Supporting Information

Reversing the relative ^{3}MLCT-^{3}MC order in Fe(II) complexes using cyclometallating ligands : a computational study aiming at luminescent Fe(II) complexes

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1. Computational details

Geometry optimization was performed with Orca 2.8 using the PBE0 functional, the def2-TZVP(-f) basis set, Grimme's empirical correction for dispersion VDW06 and ZORA scalar relativity, followed by a frequency calculation at the same level of calculation. Energies were then computed by single point calculations with B3LYP*, at the PBE0 geometries.

For each complex, singlet, triplet and quintet states were optimized by DFT but no ^{5}MLCT minima were found for the FeN_5C^+ complexes **2** and **3**, and no ^{5}MC minimum was found for complex **4**. Unrestricted Natural Orbitals (UNOs) were computed with B3LYP* to view the singly occupied orbitals of all excited states.

^{7}MLCT states were optimized when $S^2(^5MC) > 6.10$, *i.e.* for complexes **6** and **7**.

The ^{3}MLCT-^{3}MC pathway was explored using the Nudged Elastic Band method to perform minimum energy path optimizations with NWChem version 6.5 and the PBE0 functional.

The minimum energy crossing points between the ^{3}MC and the ground state surfaces were optimized with B3LYP*. Due to the fact that the S^2 values of the ^{3}MC and triplet state in the MECP search were very similar, identical energy corrections were applied to account for spin contamination.

2. Geometries and electronic energies

Main geometrical parameters (distances in Å, and angles in degrees). MPA is the angle between the mean planes of the ligands. In parentheses, Mulliken spin population on the metal centre. Uncorrected electronic energies (see section 3 for corrections).

$Fe(tpy)_2^{2+}$ 1	**GS**	**^{3}MC** (2.03)	**^{5}MC** (3.76)
Energy (au)	-2762.067953	-2762.035097	-2762.036697
S^2	-	2.05	6.03
Fe-N1	1.971	2.108	2.189
Fe-N2	1.882	1.910	2.132
Fe-N3	1.971	2.105	2.171
Fe-N4	1.971	2.106	2.167
Fe-N5	1.881	1.909	2.135
Fe-N6	1.970	2.104	2.169
∑ (Fe-X)	11.646	12.242	12.963
N2-Fe-N5	179.8	179.5	169.0
MPA	89.88	89.96	89.91

$Fe(tpy)(NCN)^+$ 2	**GS**	**^{3}MLCT** (1.11)	**^{3}MC** (2.36)	**^{5}MC** (3.75)
Energy (au)	-2745.640140	-2745.599693	-2745.612022	-2745.595361
S^2	-	2.02	2.23	6.07
Fe-N1	1.961	1.961	2.105	2.172
Fe-N2	1.894	1.902	1.905	2.189
Fe-N3	1.961	1.983	2.104	2.165
Fe-N4	1.987	1.986	2.119	2.243
Fe-C5	1.862	1.884	1.890	2.030
Fe-N6	1.988	1.987	2.115	2.323
∑ (Fe-X)	11.653	11.703	12.238	13.122
N2-Fe-C5	179.5	177.0	179.4	158.9
MPA	89.92	89.29	89.72	78.71

$Fe(tpy)(NNC)^+$ 3	**GS**	**^{3}MLCT** (1.22)	**^{3}MC** (2.22)	**^{5}MC** (3.78)
Energy (au)	-2745.643567	-2745.605072	-2745.609017	-2745.596813
S^2	-	2.03	2.14	6.09
Fe-N1	1.948	1.948	2.188	2.198
Fe-N2	1.848	1.861	1.966	2.157
Fe-N3	1.946	1.963	2.186	2.193
Fe-N4	1.997	2.105	2.044	2.305
Fe-N5	1.904	1.949	1.909	2.145
Fe-C6	1.944	1.923	1.975	2.067
∑ (Fe-X)	11.587	11.749	12.268	13.065
N2-Fe-N5	177.7	178.0	174.5	153.5
MPA	89.96	89.19	89.83	77.43

Fe(tpy)(CNC) 4	**GS**	**^{3}MLCT** (1.08)	**^{3}MC** (2.52)	**^{5}MLCT** (2.96)
Energy (au)	-2729.110302	-2729.075511	-2729.070783	-2729.049363
S^2	**-**	2.02	2.38	6.06
Fe-N1	1.925	1.939	2.134	2.219
Fe-N2	1.809	1.867	1.965	2.019
Fe-N3	1.923	1.960	2.132	2.105
Fe-C4	1.966	1.984	1.980	2.000
Fe-N5	1.946	1.931	2.007	1.963
Fe-C6	1.968	1.985	1.985	2.000
∑ (Fe-X)	11.537	11.666	12.203	12.306
N2-Fe-C5	179.5	178.4	179.7	166.8
MPA	89.98	89.81	89.72	89.82

$Fe(NCN)_2$ 5	**GS**	**^{3}MLCT** (1.12)	**^{3}MC** (2.33)	**^{5}MLCT** (3.02)	**^{5}MC** (3.86)
Energy (au)	-2729.095832	-2729.048077	-2729.069536	-2729.035400	-2729.044550
S^2	-	2.02	2.14	6.07	6.08
Fe-N1	1.982	1.968	2.139	2.183	2.265
Fe-C2	1.880	1.908	1.903	1.968	2.068
Fe-N3	1.983	2.004	2.139	2.183	2.354
Fe-N4	1.983	2.006	2.137	2.040	2.346
Fe-C5	1.880	1.908	1.903	1.920	2.068
Fe-N6	1.982	1.967	2.139	2.040	2.267
∑ (Fe-X)	11.690	11.761	12.360	12.334	13.368
C2-Fe-C5	179.8	175.5	179.8	179.9	159.9
MPA	90.00	87.20	89.83	89.94	63.81

Fe(NNC)(NCN) 6	**GS**	**^{3}MLCT** (1.17)	**^{3}MC** (2.67)	**^{5}MLCT** (3.03)	**^{5}MC** (3.85)	**^{7}MLCT** (4.25)
Energy (au)	-2729.105131	-2729.076253	-2729.073848	-2729.056560	-2729.051249	-2729.024390
S^2	-	2.03	2.54	6.07	6.18	12.02
Fe-N1	1.976	2.016	2.014	2.030	2.273	2.153
Fe-N2	1.917	1.939	1.894	1.926	2.182	2.117
Fe-C3	1.939	1.944	1.985	1.983	2.096	2.070
Fe-N4	1.965	1.997	2.233	2.242	2.328	2.266
Fe-C5	1.838	1.859	1.934	1.935	2.061	2.052
Fe-N6	1.967	1.960	2.256	2.246	2.291	2.225
∑ (Fe-X)	11.602	11.715	12.316	12.362	13.231	12.883
N2-Fe-C5	179.4	177.5	173.2	170.9	150.1	158.7
MPA	86.09	87.50	88.56	89.05	68.06	82.33

$Fe(NNC)_2$ 7	**GS**	**^{3}MLCT** (1.15)	**^{3}MC** (2.67)	**^{5}MLCT** (3.06)	**^{5}MC** (3.86)	**^{7}MLCT** (4.26)
Energy (au)	-2729.109768	-2729.083056	-2729.064505	-2729.048288	-2729.050422	-2729.026409
S^2	-	2.02	2.53	6.08	6.24	12.02
Fe-N1	1.959	2.025	2.335	2.054	2.261	2.223
Fe-N2	1.875	1.886	2.181	2.001	2.175	2.138
Fe-C3	1.928	1.927	1.969	1.969	2.098	2.074
Fe-N4	1.957	2.020	2.006	2.365	2.243	2.222
Fe-N5	1.875	1.886	1.973	2.197	2.174	2.138
Fe-C6	1.928	1.930	1.961	1.964	2.097	2.074
∑ (Fe-X)	11.522	11.674	12.425	12.550	13.048	12.869
N2-Fe-N5	178.2	178.1	150.7	150.0	151.1	154.9
MPA	89.05	88.65	78.78	75.72	86.22	72.61

^{3}MC-GS MECP geometries and energies (see section 3 for details on the correction)

Fe(NNC)(NCN) 6	**MECP**
Fe-N1	2.05
Fe-N2	1.92
Fe-C3	2.00
Fe-N4	2.28
Fe-C5	1.94
Fe-N6	2.29
Energy	–2729.058650 au
Corrected energy	–2729.061463 au

$Fe(NNC)_2$ 7	**MECP**
Fe-N1	2.23
Fe-N2	2.14
Fe-C3	1.97
Fe-N4	2.07
Fe-N5	2.04
Fe-C6	1.97
Energy	–2729.067374 au
Corrected energy	–2729.070392 au

3. Treatment of spin contamination

For indicative purposes, classical DFT codes calculate an S^2 value for open-shell species. Finding $S^2 = 2.5$ for a triplet state, or 6.3 for a quintet state, is not so worrying since it is the gap to the state of higher multiplicity that should be considered (how close S^2 is from 6 for a triplet state, or how close S^2 is from 12 for a quintet state). Nevertheless, we have derived from Ovchinnikov and Labanowski (OL) (*Phys. Rev. A* **1996**, *53*, 3946, equation 25) a correction for quintet states (Q) and for triplet states (T). This correction has been applied when $S^2(T) > 2.10$ and $S^2(Q) > 6.10$. The heptet (H) contaminating the quintet is considered to be pure ; the quintet is contaminated by H ; the triplet is contaminated by Q and H. N is the norm as defined in OL's equation 25.

<u>For the quintet state</u>, as proposed by OL, the correction should read as :

$$E_{corr}(Q) = \frac{1}{N}\left[E_{uncorr}(Q) - A_Q(H) E_{corr}(H) \right]$$

with, as said before, the approximation that $E_{corr}(H) = E_{uncorr}(H)$ (heptet energy at the quintet geometry).

Following OL's notation, $A_Q(H) = \frac{B_1}{6}$, B_1 being related to the trace of $S_{ij}^{\alpha\beta}$, the overlap integral between the i^{th} α and the j^{th} β molecular spin orbital. In this simple case, B_1 is the spin contamination $S^2 - 4$.

<u>For the triplet state :</u>

$$E_{corr}(T) = \frac{1}{N}\left[E_{uncorr}(T) - A_T(Q) E_{corr}(Q) - A_T(H) E_{corr}(H) \right]$$

with $E_{corr}(H) = E_{uncorr}(H)$, $A_T(H) = \frac{B_2}{60}$ and $A_T(Q) = \frac{6B_1 - B_2}{24}$.

In this case, one needs B_1 and also B_2, which is related to the variance of the $S_{ij}^{\alpha\beta}$ matrix. In Orca we don't have access to this matrix, and knowing that $B_2 \ll B_1$, we have set B_2 to zero. Thus, to correct the energy of the triplet, one first corrects the energy of the quintet (at the triplet geometry) and uses this corrected quintet energy :

$$E_{corr}(T) = \frac{1}{N}\left[E_{uncorr}(T) - \frac{B_1}{4} E_{corr}(Q) \right]$$

It is important to note that this correction has no incidence on the ordering of the states because it is small in comparison with the energy gaps between the states. For the most 'severe' case (^{3}MC state with S^2=2.54), the correction on the energy is –0.079 eV and the contribution to the wavefunction of the states of higher multiplicity is 13.5%. For the least 'severe' case (^{3}MC state with S^2=2.14), the correction on the energy is –0.039 eV and the contribution of the states of higher multiplicity is 3.5%. With this proportion of mixing states, we are still on the safe side of DFT.

Complex	State	S^2	uncorrected energy (au)	corrected energy (au)	correction
2	^{3}MC	2.23	-2745.612022389	-2745.61402324	–0.054 eV
3	^{3}MC	2.14	-2745.609017132	-2745.61032604	–0.035 eV
4	^{3}MC	2.38	-2729.070782735	-2729.0735571	–0.075 eV
5	^{3}MC	2.14	-2729.069536077	-2729.07097831	–0.039 eV
6	^{3}MC	2.54	-2729.073848289	-2729.07675227	–0.079 eV
6	^{5}MC	6.18	-2729.051249515	-2729.05237872	–0.031 eV
7	^{3}MC	2.53	-2729.064505204	-2729.06722065	–0.074 eV
7	^{5}MC	6.24	-2729.050421685	-2729.0516105	–0.032 eV

4. Contribution from spin polarization

Considering that the UKS energy of an open-shell state can be expressed as :

E(UKS) = E(ROKS) + pol + contam

with pol = contribution from spin polarization

and contam = correction for spin contamination (taken as zero for a ^{3}MLCT state),

one can calculate the contribution from spin polarization.

As an example, for the ^{3}MLCT state of complex **6** :

E(UKS) = –2729.076253548 au

E(ROKS) = –2729.073942726 au

therefore pol = –0.06 eV

For the ^{3}MC state of complex **6 :**

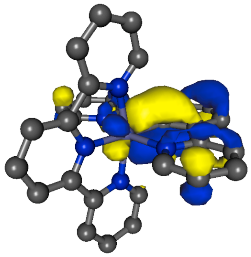
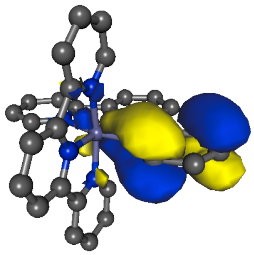
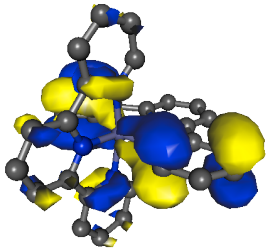
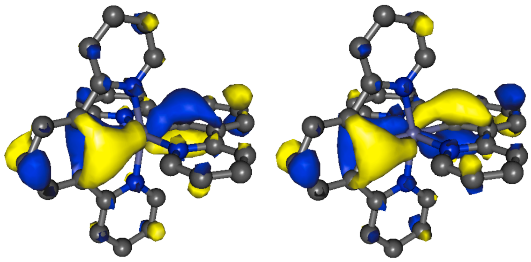
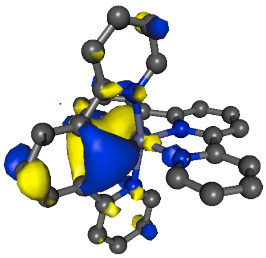
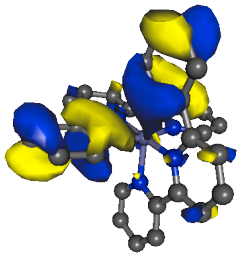
E(UKS) = –2729.073848289 au

E(ROKS) = –2729.061846768 au

contam = –0.08 eV

therefore pol = –0.24 eV

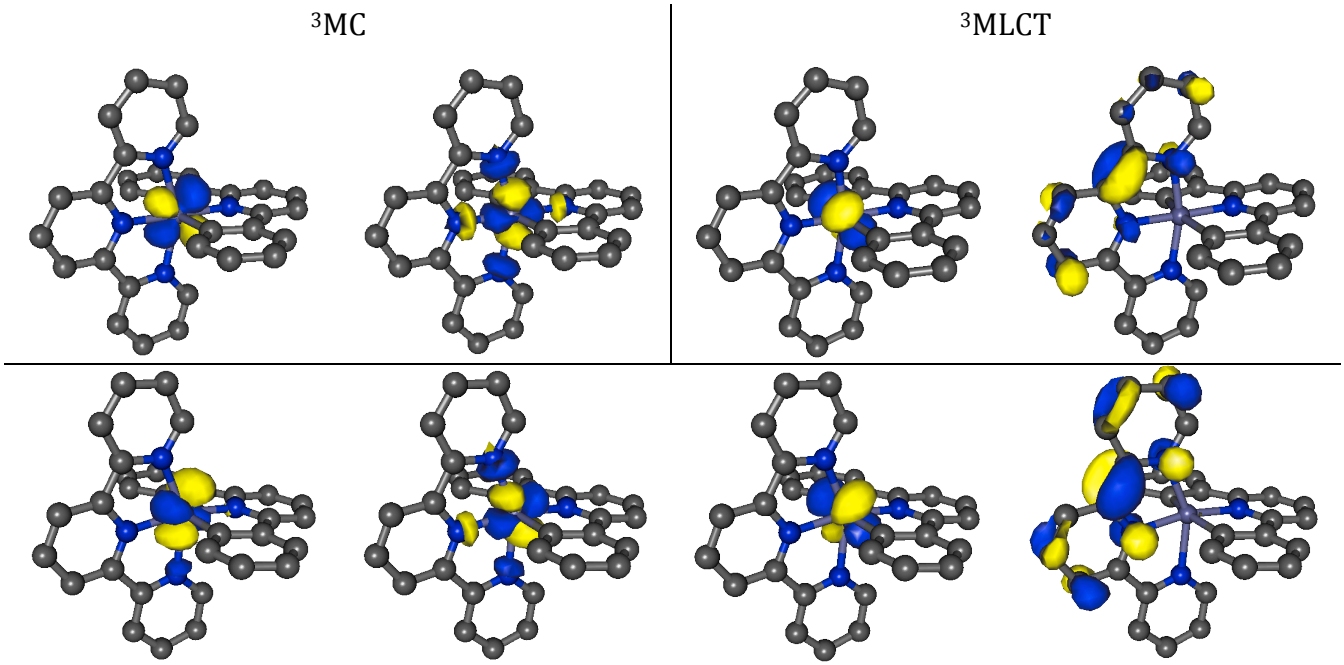
5. Fe-Ph π bonding interactions in ground state Kohn-Sham orbitals

		covalent Fe-Ph π interaction
Fe(tpy)(NCN)⁺ **2**	HO-4	
Fe(tpy)(NNC)⁺ **3**	HO-4	
Fe(tpy)(CNC) **4**	HO-6	
$Fe(NCN)_2$ **5**	HO-6 HO-7	
Fe(NCN)(NNC) **6**	HO-5	
$Fe(NNC)_2$ **7**	HO-3	

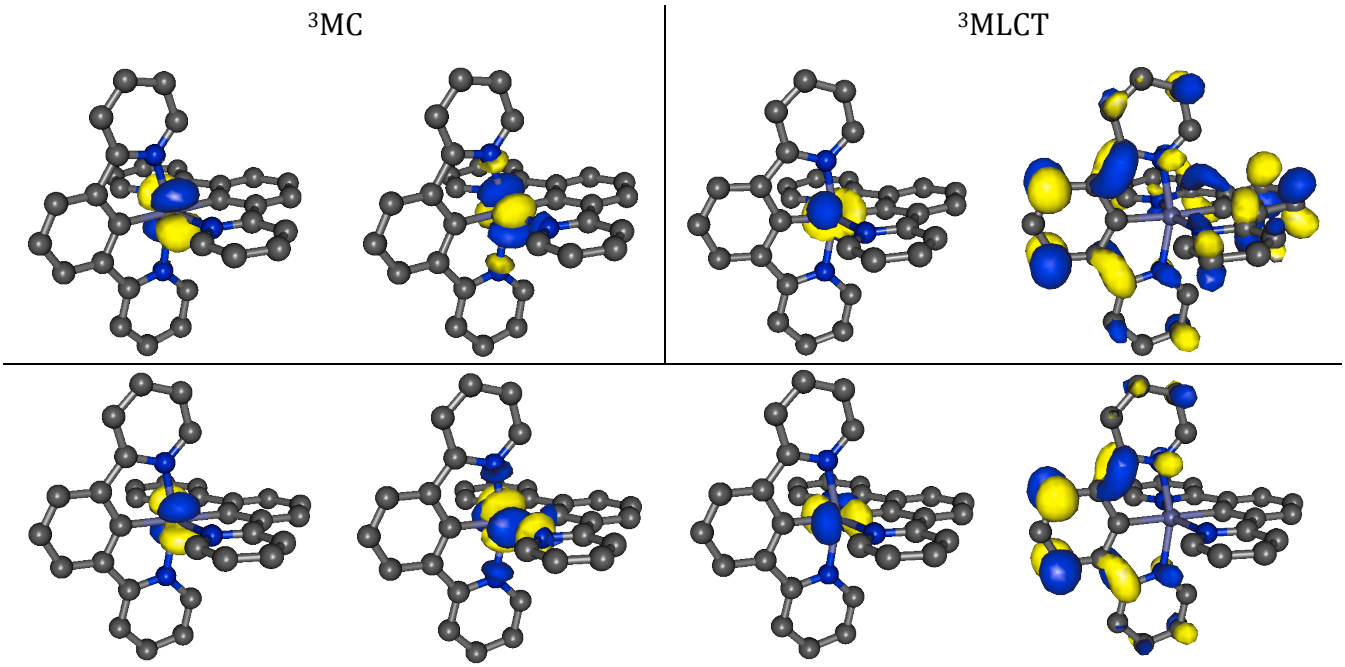
6. Orbital parentage (UNOs) between the ^{5}MLCT states and the ^{3}MLCT/^{3}MC states.

Natural SOMO / SOMO+1 for the triplet states and SOMO / SOMO+1 / SOMO+2 / SOMO+3 for the quintet states of complexes **4**-**7**.

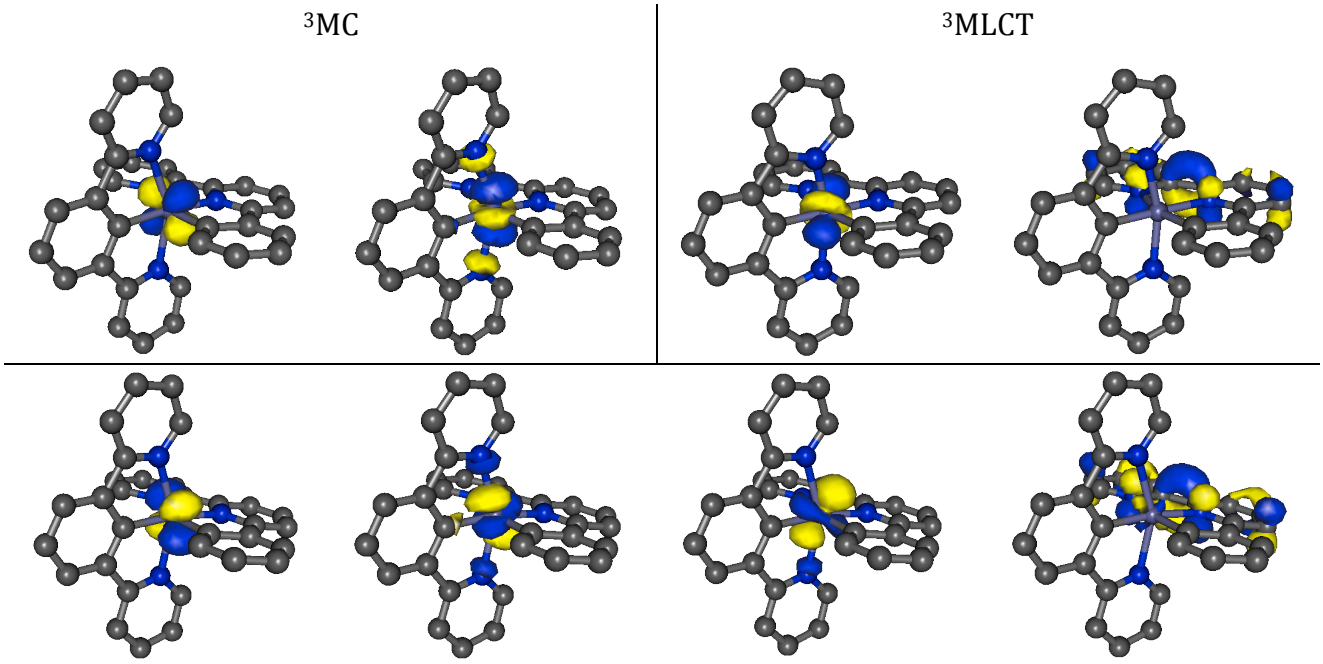
Fe(tpy)(CNC) 4



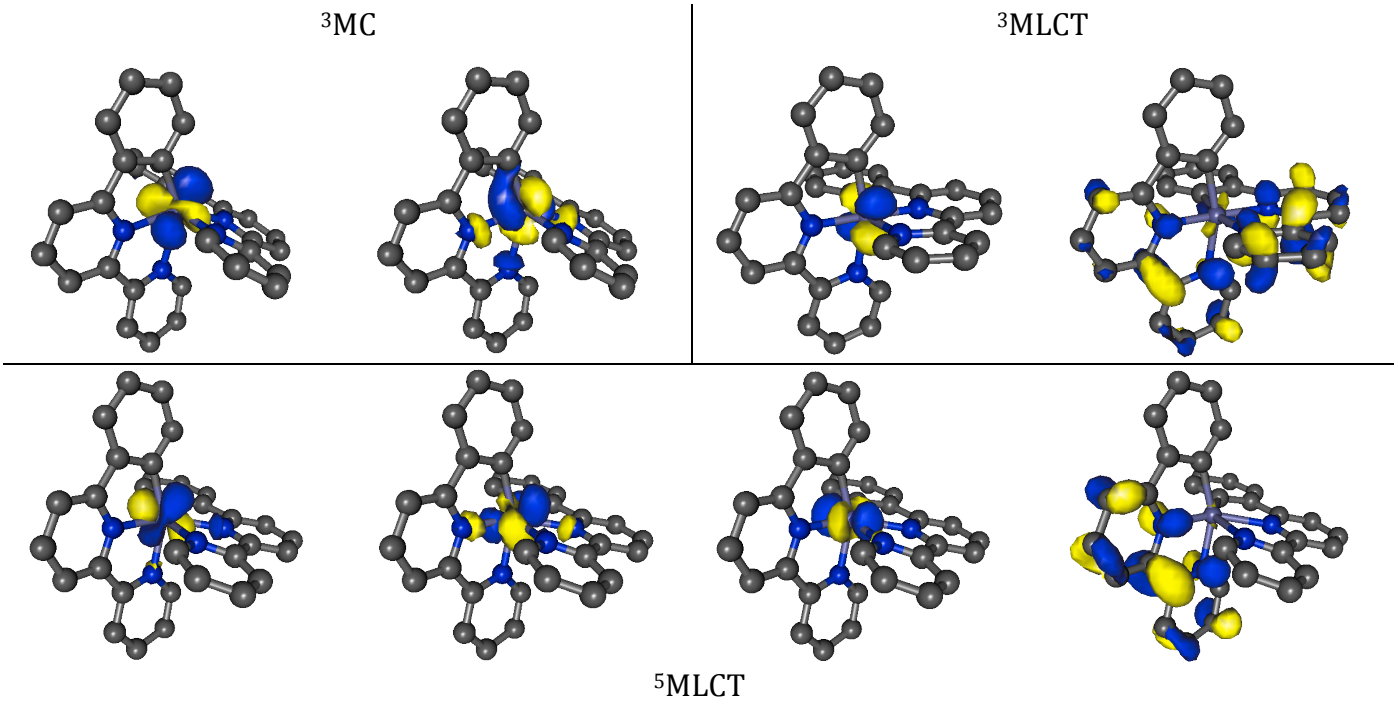
Fe(NCN)$_2$ 5



Fe(NCN)(NNC) 6

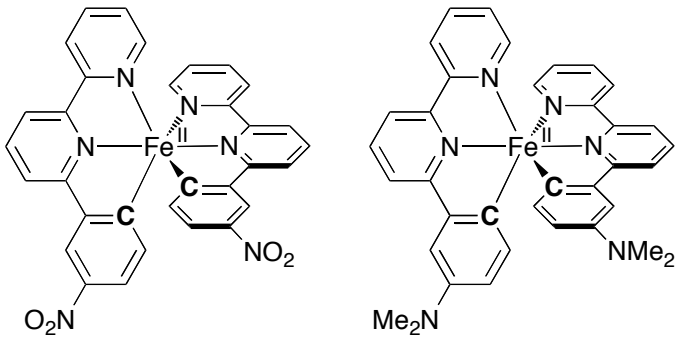


Fe(NNC)$_2$ 7



7. $Fe(NNC)_2$ derivatives

Ground, ^{3}MLCT and ^{3}MC states were optimized following the same procedure as described in the Computational details.



7a **7b**

Eigenvalues (eV) for selected ground state orbitals

	7	**7a**	**7b**
HOMO	–4.15	–4.89	–3.65
LUMO	–1.96	–2.56	–1.75
d_σ*	+0.95	+0.43	+1.21

Absolute energies (au) and energy gaps (eV)

	7	**7a**	**7b**
GS	-2729.109768	-3138.389312	-2997.006452
^{3}MLCT	-2729.083056	-3138.356633	-2996.984256
^{3}MC[a]	-2729.064505	-3138.340601	-
GS-^{3}MLCT	0.73	0.89	0.60
GS-^{3}MC[a]	1.23	1.32	-
^{3}MLCT-^{3}MC[a]	0.50	0.43	-

[a] ^{3}MC energy uncorrected for spin contamination

8. Cartesian coordinates

$Fe(tpy)_2^{2+}$ 1

GS				^{3}MC				^{5}MC			
Fe	5.442593	8.549498	4.751188	Fe	5.448013	8.547635	4.751167	Fe	5.436714	8.701228	4.823648
N	4.644908	6.747156	4.780257	N	4.592214	6.623243	4.850851	N	4.852127	6.752031	4.016622
N	5.245670	8.350327	6.611918	N	5.248281	8.348617	6.640133	N	3.932582	9.097065	3.364932
N	6.174569	10.288825	5.321230	N	6.212627	10.393233	5.415141	N	5.245506	10.862423	4.750010
N	3.692466	9.361224	4.346983	N	3.589718	9.407974	4.257684	N	7.281824	8.718562	3.687125
N	5.641592	8.754043	2.892158	N	5.651361	8.761547	2.865190	N	6.934538	7.924908	6.132314
N	7.252604	7.795654	4.555144	N	7.375622	7.748992	4.477912	N	4.470482	8.432857	6.746816
C	4.363772	5.977814	3.731255	C	4.282358	5.811257	3.846420	C	5.374957	5.594828	4.406071
H	4.607853	6.392100	2.760756	H	4.507631	6.178868	2.851155	H	6.165761	5.654154	5.146284
C	3.793805	4.722234	3.858289	C	3.705680	4.567815	4.044343	C	4.949628	4.372716	3.910065
H	3.583643	4.134651	2.974285	H	3.467198	3.937038	3.198042	H	5.405097	3.455457	4.259197
C	3.503546	4.245219	5.126792	C	3.445334	4.160577	5.344011	C	3.937470	4.362337	2.964426
H	3.058022	3.267366	5.260945	H	2.995282	3.194737	5.538637	H	3.575862	3.428952	2.551253
C	3.792171	5.040278	6.224378	C	3.765977	5.003919	6.395969	C	3.390810	5.567244	2.551050
H	3.579295	4.700058	7.229228	H	3.570537	4.705979	7.417140	H	2.599749	5.581393	1.813254
C	4.361860	6.285020	6.020314	C	4.339698	6.234406	6.114108	C	3.871372	6.746576	3.099353
C	4.713488	7.220274	7.090595	C	4.717712	7.218119	7.137505	C	3.355655	8.078752	2.725746
C	4.548456	7.043919	8.456094	C	4.557092	7.048824	8.504631	C	2.355260	8.304980	1.789310
H	4.115506	6.133205	8.848252	H	4.127899	6.137851	8.898501	H	1.883461	7.485077	1.266886
C	4.949012	8.065967	9.306743	C	4.952750	8.068149	9.356118	C	1.972328	9.612432	1.534539
H	4.828050	7.954718	10.377348	H	4.834009	7.958867	10.427105	H	1.193609	9.816217	0.809283
C	5.502781	9.230686	8.791049	C	5.499268	9.228922	8.831322	C	2.585161	10.660062	2.204489
H	5.817464	10.032058	9.446101	H	5.811478	10.033056	9.483361	H	2.292127	11.681836	2.007846
C	5.639921	9.343648	7.415803	C	5.636992	9.343209	7.456196	C	3.577329	10.361237	3.127526
C	6.186827	10.472948	6.661947	C	6.191114	10.509311	6.755749	C	4.322829	11.365355	3.913571
C	6.677369	11.632627	7.236532	C	6.658081	11.647593	7.394523	C	4.103568	12.729880	3.805968
H	6.675913	11.747117	8.313117	H	6.635356	11.725290	8.473687	H	3.359122	13.117478	3.124696
C	7.166340	12.635530	6.414898	C	7.155050	12.688329	6.626159	C	4.854497	13.595323	4.586261
H	7.555728	13.552051	6.840794	H	7.524532	13.588509	7.102280	H	4.698313	14.665351	4.518800
C	7.147968	12.445124	5.042344	C	7.172313	12.563525	5.245364	C	5.804723	13.072519	5.447810
H	7.517776	13.202983	4.363978	H	7.550805	13.356082	4.612876	H	6.414285	13.711505	6.073630
C	6.643976	11.257283	4.538829	C	6.689467	11.393360	4.683131	C	5.966218	11.697036	5.492334
H	6.611347	11.064162	3.473953	H	6.680259	11.242649	3.609256	H	6.701903	11.240762	6.146372
C	2.717928	9.639719	5.209294	C	2.576612	9.692215	5.067859	C	7.385165	9.192578	2.450276
H	2.916172	9.391364	6.244485	H	2.723504	9.450136	6.114680	H	6.481416	9.619205	2.027528
C	1.518323	10.212431	4.820341	C	1.398548	10.263135	4.615343	C	8.566073	9.152502	1.727314
H	0.757313	10.422192	5.560592	H	0.596910	10.480337	5.309209	H	8.601829	9.549835	0.721564
C	1.320999	10.506736	3.480652	C	1.278851	10.546081	3.263345	C	9.686015	8.597162	2.325217
H	0.394866	10.956157	3.143843	H	0.373201	10.994098	2.872495	H	10.629281	8.549389	1.794712
C	2.330038	10.218284	2.575969	C	2.332487	10.250166	2.413385	C	9.585288	8.104891	3.616603
H	2.211101	10.435759	1.522487	H	2.259743	10.463276	1.355349	H	10.448535	7.675363	4.106640
C	3.503051	9.647051	3.037973	C	3.478715	9.678710	2.944251	C	8.365187	8.180176	4.270246
C	4.642045	9.296411	2.188571	C	4.658332	9.315515	2.148981	C	8.153232	7.690552	5.645089
C	4.759575	9.468222	0.817618	C	4.787094	9.502944	0.780895	C	9.105313	7.023433	6.406807
H	3.952788	9.903872	0.243513	H	3.984088	9.947660	0.209438	H	10.094182	6.827276	6.017708
C	5.937076	9.067557	0.199913	C	5.961599	9.110655	0.158496	C	8.755763	6.605835	7.681345
H	6.054732	9.192339	-0.869665	H	6.084871	9.250183	-0.908546	H	9.478195	6.081350	8.295251
C	6.964637	8.507072	0.947321	C	6.977797	8.538246	0.907188	C	7.481255	6.854609	8.172034
H	7.885964	8.192103	0.476155	H	7.900274	8.227127	0.437088	H	7.199560	6.526057	9.162692
C	6.782042	8.360823	2.314215	C	6.793107	8.373004	2.271798	C	6.583267	7.528177	7.356717
C	7.720091	7.795217	3.285352	C	7.772328	7.780530	3.192310	C	5.191769	7.861991	7.725119
C	8.969201	7.291657	2.966045	C	9.004128	7.280481	2.798252	C	4.655727	7.625616	8.980362
H	9.312286	7.304929	1.939943	H	9.305874	7.310065	1.760021	H	5.254216	7.172943	9.759272
C	9.762864	6.772113	3.976189	C	9.841989	6.736893	3.759258	C	3.340513	7.990037	9.227640
H	10.743103	6.370620	3.750843	H	10.808367	6.338132	3.475733	H	2.901980	7.817372	10.202890
C	9.280481	6.773849	5.275364	C	9.427806	6.708062	5.082333	C	2.601335	8.579936	8.215352
H	9.866384	6.377311	6.094070	H	10.054748	6.291427	5.859732	H	1.573373	8.881347	8.368966
C	8.021280	7.295502	5.519415	C	8.182440	7.227312	5.394845	C	3.211573	8.781726	6.988057
H	7.603187	7.316953	6.518483	H	7.808697	7.228136	6.413070	H	2.676621	9.239944	6.162462

$Fe(tpy)(NCN)^+$ 2

GS	^{3}MLCT	^{3}MC	^{5}MC
Fe 5.432603 8.550271 4.748035	Fe 5.385528 8.538833 4.742432	Fe 5.429934 8.547096 4.755875	Fe 5.236862 8.856992 4.751866
N 4.636839 6.758497 4.794284	N 4.587525 6.750102 4.831436	N 4.576684 6.625401 4.862599	N 4.409002 6.862865 4.987148

N 5.239912 8.347768 6.621644	N 5.188979 8.374855 6.627111	N 5.244564 8.335228 6.640406	N 5.372027 8.331555 6.872452
N 6.157269 10.276787 5.330696	N 6.133200 10.293051 5.285857	N 6.180358 10.388885 5.441573	N 5.841393 10.639977 5.821711
N 3.678905 9.372318 4.306290	N 3.625865 9.315934 4.247430	N 3.566387 9.408279 4.231033	N 3.409110 9.808927 3.866658
C 5.637505 8.750639 2.908230	C 5.636203 8.779255 2.890576	C 5.633262 8.760965 2.888790	C 5.579438 8.767183 2.752608
N 7.258314 7.793899 4.532054	N 7.191219 7.737722 4.528447	N 7.371882 7.763005 4.460835	N 7.317299 7.844949 4.547694
C 4.345140 5.995466 3.740906	C 4.271588 5.984550 3.781962	C 4.258216 5.828789 3.846760	C 3.914712 6.191750 3.954112
H 4.584001 6.426891 2.776652	H 4.481537 6.418498 2.811682	H 4.475380 6.223436 2.859965	H 3.843005 6.750712 3.026632
C 3.777691 4.739508 3.866879	C 3.719085 4.730965 3.916014	C 3.688833 4.582706 4.032919	C 3.532470 4.862773 4.044650
H 3.559506 4.159423 2.979914	H 3.480452 4.151210 3.034867	H 3.442341 3.964031 3.180198	H 3.132223 4.354324 3.177160
C 3.500586 4.250253 5.134681	C 3.479466 4.237048 5.202696	C 3.445468 4.154718 5.332582	C 3.675306 4.213183 5.260053
H 3.058206 3.270551 5.265234	H 3.047140 3.254088 5.342048	H 3.001259 3.184188 5.517264	H 3.386121 3.175121 5.369760
C 3.798132 5.036397 6.234089	C 3.796880 5.015914 6.291276	C 3.773790 4.979851 6.392013	C 4.196634 4.910065 6.338306
H 3.596346 4.690922 7.239500	H 3.621235 4.667217 7.300670	H 3.591860 4.667933 7.411634	H 4.319576 4.426553 7.298278
C 4.363849 6.285059 6.033756	C 4.352638 6.279936 6.094617	C 4.341493 6.220754 6.125236	C 4.554154 6.238666 6.163523
C 4.720922 7.211803 7.106568	C 4.725956 7.199028 7.137606	C 4.727593 7.190035 7.149020	C 5.130045 7.074803 7.233054
C 4.577705 7.026137 8.473099	C 4.684319 7.015560 8.504392	C 4.596256 7.006905 8.514528	C 5.436941 6.631719 8.516014
H 4.155809 6.109887 8.864870	H 4.312507 6.089172 8.923242	H 4.180337 6.086581 8.902167	H 5.246199 5.610129 8.813665
C 4.986535 8.044207 9.325299	C 5.142493 8.042455 9.336334	C 5.001892 8.016660 9.377255	C 6.005645 7.530898 9.402824
H 4.882990 7.925647 10.396692	H 5.116998 7.915983 10.410839	H 4.904943 7.893165 10.448187	H 6.259491 7.212741 10.406594
C 5.528860 9.213669 8.806973	C 5.656982 9.224580 8.787482	C 5.532830 9.186920 8.850427	C 6.257737 8.837406 9.006975
H 5.853328 10.012072 9.461139	H 6.038376 10.007834 9.429775	H 5.855567 9.986154 9.504182	H 6.709243 9.543122 9.690869
C 5.644480 9.335529 7.430731	C 5.681492 9.369955 7.417478	C 5.644846 9.322782 7.477764	C 5.921285 9.205383 7.710836
C 6.181031 10.463741 6.672142	C 6.195043 10.473132 6.642895	C 6.179959 10.492556 6.784221	C 6.141738 10.544256 7.124507
C 6.674681 11.625892 7.242384	C 6.720294 11.646008 7.182037	C 6.656475 11.633348 7.419956	C 6.612568 11.629341 7.846406
H 6.680944 11.738577 8.319198	H 6.759231 11.762595 8.257762	H 6.651958 11.702340 8.500074	H 6.844563 11.531690 8.898604
C 7.153826 12.628011 6.416886	C 7.178969 12.636487 6.343560	C 7.134394 12.676886 6.649546	C 6.774083 12.843173 7.196985
H 7.545411 13.545609 6.838370	H 7.590289 13.551429 6.751894	H 7.509778 13.575642 7.123952	H 7.139590 13.707019 7.738817
C 7.122945 12.435357 5.043901	C 7.105149 12.445170 4.960696	C 7.127502 12.561376 5.264684	C 6.458728 12.936266 5.851309
H 7.485008 13.193043 4.361247	H 7.450807 13.198821 4.266184	H 7.491779 13.359084 4.630570	H 6.568675 13.866155 5.308738
C 6.618186 11.247793 4.542728	C 6.578899 11.265776 4.483663	C 6.640045 11.394948 4.704205	C 5.991909 11.803809 5.202528
H 6.572435 11.042693 3.480583	H 6.502546 11.066345 3.422310	H 6.607385 11.238354 3.631463	H 5.727932 11.812965 4.150075
C 2.713813 9.650044 5.182163	C 2.640773 9.519180 5.119559	C 2.567714 9.681930 5.064153	C 2.387611 10.349634 4.521810
H 2.927597 9.393968 6.213140	H 2.841765 9.197632 6.133912	H 2.743198 9.435023 6.106079	H 2.444642 10.313402 5.605957
C 1.511220 10.227396 4.820551	C 1.443500 10.104770 4.753271	C 1.376827 10.244697 4.643758	C 1.300416 10.928298 3.890956
H 0.763065 10.434499 5.574168	H 0.668885 10.255098 5.493268	H 0.589834 10.453362 5.356325	H 0.490853 11.351461 4.471411
C 1.298538 10.529524 3.481965	C 1.268379 10.487136 3.430236	C 1.229016 10.530967 3.292286	C 1.287685 10.940415 2.503570
H 0.368680 10.984001 3.161217	H 0.341736 10.949535 3.111660	H 0.311284 10.974108 2.923535	H 0.457533 11.381536 1.964136
C 2.290972 10.244518 2.563553	C 2.288365 10.271824 2.520982	C 2.263332 10.247145 2.420180	C 2.349108 10.383320 1.813915
H 2.163249 10.467096	H 2.185285 10.556813	H 2.175666 10.460513	H 2.363535 10.388623

1.511835	1.481978	1.362692	0.731800
C 3.478945 9.665418 2.992624	C 3.467425 9.680296 2.949913	C 3.433532 9.680890 2.913984	C 3.409647 9.817832 2.516771
C 4.613219 9.312533 2.152334	C 4.634091 9.372000 2.136757	C 4.607712 9.322951 2.126416	C 4.587323 9.199050 1.877292
C 4.761607 9.473099 0.776853	C 4.834813 9.598310 0.776971	C 4.760931 9.493079 0.752171	C 4.722702 9.010005 0.501392
H 3.973475 9.906442 0.169514	H 4.065052 10.054510 0.163752	H 3.967727 9.926925 0.152562	H 3.958637 9.332640 -0.197708
C 5.949796 9.067452 0.172543	C 6.046205 9.226370 0.199974	C 5.946482 9.101916 0.140513	C 5.860461 8.378637 0.014393
H 6.072150 9.191455 -0.896616	H 6.207080 9.400557 -0.856751	H 6.068819 9.235701 -0.927357	H 5.971525 8.225358 -1.052511
C 6.984057 8.505193 0.918118	C 7.053710 8.630298 0.954217	C 6.976670 8.539445 0.885931	C 6.852395 7.927944 0.877505
H 7.898254 8.198948 0.419979	H 7.985809 8.346179 0.477889	H 7.894105 8.239564 0.390916	H 7.718242 7.424144 0.462171
C 6.819333 8.348929 2.292271	C 6.841285 8.406786 2.312581	C 6.816931 8.369338 2.259307	C 6.703857 8.120063 2.251361
C 7.747974 7.788455 3.262574	C 7.736814 7.802280 3.287592	C 7.793034 7.791741 3.176783	C 7.665413 7.637906 3.262551
C 9.010416 7.278045 2.986406	C 9.011870 7.311324 3.049371	C 9.044286 7.294817 2.828251	C 8.858436 6.991906 2.945217
H 9.369935 7.288604 1.965546	H 9.425581 7.375210 2.051364	H 9.362903 7.324585 1.794530	H 9.128155 6.835206 1.909497
C 9.780194 6.765237 4.013100	C 9.726032 6.745325 4.089897	C 9.859621 6.765934 3.811644	C 9.692979 6.556421 3.957738
H 10.765514 6.362751 3.810891	H 10.722228 6.355379 3.919185	H 10.836425 6.372844 3.555631	H 10.622901 6.053274 3.720160
C 9.271906 6.772427 5.305305	C 9.152256 6.679544 5.352037	C 9.415081 6.741326 5.127851	C 9.322788 6.772320 5.276764
H 9.838164 6.380690 6.139644	H 9.676008 6.240925 6.190563	H 10.024469 6.335237 5.924111	H 9.943361 6.449544 6.102412
C 8.010441 7.296668 5.513236	C 7.879760 7.188613 5.527053	C 8.160568 7.253670 5.401484	C 8.124071 7.423207 5.512797
H 7.571400 7.324307 6.503910	H 7.380224 7.166624 6.487986	H 7.758039 7.261404 6.409292	H 7.793828 7.613405 6.529710

Fe(tpy)(NNC)⁺ 3

GS	^{3}MLCT	^{3}MC	^{5}MC
Fe 5.353748 8.591769 4.770837	Fe 5.315482 8.591258 4.809674	Fe 5.341380 8.599655 4.654841	Fe 5.691579 8.218516 4.745594
N 4.598217 6.796601 4.780269	N 4.556702 6.797760 4.832250	N 4.265616 6.707432 4.873001	N 4.639931 6.345950 5.213012
N 5.196143 8.375007 6.599418	N 5.046912 8.434503 6.644569	N 5.243153 8.351444 6.602419	N 5.045123 8.366513 6.797754
N 6.110347 10.297512 5.324738	N 6.044168 10.339399 5.326089	N 5.923395 10.554346 5.442504	N 6.222411 10.235422 5.422486
N 3.602921 9.418829 4.284204	N 3.478137 9.411601 4.192122	N 3.568416 9.443310 4.085527	N 3.672384 9.197223 4.219426
N 5.587367 8.783352 2.890710	N 5.568415 8.815974 2.890229	N 5.614767 8.800389 2.776614	N 5.751021 8.862563 2.699993
C 7.140707 7.836094 4.645842	C 7.057876 7.788775 4.674422	C 7.152869 7.816653 4.575440	C 7.485930 7.415152 4.108265
C 4.330810 6.032111 3.721935	C 4.266919 6.042813 3.768893	C 3.873840 5.912965 3.885304	C 4.596455 5.322303 4.369024
H 4.549058 6.473329 2.757630	H 4.437086 6.505239 2.804447	H 3.842261 6.364682 2.898754	H 4.941999 5.527674 3.362192
C 3.819949 4.752912 3.836466	C 3.790880 4.756325 3.879274	C 3.527392 4.588254 4.085639	C 4.154895 4.063260 4.744395
H 3.623003 4.172747 2.944637	H 3.567310 4.186400 2.987717	H 3.210201 3.974373 3.252783	H 4.133727 3.257833 4.021841
C 3.575923 4.236910 5.101551	C 3.612198 4.214641 5.154843	C 3.599615 4.076577 5.374143	C 3.755095 3.867683 6.056425
H 3.179361 3.236953 5.224214	H 3.242273 3.204158 5.275650	H 3.344453 3.042510 5.571659	H 3.411488 2.896052 6.389930
C 3.853560 5.021593 6.205791	C 3.912522 4.980882 6.257486	C 4.010598 4.900813 6.406538	C 3.811645 4.930422 6.943680
H 3.684438 4.655089 7.209726	H 3.785611 4.595583 7.260597	H 4.091403 4.519789 7.415388	H 3.526423 4.798880 7.978991
C 4.363873 6.295854 6.015550	C 4.386837 6.279446 6.079446	C 4.335739 6.220968 6.117805	C 4.260597 6.159881 6.484625
C 4.723540 7.216191 7.085866	C 4.760584 7.187814 7.129321	C 4.798760 7.189886 7.115770	C 4.384479 7.349258 7.349674

C 4.651077 6.998584 8.452351	C 4.912960 6.909994 8.470987	C 4.793680 6.954977 8.483075	C 3.842417 7.451619 8.622872
H 4.269223 6.062535 8.838041	H 4.667084 5.927726 8.852789	H 4.419637 6.018252 8.872145	H 3.293058 6.629199 9.060183
C 5.086170 7.999469 9.310416	C 5.430857 7.895967 9.313817	C 5.259135 7.939137 9.338109	C 4.001285 8.644327 9.311785
H 5.039180 7.852812 10.382124	H 5.564340 7.692764 10.368090	H 5.255452 7.782074 10.409538	H 3.582782 8.757454 10.304293
C 5.595472 9.182700 8.792356	C 5.851575 9.116855 8.777860	C 5.723802 9.129443 8.804498	C 4.683335 9.695536 8.723636
H 5.957064 9.965116 9.446281	H 6.338230 9.853605 9.403911	H 6.086707 9.917556 9.449910	H 4.798776 10.635467 9.245666
C 5.643364 9.341308 7.416702	C 5.680017 9.358549 7.432546	C 5.706886 9.306315 7.428967	C 5.200240 9.520137 7.444450
C 6.173244 10.471017 6.665701	C 6.163176 10.486310 6.676527	C 6.184804 10.517403 6.754567	C 5.934759 10.553774 6.692965
C 6.718231 11.611730 7.233238	C 6.723566 11.639358 7.222159	C 6.874204 11.542243 7.391523	C 6.327681 11.762067 7.252312
H 6.756893 11.710463 8.310700	H 6.806789 11.732915 8.297404	H 7.098319 11.484958 8.448283	H 6.096263 11.994869 8.282954
C 7.212383 12.604008 6.406603	C 7.160849 12.641163 6.385451	C 7.290862 12.628342 6.642972	C 7.037214 12.660454 6.473375
H 7.646904 13.502973 6.825791	H 7.600366 13.542227 6.795349	H 7.835267 13.438155 7.113523	H 7.357668 13.608442 6.887331
C 7.146986 12.421929 5.032392	C 7.032019 12.480713 5.003252	C 7.012250 12.661943 5.283540	C 7.336012 12.323790 5.162317
H 7.526275 13.168918 4.347373	H 7.364655 13.243611 4.312495	H 7.322961 13.494637 4.665739	H 7.891221 12.995092 4.519797
C 6.591138 11.257507 4.535745	C 6.473816 11.317270 4.524326	C 6.326620 11.596125 4.727329	C 6.908150 11.097298 4.680536
H 6.530289 11.064391 3.472486	H 6.364103 11.137653 3.462475	H 6.089307 11.563456 3.668643	H 7.120041 10.783168 3.665049
C 2.609330 9.713422 5.119826	C 2.454781 9.687998 4.988396	C 2.537390 9.730004 4.878226	C 2.621297 9.281571 5.027438
H 2.787380 9.473254 6.161535	H 2.580209 9.395820 6.025404	H 2.669528 9.480133 5.924587	H 2.716133 8.789438 5.987573
C 1.423544 10.288152 4.698217	C 1.306812 10.310403 4.524650	C 1.373027 10.306915 4.408610	C 1.457961 9.952662 4.692886
H 0.646410 10.510923 5.417582	H 0.490965 10.520388 5.203916	H 0.562156 10.523341 5.091808	H 0.630436 9.989347 5.389810
C 1.261202 10.568157 3.349197	C 1.234546 10.652348 3.182801	C 1.273751 10.599316 3.053511	C 1.388109 10.564940 3.450838
H 0.346446 11.019468 2.984847	H 0.353198 11.142492 2.786926	H 0.375992 11.053658 2.652211	H 0.496078 11.098873 3.146023
C 2.288552 10.263132 2.473969	C 2.303677 10.363097 2.350701	C 2.337536 10.302615 2.223015	C 2.476249 10.480236 2.602341
H 2.199001 10.468404 1.415251	H 2.277353 10.621932 1.300531	H 2.293673 10.517055 1.163306	H 2.442867 10.940317 1.624758
C 3.448669 9.688989 2.970504	C 3.416287 9.738275 2.891664	C 3.475321 9.722218 2.768849	C 3.608433 9.786815 3.017101
C 4.605628 9.319004 2.154894	C 4.616712 9.371006 2.131067	C 4.663511 9.353455 2.008534	C 4.806248 9.635939 2.172454
C 4.735756 9.472550 0.785237	C 4.801857 9.542391 0.770647	C 4.851422 9.524254 0.643858	C 4.969268 10.237665 0.932519
H 3.937235 9.902583 0.196231	H 4.028285 9.983849 0.157580	H 4.077713 9.967115 0.031617	H 4.202976 10.871166 0.508083
C 5.922923 9.054268 0.192874	C 6.005562 9.120635 0.213955	C 6.053110 9.109671 0.091703	C 6.155608 10.009772 0.251698
H 6.057725 9.160843 -0.876966	H 6.178113 9.241064 -0.848962	H 6.230010 9.229545 -0.970408	H 6.320411 10.467445 -0.716331
C 6.930785 8.502024 0.963671	C 6.976926 8.541580 1.008920	C 7.030373 8.540508 0.896878	C 7.130258 9.202643 0.810308
H 7.858266 8.172029 0.515361	H 7.913662 8.200838 0.589364	H 7.972723 8.213364 0.479095	H 8.061920 9.027706 0.290081
C 6.742894 8.369804 2.339117	C 6.734152 8.392142 2.373804	C 6.790688 8.391018 2.256088	C 6.904148 8.625215 2.059921
C 7.649666 7.819987 3.328504	C 7.600943 7.805628 3.377471	C 7.676329 7.819865 3.264751	C 7.847610 7.769513 2.792461
C 8.910848 7.309464 3.024052	C 8.863617 7.277425 3.115785	C 8.936363 7.307108 2.972791	C 9.035804 7.327116 2.209384
H 9.273434 7.309286 2.001383	H 9.269559 7.292550 2.110150	H 9.318048 7.318485 1.957442	H 9.296359 7.597757 1.192140
C 9.699276 6.799436 4.039152	C 9.598316 6.732950 4.153326	C 9.706780 6.774450 3.994201	C 9.894272 6.516755 2.932280
H 10.680758 6.398194 3.818685	H 10.581474 6.320471 3.963927	H 10.688850 6.371126 3.779113	H 10.817129 6.168160 2.484893
C 9.220858 6.804616	C 9.070747 6.716089	C 9.213698 6.759095	C 9.563536 6.150032

5.346584	5.441192	5.293000	4.231259
H 9.840110 6.403772 6.142059	H 9.651584 6.288325 6.250758	H 9.818509 6.340902 6.090295	H 10.236157 5.514729 4.798109
C 7.961898 7.316370 5.641312	C 7.808152 7.237474 5.701296	C 7.951786 7.276117 5.574465	C 8.375249 6.596600 4.801024
H 7.621393 7.302489 6.673510	H 7.415058 7.212523 6.712542	H 7.594812 7.248536 6.600249	H 8.146255 6.289243 5.818399

Fe(tpy)(CNC) 4

GS	^{3}MLCT	^{3}MC	^{5}MLCT
Fe 5.428482 8.550449 4.821167	Fe 5.425719 8.542362 4.794810	Fe 5.453838 8.552235 4.704508	Fe 5.676387 8.708695 4.749048
N 4.649703 6.789930 4.815476	N 4.638640 6.770557 4.841826	N 4.575413 6.616683 4.893953	N 3.583508 7.970312 4.762506
N 5.244720 8.351525 6.610136	N 5.240987 8.349658 6.642717	N 5.245085 8.344406 6.647606	N 5.824483 6.696219 4.816136
N 6.147211 10.252837 5.353106	N 6.164112 10.288432 5.291236	N 6.212145 10.391255 5.471915	N 7.762237 8.426618 4.768813
C 3.692839 9.363927 4.383336	C 3.637396 9.285805 4.365318	C 3.709639 9.367956 4.242258	C 5.506009 9.048429 6.712154
N 5.640243 8.756440 2.897334	N 5.651553 8.782345 2.892295	N 5.666168 8.774011 2.721089	N 5.088731 10.581023 4.683440
C 7.233577 7.797615 4.604092	C 7.215736 7.708563 4.590701	C 7.273123 7.800582 4.447807	C 5.521709 8.915246 2.765791
C 4.364750 6.037737 3.747725	C 4.348290 6.012032 3.785886	C 4.262828 5.806058 3.887202	C 2.491045 8.722269 4.730151
H 4.605172 6.481551 2.790430	H 4.584915 6.445941 2.822698	H 4.488700 6.184029 2.894876	H 2.656161 9.794365 4.694727
C 3.803699 4.782685 3.850157	C 3.783695 4.758761 3.910046	C 3.688745 4.566356 4.077117	C 1.217376 8.186626 4.739619
H 3.593896 4.216902 2.951768	H 3.565056 4.178994 3.023106	H 3.449265 3.940121 3.227672	H 0.351436 8.835287 4.711136
C 3.518421 4.267734 5.112080	C 3.508370 4.270032 5.182021	C 3.429393 4.152316 5.383889	C 1.089548 6.803943 4.785855
H 3.079084 3.284115 5.222399	H 3.066376 3.289644 5.311456	H 2.979923 3.185440 5.576213	H 0.109414 6.341767 4.795108
C 3.805318 5.036264 6.220815	C 3.805113 5.053517 6.279562	C 3.749860 4.988889 6.430829	C 2.227021 6.021698 4.819830
H 3.600654 4.678823 7.221807	H 3.607723 4.715707 7.288094	H 3.558338 4.692092 7.453473	H 2.153420 4.943114 4.856023
C 4.369706 6.293849 6.045903	C 4.371408 6.306345 6.083330	C 4.326692 6.230531 6.157753	C 3.474556 6.638551 4.806270
C 4.720329 7.209180 7.109760	C 4.729380 7.233887 7.145436	C 4.703844 7.208392 7.164575	C 4.750057 5.906885 4.835638
C 4.574973 7.029261 8.474021	C 4.583801 7.048151 8.516434	C 4.538332 7.044084 8.526354	C 4.840956 4.529458 4.877129
H 4.149192 6.109817 8.855420	H 4.162801 6.138749 8.919850	H 4.102018 6.131411 8.910869	H 3.957312 3.908805 4.892871
C 4.978625 8.042165 9.335720	C 5.007909 8.107919 9.345789	C 4.930256 8.059877 9.393617	C 6.131768 3.955963 4.898095
H 4.870240 7.922563 10.406265	H 4.909422 8.012362 10.421179	H 4.803963 7.950726 10.463043	H 6.246824 2.879005 4.930144
C 5.523142 9.209338 8.813253	C 5.542945 9.257174 8.820972	C 5.483767 9.219554 8.860021	C 7.236993 4.761931 4.876698
H 5.847618 10.011780 9.463286	H 5.865216 10.062695 9.467858	H 5.795753 10.027296 9.509291	H 8.229304 4.330629 4.891474
C 5.646787 9.339608 7.441179	C 5.669204 9.387984 7.415399	C 5.631446 9.339584 7.491081	C 7.088078 6.164350 4.835043
C 6.178395 10.457342 6.693495	C 6.185184 10.465418 6.662540	C 6.186774 10.497110 6.812703	C 8.143536 7.109618 4.810241
C 6.675923 11.630606 7.247269	C 6.700968 11.661432 7.200756	C 6.664726 11.641966 7.453046	C 9.518977 6.786745 4.826683
H 6.684632 11.750599 8.323623	H 6.719159 11.790306 8.276087	H 6.639454 11.711436 8.533105	H 9.823813 5.749081 4.859484
C 7.149869 12.620842 6.412302	C 7.170850 12.637568 6.364633	C 7.165870 12.677252 6.694771	C 10.453642 7.784487 4.802346
H 7.543971 13.543883 6.819562	H 7.569946 13.557616 6.776035	H 7.540485 13.573945 7.174187	H 11.508898 7.536495 4.815536
C 7.110908 12.408765 5.036651	C 7.134092 12.440699 4.970651	C 7.184242 12.555993 5.304747	C 10.040019 9.132748 4.760700
H 7.468960 13.157962 4.342344	H 7.492494 13.189653 4.278455	H 7.566891 13.347380 4.673166	H 10.749099 9.948756 4.740468
C 6.605469 11.220557 4.553024	C 6.621808 11.250614 4.498974	C 6.696337 11.393940 4.744498	C 8.685349 9.382426 4.745582

H 6.554625 11.008317 3.493352	H 6.570322 11.042627 3.436984	H 6.683519 11.240160 3.670133	H 8.304783 10.399169 4.713582
C 2.640140 9.678503 5.241708	C 2.562824 9.526189 5.212446	C 2.655855 9.672865 5.100068	C 5.752865 8.196301 7.779696
H 2.734801 9.468546 6.304412	H 2.639612 9.257708 6.262391	H 2.754205 9.456902 6.160275	H 6.074054 7.177688 7.583031
C 1.466614 10.255391 4.770000	C 1.394295 10.112320 4.737647	C 1.480742 10.246850 4.628150	C 5.603786 8.631193 9.092878
H 0.663248 10.492185 5.461211	H 0.567016 10.299981 5.414908	H 0.675629 10.476180 5.319448	H 5.808934 7.953274 9.915153
C 1.309025 10.536972 3.414809	C 1.274611 10.465677 3.396047	C 1.323517 10.534484 3.274639	C 5.191566 9.932663 9.365038
H 0.392201 10.988500 3.053303	H 0.360978 10.922675 3.033440	H 0.405097 10.983472 2.914338	H 5.074085 10.262662 10.390681
C 2.332802 10.235287 2.534068	C 2.326923 10.232921 2.527209	C 2.349465 10.242112 2.393232	C 4.934368 10.805918 8.321506
H 2.220400 10.451598 1.475897	H 2.238739 10.508156 1.480920	H 2.237083 10.462994 1.336132	H 4.614174 11.822060 8.530719
C 3.505411 9.657703 3.018328	C 3.495467 9.650240 3.013585	C 3.524062 9.667263 2.875439	C 5.096477 10.366101 7.009823
C 4.639240 9.299082 2.181859	C 4.659358 9.354753 2.190002	C 4.655886 9.320773 2.026773	C 4.842502 11.208880 5.845173
C 4.763896 9.455795 0.804782	C 4.820714 9.590581 0.828876	C 4.779954 9.490017 0.650455	C 4.365217 12.515032 5.823853
H 3.953062 9.890063 0.235251	H 4.022315 10.050167 0.261865	H 3.971119 9.926791 0.080456	H 4.162930 13.035905 6.749555
C 5.936966 9.044618 0.190956	C 6.013651 9.222673 0.225863	C 5.956953 9.085325 0.039148	C 4.145193 13.118561 4.594119
H 6.055080 9.159280 -0.881113	H 6.159934 9.401843 -0.833548	H 6.074094 9.210262 -1.032081	H 3.773623 14.136487 4.558076
C 6.959692 8.486152 0.941903	C 7.018922 8.620650 0.967061	C 6.987334 8.521881 0.778128	C 4.376169 12.434189 3.409542
H 7.882274 8.158043 0.482281	H 7.952200 8.319773 0.510796	H 7.908140 8.203264 0.308933	H 4.183361 12.892329 2.449291
C 6.782669 8.349838 2.315517	C 6.809516 8.403880 2.324799	C 6.812845 8.372334 2.150518	C 4.852496 11.129356 3.479925
C 7.715755 7.790108 3.280540	C 7.717902 7.780808 3.278273	C 7.746748 7.808241 3.118357	C 5.114410 10.209495 2.376671
C 8.970646 7.282542 2.947347	C 8.974774 7.281098 2.942738	C 9.001667 7.309667 2.773742	C 4.957760 10.558011 1.036907
H 9.311790 7.289558 1.916719	H 9.340912 7.343639 1.922911	H 9.337064 7.327475 1.741487	H 4.638395 11.557125 0.757133
C 9.781727 6.766132 3.942939	C 9.756749 6.700585 3.927084	C 9.820604 6.788131 3.760662	C 5.216683 9.613750 0.057401
H 10.759361 6.367110 3.698560	H 10.737162 6.309455 3.681297	H 10.798730 6.396395 3.507039	H 5.101637 9.871846 -0.989017
C 9.330347 6.762207 5.260864	C 9.280089 6.622673 5.233235	C 9.377197 6.770148 5.080389	C 5.626237 8.333517 0.420202
H 9.966607 6.357123 6.041878	H 9.898771 6.169559 6.001299	H 10.019803 6.361572 5.853978	H 5.831525 7.599664 -0.352574
C 8.077189 7.271175 5.581296	C 8.022165 7.119534 5.556598	C 8.123048 7.269777 5.414092	C 5.771389 7.990735 1.760842
H 7.751737 7.253542 6.618909	H 7.667624 7.050937 6.581605	H 7.800147 7.243764 6.451306	H 6.090117 6.987427 2.028552

$Fe(NCN)_2$ 5

GS	^{3}MLCT	^{3}MC	^{5}MLCT	^{5}MC
Fe 6.261836 3.128757 5.140752	Fe 6.222558 3.033886 5.141391	Fe 6.262326 3.129888 5.141444	Fe 6.264268 3.129782 5.225724	Fe 6.138587 2.754138 5.147654
N 6.964699 1.309367 4.788795	N 6.873321 1.220574 4.741196	N 7.008033 1.173786 4.700169	N 7.026468 1.145982 4.726442	N 6.704112 0.725752 4.313695
C 6.262468 3.131228 3.260524	C 6.251156 3.104615 3.235136	C 6.264446 3.133434 3.238207	C 6.263146 3.132550 3.257401	C 6.345865 3.057894 3.112477
C 7.310106 0.428317 5.728121	C 7.118827 0.301395 5.668207	C 7.365495 0.251569 5.586461	C 7.387910 0.224658 5.610269	C 6.754352 -0.404960 5.003695
C 7.809382 -0.828767 5.438235	C 7.614371 -0.955469 5.359859	C 7.861098 -0.988475 5.222155	C 7.881993 -1.012049 5.230344	C 7.002062 -1.637314 4.421803
C 7.957328 -1.195094 4.106628	C 7.863867 -1.256064 4.023886	C 7.985740 -1.270509 3.866665	C 7.997273 -1.282134 3.873519	C 7.200450 -1.676651 3.049375
C 7.601069 -0.292817 3.122682	C 7.605682 -0.310384 3.053385	C 7.614542 -0.316991 2.938288	C 7.618940 -0.321347 2.952032	C 7.138593 -0.501107 2.323760
C 7.106567 0.957492 3.478337	C 7.098716 0.937129 3.423021	C 7.123527 0.911640 3.376847	C 7.130964 0.899962 3.405095	C 6.884943 0.701348 2.979811
C 6.699451	C 6.753710	C 6.700555	C 6.698276	C 6.766789

2.007692 2.557117	2.021274 2.531554	2.011733 2.516046	2.011594 2.552005	2.007096 2.301544
C 6.706952	C 6.879061	C 6.705906	C 6.698083	C 7.060426
2.002018 1.165078	2.103897 1.133650	2.010958 1.123864	2.008286 1.158265	2.208068 0.951958
C 6.274236	C 6.500111	C 6.275319	C 6.262115	C 6.919104
3.138766 0.481314	3.285766 0.503423	3.142347 0.435223	3.136628 0.472210	3.479527 0.410638
N 8.082613	N 8.073944	N 8.215432	N 8.141401	N 8.146396
3.831925 5.488535	3.756542 5.410691	3.880950 5.575331	3.852205 5.566200	3.893616 5.566644
C 6.263391	C 6.258074	C 6.263921	C 6.264434	C 6.187316
3.131005 7.020980	3.099758 7.047529	3.130364 7.044095	3.130194 7.145269	3.124537 7.181994
C 8.962196	C 8.931757	C 9.132142	C 9.034618	C 8.984029
4.176502 4.547507	4.073244 4.448565	4.244143 4.685615	4.207249 4.649040	4.321100 4.634930
C 10.219967	C 10.168580	C 10.371461	C 10.283364	C 9.956754
4.675481 4.834932	4.646755 4.701518	4.744733 5.045509	4.708681 4.962912	5.279201 4.875454
C 10.588752	C 10.515934	C 10.658829	C 10.611558	C 10.046301
4.824063 6.165762	4.900142 6.026571	4.868173 6.399977	4.845642 6.319098	5.806316 6.155199
C 9.688045	C 9.633888	C 9.710949	C 9.700475	C 9.167007
4.468719 7.151466	4.577283 7.035106	4.491344 7.331864	4.483054 7.281942	5.367664 7.129069
C 8.436944	C 8.400749	C 8.482605	C 8.445949	C 8.213076
3.974479 6.798265	3.997603 6.719749	3.995770 6.897831	3.979388 6.904575	4.405295 6.806602
C 7.388435	C 7.379498	C 7.387536	C 7.405732	C 7.174482
3.568209 7.721800	3.625467 7.672580	3.567893 7.762555	3.571388 7.803426	3.930758 7.743604
C 7.397024	C 7.377887	C 7.393892	C 7.409017	C 7.114317
3.576380 9.113799	3.770619 9.072029	3.570695 9.154630	3.571049 9.224534	4.305810 9.085635
C 6.261656	C 6.234064	C 6.266216	C 6.263627	C 6.040601
3.144163 9.800194	3.393146 9.778233	3.136019 9.846983	3.133626 9.884828	3.890300 9.864502
H 7.173377	H 6.907367	H 7.242740	H 7.271056	H 6.583609 -
0.768276 6.747828	0.607410 6.686257	0.539652 6.625706	0.507220 6.651928	0.309488 6.072254
H 8.075807 -	H 7.804032 -	H 8.141968 -	H 8.168545 -	H 7.036084 -
1.499997 6.244254	1.669351 6.149790	1.708765 5.979571	1.738530 5.979357	2.533655 5.027819
H 8.347168 -	H 8.258435 -	H 8.372211 -	H 8.382127 -	H 7.394618 -
2.171217 3.841780	2.226910 3.746091	2.229009 3.538613	2.237617 3.535753	2.618007 2.547723
H 7.701219 -	H 7.786133 -	H 7.702574 -	H 7.700896 -	H 7.273389 -
0.536461 2.072197	0.512818 2.005269	0.508515 1.876115	0.506845 1.888595	0.509804 1.249685
H 7.042103	H 7.262109	H 7.040658	H 7.032247	H 7.407635
1.135186 0.602343	1.276399 0.545533	1.142314 0.564382	1.139809 0.599787	1.399096 0.316769
H 6.278889	H 6.594845	H 6.279674	H 6.261696	H 7.139645
3.141748 -0.602708	3.358597 -0.574617	3.145884 -0.648679	3.138217 -0.611643	3.645402 -0.637823
H 8.620775	H 8.601217	H 8.839971	H 8.715309	H 8.847455
4.039452 3.528340	3.855615 3.439945	4.122019 3.647435	4.076778 3.620367	3.885205 3.649885
H 10.889834	H 10.831171	H 11.087189	H 10.973544	H 10.616398
4.941163 4.027532	4.884669 3.880840	5.030121 4.285477	4.983645 4.177281	5.602300 4.080042
H 11.565502	H 11.473210	H 11.617024	H 11.579909	H 10.787268
5.213659 6.428648	5.350078 6.265234	5.258287 6.724572	5.238131 6.609237	6.562737 6.389476
H 9.933525	H 9.871297	H 9.906455	H 9.927150	H 9.202770
4.569304 8.201473	4.765124 8.074389	4.578680 8.393349	4.581254 8.336179	5.783013 8.127762
H 8.265069	H 8.233306	H 8.263945	H 8.273742	H 7.886052
3.911742 9.674530	4.172041 9.605003	3.906544 9.711251	3.898470 9.790228	4.920393 9.537898
H 6.260963	H 6.227559	H 6.267042	H 6.263323	H 5.984451
3.149369 10.884217	3.507652 10.857123	3.138353 10.930893	3.134933 10.970759	4.189487 10.904887
N 5.558014	N 5.503538	N 5.509738	N 5.501289	N 5.551726
4.949201 4.792766	4.883693 4.860792	5.084089 4.706802	5.114801 4.732770	4.996475 4.738930
C 5.207122	C 5.140897	C 5.144846	C 5.140226	C 5.276921
5.826419 5.733658	5.719070 5.826751	6.000437 5.596137	6.033273 5.619708	5.892827 5.674147
C 4.707985	C 4.706901	C 4.650922	C 4.645179	C 5.286748
7.084082 5.446059	7.012404 5.573709	7.242317 5.235783	7.270856 5.243869	7.259035 5.437319
C 4.566514	C 4.658292	C 4.536511	C 4.528541	C 5.602139
7.455527 4.115185	7.443438 4.252930	7.532739 3.881157	7.544929 3.887963	7.694433 4.158355
C 4.928117	C 5.037174	C 4.915430	C 4.906457	C 5.897722
6.557150 3.129628	6.583569 3.241595	6.585287 2.949666	6.587049 2.963254	6.760732 3.180749
C 5.421468	C 5.458850	C 5.403910	C 5.395368	C 5.867844
5.305744 3.482988	5.291024 3.557272	5.354275 3.384274	5.364649 3.412281	5.404461 3.498988
C 5.832168	C 5.888077	C 5.833686	C 5.827530	C 6.232527
4.258842 2.559574	4.285434 2.604521	4.259650 2.519815	4.255591 2.555592	4.329555 2.554327
C 5.836204	C 6.007558	C 5.839214	C 5.826688	C 6.505416
4.271982 1.167593	4.384363 1.210913	4.269306 1.127715	4.262975 1.161900	4.544408 1.203048
H 5.506850	H 5.734517	H 5.508714	H 5.492095	H 6.402438
5.142288 0.606811	5.289558 0.678623	5.141480 0.571226	5.133089 0.606245	5.526940 0.753888
H 4.832742	H 5.012820	H 4.835404	H 4.823376	H 6.169307
6.804516 2.079582	6.887226 2.203095	6.783338 1.888079	6.775602 1.900454	7.077035 2.182182
H 4.177386	H 4.324510	H 4.151952	H 4.142897	H 5.629036
8.432420 3.852149	8.447435 4.015892	8.493028 3.556124	8.501217 3.553385	8.753454 3.926636
H 4.437061	H 4.416772	H 4.363776	H 4.358904	H 5.057379
7.751958 6.253359	7.653415 6.394800	7.957682 5.995504	7.994957 5.995294	7.955393 6.233960
H 5.339358	H 5.206019	H 5.260045	H 5.258177	H 5.059572
5.483265 6.752878	5.324051 6.833363	5.705976 6.634469	5.747578 6.660390	5.489249 6.658521
N 4.442752	N 4.439340	N 4.309712	N 4.387191	N 4.262041
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C 3.564040 2.073669 4.553721	C 3.590445 1.866587 4.614159	C 3.391171 2.010737 4.694675	C 3.493862 2.052039 4.649954	C 3.404237 1.048476 5.260595
C 2.307006 1.574380 4.843780	C 2.333594 1.373063 4.924873	C 2.152499 1.511226 5.058267	C 2.244643 1.552051 4.964243	C 2.305377 0.421231 5.825055
C 1.937991 1.433613 6.175433	C 1.951920 1.343202 6.265558	C 1.867631 1.391587 6.413653	C 1.915957 1.417392 6.320571	C 2.109368 0.564775 7.191300
C 2.837964 1.796053 7.159233	C 2.825563 1.790559 7.232629	C 2.817342 1.770971 7.342600	C 2.827109 1.780593 7.283119	C 3.008281 1.314376 7.928861
C 4.088638 2.289519 6.803420	C 4.087348 2.267357 6.860755	C 4.044898 2.265288 6.904743	C 4.082245 2.282514 6.905349	C 4.089138 1.918625 7.289303
C 5.137258 2.700997 7.724520	C 5.119582 2.736951 7.750102	C 5.141565 2.695668 7.766060	C 5.122551 2.691059 7.803842	C 5.114893 2.727593 7.977578
C 5.127027 2.705719 9.116546	C 5.100490 2.881645 9.153342	C 5.137519 2.698579 9.158249	C 5.118568 2.694710 9.224960	C 5.030357 3.109429 9.317230
H 4.257909 2.376637 9.679332	H 4.231506 2.610014 9.743204	H 4.268265 2.365228 9.717625	H 4.253440 2.368892 9.790979	H 4.187988 2.822701 9.939597
H 2.592409 1.701173 8.209759	H 2.561913 1.776094 8.282546	H 2.623863 1.686687 8.404726	H 2.600039 1.684205 8.337449	H 2.883767 1.426991 8.998397
H 0.961678 1.044357 6.440432	H 0.974782 0.967684 6.547840	H 0.910006 1.002477 6.741147	H 0.947163 1.026227 6.611036	H 1.264859 0.091187 7.679089
H 1.637744 1.302775 4.037860	H 1.677489 1.030387 4.136693	H 1.435259 1.223857 4.300400	H 1.554408 1.276564 4.178838	H 1.627499 - 0.157810 5.210625
H 3.905751 2.205543 3.533961	H 3.950172 1.926292 3.593401	H 3.681210 2.129979 3.655560	H 3.813451 2.180958 3.621170	H 3.614992 0.969511 4.197837

Fe(NNC)(NCN) 6

GS	^{3}MLCT	^{3}MC	^{5}MLCT	^{5}MC	^{7}MLCT
Fe 5.482925 8.534531 4.785217	Fe 5.412543 8.513884 4.782341	Fe 5.472308 8.445345 4.634510	Fe 5.440196 8.401310 4.630105	Fe 5.224221 8.350432 4.353995	Fe 5.372733 8.343497 4.482762
N 4.659046 6.748766 4.822830	N 4.542840 6.759517 4.865028	N 4.634838 6.371486 4.928347	N 4.589226 6.344241 4.931631	N 4.687260 6.142240 4.064924	N 4.859733 6.206297 4.135759
C 5.276950 8.340130 6.601390	C 5.258341 8.334076 6.626531	C 5.239935 8.332338 6.551269	C 5.210473 8.314889 6.549919	C 4.003452 7.874992 5.945412	C 3.963325 7.915609 5.911530
N 6.182411 10.274813 5.371877	N 6.136844 10.291529 5.334891	N 6.376343 10.354404 5.360076	N 6.344070 10.330952 5.326631	N 5.159073 10.256216 5.689069	N 5.147343 10.243383 5.697468
C 3.753770 9.333340 4.419797	C 3.675014 9.278189 4.363095	C 3.679798 9.230148 4.301354	C 3.669578 9.231589 4.300254	C 4.679934 8.925894 2.413059	C 4.637239 9.018383 2.669888
N 5.677578 8.743749 2.889424	N 5.644058 8.747983 2.871198	N 5.699689 8.777852 2.784296	N 5.682299 8.788742 2.758577	N 7.038362 9.278599 3.573481	N 7.068767 9.244940 3.593016
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C 4.356254 6.014496 3.751749	C 4.202055 6.048491 3.792883	C 4.290162 5.511187 3.981097	C 4.262573 5.465487 3.994995	C 4.970371 5.429347 2.984575	C 5.355082 5.466477 3.153369
H 4.602332 6.462016 2.796276	H 4.402171 6.524719 2.840641	H 4.620000 5.759295 2.976682	H 4.571812 5.714896 2.984503	H 5.687435 5.875943 2.303189	H 6.106630 5.946209 2.535050
C 3.759666 4.770913 3.832454	C 3.629701 4.794778 3.889230	C 3.554607 4.367036 4.237783	C 3.569374 4.300119 4.272141	C 4.387850 4.201834 2.715213	C 4.940950 4.167420 2.916193
H 3.535590 4.221933 2.927211	H 3.370682 4.251364 2.990465	H 3.292780 3.691347 3.433845	H 3.320875 3.608089 3.478069	H 4.650060 3.657081 1.817325	H 5.370535 3.597863 2.102666
C 3.456177 4.258929 5.088700	C 3.397263 4.264462 5.152209	C 3.167326 4.123468 5.549363	C 3.206609 4.057187 5.590558	C 3.462725 3.708947 3.623475	C 3.962553 3.635693 3.744104
H 2.987137 3.287395 5.190422	H 2.950143 3.283592 5.262003	H 2.585946 3.242051 5.795451	H 2.658369 3.159241 5.852174	H 2.975713 2.755912 3.450825	H 3.604450 2.624298 3.590356
C 3.755608 5.012699 6.206195	C 3.738434 5.003768 6.268494	C 3.519899 5.021338 6.538742	C 3.542474 4.974473 6.568132	C 3.153348 4.455812 4.745244	C 3.439805 4.409958 4.763784
H 3.529223 4.656912 7.203533	H 3.568923 4.627089 7.269126	H 3.214523 4.862395 7.564715	H 3.258906 4.812430 7.599728	H 2.413705 4.108166 5.455445	H 2.667917 4.020775 5.414521
C 4.355850 6.258646	C 4.312665 6.258263	C 4.259054 6.153655	C 4.240575 6.126466	C 3.778647 5.683912	C 3.905695 5.708641

6.057942	6.106470	6.200138	6.211200	4.944670	4.943806
C 4.711782	C 4.712746	C 4.664799	C 4.636242	C 3.486892	C 3.416662
7.173287	7.173701	7.200992	7.188027	6.586342	6.639484
7.125318	7.161407	7.139714	7.141430	6.073507	5.971795
C 4.537030	C 4.594515	C 4.492920	C 4.462551	C 2.775140	C 2.485145
7.027735	7.035513	7.123609	7.126623	6.200414	6.312619
8.497761	8.542872	8.520842	8.523485	7.208863	6.956280
H 4.090242	H 4.164169	H 4.053080	H 4.022607	H 2.383323	H 2.054709
6.130864	6.143178	6.242941	6.251670	5.193952	5.318834
8.917682	8.987031	8.977460	8.990360	7.318364	7.022872
C 4.934389	C 5.024827	C 4.896968	C 4.862963	C 2.584064	C 2.105988
8.060006	8.074868	8.179377	8.193415	7.119235	7.281737
9.347342	9.363481	9.327074	9.316472	8.234088	7.876821
H 4.795561	H 4.929222	H 4.764030	H 4.726799	H 2.036995	H 1.382264
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10.416853	10.438430	10.400925	10.390495	9.123380	8.645305
C 5.499968	C 5.570934	C 5.473652	C 5.441546	C 3.099512	C 2.647539
9.230615	9.243811	9.309723	9.317771	8.405624	8.561731
8.841787	8.830684	8.761050	8.740250	8.134380	7.829419
H 5.792160	H 5.889092	H 5.788532	H 5.754094	H 2.946537	H 2.337356
10.022326	10.038524	10.124650	10.139709	9.096244	9.295706
9.525588	9.498161	9.404783	9.375834	8.957794	8.566066
C 5.668323	C 5.686077	C 5.648157	C 5.619488	C 3.810436	C 3.580805
9.364936	9.368730	9.382832	9.376965	8.776343	8.872740
7.467540	7.450787	7.381406	7.360319	6.991363	6.842229
C 6.196375	C 6.216738	C 6.242177	C 6.222169	C 4.423646	C 4.246874
10.488221	10.484819	10.526719	10.510544	10.104130	10.176481
6.718139	6.676308	6.685208	6.651164	6.806299	6.695342
C 6.665560	C 6.772092	C 6.639774	C 6.644270	C 4.272231	C 3.999110
11.685735	11.648477	11.719629	11.698374	11.160335	11.280954
7.247797	7.189786	7.285802	7.243567	7.705219	7.503824
H 6.661655	H 6.827945	H 6.521281	H 6.536964	H 3.678073	H 3.270451
11.819905	11.779318	11.855630	11.841092	11.026753	11.212827
8.322844	8.263268	8.353464	8.311463	8.599316	8.301087
C 7.117782	C 7.247341	C 7.171870	C 7.190533	C 4.877667	C 4.690953
12.679402	12.614781	12.725435	12.689846	12.375047	12.457169
6.402033	6.320999	6.500606	6.449189	7.443001	7.274564
H 7.484078	H 7.685300	H 7.482178	H 7.521669	H 4.761604	H 4.506789
13.617875	13.527986	13.661071	13.621479	13.203540	13.327461
6.801779	6.707181	6.951845	6.893713	8.133017	7.894253
C 7.088374	C 7.159737	C 7.298589	C 7.306783	C 5.627191	C 5.619102
12.457345	12.401170	12.531383	12.485980	12.519472	12.508960
5.030223	4.953057	5.130754	5.080213	6.284316	6.245942
H 7.421740	H 7.517503	H 7.704694	H 7.725195	H 6.114849	H 6.182303
13.209350	13.132628	13.298772	13.241637	13.452975	13.408159
4.326844	4.240750	4.484270	4.427876	6.033978	6.033138
C 6.612553	C 6.592757	C 6.880835	C 6.862530	C 5.736420	C 5.813777
11.245757	11.221477	11.319801	11.280421	11.424764	11.370085
4.566015	4.503301	4.606925	4.563534	5.442575	5.481095
H 6.559127	H 6.489688	H 6.944721	H 6.915569	H 6.312311	H 6.526318
11.027814	10.994740	11.101804	11.053841	11.488700	11.353238
3.506457	3.449427	3.544718	3.502804	4.525089	4.664382
C 2.699571	C 2.605221	C 2.591075	C 2.586465	C 3.502660	C 3.355646
9.648772	9.520944	9.413014	9.419246	8.649923	8.831245
5.281083	5.218614	5.146108	5.149803	1.719485	2.161350
H 2.807359	H 2.698729	H 2.669901	H 2.658773	H 2.740334	H 2.640906
9.436312	9.269001	9.104560	9.092039	8.031648	8.226151
6.340591	6.270376	6.183760	6.181863	2.188773	2.714717
C 1.523397	C 1.422066	C 1.407315	C 1.414196	C 3.261257	C 2.960593
10.222805	10.080183	9.981262	10.017969	9.138916	9.406371
4.818426	4.748287	4.686500	4.698895	0.439974	0.957595
H 0.725573	H 0.601692	H 0.569504	H 0.579321	H 2.331461	H 1.955660
10.456632	10.265912	10.115467	10.156121	8.902463 -	9.247747
5.517122	5.434405	5.363511	5.378541	0.068576	0.580013
C 1.349953	C 1.279966	C 1.291019	C 1.306969	C 4.210111	C 3.855374
10.507410	10.406080	10.384851	10.446401	9.932881 -	10.188118
3.463902	3.402824	3.360527	3.380499	0.195297	0.236047
H 0.428457	H 0.355134	H 0.367951	H 0.392801	H 4.026542	H 3.550921
10.957115	10.842077	10.829749	10.914940	10.313137 -	10.636243 -
3.112070	3.042321	3.005811	3.033436	1.193821	0.702988
C 2.365719	C 2.325382	C 2.357177	C 2.370873	C 5.395766	C 5.139871
10.209650	10.168701	10.215780	10.273077	10.227940	10.391283
2.575977	2.526371	2.492251	2.509576	0.454879	0.716790
H 2.244357	H 2.224375	H 2.267513	H 2.290261	H 6.144695	H 5.838779
10.426912	10.417093	10.527179	10.603637	10.830636 -	10.993894
1.518643	1.474672	1.456431	1.479293	0.050113	0.145729
C 3.545780	C 3.510137	C 3.537909	C 3.540671	C 5.621283	C 5.528073

9.633681	9.611442	9.642750	9.670329	9.727094	9.809043
3.049484	3.000325	2.956650	2.961240	1.737554	1.920410
C 4.661404	C 4.663777	C 4.708552	C 4.709600	C 6.873680	C 6.878252
9.287284	9.314923	9.418460	9.448295	9.998600	9.973555
2.189373	2.156090	2.108723	2.105414	2.455976	2.484382
C 4.784156	C 4.824634	C 4.889435	C 4.894395	C 7.837164	C 7.873235
9.442902	9.557875	9.784398	9.847380	10.935490	10.796126
0.810828	0.802289	0.796944	0.798937	2.087110	1.995047
H 3.969416	H 4.031707	H 4.098098	H 4.118539	H 7.698714	H 7.714349
9.875772	10.012441	10.294691	10.382694	11.535695	11.388502
0.244923	0.224918	0.263839	0.269634	1.198010	1.105227
C 5.952498	C 6.053486	C 6.116464	C 6.132443	C 8.961261	C 9.099883
9.037932	9.195277	9.494028	9.545616	11.099858	10.846529
0.181297	0.211952	0.165120	0.182860	2.881775	2.696524
H 6.058409	H 6.211032	H 6.271636	H 6.302893	H 9.715553	H 9.896917
9.156529 -	9.373771 -	9.779595 -	9.845768 -	11.830426	11.488148
0.890909	0.845977	0.868345	0.844794	2.611282	2.338265
C 6.987362	C 7.057243	C 7.119233	C 7.126114	C 9.115449	C 9.290276
8.479267	8.621258	8.859312	8.890059	10.338377	10.095771
0.920452	0.954320	0.860139	0.865254	4.028635	3.826905
H 7.905548	H 7.999258	H 8.071603	H 8.076181	H 9.981706	H 10.226680
8.156022	8.347015	8.640702	8.675001	10.460228	10.136438
0.448394	0.497011	0.393965	0.392839	4.665117	4.369077
C 6.807933	C 6.848393	C 6.898940	C 6.902751	C 8.112843	C 8.241756
8.346523	8.393316	8.503888	8.508955	9.427964	9.272018
2.290302	2.330009	2.196403	2.203893	4.344149	4.286641
C 7.751631	C 7.745069	C 7.812318	C 7.803009	C 8.105998	C 8.249529
7.782634	7.829831	7.865414	7.873722	8.570046	8.444016
3.249919	3.269686	3.088814	3.094183	5.535298	5.436699
C 9.001010	C 9.048070	C 9.100880	C 9.111002	C 9.167543	C 9.350933
7.274309	7.376242	7.427247	7.460113	8.493788	8.259334
2.920808	2.978423	2.757136	2.771382	6.432481	6.297551
H 9.328906	H 9.418487	H 9.467206	H 9.484938	H 10.060855	H 10.276731
7.288263	7.460794	7.575105	7.629075	9.082755	8.782107
1.889449	1.964298	1.749136	1.769275	6.273224	6.092312
C 9.802739	C 9.823143	C 9.873462	C 9.886663	C 9.064940	C 9.245201
6.756049	6.837232	6.812318	6.850566	7.649662	7.420742
3.920251	3.967607	3.710148	3.719185	7.521895	7.372689
H 10.780612	H 10.824292	H 10.870975	H 10.892394	H 9.878838	H 10.092394
6.352862	6.487855	6.467540	6.530571	7.572227	7.272540
3.686460	3.743214	3.465232	3.472734	8.233639	8.032551
C 9.329316	C 9.308862	C 9.355421	C 9.370368	C 7.903719	C 8.024493
6.761318	6.738700	6.634151	6.642426	6.904235	6.747826
5.226920	5.280583	5.005168	5.017874	7.686208	7.613772
H 9.921206	H 9.887897	H 9.934241	H 9.955247	H 7.777981	H 7.897674
6.365692	6.315989	6.155151	6.167473	6.231872	6.081511
6.042175	6.089947	5.783705	5.793504	8.525612	8.456365
C 8.076125	C 8.032459	C 8.087251	C 8.089144	C 6.892993	C 6.985235
7.284265	7.197846	7.088761	7.069026	7.042191	6.972306
5.482672	5.509119	5.272169	5.278464	6.751330	6.742770
H 7.654721	H 7.583945	H 7.634182	H 7.635800	H 5.957112	H 6.018836
7.314481	7.149065	6.986936	6.944451	6.503058	6.498278
6.480657	6.496061	6.252359	6.256760	6.844608	6.885673

$Fe(NNC)_2$ 7

GS	^{3}MLCT	^{3}MC	^{5}MLCT	^{5}MC	^{7}MLCT
Fe 5.478079	Fe 5.462033	Fe 5.465417	Fe 5.092367	Fe 5.290069	Fe 5.276309
8.459160	8.507974	8.979714	8.887897	8.994283	9.019540
4.744803	4.748157	4.644393	4.904271	4.773703	4.777370
N 4.633984	N 4.581688	N 4.525533	N 4.361822	N 4.492582	N 4.574576
6.692934	6.684249	6.844193	6.967798	6.880917	6.912158
4.814058	4.762007	4.728591	4.912815	4.877588	4.868160
N 5.275189	N 5.278527	N 5.332070	N 5.343493	N 5.373725	N 5.316494
8.285453	8.276690	8.288705	8.348200	8.309861	8.404806
6.601165	6.611024	6.709084	6.814881	6.835992	6.825205
C 6.146285	C 6.080109	C 6.025896	C 5.654298	C 6.163875	C 6.012012
10.198735	10.255367	10.576846	10.615853	10.614071	10.702992
5.237859	5.276327	5.650894	5.663423	5.779877	5.739052
C 3.776881	C 3.784873	C 3.843336	C 3.593501	C 3.499561	C 3.544569
9.305579	9.392230	9.929305	9.790335	9.697051	9.837966
4.418737	4.390064	4.085587	4.012819	3.937989	3.981783
N 5.667434	N 5.671037	N 5.541539	N 5.620084	N 5.572644	N 5.568541
8.689164	8.682083	8.611124	8.673785	8.661329	8.767284
2.894062	2.881648	2.707783	2.781959	2.644294	2.674311

N 7.293589 7.763788 4.517122	N 7.337833 7.779463 4.571054	N 7.290356 8.174508 4.435778	N 7.231431 7.908454 4.663484	N 7.290782 8.032548 4.454573	N 7.207696 7.961245 4.485191
C 4.294454 5.938007 3.765826	C 4.165957 5.979147 3.716423	C 4.191771 6.139017 3.654105	C 3.758728 6.349261 3.898353	C 3.952352 6.248976 3.839017	C 4.232122 6.208202 3.790496
H 4.537019 6.356106 2.796173	H 4.378610 6.419567 2.748206	H 4.152413 6.678765 2.716565	H 3.569842 6.970074 3.028074	H 3.987705 6.774944 2.893157	H 4.124587 6.772703 2.871738
C 3.667495 4.715207 3.897491	C 3.509358 4.771127 3.841426	C 3.905307 4.784368 3.696803	C 3.393296 5.023730 3.923590	C 3.368374 4.999911 3.932316	C 4.020601 4.847096 3.815185
H 3.411977 4.145541 3.013410	H 3.207453 4.222548 2.959844	H 3.635405 4.262207 2.788001	H 2.911431 4.574699 3.065696	H 2.947347 4.533216 3.051077	H 3.737747 4.326220 2.909979
C 3.372273 4.243601 5.172133	C 3.251586 4.289496 5.130652	C 3.979334 4.129602 4.915510	C 3.655127 4.288565 5.099399	C 3.334580 4.374488 5.172611	C 4.170141 4.173588 5.033126
H 2.880848 3.288247 5.309026	H 2.728507 3.351059 5.270733	H 3.778388 3.067291 4.989823	H 3.373220 3.244251 5.166845	H 2.884774 3.395975 5.289600	H 4.017555 3.102710 5.095970
C 3.709547 5.021870 6.262493	C 3.654651 5.024325 6.221505	C 4.320363 4.857884 6.040695	C 4.251201 4.908935 6.163750	C 3.876108 5.030414 6.260378	C 4.517002 4.892553 6.154761
H 3.489101 4.699150 7.271778	H 3.447307 4.687242 7.228910	H 4.399437 4.379480 7.007653	H 4.441104 4.372922 7.085791	H 3.845704 4.581053 7.243952	H 4.644602 4.397434 7.108474
C 4.336374 6.243151 6.055384	C 4.330616 6.231319 6.022159	C 4.577737 6.216927 5.911140	C 4.608078 6.267706 6.076862	C 4.448617 6.286755 6.080263	C 4.714691 6.270945 6.054135
C 4.710626 7.177733 7.106038	C 4.761496 7.118625 7.074163	C 4.928346 7.072186 7.055036	C 5.200034 7.026379 7.118591	C 5.003397 7.078140 7.183730	C 5.108237 7.115859 7.158963
C 4.505791 7.024544 8.469507	C 4.648001 6.909938 8.449007	C 4.837992 6.686471 8.385378	C 5.667968 6.567449 8.366541	C 5.128119 6.621593 8.492619	C 5.308053 6.683740 8.472800
H 4.041549 6.128033 8.858854	H 4.239996 5.982900 8.829730	H 4.484807 5.702628 8.662190	H 5.586022 5.519456 8.626556	H 4.837129 5.617146 8.766511	H 5.129732 5.652709 8.746013
C 4.896695 8.058673 9.308834	C 5.059174 7.914069 9.306980	C 5.196587 7.614777 9.353906	C 6.242841 7.464052 9.232331	C 5.646335 7.492665 9.435638	C 5.744662 7.597208 9.408899
H 4.744719 7.974328 10.378489	H 4.975941 7.771156 10.378160	H 5.137101 7.350810 10.403548	H 6.608359 7.119035 10.192596	H 5.759228 7.172636 10.465044	H 5.906960 7.284815 10.433819
C 5.468073 9.205485 8.777277	C 5.571142 9.110571 8.804895	C 5.620414 8.877527 8.982173	C 6.380943 8.829387 8.884430	C 6.030015 8.771334 9.062645	C 6.001438 8.918506 9.034363
H 5.762795 10.028513 9.415373	H 5.884693 9.908642 9.464123	H 5.901726 9.607393 9.729094	H 6.840904 9.537519 9.560031	H 6.445894 9.452319 9.792162	H 6.380704 9.634426 9.750067
C 5.648910 9.307394 7.401496	C 5.667790 9.267093 7.427417	C 5.674209 9.201231 7.624303	C 5.926072 9.227164 7.643345	C 5.888844 9.166006 7.732294	C 5.787730 9.293274 7.715240
C 6.179423 10.414821 6.635582	C 6.148020 10.414656 6.676279	C 6.087281 10.479303 7.053840	C 6.054835 10.545744 7.015417	C 6.298335 10.462386 7.174788	C 6.089689 10.609191 7.139417
C 6.656932 11.597361 7.200624	C 6.630562 11.585895 7.255449	C 6.520848 11.546915 7.844473	C 6.550375 11.664944 7.675090	C 6.801752 11.478949 7.990850	C 6.444648 11.704844 7.925287
H 6.666199 11.728350 8.279193	H 6.675579 11.686303 8.335740	H 6.557496 11.453118 8.925224	H 6.850228 11.592064 8.715342	H 6.886800 11.346366 9.065005	H 6.485527 11.621599 9.006667
C 7.118052 12.605999 6.376101	C 7.052869 12.621741 6.441350	C 6.909736 12.731086 7.249836	C 6.660904 12.870234 7.000311	C 7.190005 12.681371 7.428041	C 6.734165 12.916183 7.321079
H 7.492230 13.531542 6.798073	H 7.430150 13.538958 6.878608	H 7.246119 13.562856 7.857722	H 7.046781 13.745207 7.510885	H 7.576213 13.476985 8.055200	H 7.007530 13.772678 7.926765
C 7.090671 12.423570 4.992781	C 6.989038 12.482637 5.055951	C 6.858027 12.847846 5.862323	C 6.267798 12.955456 5.669866	C 7.070062 12.863031 6.053582	C 6.661830 13.032511 5.936780
H 7.445136 13.219578 4.344634	H 7.316825 13.300269 4.421959	H 7.155484 13.779132 5.390938	H 6.346011 13.902037 5.144935	H 7.370813 13.806916 5.609021	H 6.885419 13.983690 5.464549
C 6.613719 11.244352	C 6.506984 11.313715	C 6.416331 11.789554	C 5.758527 11.839223	C 6.562221 11.844451	C 6.295695 11.937854

4.439128	4.482821	5.082532	5.014620	5.255988	5.163200
H 6.597441	H 6.455988	H 6.361961	H 5.426560	H 6.468428	H 6.223137
11.138004	11.224606	11.915042	11.927243	12.025424	12.059873
3.357704	3.402138	4.005227	3.985275	4.187652	4.085405
C 2.746806	C 2.774632	C 2.938238	C 2.519044	C 2.411765	C 2.513570
9.631632	9.754796	10.624260	10.383559	10.282105	10.460628
5.303699	5.274040	4.878951	4.673486	4.587033	4.679403
H 2.870595	H 2.910396	H 3.164313	H 2.513281	H 2.425709	H 2.533696
9.427039	9.586125	10.782110	10.417775	10.377482	10.479830
6.363812	6.338074	5.928812	5.758611	5.670404	5.766177
C 1.570527	C 1.600770	C 1.759795	C 1.460079	C 1.302608	C 1.452837
10.221182	10.336593	11.135287	10.942450	10.758419	11.068395
4.863351	4.814065	4.345441	3.973134	3.898190	4.018311
H 0.789706	H 0.824176	H 1.064346	H 0.633342	H 0.472202	H 0.653694
10.466993	10.617197	11.671887	11.392754	11.202120	11.536754
5.576849	5.518280	4.982953	4.513026	4.439526	4.584074
C 1.376381	C 1.410233	C 1.474645	C 1.455425	C 1.251302	C 1.414792
10.510152	10.571404	10.980540	10.942810	10.672733	11.084877
3.512069	3.453791	2.992735	2.580038	2.510162	2.627563
H 0.455406	H 0.492378	H 0.561774	H 0.630780	H 0.391493	H 0.594331
10.974581	11.030145	11.392287	11.387365	11.050603	11.569026
3.178936	3.104452	2.578124	2.035202	1.968361	2.110015
C 2.372857	C 2.398235	C 2.364734	C 2.514690	C 2.312126	C 2.434001
10.204053	10.219187	10.302951	10.376603	10.108353	10.489020
2.604935	2.551346	2.175060	1.897913	1.825044	1.904720
H 2.237839	H 2.258828	H 2.148614	H 2.515966	H 2.274224	H 2.410036
10.428866	10.399075	10.181434	10.382479	10.057477	10.520350
1.550929	1.489960	1.118092	0.812551	0.740991	0.820039
C 3.551992	C 3.573867	C 3.533441	C 3.572769	C 3.415948	C 3.484664
9.610968	9.635230	9.774529	9.801304	9.626327	9.865896
3.056070	3.016816	2.715514	2.606097	2.532812	2.578004
C 4.666082	C 4.679709	C 4.514605	C 4.711508	C 4.549107	C 4.573771
9.270019	9.230377	9.018813	9.175413	8.994907	9.180495
2.197952	2.164490	1.936353	1.941723	1.843999	1.872731
C 4.812268	C 4.799073	C 4.467795	C 4.898429	C 4.604272	C 4.597653
9.485955	9.349573	8.669663	9.050461	8.680210	8.887723
0.831272	0.785910	0.603682	0.562252	0.486671	0.516763
H 4.007983	H 3.996772	H 3.638420	H 4.167571	H 3.780416	H 3.793867
9.951838	9.786784	8.984236 -	9.450517 -	8.935391 -	9.218168 -
0.276716	0.207314	0.016015	0.127187	0.165753	0.126382
C 5.991338	C 5.972370	C 5.515688	C 6.027517	C 5.713335	C 5.656694
9.114101	8.896056	7.891176	8.404563	8.013553 -	8.131744
0.202602	0.177336	0.074341	0.098670	0.011012	0.010147
H 6.116836	H 6.087430	H 5.494683	H 6.191578	H 5.760306	H 5.689990
9.284256 -	8.977405 -	7.603784 -	8.299783 -	7.750489 -	7.886016 -
0.860314	0.897511	0.970319	0.967843	1.061566	1.044987
C 7.016937	C 6.992240	C 6.567497	C 6.955198	C 6.752782	C 6.643615
8.535595	8.351112	7.498305	7.887019	7.667908	7.669716
0.937552	0.933297	0.869874	0.994025	0.835684	0.854800
H 7.952585	H 7.907136	H 7.382289	H 7.844176	H 7.615666	H 7.452166
8.252878	8.006251	6.908960	7.384218	7.129599	7.057511
0.474078	0.470034	0.468467	0.640374	0.467811	0.479538
C 6.816975	C 6.825007	C 6.567725	C 6.703699	C 6.641483	C 6.571068
8.339572	8.255084	7.879125	8.043247	8.018014	7.996406
2.296333	2.317713	2.218924	2.349426	2.177651	2.210877
C 7.766673	C 7.779353	C 7.557912	C 7.580311	C 7.655286	C 7.481045
7.786633	7.774703	7.605370	7.542738	7.731881	7.525064
3.249415	3.277537	3.212085	3.425160	3.198190	3.230626
C 9.041427	C 9.085712	C 8.729480	C 8.685295	C 8.919037	C 8.544991
7.336160	7.369190	6.869444	6.739102	7.230549	6.654900
2.933557	2.977294	3.001861	3.174983	2.898469	2.986242
H 9.380395	H 9.426983	H 8.905610	H 8.933626	H 9.189553	H 8.741663
7.371808	7.389260	6.426547	6.446397	7.012031	6.310768
1.906371	1.950352	2.029378	2.164055	1.873955	1.979429
C 9.855407	C 9.918217	C 9.635135	C 9.453508	C 9.824855	C 9.328969
6.854012	6.964029	6.721570	6.308262	7.035573	6.231275
3.940401	3.992513	4.021913	4.242441	3.923037	4.035810
H 10.853855	H 10.930350	H 10.545939	H 10.317323	H 10.814038	H 10.154103
6.498064	6.646667	6.154905	5.675620	6.646029	5.550854
3.717789	3.770921	3.871244	4.074856	3.714264	3.862421
C 9.369230	C 9.451893	C 9.365349	C 9.096400	C 9.447650	C 9.040351
6.841334	6.978015	7.329002	6.696900	7.362443	6.690418
5.243413	5.316046	5.263956	5.521301	5.220498	5.326719
H 9.973111	H 10.075872	H 10.060135	H 9.665349	H 10.126143	H 9.633968
6.481126	6.664772	7.255473	6.388338	7.237627	6.392339
6.066242	6.141731	6.090633	6.388498	6.054781	6.180638
C 8.091435	C 8.160951	C 8.198905	C 7.974985	C 8.176189	C 7.976567

7.304317	7.407059	8.034494	7.498009	7.860904	7.550906
5.484665	5.545153	5.414277	5.682397	5.432720	5.492990
H 7.669683	H 7.746836	H 7.947988	H 7.667792	H 7.843936	H 7.717322
7.324910	7.460269	8.528062	7.819274	8.145783	7.936543
6.482579	6.546616	6.345991	6.669118	6.423393	6.471551

^{3}MC-GS MECP Cartesian coordinates

Fe(NNC)(NCN) 6			
Fe	5.481333	8.480145	4.668732
N	4.634897	6.464890	4.892847
C	5.250215	8.339424	6.565470
N	6.338183	10.360235	5.382565
C	3.698068	9.274608	4.328461
N	5.693274	8.762060	2.806732
N	7.326111	7.726017	4.395230
C	4.299889	5.637943	3.912249
H	4.605558	5.942904	2.916047
C	3.602140	4.462532	4.128534
H	3.347425	3.816496	3.298449
C	3.243581	4.147663	5.433372
H	2.693897	3.238063	5.647271
C	3.585078	5.010133	6.457520
H	3.305049	4.796660	7.480992
C	4.284712	6.178071	6.160780
C	4.678439	7.196164	7.133385
C	4.502901	7.095928	8.511795
H	4.060345	6.208814	8.953867
C	4.902739	8.142272	9.334646
H	4.766352	8.067172	10.407029
C	5.476605	9.285064	8.788566
H	5.784921	10.092222	9.445590
C	5.651634	9.379499	7.410521
C	6.231275	10.526983	6.713817
C	6.639714	11.716687	7.312452
H	6.543147	11.842214	8.383791
C	7.153124	12.728784	6.523385
H	7.471497	13.662196	6.973552
C	7.250616	12.542540	5.149851
H	7.640920	13.314332	4.498958
C	6.825602	11.333563	4.626819
H	6.868096	11.123620	3.562248
C	2.620414	9.504351	5.178058
H	2.707548	9.234051	6.225964
C	1.437788	10.069903	4.713383
H	0.611681	10.240182	5.396844
C	1.305376	10.424410	3.374304
H	0.382577	10.866920	3.015991
C	2.356973	10.208404	2.499718
H	2.256890	10.481534	1.453835
C	3.537736	9.639410	2.971300
C	4.692171	9.370077	2.117815
C	4.852017	9.664329	0.782162
H	4.052056	10.148292	0.237347
C	6.061315	9.334974	0.144849
H	6.198851	9.565238	-0.904898
C	7.073756	8.727337	0.854624
H	8.014763	8.474628	0.383016
C	6.872085	8.445733	2.208640
C	7.798317	7.835725	3.117189
C	9.073283	7.370264	2.780247
H	9.421585	7.467902	1.759871
C	9.859804	6.791186	3.746922
H	10.848881	6.424682	3.499557
C	9.364839	6.679879	5.055037
H	9.952758	6.231173	5.844802
C	8.104743	7.159326	5.324486
H	7.668268	7.106208	6.315888

$Fe(NNC)_2$ 7			
Fe	5.503636	8.799181	4.684575
N	4.604510	6.796429	4.780529
N	5.307113	8.295191	6.723037
C	6.098462	10.467808	5.538187
C	3.834175	9.705603	4.220320
N	5.605850	8.629781	2.713292
N	7.330722	8.048276	4.423346
C	4.295544	6.068699	3.711403
H	4.388994	6.568638	2.755443
C	3.879683	4.751587	3.791648
H	3.636079	4.207707	2.888295
C	3.788415	4.158131	5.043125
H	3.479709	3.124793	5.146408
C	4.101224	4.910411	6.160341
H	4.047062	4.482779	7.152770
C	4.497894	6.230957	5.996371
C	4.817272	7.123140	7.116697
C	4.614039	6.839214	8.459605
H	4.199370	5.891621	8.776274
C	4.939620	7.824579	9.383774
H	4.789921	7.641061	10.441571
C	5.438346	9.044776	8.959363
H	5.684299	9.820417	9.672304
C	5.610927	9.266231	7.591689
C	6.096812	10.480684	6.948315
C	6.534192	11.591582	7.673405
H	6.523731	11.578294	8.759181
C	6.987523	12.712697	7.006722
H	7.327832	13.579078	7.561892
C	7.000380	12.719904	5.612673
H	7.350831	13.601690	5.085261
C	6.560336	11.616911	4.896713
H	6.565484	11.654902	3.811023
C	2.879206	10.250956	5.070505
H	3.076234	10.284821	6.138307
C	1.687013	10.768406	4.577890
H	0.955321	11.188089	5.260924
C	1.429832	10.768005	3.209984
H	0.504226	11.183901	2.828965
C	2.365285	10.238235	2.337059
H	2.171400	10.234543	1.268757
C	3.551539	9.704086	2.834712
C	4.576080	9.095781	1.984439
C	4.578151	8.935220	0.611394
H	3.751458	9.298888	0.015678
C	5.671092	8.287260	0.013562
H	5.688900	8.151432	-1.061802
C	6.724946	7.829025	0.776353
H	7.575499	7.339403	0.319424
C	6.671477	8.018715	2.162175
C	7.652655	7.656682	3.147436
C	8.855390	7.001812	2.875067
H	9.071280	6.698267	1.858109
C	9.744176	6.753836	3.893611
H	10.679453	6.244323	3.697024
C	9.419648	7.181794	5.192359
H	10.095860	7.024697	6.022683
C	8.221284	7.817435	5.400863
H	7.926428	8.173661	6.381444