.16180700	-2.02842200
H	2.35534400	3.99266600	-2.19004800
C	0.00336700	-3.11224700	-1.61671800
H	-1.99783100	-4.96839300	-0.86279200
C	1.97427700	-0.20615200	-1.99056200
H	3.14278000	1.51393000	-2.41335100
C	0.96037600	-2.13981700	-1.85498400
H	0.22584400	-4.13032800	-1.92084800
N	0.81731200	-0.80709700	-1.55162000
C	2.88253500	-1.18813100	-2.53280900
C	2.24375200	-2.38815900	-2.46411200
H	3.85978800	-0.96346900	-2.94118800
H	2.58946800	-3.35870900	-2.79689400
Fe	-0.67862100	0.06419000	-0.51295200
C	0.98304300	-0.75233900	1.50888700
C	1.92625400	-0.18336800	2.42292300
C	1.92589200	-2.84583700	1.70571900
C	2.92682500	-1.02844900	2.90480000
H	1.87807200	-3.89938400	1.43222500
C	2.93887900	-2.37636100	2.55056400
H	3.68121100	-0.63030600	3.57938500
H	3.69967000	-3.05258800	2.92897400
N	0.98853800	-2.06668300	1.18043600
C	2.22912600	2.26883500	1.72626200
C	3.62781700	2.05214800	1.14492100
H	2.15163300	3.28218600	2.14216400
H	1.48170800	2.19647900	0.93258800
C	1.85140900	1.26530700	2.83617400
H	2.51027700	1.41648900	3.70203500
H	3.85544500	2.81181100	0.38884900
H	4.39994700	2.10689800	1.92378200
H	3.70516700	1.07104200	0.66285600
H	0.82466400	1.48261900	3.15449700

¹Nl_{oss}

N	-0.09561400	-0.08273500	1.00316100
H	4.51627600	-3.09064900	1.38175900
C	4.02946700	-2.16296700	1.10838900
C	4.43629500	-0.88690700	1.34696800

C	2.78195600	-2.07237900	0.38523200
C	3.44095500	-0.02104600	0.75974400
H	5.32876100	-0.54442400	1.85525500
N	2.43878500	-0.75835400	0.18143300
C	2.04600400	-3.16489100	-0.04435800
C	3.51141500	1.36274800	0.73506900
C	0.84058400	-3.09479500	-0.72746600
H	2.43264600	-4.15319400	0.18523700
C	2.60250600	2.18327100	0.08616100
H	4.35672100	1.83742600	1.22354600
N	0.19056700	-1.93567900	-1.09584300
C	0.05850100	-4.24778000	-1.09207500
N	1.46564300	1.76555000	-0.58099800
C	2.74241200	3.61176800	-0.00965100
C	-1.01121800	-2.34540900	-1.63614500
C	-1.09363200	-3.78239900	-1.65104200
H	0.36055900	-5.27348500	-0.92217800
C	0.88374400	2.91834100	-1.07167300
C	1.68659800	4.06443800	-0.74102600
H	3.55683000	4.17785100	0.42435100
C	-2.02545700	-1.50457700	-2.06904100
H	-1.93397900	-4.34568900	-2.03653000
C	-0.32680800	2.99590200	-1.73736500
H	1.44923300	5.08133700	-1.02685500
C	-1.95139600	-0.12140000	-2.07851200
H	-2.92858700	-1.96509100	-2.45706000
C	-1.16487300	1.91749900	-1.96521700
H	-0.66015700	3.97597800	-2.06406700
N	-0.87859100	0.61592000	-1.63121000
C	-2.95138800	0.74087300	-2.66222400
C	-2.45516200	2.00645600	-2.60505800
H	-3.88794300	0.39874400	-3.08409600
H	-2.90168400	2.92530700	-2.96356400
Fe	0.69713000	-0.05298000	-0.56364900
C	-1.03742100	0.73264600	1.51420100
C	-1.92095200	0.15208300	2.49445200
C	-2.05856100	2.79564200	1.71300000
C	-2.90680800	0.97668200	3.03004100
H	-2.08143600	3.84013400	1.40187800
C	-2.98986700	2.31638100	2.64711900
H	-3.60582000	0.56913300	3.75688000
H	-3.74625100	2.97665800	3.06060400
N	-1.12239300	2.04574700	1.15299900
C	-2.15236100	-2.30167800	1.77678500
C	-3.54663200	-2.09719600	1.18011400
H	-2.06941200	-3.31501900	2.19186500
H	-1.39851800	-2.21846800	0.99044800

C	-1.79737900	-1.29682700	2.89530500
H	-2.44630800	-1.47564200	3.76338300
H	-3.76128500	-2.86229600	0.42548400
H	-4.32739700	-2.15238600	1.95028000
H	-3.62534400	-1.11927400	0.69178400
H	-0.76417400	-1.48948400	3.20933000

³Ni

N	-0.01057200	-0.23298100	0.83982500
H	3.99111500	3.69555500	0.65530100
C	2.94975200	3.42120000	0.54317300
C	1.84351600	4.08634800	0.97547200
C	2.48443000	2.22672600	-0.11722500
C	0.70481900	3.29926500	0.57332400
H	1.78457400	5.02254600	1.51600600
N	1.10869900	2.17576500	-0.10989600
C	3.32337400	1.26012700	-0.64984500
C	-0.61188800	3.63335700	0.85004500
C	2.90161900	0.08723000	-1.25583000
H	4.39333900	1.42944700	-0.57670100
C	-1.71253600	2.89622000	0.44715500
H	-0.79458100	4.54998500	1.40229800
N	1.59035600	-0.29185000	-1.43234800
C	3.79319000	-0.91995500	-1.77741300
N	-1.66849200	1.71296000	-0.25918500
C	-3.07886600	3.30170400	0.66565100
C	1.64325400	-1.52472900	-2.03942400
C	3.01114800	-1.92435700	-2.26002100
H	4.87342100	-0.85004700	-1.76461900
C	-2.98252100	1.37738400	-0.49577900
C	-3.86607500	2.36438400	0.07204900
H	-3.37511200	4.20034000	1.19170600
C	0.53635800	-2.27761000	-2.39753800
H	3.31345800	-2.85163600	-2.72982100
C	-3.40776200	0.25964100	-1.19078100
H	-4.94633300	2.32762300	0.01135000
C	-0.77677200	-1.87502800	-2.22255100
H	0.70923200	-3.23940700	-2.87021400
C	-2.56445700	-0.71057000	-1.70206600
H	-4.47644000	0.11593800	-1.31411200
N	-1.18697800	-0.69295600	-1.63639700
C	-1.91481600	-2.63465600	-2.66987400
C	-3.02180800	-1.90639600	-2.35847700
H	-1.85343500	-3.59358000	-3.16860000
H	-4.06178600	-2.14475500	-2.54182000
Fe	-0.05427400	0.60497100	-0.64998000
C	-0.72190800	-1.12077900	1.55325600

C	-0.01081500	-1.80739900	2.59976000
C	-2.68174000	-2.22102700	2.05354000
C	-0.72989000	-2.72295700	3.35747100
H	-3.73620700	-2.36628500	1.81935000
C	-2.08595800	-2.94384600	3.09442700
H	-0.22800400	-3.26687200	4.15506700
H	-2.66636600	-3.65328700	3.67624300
N	-2.04033400	-1.33600600	1.29807800
C	2.33463200	-2.20592800	1.70556900
C	3.80926900	-1.81583600	1.82946800
H	1.95845800	-1.89502400	0.72622800
H	2.22371800	-3.29759700	1.75888700
C	1.46172300	-1.55556600	2.80048500
H	1.76953300	-1.93193200	3.78531200
H	4.40772900	-2.28961800	1.04336000
H	3.92797200	-0.73030200	1.72714900
H	4.22522100	-2.11240500	2.80101500
H	1.64723500	-0.47413800	2.79142900

⁵Ni

N	-0.34625100	-0.08843600	-1.21394100
H	3.69794500	4.21329900	-1.19340000
C	3.47746600	3.16892900	-1.01085600
C	4.22292100	2.07693600	-1.34717300
C	2.30357000	2.68038300	-0.32401700
C	3.50692700	0.91647200	-0.86837000
H	5.17546300	2.04781300	-1.86138200
N	2.34301400	1.30958400	-0.25657900
C	1.30118000	3.48610900	0.21663500
C	3.94790400	-0.40220400	-0.98683800
C	0.19200200	3.05510400	0.94388800
H	1.41056000	4.55850200	0.08223800
C	3.30827800	-1.53378400	-0.48250300
H	4.89347900	-0.55907200	-1.49786300
N	-0.11817200	1.74472700	1.21608100
C	-0.80360800	3.92266000	1.53169800
N	2.11031300	-1.53150600	0.18638800
C	3.81504600	-2.88564800	-0.57143500
C	-1.27696000	1.75547200	1.95169200
C	-1.71226900	3.11848900	2.15612800
H	-0.79284100	5.00395800	1.47524200
C	1.84254100	-2.83356700	0.52537500
C	2.90792200	-3.68973900	0.05271200
H	4.74755100	-3.16703600	-1.04459500
C	-1.93760200	0.62024400	2.42156700
H	-2.59376800	3.40940100	2.71367200
C	0.72210000	-3.26564000	1.23163800

H	2.94851400	-4.76249300	0.19462000
C	-1.51110400	-0.69868100	2.27405800
H	-2.85989900	0.78052100	2.97224300
C	-0.29847200	-2.46149900	1.73624100
H	0.63929100	-4.33304800	1.41459400
N	-0.36536900	-1.09434600	1.62561200
C	-2.19167500	-1.85592500	2.80765200
C	-1.43970900	-2.94541400	2.47743500
H	-3.11570500	-1.82430500	3.37146800
H	-1.62536200	-3.98520600	2.71628000
Fe	0.73175300	0.05828300	0.26059500
C	-1.39989100	-0.80769200	-1.58234000
C	-2.49895500	-0.17359100	-2.27253200
C	-2.46690600	-2.86348900	-1.63849400
C	-3.59514200	-0.96752700	-2.60950600
H	-2.44136400	-3.92421800	-1.38912800
C	-3.59579300	-2.32341000	-2.29221800
H	-4.44577400	-0.52082900	-3.11893600
H	-4.43892700	-2.96050500	-2.54264400
N	-1.40804500	-2.15809500	-1.29573300
C	-2.65938300	2.19806500	-1.33932800
H	-2.61314800	3.24404100	-1.66912900
H	-1.81283900	2.04000700	-0.66856500
C	-2.46488600	1.29946500	-2.58199000
H	-3.24569700	1.52472500	-3.32082300
C	-3.97015700	1.94760400	-0.59051700
H	-4.06886700	2.64078500	0.25168700
H	-4.84161100	2.08082300	-1.24538900
H	-4.00587400	0.92932300	-0.18652800
H	-1.49723200	1.54593700	-3.03353000

¹TS2_{css}

N	0.02939900	0.01117500	1.04113900
H	4.61120100	2.90195700	0.93506500
C	3.56358300	2.79363700	0.68314500
C	2.55482300	3.69468100	0.83509700
C	2.97624000	1.61412300	0.08993300
C	1.35684300	3.06483400	0.32782500
H	2.60079100	4.69933700	1.23656000
N	1.63200200	1.79875200	-0.12257000
C	3.67144800	0.45581100	-0.22332400
C	0.11236900	3.67660000	0.26568900
C	3.10545400	-0.68477800	-0.77840100
H	4.73953600	0.43854000	-0.02747900
C	-1.02702200	3.10951600	-0.28452100
H	0.03220400	4.69165500	0.64333000
N	1.76474900	-0.86316300	-1.06521400

C	3.85333900	-1.86668400	-1.12115100
N	-1.12529400	1.83164000	-0.79316100
C	-2.28382200	3.80461600	-0.42371300
C	1.66277400	-2.14608000	-1.56378200
C	2.95910800	-2.77159800	-1.61274500
H	4.92437800	-1.97237900	-1.00174100
C	-2.42385500	1.71010000	-1.23621400
C	-3.14554500	2.94075500	-1.02582500
H	-2.45989100	4.82478000	-0.10633600
C	0.48300900	-2.77711200	-1.93196600
H	3.14392300	-3.77552800	-1.97402300
C	-2.98882500	0.56381000	-1.77074600
H	-4.18042200	3.10041200	-1.30151800
C	-0.76464000	-2.17377400	-1.94996200
H	0.55153500	-3.80536500	-2.27445100
C	-2.32939100	-0.64662400	-1.91101400
H	-4.02936800	0.61150900	-2.07757000
N	-1.01153000	-0.86916400	-1.59277300
C	-1.96419700	-2.79924900	-2.45848500
C	-2.93368000	-1.84529200	-2.44431800
H	-2.02640900	-3.82344300	-2.80445300
H	-3.96324700	-1.92254700	-2.77082600
Fe	0.26867000	0.40724400	-0.69796200
C	-1.06101600	-0.53662300	1.68511400
C	-0.86145100	-1.17571400	2.94896500
C	-3.33666600	-0.81215100	1.84714300
C	-1.97213100	-1.65077900	3.62423700
H	-4.30670200	-0.63769400	1.38309700
C	-3.24701500	-1.47591800	3.06973400
H	-1.84744700	-2.15398800	4.58064900
H	-4.13649800	-1.84942700	3.56710900
N	-2.28501300	-0.36863600	1.15558800
C	1.52348500	-1.50641700	2.33725400
H	2.52026400	-1.07074400	2.44193200
H	0.98140500	-0.43801000	1.52273400
C	0.55428100	-1.23865800	3.47452000
H	0.63978600	-2.00979600	4.25628900
C	1.46767700	-2.86011500	1.70461000
H	2.18547300	-2.96152000	0.89026400
H	1.69936800	-3.63208100	2.45882500
H	0.46094100	-3.07769300	1.32670700
H	0.81250400	-0.27604700	3.93916700

¹TS_{2oss}

N	-0.01653300	-0.09835000	0.99690700
H	4.76354600	2.68927500	0.89213700
C	3.70447100	2.62632300	0.67601600

C	2.72752600	3.53848000	0.93617200
C	3.06306300	1.50306100	0.03842900
C	1.49371500	2.97834500	0.44142500
H	2.81749400	4.50944300	1.40673400
N	1.71554900	1.73883800	-0.11083800
C	3.71336600	0.33642800	-0.33302800
C	0.26856800	3.62754000	0.48139600
C	3.08670700	-0.78076000	-0.86470600
H	4.78583000	0.28287400	-0.17266600
C	-0.90248300	3.14431200	-0.08080500
H	0.23549000	4.61013400	0.94208200
N	1.73316100	-0.89870400	-1.10523600
C	3.76627200	-2.00347600	-1.20881500
N	-1.04794100	1.92244000	-0.69960300
C	-2.13171900	3.89542500	-0.15590000
C	1.55229900	-2.18157300	-1.57398700
C	2.81280500	-2.87541500	-1.64303100
H	4.83429800	-2.15838300	-1.12191900
C	-2.34470800	1.89410500	-1.16084600
C	-3.02063000	3.12631400	-0.84165000
H	-2.27073700	4.88809100	0.25336600
C	0.33632400	-2.73047500	-1.95221100
H	2.93548100	-3.89470500	-1.98677000
C	-2.93922800	0.82241900	-1.80401400
H	-4.04586100	3.35100400	-1.10705900
C	-0.85747300	-2.03000800	-2.01544400
H	0.33143900	-3.76543500	-2.27994100
C	-2.32646100	-0.40281800	-2.00261000
H	-3.97249900	0.92947300	-2.11894300
N	-1.02379000	-0.70574600	-1.67318900
C	-2.08174500	-2.57033800	-2.55300600
C	-2.98737000	-1.55465600	-2.56136000
H	-2.20468300	-3.58970400	-2.89650000
H	-4.01382900	-1.56660100	-2.90533100
Fe	0.28532000	0.43716000	-0.69047300
C	-1.12981400	-0.60869300	1.61935400
C	-0.95834600	-1.25488300	2.88766000
C	-3.40954000	-0.91797300	1.70838300
C	-2.08900900	-1.75442500	3.51445100
H	-4.36725500	-0.75277800	1.21506400
C	-3.34932100	-1.59322700	2.92554500
H	-1.98818900	-2.26378000	4.47089300
H	-4.24897400	-1.97712400	3.39615500
N	-2.34356200	-0.44571000	1.05869700
C	1.48560300	-1.53525500	2.42134300
H	2.46287300	-1.10168100	2.65034700
H	0.97851200	-0.70064500	1.53368100

C	0.42674700	-1.30939000	3.49442500
H	0.47071300	-2.09004000	4.26871600
C	1.53791600	-2.91649900	1.81549600
H	2.28535400	-2.97960800	1.02130600
H	1.79242100	-3.66525900	2.58250400
H	0.56443400	-3.19619500	1.39551700
H	0.63241000	-0.35122600	3.99367500

³TS2

N	-0.00346500	-0.13439200	0.91055200
H	4.49934900	3.12127400	0.46847200
C	3.44930100	2.94177200	0.27469500
C	2.39693600	3.79024000	0.43902900
C	2.90737600	1.69873600	-0.21564500
C	1.21541800	3.07000500	0.03272800
H	2.40273900	4.81399100	0.79145400
N	1.54289300	1.79769400	-0.37489100
C	3.65859200	0.55492200	-0.44016200
C	-0.06409500	3.60714600	0.02825300
C	3.13522500	-0.67255900	-0.81889600
H	4.72995600	0.61567200	-0.27459200
C	-1.19406400	2.95739700	-0.44179300
H	-0.18075800	4.62939900	0.37498400
N	1.80268200	-0.92877100	-1.05512400
C	3.91485300	-1.87562300	-0.97492600
N	-1.23280300	1.66525200	-0.91826800
C	-2.49074400	3.57735200	-0.56583900
C	1.72938800	-2.27269700	-1.33882300
C	3.03967200	-2.87218700	-1.28806100
H	4.98923300	-1.93292400	-0.85349100
C	-2.52607300	1.46674900	-1.34535900
C	-3.31238100	2.65743200	-1.14072500
H	-2.71762700	4.59209400	-0.26413300
C	0.56720600	-2.95570800	-1.66710300
H	3.24654100	-3.91729000	-1.48087600
C	-3.01945300	0.28579200	-1.87316800
H	-4.35802000	2.75539000	-1.40363000
C	-0.67624300	-2.36679400	-1.82980000
H	0.64756500	-4.02079900	-1.86172400
C	-2.29073200	-0.88715100	-1.97283600
H	-4.06178000	0.26180900	-2.17518200
N	-0.96294300	-1.03172400	-1.63682100
C	-1.84538100	-3.06857500	-2.29779100
C	-2.84142200	-2.14698200	-2.40245200
H	-1.87546100	-4.12615800	-2.52763300
H	-3.86372900	-2.29057200	-2.72858600
Fe	0.22785700	0.31869800	-0.79500000

C	-1.05895400	-0.48516800	1.70387700
C	-0.81334800	-0.75408000	3.09189000
C	-3.30077800	-0.94571200	1.94889000
C	-1.89020900	-1.15884100	3.86517900
H	-4.27536300	-0.99748600	1.46386400
C	-3.16686000	-1.26342800	3.29934300
H	-1.73507400	-1.38437800	4.91851200
H	-4.02408500	-1.57644000	3.88691000
N	-2.29047000	-0.57475600	1.16034200
C	1.65467700	-0.86313900	2.63481500
H	2.56282100	-0.26090600	2.71480500
H	1.04105500	-0.37610700	1.56517800
C	0.57643900	-0.53214000	3.65594500
H	0.70489500	-1.12481000	4.57449500
C	1.88660000	-2.32440900	2.33163100
H	2.58598400	-2.45462300	1.50076000
H	2.29938100	-2.84450300	3.21030100
H	0.94524700	-2.82020600	2.06683900
H	0.67591300	0.52420400	3.94537500

⁵TS2

N	-0.20792500	-0.30556600	1.08558200
H	4.97684400	1.95405300	1.42675800
C	3.94182200	2.07322500	1.13193800
C	3.10152100	3.11523200	1.38222500
C	3.19291600	1.10875700	0.36439900
C	1.83978000	2.78878900	0.76548300
H	3.30205000	4.03017200	1.92513200
N	1.91246400	1.56092000	0.14830300
C	3.70972200	-0.09506100	-0.09319700
C	0.72396300	3.61236200	0.78946500
C	3.00513400	-1.02755300	-0.84161200
H	4.74716400	-0.31678700	0.13712200
C	-0.48599500	3.32606500	0.17466000
H	0.80858600	4.55784800	1.31606900
N	1.67895200	-0.92654900	-1.20102600
C	3.56636800	-2.25289600	-1.34887800
N	-0.77241300	2.17802900	-0.52837900
C	-1.62581700	4.20783300	0.17856400
C	1.39551300	-2.06948900	-1.91685100
C	2.56685200	-2.90025900	-2.01443800
H	4.59398300	-2.56334900	-1.20753300
C	-2.07033100	2.31616300	-0.95887500
C	-2.60770700	3.58210800	-0.52850600
H	-1.65250300	5.17655200	0.66120000
C	0.16279400	-2.38724400	-2.46924300
H	2.60524100	-3.85103200	-2.53074900

C	-2.77886700	1.37816500	-1.69372500
H	-3.61010700	3.92942300	-0.74468400
C	-0.95283000	-1.56486400	-2.43655500
H	0.07350500	-3.33706300	-2.98702100
C	-2.28098100	0.14945800	-2.09595500
H	-3.80275500	1.61824500	-1.96213200
N	-1.01211400	-0.32050100	-1.84955100
C	-2.21357900	-1.88538200	-3.05784300
C	-3.03507100	-0.81966600	-2.85044500
H	-2.42062700	-2.80619000	-3.58824400
H	-4.05995300	-0.68426400	-3.17206800
Fe	0.36952200	0.51963200	-0.65503000
C	-1.33150800	-0.79505000	1.65728400
C	-1.25113300	-1.64328200	2.81440300
C	-3.63333000	-0.92542300	1.65262700
C	-2.43610600	-2.13408800	3.34084500
H	-4.56531800	-0.61791300	1.17813500
C	-3.65916000	-1.77925300	2.76023300
H	-2.40782900	-2.78966300	4.20925100
H	-4.60091800	-2.15063700	3.15215900
N	-2.52234500	-0.44472900	1.10059600
C	1.18855300	-1.98965400	2.34379400
H	2.18052400	-1.67174300	2.67507500
H	0.75729100	-1.01150500	1.59341100
C	0.11022900	-1.91351300	3.41970300
H	0.07980600	-2.83729400	4.01718700
C	1.18384900	-3.23365800	1.48493700
H	1.93894800	-3.18168700	0.69723200
H	1.38901100	-4.12732200	2.09497300
H	0.20541500	-3.37595800	1.01114100
H	0.35810900	-1.09646200	4.11306800

¹H_{loss}

N	0.08300100	-0.20732600	0.94400500
H	4.53976600	3.05542000	1.07295100
C	3.48683900	2.92191600	0.85903200
C	2.44198700	3.72884000	1.19257400
C	2.93206400	1.79893700	0.14546900
C	1.25157100	3.10624100	0.66868200
H	2.45812100	4.66638200	1.73385600
N	1.56624200	1.93304100	0.02169200
C	3.67049300	0.71345700	-0.30031900
C	-0.02265500	3.64374400	0.77545800
C	3.13207600	-0.41140500	-0.90679500
H	4.74284300	0.72967300	-0.13127000
C	-1.15993600	3.10684600	0.19412500
H	-0.12885900	4.57995100	1.31493900

N	1.79485100	-0.60024300	-1.18577300
C	3.89606600	-1.57000900	-1.29465300
N	-1.21104400	1.93386400	-0.52662100
C	-2.45178100	3.74858900	0.20478900
C	1.70544600	-1.86587700	-1.72078100
C	3.00930000	-2.47586300	-1.79390500
H	4.96969200	-1.66198800	-1.18965000
C	-2.51112400	1.83005800	-0.96827500
C	-3.28548700	2.96400700	-0.53064800
H	-2.66795900	4.68582400	0.70183000
C	0.53508600	-2.46993800	-2.15496900
H	3.20353400	-3.46555300	-2.18771400
C	-3.02385000	0.77180300	-1.69806000
H	-4.33259500	3.11753900	-0.75877600
C	-0.70831500	-1.85920700	-2.17755900
H	0.60680500	-3.47939400	-2.54802400
C	-2.31029400	-0.37079600	-2.01701800
H	-4.06928700	0.81407000	-1.98723000
N	-0.98018400	-0.58426000	-1.73037000
C	-1.89008200	-2.45588300	-2.74969600
C	-2.87923400	-1.52513700	-2.66508600
H	-1.93200500	-3.45134100	-3.17338400
H	-3.90688000	-1.59835400	-2.99770100
Fe	0.24411400	0.58419000	-0.67708000
C	-0.97247500	-0.81273300	1.56967900
C	-0.74113200	-1.62063100	2.73109900
C	-3.24114500	-1.20825600	1.67164200
C	-1.84615900	-2.22345500	3.31620500
H	-4.21544100	-1.01319500	1.22339100
C	-3.12875100	-2.03013300	2.79010400
H	-1.70370400	-2.85073200	4.19422100
H	-4.00225000	-2.49664400	3.23433900
N	-2.20785000	-0.61412400	1.07439700
C	1.68693500	-2.33626700	2.37498000
C	1.37771700	-3.44761400	1.42911500
H	2.72830800	-2.10962100	2.59405700
H	0.98978400	-0.46700200	1.32484300
C	0.64990900	-1.78116800	3.31521100
H	0.57022200	-2.43182700	4.20584200
H	2.19342200	-3.60115100	0.71624500
H	1.21196500	-4.40283900	1.96051900
H	0.46322700	-3.24511000	0.85803600
H	1.00080900	-0.81013200	3.69906500
³M			
N	0.08424100	-0.21624300	0.93021200
H	4.49917600	3.10935600	1.00229100

C	3.44738800	2.95841000	0.79443700
C	2.39242400	3.75367900	1.12435900
C	2.90590400	1.81973600	0.09580700
C	1.20886500	3.10862100	0.61246700
H	2.39745700	4.69702700	1.65568400
N	1.53772900	1.93317100	-0.02363100
C	3.65822500	0.73927600	-0.33921400
C	-0.07256100	3.62890200	0.71955700
C	3.13344100	-0.40221100	-0.92621200
H	4.73095800	0.77357400	-0.17532800
C	-1.20447400	3.06998000	0.14848200
H	-0.18972400	4.56925800	1.24947200
N	1.79796600	-0.61402100	-1.19531300
C	3.91169700	-1.55667200	-1.29877500
N	-1.24142100	1.88887800	-0.55948200
C	-2.50496800	3.69427400	0.15517500
C	1.72343600	-1.88884100	-1.70977900
C	3.03504600	-2.48288300	-1.77818800
H	4.98697700	-1.63227300	-1.19753200
C	-2.54033000	1.76332900	-0.99856500
C	-3.32920700	2.89118800	-0.57091600
H	-2.73291000	4.63366600	0.64279900
C	0.55941200	-2.51313200	-2.13268300
H	3.24093000	-3.47641900	-2.15603100
C	-3.03899400	0.69158500	-1.71854000
H	-4.37858100	3.02850300	-0.79896600
C	-0.69067100	-1.91632000	-2.16545200
H	0.64221900	-3.52749900	-2.51066000
C	-2.31053300	-0.44472400	-2.02610400
H	-4.08502700	0.71702500	-2.00751800
N	-0.97766700	-0.63799000	-1.73746100
C	-1.86502900	-2.53464600	-2.72949000
C	-2.86514500	-1.61443200	-2.65853400
H	-1.89522300	-3.53653800	-3.13876700
H	-3.89178800	-1.70473200	-2.99005400
Fe	0.23101000	0.55829700	-0.70037600
C	-0.96363500	-0.80029700	1.58530100
C	-0.72574500	-1.53893400	2.79186900
C	-3.22508600	-1.23800400	1.69137700
C	-1.82354100	-2.13626300	3.39684100
H	-4.19957300	-1.08622400	1.22699800
C	-3.10495700	-1.99931000	2.85140800
H	-1.67639500	-2.71263100	4.30834400
H	-3.97217100	-2.46087000	3.31278300
N	-2.19951400	-0.65481400	1.07140200
C	1.74775700	-2.13839900	2.50583700
C	1.52291600	-3.26667200	1.55577300

H	2.76854300	-1.84793700	2.74459600
H	0.99502800	-0.44647600	1.32401000
C	0.65785800	-1.62718000	3.40934600
H	0.58691400	-2.27065400	4.30582700
H	2.37459000	-3.39543400	0.88108700
H	1.36595100	-4.22301000	2.08728800
H	0.62932600	-3.10114000	0.94103000
H	0.95076200	-0.63553200	3.78883900

⁵M

N	0.27489000	0.09502700	1.09022500
H	-1.47676600	5.16931800	0.18224100
C	-1.70470300	4.11217100	0.23393500
C	-2.75533900	3.50178700	0.85159000
C	-0.92670200	3.07743600	-0.40187100
C	-2.63234600	2.08754700	0.59760000
H	-3.56516400	3.95683100	1.40767200
N	-1.49827400	1.84754100	-0.14822200
C	0.18229900	3.31755300	-1.20919200
C	-3.57925400	1.13755800	0.97210000
C	0.93413400	2.35215200	-1.87036600
H	0.48523400	4.35347000	-1.32864800
C	-3.53357100	-0.21925800	0.67134800
H	-4.43503700	1.49412200	1.53739800
N	0.70940600	1.00286000	-1.78257000
C	2.11916400	2.60423200	-2.65826200
N	-2.50790500	-0.83286200	-0.00099000
C	-4.50995400	-1.20256200	1.08078100
C	1.74215900	0.39148000	-2.44131800
C	2.62440300	1.38639300	-3.00799900
H	2.51268100	3.58623200	-2.88899700
C	-2.77454200	-2.17551800	0.01967400
C	-4.03955300	-2.41653100	0.67507000
H	-5.42284100	-0.98117900	1.61924500
C	1.92939300	-0.98722800	-2.49654000
H	3.51424400	1.16876800	-3.58513300
C	-1.90703000	-3.15755100	-0.44998600
H	-4.48772600	-3.39209700	0.81518700
C	1.07664600	-1.94504000	-1.96018300
H	2.81005700	-1.35034000	-3.01754900
C	-0.66815300	-2.93203800	-1.03650800
H	-2.21978200	-4.19161900	-0.34224500
N	-0.10720800	-1.70266800	-1.29995100
C	1.27171200	-3.36801300	-2.10005300
C	0.19400200	-3.97627900	-1.53401400
H	2.11922800	-3.82381600	-2.59599600
H	-0.02524800	-5.03438900	-1.46870900

Fe	-0.69668200	0.03863500	-0.53760900
C	1.26723500	-0.68679000	1.61890700
C	2.17527300	-0.15288100	2.59327900
C	2.30575200	-2.74924900	1.71225900
C	3.15826100	-1.00108000	3.08784400
H	2.32123900	-3.77186100	1.33534300
C	3.24534700	-2.32643500	2.65093400
H	3.86551900	-0.61984700	3.82228000
H	4.00924600	-3.00103400	3.02444800
N	1.34824300	-1.97039800	1.21172200
C	2.13373500	2.32790400	2.00841900
C	3.06657400	2.18498500	0.85282700
H	1.61791200	3.27030700	2.17335200
H	0.31643200	1.04982200	1.43942100
C	2.05622200	1.27887700	3.08372400
H	2.85783000	1.44739600	3.82651600
H	3.05587100	3.06936300	0.21036600
H	4.10440200	2.01407200	1.18590300
H	2.79996800	1.32091700	0.22751600
H	1.11539500	1.40282600	3.64274100

PC

C	-0.22101500	0.77010600	-0.19953500
C	-0.21134600	-0.64031900	-0.27139900
C	-2.41128800	-0.79689400	0.21463800
C	-2.54757500	0.58561400	0.30670900
C	-1.41459800	1.39592400	0.09556100
C	2.03571900	-0.02307400	-0.34264300
H	-3.27237300	-1.44180600	0.38207400
H	-3.51097800	1.02439200	0.54576500
H	-1.48189000	2.47886700	0.17097900
H	2.82560200	-0.06022300	-1.10050300
H	1.28903200	-2.03978100	-0.30557600
N	-1.25694200	-1.43537700	-0.06742700
N	1.05646500	-1.09858700	-0.60058900
C	2.65873600	-0.13403800	1.05423100
H	3.17830000	-1.09169500	1.17891800
H	3.38637500	0.66926800	1.22022400
H	1.88182900	-0.06220400	1.82464100
C	1.17161500	1.26730500	-0.50248400
H	1.23321300	1.64404300	-1.53240700
H	1.51274600	2.06914800	0.16152700

³Nl'

N	0.31193300	-0.07336100	-0.76526800
H	5.07888300	2.22823900	-2.48039100
C	4.56585900	1.47108600	-1.90099100

C	4.86399400	0.14973800	-1.77435800
C	3.40206600	1.71516000	-1.08307600
C	3.88081200	-0.41116200	-0.88028400
H	5.67276800	-0.40889900	-2.22800800
N	2.99664300	0.55413200	-0.46439600
C	2.80434100	2.95560700	-0.93446800
C	3.84336200	-1.73829000	-0.48442300
C	1.70989700	3.21888200	-0.12437800
H	3.23060600	3.78734300	-1.48712700
C	2.91127400	-2.26879000	0.38978200
H	4.59485200	-2.40964200	-0.88782500
N	1.04326800	2.28907700	0.64087700
C	1.10331300	4.51904600	0.01386400
N	1.88655800	-1.57263400	1.00015700
C	2.88057700	-3.65361400	0.77897300
C	0.00844000	2.97894700	1.23268900
C	0.04603800	4.37003700	0.85889600
H	1.45330200	5.41683100	-0.47983400
C	1.19013400	-2.51571600	1.72901200
C	1.81534700	-3.80582700	1.61099300
H	3.59211500	-4.39859400	0.44626100
C	-0.96534500	2.41960800	2.04627900
H	-0.65606700	5.11858400	1.20356900
C	0.03675600	-2.28847600	2.45735600
H	1.46506500	-4.70301600	2.10533700
C	-1.03569800	1.07986100	2.38815700
H	-1.73141900	3.07938400	2.44131200
C	-0.59248900	-1.05947500	2.56838500
H	-0.40294900	-3.13157000	2.98073700
N	-0.16127300	0.10000600	1.96612800
C	-2.03955300	0.51879200	3.25774500
C	-1.76501100	-0.80960800	3.36957100
H	-2.84164500	1.08484000	3.71327100
H	-2.28891400	-1.56280600	3.94415900
Fe	1.30326500	0.26860600	0.59047300
C	-0.32243800	-1.09015300	-1.36878000
C	-1.30814300	-0.72670200	-2.35372300
C	-0.73629000	-3.33823100	-1.67815100
C	-2.00494300	-1.76135800	-2.96565400
H	-0.48674300	-4.36121800	-1.39732600
C	-1.72664600	-3.09091100	-2.63767500
H	-2.77541100	-1.52476900	-3.69559700
H	-2.26120100	-3.91229400	-3.10454900
N	-0.05120600	-2.38801200	-1.05494000
C	-2.25321800	1.49796000	-1.48276900
H	-2.48218700	2.51176400	-1.83476300
H	-1.51319300	1.59215900	-0.68442900

C	-1.60052600	0.72076400	-2.66042100
H	-2.26513200	0.76916700	-3.53192400
H	-0.66861100	1.23598600	-2.92474400
C	-3.50233700	0.83248900	-0.95469700
C	-4.76196100	1.11449100	-1.49923100
C	-3.41615800	-0.12269800	0.06856700
C	-5.90711700	0.46348800	-1.03520600
H	-4.84548200	1.85536900	-2.29238400
C	-4.55743100	-0.77301500	0.53800100
H	-2.44740400	-0.35558900	0.49753700
C	-5.80803300	-0.48342700	-0.01295100
H	-6.87641500	0.69942400	-1.46772000
H	-4.46567300	-1.50206300	1.33906800
H	-6.69874500	-0.98786400	0.35296100

⁵Ni'

N	0.30698700	-0.18783700	-1.17229900
H	5.07356800	3.18372700	-1.96036100
C	4.64711100	2.28361200	-1.53546800
C	5.16041100	1.01932200	-1.54603200
C	3.39411700	2.22236000	-0.81898200
C	4.22193100	0.17872900	-0.83906700
H	6.09103700	0.67738200	-1.98144000
N	3.15848900	0.93286200	-0.40875600
C	2.56522300	3.31493900	-0.56186500
C	4.38061200	-1.19084800	-0.62110700
C	1.39212900	3.30499700	0.19296000
H	2.88596900	4.27501100	-0.95612900
C	3.51246700	-2.02182000	0.08503500
H	5.27390300	-1.65124300	-1.03337900
N	0.83658900	2.19324500	0.77414500
C	0.60316500	4.47271100	0.51903500
N	2.34394000	-1.62004500	0.68019100
C	3.70986700	-3.43845300	0.30500000
C	-0.26735000	2.61928100	1.46767900
C	-0.42282800	4.04843500	1.31145900
H	0.82552800	5.48102600	0.19261000
C	1.79076500	-2.73138200	1.25914100
C	2.64282900	-3.87761300	1.03047600
H	4.56011600	-4.00725200	-0.05016100
C	-1.11330000	1.79483000	2.21013200
H	-1.21153400	4.63801100	1.76183900
C	0.59592000	-2.75032400	1.97550800
H	2.44276700	-4.87919900	1.39024500
C	-0.97688800	0.41907500	2.38622400
H	-1.95773800	2.26908300	2.70107600
C	-0.21565300	-1.65141300	2.25725000

H	0.28040700	-3.70733500	2.38080200
N	0.01176700	-0.36311900	1.83270700
C	-1.86182200	-0.40536200	3.17485200
C	-1.39580700	-1.68557100	3.08944000
H	-2.72749300	-0.04056900	3.71267300
H	-1.79511300	-2.57618800	3.55847800
Fe	1.33081600	0.18512200	0.29447100
C	-0.55532500	-1.08581200	-1.62834300
C	-1.70982200	-0.64840900	-2.37721200
C	-1.19072400	-3.30274800	-1.82592700
C	-2.59708200	-1.62162200	-2.83212200
H	-0.97981400	-4.34815700	-1.60075400
C	-2.34599300	-2.96479700	-2.56373400
H	-3.48841200	-1.32460400	-3.37879300
H	-3.02362100	-3.74268600	-2.90275300
N	-0.32117900	-2.42186600	-1.37128900
C	-2.42396000	1.53196000	-1.27556300
H	-2.58173000	2.59235800	-1.50668000
H	-1.59935200	1.47837700	-0.56131200
C	-1.96832800	0.81908700	-2.58058900
H	-2.73760000	0.94915800	-3.35157600
H	-1.05119500	1.30826200	-2.92611000
C	-3.67624700	0.93349700	-0.67877500
C	-4.94504900	1.43012900	-1.00457300
C	-3.59350500	-0.16782300	0.18620400
C	-6.10122400	0.84783700	-0.47985700
H	-5.02651800	2.28571800	-1.67241900
C	-4.74468600	-0.75094800	0.71579000
H	-2.61977200	-0.56685500	0.45030100
C	-6.00420600	-0.24553600	0.38397000
H	-7.07636000	1.25146800	-0.74104900
H	-4.65239500	-1.59651800	1.39259900
H	-6.90248400	-0.69676700	0.79752600

³TS_{2sp3}'

N	-0.16759300	-0.19218100	1.13179900
H	4.38032300	3.08329100	0.98586000
C	3.34352000	2.89655600	0.73570100
C	2.27425900	3.73079300	0.86368800
C	2.84201600	1.65914800	0.19237400
C	1.12444700	3.00972200	0.37755900
H	2.25109900	4.74740100	1.23556500
N	1.48653300	1.74732900	-0.03346600
C	3.61765000	0.53041400	-0.02863000
C	-0.15391700	3.54216800	0.28986400
C	3.12326300	-0.69724100	-0.44122300
H	4.68218400	0.60310900	0.17267500

C	-1.23851400	2.89955100	-0.28548800
H	-0.30085400	4.55844500	0.64255800
N	1.79841000	-0.97035800	-0.70499900
C	3.92079400	-1.88926200	-0.58524800
N	-1.23394500	1.61280100	-0.77830000
C	-2.51713600	3.52278900	-0.52286800
C	1.74762400	-2.31810200	-0.97535200
C	3.06393500	-2.89920000	-0.89891800
H	4.99222900	-1.93389100	-0.43665600
C	-2.48276700	1.42033000	-1.32493200
C	-3.28140900	2.61170800	-1.18515500
H	-2.77052300	4.53455800	-0.23245100
C	0.60219800	-3.01616700	-1.32775100
H	3.28262500	-3.94664800	-1.05839400
C	-2.93439400	0.23829400	-1.88688600
H	-4.29748800	2.71529200	-1.54428300
C	-0.62866100	-2.43142600	-1.57771600
H	0.69309500	-4.08659700	-1.48211600
C	-2.21234300	-0.94310600	-1.89602200
H	-3.94604400	0.21724600	-2.27975900
N	-0.91720800	-1.08856600	-1.44994400
C	-1.76640700	-3.13876900	-2.10892500
C	-2.73975400	-2.21200500	-2.32716300
H	-1.78985100	-4.20310900	-2.30606700
H	-3.73378800	-2.35820700	-2.73045600
Fe	0.20908700	0.26543100	-0.53616400
C	-1.29568400	-0.51452800	1.82917600
C	-1.17294100	-0.83759600	3.22117400
C	-3.57146700	-0.86793700	1.88911200
C	-2.32632400	-1.20442500	3.89853400
H	-4.50586900	-0.85873800	1.32825200
C	-3.55960200	-1.22466900	3.23655500
H	-2.26252000	-1.47089900	4.95173100
H	-4.47413800	-1.50651000	3.74850800
N	-2.48576600	-0.53011000	1.19230900
C	1.34954300	-1.03215000	2.96776500
H	2.21591900	-0.38947100	3.14015200
H	0.84238200	-0.55220900	1.87859100
C	0.17561900	-0.72871900	3.90245500
H	0.20078800	-1.38121900	4.78543200
H	0.29681700	0.30169100	4.26563700
C	1.71815800	-2.43515800	2.69482200
C	3.07281200	-2.79919700	2.58421300
C	0.74561800	-3.43981000	2.50898700
C	3.44706100	-4.11490100	2.31978600
H	3.83592000	-2.03474000	2.70673600
C	1.12041500	-4.75222500	2.23381200

H	-0.30699600	-3.18463200	2.57431200
C	2.47249800	-5.09906900	2.14145800
H	4.50095200	-4.37054900	2.24546300
H	0.35371000	-5.50955300	2.09118300
H	2.76172100	-6.12560000	1.93207100
⁵TS_{2sp3}'			
N	0.13878100	-0.39003100	-0.65045900
H	3.15709800	1.58167400	3.78065800
C	2.23149700	1.14566200	3.42652500
C	1.53048300	0.09796100	3.95044100
C	1.49976700	1.60261800	2.27478100
C	0.37157700	-0.08596500	3.11758800
H	1.76488900	-0.50233300	4.82038800
N	0.36387800	0.84314600	2.09971400
C	1.89883200	2.65284200	1.45928100
C	-0.57964300	-1.07980800	3.30859500
C	1.19298200	3.11324500	0.35806100
H	2.82636100	3.15823500	1.70943600
C	-1.69465900	-1.27331000	2.50734300
H	-0.44173100	-1.75188700	4.14980900
N	0.00504600	2.59603300	-0.10268800
C	1.61291700	4.21916900	-0.46771400
N	-2.02970000	-0.51573200	1.40632500
C	-2.67675300	-2.30681200	2.71909900
C	-0.32662200	3.34820700	-1.20450500
C	0.66889000	4.36590600	-1.43691800
H	2.51495300	4.79644600	-0.30926500
C	-3.20448400	-1.04992400	0.92692200
C	-3.61231900	-2.16822700	1.73914900
H	-2.64161900	-3.03246200	3.52178300
C	-1.45185900	3.16499700	-1.99422500
H	0.63271000	5.08842800	-2.24221200
C	-3.91176100	-0.58184000	-0.16949700
H	-4.50422400	-2.75759900	1.56879300
C	-2.41834400	2.19379000	-1.78248900
H	-1.58485700	3.82989600	-2.84176600
C	-3.53560200	0.50017800	-0.95046800
H	-4.82351500	-1.10470000	-0.43977800
N	-2.41133500	1.26805000	-0.76425100
C	-3.58186500	2.01571900	-2.61312100
C	-4.27557700	0.96432000	-2.09564900
H	-3.81895900	2.62285300	-3.47742300
H	-5.20083800	0.52638200	-2.44787400
Fe	-0.90923400	0.90525000	0.52415600
C	-0.24536300	-1.61639400	-1.09767900
C	0.40366000	-2.81120100	-0.63799400
C	-1.63006600	-2.83876500	-2.48077300

C	-0.00466100	-4.02131500	-1.18190500
H	-2.45041000	-2.82072800	-3.19838900
C	-1.03761200	-4.05345700	-2.12417900
H	0.47589600	-4.94381100	-0.86056600
H	-1.37666800	-4.98734300	-2.56173700
N	-1.26099200	-1.65365500	-1.99981500
C	2.23700200	-1.42595400	0.46231100
H	2.39023300	-0.99393000	1.45093100
H	1.26285100	-0.62230200	-0.02334500
C	1.44345300	-2.72654900	0.46327100
H	2.11470400	-3.59515200	0.40670300
H	0.92034400	-2.79136700	1.42692800
C	3.35558300	-1.21488700	-0.45666200
C	3.51927900	-1.96741400	-1.63874300
C	4.28252900	-0.18267600	-0.19269300
C	4.57626700	-1.70683600	-2.50759000
H	2.80691000	-2.75110300	-1.87772000
C	5.33556000	0.07631200	-1.06337700
H	4.15632900	0.41606500	0.70654900
C	5.49043200	-0.68695700	-2.22621400
H	4.68623600	-2.29980900	-3.41198600
H	6.03983900	0.87325700	-0.83804800
H	6.31269200	-0.48570600	-2.90752500

³TS_{2sp²}'

N	0.72983000	-0.79835200	-0.73345700
H	-4.04505700	-0.92627600	-3.48474400
C	-3.34563800	-0.34993600	-2.89249000
C	-2.90672500	0.92085100	-3.09306300
C	-2.70002100	-0.82794300	-1.69321300
C	-1.98676500	1.21553500	-2.02128400
H	-3.16581900	1.60979300	-3.88703900
N	-1.88297100	0.14497500	-1.16582100
C	-2.91249300	-2.08294600	-1.14796500
C	-1.28310100	2.40337800	-1.90787900
C	-2.34410000	-2.54421900	0.03087000
H	-3.59557800	-2.74707700	-1.66864500
C	-0.37184700	2.68864600	-0.90270400
H	-1.45516100	3.16494200	-2.66201900
N	-1.44413300	-1.84831700	0.80386400
C	-2.63289400	-3.82739200	0.62336700
N	-0.02803300	1.83438800	0.12100300
C	0.32350600	3.94464700	-0.76857100
C	-1.15972300	-2.67049800	1.87170600
C	-1.90062600	-3.90417700	1.76976900
H	-3.31660900	-4.55724300	0.20851400
C	0.85800200	2.53990800	0.90676400

C	1.08398000	3.85385300	0.35677700
H	0.21896400	4.78055200	-1.44859800
C	-0.26211000	-2.38045800	2.88837500
H	-1.85510000	-4.71113800	2.49018000
C	1.45480300	2.06876500	2.06629100
H	1.73639900	4.59912200	0.79409700
C	0.46243000	-1.20171300	2.99344900
H	-0.12217100	-3.12733600	3.66389000
C	1.24125300	0.81343300	2.61827900
H	2.13816600	2.73461000	2.58452900
N	0.40620600	-0.15289300	2.09995700
C	1.36499400	-0.89745800	4.07594900
C	1.84802500	0.35434100	3.84326800
H	1.57764300	-1.56086900	4.90477900
H	2.53987900	0.93357800	4.44178000
Fe	-0.55404300	-0.10378100	0.30908600
C	1.20842300	-0.19513100	-1.90314800
C	2.45647600	0.48599200	-1.86066200
C	0.91242000	0.32357900	-4.12066000
C	2.89361000	1.10487100	-3.02728000
H	0.27572800	0.23545600	-4.99995000
C	2.10987200	1.03575100	-4.18174300
H	3.84044900	1.64115100	-3.03141000
H	2.42160500	1.51542200	-5.10501600
N	0.46701300	-0.28566100	-3.01729800
C	3.25692500	0.45407700	-0.58780300
H	4.02716600	1.23394800	-0.59059000
C	3.06057300	-2.06479100	-0.84451400
C	3.38954600	-2.76310700	-1.99476900
C	1.76029900	-2.27674300	-0.23340200
C	2.54352900	-3.75110100	-2.52577900
H	4.32963600	-2.54224600	-2.49564900
C	0.98393700	-3.39757500	-0.71758800
H	1.67651300	-2.04363300	0.82348000
C	1.34412500	-4.07043900	-1.86622100
H	2.83009500	-4.27993800	-3.43036800
H	0.07930800	-3.66632700	-0.19036500
H	0.71060300	-4.86659800	-2.24833900
H	2.58797600	0.65241900	0.24866900
C	3.92958600	-0.93812100	-0.35480600
H	4.14065400	-1.04089600	0.71829000
H	4.89034000	-0.97086100	-0.88146200

⁵TS₂_{sp2}'

N	0.16663800	0.02797200	0.81646500
H	0.10900100	-5.43168500	-0.39662100
C	0.39989900	-4.43302000	-0.69665400

C	1.60915400	-3.99650600	-1.14043100
C	-0.47727500	-3.28606700	-0.69108500
C	1.47109300	-2.58338800	-1.40415000
H	2.52224600	-4.56135000	-1.27991400
N	0.19101300	-2.17085800	-1.13538800
C	-1.80512000	-3.32104400	-0.29243400
C	2.50284200	-1.77034200	-1.85074400
C	-2.66528600	-2.23107800	-0.28963200
H	-2.20573300	-4.27538500	0.03522400
C	2.39214300	-0.41147500	-2.11127700
H	3.47100100	-2.23336600	-2.01358600
N	-2.32780100	-0.94702500	-0.65329700
C	-4.05071000	-2.29003900	0.10345200
N	1.25179700	0.34094100	-1.95145900
C	3.46362400	0.40820400	-2.62044900
C	-3.47175600	-0.19818000	-0.50140300
C	-4.55198700	-1.02893100	-0.03003200
H	-4.56066800	-3.18769500	0.42946100
C	1.58014900	1.61299000	-2.36231300
C	2.95901900	1.66371000	-2.77989600
H	4.46396100	0.05124400	-2.83051200
C	-3.57997000	1.16566900	-0.74303100
H	-5.55733700	-0.67836900	0.16683300
C	0.71918600	2.70237600	-2.36720500
H	3.45841600	2.55078800	-3.14858700
C	-2.55332100	1.97649800	-1.20865600
H	-4.54715300	1.62895500	-0.57426100
C	-0.60585400	2.67064500	-1.95374800
H	1.11205600	3.65117600	-2.71932900
N	-1.26496900	1.56216900	-1.46738000
C	-2.69822600	3.37819100	-1.51430700
C	-1.49134200	3.80796300	-1.97834700
H	-3.61525200	3.94170600	-1.39638100
H	-1.21298000	4.79683300	-2.32028300
Fe	-0.47373000	-0.26277600	-1.07146000
C	1.45340000	-0.09617500	1.27667800
C	2.26060300	1.07341700	1.42217700
C	3.19479800	-1.46910600	1.87496800
C	3.58633400	0.89439300	1.79611500
H	3.53634200	-2.48850800	2.05191600
C	4.07541000	-0.39557200	2.02573700
H	4.23738600	1.76007500	1.90233200
H	5.10819600	-0.56437200	2.31558200
N	1.91630600	-1.34225900	1.51374800
C	1.63647900	2.41980800	1.16893900
H	2.40907600	3.18114500	1.00968100
C	-0.10503200	1.73256600	2.88972900

C	0.12472800	1.23798200	4.16216100
C	-0.99308100	1.00713400	2.00815800
C	-0.56720400	0.11465400	4.65031100
H	0.85286700	1.73377800	4.80027900
C	-1.78338900	-0.05934300	2.57191300
H	-1.42081200	1.55317000	1.17279600
C	-1.53351300	-0.51846600	3.84897200
H	-0.36522500	-0.24944000	5.65363000
H	-2.53046900	-0.53486000	1.94938700
H	-2.09498300	-1.36175500	4.24216400
H	1.04247400	2.36336200	0.25391600
C	0.70558500	2.87450700	2.33603400
H	0.05091200	3.67270100	1.95884900
H	1.31448700	3.30560300	3.13925300

³Ni''

N	-0.07537800	-0.15470900	0.47131100
H	3.27229900	2.16460100	-3.56894400
C	2.42731500	2.21972100	-2.89427700
C	2.02950800	3.26118500	-2.11139900
C	1.50021900	1.14150900	-2.65370000
C	0.84958000	2.82379900	-1.40911100
H	2.47631600	4.24226000	-2.01243100
N	0.52811800	1.53293500	-1.75908200
C	1.62197700	-0.12478400	-3.20557700
C	0.12430300	3.61305600	-0.52936500
C	0.77715100	-1.19131400	-2.93945600
H	2.45988800	-0.30253800	-3.87256100
C	-1.07899900	3.24206800	0.04610700
H	0.49681800	4.61105700	-0.32091300
N	-0.33886900	-1.14104700	-2.13383700
C	0.96739100	-2.52509700	-3.45446800
N	-1.70438400	2.02467700	-0.12337800
C	-1.90240500	4.12408100	0.83504700
C	-0.84276300	-2.42082500	-2.12304500
C	-0.03328900	-3.29151100	-2.93860600
H	1.77015400	-2.81882700	-4.11874300
C	-2.90932500	2.13441500	0.53316300
C	-3.04520600	3.44325800	1.12050900
H	-1.63328500	5.13784100	1.10298300
C	-1.98735400	-2.81533100	-1.44728800
H	-0.22722800	-4.34500100	-3.09503600
C	-3.85697600	1.13200000	0.63952300
H	-3.90945700	3.77712600	1.68049700
C	-2.81240600	-1.95996100	-0.73619200
H	-2.28380700	-3.85710800	-1.51930600
C	-3.68353600	-0.15829000	0.16948500

H	-4.77211000	1.35501800	1.17874600
N	-2.58833600	-0.61296700	-0.53219400
C	-4.06999300	-2.35186000	-0.15312000
C	-4.61819000	-1.23102000	0.39109600
H	-4.47415100	-3.35568000	-0.18514500
H	-5.56327500	-1.12324800	0.90799900
Fe	-0.91439500	0.38292300	-0.92120900
C	-0.32502500	-0.48848900	1.75019000
C	0.63774900	-1.31365500	2.43309100
C	-1.67233100	-0.37209400	3.62346000
C	0.35685300	-1.63498100	3.75752900
H	-2.59151700	0.01361900	4.06418300
C	-0.80463400	-1.16834400	4.37820000
H	1.05448900	-2.26107300	4.30952100
H	-1.03248200	-1.41480400	5.41061400
N	-1.45565800	-0.03754600	2.35770900
C	1.64557400	-2.64119600	0.49141900
C	2.89817300	-3.32262300	-0.06473500
H	1.20209000	-1.99754800	-0.26953400
H	0.88410300	-3.39585300	0.72836500
C	1.91546600	-1.82322900	1.77564400
H	2.36132300	-2.52187500	2.49772600
C	2.92425300	-0.68368400	1.60945600
C	3.79171500	-0.38624600	2.66949800
C	2.99715100	0.09993000	0.45051100
C	4.70414300	0.66590400	2.58346700
H	3.74826300	-0.98603800	3.57665500
C	3.90989600	1.15283300	0.35916700
H	2.33382900	-0.10117700	-0.38027100
C	4.76520100	1.44179900	1.42404300
H	5.36713500	0.87633200	3.41908600
H	3.94001100	1.74897700	-0.54787500
H	5.47450700	2.26240600	1.35091000
H	2.65225200	-3.89425500	-0.96649700
H	3.66224400	-2.58433100	-0.33070400
H	3.34029000	-4.01141500	0.66680500

⁵Ni''

N	-0.03006200	-0.49486600	-0.61894500
H	-2.85273200	4.18637400	1.79988000
C	-1.99715800	3.80359300	1.25751900
C	-1.36999900	4.34824300	0.17387700
C	-1.28797400	2.58763800	1.58507200
C	-0.27341200	3.46953100	-0.16249300
H	-1.61028100	5.26603400	-0.34806700
N	-0.25066600	2.40451000	0.70363800
C	-1.60719500	1.73659700	2.64452200

C	0.64582800	3.69439000	-1.18877900
C	-0.91618200	0.58457900	3.01970500
H	-2.46932200	2.00798200	3.24686500
C	1.76357200	2.91426000	-1.48235100
H	0.49231900	4.58082700	-1.79744800
N	0.19470400	0.08414700	2.38405900
C	-1.25625600	-0.26063800	4.14232100
N	2.11895800	1.76613000	-0.82192300
C	2.73347700	3.20129500	-2.51707700
C	0.56865000	-1.04515100	3.06797500
C	-0.33837600	-1.27015800	4.17116300
H	-2.08566100	-0.08914600	4.81691300
C	3.27629900	1.31470900	-1.40172900
C	3.67021300	2.21199000	-2.46601500
H	2.69431800	4.05445700	-3.18277300
C	1.66461700	-1.84833700	2.75001700
H	-0.26567000	-2.08941600	4.87547400
C	3.97235800	0.16928900	-1.01908200
H	4.55343200	2.09262400	-3.08101200
C	2.58367400	-1.62110500	1.72645300
H	1.83185600	-2.72093800	3.37485700
C	3.63210100	-0.70040400	0.01600100
H	4.87051300	-0.06892900	-1.58140700
N	2.54566400	-0.56740500	0.84520400
C	3.73632000	-2.44625400	1.44515600
C	4.38515300	-1.87544300	0.38961600
H	4.00864900	-3.33693400	1.99761700
H	5.29541100	-2.20554400	-0.09523100
Fe	0.88716200	0.64614700	0.46266000
C	0.04927600	-1.60278200	-1.34141700
C	-1.05397500	-2.53624200	-1.37003900
C	1.29313000	-2.92072500	-2.78590000
C	-0.90556700	-3.67821000	-2.15668900
H	2.22322800	-3.06325600	-3.33575400
C	0.27155300	-3.88950100	-2.87073000
H	-1.71321700	-4.40499700	-2.20586400
H	0.40651200	-4.77540100	-3.48424600
N	1.20117200	-1.81756100	-2.06982600
C	-2.09161100	-2.31091800	0.93563300
C	-3.38265700	-2.28208500	1.75739800
H	-1.45035700	-1.47123400	1.20618200
H	-1.52195100	-3.21809900	1.17601800
C	-2.33969300	-2.29942500	-0.59168800
H	-2.98608800	-3.16186100	-0.80928500
C	-3.07604500	-1.06577400	-1.12313100
C	-3.86843700	-1.19628400	-2.27101700
C	-2.95964300	0.19939700	-0.53413400

C	-4.52051600	-0.09386200	-2.82630200
H	-3.96963200	-2.17303700	-2.74075100
C	-3.60902300	1.30524500	-1.08530000
H	-2.35090000	0.33186200	0.34967700
C	-4.38931600	1.16418200	-2.23482700
H	-5.12853200	-0.21879100	-3.71882300
H	-3.49018800	2.27735200	-0.61493500
H	-4.89213900	2.02639600	-2.66533600
H	-3.14995400	-2.30520700	2.82719500
H	-3.95918700	-1.37316100	1.55695000
H	-4.02417000	-3.14228700	1.52631800

³TS_{2sp3}'

N	-0.08227900	-0.04012100	-0.57490100
H	2.64074900	3.26183200	3.01552200
C	2.05120700	2.37171200	2.83639100
C	2.24013200	1.11492100	3.32437600
C	0.88394300	2.31852400	1.99207500
C	1.18430500	0.29575700	2.78258000
H	3.01566000	0.75810700	3.99014600
N	0.35415100	1.04599900	1.98059300
C	0.39370000	3.39660000	1.27155000
C	1.04038200	-1.06115900	3.03416700
C	-0.69849100	3.34780800	0.41757800
H	0.91503800	4.34412300	1.36750700
C	0.00201500	-1.84850000	2.56311500
H	1.77673300	-1.53363200	3.67700700
N	-1.46570000	2.23096300	0.17243400
C	-1.17006800	4.46446600	-0.36355400
N	-1.02424200	-1.41728200	1.75066000
C	-0.19132500	-3.23077800	2.92733100
C	-2.39925800	2.62088700	-0.75936100
C	-2.22385300	4.01124400	-1.09921500
H	-0.73963000	5.45764600	-0.33978300
C	-1.86421900	-2.49935500	1.61241200
C	-1.35608900	-3.62981500	2.34817000
H	0.47865600	-3.79808900	3.56087500
C	-3.38987300	1.80452300	-1.28557400
H	-2.83992900	4.55541400	-1.80386600
C	-3.02933100	-2.51546900	0.86545000
H	-1.84103300	-4.59629900	2.40075500
C	-3.61546200	0.49023800	-0.91023900
H	-4.06260600	2.23922100	-2.01853900
C	-3.47697300	-1.45594200	0.09488800
H	-3.60558000	-3.43510300	0.84513400
N	-2.86935700	-0.22335100	0.00444500
C	-4.71303600	-0.30900100	-1.39485300

C	-4.63444000	-1.51078100	-0.76094600
H	-5.44619900	0.02846400	-2.11650100
H	-5.28568600	-2.37015800	-0.85786700
Fe	-1.13841000	0.33506100	0.80640300
C	0.12354600	-1.10078900	-1.41226300
C	1.21508300	-1.04303300	-2.33946700
C	-0.48875400	-3.18637800	-2.16855800
C	1.38930000	-2.12303400	-3.19143400
H	-1.17958000	-4.02285700	-2.06574100
C	0.52921200	-3.22433200	-3.12036200
H	2.21035400	-2.10969400	-3.90539300
H	0.64837900	-4.08066500	-3.77642900
N	-0.70343800	-2.16381600	-1.33916200
C	1.44003500	1.41787000	-1.91442000
H	2.04599700	2.12763000	-1.34755800
H	0.62726700	0.89675500	-1.00622300
C	2.17856500	0.14183000	-2.32140400
H	2.56078900	0.27259600	-3.34571400
C	0.52536900	2.03411300	-2.94574700
H	-0.04724200	2.86415200	-2.52163300
H	1.10374900	2.41959900	-3.79979500
H	-0.18191300	1.29138500	-3.33307300
C	3.37249100	-0.13484400	-1.41204500
C	3.19412800	-0.35978900	-0.03849000
C	4.67073800	-0.15769900	-1.93339300
C	4.29114600	-0.59473400	0.78830900
H	2.19558600	-0.35209600	0.38402400
C	5.77136600	-0.39689400	-1.10602700
H	4.82395600	0.01540100	-2.99671000
C	5.58474400	-0.61511000	0.25951700
H	4.12861600	-0.75964900	1.84990800
H	6.77227200	-0.41078100	-1.53016500
H	6.43890800	-0.79994200	0.90581800

⁵TS₂_{sp3}'

N	-0.05839900	-0.21674000	-0.74711800
H	2.54468000	3.27369300	2.92936900
C	1.93487000	2.39025800	2.78924800
C	2.04815600	1.17604200	3.39546500
C	0.81238800	2.30492400	1.88866100
C	1.00088700	0.34331900	2.85913000
H	2.77037300	0.85578100	4.13553300
N	0.25041500	1.04926100	1.94402700
C	0.36621200	3.35172300	1.09492800
C	0.80734500	-0.98747100	3.19971500
C	-0.74505700	3.30151500	0.26354500
H	0.91339000	4.28797000	1.14482900

C	-0.19659800	-1.79847200	2.68980000
H	1.48976500	-1.42605200	3.92106900
N	-1.55467300	2.20430700	0.07762800
C	-1.21988400	4.41018400	-0.52494200
N	-1.15681000	-1.40685900	1.78416800
C	-0.38530800	-3.18018600	3.05228000
C	-2.52932700	2.60111100	-0.81135700
C	-2.32821900	3.97602600	-1.19068100
H	-0.75795800	5.38912300	-0.55047500
C	-1.94483300	-2.51348000	1.57069000
C	-1.46991500	-3.62339600	2.35732400
H	0.23799100	-3.72330100	3.75122800
C	-3.56076900	1.80189400	-1.28370200
H	-2.96254700	4.52467200	-1.87526500
C	-3.05267500	-2.56570600	0.73851600
H	-1.92122900	-4.60744300	2.36643800
C	-3.76754300	0.47867600	-0.92357800
H	-4.25858500	2.24651600	-1.98640500
C	-3.53404600	-1.50209400	-0.00907100
H	-3.58362000	-3.50976100	0.66861500
N	-2.98326400	-0.24403000	-0.05375400
C	-4.84344000	-0.34018400	-1.42572400
C	-4.69777500	-1.56912700	-0.85845300
H	-5.60093800	-0.00155100	-2.12112700
H	-5.31051900	-2.45165300	-0.99201900
Fe	-1.23427900	0.32821300	0.76702000
C	0.34373300	-1.20798600	-1.56902300
C	1.51916500	-1.05447200	-2.37969300
C	-0.02841100	-3.32364800	-2.40130700
C	1.86676400	-2.10333400	-3.21823200
H	-0.65288300	-4.21670800	-2.38651200
C	1.08742700	-3.26364100	-3.24486000
H	2.75435200	-2.01957200	-3.84224000
H	1.33706100	-4.09821900	-3.89249600
N	-0.40835000	-2.34293100	-1.58733400
C	1.50886300	1.40200000	-1.85992800
H	2.01094500	2.13263800	-1.22280700
H	0.66577200	0.80527300	-1.08097500
C	2.37898600	0.19860400	-2.23532400
H	2.84962800	0.39480200	-3.21102900
C	0.66278600	1.99713000	-2.96281600
H	-0.02627800	2.75005700	-2.56803500
H	1.29437500	2.47883200	-3.72477500
H	0.07222000	1.22091900	-3.46329800
C	3.49298300	-0.03351000	-1.21767500
C	3.19481300	-0.28859400	0.12981500
C	4.83449700	0.00672100	-1.61351200

C	4.21840200	-0.49307600	1.05350200
H	2.16115600	-0.32929000	0.45716700
C	5.86128100	-0.20024300	-0.68851200
H	5.07964300	0.20436200	-2.65507900
C	5.55572400	-0.45078300	0.64976100
H	3.96368100	-0.68374500	2.09212100
H	6.89747500	-0.16419500	-1.01546600
H	6.35197500	-0.61206600	1.37185900

³TS_{sp2}'

N	0.10027200	-0.17942600	0.68056500
H	-2.14482200	4.78657700	2.00429400
C	-2.20267000	3.90848800	1.37362000
C	-3.30510700	3.22331700	0.96853000
C	-1.06563400	3.26325900	0.76038200
C	-2.83954100	2.13978900	0.13692500
H	-4.34447000	3.41345900	1.20461800
N	-1.47081200	2.17752300	0.01781100
C	0.22926000	3.74937500	0.82481200
C	-3.66684500	1.18226900	-0.42460500
C	1.29478300	3.24841300	0.08909500
H	0.40723100	4.63223300	1.43107500
C	-3.21827500	0.07231300	-1.12303700
H	-4.73572000	1.27740100	-0.26042400
N	1.25155400	2.12361100	-0.70307200
C	2.59207100	3.87160000	0.01112900
N	-1.90310000	-0.20346200	-1.41926600
C	-4.07699000	-0.97694600	-1.61376400
C	2.50067000	2.02881900	-1.27922000
C	3.33688300	3.12204800	-0.85047600
H	2.87431800	4.77435700	0.53796000
C	-1.92138900	-1.40195900	-2.09942500
C	-3.27102600	-1.90103500	-2.20429300
H	-5.15449400	-0.98822200	-1.50905100
C	2.92884000	0.99321600	-2.09682600
H	4.35962300	3.27700400	-1.17020500
C	-0.82314000	-2.00351700	-2.69125400
H	-3.54810900	-2.82599200	-2.69407000
C	2.14951600	-0.08881200	-2.47795500
H	3.95264400	1.02724400	-2.45666300
C	0.45010700	-1.45174300	-2.73764800
H	-0.98175300	-2.94472100	-3.20849700
N	0.82926600	-0.27838500	-2.12427800
C	2.60872600	-1.17090900	-3.31191300
C	1.55500200	-2.02047700	-3.46830800
H	3.60698900	-1.24985000	-3.72343000
H	1.50845700	-2.94168000	-4.03520000

Fe	-0.27459900	0.80422300	-0.80598200
C	-0.82619000	-0.97374000	1.34707600
C	-0.54729700	-2.33063600	1.70033400
C	-2.97261700	-1.15778600	2.18658400
C	-1.56121400	-3.07387700	2.29189200
H	-3.91695800	-0.64641300	2.37238900
C	-2.81237200	-2.49869300	2.52828700
H	-1.36755800	-4.10813900	2.57004500
H	-3.62179600	-3.06293500	2.98116900
N	-2.01674100	-0.41208600	1.63237800
C	1.11516400	-3.36582400	0.06881700
C	2.53494800	-3.89580600	-0.14487800
H	0.91718800	-2.53998200	-0.61474100
H	0.37880400	-4.14253200	-0.17414900
C	0.85096700	-2.89487900	1.51223800
H	0.96522300	-3.75907800	2.18098900
C	1.74973700	-1.78130500	1.99634200
C	2.14456800	-1.72451300	3.32340600
C	1.89971800	-0.62697600	1.13539600
C	2.73507700	-0.57255400	3.86185800
H	1.96711300	-2.58699800	3.96241700
C	2.56952200	0.51812600	1.71035700
H	2.10449400	-0.81191000	0.08543500
C	2.93440600	0.55116200	3.03993600
H	3.03880500	-0.55278800	4.90471100
H	2.80268000	1.35791800	1.07533900
H	3.41556600	1.43862700	3.44310300
H	2.68332600	-4.20326400	-1.18590000
H	3.28053800	-3.12607600	0.08513700
H	2.74122700	-4.75970200	0.49970300

⁵TS_{sp2}'

N	-0.26144700	-0.10829100	-0.90980800
H	4.79733800	2.30355100	-2.27783500
C	4.27575700	1.53912900	-1.71596700
C	4.56259400	0.21363300	-1.61363000
C	3.11229800	1.77517000	-0.89303400
C	3.57014700	-0.36138300	-0.73537100
H	5.36867100	-0.34146900	-2.07653800
N	2.68846700	0.60317700	-0.31361600
C	2.54528400	3.02351300	-0.68558700
C	3.54257700	-1.69641500	-0.36331600
C	1.47087900	3.27781400	0.15615900
H	2.99290900	3.87042200	-1.19649100
C	2.59928900	-2.26748100	0.47794600
H	4.30974600	-2.34702900	-0.77150100
N	0.76477300	2.32474900	0.85859600

C	0.92395800	4.58671800	0.40297300
N	1.55544900	-1.60236100	1.07572800
C	2.56298100	-3.66630700	0.82051600
C	-0.21474600	3.01094300	1.54147200
C	-0.12312100	4.42050700	1.26195600
H	1.30250100	5.50425200	-0.02941100
C	0.85693200	-2.55563000	1.77885100
C	1.47434400	-3.84820800	1.61986800
H	3.28014900	-4.40225000	0.47937100
C	-1.16857400	2.43868000	2.37527700
H	-0.77941700	5.17428600	1.67831900
C	-0.26628600	-2.31738600	2.55976200
H	1.11569100	-4.76220200	2.07603000
C	-1.25292000	1.08683600	2.67744100
H	-1.88857000	3.10313400	2.84276500
C	-0.83777300	-1.07070900	2.76635600
H	-0.70952900	-3.16424200	3.07428700
N	-0.43060200	0.10372200	2.16937300
C	-2.20852900	0.51402300	3.59367900
C	-1.95036800	-0.82246600	3.64968700
H	-2.96389900	1.07834100	4.12576900
H	-2.45203200	-1.58288600	4.23454800
Fe	0.99850000	0.31682000	0.75333100
C	-0.53409600	-1.35637500	-1.38587500
C	-1.85361800	-1.91063700	-1.48715600
C	0.40588100	-3.33994600	-2.12057900
C	-1.97255900	-3.23543800	-1.89269400
H	1.31947900	-3.87459500	-2.37929000
C	-0.83527400	-3.98235600	-2.20313800
H	-2.96259800	-3.68097800	-1.97041200
H	-0.90540400	-5.01926600	-2.51709500
N	0.56555100	-2.07951500	-1.73793600
C	-3.40664100	-1.07386000	0.33334700
C	-4.61056600	-0.20297500	0.69738400
H	-2.52763300	-0.74990600	0.89303800
H	-3.58630000	-2.11460200	0.63149200
C	-3.07580100	-1.06281300	-1.17606200
H	-3.93309000	-1.49077100	-1.71398400
C	-2.77786900	0.30410100	-1.74675300
C	-3.19404600	0.65803100	-3.02124900
C	-1.80240000	1.10823500	-1.06005200
C	-2.71610500	1.82014100	-3.64449900
H	-3.88958200	0.00989700	-3.55034900
C	-1.36002600	2.31562800	-1.70344600
H	-1.82284300	1.12023400	0.02501400
C	-1.78851900	2.63947700	-2.97536400
H	-3.06091500	2.08319500	-4.64055800

H	-0.67721500	2.96684700	-1.17579000
H	-1.42773100	3.54738400	-3.45198100
H	-4.80498700	-0.24454900	1.77452700
H	-4.43339400	0.84431200	0.42754300
H	-5.51620900	-0.53196100	0.17215700