

Electronic supplementary information

Mechanistic and chemoselective insights on sp^3 - and sp^2 -C-H bond aminations: Fe- vs. Ir-based catalysis

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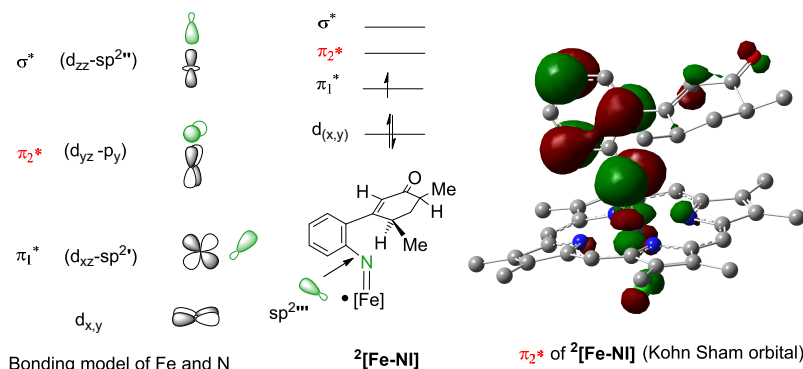
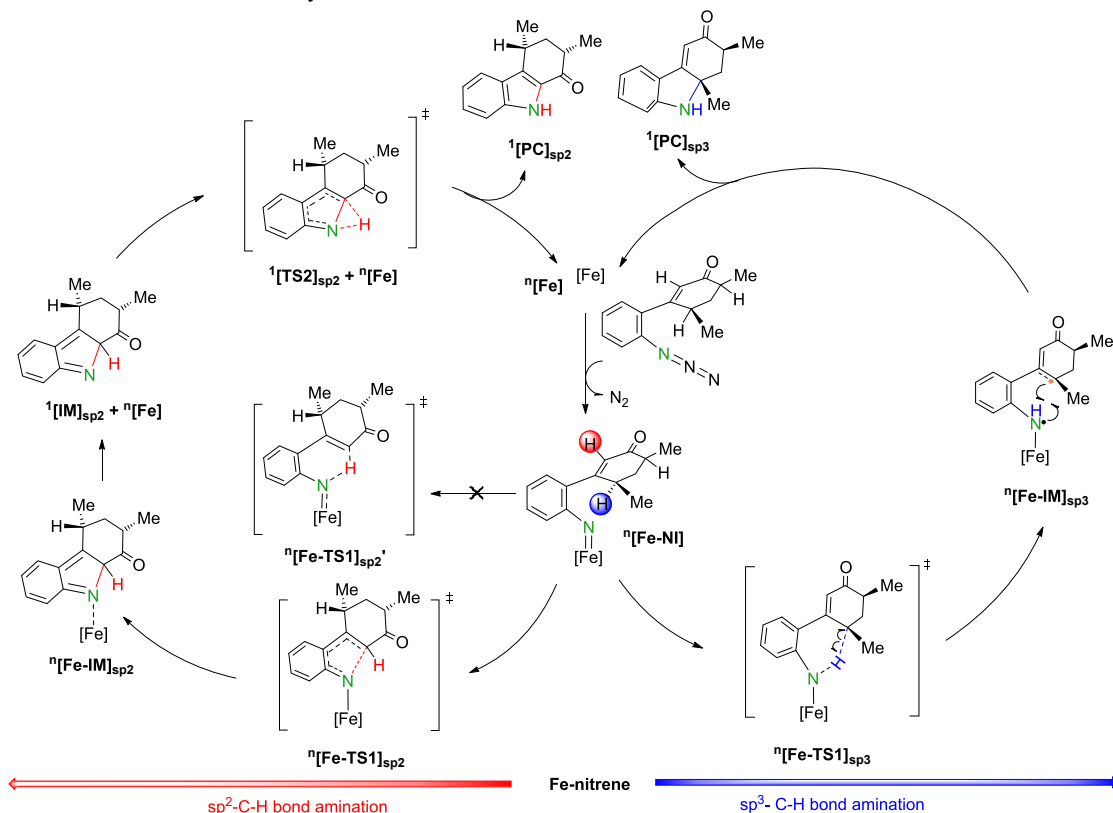
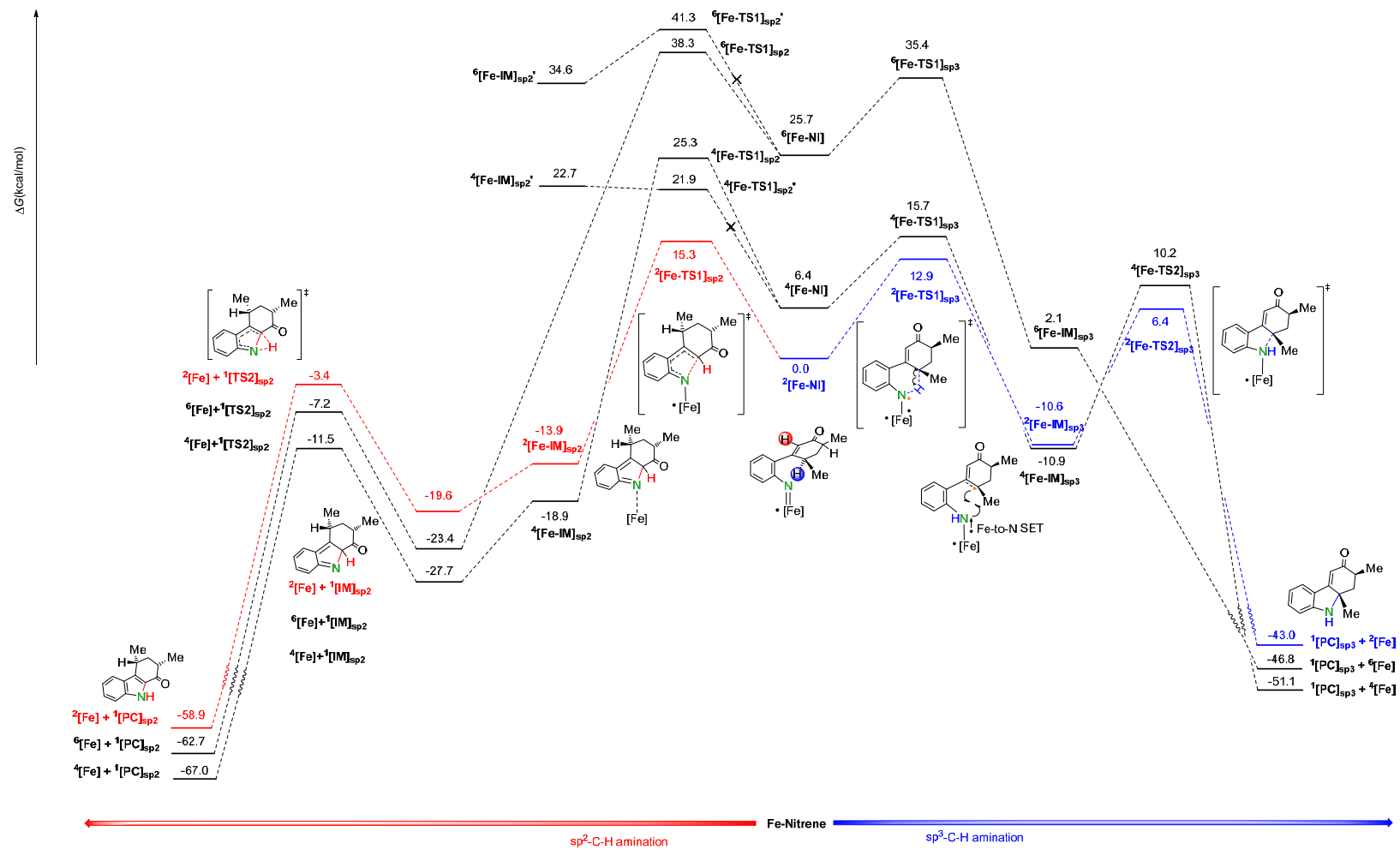


Fig. S1 Frontier molecular orbital of Fe-nitrene. The Fe center utilizes d_{zz} , d_{xz} and d_{yz} orbitals to form σ and π bonds with p_y and two orbitals of sp^2 hybrids of nitrene-N atom, respectively (another sp^2 orbital was used to form the N–C bond). The energetic ordering of important frontier orbitals of Fe-nitrene can be described as $\sigma(d_{zz}-sp^{2n}) < \pi_2(d_{xz}-sp^{2n}) < \pi_1(d_{yz}-p_y) < d_{xy} < \pi_1(d_{yz}-p_y)^* < \pi_2(d_{xz}-sp^{2n})^* < d_{xx-yy} < \sigma(d_{zz}-sp^{2n})^*$. The electronic configuration of doublet nitrene $^2[\text{Fe-NI}]$ can be described as $\sigma^2\pi_2^2\pi_1^2d_{xy}^2\pi_1^*1\pi_2^*d_{xx-yy}\sigma^*$. One electron transfers from d_{xy} to π_2^* leading to quartet $^4[\text{Fe-NI}]$, as well as two single electrons shift from d_{xy} and π_1 to π_2^* and π_1^* , respectively, receiving sextet $^6[\text{Fe-NI}]$. Obviously, Fe–N (nitrene) bonds in $^2[\text{Fe-NI}]$, $^4[\text{Fe-NI}]$ and $^6[\text{Fe-NI}]$ are of multiple-bond characters. For clarity, all H-atoms are omitted in Kohn Sham orbital diagram.

(a) Mechanistic details for Fe-catalyzed aminations.



(b) Gibbs free energy profile of doublet, quartet and sextet pathways for Fe-catalyzed aminations.



(c) Optimized structures with important geometrical parameters of the species in the Fe-catalyzed pathways (bond lengths in Å). For clarity, except for the two reactive H atoms of sp^3 - and sp^2 -C-H bonds, other H atoms are omitted.

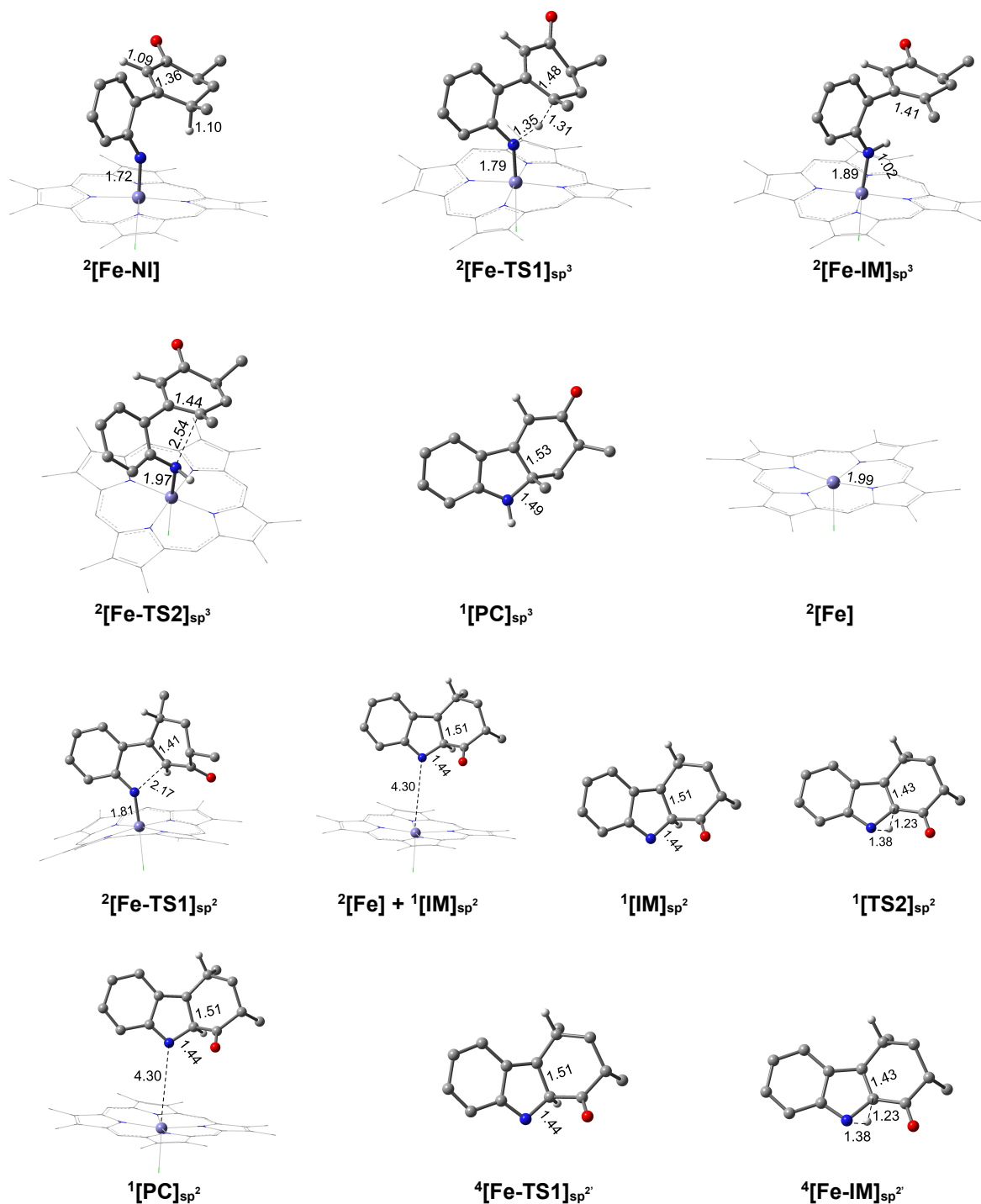


Fig. S2 Mechanistic details, free energy profiles and optimized structures of doublet, quartet and sextet pathways for Fe-catalyzed sp^3 - vs. sp^2 -C-H aminations.

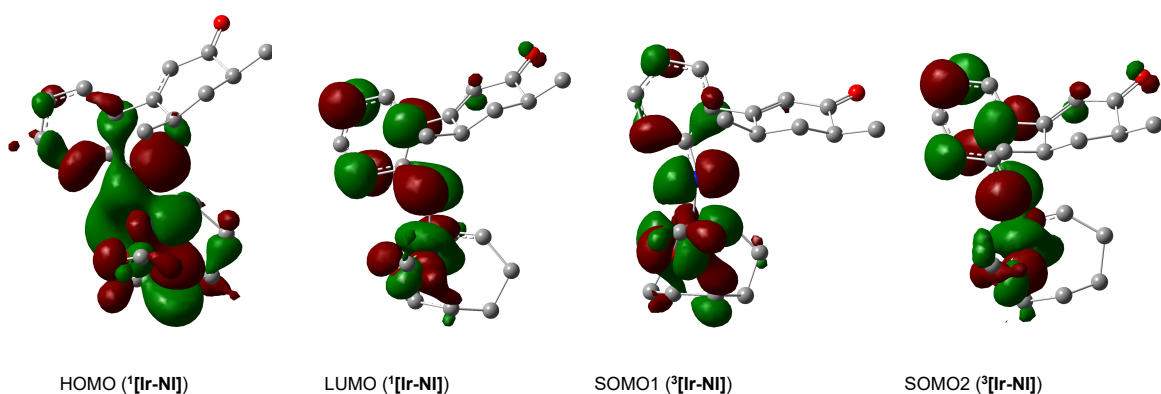
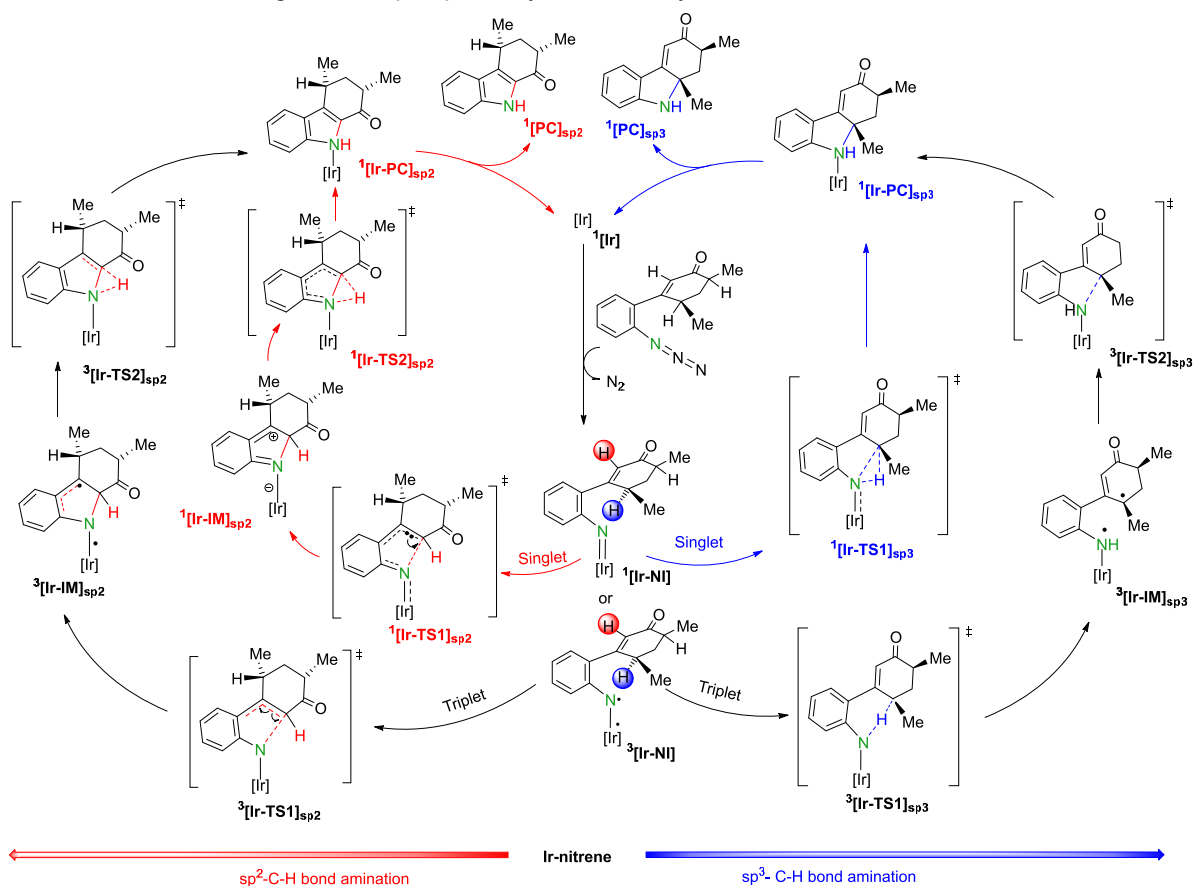
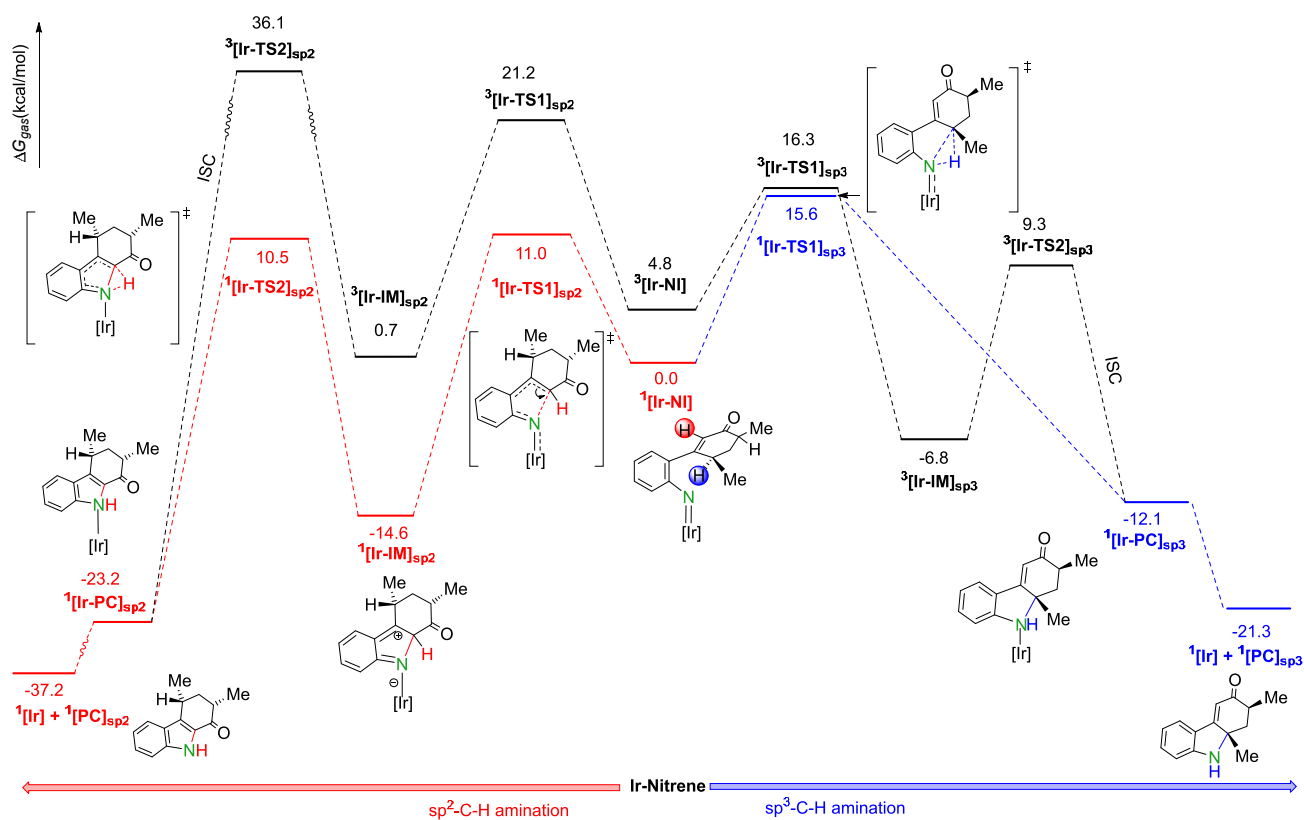


Fig. S3 Frontier molecular orbital of Ir-nitrene. For clarity, all H-atoms are omitted in Kohn Sham orbital diagram. HOMO and LUMO are the highest occupied molecular orbital and the the lowest unoccupied molecular orbital of singlet nitrene $^1[\text{Ir-NI}]$. SOMO1 and SOMO2 are two singly occupied molecular orbital of triplet nitrene $^3[\text{Ir-NI}]$. LUMO and SOMO1 and SOMO2 have a large contribution from the N p orbital, which indicates that they might accept electrons from heterolytic or homolytic cleavages of $\sigma_{\text{C-H}}/\pi_{\text{C=C}}$ bond of the substrates to trigger sp^3 - or sp^2 -C-H amination.

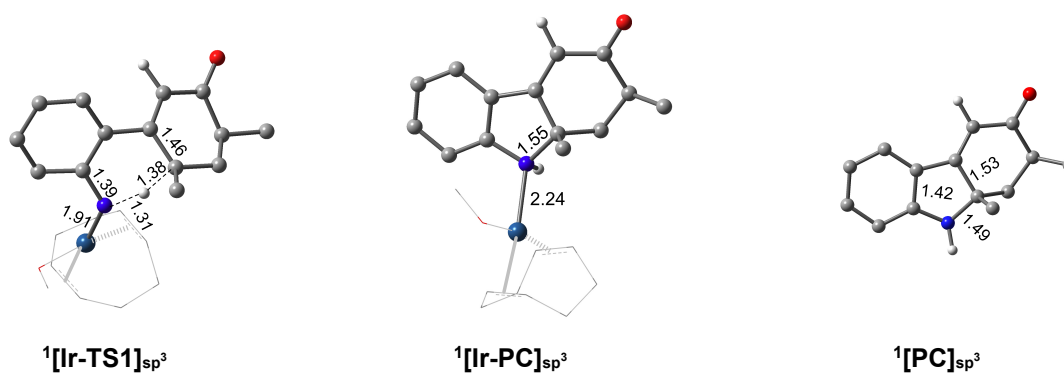
(a) Mechanistic details of singlet and triplet pathways for Ir-catalyzed aminations.



(b) Free energy profiles of singlet and triplet pathways for Ir-catalyzed aminations.



(c) Optimized structures with important geometrical parameters of the species in the Ir-catalyzed pathways (bond lengths in Å). For clarity, except for the two reactive H atoms of sp^3 - and sp^2 -C-H aminations, other H atoms are omitted.



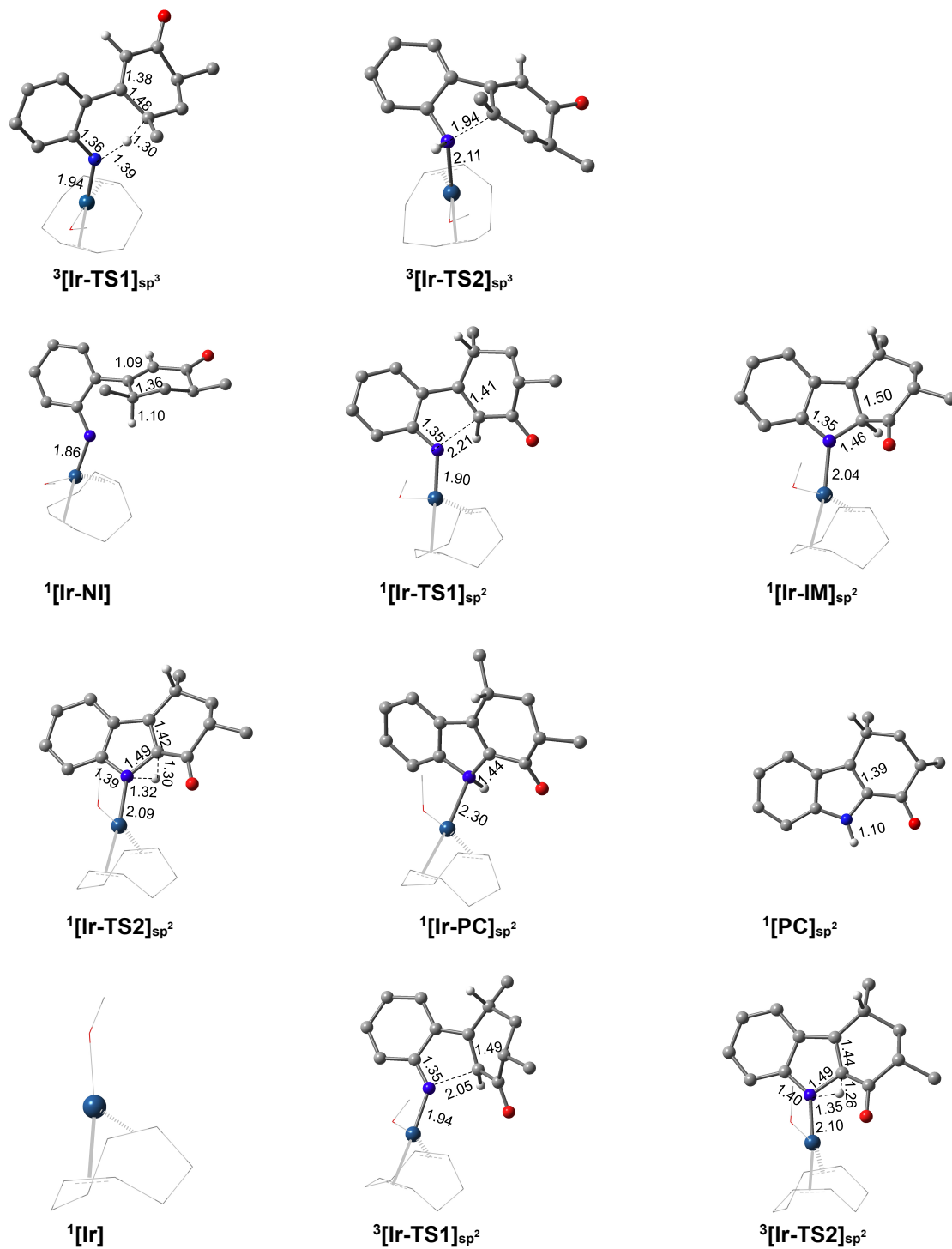


Fig. S4 Mechanistic details, free energy profiles and optimized structures of singlet and triplet pathways for Ir-catalyzed sp^3 - vs. sp^2 -C-H aminations.

Table S1(a) Energy calculations of the Fe-catalyzed system.

	Thermal Correction of Gibbs Energies	Gibbs Energies (BS1, gas)	Singlet Point Energies (BS2, gas)	Singlet Point Energies (BS2, sol)	ΔG (gas)	ΔG (sol)
²[Fe-NI]	0.651838	-2558.339976	-2559.543228	-2559.594777	0.0	0.0
⁴[Fe-NI]	0.650005	-2558.329385	-2559.531219	-2559.583139	6.4	6.2
⁶[Fe-NI]	0.644501	-2558.299862	-2559.494886	-2559.546332	25.7	25.8
²[Fe-TS1]_{sp³}	0.649731	-2558.318723	-2559.520603	-2559.569378	12.9	14.6
⁴[Fe-TS1]_{sp³}	0.648535	-2558.314278	-2559.514918	-2559.564239	15.7	17.1
⁶[Fe-TS1]_{sp³}	0.643026	-2558.283681	-2559.477937	-2559.527301	35.4	36.8
²[Fe-IM]_{sp³}	0.650070	-2558.353602	-2559.558308	-2559.610132	-10.6	-10.7
⁴[Fe-IM]_{sp³}	0.649396	-2558.354234	-2559.558172	-2559.609889	-10.9	-11.0
⁶[Fe-IM]_{sp³}	0.641294	-2558.334062	-2559.529292	-2559.585417	2.1	-0.7
²[Fe-TS2]_{sp³}	0.653791	-2558.326298	-2559.534982	-2559.579615	6.4	10.7
⁴[Fe-TS2]_{sp³}	0.649688	-2558.319545	-2559.524805	-2559.571280	10.2	13.4
¹[PC]_{sp³}	0.213954	-672.208910	-672.606384	-672.626167	—	—
²[Fe]	0.420582	-1886.196301	-1886.988047	-1887.026706	—	—
⁴[Fe]	0.419012	-1886.209070	-1886.999376	-1887.039523	—	—
⁶[Fe]	0.416181	-1886.201690	-1886.989684	-1887.027885	—	—
²[Fe-TS1]_{sp²}	0.655976	-2558.317271	-2559.522976	-2559.571985	15.3	16.9
⁴[Fe-TS1]_{sp²}	0.652279	-2558.300170	-2559.503309	-2559.552164	25.3	27.0
⁶[Fe-TS1]_{sp²}	0.646296	-2558.279218	-2559.475895	-2559.526527	38.8	39.4
⁴[Fe-TS1]_{sp^{2'}}	0.648178	-2558.305847	-2559.504726	-2559.553430	21.9	23.6
⁶[Fe-TS1]_{sp^{2'}}	0.641820	-2558.274776	-2559.467380	-2559.516305	41.3	43.0
²[Fe-IM]_{sp²}	0.643053	-2558.361368	-2559.556639	-2559.617054	-13.9	-19.5
⁴[Fe-IM]_{sp²}	0.645196	-2558.368842	-2559.566637	-2559.628161	-18.9	-25.1
⁴[Fe-IM]_{sp^{2'}}	0.651839	-2558.303827	-2559.507098	-2559.555772	22.7	24.5
⁶[Fe-IM]_{sp^{2'}}	0.642217	-2558.285753	-2559.478516	-2559.531421	34.6	33.7
¹[IM]_{sp²}	0.211760	-672.173902	-672.5669727	-672.5882334	—	—
¹[TS2]_{sp²}	0.208714	-672.148030	-672.538038	-672.558161	—	—
¹[PC]_{sp²}	0.214510	-672.235078	-672.632276	-672.650932	—	—

Table S1(b) Comparison of the energy order of doublet, quadruplet and sextet spin states using BPW91 and TPSSh functionals

	² [Fe-NI]	⁴ [Fe-NI]	⁶ [Fe-NI]	² [Fe-TS1] _{sp³}	⁴ [Fe-TS1] _{sp³}	⁶ [Fe-TS1] _{sp³}
BPW91 ^a	-2558.8914	-2558.8812	-2558.8504	-2558.8709	-2558.8664	-2558.8349
TPSSh ^b	-2559.1331	-2559.1219	-2559.0877	-2559.3645	-2559.3628	-2559.3574
Order ^c	² [Fe-NI] < ⁴ [Fe-NI] < ⁶ [Fe-NI]			² [Fe-TS1] _{sp³ < ⁴[Fe-TS1]_{sp³ < ⁶[Fe-TS1]_{sp³}}}		

^aFree energies(a.u.), BPW91/6-311+G (df,p)-LanL08(f)//BPW91/6-31g(d,p)-LanL08(f). ^bFree energies(a.u.), TPSSh/6-311+G(df,p)-LanL08(f)//TPSSh/6-31g(d,p)-LanL08(f) including dispersion correction (B3LYP-D3).

^cFree energy orders from the BPW91 functional calculations are in accord with those from the TPSSh.

Table S2 Energy calculations of the Ir-catalyzed system

	Thermal Correction of Gibbs Energies	Gibbs Energies	Singlet Point Energies (gas)	Singlet Point Energies (sol)	ΔG (gas)	ΔG (sol)
¹ [Ir-NI]	0.411549	-1203.946106	-1204.646908	-1204.674087	0.0	0.0
³ [Ir-NI]	0.408709	-1203.936598	-1204.636351	-1204.664016	4.8	4.5
¹ [Ir-TS1] _{sp²}	0.415474	-1203.930367	-1204.633286	-1204.658990	11.0	11.9
³ [Ir-TS1] _{sp²}	0.410138	-1203.912698	-1204.611792	-1204.638440	21.2	21.5
¹ [Ir-IM] _{sp²}	0.414687	-1203.970515	-1204.673285	-1204.701320	-14.6	-15.1
³ [Ir-IM] _{sp²}	0.412521	-1203.946361	-1204.646820	-1204.673016	0.7	1.3
¹ [Ir-TS2] _{sp²}	0.409828	-1203.929975	-1204.628409	-1204.657149	10.5	9.5
³ [Ir-TS2] _{sp²}	0.411056	-1203.889905	-1204.588860	-1204.614302	36.1	37.2
¹ [Ir-PC] _{sp²}	0.416662	-1203.982333	-1204.688971	-1204.718206	-23.2	-24.5
¹ [Ir]	0.179461	-531.765498	-532.056263	-532.074476	—	—
¹ [PC] _{sp²}	0.214510	-672.235078	-672.632276	-672.650932	—	—
¹ [Ir-TS1] _{sp³}	0.408849	-1203.920240	-1204.619360	-1204.645856	15.6	16.0
³ [Ir-TS1] _{sp³}	0.405371	-1203.919049	-1204.614721	-1204.643257	16.3	15.5
³ [Ir-IM] _{sp³}	0.408328	-1203.952912	-1204.654537	-1204.682663	-6.8	-7.4
³ [Ir-TS2] _{sp³}	0.412331	-1203.886931	-1204.632793	-1204.667597	9.3	4.6
¹ [Ir-PC] _{sp³}	0.417094	-1203.962279	-1204.671700	-1204.701660	-12.1	-13.8
¹ [PC] _{sp³}	0.213954	-672.208910	-672.606384	-672.626167	—	—

Cartesian coordinates of species of reaction pathways for Fe-catalyzed system

²[Fe-NI]

C	1.88812200	0.07762600	-2.17136600
N	0.78908500	0.71216600	-1.64570800
C	1.00821800	2.05912400	-1.80577100
C	2.29323200	2.29524500	-2.45474500
C	2.83593800	1.05253400	-2.70173000
N	-1.74875100	1.62829200	-0.69852600
C	-3.07266200	1.86823000	-0.40615000
C	-3.36758800	3.29069200	-0.50256600
C	-2.18649000	3.91008800	-0.85318800
C	-1.19278900	2.85371300	-0.99572600
C	0.49937000	-4.25164300	-0.82882600
C	-0.42329500	-3.17308300	-0.49956700
N	0.05460400	-1.96879700	-0.96169100
C	1.25020600	-2.24497800	-1.58679900
C	1.53926200	-3.67262600	-1.52515200
C	-3.71094800	-0.45653200	0.15755200
N	-2.47492400	-1.04133100	-0.03806900
C	-2.62367600	-2.36994100	0.29562900
C	-3.98190400	-2.63201200	0.75085300
C	-4.66672900	-1.43949400	0.64585100
C	2.84507600	3.65008200	-2.78809800
H	3.84287200	3.57592100	-3.24298100
H	2.19861900	4.18957900	-3.50074300
H	2.94054000	4.28389000	-1.89072100
C	4.12613800	0.70613300	-3.38601000
H	4.78367500	0.09520200	-2.74526500
H	3.95206200	0.13175300	-4.31151900
H	4.68818100	1.60948000	-3.66180600
C	-1.92237700	5.36759100	-1.09354300
H	-2.81065700	5.97727400	-0.87575200
H	-1.10169600	5.74409500	-0.46040200
H	-1.63948900	5.56305300	-2.14161700
C	-4.71767000	3.90004900	-0.26139200
H	-5.08845000	3.68958900	0.75608800
H	-4.69151800	4.99239700	-0.38046900
H	-5.47057000	3.51126600	-0.96737800
C	-6.10739800	-1.14934900	0.95015200
H	-6.64921700	-0.80320400	0.05407300
H	-6.62693900	-2.04396900	1.32134300
H	-6.21622800	-0.36440800	1.71761000
C	-4.48768600	-3.97257000	1.19697600
H	-4.45624900	-4.71250900	0.37947600
H	-3.88722800	-4.38070800	2.02712400
H	-5.52891300	-3.91321900	1.54408800

C	0.28343500	-5.69589300	-0.48287700
H	-0.61009000	-6.10547600	-0.98366900
H	1.14005200	-6.31391200	-0.78708700
H	0.14204000	-5.84104300	0.60122400
C	2.74733300	-4.32633900	-2.12981200
H	2.77210800	-4.19852100	-3.22503400
H	3.68606000	-3.90367100	-1.73390300
H	2.76331800	-5.40640200	-1.92619900
Fe	-0.82375500	-0.16136600	-0.74827500
Cl	-1.70215000	-0.41054200	-2.87089500
C	0.69684600	1.39311700	4.13626800
H	1.57355700	1.55764300	4.76684800
C	-0.58056900	1.71569100	4.61935400
H	-0.68657800	2.13810700	5.62170400
C	-1.72012700	1.48732900	3.82430900
H	-2.71393800	1.73413400	4.20574500
C	-1.58022400	0.95862600	2.54690400
H	-2.44738500	0.79222800	1.91127700
C	-0.28795600	0.61068300	2.02370900
C	0.88192900	0.82578900	2.86513400
C	2.25922700	0.50017400	2.41232000
H	2.94313300	2.48920200	2.81531300
C	3.20120400	1.48694700	2.46063300
C	4.59126200	1.32967500	1.97962300
O	5.41377300	2.24263100	2.10983700
C	6.42709800	-0.24979900	1.20559300
H	6.64658500	-1.12826700	0.57949400
H	6.95017400	0.62319000	0.79215700
H	6.83997800	-0.43503700	2.21002200
C	1.89570700	-2.00199500	2.76847200
H	2.17452800	-1.93489700	3.83264500
H	0.80198900	-1.93696700	2.69221600
H	2.19525200	-2.99573100	2.40250700
C	4.12682100	-1.13250800	1.94234800
H	4.47145800	-1.24231600	2.98829200
H	4.35065100	-2.08843900	1.43934700
C	4.91764900	0.00810900	1.27535500
H	4.52423900	0.12882900	0.24489400
C	2.60067000	-0.90920600	1.93797500
H	2.22924300	-0.98765600	0.89874300
N	-0.11026500	0.10551700	0.79276000
C	0.10326200	3.06232700	-1.46388000
H	0.40468500	4.09323400	-1.65395500
C	-3.99890200	0.89382200	-0.03262300
H	-5.02153100	1.22072900	0.15956700
C	-1.65164300	-3.35540500	0.13254500
H	-1.90987600	-4.36827900	0.44421600

C	2.09669100	-1.30068800	-2.16577400
H	3.01294900	-1.66941200	-2.62895200

⁴[Fe-Ni]

C	1.76184800	-0.30179500	-2.32043500
N	0.80302600	0.47455700	-1.70703800
C	1.23170800	1.77264000	-1.81267200
C	2.50801200	1.83710900	-2.51620300
C	2.82137800	0.54016900	-2.86673400
N	-1.57491100	1.65666900	-0.83003000
C	-2.89798900	2.02893300	-0.68518000
C	-3.03209400	3.47306400	-0.79656700
C	-1.75840500	3.97455900	-0.97453000
C	-0.86568000	2.82684200	-1.03070100
C	0.13973200	-4.32833200	-0.43597200
C	-0.65165600	-3.13567700	-0.15566100
N	-0.14882900	-2.05279000	-0.82953100
C	0.92518600	-2.51019200	-1.55048100
C	1.10907300	-3.94213900	-1.33956300
C	-3.75718200	-0.18393000	0.02055500
N	-2.54765100	-0.83949300	-0.00220900
C	-2.76771900	-2.07323400	0.57266200
C	-4.15320600	-2.19063900	1.00870200
C	-4.78159200	-1.02254800	0.62815300
C	3.25883500	3.10328900	-2.80533300
H	4.21064300	2.89774200	-3.31459800
H	2.67974400	3.78218700	-3.45401100
H	3.49443800	3.65578800	-1.88077800
C	4.00401700	0.03139100	-3.63778300
H	4.60552600	-0.68072300	-3.04833800
H	3.69210700	-0.49023100	-4.55796800
H	4.67081900	0.85254600	-3.93542300
C	-1.32142500	5.39994400	-1.14092300
H	-2.16053400	6.09574900	-1.00203000
H	-0.54201200	5.67300800	-0.41050700
H	-0.90521300	5.58442200	-2.14583000
C	-4.33257600	4.21497700	-0.70233000
H	-4.81823500	4.06753500	0.27724900
H	-4.18854400	5.29600600	-0.83670200
H	-5.04629700	3.87959900	-1.47310400
C	-6.21897600	-0.62564700	0.79485700
H	-6.69579900	-0.41617600	-0.17711600
H	-6.80088700	-1.42114700	1.28089300
H	-6.32623900	0.28249100	1.41201200
C	-4.73551600	-3.39702400	1.68489700
H	-4.71388100	-4.28366900	1.02884000
H	-4.18194500	-3.65681000	2.60242100

H	-5.78321200	-3.22884000	1.97095700
C	-0.13113200	-5.68965900	0.13451200
H	-1.09952800	-6.09161100	-0.20877000
H	0.64391200	-6.40996900	-0.16295800
H	-0.15812400	-5.67289300	1.23662300
C	2.17073700	-4.77451900	-1.99660100
H	2.06558200	-4.77228100	-3.09433000
H	3.18438400	-4.40536300	-1.76656600
H	2.12150800	-5.82128800	-1.66532600
Fe	-0.84877300	-0.15363000	-0.77830800
Cl	-1.77961600	-0.58661500	-2.87277600
C	0.77879200	1.56873800	4.09057600
H	1.67039700	1.73664400	4.70027900
C	-0.48018200	1.95129700	4.57800900
H	-0.56584000	2.42327300	5.55927500
C	-1.62582500	1.71194200	3.79517200
H	-2.61277800	2.00470800	4.16417700
C	-1.51528700	1.10570400	2.54935300
H	-2.39562700	0.93145800	1.93355900
C	-0.23918500	0.70045900	2.01980500
C	0.94119200	0.94251700	2.84422600
C	2.30575900	0.57600900	2.38797400
H	3.05494500	2.54804500	2.74243800
C	3.28207000	1.53227100	2.40546600
C	4.65300400	1.33275500	1.89990800
O	5.49973000	2.23252700	1.96978400
C	6.43987300	-0.31451700	1.14878500
H	6.63481100	-1.20610700	0.53277000
H	6.98288500	0.54064200	0.72380000
H	6.85165700	-0.49847700	2.15405600
C	1.88774600	-1.90629600	2.80374500
H	2.19147000	-1.82150800	3.85963000
H	0.79554300	-1.80714300	2.75002400
H	2.15240800	-2.91677600	2.45554100
C	4.12306400	-1.12003000	1.91557700
H	4.48010900	-1.22213400	2.95815200
H	4.31143900	-2.09157700	1.42696700
C	4.93797500	-0.01496000	1.22149600
H	4.54551400	0.09617800	0.18943900
C	2.60435000	-0.85092700	1.93545200
H	2.20884600	-0.94369500	0.90568900
N	-0.10133200	0.14336200	0.81223000
C	0.46982500	2.87988100	-1.42730900
H	0.90864000	3.86753500	-1.57683700
C	-3.92917800	1.15371200	-0.34654300
H	-4.93277800	1.57272600	-0.25917800
C	-1.84879300	-3.12341200	0.56703400

H	-2.15498600	-4.05626800	1.04344500
C	1.79225200	-1.69538600	-2.28644400
H	2.61973500	-2.18713800	-2.80064100

⁶[Fe-NI]

C	1.94892400	-0.29727700	-2.13007800
N	0.90359300	0.49978800	-1.71447500
C	1.21928600	1.78642500	-2.04432500
C	2.52815400	1.83308800	-2.69994300
C	2.98022400	0.52928400	-2.76014100
N	-1.57792100	1.76549800	-0.79748100
C	-2.85297900	2.15716200	-0.45084100
C	-3.00113800	3.59412300	-0.66339600
C	-1.79342300	4.04932700	-1.15739400
C	-0.91608700	2.88681200	-1.25647400
C	0.01715700	-4.43225100	-0.61938500
C	-0.79295300	-3.23680500	-0.37270200
N	-0.13317500	-2.12562600	-0.82723000
C	1.04642100	-2.54188900	-1.36759000
C	1.16830500	-3.99713600	-1.24897900
C	-3.79122400	-0.09511800	0.22720400
N	-2.65476200	-0.83777700	0.04569000
C	-2.96054600	-2.13733600	0.34807700
C	-4.35666500	-2.23096600	0.77891900
C	-4.87902600	-0.95368000	0.69496100
C	3.18981300	3.08406900	-3.19652300
H	4.17191600	2.87279000	-3.64208700
H	2.58090900	3.58762800	-3.96644800
H	3.34889500	3.80979900	-2.38129200
C	4.25158100	0.00376700	-3.35997100
H	4.84752800	-0.56557400	-2.62743200
H	4.04926000	-0.67186000	-4.20830200
H	4.88741600	0.81827000	-3.73418800
C	-1.40824000	5.44293600	-1.55766600
H	-2.22118000	6.15719600	-1.36621600
H	-0.52298600	5.79510100	-1.00217700
H	-1.16376000	5.50443100	-2.63160100
C	-4.25629400	4.36973000	-0.39207000
H	-4.56515600	4.28871400	0.66378200
H	-4.12657200	5.43806400	-0.61445700
H	-5.09828100	4.00692800	-1.00556500
C	-6.27303400	-0.48529400	0.99357600
H	-6.76667300	-0.08016500	0.09412600
H	-6.90176800	-1.30446900	1.37003800
H	-6.28317800	0.31203800	1.75580700
C	-5.04317200	-3.50004600	1.19132600
H	-5.09309300	-4.22456400	0.36095400

H	-4.51773000	-3.99631100	2.02442700
H	-6.07441400	-3.31132700	1.52158800
C	-0.38537400	-5.83264300	-0.26091300
H	-1.29182100	-6.14782100	-0.80496600
H	0.40731600	-6.55446500	-0.50346600
H	-0.60187100	-5.93268800	0.81589200
C	2.32973300	-4.80615100	-1.74781900
H	2.43693100	-4.73155700	-2.84320400
H	3.28314100	-4.47150100	-1.30555900
H	2.21319600	-5.87154700	-1.50371700
Fe	-0.83324800	-0.11706500	-0.72374800
Cl	-1.77524800	-0.58787400	-2.80393700
C	0.83504000	1.54668000	4.14057700
H	1.73799700	1.72452100	4.73036600
C	-0.41708900	1.91340600	4.65708800
H	-0.48609300	2.38533500	5.63969200
C	-1.57717100	1.65163200	3.90354800
H	-2.56019500	1.92305900	4.29839600
C	-1.48635100	1.04600700	2.65627800
H	-2.37953600	0.84657200	2.06940200
C	-0.21837600	0.66657600	2.08923200
C	0.97786900	0.92363900	2.89052700
C	2.33845400	0.56193400	2.42051900
H	3.07445200	2.54552600	2.73935400
C	3.30740900	1.52619200	2.41768100
C	4.68146600	1.32479700	1.92158000
O	5.52356700	2.22951400	1.98103400
C	6.48310300	-0.32706600	1.21854000
H	6.68773500	-1.23190500	0.62532800
H	7.02409500	0.52108800	0.77728100
H	6.88900400	-0.48489000	2.23059200
C	1.92296900	-1.92093300	2.85477100
H	2.21391300	-1.82890500	3.91363900
H	0.83113300	-1.82694900	2.78725500
H	2.19471200	-2.93285900	2.51617400
C	4.16513600	-1.13092000	1.98496400
H	4.51497500	-1.21117700	3.03185800
H	4.36238100	-2.11071900	1.51660900
C	4.97895100	-0.03531000	1.27448400
H	4.59207600	0.05215200	0.23802700
C	2.64508300	-0.86903800	1.98714500
H	2.26178900	-0.97159800	0.95410300
N	-0.09127000	0.10037700	0.88428800
C	0.37374500	2.88857900	-1.80708400
H	0.75171000	3.86113400	-2.13031300
C	-3.86513500	1.29323900	0.00428700
H	-4.83235800	1.76009700	0.20455100

C	-2.07982300	-3.22638300	0.19299800
H	-2.47389800	-4.19992400	0.49476400
C	2.00342800	-1.68720200	-1.96332900
H	2.89904000	-2.17779300	-2.35240700

²[Fe-TS1]_{sp}³

C	-0.25294800	-2.13722900	4.04791800
H	-1.04495800	-2.39253100	4.75661300
C	1.04856200	-2.60664900	4.25547000
H	1.27720900	-3.23293300	5.12025000
C	2.05413500	-2.25075500	3.33925700
H	3.07945300	-2.59977300	3.48857600
C	1.77240700	-1.44865900	2.23533500
H	2.56358700	-1.16744000	1.54707000
C	0.46077900	-0.93485300	2.00991500
N	0.19482700	-0.07985000	0.97587200
C	-0.57352400	-1.31187800	2.95805600
C	-1.94585000	-0.87269100	2.66857700
C	-4.37075800	-1.35677800	2.30457100
O	-5.38464700	-1.97348100	2.65429800
C	-5.79833900	0.16531000	0.84903900
H	-5.79797700	0.82245700	-0.03380900
H	-6.46400800	-0.68704800	0.65830600
H	-6.22230300	0.72953300	1.69481900
C	-1.45252900	1.61092300	2.88727000
H	-2.07438900	1.78154000	3.78347400
H	-0.42838400	1.39426300	3.21675900
H	-1.43784100	2.54068000	2.30005700
C	-3.41436600	0.84627800	1.46776800
H	-3.90373100	1.52401400	2.19539500
H	-3.27133600	1.45101800	0.55623100
C	-4.37948900	-0.31919700	1.17199100
H	-3.98263400	-0.86748100	0.29457100
C	-2.05686800	0.46911200	2.05608000
H	-1.08425800	0.30887400	1.19758800
C	-3.04072800	-1.68035700	2.84936100
H	-2.94683300	-2.64815800	3.35078700
C	0.80892500	-2.71323900	-1.24597100
N	1.47149700	-1.54941500	-0.93796300
C	2.81148600	-1.87346600	-0.88808500
C	3.00175000	-3.29307700	-1.15440700
C	1.74444000	-3.82569800	-1.34933800
N	2.44327900	0.97652400	-0.08426500
C	2.69122000	2.22103200	0.44112700
C	4.10479100	2.36440900	0.77112200
C	4.71445800	1.18931200	0.38461100
C	3.65758100	0.33000200	-0.13542300

C	-3.11927800	-0.47894200	-2.58015200
C	-2.09813200	0.37377600	-1.98714800
N	-1.05706100	-0.38733500	-1.49871200
C	-1.38756300	-1.70163400	-1.76387400
C	-2.69086300	-1.78011400	-2.40845500
C	0.47494800	3.21951900	-0.03190100
N	-0.10944200	2.11864300	-0.62520200
C	-1.28506500	2.56696500	-1.18587000
C	-1.46823400	3.98772400	-0.92559700
C	-0.37904500	4.39054000	-0.17895200
C	4.33330200	-3.98415000	-1.18845300
H	4.22385600	-5.05446800	-1.41289400
H	4.99428500	-3.55302700	-1.95875200
H	4.86283000	-3.90350900	-0.22409300
C	1.35637600	-5.24269800	-1.65395600
H	0.62920100	-5.63209000	-0.92211400
H	0.89460800	-5.33448600	-2.65159500
H	2.22925200	-5.91037300	-1.63572700
C	6.16348500	0.80725500	0.46285600
H	6.57644000	0.57759000	-0.53364900
H	6.76996000	1.61865500	0.88929600
H	6.32002800	-0.08512200	1.09224000
C	4.72098800	3.59313200	1.37292200
H	5.79272900	3.44912700	1.56978200
H	4.62492900	4.46650500	0.70587500
H	4.24429900	3.86190700	2.33042000
C	-0.05648700	5.75660900	0.35276100
H	0.83527400	6.18373400	-0.13651100
H	-0.88665000	6.45781100	0.18753900
H	0.14672600	5.73719100	1.43631500
C	-2.63357300	4.80137900	-1.40739700
H	-2.68444000	4.82207300	-2.50899300
H	-3.59474200	4.39817500	-1.04675700
H	-2.56584000	5.84320500	-1.06386600
C	-4.36354600	0.02002200	-3.25464700
H	-4.12395200	0.59901500	-4.16243500
H	-5.01633800	-0.81040600	-3.55805300
H	-4.95505100	0.67877900	-2.59794400
C	-3.35804000	-3.05526100	-2.83442800
H	-2.79170500	-3.56447100	-3.63249700
H	-3.45149700	-3.76662100	-1.99735500
H	-4.37026700	-2.86881100	-3.21990600
Fe	0.65070400	0.27042100	-0.71924300
Cl	1.40240100	0.72571200	-2.83761200
C	-0.54785200	-2.79540500	-1.56420900
H	-0.94656400	-3.78197700	-1.80432500
C	3.83819000	-0.98871600	-0.55598000

H	4.85667500	-1.37951500	-0.55911200
C	1.75206100	3.24996300	0.52650800
H	2.08478900	4.19497200	0.95850700
C	-2.19778400	1.75945400	-1.86502600
H	-3.07822700	2.24131500	-2.29230800

⁴[Fe-TS1]_{sp³}

C	-0.37980100	-1.64742500	4.25673500
H	-1.16700800	-1.79424700	5.00085200
C	0.92327300	-2.08632000	4.52242300
H	1.15548400	-2.57741200	5.46986900
C	1.92679400	-1.87826300	3.55705200
H	2.94953200	-2.21276100	3.75127800
C	1.64237600	-1.23816900	2.35467900
H	2.42767500	-1.07657400	1.62147800
C	0.32788800	-0.75342200	2.05703400
N	0.02276500	-0.10551900	0.90514200
C	-0.70925300	-0.99258400	3.06062700
C	-2.08878900	-0.61511800	2.71827600
C	-4.48569700	-1.23857500	2.37649000
O	-5.47927300	-1.87396200	2.75470200
C	-5.95146500	0.07254100	0.75999100
H	-5.96850800	0.62473000	-0.19224800
H	-6.57866000	-0.82394000	0.66393500
H	-6.40890800	0.71080800	1.53276000
C	-1.63644300	1.88194500	2.61856900
H	-2.24472600	2.14853100	3.50068700
H	-0.60194200	1.72701200	2.95245200
H	-1.65025700	2.73610900	1.92554600
C	-3.61102500	0.91585600	1.35398000
H	-4.12649500	1.61178100	2.04643600
H	-3.50807700	1.46898500	0.40461100
C	-4.51884900	-0.31224900	1.14802900
H	-4.08083500	-0.92038300	0.33131600
C	-2.22534300	0.63614000	1.93629600
H	-1.29456700	0.35356700	1.09719400
C	-3.15947100	-1.43767000	2.97816900
H	-3.03498500	-2.34338100	3.57904500
C	0.85067500	-2.79529600	-1.10757000
N	1.53009000	-1.60793600	-0.87950600
C	2.86786100	-1.94409400	-0.81445700
C	3.04365900	-3.37722900	-0.98735800
C	1.78020800	-3.91348900	-1.13379800
N	2.46237300	0.90003100	-0.07540900
C	2.68843600	2.15290100	0.47298900
C	4.08861200	2.30072800	0.83915200
C	4.72287800	1.14135100	0.44117200

C	3.69290700	0.27527000	-0.11139200
C	-3.01266200	-0.60583200	-2.67467000
C	-1.97352000	0.26088600	-2.12705500
N	-0.95740100	-0.49276900	-1.58758900
C	-1.32139200	-1.80334000	-1.74889200
C	-2.61961600	-1.90174700	-2.40546000
C	0.51535800	3.16553500	-0.13496200
N	-0.01477100	2.06272800	-0.75162100
C	-1.16052300	2.48632000	-1.38435000
C	-1.36212700	3.91472500	-1.16719700
C	-0.32540900	4.33524400	-0.35764500
C	4.36999600	-4.07791400	-0.97772800
H	4.25530100	-5.15818200	-1.14315500
H	5.03639800	-3.69268400	-1.76740400
H	4.89540900	-3.94614500	-0.01662500
C	1.38384400	-5.34618700	-1.33672000
H	0.64805500	-5.67419800	-0.58400200
H	0.92890600	-5.50712200	-2.32873800
H	2.25124700	-6.01682300	-1.26237300
C	6.17427800	0.77660100	0.54524600
H	6.60677700	0.55418100	-0.44448700
H	6.76368700	1.59318600	0.98499400
H	6.32843500	-0.11629300	1.17463500
C	4.67847900	3.52469200	1.47580000
H	5.74238300	3.38134400	1.71092900
H	4.60452200	4.40449500	0.81436900
H	4.16494800	3.78124300	2.41719400
C	-0.03802900	5.71017800	0.17128700
H	0.88383200	6.13076100	-0.26509500
H	-0.85547900	6.40768300	-0.05978700
H	0.09240900	5.70870300	1.26613100
C	-2.49472200	4.71653800	-1.73852100
H	-2.47526500	4.71551200	-2.84117000
H	-3.47672200	4.31983000	-1.43096000
H	-2.44869500	5.76484000	-1.41158600
C	-4.23937100	-0.12480600	-3.39257400
H	-4.82144600	0.58748500	-2.78514500
H	-3.97996400	0.38830100	-4.33388700
H	-4.90786100	-0.95908600	-3.64729000
C	-3.31231800	-3.18910800	-2.74490900
H	-2.74878800	-3.77050100	-3.49429400
H	-3.43543200	-3.83285300	-1.85844900
H	-4.31424200	-3.00799100	-3.15878900
Fe	0.76407800	0.19298500	-0.76980900
Cl	1.46974000	0.63025600	-2.91638300
C	-0.49626900	-2.89102200	-1.44473900
H	-0.89857900	-3.89026400	-1.61747000

C	3.89142400	-1.04690400	-0.50991300
H	4.91119300	-1.43335100	-0.48780900
C	1.75708100	3.18660700	0.50889300
H	2.07473600	4.13012100	0.95532100
C	-2.05257000	1.65334000	-2.06369200
H	-2.92046600	2.12517300	-2.52717300

⁶[Fe-TS1]_{sp³}

C	0.36938300	1.78028900	4.28811500
H	1.16379600	1.95977700	5.01722300
C	-0.93698700	2.20295500	4.56002000
H	-1.16549200	2.71951100	5.49464000
C	-1.94849400	1.93737500	3.61917500
H	-2.97714000	2.25030700	3.81830000
C	-1.66692600	1.26225200	2.43438400
H	-2.46123200	1.05320700	1.72466400
C	-0.34769100	0.80941600	2.12500600
N	-0.03906600	0.13465900	0.98370600
C	0.69559700	1.09676500	3.10641400
C	2.07413200	0.71304300	2.77336200
C	4.47801100	1.30528700	2.42882700
O	5.47528600	1.93922200	2.79901200
C	5.94492000	-0.06879400	0.86661800
H	5.96323200	-0.66009000	-0.06186900
H	6.58003200	0.81780500	0.73739400
H	6.39263800	-0.67843100	1.66759700
C	1.61402100	-1.78887200	2.75724000
H	2.22343700	-2.03138500	3.64526200
H	0.58152500	-1.61757000	3.08874900
H	1.62148700	-2.66316200	2.08985400
C	3.59205700	-0.87075200	1.46345700
H	4.09847900	-1.55801400	2.17074900
H	3.48502500	-1.44377400	0.52562400
C	4.51290500	0.34209700	1.22951100
H	4.08820100	0.93075500	0.39168200
C	2.20860100	-0.56738800	2.03553300
H	1.29340500	-0.31533100	1.18623000
C	3.14859600	1.53578800	3.01152200
H	3.02849800	2.45862800	3.58655100
C	-0.93868000	2.80703700	-1.29943600
N	-1.57726500	1.66145500	-0.86305700
C	-2.90423600	1.97673800	-0.67863800
C	-3.11868900	3.39142400	-0.96611700
C	-1.89258300	3.91130100	-1.33852700
N	-2.51708800	-0.96155300	-0.01774900
C	-2.75129700	-2.27245600	0.33922400
C	-4.15886800	-2.43903900	0.69449200

C	-4.76595200	-1.21246400	0.49787000
C	-3.72143800	-0.29822500	0.04485400
C	3.11272100	0.63716900	-2.65730600
C	2.12698600	-0.23304600	-2.01036800
N	1.06168200	0.51330500	-1.57794300
C	1.30308400	1.81185000	-1.92488000
C	2.60258000	1.92067800	-2.59112300
C	-0.49546500	-3.26028700	-0.24957200
N	0.12313800	-2.12820700	-0.70389200
C	1.32624100	-2.50467900	-1.24018100
C	1.50430100	-3.95084700	-1.09631600
C	0.36687800	-4.42318400	-0.46706300
C	-4.44370000	4.08808500	-0.86868600
H	-4.35904700	5.15489700	-1.11859600
H	-5.18470200	3.64731700	-1.55677000
H	-4.86568300	4.02076100	0.14833800
C	-1.55558100	5.31508400	-1.74695200
H	-0.75716100	5.74078800	-1.11654300
H	-1.20412300	5.36115300	-2.79159700
H	-2.42725100	5.97950000	-1.66592700
C	-6.20622800	-0.83568600	0.68364000
H	-6.66072800	-0.49469800	-0.26185100
H	-6.80293600	-1.68447800	1.04604100
H	-6.32312900	-0.01624700	1.41294700
C	-4.77795200	-3.72897800	1.14615400
H	-5.84144400	-3.60220500	1.39286700
H	-4.71274800	-4.50601300	0.36577200
H	-4.27713200	-4.12824200	2.04400000
C	0.01790100	-5.83426100	-0.09319500
H	-0.85670600	-6.20042700	-0.65723900
H	0.84940300	-6.52325300	-0.29873900
H	-0.22637100	-5.92543800	0.97839700
C	2.69957600	-4.72151400	-1.57594400
H	2.80966500	-4.65846900	-2.67172200
H	3.63666600	-4.34304400	-1.13434300
H	2.62322700	-5.78701300	-1.31683000
C	4.39147000	0.16897800	-3.28801400
H	4.19772600	-0.47259600	-4.16441000
H	5.00504200	1.01401200	-3.63092400
H	5.00645400	-0.41834800	-2.58675400
C	3.19712300	3.19647300	-3.11156900
H	2.58978800	3.62666300	-3.92598500
H	3.27228700	3.96309900	-2.32243500
H	4.20931800	3.03678400	-3.50924500
Fe	-0.74584800	-0.18479300	-0.69791700
Cl	-1.39827800	-0.67014000	-2.86330400
C	0.38959300	2.87101600	-1.74237800

H	0.73213500	3.85588800	-2.06798000
C	-3.89184700	1.05998000	-0.27512500
H	-4.90656100	1.45376700	-0.18593400
C	-1.80468300	-3.30589200	0.27062700
H	-2.15684600	-4.29143000	0.58415800
C	2.24457600	-1.62445300	-1.84487900
H	3.15191600	-2.08091900	-2.24755700

²[Fe-IM]_{sp³}

C	-0.62621400	-0.63176100	4.40707400
H	-1.47006400	-0.68828000	5.10017800
C	0.68145500	-0.84046700	4.87523400
H	0.85774300	-1.05987500	5.93058200
C	1.75358800	-0.75833500	3.96990100
H	2.77760800	-0.91390400	4.31963700
C	1.52984000	-0.48258500	2.62248300
H	2.36435300	-0.42599800	1.92817000
C	0.21114700	-0.27564400	2.12353700
N	-0.04042300	-0.02691000	0.80321900
C	-0.88563400	-0.34113500	3.06136200
C	-2.30382800	-0.14628700	2.60922600
C	-4.48908800	-1.25224400	1.96921800
O	-5.21985700	-2.25767100	1.96098700
C	-6.45329400	0.18673000	1.20738300
H	-6.74136000	1.07183100	0.61921200
H	-6.85320300	-0.71266300	0.72023000
H	-6.93072200	0.26330300	2.19734200
C	-2.04821800	2.40178800	2.56805100
H	-2.55401000	3.07125900	3.28792000
H	-1.02603800	2.21852400	2.92213100
H	-1.99142500	2.96109000	1.61742900
C	-4.30721300	1.27942000	2.09125600
H	-4.83725900	1.41261700	3.05890700
H	-4.48918300	2.21269600	1.53097700
C	-4.93059300	0.08356500	1.34228700
H	-4.48278100	0.07160700	0.32721600
C	-2.83445600	1.13714500	2.39155300
H	-1.04267800	0.08535700	0.62568500
C	-3.12851200	-1.29095200	2.49130200
H	-2.74113300	-2.27182000	2.77686500
C	1.53675100	-2.89459400	-0.59309900
N	1.94972900	-1.57718800	-0.49580400
C	3.29292000	-1.62646200	-0.18399300
C	3.74212400	-3.00486300	-0.06477100
C	2.63703300	-3.79786800	-0.29677900
N	2.34532800	1.19522000	-0.18975200
C	2.31909600	2.56591000	0.00129200

C	3.61818400	3.04465200	0.44486100
C	4.45167400	1.94504400	0.47295300
C	3.64062500	0.80295000	0.08224100
C	-2.60456300	-1.82611200	-2.59476200
C	-1.78369700	-0.68510800	-2.20720100
N	-0.64066800	-1.10881200	-1.56607300
C	-0.71538400	-2.48178100	-1.52303000
C	-1.94437200	-2.95126000	-2.14636200
C	0.06890000	2.99863100	-0.92547500
N	-0.24237900	1.69942700	-1.25377900
C	-1.43849200	1.75307400	-1.93432700
C	-1.89942500	3.13073700	-2.04802100
C	-0.96244700	3.91032300	-1.39947300
C	5.14755900	-3.41778400	0.25876700
H	5.24742800	-4.51171100	0.29166200
H	5.86272200	-3.04450700	-0.49319400
H	5.47344500	-3.02787300	1.23786800
C	2.53546700	-5.29489900	-0.29433700
H	1.76107700	-5.64905100	0.40617400
H	2.27592500	-5.68767600	-1.29184800
H	3.48516400	-5.76085600	0.00376700
C	5.90685700	1.87390800	0.83070200
H	6.51084800	1.48462300	-0.00589300
H	6.30607800	2.86440900	1.09018700
H	6.08408900	1.21092800	1.69435100
C	3.93916000	4.47641300	0.75923000
H	4.97197100	4.58634800	1.11861100
H	3.82992100	5.12302500	-0.12776100
H	3.27452300	4.88131700	1.54048400
C	-0.93246300	5.40144100	-1.22788100
H	-0.09600400	5.85801400	-1.78367700
H	-1.85899500	5.86623700	-1.59379200
H	-0.81458800	5.69185200	-0.17071500
C	-3.15187300	3.55795500	-2.75575000
H	-3.11017700	3.31941300	-3.83178000
H	-4.04633000	3.05721600	-2.34884600
H	-3.31370800	4.64155800	-2.66728300
C	-3.90705100	-1.73047700	-3.33336700
H	-3.78273300	-1.23694100	-4.31170900
H	-4.33582900	-2.72506400	-3.51919200
H	-4.65795900	-1.15138100	-2.77012400
C	-2.34698400	-4.39185800	-2.26377500
H	-1.61589400	-4.97348100	-2.85003500
H	-2.42979600	-4.87280800	-1.27494700
H	-3.32221400	-4.49637600	-2.75944200
Fe	0.86665500	0.04694700	-0.84971100
Cl	1.69347400	0.16128900	-2.95310400

C	0.28119100	-3.31655200	-1.01910800
H	0.09606300	-4.39102900	-1.04522600
C	4.09721600	-0.51334000	0.05186700
H	5.14763000	-0.68939400	0.28600400
C	1.24423800	3.39977600	-0.29092000
H	1.36915500	4.46502000	-0.09237200
C	-2.14678500	0.64654400	-2.40287800
H	-3.08263600	0.83730600	-2.92987500

⁴[Fe-IM]_{sp³}

C	-0.65069200	-0.84112100	4.36710300
H	-1.49691300	-0.92614500	5.05436500
C	0.65222900	-1.09505600	4.82503300
H	0.82233000	-1.37844900	5.86607000
C	1.72821000	-0.97438900	3.92834900
H	2.74913900	-1.16392200	4.27021900
C	1.51115800	-0.61716500	2.59950400
H	2.34799500	-0.53049000	1.91115400
C	0.19680500	-0.36204200	2.10982100
N	-0.04092000	-0.03006900	0.80567200
C	-0.90403100	-0.46764900	3.04017000
C	-2.32039900	-0.23151600	2.60402100
C	-4.52744600	-1.28414300	1.94822000
O	-5.28157500	-2.27218500	1.93341400
C	-6.45570200	0.20270600	1.18723600
H	-6.72106300	1.10044100	0.60758100
H	-6.87086400	-0.68231300	0.68666900
H	-6.93866700	0.27751800	2.17461100
C	-2.01433300	2.31020000	2.60469600
H	-2.54051300	3.00785500	3.28112700
H	-1.01924500	2.10351200	3.01881800
H	-1.88307200	2.84924000	1.64930300
C	-4.29348000	1.24102400	2.09745400
H	-4.82789700	1.37682600	3.06230300
H	-4.45117400	2.18312800	1.54456200
C	-4.93655300	0.06646900	1.33167000
H	-4.48140300	0.05550400	0.31988900
C	-2.82613600	1.06486200	2.40671600
H	-1.03916100	0.11568300	0.62982100
C	-3.16966700	-1.35750800	2.47372900
H	-2.80422000	-2.34911500	2.75103700
C	1.45478200	-2.88878700	-0.69187100
N	1.90605700	-1.58802900	-0.54841100
C	3.24745100	-1.68749500	-0.23951700
C	3.65592000	-3.08163600	-0.16934200
C	2.52806100	-3.83343500	-0.42812000
N	2.38271000	1.15841500	-0.14336500

C	2.39524600	2.52120000	0.09863200
C	3.70743600	2.94608300	0.55864000
C	4.50932900	1.82304600	0.54501400
C	3.66601500	0.71967400	0.11302800
C	-2.64701700	-1.62939400	-2.66256200
C	-1.79447100	-0.52746700	-2.23219800
N	-0.66698500	-1.00732900	-1.60322000
C	-0.78243400	-2.37797800	-1.60874400
C	-2.02242000	-2.78869000	-2.25171800
C	0.15856000	3.05154100	-0.81012300
N	-0.18862400	1.77490200	-1.18741200
C	-1.38061800	1.88800300	-1.86790000
C	-1.80239300	3.28140900	-1.92985400
C	-0.84576200	4.00916000	-1.25039500
C	5.04853800	-3.54678400	0.13833800
H	5.11671300	-4.64360300	0.13053700
H	5.77483200	-3.16663900	-0.59935900
H	5.38468400	-3.20312700	1.13120900
C	2.38291900	-5.32601600	-0.47805600
H	1.59883200	-5.68173700	0.21076400
H	2.11155300	-5.67574700	-1.48835000
H	3.31874100	-5.82962900	-0.19787500
C	5.96183100	1.69724100	0.89856100
H	6.55415000	1.31990900	0.04826800
H	6.38969800	2.66610500	1.19186000
H	6.11983400	0.99976000	1.73845800
C	4.06879300	4.35539200	0.92615500
H	5.10449800	4.42256900	1.28773200
H	3.97725700	5.03785300	0.06438700
H	3.41630600	4.74902900	1.72324800
C	-0.77518500	5.49104000	-1.02079200
H	0.07635500	5.94534700	-1.55509900
H	-1.68664900	5.99543100	-1.37179000
H	-0.65461300	5.73647100	0.04741800
C	-3.04067100	3.77023000	-2.62247900
H	-3.00500100	3.56767200	-3.70605700
H	-3.95023800	3.28297000	-2.23301400
H	-3.16987800	4.85451700	-2.49674300
C	-3.94201400	-1.46929600	-3.40332400
H	-3.79597200	-0.95448100	-4.36763100
H	-4.40383800	-2.44319700	-3.61743200
H	-4.67539300	-0.87964400	-2.82812700
C	-2.46677200	-4.21175800	-2.42099500
H	-1.75236700	-4.79298200	-3.02788300
H	-2.56449400	-4.72539000	-1.45014000
H	-3.44410400	-4.26985000	-2.92013200
Fe	0.87210600	0.07723400	-0.84404000

Cl	1.70313000	0.24524200	-2.94227900
C	0.18800100	-3.25877900	-1.13277800
H	-0.02841800	-4.32580600	-1.19661200
C	4.08402600	-0.60749000	0.03483900
H	5.12875700	-0.82254000	0.26173100
C	1.34433600	3.39531300	-0.16119400
H	1.49900600	4.44844300	0.07707700
C	-2.11817600	0.82042700	-2.37973400
H	-3.04617600	1.05752500	-2.90176100

⁶[Fe-IM]_{sp³}

C	-1.39031200	-1.33650700	4.39160700
H	-2.29600100	-1.48568300	4.98559100
C	-0.13715700	-1.67507900	4.93636200
H	-0.08104100	-2.08907100	5.94590900
C	1.04130900	-1.46997800	4.18604600
H	2.01233600	-1.72911000	4.61494300
C	0.96724300	-0.94610600	2.90433700
H	1.85923000	-0.79079600	2.29603900
C	-0.29977900	-0.60225000	2.30938000
N	-0.29819100	-0.14871000	1.04628900
C	-1.50510500	-0.78889400	3.10957600
C	-2.85303200	-0.44843900	2.55955000
C	-5.06311800	-1.34486100	1.71103900
O	-5.88996000	-2.27014500	1.65084400
C	-6.77723900	0.26272000	0.71842700
H	-6.90708400	1.16459500	0.10054800
H	-7.20620900	-0.59802700	0.18819500
H	-7.35460600	0.39703600	1.64692700
C	-2.37097400	2.07170500	2.58296300
H	-2.94099700	2.82757900	3.15197400
H	-1.46563400	1.81838600	3.14914800
H	-2.05691500	2.56595600	1.64606800
C	-4.64655900	1.15474300	1.83475200
H	-5.26505100	1.35727000	2.73551300
H	-4.67164400	2.09143800	1.25162400
C	-5.29747100	0.01335800	1.02678000
H	-4.74053700	-0.06077500	0.06998600
C	-3.23669400	0.87917800	2.29919800
H	-1.26014700	0.02620700	0.72194100
C	-3.77079000	-1.51046100	2.36677800
H	-3.51102600	-2.52221400	2.68717200
C	1.77890300	-2.80124800	-0.90326000
N	2.12741900	-1.51319000	-0.54835200
C	3.37020100	-1.61486900	0.04465300
C	3.82092700	-2.99744700	0.06866500
C	2.81923300	-3.74274600	-0.51949200

N	2.46715000	1.23520000	0.08845700
C	2.44867600	2.59267400	0.34030900
C	3.65297900	3.00415500	1.04474100
C	4.41762400	1.86638800	1.20542500
C	3.66235800	0.77793200	0.60542100
C	-2.25748000	-1.52907100	-3.02757200
C	-1.49833200	-0.43923700	-2.43594700
N	-0.35843200	-0.91505500	-1.81543600
C	-0.37789400	-2.28230700	-2.00116800
C	-1.55834100	-2.68654300	-2.74818300
C	0.30253900	3.11951400	-0.77659100
N	-0.01323400	1.84166800	-1.18965300
C	-1.19478300	1.95814600	-1.89470800
C	-1.64028000	3.34174300	-1.93079500
C	-0.70347700	4.07038000	-1.22340600
C	5.13292700	-3.46045300	0.63068900
H	5.23910400	-4.55190100	0.55666400
H	5.98493800	-3.01027800	0.09426800
H	5.24144600	-3.19123400	1.69488700
C	2.76409700	-5.22311300	-0.75799900
H	1.87874400	-5.68018100	-0.28522300
H	2.71576200	-5.45944400	-1.83420500
H	3.65103900	-5.72923700	-0.35147500
C	5.76432600	1.71995100	1.85086200
H	6.52001500	1.35722000	1.13413200
H	6.12531200	2.67833000	2.24994700
H	5.74172500	1.00275300	2.68862600
C	3.95738500	4.41017800	1.47153600
H	4.91195900	4.46808200	2.01333700
H	4.02948200	5.09056600	0.60645300
H	3.17630300	4.81371800	2.13753000
C	-0.66218300	5.54802600	-0.96355900
H	0.20443500	6.02141600	-1.45499700
H	-1.56510800	6.04853800	-1.34112300
H	-0.58617900	5.77404600	0.11315500
C	-2.87412200	3.82761600	-2.63376700
H	-2.80816900	3.66788200	-3.72309300
H	-3.78024600	3.30406300	-2.28558700
H	-3.03337500	4.90290000	-2.47035900
C	-3.53891400	-1.36563700	-3.79111300
H	-3.39805400	-0.74161900	-4.68949600
H	-3.93449700	-2.33535200	-4.12411700
H	-4.32240400	-0.88477600	-3.18175600
C	-1.89008100	-4.10033700	-3.12503600
H	-1.11505700	-4.53944200	-3.77534300
H	-1.97604000	-4.74936500	-2.23757400
H	-2.84442000	-4.15887000	-3.66689400

Fe	1.12989800	0.18096000	-0.99172400
Cl	2.24489400	0.51631900	-3.04037500
C	0.60814700	-3.16388800	-1.56420800
H	0.46493600	-4.22268200	-1.78354700
C	4.09144700	-0.54819300	0.57754200
H	5.06481500	-0.77005100	1.01706900
C	1.43842700	3.46872200	-0.04878300
H	1.56216400	4.52090000	0.21115700
C	-1.88617200	0.89820500	-2.48022700
H	-2.80790500	1.13460400	-3.01364500

²[Fe-TS2]_{sp³}

C	-0.22288700	-3.15590500	3.03596400
H	-1.07277500	-3.74743600	3.38567100
C	1.08782300	-3.56967400	3.30647100
H	1.26720000	-4.50967800	3.83385700
C	2.16452400	-2.74423100	2.94453900
H	3.18723500	-3.04177200	3.19104000
C	1.94686900	-1.53733800	2.26507900
H	2.79080300	-0.90809000	1.98181300
C	0.63577700	-1.14283900	1.92436200
N	0.30642200	0.04956700	1.22250700
C	-0.45391200	-1.93733600	2.37515400
C	-1.78153200	-1.31228400	2.21463200
C	-4.20116400	-1.40467400	1.55081500
O	-5.21679800	-2.08723600	1.33952600
C	-5.60818000	0.71703800	1.63099200
H	-5.64319200	1.77773700	1.33868000
H	-6.35646400	0.16110900	1.05078400
H	-5.89301300	0.64614900	2.69348100
C	-1.06393600	0.71123800	3.65643800
H	-1.67578700	0.69264600	4.57913500
H	-0.12524100	0.19013700	3.87596500
H	-0.85328900	1.77216100	3.44710300
C	-3.12671400	0.84393100	2.22336400
H	-3.56017400	1.14328400	3.20091800
H	-2.85614400	1.80025100	1.73923900
C	-4.21194400	0.12345000	1.39563600
H	-3.95535700	0.26554000	0.32975400
C	-1.86353200	0.08601500	2.53831400
H	0.80401600	0.84765600	1.63722800
C	-2.89956700	-2.02022900	1.80058500
H	-2.82936700	-3.09587400	1.61974500
C	-0.74806700	-2.19055300	-1.53331900
N	0.40817000	-1.54167500	-1.14404000
C	1.41118200	-2.49330900	-1.21885500
C	0.86588700	-3.78391700	-1.60016500

C	-0.48950800	-3.59687800	-1.78753200
N	2.59861100	0.10470700	-0.37777200
C	3.51167600	1.03649700	0.06443500
C	4.85610100	0.47041200	0.09094600
C	4.73823400	-0.82701900	-0.35916400
C	3.32161200	-1.03756900	-0.63138700
C	-3.27050900	1.79321700	-1.84392500
C	-1.94949500	1.93117400	-1.24067000
N	-1.31167500	0.70999600	-1.16815100
C	-2.20264100	-0.20338300	-1.68635800
C	-3.43225300	0.45214000	-2.11886800
C	1.95238400	2.94532800	0.30640600
N	0.81273800	2.32072500	-0.16875900
C	-0.14881200	3.30688800	-0.24841500
C	0.37492800	4.57608100	0.22597100
C	1.69021300	4.34754700	0.58259600
C	1.67203800	-5.03908600	-1.76076300
H	1.03483400	-5.89354500	-2.02859400
H	2.43154700	-4.93588800	-2.55396800
H	2.20492800	-5.30231100	-0.83201400
C	-1.52805100	-4.59435500	-2.20912100
H	-2.37554300	-4.62321200	-1.50501100
H	-1.94128600	-4.35562400	-3.20383900
H	-1.11040100	-5.60946500	-2.26471200
C	5.80905500	-1.85985300	-0.55552600
H	5.88439800	-2.16932600	-1.61139800
H	6.79516300	-1.47831100	-0.25497200
H	5.61530200	-2.77103300	0.03522600
C	6.08920600	1.21665800	0.50901500
H	6.97612000	0.56754500	0.49170200
H	6.29380200	2.07020600	-0.15905200
H	5.99837000	1.62048400	1.53145400
C	2.70284900	5.31941700	1.11417900
H	3.53534600	5.46741100	0.40571500
H	2.25402400	6.30536100	1.30025400
H	3.14363300	4.97378600	2.06407400
C	-0.40289500	5.85881900	0.27302700
H	-0.70049100	6.19039000	-0.73613800
H	-1.32729600	5.75672000	0.86555800
H	0.18698500	6.67045900	0.72182000
C	-4.21245400	2.93097900	-2.10902200
H	-3.78470600	3.65080200	-2.82691900
H	-5.16372400	2.57429400	-2.52828900
H	-4.44985100	3.49347700	-1.19044800
C	-4.60266700	-0.25445400	-2.73773700
H	-4.31828500	-0.76879200	-3.67065800
H	-5.02366700	-1.01597000	-2.05986300

H	-5.41128800	0.44817400	-2.98358200
Fe	0.61016800	0.37984700	-0.69328200
Cl	1.15814600	0.88747100	-2.84092300
C	-1.97006200	-1.57123200	-1.78567900
H	-2.78346000	-2.19695100	-2.15432700
C	2.76666400	-2.25652600	-1.01310200
H	3.44688400	-3.09803800	-1.14974000
C	3.20467600	2.34532500	0.43151400
H	4.02273600	2.96937500	0.79394300
C	-1.43015900	3.13380900	-0.77090100
H	-2.06535400	4.01788800	-0.84185700

⁴[Fe-TS2]_{sp³}

C	-0.27514800	-3.26331000	2.96707600
H	-1.11407100	-3.89923100	3.26156900
C	1.04367000	-3.67586000	3.20335700
H	1.23948200	-4.65359700	3.65003200
C	2.10858100	-2.80154200	2.91890100
H	3.13468800	-3.10501300	3.14395900
C	1.87368600	-1.54268400	2.35548300
H	2.70870800	-0.87694400	2.13099300
C	0.55318900	-1.13700900	2.03559000
N	0.18871100	0.05788700	1.40127800
C	-0.52571700	-1.99568800	2.42049800
C	-1.85463900	-1.37224100	2.28977100
C	-4.22622900	-1.38268800	1.45586900
O	-5.21536400	-2.02394400	1.05913400
C	-5.63998400	0.72789200	1.65913100
H	-5.65415700	1.81597000	1.49141200
H	-6.33314400	0.24769000	0.95598500
H	-6.01532600	0.53546400	2.67759500
C	-1.17972700	0.51208000	3.92995400
H	-1.79935000	0.39558100	4.84054900
H	-0.23495000	-0.01409300	4.10465400
H	-0.98385400	1.59057700	3.82411600
C	-3.22395000	0.75442000	2.48089200
H	-3.72644500	0.87662200	3.46444300
H	-2.95382700	1.78407200	2.18364600
C	-4.22718500	0.15548700	1.47735800
H	-3.87651600	0.42100100	0.46229500
C	-1.95926100	-0.01592000	2.75027800
H	0.83863400	0.80046600	1.70290500
C	-2.95556000	-2.03168300	1.75294300
H	-2.87328900	-3.08433500	1.47074700
C	-0.61419700	-2.21248400	-1.62384900
N	0.51676500	-1.52889000	-1.22125100
C	1.54523300	-2.45002200	-1.27063100

C	1.05039300	-3.75396000	-1.67835400
C	-0.30635600	-3.60846300	-1.88732300
N	2.60624200	0.17443900	-0.32239600
C	3.47489300	1.12587300	0.17913800
C	4.82021200	0.58598000	0.28622200
C	4.75816900	-0.71272700	-0.18153500
C	3.37179000	-0.95382600	-0.54291900
C	-3.28949500	1.67514400	-1.88197500
C	-1.95854300	1.87057000	-1.32632500
N	-1.27776900	0.67288500	-1.25544900
C	-2.15029300	-0.28176300	-1.73038200
C	-3.41631400	0.32018500	-2.12191600
C	1.87593500	3.00960900	0.30714100
N	0.78134900	2.35537900	-0.22446400
C	-0.20331200	3.31445800	-0.34882600
C	0.26740300	4.60111900	0.13713500
C	1.56809700	4.40760700	0.55946900
C	1.89945300	-4.98161100	-1.82865500
H	1.29955400	-5.84908600	-2.13750000
H	2.68672700	-4.84031800	-2.58801300
H	2.40187700	-5.24709900	-0.88359700
C	-1.30664300	-4.63606600	-2.32813800
H	-2.15031200	-4.71269300	-1.62278500
H	-1.73144000	-4.39203200	-3.31644100
H	-0.85034800	-5.63288700	-2.40564300
C	5.86466700	-1.71700700	-0.31849500
H	6.01671900	-2.00914500	-1.37091100
H	6.81908600	-1.31707600	0.05176300
H	5.65291900	-2.64016800	0.24643200
C	6.01130400	1.35080600	0.78464300
H	6.90683800	0.71523200	0.82915200
H	6.24733300	2.20577200	0.12904400
H	5.84455400	1.75487400	1.79711600
C	2.52889600	5.40464200	1.13798000
H	3.40228200	5.55548300	0.48137100
H	2.05345400	6.38545700	1.27926100
H	2.91345700	5.08096100	2.11960800
C	-0.54443300	5.86318800	0.14104900
H	-0.82579400	6.16707500	-0.88119600
H	-1.47989500	5.74715900	0.71345700
H	0.01275600	6.69837500	0.58824600
C	-4.28278100	2.77174500	-2.13211500
H	-3.89660900	3.50765000	-2.85693300
H	-5.22466700	2.37478100	-2.53557900
H	-4.52841000	3.32391300	-1.20956200
C	-4.59300300	-0.43788800	-2.66289900
H	-4.32282800	-1.02277000	-3.55727000

H	-4.99540500	-1.14187700	-1.91561300
H	-5.40915700	0.24016000	-2.94930600
Fe	0.67028100	0.42029600	-0.80337700
Cl	1.25437900	0.96529400	-3.01161500
C	-1.86259000	-1.63933900	-1.84793500
H	-2.66055800	-2.29368200	-2.19981000
C	2.88034000	-2.17779500	-0.98791900
H	3.59356100	-2.99509700	-1.09939900
C	3.12745100	2.43253700	0.51625300
H	3.91219600	3.07080000	0.92415700
C	-1.46949100	3.09866200	-0.88814700
H	-2.13147800	3.96139700	-0.97353900

¹[PC]_{sp³}

C	-2.38060900	1.60134400	0.20361300
H	-2.03375700	2.61851700	0.40181700
C	-3.74827500	1.31985600	0.10965300
H	-4.48112500	2.12064700	0.22777700
C	-4.18628000	-0.00044400	-0.13199200
H	-5.25826700	-0.20465200	-0.19721800
C	-3.28316500	-1.05956100	-0.29224300
H	-3.63787000	-2.07447000	-0.48718100
C	-1.90850000	-0.77467400	-0.20115300
N	-0.83115800	-1.63253000	-0.38857700
C	-1.45521700	0.55207400	0.06270500
C	-0.00371000	0.51477300	0.07646600
C	2.35550300	1.22915900	-0.15086000
O	3.22127900	2.10355700	-0.00495400
C	3.91473600	-0.74518300	0.23361900
H	4.36628300	-1.63234300	-0.23714200
H	4.68991800	0.02485100	0.35172100
H	3.57072300	-1.03624000	1.23747400
C	0.71720600	-1.41079100	1.52901000
H	1.54928200	-0.83294700	1.95457800
H	-0.16254300	-1.25793100	2.17239100
H	0.99107700	-2.47864100	1.55015200
C	1.59356900	-1.16392900	-0.88720000
H	1.95023200	-2.20770300	-0.83612400
H	1.19549700	-1.01540300	-1.90342600
C	2.77534900	-0.18356800	-0.64315200
H	3.23054600	0.02597400	-1.62825900
C	0.41011700	-0.95764300	0.08034300
H	-0.94880500	-2.61161800	-0.13444100
C	0.92890200	1.51117300	0.04044700
H	0.64892700	2.56569400	0.11201500

²[Fe]

C	2.78877500	-1.21484200	-0.25870500
N	1.41544100	-1.39244400	-0.17184400
C	1.24676300	-2.76422300	-0.07253700
C	2.52259200	-3.45843400	-0.11085700
C	3.49032000	-2.48544300	-0.24024700
N	-1.40037000	-1.40752700	-0.17275200
C	-2.77555000	-1.24461700	-0.25967100
C	-3.46339600	-2.52268000	-0.24182000
C	-2.48528300	-3.48527400	-0.11249300
C	-1.21703500	-2.77745400	-0.07348800
C	2.48527500	3.48534900	-0.11234700
C	1.21702500	2.77752200	-0.07335500
N	1.40039500	1.40757300	-0.17256300
C	2.77557000	1.24470800	-0.25957200
C	3.46339500	2.52277200	-0.24177600
C	-2.78883500	1.21494300	-0.25862400
N	-1.41547600	1.39249600	-0.17179200
C	-1.24677000	2.76428800	-0.07255000
C	-2.52257800	3.45851500	-0.11084300
C	-3.49034300	2.48553200	-0.24019900
Fe	0.00002800	0.00004900	0.03614100
Cl	0.00000600	-0.00062700	2.25135000
C	-3.42382400	-0.01827400	-0.32041700
H	-4.51266500	-0.02413200	-0.38382300
C	-0.01826700	3.40840000	0.00052900
H	-0.02408800	4.49658500	0.07571100
C	3.42381200	0.01834700	-0.32044600
H	4.51264600	0.02416000	-0.38392800
C	0.01826200	-3.40833100	0.00052200
H	0.02407500	-4.49651200	0.07575800
C	2.63448600	4.97612800	-0.03466400
H	2.11964700	5.48256200	-0.86851600
H	2.21055900	5.37818500	0.90065000
H	3.69109500	5.27628900	-0.07103400
C	4.95077300	2.69455200	-0.34067500
H	5.47450100	2.20248400	0.49612000
H	5.35092900	2.26262700	-1.27333800
H	5.23378000	3.75643300	-0.32424700
C	4.97950300	-2.64132800	-0.33853200
H	5.37533300	-2.20596600	-1.27144300
H	5.49763000	-2.14294400	0.49800900
H	5.27380300	-3.70011500	-0.32104700
C	2.68759200	-4.94753000	-0.03302000
H	2.26717400	-5.35412500	0.90191100
H	2.17888400	-5.45931800	-0.86736600
H	3.74735400	-5.23649600	-0.06849300
C	-2.63450000	-4.97605800	-0.03493600

H	-2.11958400	-5.48241500	-0.86878600
H	-2.21065500	-5.37819800	0.90038000
H	-3.69110700	-5.27621500	-0.07141400
C	-4.95078700	-2.69443100	-0.34056400
H	-5.47439400	-2.20268200	0.49649700
H	-5.35109000	-2.26216100	-1.27300300
H	-5.23379300	-3.75631800	-0.32449000
C	-4.97951800	2.64147100	-0.33847000
H	-5.37532900	2.20664100	-1.27164100
H	-5.49768200	2.14259600	0.49775500
H	-5.27382400	3.70024500	-0.32038800
C	-2.68756500	4.94760700	-0.03293800
H	-2.26679400	5.35417800	0.90184600
H	-2.17916900	5.45944500	-0.86744800
H	-3.74733700	5.23657700	-0.06801700

⁴[Fe]

C	-2.57331000	1.62839000	-0.17856500
N	-1.18915300	1.60493700	-0.16861700
C	-0.80853200	2.93595100	-0.17959300
C	-1.96587400	3.81213100	-0.20183300
C	-3.07453800	2.99070800	-0.20112800
N	1.60497100	1.18913300	-0.16859600
C	2.93598900	0.80853300	-0.17852100
C	3.81216800	1.96587400	-0.20112000
C	2.99071900	3.07451700	-0.20194400
C	1.62839900	2.57328300	-0.17965700
C	-2.99072500	-3.07451300	-0.20197000
C	-1.62839900	-2.57328300	-0.17971600
N	-1.60496800	-1.18913600	-0.16859900
C	-2.93599500	-0.80852900	-0.17846200
C	-3.81216900	-1.96586800	-0.20105500
C	2.57330500	-1.62838600	-0.17852400
N	1.18914200	-1.60494400	-0.16858200
C	0.80852800	-2.93595600	-0.17962700
C	1.96587800	-3.81213200	-0.20186000
C	3.07453500	-2.99070500	-0.20110200
C	-1.90390300	5.31112000	-0.22185100
H	-1.36551200	5.68577100	-1.10853500
H	-2.90951600	5.75412200	-0.23775400
H	-1.38409500	5.70790500	0.66606800
C	-4.52662700	3.36783100	-0.22038700
H	-4.65770800	4.45884800	-0.23676800
H	-5.04230600	2.96138200	-1.10656300
H	-5.05701500	2.98650200	0.66804800
C	3.36782000	4.52660000	-0.22225100
H	2.98651400	5.05762000	0.66582000

H	4.45883400	4.65768900	-0.23876800
H	2.96132500	5.04163500	-1.10877700
C	5.31116900	1.90390900	-0.22011500
H	5.75416500	2.90951500	-0.23665300
H	5.70738100	1.38492300	0.66854100
H	5.68641000	1.36471300	-1.10605900
C	4.52663100	-3.36782400	-0.22026000
H	5.05697500	-2.98634600	0.66813400
H	4.65771700	-4.45884400	-0.23645900
H	5.04235300	-2.96151700	-1.10647800
C	1.90390800	-5.31112400	-0.22186700
H	1.38391600	-5.70788600	0.66595200
H	1.36569900	-5.68581400	-1.10864700
H	2.90952500	-5.75413000	-0.23755200
C	-3.36783300	-4.52659300	-0.22232900
H	-4.45884900	-4.65767700	-0.23879000
H	-2.96139800	-5.04158300	-1.10891100
H	-2.98647700	-5.05767000	0.66568500
C	-5.31117200	-1.90390100	-0.21994500
H	-5.75417400	-2.90950600	-0.23639900
H	-5.70730800	-1.38487200	0.66871900
H	-5.68647700	-1.36474200	-1.10588400
Fe	-0.00001200	-0.00000800	0.11348200
Cl	0.00003700	0.00000600	2.41394100
C	3.39079300	-0.50459800	-0.17545400
H	4.46933500	-0.66514000	-0.18071000
C	-0.50460100	-3.39076200	-0.17745400
H	-0.66513900	-4.46930000	-0.18360800
C	-3.39079800	0.50459800	-0.17543000
H	-4.46933900	0.66514300	-0.18066900
C	0.50459600	3.39075300	-0.17736300
H	0.66513000	4.46929300	-0.18346100

⁶[Fe]

H	2.89252000	3.48545300	-0.22554700
C	2.19573200	2.64575500	-0.19942700
C	0.83333100	2.95968200	-0.19605300
C	2.75531600	1.36457400	-0.19603300
N	-0.18873500	2.03070700	-0.16448700
C	0.29329900	4.31099800	-0.24281400
C	4.18299800	1.08302400	-0.24271200
N	2.03072000	0.18872900	-0.16425500
C	-1.36459100	2.75531700	-0.19595500
Fe	0.00000500	0.00006100	0.32464800
C	-1.08305100	4.18298200	-0.24270700
C	4.31101700	-0.29331600	-0.24247100
C	2.95969900	-0.83335600	-0.19563100

C	-2.64577800	2.19572700	-0.19903900
Cl	0.00008800	-0.00003100	2.57818600
N	-2.03074700	-0.18875000	-0.16392200
N	0.18874100	-2.03072700	-0.16386300
C	2.64576300	-2.19573700	-0.19889700
C	-2.95972300	0.83334300	-0.19562100
H	-3.48547300	2.89252600	-0.22506500
C	-2.75534700	-1.36457600	-0.19570000
C	-0.83336200	-2.95969500	-0.19568600
C	1.36456300	-2.75531600	-0.19573400
H	3.48545300	-2.89254000	-0.22489900
C	-4.31101700	0.29331300	-0.24258900
C	-4.18301300	-1.08304100	-0.24263800
C	-2.19573700	-2.64576600	-0.19897300
C	-0.29331700	-4.31099400	-0.24287100
C	1.08302600	-4.18298300	-0.24285000
H	-2.89252300	-3.48546800	-0.22511000
C	2.12647100	-5.26037100	-0.28741500
H	2.77183100	-5.16588400	-1.17693200
H	2.78516200	-5.22415100	0.59637300
H	1.67254600	-6.26089200	-0.31679400
C	-1.11992500	-5.56249600	-0.28742700
H	-1.77462800	-5.64802000	0.59591800
H	-1.77094600	-5.58928900	-1.17743800
H	-0.48903900	-6.46203100	-0.31579400
C	-5.26039600	-2.12649400	-0.28695400
H	-5.16506200	-2.77295300	-1.17557400
H	-5.22507100	-2.78409600	0.59768900
H	-6.26087900	-1.67258100	-0.31789400
C	-5.56254500	1.11989900	-0.28696800
H	-5.64777800	1.77485900	0.59621500
H	-5.58964000	1.77067400	-1.17715100
H	-6.46207600	0.48899100	-0.31482100
C	-2.12648800	5.26039500	-0.28688000
H	-2.77192300	5.16611300	-1.17636500
H	-2.78510600	5.22397000	0.59695300
H	-1.67254400	6.26091100	-0.31607600
C	1.11992100	5.56249400	-0.28720100
H	1.77588800	5.64704000	0.59528600
H	1.76966400	5.59018500	-1.17813100
H	0.48906000	6.46210400	-0.31372300
C	5.26039300	2.12646800	-0.28713300
H	5.16634600	2.77148900	-1.17694600
H	5.22370800	2.78549500	0.59638300
H	6.26093700	1.67255000	-0.31582700
C	5.56253400	-1.11993100	-0.28646300
H	5.64798300	-1.77415900	0.59724200

H	5.58941500	-1.77142800	-1.17612100
H	6.46206300	-0.48904900	-0.31509600

²[Fe-TS1]_{sp²}

C	-0.25338800	0.27457400	4.60587900
H	0.40867600	0.45762700	5.45440600
C	-1.59286500	0.00566800	4.81930300
H	-1.99442900	-0.02536700	5.83478000
C	-2.45331400	-0.21740000	3.70682800
H	-3.51118000	-0.43148400	3.88203800
C	-1.98884200	-0.17168300	2.40714000
H	-2.66116300	-0.36933000	1.58069300
C	-0.59577300	0.07586900	2.13208200
N	-0.03072500	-0.01490100	0.92196700
C	0.27220900	0.34237000	3.28383800
C	1.62727700	0.54132800	2.94045800
H	1.41341100	1.57265700	1.00811900
C	1.89407400	0.75880900	1.56448300
C	3.22946000	0.33228200	1.04917200
O	3.77359100	0.85220400	0.07214800
C	5.24794100	-1.20398000	1.31595900
H	5.72979600	-1.94184300	1.97616300
H	5.09132100	-1.66851500	0.33260800
H	5.93738500	-0.35816800	1.17575800
C	2.96551800	1.67466500	4.76682000
H	3.26450200	2.49620800	4.09751000
H	2.05736000	1.99077200	5.30047900
H	3.76658600	1.52971000	5.50943100
C	4.08810900	-0.07430900	3.30046200
H	4.75263600	0.79990100	3.18073200
H	4.60886100	-0.76740400	3.98156800
C	3.91935200	-0.73348900	1.91042100
H	3.22389300	-1.58763800	2.00933700
C	2.74986100	0.37089000	3.95672300
H	2.43230500	-0.41701900	4.66245900
C	1.10175400	-2.56049300	-1.07444500
N	0.98279300	-1.20814600	-1.31310900
C	2.08997100	-0.84343100	-2.04238300
C	2.95570600	-1.99234100	-2.26069000
C	2.35517900	-3.06096400	-1.62281200
N	0.48795400	1.56089900	-1.33324800
C	0.14375100	2.88036900	-1.11451400
C	1.15639000	3.76842200	-1.67091400
C	2.08303100	2.95914800	-2.29347400
C	1.65727400	1.58604800	-2.06205000
C	-3.48235400	-3.12549900	-0.18263200
C	-3.04970800	-1.74881800	-0.38978500

N	-1.67707500	-1.68286200	-0.46155400
C	-1.21959300	-2.97141800	-0.32724400
C	-2.33466100	-3.88724300	-0.11095100
C	-2.17333500	2.47476300	-0.36438800
N	-2.15447200	1.10264700	-0.47563200
C	-3.47371000	0.69128300	-0.41238100
C	-4.34996500	1.83724100	-0.23364500
C	-3.53368100	2.95048100	-0.16781500
C	4.24307300	-1.95362000	-3.03065100
H	4.94550900	-1.21779700	-2.60580100
H	4.74435400	-2.93205000	-3.02863200
H	4.07565900	-1.67303900	-4.08412900
C	2.81849700	-4.48615500	-1.53765200
H	3.82946500	-4.60457000	-1.95289800
H	2.84585900	-4.84691500	-0.49593000
H	2.15330800	-5.16538800	-2.09760200
C	3.32771600	3.34667400	-3.03463600
H	3.33187600	2.94428600	-4.06128200
H	3.42873600	4.43869300	-3.11004900
H	4.22823000	2.96229500	-2.52741800
C	1.11497500	5.26633500	-1.58962500
H	2.00976800	5.71654200	-2.04222000
H	0.23760100	5.68022500	-2.11521500
H	1.06255200	5.61820400	-0.54552400
C	-3.91845300	4.39002600	0.01037700
H	-3.68850600	4.98840900	-0.88752700
H	-4.99464300	4.49684300	0.20719900
H	-3.38206000	4.85384900	0.85493300
C	-5.84582400	1.76150900	-0.13813600
H	-6.28785400	1.32602100	-1.04981900
H	-6.17273900	1.13666400	0.71028400
H	-6.29082200	2.75731200	-0.00202600
C	-4.91376600	-3.56259300	-0.07141700
H	-4.99102500	-4.64679900	0.09274600
H	-5.43227900	-3.06593300	0.76628200
H	-5.48152100	-3.32823700	-0.98755400
C	-2.19712200	-5.36797100	0.09068300
H	-3.17043800	-5.83797200	0.29145500
H	-1.77145100	-5.86369400	-0.79833400
H	-1.53604100	-5.60470500	0.94115100
Fe	-0.55807200	-0.03936500	-0.81462600
Cl	-1.27439300	-0.22051600	-2.99424500
C	-1.06966800	3.30518400	-0.57492900
H	-1.21898600	4.37942100	-0.45693000
C	-3.89802000	-0.63892500	-0.42125800
H	-4.97179700	-0.82369300	-0.36704100
C	0.10278700	-3.37070800	-0.53276900

H	0.33220200	-4.42965100	-0.40415900
C	2.37996200	0.45945700	-2.44520000
H	3.29263300	0.61863100	-3.01917000

⁴[Fe-TS1]_{sp²}

N	0.07233200	-0.01455100	0.98552900
C	-0.46805200	-0.48533900	2.11820700
C	0.43099000	-0.65809900	3.26936800
C	1.76578800	-0.30326200	2.98117300
C	1.95245500	0.43475000	1.77035400
C	-1.84594100	-0.85271300	2.32363400
C	-0.04678000	-1.23055800	4.48188500
H	0.64768500	-1.37822100	5.31194100
C	-1.37835100	-1.58269900	4.62075400
H	-1.74584200	-2.00625900	5.55806700
C	-2.27051500	-1.37693800	3.53111600
H	-3.32506100	-1.64382100	3.64624700
H	-2.55402200	-0.72025200	1.51432800
C	3.25528300	0.26638700	1.06700300
H	1.50079000	1.42582700	1.64819000
H	3.16276500	1.60640800	-2.74162900
C	2.25849100	1.25694900	-2.24364900
C	2.03731000	-0.11733100	-2.21153400
C	1.48331700	2.21057000	-1.58192700
N	0.97115200	-0.73532300	-1.59215200
C	2.96615400	-1.11253000	-2.72786300
C	1.84648100	3.61293000	-1.42840700
N	0.30871300	1.94510400	-0.92642300
C	1.19757100	-2.08601800	-1.68801700
Fe	-0.64949700	0.16012300	-0.82976200
C	2.45838700	-2.34628000	-2.36847200
C	0.86627700	4.18461800	-0.64118700
C	-0.10324600	3.13057700	-0.36977500
C	0.28121200	-3.06839500	-1.30453000
Cl	-1.35116600	0.57177800	-3.01891300
N	-1.59503800	-1.55063600	-0.80349500
N	-2.29048900	1.09754400	-0.20219800
C	-1.34586000	3.32999300	0.23819900
C	-1.04458000	-2.81329100	-0.96316200
H	0.57861400	-4.11123500	-1.42237100
C	-2.96679200	-1.73980400	-0.72335400
C	-3.57546200	0.60104900	-0.22178000
C	-2.38933100	2.40601700	0.23336500
H	-1.56287400	4.32853300	0.62057300
C	-2.08356800	-3.82604500	-0.91402400
C	-3.28614400	-3.15316900	-0.80162000
C	-3.90019600	-0.72581700	-0.51465500

C	-4.51972300	1.61336000	0.22236600
C	-3.77310800	2.73115100	0.54208600
H	-4.95362000	-1.00701500	-0.48869700
O	3.72209100	1.11379100	0.29747200
C	4.02235000	-1.00613600	1.45681800
H	3.35905900	-1.87083100	1.26823900
C	5.32851500	-1.16902100	0.67745500
H	5.87143300	-2.06746200	1.01056000
H	5.13020100	-1.26308900	-0.39896600
H	5.98149100	-0.29468200	0.81799600
C	2.94225300	-0.79084800	3.81244900
H	2.68535800	-1.80199600	4.17723400
C	3.16568100	0.11374500	5.05175000
H	2.27899000	0.15679200	5.70080400
H	4.01100600	-0.26421000	5.64941100
H	3.40255100	1.14212300	4.73735100
C	4.25304500	-0.88986600	2.98277100
H	4.87674100	0.00412500	3.16273700
H	4.84007300	-1.75245500	3.33967500
C	-6.00418900	1.41409800	0.31024300
H	-6.43644300	1.15859800	-0.67158700
H	-6.26803300	0.59696700	1.00301400
H	-6.51170500	2.32176700	0.66589700
C	-4.24414100	4.05937600	1.05766500
H	-3.72491600	4.34203100	1.98846400
H	-4.06571600	4.86695500	0.32770600
H	-5.32163000	4.04651900	1.27432300
C	-4.67634300	-3.71524000	-0.75342800
H	-5.18813200	-3.46081500	0.19011300
H	-5.29876400	-3.32380600	-1.57534200
H	-4.67104100	-4.81084700	-0.83924000
C	-1.84087700	-5.30230300	-1.02716900
H	-1.42212800	-5.57203900	-2.01156200
H	-1.12878400	-5.65617800	-0.26337000
H	-2.77093600	-5.87381500	-0.89966600
C	3.01352900	-3.71243500	-2.64745100
H	3.10272900	-4.31400000	-1.72756600
H	2.37166000	-4.27871600	-3.34362600
H	4.01381000	-3.65445300	-3.09948700
C	4.21991100	-0.79367400	-3.48796000
H	3.99628700	-0.27523200	-4.43532100
H	4.88900600	-0.13739300	-2.90755200
H	4.78256900	-1.70442900	-3.73759000
C	3.08386500	4.23827400	-1.99868700
H	3.99004700	3.77252500	-1.57758600
H	3.13166100	4.12239500	-3.09419700
H	3.12930400	5.31471300	-1.78070900

C	0.74796000	5.60235400	-0.16408400
H	-0.14976700	6.09750000	-0.57158800
H	0.67923500	5.65966300	0.93519900
H	1.61791000	6.20076700	-0.46924800

⁶[Fe-TS1]_{sp²}

N	0.10819100	-0.11068200	1.00912700
C	-0.29798300	-0.55922100	2.18281200
C	0.70469300	-0.83793000	3.23786000
C	2.03295500	-0.46342500	2.92526200
C	2.24739500	0.34970900	1.79047000
C	-1.68273300	-0.83106200	2.52308600
C	0.29830700	-1.48718800	4.43905300
H	1.05113800	-1.73276200	5.19036900
C	-1.02828700	-1.79401100	4.67721200
H	-1.32376500	-2.28006300	5.60951100
C	-2.01683300	-1.44372000	3.70932000
H	-3.06844000	-1.66448500	3.91359800
H	-2.44508000	-0.58277000	1.79275200
C	3.52847400	0.26813700	1.05716400
H	1.62435400	1.22647500	1.58424600
H	3.21704400	1.45828700	-2.66543900
C	2.28129800	1.14928800	-2.19709100
C	1.98327200	-0.21984800	-2.26016300
C	1.53795900	2.17145100	-1.57523700
N	0.86676100	-0.80919800	-1.71342700
C	2.82066700	-1.24157400	-2.88553800
C	1.93084700	3.57732700	-1.49601600
N	0.34211300	1.98660300	-0.94045000
C	0.94446200	-2.15245000	-1.96660700
Fe	-0.73510400	0.17496300	-0.80701800
C	2.17907800	-2.45186900	-2.68934900
C	0.92507200	4.22556700	-0.80090500
C	-0.07521900	3.20711600	-0.47862200
C	-0.06524700	-3.07989800	-1.64627400
Cl	-1.57474700	0.69200500	-2.95654500
N	-1.79399900	-1.56280600	-0.74438100
N	-2.35678300	1.21432200	-0.01466700
C	-1.32404200	3.45079000	0.12371500
C	-1.33961700	-2.81162700	-1.12532300
H	0.13147400	-4.11950300	-1.91729800
C	-3.14209300	-1.68400000	-0.46336200
C	-3.62957100	0.72000800	0.13634800
C	-2.39567300	2.55601700	0.28826500
H	-1.51807600	4.48490400	0.41795700
C	-2.42722900	-3.77675000	-1.02555400
C	-3.55167600	-3.07244200	-0.62966200

C	-3.98350700	-0.62575100	-0.08005500
C	-4.52217000	1.78294500	0.58692300
C	-3.74841900	2.92573500	0.69719000
H	-5.03174700	-0.88259600	0.08706500
O	3.90423500	1.13670000	0.25952100
C	4.37652400	-0.96609800	1.40054000
H	3.78092700	-1.85719000	1.12471500
C	5.71292700	-0.98644800	0.65549000
H	6.29422800	-1.88234200	0.92368100
H	5.55526400	-0.98726600	-0.43157100
H	6.31357300	-0.09696500	0.89904000
C	3.22140900	-0.97599200	3.73659600
H	3.00238700	-2.02291000	4.01279700
C	3.39299600	-0.15930700	5.04327000
H	2.50290900	-0.19786200	5.68692000
H	4.24990000	-0.54558200	5.61823200
H	3.58994000	0.89794000	4.80719200
C	4.55302300	-0.94910200	2.93501600
H	5.12164400	-0.03897200	3.19772900
H	5.17599800	-1.80215600	3.25125700
C	-5.98931600	1.61343600	0.85278300
H	-6.53313900	1.30940800	-0.05751400
H	-6.18057000	0.84056600	1.61654500
H	-6.44642100	2.54697700	1.21038400
C	-4.17213300	4.30549200	1.10824200
H	-3.56520400	4.68517400	1.94718400
H	-4.06677200	5.02662000	0.28003200
H	-5.22362700	4.32703100	1.42815900
C	-4.94709600	-3.58079200	-0.41557800
H	-5.30144300	-3.38140800	0.60995100
H	-5.66263600	-3.09988100	-1.10374700
H	-5.01298200	-4.66546000	-0.58063400
C	-2.30392700	-5.23721200	-1.34692500
H	-2.04425100	-5.39893100	-2.40691100
H	-1.51747900	-5.72104700	-0.74378700
H	-3.24314500	-5.77493500	-1.15481600
C	2.59962800	-3.82035400	-3.13922600
H	2.62938200	-4.53555800	-2.30001800
H	1.90439300	-4.23301300	-3.89020800
H	3.60013600	-3.80646300	-3.59470400
C	4.10743300	-0.96932800	-3.60800000
H	3.93567900	-0.40089200	-4.53798600
H	4.80183100	-0.37574000	-2.99132100
H	4.62222600	-1.90059800	-3.88481400
C	3.20451700	4.14007800	-2.05189800
H	4.08068800	3.65724600	-1.58886800
H	3.27900900	3.98314500	-3.14108400

H	3.28374400	5.22157200	-1.87093100
C	0.81905900	5.67917500	-0.44384400
H	-0.05817700	6.15211300	-0.91713100
H	0.71822900	5.82686200	0.64470900
H	1.70705500	6.23939200	-0.76941100

⁴[Fe-TS1]_{sp²}

C	-0.56147900	0.32468800	4.44918700
H	-1.36614700	0.40248600	5.18287600
C	0.75791300	0.31320400	4.90246200
H	0.97191100	0.38312900	5.97112800
C	1.80507800	0.21150500	3.96410400
H	2.84472100	0.20256200	4.30244800
C	1.53623400	0.12011000	2.60501600
H	2.35032600	0.03927700	1.89172300
C	0.19543300	0.12226800	2.10311100
N	-0.08353100	0.02392500	0.78320100
C	-0.89091600	0.23739800	3.07828900
C	-2.27118300	0.25879300	2.61093000
C	-2.54167300	0.12953700	1.27985200
H	-1.26196300	0.01567200	0.65881800
C	-3.85267500	0.09484600	0.64775800
C	4.05642900	2.56805400	0.20020500
C	3.03559400	3.49324600	0.09783300
C	3.46325600	1.26732300	-0.05677700
C	1.84200300	2.75408200	-0.27575600
N	2.11589700	1.39533700	-0.33432000
C	4.13003800	0.04818500	0.06483700
C	0.64627600	3.34712000	-0.67027900
C	3.50495500	-1.19822800	0.03994000
H	5.19718500	0.07487000	0.28851300
C	-0.39188900	2.68344500	-1.33042000
H	0.56894700	4.43101500	-0.57346600
N	2.16122500	-1.39368400	-0.22215000
C	4.14070400	-2.45316000	0.40166500
N	-0.42923500	1.33036500	-1.54659800
C	-1.51219600	3.33931800	-1.99190600
C	1.93342900	-2.75206100	-0.04827000
C	3.15114600	-3.41697000	0.38097500
C	-1.52310500	1.09444500	-2.34505600
C	-2.20557000	2.34511800	-2.65234600
C	0.75771700	-3.41355400	-0.38793100
C	-1.98219400	-0.16819100	-2.71661900
C	-0.30030500	-2.83931400	-1.09859400
H	0.71377800	-4.48735000	-0.20058200
C	-1.48043400	-1.37761500	-2.24086100
H	-2.87589400	-0.21087000	-3.33859500

N	-0.37874100	-1.51051300	-1.42752700
C	-1.39896800	-3.58294300	-1.69966000
C	-2.12268200	-2.67045000	-2.43964500
Fe	0.87732700	-0.04595800	-0.83874700
Cl	1.78552300	-0.10412100	-2.93423800
O	-4.10590900	-0.30104500	-0.49599100
C	-5.03546300	0.62055400	1.52875500
H	-5.41881400	1.47974100	0.94816800
C	-3.44546400	0.37058700	3.59319200
H	-3.11979100	0.99060400	4.44614500
C	-4.59789400	1.14422000	2.91391000
H	-4.26080100	2.18848600	2.80140300
H	-5.46902700	1.17149500	3.59166700
C	-3.83382200	-1.01712300	4.15115700
H	-4.09350400	-1.71721200	3.34451000
H	-2.99874500	-1.46197600	4.71320600
H	-4.69732900	-0.93406900	4.83056900
C	-6.16499300	-0.43036200	1.55367500
H	-7.06981700	-0.00754300	2.01832500
H	-6.40580100	-0.73628900	0.52637700
H	-5.88505200	-1.33008900	2.12078100
C	3.26135400	-4.88318800	0.68035500
H	2.54050100	-5.19520300	1.45419000
H	3.06422800	-5.49791900	-0.21420100
H	4.26554800	-5.14486700	1.04237800
C	5.59452400	-2.60266400	0.74025800
H	6.23906700	-2.28099600	-0.09478300
H	5.87507900	-1.99601900	1.61809400
H	5.84948300	-3.64706600	0.96827500
C	5.50318600	2.79337600	0.52705800
H	5.79925800	2.27382900	1.45426200
H	6.16165100	2.42275700	-0.27621700
H	5.72314000	3.86127000	0.66504200
C	3.09604800	4.98214400	0.27430100
H	2.88008100	5.51367100	-0.66794300
H	2.36391800	5.33304700	1.02043700
H	4.09031500	5.30641100	0.61230500
C	-1.78447800	4.81460700	-1.95313500
H	-1.89440800	5.18335300	-0.91948700
H	-0.96899600	5.39356500	-2.41898900
H	-2.71012000	5.06490800	-2.49053000
C	-3.44248100	2.45393500	-3.49375600
H	-3.27482800	2.07399200	-4.51529300
H	-4.27203800	1.87146000	-3.05977700
H	-3.77826000	3.49685700	-3.58288900
C	-3.36390900	-2.88500800	-3.25261000
H	-4.21308900	-2.32776200	-2.82412700

H	-3.23485500	-2.54407700	-4.29318900
H	-3.64385400	-3.94742700	-3.28761400
C	-1.62894800	-5.05607800	-1.53035500
H	-0.78398300	-5.64984800	-1.91842800
H	-1.75868500	-5.33020700	-0.46986300
H	-2.53133300	-5.38353300	-2.06560800
⁶ [Fe-TS1] _{sp²}			
C	-0.55874400	0.80529500	4.46787100
H	-1.35941200	0.96332700	5.19304300
C	0.76290500	0.85430900	4.90568500
H	0.98887200	1.05126000	5.95565000
C	1.79779900	0.64348900	3.97186200
H	2.84172400	0.67320600	4.29557200
C	1.51700200	0.39279700	2.63549500
H	2.32515600	0.22551600	1.93214900
C	0.17460000	0.33330300	2.14858000
N	-0.11918700	0.08561600	0.84962900
C	-0.89827300	0.55383500	3.11869500
C	-2.27584400	0.50410700	2.66211500
C	-2.55707400	0.20811600	1.36243600
H	-1.27910000	0.03691900	0.72361600
C	-3.86214000	0.04756300	0.74235100
C	3.99713100	2.70710100	0.01868700
C	2.98797400	3.59254800	-0.32009400
C	3.42091400	1.37012900	-0.04430800
C	1.80681200	2.79175400	-0.61896400
N	2.09406300	1.45579000	-0.40817700
C	4.09136000	0.17039300	0.25160200
C	0.60946800	3.28954200	-1.15256700
C	3.54775900	-1.12564100	0.26928000
H	5.14398200	0.25935600	0.52776500
C	-0.47073300	2.55765800	-1.68325100
H	0.55019800	4.37523900	-1.25660500
N	2.23950500	-1.42300100	-0.04631500
C	4.24835400	-2.34499500	0.65392600
N	-0.56191100	1.19346500	-1.66930300
C	-1.60186500	3.12267000	-2.41958000
C	2.08333100	-2.79002100	0.08729700
C	3.33110800	-3.37804400	0.55897500
C	-1.67499200	0.84416900	-2.38690100
C	-2.34912000	2.04901300	-2.86972200
C	0.93863700	-3.50455300	-0.28864900
C	-2.11312000	-0.47537600	-2.57935200
C	-0.19740800	-3.01866500	-0.96564600
H	0.97137500	-4.58352900	-0.12245400
C	-1.54901900	-1.64968900	-2.05832800
H	-3.02947300	-0.60032900	-3.15779400

N	-0.41172100	-1.70562600	-1.29101700
C	-1.26713500	-3.84707000	-1.51805600
C	-2.10531800	-2.99245300	-2.21053300
Fe	0.85739300	-0.11448200	-0.79213900
Cl	1.76404100	-0.31389000	-2.88728400
O	-4.12307400	-0.51237600	-0.32591400
C	-5.04895100	0.67505600	1.55929700
H	-5.43966300	1.44463400	0.86859800
C	-3.45033200	0.72031900	3.62867700
H	-3.12826200	1.44820400	4.39298300
C	-4.61410600	1.38318500	2.85977900
H	-4.29257200	2.40810500	2.60986100
H	-5.48393800	1.48598500	3.53169000
C	-3.81241800	-0.59245600	4.35830700
H	-4.06246100	-1.39307300	3.64803600
H	-2.96836700	-0.94831700	4.96796100
H	-4.67514900	-0.43762300	5.02589700
C	-6.16484900	-0.37647000	1.72734100
H	-7.07287300	0.09629600	2.13392300
H	-6.40461800	-0.82004000	0.75154200
H	-5.87401200	-1.18823000	2.40969700
C	3.53622600	-4.83893800	0.83325600
H	2.81422600	-5.21787900	1.57578900
H	3.40971300	-5.44512500	-0.07977100
H	4.54426400	-5.04018600	1.22258900
C	5.69197700	-2.40655100	1.05757200
H	6.35424600	-2.06630100	0.24363000
H	5.89902200	-1.76536800	1.93122600
H	5.99593300	-3.42927500	1.32165500
C	5.42216200	3.00388400	0.38261200
H	5.67089800	2.63517700	1.39229000
H	6.12677800	2.52576700	-0.31853800
H	5.62746200	4.08355900	0.36804300
C	3.05156400	5.08861800	-0.41747700
H	2.87494800	5.43672000	-1.44928900
H	2.29201800	5.56982600	0.22113700
H	4.03328800	5.47269500	-0.10623700
C	-1.83964000	4.58860300	-2.63652700
H	-1.89659800	5.13959800	-1.68262100
H	-1.03054500	5.04983700	-3.22821300
H	-2.78051100	4.76873900	-3.17598900
C	-3.61242100	2.05393500	-3.67882100
H	-3.47480800	1.55090900	-4.65086600
H	-4.42608400	1.52702000	-3.15327100
H	-3.95767900	3.07704300	-3.88582400
C	-3.36679600	-3.31111500	-2.95592000
H	-4.22788300	-2.78371900	-2.51360100

H	-3.30325700	-3.00715800	-4.01421900
H	-3.58797100	-4.38782100	-2.93695200
C	-1.37409800	-5.33452500	-1.34978100
H	-0.51020700	-5.85881000	-1.79265500
H	-1.41781700	-5.62336400	-0.28607400
H	-2.27852700	-5.72979100	-1.83365500

²[Fe-IM]_{sp²}

C	-4.12985600	-4.26634500	0.70980600
H	-5.18170700	-4.54561800	0.60286700
C	-3.17311200	-5.21232300	0.99220900
H	-3.46181200	-6.25922200	1.11645300
C	-1.77420300	-4.86213800	1.12745900
H	-1.06234200	-5.66292500	1.34628700
C	-1.32421100	-3.57183700	0.99104800
H	-0.27019700	-3.30572900	1.08617100
C	-2.28590700	-2.53561900	0.70266000
N	-2.03306500	-1.24633800	0.55353700
C	-3.71433800	-2.90049500	0.54918300
C	-4.37864200	-1.72659000	0.25425400
C	2.37482100	0.26754500	2.67708500
N	1.71171500	0.99733500	1.70630100
C	1.18766600	2.08691700	2.38270300
C	1.49912400	2.03094400	3.79998600
C	2.25648000	0.89440800	3.98318300
N	0.59811400	2.29339200	-0.52123000
C	0.17970100	2.82772400	-1.72723300
C	-0.46477700	4.11686200	-1.53861300
C	-0.44411300	4.36548500	-0.18268000
C	0.22921100	3.23262600	0.42747900
C	3.47416300	-3.26279100	-0.25535500
C	2.74906700	-2.15760900	-0.85665300
N	2.50431300	-1.15322400	0.06696500
C	3.07954400	-1.60695700	1.24164200
C	3.69046000	-2.91311600	1.06112600
C	0.83416300	0.92955400	-3.15662300
N	1.36570500	0.13014400	-2.15785100
C	1.73863700	-1.03891800	-2.80272300
C	1.41834300	-0.98674000	-4.21739000
C	0.85969100	0.25402600	-4.44195000
Fe	1.73178000	0.65886500	-0.26619400
Cl	3.67529500	1.69947600	-0.64899500
C	0.30700500	2.20012700	-2.96090700
H	-0.07009400	2.72945400	-3.83705100
C	2.37370200	-2.11396200	-2.19340800
H	2.62245100	-2.97360900	-2.81688800
C	3.03851300	-0.93320600	2.45587300

H	3.52754300	-1.40324100	3.31007900
C	0.48590900	3.12690100	1.78823500
H	0.13372900	3.93216600	2.43382500
C	-3.31747800	-0.64753800	0.28576900
C	-3.79907700	0.41908000	1.33422400
C	-5.22283100	0.94601000	1.05930500
C	-6.23513400	-0.22763200	0.96335600
C	-5.83192300	-1.42260500	0.04360400
H	-5.47342500	1.52864900	1.96091500
H	-3.26146700	-0.08469500	-0.66762800
H	-6.36622600	-0.62680200	1.98301400
H	-7.21852000	0.16500900	0.65146800
H	-6.42353400	-2.29355100	0.37803800
O	-3.12875500	0.78643200	2.27854800
C	-6.17444400	-1.20860000	-1.45298400
H	-5.97402500	-2.12644000	-2.02570600
H	-7.24032700	-0.95611700	-1.57178700
H	-5.58293000	-0.40136400	-1.90785700
C	-5.23414200	1.92548300	-0.13669800
H	-6.25083600	2.31854600	-0.29259100
H	-4.56653300	2.77840900	0.05753000
H	-4.91237900	1.45868200	-1.07858900
C	3.88700400	-4.51013800	-0.98044900
H	3.01979400	-5.04082600	-1.40821600
H	4.57432200	-4.28775600	-1.81396900
H	4.40271400	-5.21211500	-0.31000200
C	4.39890200	-3.68239000	2.13718500
H	5.26341000	-3.12352100	2.53291600
H	3.73475300	-3.89841900	2.99102300
H	4.77488000	-4.64476100	1.76216400
C	2.84957500	0.35079800	5.24936000
H	2.43327600	-0.63886100	5.50294500
H	3.94302400	0.23265100	5.16828100
H	2.65415200	1.01650100	6.10179500
C	1.05063700	3.04085800	4.81466200
H	1.41845000	4.05262100	4.57463100
H	-0.04936400	3.09777200	4.87026900
H	1.41742200	2.78939300	5.81981900
C	-0.97723800	5.55009400	0.56872600
H	-1.70272200	5.25010400	1.34329900
H	-0.17154900	6.10543000	1.07798300
H	-1.48628800	6.25606800	-0.10282100
C	-1.02650100	4.96258900	-2.64355300
H	-0.24700100	5.25540600	-3.36682400
H	-1.80967600	4.43102900	-3.21030500
H	-1.47448600	5.88744800	-2.25340000
C	0.35617100	0.84165500	-5.72750400

H	-0.71659400	1.09252100	-5.67086200
H	0.89252900	1.76967000	-5.98735600
H	0.48553100	0.14321100	-6.56628400
C	1.67743500	-2.09553600	-5.19477800
H	2.75281100	-2.32904400	-5.27074000
H	1.16313400	-3.02627700	-4.90196700
H	1.32839100	-1.83163800	-6.20311900

⁴[Fe-IM]_{sp²}

C	4.36805500	4.16593800	0.21131800
H	5.40759900	4.40196500	-0.03257700
C	3.46801200	5.16247700	0.50587300
H	3.79031000	6.20692400	0.50095100
C	2.08542900	4.86906500	0.82254200
H	1.41898400	5.70780900	1.04222800
C	1.59628200	3.58622400	0.85469100
H	0.55401900	3.36258600	1.08887800
C	2.49828500	2.49896700	0.56066800
N	2.20311800	1.21014700	0.55786100
C	3.90888900	2.80467800	0.22286600
C	4.51208500	1.58924800	-0.03218100
C	-2.05444600	-0.23779700	2.85505300
N	-1.60280800	-1.00686200	1.79771300
C	-1.09670600	-2.15474500	2.38021800
C	-1.22422500	-2.10963200	3.82624900
C	-1.82602200	-0.90529200	4.12455200
N	-0.74328000	-2.27926400	-0.57501300
C	-0.37787500	-2.75177500	-1.82334600
C	0.23508700	-4.06444900	-1.72708900
C	0.24017600	-4.39306900	-0.38680400
C	-0.36933400	-3.27469500	0.31010000
C	-3.47414200	3.32563500	0.10202200
C	-2.87292900	2.20352300	-0.59628400
N	-2.49787500	1.20797600	0.28883600
C	-2.85353000	1.68491500	1.53814500
C	-3.46131200	3.00018500	1.44308000
C	-1.12698900	-0.80531000	-3.13623100
N	-1.61975800	-0.05519800	-2.08290300
C	-2.09407900	1.10863800	-2.66200200
C	-1.89148800	1.09884300	-4.09967500
C	-1.28378500	-0.10353200	-4.39756700
Fe	-1.85511100	-0.64747700	-0.16773000
Cl	-3.92887900	-1.63431100	-0.40336500
C	-0.55635000	-2.06748700	-3.01998500
H	-0.21964200	-2.55505600	-3.93555500
C	-2.68965800	2.15873600	-1.97321200
H	-3.02983500	3.01557800	-2.55564900

C	-2.65011600	1.01196400	2.73710500
H	-2.97239100	1.50575400	3.65436800
C	-0.53508200	-3.22092900	1.68886100
H	-0.18613800	-4.07282900	2.27310800
C	3.43789200	0.55079400	0.20983200
C	4.00326400	-0.43889600	1.29186900
C	5.38283900	-1.02464000	0.92546500
C	6.40115300	0.10614100	0.61648300
C	5.92709700	1.22230700	-0.36599900
H	5.71515100	-1.52870300	1.84779800
H	3.26632800	-0.09014600	-0.67843800
H	6.64479000	0.59376200	1.57518900
H	7.33952400	-0.34106100	0.24499800
H	6.56975300	2.10154300	-0.18072700
O	3.42094400	-0.71338700	2.32223400
C	6.10112500	0.85928000	-1.86282900
H	5.85930600	1.72559800	-2.49657100
H	7.14224700	0.56354000	-2.06909400
H	5.44687300	0.03210500	-2.17289200
C	5.25206700	-2.11083400	-0.16706600
H	6.24067200	-2.54009800	-0.39251400
H	4.59869200	-2.92646300	0.17765800
H	4.83585200	-1.72646000	-1.10920200
C	-3.99071800	4.56879400	-0.56079200
H	-3.20080900	5.08737700	-1.12971600
H	-4.80544900	4.34273800	-1.26885300
H	-4.38606100	5.28200500	0.17616100
C	-3.95984500	3.79907600	2.61139000
H	-4.76194900	3.26980800	3.15238800
H	-3.15718400	4.00306900	3.33982400
H	-4.36607000	4.76871100	2.29067700
C	-2.18688100	-0.33883100	5.46602300
H	-1.64905300	0.60270600	5.66796400
H	-3.26539100	-0.12072300	5.53920300
H	-1.93813100	-1.03820700	6.27648900
C	-0.75887000	-3.18757200	4.75985800
H	-1.23848500	-4.15510600	4.53651700
H	0.33144100	-3.33902100	4.69190400
H	-0.99118200	-2.94032800	5.80523400
C	0.75070500	-5.63874800	0.27606700
H	1.51890700	-5.41313800	1.03451800
H	-0.05828000	-6.18655600	0.78773000
H	1.20091700	-6.32668400	-0.45352800
C	0.73864900	-4.86197400	-2.89432400
H	-0.07345900	-5.10694300	-3.59920000
H	1.50767600	-4.31394500	-3.46438500
H	1.18638200	-5.81152400	-2.56863600

C	-0.85158000	-0.63520700	-5.73254800
H	0.23238000	-0.83756400	-5.76090300
H	-1.36470800	-1.57972400	-5.97929700
H	-1.07291400	0.07768800	-6.53929300
C	-2.28810300	2.20948300	-5.02735800
H	-3.37408800	2.39856900	-4.99374500
H	-1.78512400	3.15648400	-4.76912300
H	-2.02910400	1.97415600	-6.06927900

⁴[Fe-IM]_{sp²}

C	-0.75939000	-0.04592700	4.39605500
H	-1.58850500	-0.04737300	5.10512200
C	0.53901300	-0.09184200	4.90095700
H	0.70616100	-0.12507500	5.97968400
C	1.62593300	-0.09147000	4.00278900
H	2.65109400	-0.12126700	4.38124200
C	1.40858000	-0.05627900	2.63338700
H	2.24936100	-0.05909500	1.94651600
C	0.09014200	-0.02320800	2.07884200
N	-0.10215100	-0.00838700	0.73959100
C	-1.04119800	-0.00263500	3.00890300
C	-2.41992100	0.06706300	2.52963400
C	-2.75558600	0.05401600	1.21229500
H	-1.13086800	-0.00271700	0.49915900
C	-4.05234400	0.11636800	0.57048500
C	4.09618800	2.55102800	0.48818200
C	3.09910600	3.49545000	0.34202000
C	3.50265700	1.26845600	0.15224400
C	1.92178800	2.78494100	-0.12573700
N	2.17841100	1.42466200	-0.20838000
C	4.15628700	0.04185300	0.25810800
C	0.75315800	3.41022600	-0.54794700
C	3.53796300	-1.19781300	0.10765800
H	5.20691000	0.05145700	0.55017700
C	-0.28240300	2.78140400	-1.24094300
H	0.68857500	4.49150300	-0.41975400
N	2.21562800	-1.37974500	-0.25390000
C	4.16800600	-2.47342600	0.39959500
N	-0.34266400	1.43372800	-1.49811600
C	-1.39994600	3.47368700	-1.86646600
C	1.99790400	-2.74919600	-0.21177700
C	3.19671000	-3.44033700	0.22803800
C	-1.45680600	1.24087900	-2.28188200
C	-2.12538900	2.50987400	-2.53689500
C	0.84370400	-3.39261800	-0.64516800
C	-1.93941700	0.00253300	-2.69885600
C	-0.21070000	-2.77041300	-1.31482500

H	0.80692400	-4.47829000	-0.54713600
C	-1.42566900	-1.23231700	-2.31142100
H	-2.84835700	-0.00254800	-3.29908500
N	-0.30332000	-1.41785100	-1.53644300
C	-1.31458100	-3.47271400	-1.95262000
C	-2.06550700	-2.50996700	-2.59506200
Fe	0.94803200	0.01255300	-0.84331900
Cl	1.91134000	0.06603600	-2.89470000
O	-4.30951000	-0.14127900	-0.61194800
C	-5.21967600	0.56398800	1.51342200
H	-5.61010700	1.47321200	1.02076400
C	-3.59959700	0.11306900	3.52756000
H	-3.26110400	0.65820900	4.42474400
C	-4.74877800	0.95711000	2.93037600
H	-4.39693700	2.00218200	2.90142000
H	-5.60751100	0.93944600	3.62396000
C	-4.00026700	-1.31211100	3.96777000
H	-4.27080700	-1.93837000	3.10601000
H	-3.16884700	-1.81276300	4.48644900
H	-4.86050500	-1.27714900	4.65550000
C	-6.34995000	-0.48494800	1.46075900
H	-7.24437600	-0.10851300	1.98198600
H	-6.61278800	-0.68978100	0.41378900
H	-6.06069100	-1.43530500	1.93233700
C	3.30918900	-4.92650300	0.40221500
H	2.55056000	-5.31244300	1.10322800
H	3.17035200	-5.46049400	-0.55298900
H	4.29499500	-5.21116800	0.79611400
C	5.59997200	-2.63989600	0.81478900
H	6.29100700	-2.24640200	0.05067900
H	5.81846600	-2.10538700	1.75484400
H	5.85291100	-3.69773000	0.97237900
C	5.52126400	2.74370300	0.91569900
H	5.75104800	2.18455300	1.83854300
H	6.22635700	2.39576400	0.14234900
H	5.74352100	3.80240500	1.10965400
C	3.16927400	4.97793200	0.56358800
H	3.01902900	5.53808700	-0.37477100
H	2.39781800	5.32021200	1.27324200
H	4.14538500	5.27723400	0.97059400
C	-1.64633100	4.95161700	-1.78194300
H	-1.73916900	5.29221500	-0.73700600
H	-0.82566400	5.52954100	-2.23973600
H	-2.57301000	5.23287400	-2.30193500
C	-3.37986400	2.66053100	-3.34486300
H	-3.23992400	2.31567300	-4.38293900
H	-4.20340700	2.06947100	-2.91131300

H	-3.70710100	3.70904200	-3.38880300
C	-3.32532700	-2.66813600	-3.39223800
H	-4.16014800	-2.13003300	-2.91415900
H	-3.21528200	-2.26752000	-4.41368200
H	-3.61444200	-3.72475700	-3.48324300
C	-1.52819500	-4.95711400	-1.90038000
H	-0.68868100	-5.50744700	-2.35794300
H	-1.62756700	-5.31982400	-0.86348200
H	-2.44149200	-5.24835600	-2.43809300

⁶[Fe-IM]_{sp²}

C	-1.69857800	2.91573800	3.42061200
H	-2.62127500	3.33713900	3.82482400
C	-0.47694900	3.42766500	3.87411900
H	-0.47129500	4.23309200	4.61231900
C	0.74556400	2.90822700	3.38216400
H	1.69385900	3.31624900	3.74041300
C	0.73985500	1.88515400	2.45227800
H	1.66331700	1.46383600	2.05382200
C	-0.49820800	1.32053700	1.96104900
N	-0.42126700	0.31575900	1.09623400
C	-1.76616300	1.87844900	2.46945500
C	-3.02950100	1.33655700	1.98371200
C	-3.05481600	0.29660700	1.10557600
H	-1.42217000	-0.00775700	0.83171800
C	-4.21187800	-0.37446500	0.53570200
C	3.17332500	3.33795200	-1.06041000
C	2.06894100	3.60075000	-1.84552100
C	3.01848800	1.97571100	-0.57964600
C	1.26399300	2.39132000	-1.83804100
N	1.85049200	1.41210100	-1.05720600
C	3.92559700	1.34029400	0.26516300
C	0.07769300	2.24366500	-2.55012900
C	3.78114900	0.05216800	0.77536900
H	4.81355700	1.90070300	0.56072100
C	-0.69095000	1.08406900	-2.59825900
H	-0.26772100	3.09914100	-3.13202400
N	2.72177800	-0.79336900	0.50313500
C	4.72065500	-0.57038000	1.69223700
N	-0.39608000	-0.08939100	-1.93155700
C	-1.90945100	0.94616000	-3.37791600
C	2.97461000	-1.94233900	1.22728500
C	4.21052900	-1.82044600	1.98115000
C	-1.40242300	-0.97248300	-2.28069700
C	-2.35494800	-0.34538800	-3.18000200
C	2.17334100	-3.08098000	1.22685100
C	-1.51515000	-2.27760900	-1.81646800

C	1.01413000	-3.24658800	0.47500100
H	2.48854100	-3.91645700	1.85323300
C	-0.64672000	-2.88729700	-0.91483400
H	-2.37432100	-2.85629600	-2.15338500
N	0.48211500	-2.30248100	-0.37980100
C	0.20465700	-4.45456700	0.48467300
C	-0.83816300	-4.22919900	-0.39043300
Fe	1.25749900	-0.50487600	-0.85550200
Cl	2.50484400	-1.29070400	-2.67732000
O	-4.20310100	-1.48912500	-0.00115600
C	-5.55378100	0.42036400	0.63422400
H	-5.82949700	0.59695700	-0.42175300
C	-4.38153600	1.88310400	2.47588200
H	-4.25602500	2.95708900	2.69821800
C	-5.40719900	1.80020800	1.31951000
H	-5.09205400	2.53501400	0.55966500
H	-6.39292200	2.13698000	1.68447100
C	-4.81875700	1.18450000	3.78216800
H	-4.89440700	0.09574200	3.65039700
H	-4.09228800	1.36587400	4.58897300
H	-5.79872800	1.56258000	4.11469300
C	-6.64811900	-0.49085000	1.22884500
H	-7.63502500	-0.00991500	1.14149400
H	-6.67033100	-1.44437100	0.68366100
H	-6.47345900	-0.71034000	2.29234600
C	4.77829000	-2.88550800	2.87278900
H	4.07314600	-3.16713600	3.67266700
H	5.01385600	-3.80389700	2.30941400
H	5.70678900	-2.55149300	3.35698300
C	5.98497200	0.06824800	2.18776600
H	6.67417900	0.29994700	1.35854100
H	5.78640200	1.01481300	2.71826800
H	6.52140700	-0.59096400	2.88468700
C	4.33298300	4.23334000	-0.73619900
H	4.43236900	4.39852900	0.34995300
H	5.28668600	3.80518900	-1.08753500
H	4.22336100	5.21968800	-1.20859900
C	1.72183900	4.85521900	-2.59218800
H	1.66147300	4.67753700	-3.67901000
H	0.74724900	5.26297600	-2.27526500
H	2.47388700	5.64033300	-2.43046600
C	-2.51180900	2.02995100	-4.22301300
H	-2.74311600	2.93133500	-3.63074700
H	-1.82938000	2.34047700	-5.03203700
H	-3.44726300	1.69710300	-4.69446100
C	-3.57513300	-1.02133700	-3.73156800
H	-3.31062300	-1.89127100	-4.35572200

H	-4.22634200	-1.38517800	-2.92008400
H	-4.16654300	-0.33755600	-4.35703000
C	-1.98380100	-5.12805400	-0.74963900
H	-2.95026400	-4.65599600	-0.50805000
H	-1.99414700	-5.36416600	-1.82690700
H	-1.93297900	-6.08166900	-0.20540800
C	0.49587300	-5.67470500	1.30781400
H	1.47313100	-6.11601000	1.04948800
H	0.51777400	-5.44464500	2.38630600
H	-0.26532100	-6.45237800	1.15373200

¹[IM]_{sp²}

C	2.31828800	1.41968200	-0.51456900
H	2.03342200	2.41764400	-0.85901500
C	3.63289100	1.01767900	-0.52499000
H	4.40877900	1.69876400	-0.88367300
C	4.02841100	-0.29839300	-0.06806500
H	5.09024600	-0.55740800	-0.10216800
C	3.11948900	-1.21723200	0.39640500
H	3.41808100	-2.21091000	0.73606000
C	1.72390300	-0.85135400	0.42898400
N	0.71975800	-1.61068900	0.83437300
C	1.32573100	0.50008200	-0.03205900
C	-0.04371300	0.56933400	0.12969300
C	-0.45321900	-0.78976000	0.65411300
C	-1.52454000	-1.35989800	-0.34675300
C	-2.69833500	-0.39352000	-0.60510700
C	-2.18460500	0.99891000	-1.06081600
C	-1.04185600	1.63563400	-0.20903200
H	-3.23654900	-0.84418800	-1.45499000
H	-0.99919000	-0.71697600	1.61665900
H	-1.80260100	0.88288700	-2.08881500
H	-3.03623300	1.69858300	-1.12012800
H	-0.54800700	2.38597900	-0.85195500
O	-1.43733400	-2.45293300	-0.86944900
C	-1.54098500	2.39413400	1.04710000
H	-0.70411900	2.91269900	1.53836400
H	-2.29431500	3.14783500	0.76740800
H	-1.99454200	1.72321000	1.79044700
C	-3.67355800	-0.37768000	0.59500600
H	-4.52131800	0.29215300	0.38330400
H	-4.07615000	-1.38572300	0.77652700
H	-3.20455100	-0.03197300	1.52748000

¹[TS2]_{sp²}

C	-2.44030500	-1.38419700	-0.29882100
H	-2.19362000	-2.42660300	-0.51604900

C	-3.75854000	-0.97659300	-0.18739300
H	-4.56335400	-1.70411600	-0.32031700
C	-4.10037600	0.38292500	0.10389300
H	-5.15626800	0.65457300	0.18069900
C	-3.12853700	1.35204100	0.28706300
H	-3.38098300	2.39182500	0.50428900
C	-1.76505400	0.96761600	0.15321400
N	-0.68752400	1.80409600	0.23786200
C	-1.41165000	-0.41149400	-0.12400900
C	-0.00209600	-0.47102400	-0.14413000
C	0.45099600	0.86718000	0.10441900
C	1.83566200	1.33009000	-0.25178100
C	2.85922100	0.18856500	-0.41213900
C	2.24800400	-1.10044400	-1.01920900
C	0.93200700	-1.62778000	-0.37990900
H	3.60030200	0.57781300	-1.13047300
H	0.16582700	1.31224700	1.21178400
H	2.03369100	-0.88991900	-2.08114100
H	3.00861400	-1.90014000	-1.01178300
H	0.46227200	-2.29602100	-1.12496900
O	2.14742600	2.51064400	-0.35540000
C	1.13587700	-2.48206800	0.89724800
H	0.17821400	-2.90723400	1.23379900
H	1.82739800	-3.31578000	0.69654900
H	1.54531300	-1.89286000	1.72956000
C	3.59897600	0.00046700	0.93536600
H	4.34183400	-0.80856200	0.85729200
H	4.12509900	0.92751300	1.20679700
H	2.91382200	-0.24824400	1.75925900

¹[PC]_{sp²}

C	2.44950500	1.39574000	-0.16589100
H	2.20707000	2.45064100	-0.31659700
C	3.77392900	0.98903400	-0.01469100
H	4.57557900	1.73075600	-0.04403300
C	4.10287100	-0.37796200	0.17669500
H	5.15128300	-0.66354000	0.29259800
C	3.11919100	-1.36736500	0.21741000
H	3.37913200	-2.41876700	0.36116400
C	1.78129600	-0.95946900	0.06475600
N	0.61945800	-1.69772800	0.05296100
C	1.42221100	0.42312100	-0.12515900
C	-0.00808100	0.47059800	-0.25204800
C	-0.45771300	-0.84517800	-0.13696900
C	-1.83718800	-1.30775000	-0.18683900
C	-2.88773200	-0.19667900	-0.34998000
C	-2.30613900	1.08588200	-1.00635600

C	-0.95425000	1.62556600	-0.45379700
H	-3.64211900	-0.60963300	-1.04258900
H	0.51053100	-2.70062100	0.16220800
H	-2.14990100	0.86034800	-2.07538200
H	-3.06427700	1.88694400	-0.96855400
H	-0.53476500	2.28165600	-1.23967000
O	-2.13835000	-2.50466300	-0.06108600
C	-1.08494900	2.50077800	0.81720000
H	-0.10948900	2.92439200	1.10052400
H	-1.78044800	3.33705600	0.64212400
H	-1.45281100	1.92278500	1.67646700
C	-3.60416500	0.01735300	1.00462400
H	-4.38801400	0.78510100	0.91089000
H	-4.07440000	-0.92243400	1.32897500
H	-2.90948900	0.33470600	1.79611000

Cartesian coordinates of species of reaction pathways for Ir-catalyzed system

¹[Ir-NI]

N	0.12244000	0.45424000	0.20775600
C	0.68220100	1.65075700	-0.14671300
C	2.11537000	1.72052300	-0.33945500
C	2.99331100	0.53398700	-0.14083000
C	3.77210700	0.12140900	-1.18235600
C	-0.08588800	2.83862900	-0.37683100
C	2.68750600	2.93415400	-0.76160300
H	3.76988500	2.98236500	-0.90382300
C	1.90218400	4.07358500	-0.99170100
H	2.37941800	5.00213300	-1.31501600
C	0.50891400	4.02487800	-0.79835000
H	-0.10135300	4.91494100	-0.97123200
H	-1.16514500	2.76715700	-0.21853300
C	4.61838000	-1.09063500	-1.15580500
H	3.75370500	0.65510300	-2.13736200
H	-0.15757800	-1.68034400	-1.21808500
C	-1.24457800	-1.54944000	-1.19523800
C	-1.74972000	-0.37645800	-1.84025100
C	-2.01755800	-2.83824800	-0.96900200
C	-3.15285400	-0.24404500	-2.43440000
H	-1.00221500	0.29104800	-2.28263700
C	-3.44954800	-2.58614900	-0.44243300
H	-2.03077900	-3.44349600	-1.89622900
H	-1.45645600	-3.42896800	-0.22600100
C	-4.15249400	0.34951200	-1.41328900
H	-3.10486100	0.40499200	-3.32299100
H	-3.49777300	-1.22434700	-2.79814000
C	-3.49216500	-1.35374300	0.45394200
H	-3.79076000	-3.46469000	0.12822900

H	-4.16051800	-2.47813300	-1.27637100
C	-3.81184800	-0.03578000	0.01823700
H	-4.12177900	1.44957400	-1.47602100
H	-5.19064700	0.05513200	-1.66014900
H	-3.61467700	-1.55319700	1.52329200
H	-4.20696600	0.64685000	0.77890900
Ir	-1.65735300	-0.06304700	0.32840800
O	-2.13725700	0.63550600	2.07974700
H	-1.77588400	0.69869600	4.09952000
C	-1.41186700	0.16213100	3.20552000
H	-0.32434300	0.33942500	3.09223700
H	-1.55889400	-0.92283500	3.37034800
C	3.02174500	-0.18007300	1.20712900
H	2.10187100	-0.79492700	1.23828900
C	4.25562000	-1.09682600	1.32586200
H	4.15249700	-1.72808200	2.22510700
H	5.15343000	-0.47037900	1.48750200
C	4.48752600	-1.98152100	0.08723200
H	3.56462900	-2.57573600	-0.07984500
O	5.34504600	-1.38160500	-2.11212900
C	2.96503400	0.80194000	2.39600300
H	2.05090800	1.41173900	2.38294100
H	2.98694500	0.24368000	3.34499800
H	3.83004900	1.48464400	2.38864400
C	5.67214300	-2.94335900	0.23338700
H	5.49330500	-3.66595800	1.04432300
H	5.84187300	-3.49166500	-0.70315300
H	6.59774200	-2.39233900	0.46423400

³[Ir-Ni]

N	0.01194900	0.78284400	0.39745100
C	0.69266900	1.86622400	-0.00371900
C	2.11555800	1.80535100	-0.29390500
C	2.88663800	0.54077400	-0.15768700
C	3.56047900	0.05960700	-1.24288000
C	0.01526900	3.12396700	-0.18345100
C	2.75113200	2.96237400	-0.77268200
H	3.81843000	2.90621500	-1.00130000
C	2.06785200	4.17846500	-0.93307100
H	2.60408600	5.06149400	-1.28718300
C	0.69535100	4.25316500	-0.62502400
H	0.15735700	5.19798100	-0.73852600
H	-1.04989000	3.15754200	0.05537000
C	4.27786900	-1.23209300	-1.26978900
H	3.53761000	0.59935200	-2.19439600
H	-0.26011500	-0.26622300	-1.95787900
C	-1.29031200	-0.54187600	-1.70607800

C	-2.21612600	0.54264100	-1.58615200
C	-1.62805200	-1.98248300	-2.06709900
C	-3.71842900	0.41012300	-1.86949500
H	-1.80325900	1.54465200	-1.75193700
C	-2.84473500	-2.52956600	-1.28601100
H	-1.77931400	-2.08632500	-3.15912900
H	-0.74349400	-2.59323300	-1.82262400
C	-4.52460100	0.04953400	-0.59926000
H	-4.09293600	1.35952100	-2.28354100
H	-3.87548700	-0.34238000	-2.65931600
C	-2.94902900	-1.91894700	0.10869800
H	-2.76381000	-3.62452400	-1.19680000
H	-3.77886000	-2.33680900	-1.83757100
C	-3.71229200	-0.75809300	0.40408900
H	-4.83351800	0.97772300	-0.09230400
H	-5.45900900	-0.48282600	-0.86208200
H	-2.71435100	-2.58151400	0.94805800
H	-4.01657700	-0.64141100	1.45099100
Ir	-1.62799900	-0.13675300	0.38808500
O	-1.81973800	-0.29061500	2.34113700
H	-1.11529600	0.04471100	4.24003700
C	-0.73138400	-0.23810200	3.24303700
H	0.03767000	0.49234000	2.93168100
H	-0.24218400	-1.22778300	3.33986200
C	2.92809600	-0.17860800	1.18805200
H	1.95586000	-0.69713300	1.29939400
C	4.06029400	-1.22592900	1.22768100
H	3.94427300	-1.85038800	2.13004200
H	5.02740400	-0.69946400	1.33653900
C	4.12446400	-2.11768600	-0.02504700
H	3.13634700	-2.61050600	-0.14072800
O	4.91098600	-1.59040500	-2.26912000
C	3.07187200	0.80627200	2.36770500
H	2.23938800	1.52223900	2.41181600
H	3.09701100	0.25348600	3.31970700
H	4.00840400	1.38116400	2.28725800
C	5.20785900	-3.19975500	0.04861900
H	4.99970300	-3.90930100	0.86408000
H	5.26658300	-3.75140600	-0.89940600
H	6.19758900	-2.75114100	0.22986500

¹[Ir-TS1]_{sp²}

N	-0.39425000	0.46870800	-0.22506300
C	-1.05670500	1.62106300	0.02492800
C	-2.46575800	1.56493800	0.41206300
C	-2.98863200	0.24950400	0.51900300
C	-2.03121900	-0.79056600	0.57010400

C	-0.45953600	2.90715100	-0.22259100
C	-3.20773600	2.78104200	0.47725400
H	-4.26186500	2.75274600	0.75814100
C	-2.60364800	3.99746400	0.20663000
H	-3.18181200	4.92163500	0.28305600
C	-1.22585000	4.05532400	-0.14794200
H	-0.76159600	5.02529300	-0.34534300
H	0.58988200	2.93300600	-0.52262100
C	-2.30045000	-2.08554200	-0.09925600
H	-1.24004600	-0.79710500	1.32601800
H	0.35160000	-2.14342300	0.65668000
C	1.37127300	-1.75015000	0.75874800
C	1.60014400	-0.75102800	1.75741600
C	2.41889100	-2.71016700	0.21399400
C	2.93719600	-0.52316400	2.46830700
H	0.72312700	-0.41711100	2.32757500
C	3.75906600	-2.01450200	-0.12947600
H	2.57464300	-3.54742400	0.92134300
H	1.99761200	-3.15745200	-0.70055400
C	3.78943100	0.54780800	1.74565600
H	2.74870400	-0.20542500	3.50610300
H	3.48466300	-1.47617300	2.54042700
C	3.53681400	-0.58306100	-0.60555200
H	4.27595200	-2.58415800	-0.91811800
H	4.43636700	-2.02168600	0.73965400
C	3.55003100	0.55884500	0.24295200
H	3.51630000	1.54436800	2.12902000
H	4.86562300	0.41443800	1.96844500
H	3.70750300	-0.39627600	-1.66996600
H	3.76233800	1.51623200	-0.24686200
Ir	1.47886900	0.15657700	-0.20919300
O	1.82620200	1.42028000	-1.70338000
H	1.36297000	2.04595800	-3.60530800
C	1.16211800	1.19027500	-2.93449700
H	0.06537800	1.08776500	-2.80680400
H	1.52152800	0.27182600	-3.44034000
C	-4.47316600	-0.06090500	0.36091800
H	-4.87170500	0.59810700	-0.43289000
C	-4.71674500	-1.53448600	-0.05503300
H	-5.68164600	-1.60139700	-0.58429800
H	-4.81846800	-2.16015200	0.85065600
C	-3.59270900	-2.13345100	-0.92585800
H	-3.43058900	-1.46177700	-1.79253800
O	-1.52505100	-3.04723700	-0.02529700
C	-5.25422100	0.23548800	1.66658700
H	-5.17725600	1.28604400	1.98007200
H	-6.32188400	-0.00056600	1.52902200

H	-4.87064600	-0.38693000	2.48998700
C	-3.90510400	-3.54514700	-1.43092300
H	-4.79263200	-3.53703500	-2.08209200
H	-3.05660500	-3.95558300	-1.99517300
H	-4.10074600	-4.22989400	-0.59116200

³[Ir-TS1]_{sp²}

N	0.43366800	0.55721500	-0.07829700
C	1.10769800	1.72494400	-0.02885700
C	2.53707600	1.68359400	-0.31897100
C	2.99346000	0.33762600	-0.54565200
C	1.94749300	-0.56740700	-0.88823600
C	0.51467600	2.97098300	0.34230400
C	3.29803700	2.86744400	-0.19337600
H	4.37222500	2.84530200	-0.38571000
C	2.68704800	4.07609200	0.15320900
H	3.28433600	4.98775300	0.22467800
C	1.29719500	4.12067400	0.41231700
H	0.82939900	5.07071300	0.68449000
H	-0.55246400	2.98978100	0.57314800
C	1.99904200	-1.98354600	-0.43809600
H	1.34503300	-0.40544700	-1.78844700
H	-0.68534500	-0.59910400	-2.23885000
C	-1.66598100	-0.51453500	-1.75589700
C	-2.16167500	0.81244600	-1.54990700
C	-2.50707900	-1.77401200	-1.90575900
C	-3.64744100	1.18015400	-1.48710500
H	-1.49983400	1.63009900	-1.85858900
C	-3.64076100	-1.85670400	-0.85572900
H	-2.91199200	-1.85616800	-2.93324000
H	-1.82313600	-2.62647500	-1.76895400
C	-4.18364500	1.15818900	-0.03449100
H	-3.79016200	2.18525800	-1.91488100
H	-4.22753300	0.49744100	-2.12795900
C	-3.22137900	-1.22143700	0.46602300
H	-3.90309300	-2.91225700	-0.68108500
H	-4.55731200	-1.37319700	-1.22908700
C	-3.46988200	0.13100800	0.83336500
H	-4.02075900	2.14590300	0.42679900
H	-5.27733200	0.98766100	-0.01941500
H	-3.01775500	-1.91871600	1.28563700
H	-3.48443200	0.34461600	1.90901500
Ir	-1.38367100	-0.00006900	0.30561500
O	-1.11905600	-0.16991000	2.24447800
H	0.05885200	-0.61399400	3.86659600
C	0.04066800	-0.78264500	2.77473600
H	0.96455100	-0.36249300	2.33096000

H	0.04835900	-1.87548500	2.59619100
C	4.38695800	-0.15619200	-0.19718200
H	4.66840400	0.29677600	0.77363900
C	4.43362500	-1.69889600	-0.05577800
H	5.30064700	-1.97236300	0.56849400
H	4.61402000	-2.15118600	-1.04845400
C	3.14538200	-2.31930800	0.52742300
H	2.91913200	-1.80514600	1.48263500
O	1.15447100	-2.81121900	-0.79875000
C	5.44087500	0.28855500	-1.24503100
H	5.52474300	1.38076500	-1.32840600
H	6.43238300	-0.10535100	-0.96887500
H	5.18149000	-0.10553300	-2.23990800
C	3.26207100	-3.82548200	0.78056500
H	4.04087200	-4.03639100	1.52949400
H	2.30793100	-4.23736100	1.13679300
H	3.52164700	-4.36083300	-0.14601300

¹[Ir-IM]_{sp²}

N	0.63488200	0.41637400	0.03170400
C	1.23410000	1.63056000	0.03439000
C	2.66779300	1.53874600	-0.26056200
C	2.96327400	0.20218300	-0.47013700
C	1.67950800	-0.55288200	-0.28684200
C	0.63113800	2.89474100	0.30445100
C	3.46119200	2.73575300	-0.26534900
H	4.53108500	2.68726800	-0.48056600
C	2.84595000	3.93935000	0.00304700
H	3.43294200	4.86137700	0.00079700
C	1.43769600	4.01716400	0.28631900
H	0.99928100	4.99624300	0.49472300
H	-0.43213500	2.93652100	0.54405800
C	1.85724700	-1.71122100	0.75113300
H	1.39473100	-1.08627300	-1.22030200
H	-0.39711800	-1.90094800	-1.36577300
C	-1.39271700	-1.45114400	-1.23152700
C	-1.61751200	-0.19469600	-1.89604200
C	-2.45293700	-2.50724400	-0.93586200
C	-2.98700400	0.25984100	-2.41776600
H	-0.76257300	0.22897300	-2.44038100
C	-3.71816500	-1.89037700	-0.29295000
H	-2.70982900	-3.08421000	-1.84613500
H	-2.00590600	-3.22518300	-0.22847900
C	-3.75586200	1.08928100	-1.35856100
H	-2.84929100	0.86593400	-3.32775900
H	-3.57910800	-0.61601900	-2.73003500
C	-3.36581000	-0.66464200	0.55082400

H	-4.21502100	-2.64127400	0.34222900
H	-4.45343700	-1.61646500	-1.06673400
C	-3.40766400	0.67731400	0.06576700
H	-3.48514700	2.15254800	-1.46652000
H	-4.84896900	1.03022500	-1.52639100
H	-3.47020400	-0.78908400	1.63468800
H	-3.55349600	1.46008500	0.82075400
Ir	-1.37261000	0.08834100	0.21456800
O	-1.43536200	1.02027100	1.96827700
H	-0.51508600	1.59661400	3.71656800
C	-0.51365200	0.74881300	3.00468600
H	0.52284700	0.60348700	2.64282000
H	-0.78936300	-0.16411700	3.56973600
C	4.25547600	-0.51565100	-0.74664000
H	5.01298300	-0.15569900	-0.02227400
C	4.05669700	-2.03427600	-0.51621000
H	5.03976600	-2.52978000	-0.46326500
H	3.54146300	-2.47632700	-1.38943600
C	3.25455400	-2.35480200	0.76107600
H	3.76130500	-1.85066000	1.61075400
O	0.95319900	-2.06695100	1.48499100
C	4.80552600	-0.23493600	-2.16620600
H	4.98648300	0.83861100	-2.31984300
H	5.75544900	-0.77006300	-2.32620100
H	4.09103100	-0.56771200	-2.93538500
C	3.17075300	-3.85767600	1.07519800
H	4.17294700	-4.27079900	1.26272400
H	2.54403200	-4.03105100	1.96006600
H	2.72694000	-4.41085000	0.23231000

³[Ir-IM]_{sp²}

N	0.63178400	0.41052800	-0.05447900
C	1.26065800	1.65208200	-0.01178300
C	2.68371400	1.52815300	-0.24313700
C	2.95941200	0.15967200	-0.46900800
C	1.65723100	-0.59472100	-0.35828200
C	0.68162800	2.90493500	0.23050300
C	3.50126500	2.68038600	-0.19575600
H	4.58049100	2.60000000	-0.34717600
C	2.90803200	3.93191000	0.05255000
H	3.53271300	4.82803700	0.08367400
C	1.52232700	4.04105900	0.25966500
H	1.08047100	5.02262800	0.44804000
H	-0.39122400	2.98834700	0.40656900
C	1.79623400	-1.73060700	0.69701100
H	1.40831600	-1.12786500	-1.30914100
H	-0.44107700	-1.88175500	-1.40484900

C	-1.43532300	-1.44959600	-1.24149400
C	-1.71654200	-0.21291500	-1.90738800
C	-2.46960300	-2.49916100	-0.85253900
C	-3.10588300	0.22837700	-2.37612300
H	-0.88497600	0.24010100	-2.46000400
C	-3.71955200	-1.87282900	-0.19025400
H	-2.74996000	-3.11704300	-1.72785200
H	-1.98481100	-3.17903000	-0.13340500
C	-3.81116000	1.10040800	-1.30937900
H	-3.00745800	0.80068000	-3.31228300
H	-3.71585000	-0.65376000	-2.62674400
C	-3.35228800	-0.62320700	0.60872000
H	-4.18719600	-2.60862600	0.48305400
H	-4.48274500	-1.62821500	-0.94562700
C	-3.41238000	0.70932000	0.10550000
H	-3.52055000	2.15386900	-1.45313500
H	-4.91110900	1.06298000	-1.42961600
H	-3.40773100	-0.73022900	1.69759500
H	-3.52898100	1.50449800	0.85176000
Ir	-1.34924600	0.12466800	0.19991500
O	-1.35997800	1.04171600	1.93494800
H	-0.55093700	1.41788000	3.78394600
C	-0.47662300	0.66660200	2.97779100
H	0.57077200	0.61172100	2.62798700
H	-0.73650100	-0.32413400	3.39507600
C	4.25694800	-0.56154000	-0.69447400
H	4.98104200	-0.22372800	0.07572600
C	4.03307200	-2.08217000	-0.50367500
H	5.00630600	-2.59469100	-0.42769300
H	3.54224900	-2.49682800	-1.40400600
C	3.17902600	-2.41328300	0.73718000
H	3.67301800	-1.95344500	1.61834600
O	0.88921000	-2.04628400	1.45467900
C	4.88651700	-0.25659400	-2.07685200
H	5.07088800	0.82013500	-2.20202400
H	5.84629000	-0.78584900	-2.19375900
H	4.21695800	-0.57808700	-2.89024900
C	3.04189200	-3.92199700	1.00437300
H	4.02340200	-4.37143000	1.21748400
H	2.37691400	-4.09919900	1.86039800
H	2.61524900	-4.43923000	0.12991100

¹[Ir-TS2]_{sp²}

N	0.65051700	0.42227300	-0.02014100
C	1.20077500	1.70291600	-0.03137600
C	2.63807700	1.66654700	-0.07936600
C	3.02883500	0.30247400	-0.17079400

C	1.83719000	-0.47024600	-0.13671500
C	0.48181300	2.91575800	0.02641200
C	3.35365100	2.89784200	-0.04145700
H	4.44475800	2.91070700	-0.05344000
C	2.63866700	4.08447000	0.03612100
H	3.17679500	5.03474300	0.07681000
C	1.21438800	4.09603500	0.06711400
H	0.69125000	5.05302300	0.13005700
H	-0.60905000	2.88682500	0.06831900
C	1.79573300	-1.92269800	0.21278800
H	1.03501400	-0.19599000	-1.12126700
H	-0.51636200	-1.21775400	-1.99955700
C	-1.50633100	-0.91460000	-1.60836100
C	-1.83290300	0.48730400	-1.73199800
C	-2.50476000	-2.06880100	-1.61717900
C	-3.26467700	1.00690000	-1.92786300
H	-1.05751300	1.12562500	-2.18207900
C	-3.69526200	-1.80775200	-0.65913400
H	-2.86372300	-2.28953600	-2.64189700
H	-1.96203200	-2.96480100	-1.27522700
C	-3.92812800	1.35309200	-0.57146200
H	-3.24994400	1.90315300	-2.56964600
H	-3.86537000	0.26145500	-2.47479000
C	-3.27985700	-0.94017200	0.53435200
H	-4.08895400	-2.76836700	-0.28980500
H	-4.52865400	-1.32763200	-1.19776000
C	-3.40407400	0.48609500	0.56651900
H	-3.70374400	2.40204500	-0.31441300
H	-5.03163500	1.28315200	-0.63804500
H	-3.26911100	-1.44274700	1.50837100
H	-3.48434000	0.93758100	1.56325400
Ir	-1.37431500	-0.02761600	0.28525100
O	-1.23929100	0.06553200	2.26429700
H	0.77302200	0.67113100	2.52660400
C	-0.02651200	0.04656800	2.97960000
H	0.37922100	-0.98060200	3.09321500
H	-0.20161000	0.44252900	3.99928900
C	4.38675100	-0.34381000	-0.31121700
H	4.92559800	-0.19757400	0.64720800
C	4.22157100	-1.86546600	-0.53774100
H	5.20086700	-2.35684400	-0.41529200
H	3.91645300	-2.04010900	-1.58626300
C	3.19347200	-2.53796700	0.39704600
H	3.47044100	-2.28557400	1.44211300
O	0.75317800	-2.54950400	0.37409600
C	5.24970900	0.27266000	-1.43462500
H	5.45866400	1.33763800	-1.26480600

H	6.21563600	-0.25218400	-1.50085500
H	4.74454400	0.18049100	-2.40866600
C	3.15578000	-4.06565400	0.25579800
H	4.12283900	-4.50432600	0.54367900
H	2.36842600	-4.49409000	0.88986500
H	2.94257500	-4.35866800	-0.78424500

³[Ir-TS2]_{sp²}

N	0.72763300	0.62081900	-0.26881300
C	1.58361200	1.72989700	-0.25578500
C	2.97162900	1.30453700	-0.18940700
C	3.00726200	-0.11635500	-0.17220800
C	1.64004400	-0.55898900	-0.20840800
C	1.21575300	3.07982700	-0.31505200
C	3.97275900	2.31786900	-0.16359900
H	5.02873800	2.04961600	-0.09866000
C	3.59189800	3.66066600	-0.20368000
H	4.36376400	4.43440600	-0.17327100
C	2.23395700	4.04602900	-0.27900800
H	1.97234500	5.10627300	-0.30282100
H	0.16144200	3.36140100	-0.35414300
C	1.10738200	-1.80654800	0.21974100
H	1.08529200	-0.19695000	-1.27897900
H	-0.70152000	-0.64624500	-2.29773700
C	-1.63246500	-0.46547400	-1.73719400
C	-1.99708000	0.92205100	-1.55953800
C	-2.61027300	-1.63358200	-1.81347500
C	-3.45857900	1.39261700	-1.48540800
H	-1.29628300	1.65644500	-1.97669400
C	-3.64391100	-1.60930900	-0.66044700
H	-3.11675400	-1.67093700	-2.79701300
H	-2.01292700	-2.55524400	-1.73422800
C	-3.96406400	1.45796300	-0.02542200
H	-3.54449600	2.38713700	-1.95105400
H	-4.09066000	0.72214200	-2.09021900
C	-3.08590000	-0.93388600	0.59661700
H	-3.94452200	-2.63926900	-0.41258500
H	-4.56533600	-1.09198400	-0.97417200
C	-3.25890500	0.45520500	0.88154600
H	-3.76578600	2.46219300	0.38262500
H	-5.06073800	1.31555200	0.02530300
H	-2.91914200	-1.59037200	1.45785400
H	-3.20362600	0.74101400	1.93825500
Ir	-1.24295200	0.12477800	0.25861300
O	-0.91984900	0.45855300	2.20070600
H	1.16658600	0.80435400	2.23287100
C	0.34832000	0.33534600	2.81053500

H	0.60711900	-0.72868500	2.97828700
H	0.30257400	0.82523700	3.80044100
C	4.07298900	-1.17895500	-0.03274500
H	4.41530100	-1.19089700	1.02367400
C	3.44860500	-2.57281100	-0.34261700
H	4.19358200	-3.35377300	-0.11525700
H	3.26075600	-2.63073800	-1.43078300
C	2.12568400	-2.92352300	0.39483500
H	2.34119900	-2.97140200	1.48341200
O	-0.15753100	-1.94408300	0.47857500
C	5.31613800	-0.94929300	-0.91762800
H	5.82092900	-0.00364900	-0.67408600
H	6.04696100	-1.76238000	-0.78040900
H	5.03712400	-0.91577000	-1.98264000
C	1.57381400	-4.29640300	-0.03144900
H	2.28526500	-5.09888100	0.21742800
H	0.62119700	-4.50351500	0.47554600
H	1.39254000	-4.32576200	-1.11790700

¹[Ir-PC]_{sp}²

N	0.67536000	0.22518200	-0.88089500
C	1.06857600	1.60497900	-0.79683400
C	2.36922700	1.68737600	-0.22160400
C	2.83633400	0.32422000	-0.02408600
C	1.83155500	-0.51841900	-0.46222000
C	0.33690100	2.73041200	-1.18540400
C	2.92662300	2.96839000	0.00203800
H	3.90674300	3.08220800	0.46458600
C	2.20120100	4.09836100	-0.38110700
H	2.62697400	5.09067100	-0.21481700
C	0.92633900	3.98368300	-0.97873500
H	0.38458100	4.88526100	-1.27293300
H	-0.66067100	2.62859100	-1.61308100
C	1.92493900	-1.96978000	-0.61906800
H	0.32200500	-0.08164200	-1.79524700
H	-1.11372000	-1.68473900	-1.84058900
C	-1.95537700	-1.24359700	-1.28573200
C	-2.28916600	0.13224700	-1.57275000
C	-2.94427600	-2.30244100	-0.80450400
C	-3.71414400	0.69559100	-1.45414400
H	-1.69104500	0.61968100	-2.36118000
C	-3.78351600	-1.81035600	0.40064000
H	-3.59958200	-2.64424200	-1.62934600
H	-2.35291200	-3.18041100	-0.49743600
C	-3.95544600	1.31600700	-0.05526500
H	-3.88006000	1.46080700	-2.23017500
H	-4.45088900	-0.09838400	-1.66039200

C	-3.01246100	-0.77801900	1.22968800
H	-4.05180200	-2.66512100	1.04199100
H	-4.73821800	-1.37675600	0.06008600
C	-3.11703200	0.64633500	1.02605000
H	-3.67517400	2.38243900	-0.07455900
H	-5.02929800	1.28612000	0.21474100
H	-2.73169900	-1.09077600	2.24251700
H	-2.92126500	1.27001400	1.90733100
Ir	-1.27923700	-0.03530800	0.29869600
O	-0.64005800	0.28278000	2.15644100
H	1.13134600	1.42826600	2.12724300
C	0.67294400	0.53092700	2.58976600
H	1.36134600	-0.32411000	2.41504900
H	0.65355400	0.70713900	3.68350500
C	4.12505400	-0.22854000	0.54583800
H	3.98194800	-0.30094300	1.64383100
C	4.35447500	-1.66353000	0.00759800
H	5.19899700	-2.11827300	0.55238800
H	4.66489000	-1.59696300	-1.05184700
C	3.12434500	-2.59508100	0.10632500
H	2.82256400	-2.64017900	1.17358100
O	1.11448000	-2.62110600	-1.29123800
C	5.37285500	0.64014400	0.29201700
H	5.34237600	1.58795700	0.84664200
H	6.27393400	0.10056800	0.62251100
H	5.49117600	0.86989200	-0.77817200
C	3.41084000	-4.01770400	-0.38802600
H	4.18788100	-4.49441500	0.22838400
H	2.50145400	-4.63235300	-0.34936800
H	3.75820000	-4.00847900	-1.43306900

¹[Ir]

H	-1.31713900	-0.18881300	-2.35457100
C	-1.43571700	-0.07163900	-1.26766000
C	-2.24506500	1.16249800	-0.84440000
C	-1.37563700	-1.28161300	-0.48473000
C	-1.35016700	2.16763600	-0.07684800
H	-2.67104800	1.65068400	-1.73508200
H	-3.10727100	0.85941500	-0.22835000
C	-2.07391400	-1.47194400	0.86153100
H	-1.23571500	-2.21870900	-1.04702100
C	-0.20424000	1.46128500	0.63631500
H	-0.90166200	2.88023800	-0.78842800
H	-1.93911000	2.77411200	0.63853700
C	-1.73755900	-0.32240200	1.84327800
H	-3.16881900	-1.57646400	0.73883400
H	-1.71873600	-2.42473500	1.28732300

C	-0.36922800	0.29187500	1.50966000
H	0.63901300	2.12837400	0.87268800
H	-1.72550900	-0.70047900	2.87764300
H	-2.51235800	0.46107000	1.81476900
H	0.37743500	0.18059600	2.30971300
Ir	0.45365000	-0.24686300	-0.30633000
O	2.35928600	-0.15131400	-0.14886800
H	3.24701000	1.57724700	0.63383900
C	3.26994400	0.47533600	0.73517900
H	4.29219800	0.13534700	0.49339200
H	3.06584200	0.21491700	1.79115000

¹[PC]_{sp²}

C	2.44950500	1.39574000	-0.16589100
H	2.20707000	2.45064100	-0.31659700
C	3.77392900	0.98903400	-0.01469100
H	4.57557900	1.73075600	-0.04403300
C	4.10287100	-0.37796200	0.17669500
H	5.15128300	-0.66354000	0.29259800
C	3.11919100	-1.36736500	0.21741000
H	3.37913200	-2.41876700	0.36116400
C	1.78129600	-0.95946900	0.06475600
N	0.61945800	-1.69772800	0.05296100
C	1.42221100	0.42312100	-0.12515900
C	-0.00808100	0.47059800	-0.25204800
C	-0.45771300	-0.84517800	-0.13696900
C	-1.83718800	-1.30775000	-0.18683900
C	-2.88773200	-0.19667900	-0.34998000
C	-2.30613900	1.08588200	-1.00635600
C	-0.95425000	1.62556600	-0.45379700
H	-3.64211900	-0.60963300	-1.04258900
H	0.51053100	-2.70062100	0.16220800
H	-2.14990100	0.86034800	-2.07538200
H	-3.06427700	1.88694400	-0.96855400
H	-0.53476500	2.28165600	-1.23967000
O	-2.13835000	-2.50466300	-0.06108600
C	-1.08494900	2.50077800	0.81720000
H	-0.10948900	2.92439200	1.10052400
H	-1.78044800	3.33705600	0.64212400
H	-1.45281100	1.92278500	1.67646700
C	-3.60416500	0.01735300	1.00462400
H	-4.38801400	0.78510100	0.91089000
H	-4.07440000	-0.92243400	1.32897500
H	-2.90948900	0.33470600	1.79611000

¹[Ir-TS1]_{sp³}

C	2.86135800	3.08031400	-0.65973400
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H	3.95257400	3.09639500	-0.72289700
C	2.11904700	4.19706900	-1.07383700
H	2.63330200	5.08296000	-1.45331200
C	0.71479100	4.15584400	-1.02421000
H	0.12913900	5.01396000	-1.36386600
C	0.05541100	3.01395000	-0.56599800
H	-1.03532100	2.96427400	-0.53248100
C	0.78958800	1.90692700	-0.05441000
N	0.14358200	0.86285200	0.59343300
C	2.23350800	1.93407100	-0.15195200
C	2.95575000	0.67174600	0.14567100
C	4.31241300	-1.23217100	-0.75068000
O	5.25109300	-1.62616400	-1.45563200
C	4.12760600	-3.54790800	0.30255000
H	3.44095100	-4.25796700	0.78874500
H	4.44855700	-3.96534800	-0.66134600
H	5.02556000	-3.45259900	0.93329500
C	2.36473000	0.63073000	2.62553300
H	3.36920600	0.77340700	3.06313000
H	1.89615200	1.61921900	2.52680200
H	1.76984500	0.04456600	3.34417900
C	3.05224300	-1.50702300	1.42492200
H	3.95679900	-1.43516600	2.06481200
H	2.35727900	-2.15982700	1.98244400
C	3.45616800	-2.18508200	0.10178500
H	2.52916200	-2.32989200	-0.49258800
C	2.46860300	-0.10370100	1.28323500
H	1.13447700	0.09073000	0.96951600
C	3.85645900	0.16619200	-0.77023300
H	4.19936100	0.77707300	-1.61020100
C	-1.57406100	-2.04993900	-2.15870100
H	-1.90014200	-3.07260600	-1.91317400
H	0.16361500	-1.81092300	0.91773900
C	-0.76431500	-1.87141300	0.33407300
C	-0.66657500	-1.51320400	-1.05011600
C	-1.78942100	-2.82317400	0.93195100
H	0.31422200	-1.16683800	-1.39401700
C	-3.22262400	-2.55011800	0.41199100
H	-1.49378500	-3.87445500	0.75064800
H	-1.76902500	-2.68102500	2.02496500
C	-2.79057200	-1.12279600	-2.39447100
H	-0.99180400	-2.13590800	-3.08948900
C	-3.44015600	-1.06602400	0.13923300
H	-3.95400900	-2.89313800	1.16076800
H	-3.42535700	-3.13759600	-0.49687600
C	-3.24784800	-0.43288500	-1.11801800
H	-2.50891700	-0.33502600	-3.11163900

H	-3.62807700	-1.67866800	-2.85778700
H	-4.08118600	-0.54015100	0.85376200
H	-3.79078500	0.50613300	-1.27524100
Ir	-1.54111800	0.10583200	0.11416200
O	-2.63870900	1.67260800	0.56726200
H	-3.16654600	3.09845300	1.95011400
C	-2.58155600	2.16290300	1.89912300
H	-1.53995400	2.36663500	2.21706400
H	-3.01663600	1.44693300	2.62313300

³[Ir-TS1]_{sp³}

C	2.99650700	2.99564600	-0.70586900
H	4.08920700	3.02056200	-0.72387900
C	2.26656000	4.11829700	-1.11482600
H	2.78791800	5.01680500	-1.45169700
C	0.85752100	4.07909000	-1.08704400
H	0.28057200	4.95135500	-1.40527300
C	0.18574300	2.94271200	-0.64725000
H	-0.90459600	2.90708800	-0.60555700
C	0.90702200	1.79398900	-0.18950500
N	0.24324000	0.69331100	0.26561200
C	2.36006800	1.83116400	-0.24486600
C	3.07887900	0.58265400	0.06189000
C	4.62115900	-1.25154500	-0.65986000
O	5.67129200	-1.59743600	-1.21575300
C	4.31229800	-3.62862900	0.21725900
H	3.57038100	-4.37476100	0.54127200
H	4.79870400	-3.98457700	-0.70080900
H	5.09017000	-3.55846900	0.99395200
C	2.33619300	0.43346300	2.49403300
H	3.32545500	0.51834200	2.97645700
H	1.91269600	1.44318400	2.41124000
H	1.68900900	-0.16037700	3.15811700
C	3.02372900	-1.67607200	1.25681600
H	3.80029600	-1.66462300	2.04810700
H	2.23488800	-2.34825400	1.63806900
C	3.65301600	-2.26553300	-0.01963000
H	2.84645600	-2.38745800	-0.77163900
C	2.48009100	-0.25260600	1.12731200
H	1.26201400	-0.13973800	0.69728600
C	4.13105200	0.13453500	-0.70504100
H	4.57725300	0.77696100	-1.46983700
C	-2.53518500	-1.39332400	-2.40635300
H	-2.82237300	-2.45480600	-2.33392500
H	0.13120700	-1.96657900	-0.16521300
C	-0.93922900	-1.86887200	-0.38988700
C	-1.26556500	-1.14599500	-1.58379400

C	-1.78902300	-2.96011100	0.25128700
H	-0.42320400	-0.73026700	-2.14819800
C	-3.27790200	-2.55580100	0.38747300
H	-1.69028100	-3.91377400	-0.30235900
H	-1.37716200	-3.14490600	1.25717300
C	-3.70170000	-0.47845400	-1.95830700
H	-2.31792600	-1.21449000	-3.47109300
C	-3.44391500	-1.05161600	0.58630400
H	-3.72631200	-3.08665900	1.24202900
H	-3.84772700	-2.87297700	-0.50056100
C	-3.63218600	-0.12382600	-0.47826700
H	-3.65500200	0.46754000	-2.52152700
H	-4.67961600	-0.93501900	-2.20412300
H	-3.77056300	-0.72781800	1.57994400
H	-4.11815900	0.82055700	-0.20407600
Ir	-1.59484200	0.08333800	0.16603100
O	-2.31268000	1.59055700	1.22480600
H	-2.08053900	3.06082400	2.64087700
C	-1.67522400	2.06184300	2.39718300
H	-0.57779400	2.14244900	2.28190500
H	-1.87315600	1.39865000	3.26292500

³[Ir-IM]_{sp}³

C	2.84565700	2.88472700	-0.97304200
H	3.93214000	2.90852000	-1.09399800
C	2.07781200	4.00732300	-1.31957600
H	2.56400200	4.90255000	-1.71339500
C	0.68165600	3.96386500	-1.15514200
H	0.07201200	4.83176700	-1.41951000
C	0.06134600	2.81638800	-0.66443700
H	-1.02151200	2.77197200	-0.53250200
C	0.82503300	1.66803000	-0.30813400
N	0.20362900	0.53008500	0.16476700
C	2.25410800	1.71977100	-0.45979400
C	3.11537300	0.53577200	-0.12832300
C	4.46382800	-1.40945700	-1.03132400
O	5.05259600	-1.95506600	-1.97972400
C	5.53061700	-3.06675500	0.58979000
H	5.38860100	-3.61444200	1.53416100
H	5.55313900	-3.78537200	-0.24028100
H	6.51480100	-2.57303500	0.62377500
C	2.89469200	0.93358500	2.39151200
H	3.73468500	1.20864900	3.05463000
H	2.35885000	1.84908500	2.10993200
H	2.21800300	0.31021300	3.00418000
C	4.36876800	-0.95357200	1.46580000
H	5.38139000	-0.50796700	1.56964100

H	4.15510900	-1.41293300	2.44661900
C	4.41339500	-2.04112300	0.37269600
H	3.43793300	-2.57038000	0.40211700
C	3.39893100	0.17308500	1.20045400
H	0.88469600	-0.21419400	0.34267500
C	3.70494800	-0.17587700	-1.20190600
H	3.58295000	0.18609900	-2.22565000
C	-2.83315600	-1.47992400	-2.27853400
H	-3.19029800	-2.51357900	-2.14725500
H	-0.10521200	-2.13284000	-0.12664700
C	-1.17925500	-1.96998100	-0.30006300
C	-1.52675300	-1.27587800	-1.50558400
C	-2.05762100	-2.99280400	0.41068700
H	-0.69089600	-0.90959600	-2.11242400
C	-3.52004700	-2.50609500	0.55626600
H	-2.01532700	-3.97320800	-0.10194900
H	-1.62977100	-3.15148000	1.41463400
C	-3.91736700	-0.46373400	-1.84263100
H	-2.63652400	-1.36629300	-3.35633600
C	-3.59087000	-0.98570000	0.70112200
H	-3.97831500	-2.97536200	1.44130900
H	-4.12657600	-2.83017200	-0.30369300
C	-3.78940500	-0.07643900	-0.37654100
H	-3.80838000	0.45820100	-2.43677200
H	-4.93219600	-0.85075700	-2.05717500
H	-3.86915700	-0.62176800	1.69654500
H	-4.22144800	0.89750800	-0.11613200
Ir	-1.72366800	0.02341200	0.21286200
O	-2.27571900	1.57557000	1.29305700
H	-1.87978500	2.92019900	2.79830800
C	-1.59332500	1.89795900	2.49144200
H	-0.49356300	1.85439200	2.37217300
H	-1.86752300	1.20791200	3.31420100

³[Ir-TS2]_{sp³}

C	-3.22668100	1.60867800	2.11890800
H	-4.16994400	1.17415000	2.45837500
C	-2.68864200	2.72941200	2.76593800
H	-3.21310500	3.16233000	3.62158400
C	-1.49278400	3.31441400	2.31351900
H	-1.09078000	4.19794600	2.81479500
C	-0.80072300	2.76037900	1.21943600
H	0.14967200	3.18807600	0.88821400
C	-1.33724800	1.64413600	0.56821200
N	-0.70365600	0.95386100	-0.54084300
C	-2.57430900	1.06898000	0.99149700
C	-2.90740800	-0.07460500	0.15231300

C	-2.98161800	-2.56372300	-0.03738800
O	-3.41760800	-3.69910200	0.29779300
C	-1.85286600	-3.69886900	-2.04176500
H	-1.00952700	-3.64021400	-2.74787200
H	-1.73697200	-4.59674700	-1.41979200
H	-2.77905900	-3.82521700	-2.62483600
C	-2.85377500	1.26115200	-2.01140700
H	-3.85566800	0.99319100	-2.38589400
H	-2.95683600	2.18688800	-1.42892400
H	-2.21957700	1.45506800	-2.89292000
C	-2.15105500	-1.16755800	-1.98920500
H	-3.08187300	-1.28306800	-2.58023500
H	-1.34879100	-1.03817900	-2.73236300
C	-1.92370200	-2.44302500	-1.16710900
H	-0.95371200	-2.31065600	-0.63901400
C	-2.32254300	0.09857800	-1.16799500
H	-0.46617700	1.64062000	-1.26857600
C	-3.34619700	-1.34543200	0.61538400
H	-3.93190500	-1.42719300	1.53440500
C	2.56793500	-0.18805500	2.42157500
H	2.62663400	-1.13898700	2.97481000
H	-0.76655200	-0.95797100	1.57672800
C	0.31679700	-1.11347200	1.49721800
C	1.15722600	-0.01062800	1.85253600
C	0.74502800	-2.57198600	1.63604800
H	0.65776000	0.92258500	2.13481900
C	2.09511800	-2.86749400	0.93084500
H	0.79137600	-2.85568100	2.70470100
H	-0.04528700	-3.19975100	1.19679000
C	3.63990400	-0.13902200	1.30633400
H	2.76494500	0.60517300	3.15987400
C	2.38600200	-1.88055800	-0.20269100
H	2.08099000	-3.88975600	0.52193900
H	2.92509800	-2.84494500	1.65599900
C	3.11005300	-0.65587200	-0.02292500
H	3.95751400	0.90491700	1.14924800
H	4.54802900	-0.69559600	1.60704800
H	2.42777500	-2.31845900	-1.20803400
H	3.63060800	-0.26866900	-0.90748500
Ir	1.05175200	-0.19349200	-0.29226800
O	1.69133600	0.36762900	-2.09570200
H	1.53890700	0.98921100	-4.04201800
C	0.95079200	0.43365300	-3.28876700
H	-0.03178300	0.94134900	-3.19043900
H	0.75212300	-0.57629300	-3.70339300

¹[Ir-PC]_{sp}³

C	3.08010900	3.11106200	-0.22335900
H	4.13325900	3.23605000	0.03822000
C	2.28859100	4.21699600	-0.55126000
H	2.72507700	5.21822400	-0.54001000
C	0.93087400	4.05316600	-0.89563400
H	0.33074800	4.92934600	-1.15197100
C	0.32996600	2.78447900	-0.89968900
H	-0.72862800	2.64225200	-1.12862200
C	1.12662500	1.69047800	-0.55697000
N	0.69227900	0.29888000	-0.52351100
C	2.49337600	1.83052500	-0.23472400
C	3.05901700	0.50321900	-0.06027500
C	4.71103200	-1.33216900	-0.09268200
O	5.85093600	-1.73535900	0.16464700
C	3.58597900	-3.59442500	0.25295800
H	3.01596100	-4.38837800	-0.25324500
H	4.60909700	-3.95327100	0.43105900
H	3.11347000	-3.41009000	1.22866400
C	1.63859800	-0.94802200	1.44111800
H	2.54536800	-1.39833600	1.86844300
H	1.34906500	-0.09808000	2.07061600
H	0.81707400	-1.67928400	1.46381200
C	2.25304400	-1.68873100	-0.93175300
H	1.46931100	-2.46029600	-0.86668600
H	2.25732400	-1.31836900	-1.97251600
C	3.64135600	-2.32477700	-0.62227300
H	4.06811400	-2.64292700	-1.59118100
C	1.91038800	-0.50291400	-0.00694400
H	0.53438300	0.00588300	-1.49872300
C	4.35658700	0.09454100	-0.01628100
H	5.18855200	0.80219200	0.03526600
C	-3.48341800	-0.20733900	-2.00606700
H	-4.03577500	-1.15572200	-2.10923200
H	-0.56730000	-2.08470600	-1.38209700
C	-1.53672800	-1.68568100	-1.04433600
C	-2.00134900	-0.49498200	-1.71790700
C	-2.44339700	-2.76938000	-0.46450400
H	-1.32486900	-0.07988400	-2.48569100
C	-3.57895700	-2.17609100	0.40776600
H	-2.85842700	-3.41854400	-1.26039300
H	-1.81391300	-3.42216700	0.16395500
C	-4.10211900	0.66858600	-0.89081000
H	-3.58380200	0.30207000	-2.97844500
C	-3.16677800	-0.84456200	1.04620200
H	-3.84822600	-2.89139500	1.20126100
H	-4.49310500	-2.03481900	-0.19181000
C	-3.43155000	0.43722000	0.45595900

H	-3.96835100	1.73334400	-1.14618700
H	-5.19509100	0.50661300	-0.81509600
H	-3.06319500	-0.84967800	2.13844100
H	-3.50806100	1.27695600	1.15713900
Ir	-1.38682500	-0.02851400	0.25507000
O	-1.20587900	0.90464700	2.00966900
H	-0.68120100	2.93361900	2.00549300
C	-0.34333900	1.94680100	2.38676500
H	0.71003100	1.82694700	2.05478700
H	-0.32521400	2.01358600	3.49262100

¹[PC]_{sp³}

C	-2.38060900	1.60134400	0.20361300
H	-2.03375700	2.61851700	0.40181700
C	-3.74827500	1.31985600	0.10965300
H	-4.48112500	2.12064700	0.22777700
C	-4.18628000	-0.00044400	-0.13199200
H	-5.25826700	-0.20465200	-0.19721800
C	-3.28316500	-1.05956100	-0.29224300
H	-3.63787000	-2.07447000	-0.48718100
C	-1.90850000	-0.77467400	-0.20115300
N	-0.83115800	-1.63253000	-0.38857700
C	-1.45521700	0.55207400	0.06270500
C	-0.00371000	0.51477300	0.07646600
C	2.35550300	1.22915900	-0.15086000
O	3.22127900	2.10355700	-0.00495400
C	3.91473600	-0.74518300	0.23361900
H	4.36628300	-1.63234300	-0.23714200
H	4.68991800	0.02485100	0.35172100
H	3.57072300	-1.03624000	1.23747400
C	0.71720600	-1.41079100	1.52901000
H	1.54928200	-0.83294700	1.95457800
H	-0.16254300	-1.25793100	2.17239100
H	0.99107700	-2.47864100	1.55015200
C	1.59356900	-1.16392900	-0.88720000
H	1.95023200	-2.20770300	-0.83612400
H	1.19549700	-1.01540300	-1.90342600
C	2.77534900	-0.18356800	-0.64315200
H	3.23054600	0.02597400	-1.62825900
C	0.41011700	-0.95764300	0.08034300
H	-0.94880500	-2.61161800	-0.13444100
C	0.92890200	1.51117300	0.04044700
H	0.64892700	2.56569400	0.11201500