Supporting/Supplementary Information for the Communication

"Quantum-chemistry-aided Ligand Engineering for Potential Molecular Switches: Changing Barriers to Tune Excited State Lifetimes"

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Contents

1 A note on some terms related to spin-state transitions

Spin state transition, spin crossover, intersystem crossing, spin-forbidden transition or spin inversion: these terms related to spin-altering molecular transitions or chemical reactions are sometimes used inconsistently and confusingly, so we describe the ones relevant to this paper in a nutshell.

The photophysics of the Fe(II) polypyridil complexes involves spin-state transitions (SST), i.e. a change in

the spin state of the molecule. Other Fe(II) (or different $3d^4$...$3d^7$ transition metal) complexes can even change the spin state with temperature or pressure; when this happens in the condensed phase, the typically second-order phase transition is called[1] spin crossover (SCO). However, despite the clear former distinction, in the present literature SCO is often used to denote any molecular SST process. The SST must involve at least one intersystem crossing (ISC), which is a transition between the potentials of two states with different spin. The elementary transitions in the full photocycle for the working horse of the Fe(II) polypiridine complexes, $[Fe(bipy)_3]^{2+}$, using octahedral term symbols, are thought to be the following:[2–5]

$$^1A_1 \xrightarrow{h\nu} {}^1MLCT \xrightarrow{ISC} {}^3MLCT \longrightarrow {}^3T_1 \xrightarrow{ISC} {}^5T_2 \xrightarrow{ISC} {}^1A_1$$

The present paper deals with the final step, the quintet-singlet relaxation.

2 Computational details

Molecular geometries were optimized for all complexes with density functional theory (DFT) employing a tight optimization criterion using the ORCA 3.0 program package[6]. In all cases the TZVP basis set[7,8] and the conductor like screening model (COSMO)[9] were employed, the latter approximates the solvation effects by embedding the molecule in a polarizable medium with a dielectric constant of the solvent, in our case water. Several functionals have been tested in the literature and by us too, and the B3LYP* functional[10–13] has been found to predict the energetics of the spin state transitions in Fe(II) complexes systems satisfactorily.[14–22]

Our computational protocol was to first optimize the molecular geometry with the BP86 functional,[23,24] which is more rapid (being GGA), and which is known to provide geometries in excellent agreement with experiments. We then performed a tight geometry optimization with the B3LYP* hybrid functional, starting from the BP86 structure. This has been carried out for spin states $S = 0$, and $S = 2$. In order to determine the energy barrier between the singlet and the quintet, minimum energy crossing point calculations (MECP)[25–27] were also performed at the B3LYP*/TZVP level.

In almost all B3LYP* calculations the RIJCOSX approximation was used.[28–30] Randomly selected calculations were also carried out without this approximation, and we found that the two approaches provided very similar results. However, the ground state (singlet) structure of the $[Fe(4'\text{-}SO_2Me\text{-}terpy)_2]^{2+}$ was found slightly distorted, the main N–Fe–N axis was bent to 176°, but repeating the calculations without this approximation resulted in linear geometry (179.94°). Therefore, all states of this molecule was calculated without RIJCOSX.

3 Calculated Structures and Energies

The full optimized geometries are given in the Appendix to this document. The $r(Fe - N_{ax})$ and $r(Fe - N_{eq})$ bond lengths, and the NNN angle (the angle of the 3 nitrogen atoms in a ligand, with the axial N in the middle) for the singlet and quintet state, calculated at the BP86/TZVP and B3LYP*/TZVP levels are shown in Tables S1 and S2, respectively. The lines in the table start with the electron withdrawing groups, and going down the electron donating character of the R substituent groups increase. It is evident from both data sets, that the structure of the FeN_6 core is very similar, and the metal ligand distances and the NNN angle are not much affected by the electron donating or withdrawing properties of the substituent. For the sake of completeness, the optimized quintet-singlet MECP geometries are also shown in Table S3.

The energies of the different spin states calculated using the B3LYP* functional, and those of the singlet-quintet MECPs are listed in Table S4. The differences in the quintet-singlet energies are used in Fig. 1 of the main paper, to create a set of potential curves to obtain approximate energy barriers, using the previously calculated CASPT2 potential energy curves.[21]

4 Materials

All terpyridine derivatives were synthesized at EvoBlocks Ltd., Budapest, in 97–99+% purity, following literature methods.[31–35] The purity and the structure of these ligand materials has been verified by liquid chromatography and ^1H NMR spectroscopy.

All $[Fe(4'\text{-R-terpy})_2]^{2+}$ complexes were prepared using standard methods. 2.05 molar equivalent of the ligand was dissolved in a 3:1 mixture of water and acetonitrile then 1.0 equivalent of solid $FeCl_2 \times 4H_2O$ was added. The solution was stirred for 8 hours then filtered through paper filter to remove the excess ligand. The filtered solution was dried at 45°C, then the samples were purified by recrystallization. The synthesis route above implies that all complexes were prepared with Cl^- counterions.

4.1 Characterisation

All samples were characterized in water solution by UV-VIS spectroscopy, NMR and elemental analysis. The latter has been performed with LC-HRMS at Servier Hungária Ltd., using a Kinetex XB-C18 (50 mm×2.1 mm, 2.6 μm) cromatography column and a LC118-TOF high-resolution mass spectrometer. The chromatography revealed a single species in all cases, and the instrument derived the formula for the doubly charged complex ion by comparing numerous formula masses (calculated all possible combinations with stoichiometry numbers ("element limits") between 0 and 80

Table S1: Selected structural parameters of the FeN_6 core in the BP86/TZVP optimized molecular geometries for the singlet and quintet states of the studied $[Fe(4'\text{-R-terpy})_2]^{2+}$ complexes

	Singlet			Quintet		
R (substituent)	$r(Fe-N_{ax})$	$r(Fe-N_{eq})$	NNN	$r(Fe-N_{ax})$	$r(Fe-N_{eq})$	NNN
CN	1.879 Å	1.981 Å	102.4°	2.097 Å	2.188 Å	108.4°
SO_2Me	1.881 Å	1.981 Å	103.1°	2.100 Å	2.189 Å	107.9°
H	1.886 Å	1.979 Å	102.2°	2.100 Å	2.170 Å	108.1°
SMe	1.886 Å	1.980 Å	102.4°	2.130 Å	2.185 Å	107.7°
OMe	1.889 Å	1.979 Å	102.3°	2.138 Å	2.185 Å	107.7°
$N(CH_2CH_2OH)_2$	1.890 Å	1.979 Å	102.5°	2.114 Å	2.188 Å	108.4°

Table S2: Selected structural parameters of the FeN_6 core in the B3LYP*/TZVP optimized molecular geometries for the singlet and quintet states of the studied $[Fe(4'\text{-R-terpy})_2]^{2+}$ complexes

	Singlet			Quintet		
R (substituent)	$r(Fe-N_{ax})$	$r(Fe-N_{eq})$	NNN	$r(Fe-N_{ax})$	$r(Fe-N_{eq})$	NNN
CN	1.904 Å	2.014 Å	103.1°	2.122 Å	2.219 Å	108.6°
SO_2Me	1.907 Å	2.014 Å	103.2°	2.129 Å	2.214 Å	108.3°
H	1.909 Å	2.019 Å	103.2°	2.152 Å	2.227 Å	108.6°
SMe	1.908 Å	2.020 Å	103.5°	2.147 Å	2.233 Å	109.2°
OMe	1.911 Å	2.020 Å	103.4°	2.139 Å	2.228 Å	109.2°
$N(CH_2CH_2OH)_2$	1.913 Å	2.018 Å	103.5°	2.130 Å	2.227 Å	109.6°

for C, 0 and 120 for H, 0 and 10 for O, 0 and 10 for N, 0 and 4 for S, and 0 and 1 for Fe, 0 and 6 for Cl, 0 and 3 for F, taking into account the isotope distributions) to those corresponding for the observed characteristic peaks, using the Formula Calculator routines from Agilent Technologies. In all cases the results confirmed the expected compositions. The results are given in Table S5. The target masses represent those calculated with the isotope mass of ^{54}Fe and the most abundant isotope mass for all other elements.

The ^{1}NMR of $[Fe(terpy)_2]^{2+}$agreed with the literature spectra by Elsbernd and Beattie.[36] (See Fig. S1 for the spectra of R = H and CN.) In the case of the substituted ligands, the replacement of the 4' H resulted in the removal of the splitting of the signal from the neighbouring 3' and 5' protons. These lines, which are found at the largest chemical shifts in the spectra, reflect very clearly the variations of the substituent groups, with values of δ(3',5')= 9.35, 9.21, 8.82, 8.39, 8.40 ppm, for R=SO_2Me, CN, H, SMe, OMe, respectively.

The UV-VIS spectra showed the characteristic bands of $[Fe(terpy)_2]^{2+}$in a slightly modified form because of the substitutions, these are described in detail in the next section.

For the TOAS studies, samples were made to have an absorbance around 0.7 at the maximum of the MLCT intensity between 450 and 650 nm, this typically corresponded to a 1 mM solution. Namely, the concentrations were what follows (listed in the format 'R: c/mM'): CN: 0.76, SO_2Me: 0.4, H: 0.8, SMe: 1.0, OMe: 0.9, $N(CH_2CH_2OH)_2$: 0.7.

5 Calculated and Measured UV-vis Spectra

The theoretical UV–vis spectra were calculated for all corresponding cases with time-dependent DFT (TD-DFT) using the Tamm-Dancroft Approximation (TDA);[30,37], again with the B3LYP* functional and the TZVP basis set. The calculated UV-vis spectra were broadened by a pseudo-Voigt function (with Lorentz and Gauss FWHMs of 900 $[cm]^{-1}$and 1000 $[cm]^{-1}$, respectively; an increased broadening was applied to the 330-460 nm range so that the final curve better matches the experiment). Experimental spectra were measured using a UV-vis spectrofotometer (Jasco V-550). The calculated and measured UV-vis spectra are displayed in Figs. S2 and S3. The calculations identify that the relevant bands above 300 nm all belong to MLCT transitions of different kinds, while below 300 nm ligand-centered transitions are present. The weak $d-d$ transitions are located between 500 nm and 600 nm. These bands are clearly present in the experiment. The agreement between the two sets is qualitative only, the calculations show larger spectral weight transfer in the MLCT bands, and sharper lines than what is measured, and the positions of the bands are shifted, and intensities can differ significantly. Yet the variation of the line shapes reproduces relevant trends in shifts and broadenings.

Most importantly, the MLCT bands most sensitive to the 4'-R substitution are found in the 300-350 nm region. Previous studies on Fe(II) complexes with Py-based ligands having an ED(EW) group in the 4 (γ) position of the Py ring revealed that such substituents modify the π acceptor character of the ring, which

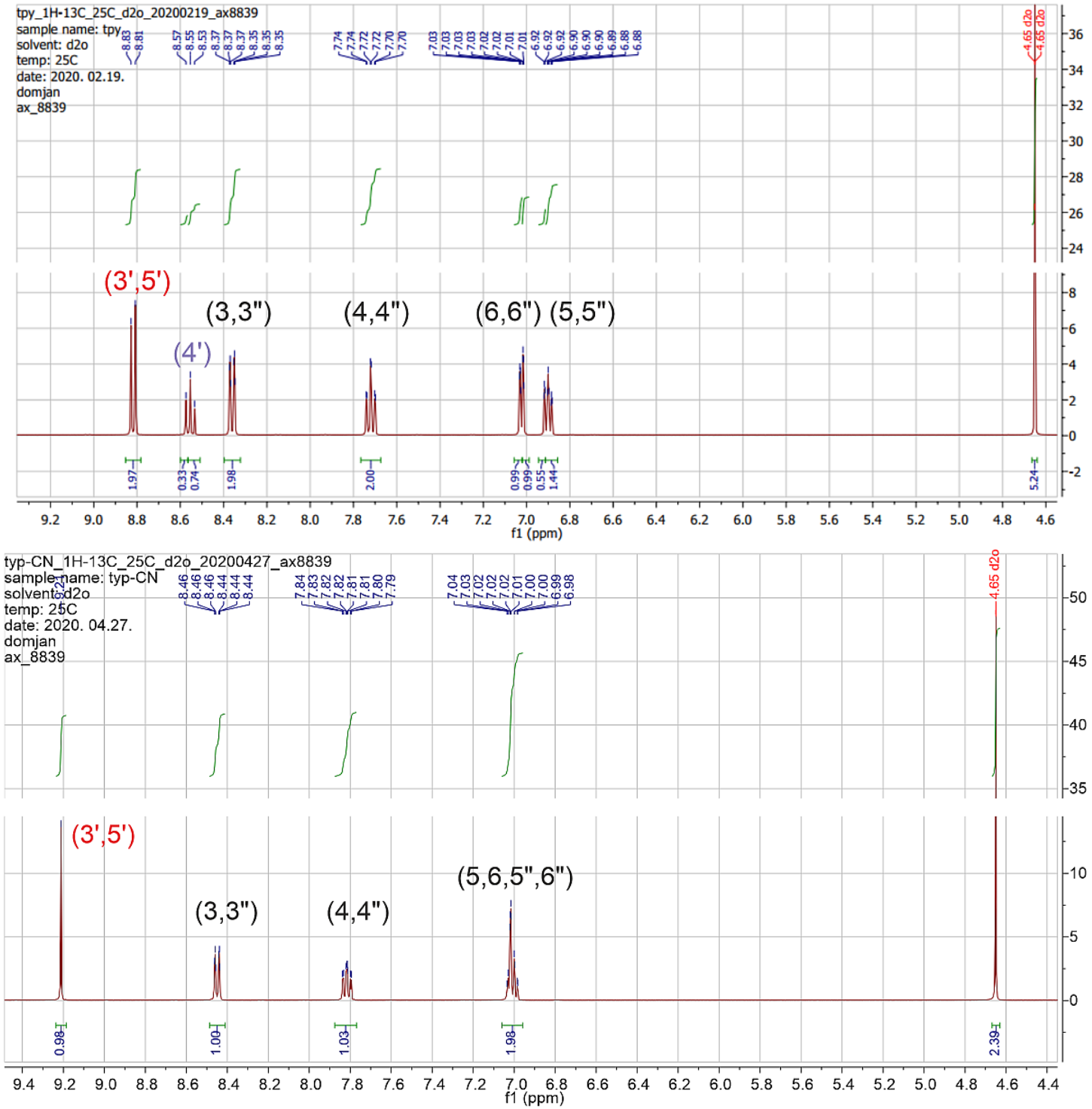

Figure S1: ^{1}H NMR spectrum of $[Fe(terpy)_2]^{2+}$(top) and $[Fe(4'\text{-}CN\text{-}terpy)_2]^{2+}$ (bottom).

Table S3: Selected structural parameters of the FeN_6 core for the MECP of the singlet and the quintet states in the studied $[Fe(4'\text{-R-terpy})_2]^{2+}$ complexes

	MECP		
R (substituent)	$r(Fe-N_{ax})$	$r(Fe-N_{eq})$	NNN
CN	2.046 Å	2.167 Å	107.40°
SO_2Me	2.053 Å	2.165 Å	107.11°
H	2.048 Å	2.168 Å	107.41°
SMe	2.038 Å	2.169 Å	107.84°
OMe	2.045 Å	2.159 Å	107.39°
$N(CH_2CH_2OH)_2$	2.036 Å	2.151 Å	107.54°

Table S4: B3LYP*/TZVP energies in atomic units for the singlet and quintet states, as well as for the singlet-quintet MECP for the studied $[Fe(4'\text{-R-terpy})_2]^{2+}$ complexes

R (substituent)	Singlet	Quintet	Singlet-Quintet MECP
CN	−2931.28856	−2931.26831	−2931.26482
SO_2Me	−3922.20927	−3922.18998	−3922.18595
H	−2746.94543	−2746.93042	−2746.92610
SMe	−3621.59477	−3621.57862	−3621.57303
OMe	−2975.83996	−2975.82583	−2975.81907
$N(CH_2CH_2OH)_2$	−3472.44405	−3472.43214	−3472.42512

Table S5: Elemental analysis for the studied complexes made with HPLC-HRMS

R (substituent)	Formula for the complex ion	Found	Target Mass	Difference (ppm)
CN	$FeC_{32}N_8H_{20}$	570.12192	570.12071	−2.13
SO_2Me	$FeC_{32}N_6O_4S_2H_{26}$	676.08511	676.08531	0.3
H	$FeC_{30}N_6H_{22}$	520.13013	520.13021	0.16
SMe	$FeC_{32}N_6S_2H_{26}$	612.10569	612.10565	−0.06
OMe	$FeC_{32}N_6O_2H_{26}$	580.15088	580.15134	0.79
$N(CH_2CH_2OH)_2$	$FeC_{38}N_8O_4H_{40}$	726.25696	726.25687	−0.14

results in blue(red) shift respectively of the affected MLCT bands in the UV-VIS spectra.[38]. The MLCT bands most sensitive to the 4'-R substitution are observed in the $300-350$ nm region of the spectra, which show systematic shifts with the substituent. Time-dependent DFT calculations (*vide supra*) confirm that in this region strong MLCT bands arise from transitions between molecular orbitals based on the Fe $3d_{xy}$ atomic orbital, which is less affected by the substitutions, and those having a strong weight from π^* orbitals on the 4'-R-substituted axial Py rings, which are largely affected, thus the energy of the transition is clearly tuned by the substituent. This MLCT band thus certainly reflects the EW/ED effect, and the experimental spectra and their variations are in agreement with theory. The transitions making up the other stronger MLCT bands have similar character ('less affected − less affected' or 'more affected − more affected') for the involved orbitals, therefore they do not show very systematic variations.

6 Transient Optical Absorption Spectroscopy

Transient absorption data were collected using a home-built pump-probe spectrometer. Laser pulses are derived from a home-built oscillator feeding a commercially-available regenerative chirped-pulse amplifier (Coherent Legend Elite He-USP). The Ti:Sa oscillator produces pulses with a central wavelength of 800 nm, 62 fs FWHM pulse duration, 400 mW power at a repetition rate of 80 MHz. After the Ti:Sa amplifier the power increases to 3 W with a reduced 1 kHz repetition rate. The beam of the pump arm is generated through second harmonic generation of the fundamental, while the white light in the probe arm is generated through supercontinuum generation, which is subsequently separated into probe and reference beams, the latter used for intensity monitoring. The pump and the probe pulse are split out from the original beam using a 25:75 (R:T) beam splitter for the pump path and a 1:99 (R:T) beam sampler for the probe path. For the pump beam, the second harmonic, at 400 nm, is generated by focusing the fundamental onto a BBO crystal (Eksma Optics, $\Theta = 29.2°$, $\phi = 90°$) with dimensions

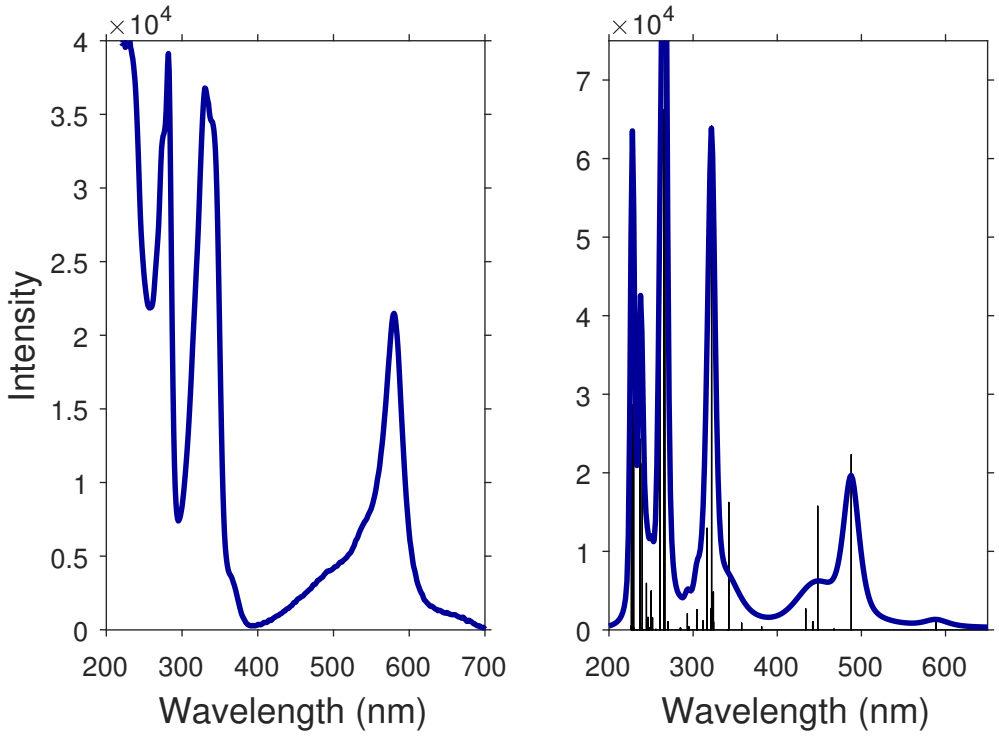

Figure S2: Experimental UV-VIS (left) and calculated (right) spectra of $[Fe(4'\text{-CN-terpy})_2]^{2+}$.

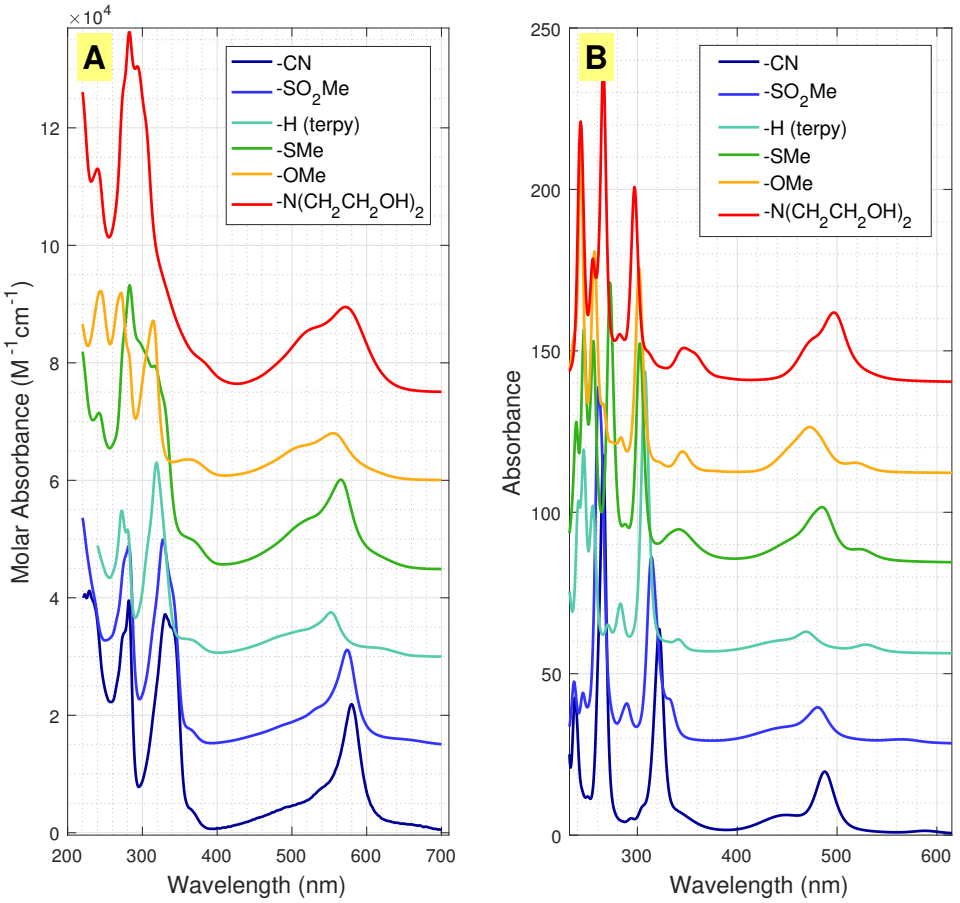

Figure S3: Experimental (A) and calculated (B) UV-VIS spectra of the studied derivatives of $[Fe(terpy)_2]^{2+}$.

$10 \times 10 \times 0.2\text{mm}^3$, cut for Type I phase matching. Second harmonic conversion efficiency is approximately 10%, resulting in approximately 35 μJ pump energy. The repetition rate of the pump pulse is reduced to 500 Hz using an optical chopper (Thorlabs, MC2000-EC), which allows only every second probe pulse to overlap with the pump pulse, leading to an alternating sequence of spectra taken with and without excitation. The pump beam is focused to a spot size of 650μm FWHM at the sample position using a 3000 mm focal length lens producing an intensity of 180 GW/cm^2.

The probe beam is directed onto two linear stages (Aerotech, ANT130-160-L-PLUS, 1 nm step size, 160 mm of travel and H2W Technologies, LSS-060-04-006-ME, 1 μm step size, 1542 mm of total travel, of which 1250 mm is currently used) which enables control of the relative time delay of the pump and probe pulses. The 1250 mm travel of the longer linear translation stage gives access to delay times up to 8 ns. When access to longer delay times is needed – as is the case some of the transients investigated here – we can shorten the path of the pump beam by approximately the same amount, which opens the 8-16 ns delay window. Accordingly, the data shown in Figure 3 of the main paper for R= H, SMe, OMe, and N(CH_2CH_2OH)$_2$ were spliced together from the results of two separate recordings (without and with shortened pump path, respectively).

A supercontinuum is generated by attenuating the probe to 1 mJ and then focusing it onto a 3 mm thick Sapphire crystal (Thorlabs) using a 150 mm focal length lens. Subsequently the white light continuum is collimated using a parabolic mirror (Altechna, 1-OPM-254-0508-26A01) and separated into the probe and the reference beams with a 50:50 (R:T) beam splitter. The reference beam is directed directly onto one of the two detectors. The probe beam is directed onto the sample position with a 500 mm focal length concave mirror to a spot size of 100μm FWHM. The pump and probe beams overlap under an angle of 4°. The relative polarization of the pump and probe beams is set to the magic angle (54.7°) by rotating the polarization of the 400 nm pump beam using a half wave plate (Thorlabs, WPH10M-405). The probe and reference spectra are detected using two identical imaging spectrographs (Horiba Jobin Yvon, CP 140-104) each equipped with a charged coupled device detector (CCD) (Hamamatsu, S7030-1006). Instrument control and data acquisition is performed with a home-developed LabView code.

The probe and reference spectra are collected for every shots. The transient absorbance is calculated from the spectra with pump on P_{ON} and pump off P_{OFF} using the equation that follows:

$$\begin{aligned}\Delta A(\lambda,t) &= A(\lambda,t)_{P_{ON}} - A(\lambda,t)_{P_{OFF}} \\ &= -log\frac{I(\lambda,t)_{ref,P_{ON}}}{I(\lambda,t)_{probe,P_{ON}}} \cdot \frac{I(\lambda,t)_{probe,P_{OFF}}}{I(\lambda,t)_{ref,P_{OFF}}}\end{aligned} \quad (1)$$

$I(\lambda,t)_{ref,P_{ON}}$ and $I(\lambda,t)_{ref,P_{OFF}}$ are the intensities of the reference beam when the sample is pumped and not pumped, and similarly $I(\lambda,t)_{probe,P_{ON}}$ and $I(\lambda,t)_{probe,P_{OFF}}$ are for the probe beam.

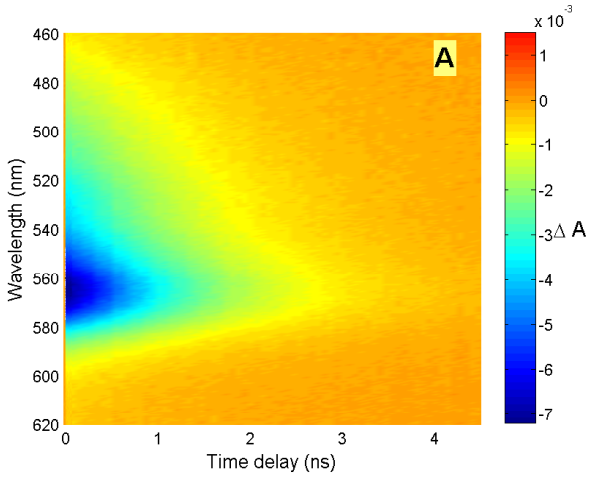

Figure S4: Transient optical absorption data of the aqueous solution of the complex with R=SO_2Me

A full set of transient data is shown in Fig. S4. Spectra from this data set at selected delays is shown in Fig. S5, together with the static GS spectrum in this region.

The lifetime of the quintet state was fitted using a single exponential curve.

$$\Delta A(\lambda,t) = \Delta A(\lambda) \cdot H(t) \cdot e^{-t/\tau} \quad (2)$$

where ΔA represents the transient absorption, H is the Heaviside step function (with which we take into account the excitation process) and τ is the lifetime of the quintet state. Points in the region of coherent artifacts were excluded from the fitting. Fig. S6 illustrates the fitting for the $[Fe(terpy)_2]^{2+}$.

7 APPENDIX A: Optimized geometries of the studied molecules (B3LYP*/TZVP)

The following lists contains the Cartesian coordinates of the studied molecules in the different spin states, and at the MECP

7.1 Singlet

7.1.1 $[Fe(terpy)_2]^{2+}$

Fe	1.000509	-0.852473	-0.227671
N	1.270093	-0.486905	-2.082363
N	2.101316	-2.467992	-0.725034
N	-0.011834	0.889815	-0.377577
N	0.718119	-1.201293	1.627914
N	-0.715831	-1.908859	-0.346111
N	2.625967	0.071562	0.533302

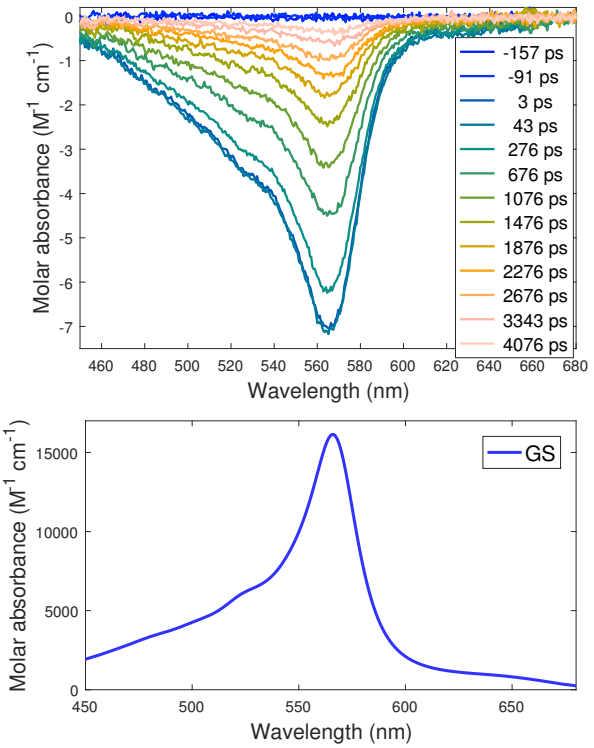

Figure S5: Comparison of the TOAS at selected delays (top), and the static absorption spectrum (bottom) for R=SO_2Me.

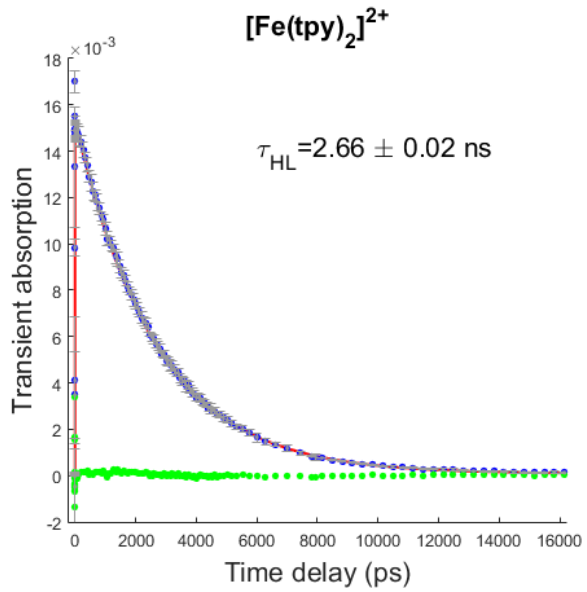

Figure S6: Example of the fitting on the $[Fe(terpy)_2]^{2+}$ data. Blue points represent the (negative) transient absorption data at the spectral maximum, the red line represents the fitted model curve (eq. 2), and the green points show the residuals. The negative data in the first picosecond is a consequence of the coherent artifacts.

H	-1.853779	4.215552	-1.108684
H	5.422125	1.826723	-0.100970
H	5.604061	1.694188	2.399817
H	-0.647276	3.022909	-2.923001
C	-1.337552	3.285082	-0.902479
C	4.673301	1.315422	0.492040
H	-1.844283	3.224344	1.199918
C	-0.663935	2.617841	-1.918480
C	4.770292	1.239745	1.876695
C	-1.335201	2.739473	0.375870
H	0.481334	1.806200	-4.411843
H	3.486679	0.761707	-1.217353
C	3.588465	0.719236	-0.139555
C	0.914440	0.917422	-3.970277
C	-0.009915	1.423327	-1.632843
C	3.780143	0.568721	2.584792
H	3.833796	0.491295	3.664107
C	-0.661814	1.544471	0.595194
C	1.667843	0.040204	-4.746184
C	0.733284	0.628036	-2.619734
H	-0.642683	1.096983	1.581480
C	2.717120	-0.004507	1.892374
C	2.213883	-1.107015	-4.176246
H	2.795873	-1.793588	-4.778152
H	2.109092	-0.559163	4.621230
C	1.990689	-1.353239	-2.823752
C	1.605968	-0.729145	2.527776
C	1.406091	-0.939125	3.890541
C	2.461714	-2.504560	-2.040380
H	3.481337	-3.563709	-3.611415
C	0.275811	-1.643958	4.298997
C	3.208294	-3.555818	-2.563421
C	-0.381538	-1.883736	2.007964
H	-0.976720	-1.924123	-2.396890
C	2.493811	-3.469686	0.075025
C	-0.629913	-2.124547	3.357060
C	-1.394572	-2.247132	-1.451619
H	2.195195	-3.406792	1.114094
C	-1.206987	-2.298911	0.865046
C	3.603247	-4.591801	-1.725928
C	3.241811	-4.547114	-0.384086
H	-1.508719	-2.672812	3.672771
H	4.185288	-5.418443	-2.117607
C	-2.577289	-2.974655	-1.411279
H	3.532001	-5.329634	0.306509
C	-2.388477	-3.025790	0.974627
H	-3.083225	-3.223309	-2.336307
H	-2.760198	-3.320780	1.948072
C	-3.083433	-3.369958	-0.178546
H	-4.004749	-3.937296	-0.112550
H	0.099151	-1.819180	5.354071
H	1.831082	0.251712	-5.796721

7.1.2 $[Fe(4'\text{-CN-terpy})_2]^{2+}$

Fe	0.000371	-0.006765	-0.000110
N	0.004813	-0.002172	-1.903511
N	1.373713	-1.445723	-0.326818
N	-1.371265	1.433846	-0.326182
N	-0.004103	-0.011519	1.903290
N	-1.440076	-1.380242	0.319424
N	1.439139	1.365071	0.333140
C	-3.209728	3.382704	-1.098047

C	3.130032	2.964464	-0.230451
C	-2.516009	2.654092	-2.057587
C	3.383737	3.204049	1.114563
C	-2.969884	3.122632	0.245709
C	2.152520	2.039781	-0.579032
C	-0.828823	0.883790	-3.946892
C	-1.603727	1.687614	-1.646250
C	2.650737	2.509966	2.070475
C	-2.045389	2.143258	0.589492
C	0.010078	0.003395	-4.639995
C	-0.807582	0.854694	-2.557684
C	1.686570	1.597374	1.654407
C	0.846499	-0.879613	-3.947253
C	0.819813	-0.856279	-2.558041
C	0.849608	0.800797	2.561709
C	0.872546	0.821380	3.951013
C	1.611951	-1.693425	-1.646999
C	-0.010671	-0.018115	4.639768
C	2.526005	-2.658067	-2.058775
C	-0.860927	-0.827033	2.553571
C	2.044114	-2.159064	0.588543
C	-0.890504	-0.854290	3.942681
C	-2.148927	-2.050597	-0.599438
C	-1.693498	-1.619280	1.638404
C	3.215491	-3.391096	-1.099550
C	2.969953	-3.137026	0.244323
C	-3.127492	-2.977559	-0.260012
C	-2.659092	-2.534443	2.045454
C	-3.387234	-3.224080	1.082600
H	-3.923644	4.140711	-1.398999
H	3.676676	3.480103	-1.010585
H	4.140056	3.918139	1.419326
H	-2.684507	2.838897	-3.111494
H	-3.485200	3.665709	1.028542
H	-1.474164	1.565331	-4.485296
H	1.935598	1.834380	-1.619768
H	2.830248	2.678575	3.125275
H	-1.839372	1.921759	1.629142
H	1.493831	-1.559058	-4.485898
H	1.551674	1.466531	4.492679
H	2.699288	-2.837926	-3.112764
H	-1.927309	-1.839753	-1.638096
H	1.833829	-1.942067	1.628288
H	-1.572244	-1.501985	4.477985
H	3.930638	-4.147778	-1.400949
H	3.481959	-3.683624	1.026880
H	-3.670258	-3.489625	-1.045197
H	-2.843501	-2.708401	3.098548
H	-4.144535	-3.940158	1.380164
C	0.012488	0.005893	-6.069789
C	-0.013931	-0.021372	6.069554
N	0.014440	0.007783	-7.225113
N	-0.016301	-0.023750	7.224875

7.1.3 $[Fe(4'\text{-}SO_2Me\text{-}terpy)_2]^{2+}$

Fe	0.917860	-0.689128	-0.204129
N	1.115393	-0.391007	-2.076565
N	2.133037	-2.231262	-0.653857
N	-0.232709	0.953540	-0.396825
N	0.719504	-0.985517	1.668508
N	-0.700934	-1.887612	-0.232691
N	2.466554	0.411015	0.466456
H	-2.339938	4.096338	-1.210989
H	5.054652	2.401692	-0.322891
H	5.309236	2.406112	2.175271
H	-1.091568	2.921648	-3.010799
C	-1.749680	3.216213	-0.982802
C	4.375632	1.847431	0.313728
H	-2.203411	3.203646	1.131953
C	-1.051786	2.560249	-1.990462
C	4.513306	1.847204	1.696502
C	-1.676655	2.725230	0.315117
H	0.084162	1.724563	-4.482649
H	3.211124	1.101768	-1.335814
C	3.341446	1.118289	-0.260907
C	0.598785	0.898415	-4.008458
C	-0.302325	1.433346	-1.671523
C	3.611816	1.116683	2.462173
H	3.696253	1.099696	3.541914
C	-0.909098	1.594098	0.565917
C	1.395153	0.032432	-4.746722
C	0.477982	0.655279	-2.641919
H	-0.834738	1.190656	1.568098
C	2.599652	0.408565	1.823779
C	2.044241	-1.049511	-4.165837
H	2.643834	-1.726108	-4.761666
H	2.146980	-0.118160	4.590595
C	1.882462	-1.237258	-2.794846
C	1.589233	-0.399755	2.517730
C	1.467713	-0.590800	3.892442
C	2.470752	-2.302597	-1.973275
H	3.554090	-3.339624	-3.516741
C	0.431845	-1.401336	4.338881
C	3.300081	-3.304784	-2.464375
C	-0.292297	-1.765750	2.102360
H	-1.032080	-1.977543	-2.272633
C	2.620126	-3.157719	0.182215
C	-0.468724	-1.996724	3.464920
C	-1.384121	-2.311058	-1.304372
H	2.335056	-3.075682	1.223718
C	-1.114626	-2.287892	1.003662
C	3.798823	-4.260862	-1.586949
C	3.453248	-4.185565	-0.243067
H	-1.282635	-2.608140	3.833552
H	4.446735	-5.050405	-1.950182
C	-2.495252	-3.139799	-1.203863
H	3.818146	-4.908079	0.476917
C	-2.218153	-3.116413	1.174429
H	-3.010395	-3.451869	-2.104305
H	-2.527621	-3.420236	2.167010
C	-2.919370	-3.548932	0.054605
H	-3.782583	-4.195017	0.166668
C	1.217365	-3.125306	6.494800
H	2.253064	-2.908358	6.233871
H	0.820357	-3.958718	5.915461
C	3.002921	1.381187	-6.704595
H	2.795612	2.308934	-6.171526
H	3.867065	0.861384	-6.291194
H	1.109581	-3.303014	7.566021

H	3.124902	1.559867	-7.774138
S	0.224614	-1.662593	6.136365
O	-1.210454	-1.980451	6.368168
O	0.827229	-0.486536	6.820443
S	1.565082	0.303640	-6.546641
O	1.877213	-1.016170	-7.158920
O	0.352747	1.042148	-6.992772

7.1.4 $[Fe(4'\text{-}SMe\text{-}terpy)_2]^{2+}$

Fe	0.991496	-0.855248	-0.229883
N	1.264979	-0.481483	-2.081502
N	2.084561	-2.472558	-0.740020
N	-0.026387	0.886130	-0.382485
N	0.722041	-1.195331	1.628072
N	-0.722721	-1.918204	-0.326356
N	2.623211	0.070094	0.522971
H	-1.861188	4.216486	-1.115546
H	5.422673	1.815526	-0.126076
H	5.605527	1.703783	2.375987
H	-0.605481	3.052764	-2.913165
C	-1.347680	3.284762	-0.908505
C	4.673365	1.310304	0.471428
H	-1.912635	3.189996	1.177422
C	-0.646486	2.632843	-1.915551
C	4.771494	1.245841	1.856428
C	-1.378510	2.719647	0.360847
H	0.551031	1.877079	-4.358015
H	3.484916	0.745630	-1.232709
C	3.586904	0.711075	-0.154713
C	0.971651	0.968953	-3.949338
C	0.002505	1.436099	-1.630428
C	3.781186	0.580718	2.569384
H	3.836303	0.512246	3.649142
C	-0.704839	1.524868	0.581362
C	1.728809	0.099777	-4.743517
C	0.760154	0.647358	-2.613348
H	-0.709344	1.063483	1.561325
C	2.717622	0.003051	1.882419
C	2.240483	-1.076884	-4.168647
H	2.829399	-1.764039	-4.764421
H	2.141890	-0.519207	4.591780
C	1.987897	-1.341005	-2.831975
C	1.607536	-0.719779	2.523857
C	1.424541	-0.916844	3.887928
C	2.445604	-2.506127	-2.055794
H	3.456844	-3.570070	-3.629653
C	0.296432	-1.622109	4.323966
C	3.182033	-3.562852	-2.582081
C	-0.375400	-1.874480	2.026488
H	-0.987486	-1.950404	-2.375661
C	2.465768	-3.482205	0.055853
C	-0.617226	-2.105849	3.370732
C	-1.400897	-2.271571	-1.427685
H	2.166062	-3.420166	1.094725
C	-1.206132	-2.304419	0.889574
C	3.565661	-4.606733	-1.748669
C	3.203186	-4.565065	-0.407011
H	-1.495554	-2.656531	3.686147
H	4.139954	-5.437397	-2.143331
C	-2.575301	-3.011803	-1.379060
H	3.484369	-5.353908	0.280246
C	-2.379507	-3.042866	1.007149
H	-3.080575	-3.273747	-2.300833
H	-2.746481	-3.335730	1.983139
C	-3.073523	-3.403356	-0.141858
H	-3.987933	-3.981036	-0.069234
S	-0.070261	-1.951670	6.022279
C	1.387391	-1.314799	6.923230
H	1.466407	-0.231027	6.836219
H	2.296855	-1.807996	6.580759
S	2.092759	0.387086	-6.451351
C	1.469753	2.080861	-6.757888
H	0.382850	2.123952	-6.683885
H	1.942094	2.792594	-6.081491
H	1.203324	-1.580338	7.964996
H	1.771047	2.303113	-7.782052

7.1.5 $[Fe(4'\text{-}OMe\text{-}terpy)_2]^{2+}$

Fe	1.081156	-0.785886	-0.206651
N	1.309103	-0.388019	-2.062304
N	2.175762	-2.390470	-0.757711
N	0.081419	0.965780	-0.311972
N	0.810527	-1.185889	1.642524
N	-0.642406	-1.834526	-0.338867
N	2.708911	0.113577	0.579572
H	-1.763852	4.310352	-0.942344
H	5.507462	1.878293	-0.019076
H	5.700986	1.675536	2.475799
H	-0.655116	3.117058	-2.816018
C	-1.245709	3.375094	-0.764442
C	4.759682	1.352974	0.563009
H	-1.648951	3.312967	1.360209
C	-0.625580	2.706922	-1.813827
C	4.862852	1.238882	1.944521
C	-1.185388	2.825783	0.510904
H	0.372113	1.892644	-4.344609
H	3.562123	0.847442	-1.155293
C	3.670343	0.776698	-0.079502
C	0.840792	1.006561	-3.940232
C	0.034204	1.507514	-1.563668
C	3.873473	0.551727	2.638738
H	3.933942	0.443717	3.715119
C	-0.515581	1.622596	0.692951
C	1.556683	0.121968	-4.757603
C	0.740200	0.714103	-2.583190
H	-0.453633	1.169053	1.674681
C	2.804734	0.001810	1.936822
C	2.140406	-1.025498	-4.196751
H	2.684270	-1.707060	-4.838351
H	2.209045	-0.592478	4.640252
C	1.992742	-1.254275	-2.841854
C	1.690488	-0.737620	2.556392
C	1.501052	-0.969344	3.915902
C	2.499394	-2.409132	-2.083042
H	3.483726	-3.438572	-3.695342
C	0.369377	-1.695376	4.312642

C	3.240116	-3.446612	-2.639982
C	-0.287900	-1.880053	2.013047
H	-0.924137	-1.788453	-2.386397
C	2.598494	-3.399648	0.017710
C	-0.534915	-2.160090	3.343701
C	-1.335339	-2.135365	-1.446842
H	2.328755	-3.350764	1.065495
C	-1.125829	-2.257459	0.863985
C	3.665286	-4.490709	-1.827927
C	3.340808	-4.465546	-0.475975
H	-1.407374	-2.717752	3.660037
H	4.242693	-5.307383	-2.246499
C	-2.523264	-2.854334	-1.417090
H	3.655683	-5.254851	0.195817
C	-2.312525	-2.976889	0.963617
H	-3.039678	-3.071500	-2.344323
H	-2.678169	-3.295737	1.931873
C	-3.021933	-3.281162	-0.191841
H	-3.947948	-3.841612	-0.133374
O	0.063427	-1.995888	5.585582
C	0.877091	-1.466193	6.650717
H	0.858059	-0.372853	6.638830
H	1.903879	-1.833075	6.574603
O	1.734438	0.280312	-6.079032
C	1.172240	1.439114	-6.728529
H	0.081922	1.437348	-6.645984
H	1.586179	2.356001	-6.301664
H	0.422652	-1.834770	7.567711
H	1.465567	1.352300	-7.772537

7.1.6 $[Fe(4'\text{-}N(CH_2CH_2OH)_2\text{-}terpy)_2]^{2+}$

Fe	0.232267	0.053031	-0.090931
N	0.182679	0.167628	-1.999405
N	1.952447	-0.900451	-0.540585
N	-1.513652	1.038083	-0.332758
N	0.259692	-0.046437	1.818568
N	-0.738154	-1.693780	0.176167
N	1.218086	1.763418	0.331192
C	-3.877787	2.367703	-0.966646
C	2.358883	3.814067	-0.149843
C	-3.014479	1.951954	-1.972787
C	2.538206	4.054377	1.207370
C	-3.542666	2.108813	0.357290
C	1.696401	2.659246	-0.544633
C	-0.938546	0.859921	-3.984422
C	-1.840573	1.285365	-1.634101
C	2.050198	3.131575	2.124379
C	-2.353131	1.446800	0.629633
C	0.082515	0.295727	-4.795668
C	-0.855057	0.777488	-2.607259
C	1.391661	1.994868	1.664862
C	1.171651	-0.314158	-4.114596
C	1.180012	-0.367153	-2.732169
C	0.824303	0.946614	2.534446
C	0.818880	0.934678	3.917657
C	2.212662	-0.985979	-1.878189
C	0.217398	-0.145878	4.615745
C	3.356565	-1.618545	-2.355348
C	-0.336766	-1.081264	2.443467
C	2.826711	-1.441700	0.320122
C	-0.382069	-1.161498	3.823387
C	-1.215382	-2.508292	-0.775871
C	-0.905048	-2.047190	1.483896
C	4.256087	-2.173950	-1.453521
C	3.985909	-2.085326	-0.092608
C	-1.871699	-3.697239	-0.487364
C	-1.557333	-3.224195	1.839120
C	-2.046729	-4.060458	0.842974
H	-4.795636	2.888057	-1.215747
H	2.724845	4.504352	-0.900245
H	3.053400	4.944336	1.550654
H	-3.252446	2.149557	-3.010821
H	-4.183660	2.415589	1.174945
H	-1.794263	1.344361	-4.429463
H	1.541861	2.439454	-1.593814
H	2.183602	3.296375	3.186282
H	-2.058850	1.234150	1.650029
H	1.989858	-0.756282	-4.663035
H	1.274865	1.753760	4.452643
H	3.543686	-1.679800	-3.420146
H	-1.065123	-2.193293	-1.801284
H	2.584508	-1.354848	1.372344
H	-0.882678	-1.999012	4.284240
H	5.150959	-2.670610	-1.811108
H	4.657082	-2.505837	0.646451
H	-2.236698	-4.317534	-1.296998
H	-1.684099	-3.487645	2.881900
H	-2.557738	-4.980009	1.104875
N	0.221662	-0.212658	5.980878
N	0.009863	0.330613	-6.156790
C	0.833090	0.842231	6.794176
H	1.157396	0.388991	7.733636
H	1.732913	1.219428	6.303882
C	-0.396133	-1.342506	6.681541
H	-0.183245	-2.271537	6.147181
H	0.082016	-1.429478	7.659096
C	-1.917981	-1.199771	6.856854
H	-2.149209	-0.383608	7.549736
H	-2.388348	-0.964832	5.899266
C	-0.112699	2.014283	7.099687
H	-0.513426	2.437130	6.174915
H	-0.958674	1.666365	7.703804
C	1.026297	-0.306788	-7.001333
H	1.369387	-1.235963	-6.539173
H	0.540509	-0.595037	-7.936884
C	-1.138609	0.929392	-6.840518
H	-0.811656	1.236287	-7.834157
H	-1.453098	1.840561	-6.327699
C	-2.322113	-0.032373	-6.963522
H	-2.040683	-0.889595	-7.587037
H	-2.609623	-0.412133	-5.974955
C	2.237129	0.572132	-7.320149
H	2.686473	0.959131	-6.402414
H	2.984990	-0.050291	-7.826850
O	1.911711	1.719473	-8.111467
H	1.692650	1.420401	-9.005875
O	-3.395987	0.700609	-7.558392

H	-4.154121	0.105961	-7.649476
O	-2.507179	-2.424319	7.300709
H	-2.267251	-2.566527	8.227918
O	0.581268	3.074351	7.761202
H	0.770970	2.801506	8.670566

7.2 Quintet

7.2.1 $[Fe(terpy)_2]^{2+}$

Fe	0.898670	-0.898856	-0.247264
N	1.255836	-0.463628	-2.323559
N	2.075367	-2.617867	-1.043389
N	-0.284290	0.939033	-0.712196
N	0.676864	-1.247688	1.865439
N	-0.962764	-2.073647	-0.018664
N	2.654453	0.065429	0.733074
H	-2.124769	4.173011	-1.747302
H	5.494260	1.768986	0.148703
H	5.646878	1.576370	2.647780
H	-0.620310	3.024378	-3.342492
C	-1.610393	3.265343	-1.452412
C	4.728244	1.262348	0.723512
H	-2.437253	3.194881	0.546414
C	-0.766183	2.619638	-2.349122
C	4.807824	1.153424	2.106590
C	-1.785563	2.728239	-0.182442
H	0.663776	1.933051	-4.607299
H	3.534647	0.764299	-1.001610
C	3.632163	0.701486	0.077257
C	1.061972	1.028166	-4.167743
C	-0.119034	1.451328	-1.952461
C	3.796690	0.489632	2.793863
H	3.848835	0.390146	3.870801
C	-1.100866	1.563221	0.144018
C	1.889490	0.196610	-4.913853
C	0.759832	0.666728	-2.854915
H	-1.212079	1.113999	1.125597
C	2.725567	-0.042557	2.078517
C	2.390452	-0.972252	-4.352489
H	3.031307	-1.621982	-4.933936
H	2.184904	-0.548305	4.789430
C	2.045072	-1.284451	-3.037812
C	1.595482	-0.762196	2.719029
C	1.455614	-0.942219	4.093731
C	2.488366	-2.508922	-2.326175
H	3.588365	-3.402278	-3.955301
C	0.347204	-1.640350	4.564380
C	3.266928	-3.496853	-2.926160
C	-0.398475	-1.923892	2.305641
H	-1.423902	-2.178140	-2.030517
C	2.431292	-3.697154	-0.336941
C	-0.590975	-2.141351	3.670965
C	-1.746280	-2.460941	-1.033608
H	2.078697	-3.742998	0.687971
C	-1.320499	-2.395549	1.245442
C	3.631907	-4.615967	-2.185935
C	3.211206	-4.719809	-0.865315
H	-1.450003	-2.688599	4.036452
H	4.237462	-5.393571	-2.638292
C	-2.916455	-3.186223	-0.845089
H	3.475676	-5.571972	-0.250750
C	-2.482705	-3.119495	1.511619
H	-3.514663	-3.478955	-1.699515
H	-2.760562	-3.370944	2.527141
C	-3.287878	-3.521335	0.452473
H	-4.192773	-4.087639	0.641865
H	0.215819	-1.794985	5.629592
H	2.146367	0.461221	-5.933258

7.2.2 $[Fe(4'\text{-}CN\text{-}terpy)_2]^{2+}$

Fe	0.991520	-0.807617	-0.215402
N	1.330116	-0.353681	-2.260927
N	2.248921	-2.470416	-0.981473
N	-0.172523	1.047649	-0.606567
N	0.755330	-1.223365	1.851159
N	-0.914342	-1.922151	-0.061748
N	2.771858	0.081433	0.765286
H	-2.021565	4.292401	-1.585165
H	5.624445	1.787256	0.260770
H	5.766232	1.492753	2.750318
H	-0.605692	3.116978	-3.236691
C	-1.501694	3.383137	-1.305060
C	4.852089	1.264876	0.812033
H	-2.228554	3.345662	0.732759
C	-0.707562	2.720511	-2.234689
C	4.925825	1.099297	2.189735
C	-1.618782	2.863544	-0.021597
H	0.596188	2.001764	-4.549266
H	3.667188	0.838007	-0.937263
C	3.756539	0.736651	0.138982
C	1.030673	1.114177	-4.110608
C	-0.056317	1.548311	-1.858467
C	3.907156	0.417819	2.847458
H	3.956096	0.277588	3.919705
C	-0.934627	1.692828	0.283993
C	1.858744	0.286954	-4.873406
C	0.790966	0.760830	-2.785298
H	-1.004839	1.253433	1.273392
C	2.834897	-0.076982	2.107984
C	2.415785	-0.865998	-4.316197
H	3.056142	-1.502039	-4.911449
H	2.295937	-0.687299	4.794441
C	2.114486	-1.166947	-2.990482
C	1.692144	-0.798229	2.717854
C	1.555422	-1.028208	4.084235
C	2.595962	-2.378738	-2.286462
H	3.605800	-3.299475	-3.959547
C	0.421103	-1.713100	4.526875
C	3.333010	-3.379794	-2.915082
C	-0.342620	-1.879624	2.265924
H	-1.368039	-1.948318	-2.077726
C	2.624989	-3.548994	-0.283357
C	-0.544749	-2.148865	3.616635
C	-1.696245	-2.264209	-1.093237
H	2.332685	-3.578234	0.760773
C	-1.278223	-2.284532	1.190602
C	3.714586	-4.499939	-2.184614

C	3.355166	-4.589861	-0.845095
H	-1.419185	-2.680988	3.965130
H	4.285045	-5.289820	-2.660042
C	-2.875936	-2.981066	-0.932250
H	3.635111	-5.442858	-0.238784
C	-2.453007	-2.994515	1.428820
H	-3.474896	-3.237602	-1.797666
H	-2.742490	-3.274858	2.433513
C	-3.259464	-3.347375	0.352375
H	-4.175252	-3.903012	0.519717
C	2.141185	0.625462	-6.234801
C	0.245586	-1.973816	5.922602
N	0.102137	-2.188444	7.048216
N	2.372232	0.898015	-7.333011

7.2.3 $[Fe(4'\text{-}SO_2Me\text{-}terpy)_2]^{2+}$

Fe	1.158612	-0.747809	-0.188628
N	1.425592	-0.221083	-2.234588
N	2.179723	-2.482552	-1.111873
N	0.289254	1.278295	-0.389339
N	0.900368	-1.273050	1.858360
N	-0.747377	-1.871072	-0.109773
N	2.927188	0.080786	0.856603
H	-1.245408	4.754656	-1.066563
H	5.833623	1.719794	0.450331
H	5.945591	1.309307	2.925226
H	-0.154997	3.495295	-2.895726
C	-0.816749	3.777694	-0.873057
C	5.042744	1.193638	0.971264
H	-1.343252	3.733190	1.225399
C	-0.202839	3.070245	-1.901215
C	5.100034	0.964222	2.340751
C	-0.873667	3.216430	0.397066
H	0.843824	2.331057	-4.352903
H	3.848268	0.902384	-0.800364
C	3.934490	0.736040	0.268138
C	1.166808	1.363257	-3.992447
C	0.340930	1.816784	-1.630051
C	4.057146	0.282769	2.959281
H	4.091106	0.095853	4.025015
C	-0.304748	1.963723	0.594466
C	1.780410	0.458859	-4.845119
C	0.995335	0.978157	-2.661424
H	-0.321451	1.495099	1.572712
C	2.981160	-0.152049	2.188787
C	2.229872	-0.776562	-4.405141
H	2.726621	-1.457800	-5.083200
H	2.446137	-0.958639	4.833425
C	2.032225	-1.091272	-3.059551
C	1.834320	-0.903266	2.750872
C	1.701120	-1.237441	4.099836
C	2.468582	-2.358857	-2.428399
H	3.365206	-3.257913	-4.176025
C	0.579252	-1.962117	4.470866
C	3.141749	-3.362130	-3.121758
C	-0.184477	-1.979315	2.218994
H	-1.208915	-1.743438	-2.119847
C	2.557699	-3.589875	-0.462763
C	-0.377963	-2.356798	3.549028
C	-1.549792	-2.103784	-1.155047
H	2.303532	-3.647243	0.590333
C	-1.122078	-2.301142	1.117689
C	3.530386	-4.510845	-2.440599
C	3.238186	-4.628720	-1.086940
H	-1.234611	-2.941889	3.856757
H	4.055546	-5.301548	-2.964617
C	-2.760658	-2.775608	-1.035012
H	3.523179	-5.506209	-0.519098
C	-2.319129	-2.986263	1.313241
H	-3.376186	-2.940889	-1.911134
H	-2.610653	-3.329143	2.297864
C	-3.147056	-3.226208	0.221648
H	-4.082529	-3.757898	0.355781
C	-0.581903	-1.098841	6.949577
H	-1.539663	-1.042837	6.432539
H	-0.010171	-0.177175	6.843123
C	0.555493	0.330857	-7.437042
H	0.498487	-0.749857	-7.307269
H	-0.308383	0.836185	-7.005308
H	-0.715624	-1.361092	8.000367
H	0.683341	0.595894	-8.487812
S	0.375142	-2.444935	6.225013
O	-0.441833	-3.688414	6.242483
O	1.732764	-2.460389	6.833748
S	2.037018	0.924355	-6.596930
O	2.067152	2.410973	-6.653388
O	3.214273	0.155849	-7.084390

7.2.4 $[Fe(4'\text{-}SMe\text{-}terpy)_2]^{2+}$

Fe	0.856275	-0.939449	-0.262655
N	1.271436	-0.447955	-2.309648
N	2.036745	-2.642505	-1.087280
N	-0.309820	0.917084	-0.719638
N	0.668274	-1.230157	1.856599
N	-1.000618	-2.113244	0.034512
N	2.652421	0.025729	0.676798
H	-2.259206	4.071696	-1.801145
H	5.500074	1.698350	0.035120
H	5.650502	1.598275	2.540939
H	-0.636438	3.014754	-3.340689
C	-1.712187	3.188289	-1.491679
C	4.732215	1.215737	0.627906
H	-2.620200	3.052687	0.467743
C	-0.799319	2.595362	-2.356491
C	4.811762	1.157224	2.013975
C	-1.915384	2.627094	-0.236406
H	0.888881	2.112871	-4.446385
H	3.538535	0.662819	-1.078032
C	3.633880	0.636159	0.002249
C	1.249180	1.169103	-4.063331
C	-0.113739	1.455396	-1.943595
C	3.798324	0.520237	2.721331
H	3.848645	0.462130	3.801026
C	-1.190658	1.491536	0.107269
C	2.130914	0.380312	-4.809884
C	0.836082	0.717667	-2.814632
H	-1.322397	1.025170	1.078155
C	2.727484	-0.037273	2.024425
C	2.553190	-0.848585	-4.277318

H	3.230895	-1.478167	-4.840583
H	2.257647	-0.486835	4.718990
C	2.103052	-1.232771	-3.023463
C	1.600152	-0.738852	2.690081
C	1.496570	-0.892422	4.068540
C	2.487540	-2.501767	-2.353922
H	3.600296	-3.375084	-3.986067
C	0.392368	-1.572453	4.593852
C	3.249546	-3.493468	-2.968958
C	-0.401526	-1.891409	2.343678
H	-1.476936	-2.282601	-1.969169
C	2.338185	-3.757416	-0.410703
C	-0.571649	-2.078324	3.706720
C	-1.792126	-2.532549	-0.961198
H	1.957441	-3.826929	0.602902
C	-1.344540	-2.393768	1.311577
C	3.556681	-4.650030	-2.260511
C	3.097479	-4.786370	-0.955527
H	-1.430089	-2.615889	4.089496
H	4.147346	-5.432172	-2.724617
C	-2.960251	-3.251472	-0.738589
H	3.317174	-5.668214	-0.365461
C	-2.503206	-3.109252	1.611649
H	-3.566109	-3.572585	-1.577231
H	-2.771939	-3.330779	2.636702
C	-3.318449	-3.544102	0.572754
H	-4.220914	-4.104703	0.788954
S	0.122590	-1.847712	6.315521
C	1.631705	-1.192999	7.114316
H	1.703962	-0.111623	6.998689
H	2.518063	-1.694230	6.726558
S	2.762739	0.828977	-6.395173
C	2.102782	2.511218	-6.684706
H	1.015844	2.499489	-6.765578
H	2.436949	3.197407	-5.906868
H	1.511840	-1.437580	8.170430
H	2.533064	2.812205	-7.640207

7.2.5 $[Fe(4'\text{-}OMe\text{-}terpy)_2]^{2+}$

Fe	0.975731	-0.910573	-0.242666
N	1.304513	-0.374929	-2.287001
N	2.169892	-2.567436	-1.127691
N	-0.147361	0.990553	-0.576868
N	0.754912	-1.255906	1.857219
N	-0.886410	-2.095461	-0.014748
N	2.747373	0.036349	0.739106
H	-1.913596	4.326858	-1.394503
H	5.624015	1.683174	0.167385
H	5.742376	1.526078	2.671146
H	-0.534121	3.190814	-3.104536
C	-1.420352	3.390282	-1.160659
C	4.842147	1.198354	0.739908
H	-2.147567	3.271268	0.874442
C	-0.646064	2.750283	-2.121931
C	4.902809	1.109630	2.125676
C	-1.552228	2.810186	0.095575
H	0.619946	2.108690	-4.444139
H	3.661392	0.694756	-0.992592
C	3.744833	0.646253	0.088243
C	1.039810	1.185641	-4.073804
C	-0.022743	1.545695	-1.802564
C	3.871366	0.473525	2.808455
H	3.909141	0.389281	3.887359
C	-0.895841	1.610055	0.342496
C	1.835670	0.375623	-4.891829
C	0.800767	0.772663	-2.767511
H	-0.972034	1.127566	1.311532
C	2.800720	-0.051906	2.086575
C	2.353954	-0.822897	-4.377873
H	2.964072	-1.446100	-5.018621
H	2.204814	-0.432364	4.776622
C	2.062884	-1.169751	-3.071126
C	1.647899	-0.744374	2.720178
C	1.482684	-0.859157	4.096625
C	2.537868	-2.417182	-2.419378
H	3.591641	-3.250794	-4.110003
C	0.350688	-1.530033	4.575340
C	3.302870	-3.380242	-3.074813
C	-0.335402	-1.910855	2.309097
H	-1.330127	-2.221216	-2.028790
C	2.554439	-3.665718	-0.465762
C	-0.569786	-2.066594	3.662294
C	-1.650413	-2.510537	-1.033075
H	2.237924	-3.743474	0.569230
C	-1.240433	-2.421083	1.247915
C	3.696282	-4.519861	-2.382089
C	3.319445	-4.667000	-1.051914
H	-1.440233	-2.585820	4.040987
H	4.290840	-5.279620	-2.877296
C	-2.797809	-3.272220	-0.847586
H	3.608222	-5.536552	-0.473583
C	-2.377459	-3.183404	1.511781
H	-3.382343	-3.587288	-1.703506
H	-2.649691	-3.444477	2.526552
C	-3.163435	-3.615231	0.449424
H	-4.048953	-4.212278	0.636463
O	0.059755	-1.703141	5.870451
C	0.948124	-1.169854	6.875796
H	1.019016	-0.082450	6.789482
H	1.937236	-1.626978	6.796102
O	2.151978	0.661558	-6.160966
C	1.652379	1.881382	-6.751795
H	0.559823	1.875490	-6.778862
H	2.018511	2.750313	-6.200213
H	0.492961	-1.437756	7.826830
H	2.049705	1.891474	-7.763876

7.2.6 $[Fe(4'\text{-}N(CH_2CH_2OH)_2\text{-}terpy)_2]^{2+}$

Fe	0.7329227	-0.6919632	-0.2149447
N	0.7828346	-0.2587256	-2.2957099
N	1.0457292	-2.6453688	-1.2540432
N	0.3640909	1.4991328	-0.4006694
N	0.8305389	-1.1750289	1.8605251
N	-1.3432190	-1.1808634	0.4041990
N	2.8621904	-0.4182836	0.3963463
H	-0.2930660	5.2574261	-1.0003873
H	5.9024699	0.5132166	-0.7014378
H	6.4706884	0.0259667	1.6978508
H	0.1874306	3.7521088	-2.9030445
C	-0.1041239	4.2037933	-0.8269077
C	5.1494920	0.1709810	-0.0015515
H	-0.3418433	4.2995868	1.3230083

C	0.1660773	3.3572003	-1.8954558
C	5.4595931	-0.0997968	1.3263953
C	-0.1346005	3.6778250	0.4602060
H	0.8968157	2.4094722	-4.3230140
H	3.5536779	0.1953586	-1.4506843
C	3.8371533	-0.0042463	-0.4223789
C	0.9560781	1.3722452	-4.0351576
C	0.4042526	2.0054353	-1.6528156
C	4.4521661	-0.5320952	2.1807130
H	4.6826224	-0.7475073	3.2159186
C	0.1030692	2.3192852	0.6248141
C	1.2920113	0.3776168	-4.9934373
C	0.7199895	1.0200907	-2.7219173
H	0.0836697	1.8678305	1.6116616
C	3.1562362	-0.6806641	1.6883738
C	1.3025492	-0.9630162	-4.5182759
H	1.5334565	-1.7782525	-5.1857427
H	3.0645164	-1.3555566	4.3529662
C	1.0581270	-1.2321492	-3.1867426
C	2.0022767	-1.1098117	2.5235652
C	2.1035544	-1.4163168	3.8669374
C	1.1195596	-2.5984851	-2.6021147
H	1.2974738	-3.7154095	-4.4429259
C	0.9497147	-1.7980450	4.6003563
C	1.2541606	-3.7602988	-3.3622008
C	-0.2842714	-1.5378534	2.5253314
H	-2.2114925	-0.8495770	-1.4394985
C	1.1214567	-3.8309360	-0.6369138
C	-0.2679433	-1.8449089	3.8723051
C	-2.4001679	-1.1627000	-0.4173916
H	1.0644568	-3.8166803	0.4466757
C	-1.5156076	-1.5603429	1.6900366
C	1.3295217	-4.9886262	-2.7155166
C	1.2664212	-5.0283369	-1.3265901
H	-1.1877541	-2.1162784	4.3659250
H	1.4357198	-5.9015920	-3.2910424
C	-3.6783207	-1.5202133	-0.0053672
H	1.3265689	-5.9632204	-0.7820548
C	-2.7676874	-1.9385122	2.1714773
H	-4.5026902	-1.4875474	-0.7077103
H	-2.8965063	-2.2542858	3.1985740
C	-3.8620313	-1.9163338	1.3149252
H	-4.8413147	-2.2097320	1.6767639
N	1.0033090	-2.0981639	5.9249769
N	1.6087245	0.6765382	-6.2765901
C	-0.1874614	-2.5084356	6.6759173
H	0.1422670	-3.1234635	7.5153330
H	-0.8261261	-3.1433414	6.0583386
C	-0.9820561	-1.3173723	7.2100397
H	-0.3396277	-0.7017978	7.8520765
H	-1.3362983	-0.6903494	6.3824218
C	2.2486664	-2.0208912	6.6948361
H	1.9900668	-1.7649850	7.7246470
H	2.8775331	-1.2103875	6.3227676
C	3.0192883	-3.3409676	6.6823003
H	2.3830227	-4.1428466	7.0770618
H	3.3062470	-3.6044846	5.6563854
C	1.6468204	2.0511255	-6.7955975
H	2.4907966	2.1175086	-7.4859382
H	1.8591210	2.7511209	-5.9872973
C	0.3770929	2.4599597	-7.5411520
H	0.1545989	1.7336205	-8.3271338
H	0.5564806	3.4295203	-8.0208073
C	1.9945098	-0.3705821	-7.2339486
H	1.8361111	0.0323436	-8.2359131
H	1.3287086	-1.2319020	-7.1418742
C	3.4390772	-0.8366670	-7.1093935
H	3.6380675	-1.2340028	-6.1072670
H	3.5931701	-1.6478322	-7.8329787
O	-0.7883606	2.5083883	-6.7086451
H	-0.7657928	3.3270546	-6.1935056
O	4.3091105	0.2663252	-7.3857915
H	5.2187948	-0.0193411	-7.2197808
O	-2.0842747	-1.8513087	7.9496155
H	-2.6101934	-1.1124584	8.2874015
O	4.1774118	-3.1612978	7.5015465
H	4.6748304	-3.9913333	7.5131599

7.3 Singlet-quintet MECP

7.3.1 $[Fe(terpy)_2]^{2+}$

Fe	0.980822	-0.861394	-0.228592
N	1.307270	-0.447485	-2.208379
N	2.139149	-2.566614	-0.909859
N	-0.075605	1.012221	-0.530217
N	0.704279	-1.216257	1.767972
N	-0.847520	-2.015453	-0.176903
N	2.684129	0.111787	0.689263
H	-1.941677	4.252244	-1.499571
H	5.545322	1.798598	0.164323
H	5.633447	1.628234	2.668169
H	-0.548524	3.064604	-3.167135
C	-1.419949	3.342763	-1.223931
C	4.763280	1.298957	0.723515
H	-2.123013	3.309830	0.823034
C	-0.638455	2.676221	-2.160399
C	4.807156	1.202294	2.110015
C	-1.523564	2.824781	0.062224
H	0.716828	1.957886	-4.483980
H	3.609663	0.797955	-1.026915
C	3.681857	0.739628	0.053842
C	1.096736	1.039884	-4.054739
C	0.018382	1.504626	-1.790257
C	3.778152	0.546976	2.776861
H	3.801943	0.455175	3.855655
C	-0.829581	1.660020	0.365780
C	1.866408	0.174925	-4.825521
C	0.829016	0.697582	-2.729444
H	-0.876167	1.230079	1.360489
C	2.723216	0.008920	2.041049
C	2.350510	-1.006435	-4.273121
H	2.949416	-1.680393	-4.871890
H	2.102903	-0.505162	4.743634
C	2.048692	-1.297173	-2.943664
C	1.589131	-0.719537	2.653525
C	1.404450	-0.910023	4.022592
C	2.495794	-2.507124	-2.216803

H	3.514082	-3.469661	-3.857624
C	0.296411	-1.633998	4.452701
C	3.238051	-3.525168	-2.812351
C	-0.374325	-1.914419	2.170171
H	-1.233960	-2.060293	-2.204940
C	2.524304	-3.619534	-0.178298
C	-0.603770	-2.147851	3.525159
C	-1.595186	-2.368675	-1.230093
H	2.220540	-3.621543	0.862640
C	-1.250410	-2.370620	1.068299
C	3.626327	-4.619146	-2.047901
C	3.268474	-4.668396	-0.705119
H	-1.463844	-2.713940	3.858874
H	4.202830	-5.419842	-2.497891
C	-2.773287	-3.093732	-1.102120
H	3.555528	-5.499367	-0.072056
C	-2.420593	-3.100419	1.270063
H	-3.342490	-3.359641	-1.984589
H	-2.733453	-3.380229	2.267929
C	-3.187928	-3.468372	0.171175
H	-4.099187	-4.038850	0.311329
H	0.133219	-1.798660	5.511833
H	2.094077	0.424139	-5.855584

7.3.2 $[Fe(4'\text{-}CN\text{-}terpy)_2]^{2+}$

Fe	1.020512	-0.806319	-0.213074
N	1.304488	-0.380980	-2.194810
N	2.222445	-2.468437	-0.908625
N	-0.087886	1.039423	-0.494587
N	0.762885	-1.203482	1.777188
N	-0.838741	-1.911019	-0.164088
N	2.761381	0.099298	0.703227
H	-2.021755	4.255950	-1.408066
H	5.611438	1.804231	0.187583
H	5.760054	1.521292	2.677464
H	-0.709890	3.056498	-3.129955
C	-1.476512	3.356087	-1.146820
C	4.840752	1.283582	0.742802
H	-2.058815	3.354856	0.937129
C	-0.741211	2.680981	-2.114995
C	4.918356	1.124698	2.121159
C	-1.500221	2.860989	0.151393
H	0.514255	1.955217	-4.483125
H	3.653396	0.851461	-1.003374
C	3.744537	0.752850	0.072669
C	0.957849	1.069875	-4.048633
C	-0.055879	1.521813	-1.761258
C	3.901604	0.445445	2.783825
H	3.950698	0.308181	3.856619
C	-0.790686	1.699429	0.433030
C	1.767182	0.234315	-4.823867
C	0.750969	0.730545	-2.715190
H	-0.789364	1.280567	1.433167
C	2.828665	-0.053096	2.048938
C	2.338161	-0.914717	-4.270180
H	2.962966	-1.557299	-4.875223
H	2.254540	-0.647264	4.741295
C	2.071821	-1.203296	-2.935346
C	1.687048	-0.771704	2.656883
C	1.526430	-0.994091	4.020928
C	2.564888	-2.399390	-2.218872
H	3.574145	-3.341265	-3.878234
C	0.384204	-1.677861	4.447638
C	3.305447	-3.406855	-2.831513
C	-0.342293	-1.861074	2.175606
H	-1.225862	-1.947962	-2.193215
C	2.608216	-3.531564	-0.192635
C	-0.566109	-2.121302	3.523586
C	-1.587074	-2.257056	-1.218674
H	2.319080	-3.543961	0.852326
C	-1.245468	-2.269742	1.078593
C	3.696870	-4.510681	-2.081993
C	3.342793	-4.577311	-0.739610
H	-1.445718	-2.653249	3.859513
H	4.270749	-5.305707	-2.544424
C	-2.772290	-2.971747	-1.091909
H	3.630001	-5.417392	-0.118871
C	-2.426951	-2.978643	1.281099
H	-3.342432	-3.230944	-1.975819
H	-2.746832	-3.254606	2.278021
C	-3.198168	-3.334651	0.180244
H	-4.119184	-3.889456	0.318990
C	2.018409	0.561543	-6.193529
C	0.183077	-1.928658	5.841138
N	0.017168	-2.135302	6.965223
N	2.224552	0.825326	-7.298905

7.3.3 $[Fe(4'\text{-}SO_2Me\text{-}terpy)_2]^{2+}$

Fe	0.915168	-0.687348	-0.203691
N	1.122352	-0.359086	-2.221109
N	2.247932	-2.270685	-0.832355
N	-0.326538	1.049761	-0.557382
N	0.709841	-1.008161	1.813013
N	-0.825814	-1.964344	-0.074763
N	2.554030	0.433640	0.648893
H	-2.403304	4.147226	-1.559929
H	5.163157	2.455769	0.017658
H	5.333369	2.352774	2.521433
H	-1.122516	2.896609	-3.271021
C	-1.820766	3.278168	-1.275562
C	4.462512	1.876789	0.607422
H	-2.322287	3.371575	0.827205
C	-1.101819	2.575892	-2.236810
C	4.552901	1.816585	1.993185
C	-1.778831	2.852766	0.046914
H	0.035443	1.720649	-4.635309
H	3.349501	1.184613	-1.104633
C	3.447714	1.167629	-0.024426
C	0.572653	0.913322	-4.154932
C	-0.358893	1.464362	-1.848026
C	3.626569	1.058003	2.700728
H	3.682576	1.003314	3.781106
C	-1.019699	1.731491	0.361475
C	1.401679	0.078812	-4.889302
C	0.457676	0.664352	-2.786638
H	-0.967419	1.365639	1.381150
C	2.633500	0.376651	2.001226
C	2.084217	-0.979744	-4.307284

H	2.707829	-1.633856	-4.902918
H	2.172267	-0.181145	4.731543
C	1.916921	-1.176250	-2.936130
C	1.592251	-0.442583	2.657186
C	1.480232	-0.635627	4.034410
C	2.549828	-2.261017	-2.154289
H	3.627179	-3.200289	-3.772015
C	0.432089	-1.422933	4.487332
C	3.389595	-3.219470	-2.715704
C	-0.309234	-1.768800	2.253635
H	-1.231016	-2.125425	-2.094381
C	2.763405	-3.229620	-0.054802
C	-0.485016	-1.996465	3.618966
C	-1.543359	-2.432630	-1.102384
H	2.496807	-3.199368	0.996007
C	-1.174692	-2.316574	1.187289
C	3.923681	-4.211071	-1.899889
C	3.604660	-4.220808	-0.547155
H	-1.308068	-2.590333	3.994525
H	4.580616	-4.964928	-2.319558
C	-2.640646	-3.268035	-0.930010
H	3.999104	-4.975179	0.122989
C	-2.264408	-3.147327	1.435263
H	-3.190704	-3.620086	-1.794094
H	-2.535243	-3.421163	2.446959
C	-3.006262	-3.627690	0.361784
H	-3.858288	-4.274919	0.536718
C	1.159093	-3.196530	6.623834
H	2.198012	-3.034187	6.336729
H	0.705035	-4.008330	6.056395
C	3.050204	1.381028	-6.844708
H	2.885137	2.308104	-6.296689
H	3.895333	0.820912	-6.445216
H	1.068625	-3.366922	7.697939
H	3.171199	1.569403	-7.912486
S	0.234709	-1.684834	6.287231
O	-1.210994	-1.933671	6.536370
O	0.903230	-0.544009	6.969745
S	1.569872	0.362261	-6.689959
O	1.822326	-0.962658	-7.318509
O	0.385293	1.153979	-7.117840

7.3.4 $[Fe(4'\text{-}SMe\text{-}terpy)_2]^{2+}$

Fe	0.955772	-0.847331	-0.228473
N	1.278700	-0.449176	-2.201567
N	2.157347	-2.527270	-0.885517
N	-0.159270	0.991504	-0.563238
N	0.696879	-1.196433	1.761837
N	-0.894436	-1.967167	-0.154377
N	2.692609	0.085327	0.672048
H	-2.051125	4.203499	-1.576054
H	5.525525	1.814554	0.131326
H	5.645685	1.619634	2.632139
H	-0.636323	3.014470	-3.221291
C	-1.520177	3.303661	-1.286720
C	4.755207	1.301526	0.694579
H	-2.229012	3.287907	0.757934
C	-0.727852	2.634491	-2.211794
C	4.817715	1.190377	2.079123
C	-1.621131	2.800625	0.005381
H	0.629908	1.923682	-4.485996
H	3.592698	0.793337	-1.048191
C	3.674521	0.732553	0.031685
C	1.050261	1.021306	-4.065607
C	-0.060745	1.474511	-1.825980
C	3.803203	0.518185	2.750815
H	3.840080	0.420541	3.828578
C	-0.919587	1.644131	0.323622
C	1.866886	0.183286	-4.832847
C	0.780066	0.674121	-2.746404
H	-0.970986	1.220932	1.321005
C	2.745790	-0.024159	2.022459
C	2.374446	-0.987731	-4.246914
H	3.010886	-1.649125	-4.821952
H	2.200395	-0.576856	4.698725
C	2.056008	-1.278268	-2.928951
C	1.608776	-0.745232	2.641285
C	1.458567	-0.951961	4.008706
C	2.514576	-2.480132	-2.192924
H	3.528621	-3.463206	-3.825102
C	0.331379	-1.640072	4.470479
C	3.247608	-3.509520	-2.780613
C	-0.397547	-1.861004	2.187004
H	-1.273951	-2.048189	-2.182424
C	2.520671	-3.585135	-0.149447
C	-0.612376	-2.097516	3.535708
C	-1.632601	-2.349456	-1.204365
H	2.217517	-3.575426	0.891660
C	-1.293640	-2.310288	1.095342
C	3.616497	-4.606330	-2.010595
C	3.247086	-4.648775	-0.670497
H	-1.489262	-2.637860	3.870768
H	4.185378	-5.415938	-2.454374
C	-2.800872	-3.088536	-1.068184
H	3.517366	-5.482761	-0.033861
C	-2.459666	-3.044213	1.306016
H	-3.363111	-3.377853	-1.947802
H	-2.774141	-3.310667	2.307093
C	-3.219399	-3.438839	0.210865
H	-4.127043	-4.013307	0.358092
S	0.006023	-1.983394	6.173030
C	1.510175	-1.406901	7.037617
H	1.617204	-0.324206	6.970611
H	2.392701	-1.917709	6.653360
S	2.311348	0.502402	-6.512948
C	1.638553	2.172092	-6.843832
H	0.548619	2.170682	-6.827409
H	2.045578	2.897538	-6.140140
H	1.353938	-1.689893	8.079200
H	1.984511	2.412242	-7.849588

7.3.5 $[Fe(4'\text{-}OMe\text{-}terpy)_2]^{2+}$

Fe	1.084320	-0.759558	-0.199469
N	1.335203	-0.345705	-2.186314
N	2.282276	-2.417238	-0.908417
N	0.035903	1.106891	-0.463429
N	0.791224	-1.200472	1.775632
N	-0.758910	-1.886330	-0.206342
N	2.771869	0.161566	0.775327
H	-1.782233	4.412395	-1.301964
H	5.622427	1.891128	0.338526

H	5.717989	1.588050	2.829647
H	-0.597855	3.152651	-3.073581
C	-1.273153	3.485626	-1.062975
C	4.843869	1.358970	0.872240
H	-1.774292	3.507002	1.042513
C	-0.608955	2.776738	-2.057971
C	4.892196	1.189208	2.251176
C	-1.271105	2.988765	0.235181
H	0.360260	1.894067	-4.494878
H	3.691130	0.941472	-0.902322
C	3.764705	0.828882	0.174267
C	0.839018	1.018881	-4.080141
C	0.035953	1.585636	-1.732228
C	3.865265	0.495898	2.883461
H	3.890585	0.347682	3.956077
C	-0.602555	1.797165	0.488928
C	1.548552	0.126863	-4.894205
C	0.756706	0.744622	-2.717807
H	-0.577405	1.378391	1.489291
C	2.812995	-0.006399	2.120852
C	2.149356	-1.005013	-4.321198
H	2.690545	-1.689430	-4.961210
H	2.191328	-0.637929	4.779024
C	2.019437	-1.213218	-2.961857
C	1.669986	-0.760872	2.692636
C	1.486754	-1.010275	4.049696
C	2.574864	-2.376590	-2.231051
H	3.569335	-3.319965	-3.896812
C	0.365622	-1.754348	4.441184
C	3.339227	-3.369190	-2.839814
C	-0.297928	-1.908490	2.141950
H	-1.127999	-1.841127	-2.237396
C	2.743188	-3.439105	-0.176326
C	-0.536574	-2.213270	3.468101
C	-1.497657	-2.191338	-1.280139
H	2.489106	-3.431557	0.877964
C	-1.177194	-2.297990	1.014620
C	3.807283	-4.430567	-2.073954
C	3.505722	-4.467982	-0.717091
H	-1.399630	-2.785552	3.782327
H	4.401656	-5.212697	-2.533113
C	-2.679797	-2.917034	-1.196783
H	3.853683	-5.273519	-0.081695
C	-2.354723	-3.024820	1.174736
H	-3.239340	-3.141578	-2.096918
H	-2.679383	-3.343103	2.157283
C	-3.114018	-3.340677	0.053899
H	-4.031681	-3.908159	0.159907
O	0.068699	-2.077471	5.706910
C	0.883251	-1.564314	6.781168
H	0.856184	-0.471429	6.791104
H	1.911405	-1.923767	6.693043
O	1.704771	0.260638	-6.217601
C	1.112131	1.392955	-6.888566
H	0.023456	1.370076	-6.791555
H	1.513466	2.327297	-6.488986
H	0.433351	-1.955181	7.690942
H	1.395164	1.285027	-7.933386

7.3.6 $[Fe(4'\text{-}N(CH_2CH_2OH)_2\text{-}terpy)_2]^{2+}$

Fe	0.969095	-0.614397	-0.168317
N	1.057232	-0.225823	-2.162490
N	1.307437	-2.554160	-1.045723
N	0.657633	1.510903	-0.281648
N	0.912682	-1.058895	1.819362
N	-1.103990	-1.038146	0.197344
N	3.008647	-0.362323	0.459097
H	0.039292	5.284137	-0.843852
H	6.094938	0.590861	-0.478738
H	6.541062	0.126129	1.949579
H	0.461919	3.784147	-2.767485
C	0.217654	4.226788	-0.681837
C	5.309176	0.245415	0.182323
H	0.028004	4.309291	1.473348
C	0.452746	3.383889	-1.761664
C	5.552424	-0.013723	1.526603
C	0.208679	3.691509	0.601856
H	0.956760	2.380229	-4.264611
H	3.792872	0.244384	-1.351702
C	4.023540	0.055020	-0.308887
C	1.062967	1.354269	-3.951444
C	0.675341	2.027363	-1.535301
C	4.505218	-0.450006	2.329183
H	4.676197	-0.654654	3.378288
C	0.432733	2.329395	0.754038
C	1.295153	0.328910	-4.909824
C	0.942798	1.041100	-2.612578
H	0.431251	1.871367	1.737500
C	3.239244	-0.613542	1.771261
C	1.407705	-0.992252	-4.394273
H	1.599893	-1.824105	-5.054072
H	2.998450	-1.383549	4.420997
C	1.287010	-1.223617	-3.037684
C	2.047520	-1.040841	2.545216
C	2.064682	-1.398764	3.880226
C	1.404435	-2.558068	-2.398194
H	1.669706	-3.732297	-4.188403
C	0.861263	-1.781864	4.530314
C	1.595624	-3.742073	-3.108190
C	-0.247236	-1.427091	2.398473
H	-1.795116	-0.691992	-1.716352
C	1.404111	-3.715659	-0.385354
C	-0.314716	-1.782589	3.732451
C	-2.082864	-0.996205	-0.715505
H	1.323604	-3.665017	0.695372
C	-1.403789	-1.408684	1.467307
C	1.691676	-4.943261	-2.415660
C	1.594782	-4.932642	-1.028332
H	-1.265822	-2.061262	4.159025
H	1.840969	-5.872494	-2.954263
C	-3.400506	-1.321625	-0.419012
H	1.666102	-5.844923	-0.448033
C	-2.704432	-1.746354	1.834187
H	-4.155849	-1.275216	-1.194552

H	-2.933989	-2.047149	2.848616
C	-3.714818	-1.703664	0.880494
H	-4.730381	-1.969536	1.152074
N	0.837867	-2.133289	5.844736
N	1.416721	0.585593	-6.237550
C	-0.387140	-2.582837	6.512997
H	-0.097142	-3.257964	7.320459
H	-1.003035	-3.167670	5.827453
C	-1.194625	-1.428079	7.104858
H	-0.550181	-0.823799	7.756000
H	-1.579647	-0.778648	6.308891
C	2.043013	-2.113347	6.679857
H	1.735708	-1.895272	7.705006
H	2.704891	-1.300684	6.376110
C	2.788406	-3.447991	6.648914
H	2.115350	-4.252834	6.970176
H	3.126522	-3.671670	5.629008
C	1.341714	1.943349	-6.797200
H	2.031718	1.986403	-7.643287
H	1.706673	2.664845	-6.065508
C	-0.052750	2.327760	-7.288965
H	-0.401938	1.599075	-8.024960
H	0.012906	3.302031	-7.787364
C	1.563842	-0.498885	-7.219181
H	1.115499	-0.158972	-8.155974
H	0.983147	-1.367148	-6.902803
C	2.999272	-0.925766	-7.492656
H	3.517201	-1.166653	-6.556114
H	2.974526	-1.830845	-8.113345
O	-1.040992	2.347242	-6.251325
H	-0.981659	3.191415	-5.783093
O	3.672770	0.137615	-8.179779
H	4.597670	-0.120842	-8.301172
O	-2.268380	-2.011913	7.849409
H	-2.836214	-1.298725	8.174001
O	3.902949	-3.334181	7.537400
H	4.390944	-4.169647	7.521865

8 APPENDIX B: Optimized geometries of the studied molecules (BP86/TZVP)

8.1 Singlet

8.1.1 $[Fe(terpy)_2]^{2+}$

Fe	0.989633	-0.844632	-0.228915
N	1.262631	-0.494933	-2.061792
N	2.061430	-2.443000	-0.692231
N	0.008213	0.868797	-0.365987
N	0.716139	-1.195014	1.603652
N	-0.694505	-1.876530	-0.359824
N	2.584087	0.072040	0.502210
H	-1.818023	4.239435	-1.035307
H	5.357228	1.863895	-0.199579
H	5.587078	1.759363	2.312899
H	-0.629091	3.055311	-2.889652
C	-1.306098	3.295303	-0.848624
C	4.621949	1.346447	0.415768
H	-1.804155	3.201934	1.266632
C	-0.643973	2.636644	-1.883753
C	4.745704	1.286308	1.806326
C	-1.300733	2.724252	0.426733
H	0.505410	1.817023	-4.411742
H	3.409943	0.760957	-1.278420
C	3.532887	0.730286	-0.196939
C	0.925012	0.914621	-3.968751
C	0.005722	1.427253	-1.622456
C	3.772451	0.609469	2.540083
H	3.839743	0.544697	3.625722
C	-0.636238	1.516309	0.627849
C	1.661909	0.017179	-4.747804
C	0.736199	0.634153	-2.612145
H	-0.614914	1.047897	1.610588
C	2.701852	0.010384	1.870805
C	2.197166	-1.138843	-4.171236
H	2.772117	-1.842299	-4.772298
H	2.150011	-0.603985	4.609526
C	1.981814	-1.376503	-2.810392
C	1.614474	-0.728056	2.514601
C	1.433161	-0.976003	3.878551
C	2.446337	-2.510709	-2.010543
H	3.497756	-3.604315	-3.546110
C	0.315876	-1.709929	4.288956
C	3.207440	-3.577423	-2.496194
C	-0.375519	-1.911162	1.991197
H	-0.948419	-1.829704	-2.424102
C	2.436122	-3.437900	0.139717
C	-0.599285	-2.184124	3.344041
C	-1.371360	-2.185936	-1.486102
H	2.115778	-3.354663	1.177086
C	-1.195700	-2.307729	0.845791
C	3.587656	-4.598655	-1.626599
C	3.194715	-4.525567	-0.287634
H	-1.471639	-2.756742	3.656756
H	4.181389	-5.437955	-1.989040
C	-2.553541	-2.923033	-1.470620
H	3.467987	-5.299226	0.429173
C	-2.377057	-3.050296	0.923053
H	-3.056812	-3.142916	-2.411577
H	-2.750267	-3.378455	1.892772
C	-3.066449	-3.363268	-0.247631
H	-3.989442	-3.941734	-0.205173
H	0.157992	-1.912972	5.347936
H	1.819512	0.219177	-5.807027

8.1.2 $[Fe(4'\text{-}CN\text{-}terpy)_2]^{2+}$

Fe	-0.00008	-0.00752	-0.00011
N	0.00431	-0.00286	-1.87871
N	1.34817	-1.42661	-0.30535
N	-1.34682	1.41317	-0.30459
N	-0.00414	-0.01173	1.87848
N	-1.42022	-1.35610	0.29865
N	1.41878	1.33969	0.31084
C	-3.20472	3.37760	-1.03327
C	3.10490	2.94078	-0.29661
C	-2.52108	2.66038	-2.01393
C	3.37672	3.20089	1.04839
C	-2.94597	3.09839	0.31048
C	2.12310	2.00760	-0.62545
C	-0.83201	0.88843	-3.93909
C	-1.59922	1.68538	-1.62775

C	2.65547	2.51684	2.02580
C	-2.01446	2.11352	0.63485
C	0.01175	0.00495	-4.63835
C	-0.81269	0.86110	-2.54610
C	1.68389	1.59322	1.63523
C	0.85177	-0.88242	-3.93955
C	0.82501	-0.86292	-2.54656
C	0.85583	0.80628	2.54979
C	0.87621	0.82626	3.94289
C	1.60715	-1.69187	-1.62867
C	-0.01022	-0.01772	4.63813
C	2.53139	-2.66442	-2.01537
C	-0.86707	-0.83258	2.54242
C	2.01145	-2.13161	0.63370
C	-0.89357	-0.85864	3.93530
C	-2.12045	-2.01995	-0.64357
C	-1.69115	-1.61542	1.62074
C	3.21051	-3.38646	-1.03509
C	2.94496	-3.11442	0.30880
C	-3.10370	-2.95453	-0.32312
C	-2.66450	-2.54067	2.00305
C	-3.38147	-3.22046	1.01954
H	-3.92794	4.14304	-1.31539
H	3.64268	3.45011	-1.09515
H	4.13949	3.92554	1.33404
H	-2.69988	2.85505	-3.07105
H	-3.45505	3.63272	1.11148
H	-1.48243	1.57551	-4.47717
H	1.89232	1.78615	-1.66602
H	2.84427	2.69684	3.08379
H	-1.79391	1.87724	1.67437
H	1.50524	-1.56632	-4.47797
H	1.56011	1.47743	4.48409
H	2.71569	-2.85335	-3.07259
H	-1.88514	-1.79402	-1.68214
H	1.78570	-1.90077	1.67333
H	-1.57987	-1.51217	4.47061
H	3.93551	-4.15002	-1.31775
H	3.45037	-3.65271	1.10948
H	-3.63796	-3.46042	-1.12619
H	-2.85800	-2.72508	3.05942
H	-4.14552	-3.94631	1.29865
C	0.01562	0.00897	-6.06700
C	-0.01339	-0.02089	6.06679
N	0.01881	0.01223	-7.23324
N	-0.01599	-0.02348	7.23303

8.1.3 $[Fe(4'\text{-}SO_2Me\text{-}terpy)_2]^{2+}$

Fe	0.917928	-0.688088	-0.203769
N	1.101047	-0.391273	-2.052760
N	2.108276	-2.209313	-0.641254
N	-0.213637	0.930413	-0.367714
N	0.731839	-0.976133	1.645711
N	-0.675530	-1.864304	-0.235683
N	2.451969	0.392650	0.429977
H	-2.326516	4.115341	-1.098554
H	5.048932	2.363192	-0.440959
H	5.357408	2.399767	2.064562
H	-1.111308	2.954490	-2.949012
C	-1.735915	3.222276	-0.895280
C	4.375343	1.819831	0.220929
H	-2.152138	3.176184	1.238404
C	-1.058219	2.576454	-1.928435
C	4.542894	1.837794	1.607452
C	-1.641712	2.705830	0.399015
H	0.059857	1.747024	-4.466297
H	3.170745	1.058262	-1.406574
C	3.323349	1.089059	-0.328666
C	0.576739	0.912053	-3.994651
C	-0.304472	1.436010	-1.642354
C	3.648604	1.122812	2.403141
H	3.751528	1.117891	3.488314
C	-0.875117	1.563524	0.623102
C	1.372095	0.044542	-4.743161
C	0.459838	0.667380	-2.623597
H	-0.786215	1.141704	1.622881
C	2.613706	0.408871	1.794427
C	2.024280	-1.045749	-4.165637
H	2.622814	-1.727967	-4.768063
H	2.180128	-0.096821	4.580434
C	1.870543	-1.240810	-2.790565
C	1.611231	-0.385322	2.503270
C	1.491305	-0.572203	3.883076
C	2.456159	-2.298951	-1.967856
H	3.551706	-3.358289	-3.498464
C	0.450081	-1.379703	4.340326
C	3.293379	-3.311894	-2.440954
C	-0.288530	-1.758453	2.098363
H	-0.988007	-1.941757	-2.291468
C	2.594440	-3.132138	0.214344
C	-0.459289	-1.978619	3.467753
C	-1.352378	-2.283825	-1.324550
H	2.300107	-3.037666	1.258120
C	-1.105886	-2.276998	1.002379
C	3.790570	-4.258311	-1.545882
C	3.434164	-4.165335	-0.198570
H	-1.281389	-2.587933	3.841534
H	4.446391	-5.055614	-1.896122
C	-2.467534	-3.115100	-1.236578
H	3.797995	-4.881192	0.537539
C	-2.215574	-3.111204	1.153319
H	-2.975440	-3.421709	-2.150006
H	-2.532975	-3.423662	2.147320
C	-2.907647	-3.536245	0.020118
H	-3.777220	-4.186072	0.118517
C	1.134014	-3.157044	6.498550
H	2.181993	-3.018939	6.208620
H	0.658398	-3.966925	5.934735
C	3.034394	1.298500	-6.730710
H	2.901357	2.237564	-6.182833
H	3.872391	0.712672	-6.336945
H	1.038305	-3.316437	7.579886
H	3.146686	1.478669	-7.806785
S	0.241445	-1.621317	6.146963
O	-1.220271	-1.840017	6.393343
O	0.941607	-0.482623	6.824007
S	1.523106	0.317498	-6.551243
O	1.736179	-1.026102	-7.179750
O	0.347166	1.147777	-6.966378

8.1.4 [Fe(4'-SMe-terpy)$_2$]$^{2+}$

Fe	1.012159	-0.831707	-0.222948
N	1.295177	-0.465826	-2.052012
N	2.080234	-2.428814	-0.699718
N	0.041007	0.888572	-0.357758
N	0.728240	-1.193548	1.605927
N	-0.675767	-1.856331	-0.364570
N	2.603413	0.073241	0.529965
H	-1.740680	4.288067	-1.003941
H	5.386844	1.864007	-0.138645
H	5.599944	1.738511	2.374264
H	-0.557052	3.110596	-2.861529
C	-1.243271	3.335285	-0.823919
C	4.645568	1.343897	0.467557
H	-1.757212	3.225001	1.286715
C	-0.582514	2.678823	-1.861256
C	4.760338	1.272209	1.858406
C	-1.254256	2.750240	0.445034
H	0.561679	1.880992	-4.366882
H	3.442502	0.774832	-1.239112
C	3.558830	0.735328	-0.156819
C	0.979162	0.966390	-3.951160
C	0.053035	1.460438	-1.609044
C	3.779543	0.592910	2.579834
H	3.840062	0.521350	3.665851
C	-0.604546	1.533175	0.637743
C	1.717158	0.072639	-4.748624
C	0.784586	0.668058	-2.601363
H	-0.596394	1.053540	1.615576
C	2.712236	0.001009	1.899427
C	2.240141	-1.099470	-4.160138
H	2.814812	-1.807068	-4.757914
H	2.156976	-0.615095	4.610042
C	2.013408	-1.342219	-2.810071
C	1.615689	-0.739348	2.529747
C	1.432353	-0.990082	3.890539
C	2.470180	-2.487716	-2.017365
H	3.525757	-3.572990	-3.556739
C	0.305975	-1.725243	4.304169
C	3.231038	-3.552291	-2.507964
C	-0.368773	-1.906869	1.988742
H	-0.916267	-1.794807	-2.428943
C	2.449751	-3.432055	0.125417
C	-0.605612	-2.187772	3.329802
C	-1.347759	-2.155557	-1.496907
H	2.123900	-3.355203	1.161316
C	-1.186128	-2.293976	0.835245
C	3.606630	-4.580932	-1.644907
C	3.208542	-4.517765	-0.306832
H	-1.486571	-2.758079	3.625117
H	4.201025	-5.418031	-2.011832
C	-2.533093	-2.887245	-1.493435
H	3.478381	-5.297172	0.405084
C	-2.371205	-3.031356	0.899992
H	-3.031402	-3.099289	-2.438685
H	-2.752379	-3.364926	1.864481
C	-3.055351	-3.333382	-0.276544
H	-3.981612	-3.906978	-0.242972
S	-0.060065	-2.123322	5.989303
C	1.314922	-1.364187	6.926653
H	1.319080	-0.274067	6.808092
H	2.278012	-1.801163	6.638428
S	2.045146	0.312945	-6.471270
C	1.236934	1.910695	-6.846790
H	0.155823	1.856014	-6.669710
H	1.694987	2.726651	-6.276143
H	1.105534	-1.612832	7.974263
H	1.420221	2.070585	-7.916154

8.1.5 [Fe(4'-OMe-terpy)$_2$]$^{2+}$

Fe	1.024544	-0.791414	-0.212597
N	1.271352	-0.412994	-2.047039
N	2.091112	-2.379719	-0.719261
N	0.044091	0.925041	-0.319785
N	0.775158	-1.163713	1.621895
N	-0.660831	-1.822563	-0.327922
N	2.624793	0.115601	0.516264
H	-1.762575	4.321767	-0.914408
H	5.391114	1.917778	-0.192980
H	5.651660	1.777277	2.314753
H	-0.611518	3.156424	-2.801269
C	-1.258305	3.369911	-0.749038
C	4.662437	1.392241	0.423759
H	-1.727677	3.248746	1.371450
C	-0.616333	2.720410	-1.802467
C	4.803393	1.312482	1.811858
C	-1.240844	2.779259	0.517398
H	0.477654	1.943400	-4.336850
H	3.428186	0.830470	-1.263340
C	3.565741	0.784549	-0.183830
C	0.907921	1.030749	-3.931185
C	0.028522	1.503105	-1.568492
C	3.837492	0.626960	2.547409
H	3.918181	0.548830	3.631790
C	-0.582965	1.563716	0.691338
C	1.636249	0.139685	-4.740681
C	0.744088	0.719560	-2.579491
H	-0.552093	1.080481	1.666941
C	2.759052	0.036344	1.883348
C	2.178655	-1.033405	-4.175189
H	2.740579	-1.721106	-4.805815
H	2.254605	-0.588645	4.606226
C	1.979734	-1.281856	-2.823275
C	1.676305	-0.709933	2.530486
C	1.521659	-0.962889	3.895410
C	2.457017	-2.429006	-2.044426
H	3.490163	-3.497724	-3.609582
C	0.400933	-1.702627	4.317089
C	3.214704	-3.486045	-2.555374
C	-0.313236	-1.882139	2.020542
H	-0.938330	-1.753947	-2.387136
C	2.481389	-3.386114	0.092471
C	-0.527886	-2.168387	3.362665
C	-1.352319	-2.119766	-1.449151

H	2.174536	-3.316503	1.134679
C	-1.148757	-2.266936	0.878900
C	3.611646	-4.518027	-1.705898
C	3.237711	-4.465106	-0.360375
H	-1.394457	-2.739845	3.693110
H	4.203780	-5.349630	-2.088730
C	-2.535181	-2.855121	-1.427675
H	3.524583	-5.247432	0.341629
C	-2.329981	-3.008428	0.961794
H	-3.049706	-3.064821	-2.364771
H	-2.692110	-3.346925	1.931931
C	-3.034421	-3.307826	-0.203482
H	-3.958250	-3.884398	-0.155754
O	0.131755	-2.014540	5.603253
C	1.045649	-1.549695	6.626970
H	1.085779	-0.450798	6.639620
H	2.049580	-1.969114	6.471233
O	1.867427	0.319882	-6.059158
C	1.340690	1.512725	-6.690895
H	0.243614	1.536271	-6.621342
H	1.773602	2.414714	-6.236332
H	0.630758	-1.918318	7.569265
H	1.647206	1.440361	-7.738363

8.1.6 $[Fe(4'\text{-}N(CH_2CH_2OH)_2\text{-}terpy)_2]^{2+}$

Fe	0.192322	0.047193	-0.085833
N	0.144048	0.141441	-1.973147
N	1.883669	-0.892125	-0.501427
N	-1.516771	1.018828	-0.318261
N	0.229443	-0.046389	1.800735
N	-0.753191	-1.672300	0.171103
N	1.152186	1.732789	0.303070
C	-3.888110	2.386406	-0.921854
C	2.278991	3.792289	-0.232727
C	-3.046431	1.950880	-1.944181
C	2.473150	4.065169	1.124375
C	-3.527712	2.128419	0.403848
C	1.617459	2.623037	-0.600637
C	-0.971705	0.832338	-3.981681
C	-1.868142	1.270055	-1.624925
C	1.999067	3.154620	2.067665
C	-2.341417	1.446290	0.662928
C	0.055658	0.258639	-4.787588
C	-0.897553	0.754161	-2.597848
C	1.342894	1.996633	1.640375
C	1.133602	-0.371893	-4.098140
C	1.143980	-0.412397	-2.709874
C	0.799644	0.955958	2.522022
C	0.818378	0.932603	3.910540
C	2.164284	-1.015979	-1.843239
C	0.241815	-0.164125	4.615411
C	3.321457	-1.661473	-2.288416
C	-0.337936	-1.103650	2.441317
C	2.758509	-1.409651	0.388758
C	-0.351672	-1.192121	3.826729
C	-1.241641	-2.477275	-0.797974
C	-0.907709	-2.058640	1.483060
C	4.215204	-2.191473	-1.358851
C	3.927214	-2.061769	0.002806
C	-1.892759	-3.676951	-0.521440
C	-1.553213	-3.251872	1.819695
C	-2.052862	-4.072598	0.809694
H	-4.810301	2.917776	-1.157196
H	2.632428	4.472723	-1.006695
H	2.985917	4.972280	1.444644
H	-3.301851	2.138140	-2.986809
H	-4.152859	2.448702	1.236622
H	-1.826904	1.325796	-4.435940
H	1.448426	2.380856	-1.649093
H	2.137479	3.341835	3.132368
H	-2.031724	1.230512	1.684555
H	1.955691	-0.826487	-4.643582
H	1.281915	1.757207	4.444882
H	3.520531	-1.748348	-3.356515
H	-1.100817	-2.139758	-1.824003
H	2.504026	-1.291615	1.441283
H	-0.815545	-2.056154	4.293711
H	5.121673	-2.696350	-1.693226
H	4.595022	-2.458509	0.766709
H	-2.265518	-4.284986	-1.344943
H	-1.663011	-3.536150	2.866018
H	-2.557198	-5.006254	1.058679
N	0.273668	-0.237073	5.984011
N	0.007727	0.309737	-6.153209
C	0.863802	0.841170	6.786369
H	1.153647	0.409437	7.753542
H	1.789520	1.197354	6.311640
C	-0.330043	-1.370473	6.694133
H	-0.111156	-2.306301	6.158672
H	0.163617	-1.445051	7.672326
C	-1.852187	-1.239422	6.892164
H	-2.076652	-0.374356	7.538727
H	-2.351355	-1.077669	5.926303
C	-0.085746	2.032523	7.015486
H	-0.453373	2.418884	6.054515
H	-0.959728	1.711755	7.607143
C	1.028371	-0.343519	-6.984441
H	1.318152	-1.305930	-6.537101
H	0.559482	-0.587137	-7.948669
C	-1.085489	0.988765	-6.857146
H	-0.700856	1.320326	-7.828991
H	-1.379935	1.896782	-6.312586
C	-2.299389	0.079248	-7.065937
H	-2.008002	-0.797946	-7.669781
H	-2.675917	-0.286840	-6.094532
C	2.282462	0.503343	-7.228613
H	2.719703	0.831442	-6.275355
H	3.027483	-0.125139	-7.747836
O	2.018595	1.708650	-7.965877
H	1.786537	1.454505	-8.878165
O	-3.296187	0.863036	-7.741826
H	-4.069652	0.290772	-7.892701
O	-2.412424	-2.444681	7.432296
H	-2.107342	-2.531771	8.354237
O	0.593943	3.125354	7.650604
H	0.803097	2.858362	8.564671

8.2 Quintet

8.2.1 $[Fe(terpy)_2]^{2+}$

Fe	0.929443	-0.882668	-0.246265
N	1.205488	-0.511864	-2.294729
N	2.187534	-2.535020	-0.952845

N	-0.179679	0.968258	-0.637294
N	0.654632	-1.253968	1.802237
N	-0.948993	-2.007783	-0.125718
N	2.660586	0.044214	0.731097
H	-1.976711	4.267304	-1.602185
H	5.444638	1.888719	0.223385
H	5.563950	1.657743	2.733948
H	-0.773029	2.942056	-3.330642
C	-1.469624	3.341773	-1.327574
C	4.685629	1.338758	0.778861
H	-1.994710	3.438717	0.781730
C	-0.796656	2.598408	-2.297377
C	4.747101	1.207805	2.168718
C	-1.482430	2.887465	-0.006182
H	0.302277	1.699634	-4.691950
H	3.545575	0.803742	-0.985908
C	3.626620	0.737485	0.100172
C	0.777409	0.835966	-4.229480
C	-0.152161	1.412287	-1.924208
C	3.747563	0.494794	2.831004
H	3.778628	0.388298	3.914509
C	-0.827543	1.693711	0.293282
C	1.564316	-0.026119	-4.995982
C	0.619277	0.569097	-2.864075
H	-0.822253	1.295390	1.309070
C	2.707306	-0.075577	2.086672
C	2.170009	-1.133475	-4.398601
H	2.785192	-1.807619	-4.992487
H	2.169350	-0.713715	4.779874
C	1.965068	-1.357925	-3.031782
C	1.579456	-0.818291	2.691649
C	1.425030	-1.056240	4.062809
C	2.510544	-2.506742	-2.275313
H	3.542735	-3.483275	-3.913595
C	0.289840	-1.740310	4.502589
C	3.285232	-3.518742	-2.855916
C	-0.446703	-1.924599	2.218829
H	-1.329015	-2.087505	-2.164698
C	2.610987	-3.564695	-0.196271
C	-0.661298	-2.178628	3.578959
C	-1.687917	-2.396285	-1.181657
H	2.327965	-3.541136	0.857235
C	-1.345978	-2.361054	1.127928
C	3.723473	-4.580040	-2.063703
C	3.377085	-4.609960	-0.710263
H	-1.548571	-2.711088	3.917834
H	4.327675	-5.375773	-2.500636
C	-2.855396	-3.146234	-1.046845
H	3.697210	-5.421206	-0.057187
C	-2.513637	-3.105504	1.337457
H	-3.420388	-3.436051	-1.932222
H	-2.825359	-3.378155	2.344820
C	-3.275974	-3.500194	0.237890
H	-4.187778	-4.080152	0.384264
H	0.146219	-1.931758	5.566116
H	1.705581	0.165120	-6.059863

8.2.2 $[Fe(4'\text{-}CN\text{-}terpy)_2]^{2+}$

Fe	1.001926	-0.803243	-0.218383
N	1.301188	-0.380530	-2.251033
N	2.239711	-2.450041	-0.955762
N	-0.087954	1.060467	-0.568328
N	0.737862	-1.222762	1.818793
N	-0.884970	-1.904108	-0.115758
N	2.744408	0.083344	0.766647
H	-1.836064	4.409045	-1.445371
H	5.549446	1.899385	0.279524
H	5.697219	1.592328	2.779322
H	-0.629547	3.128429	-3.203010
C	-1.344659	3.468655	-1.195647
C	4.788815	1.344837	0.828377
H	-1.894458	3.500886	0.908298
C	-0.668618	2.749667	-2.182353
C	4.866249	1.172049	2.212069
C	-1.379202	2.970444	0.108507
H	0.444141	1.913034	-4.589192
H	3.621242	0.881803	-0.938391
C	3.712585	0.780424	0.144020
C	0.902324	1.032508	-4.144485
C	-0.042296	1.546706	-1.839002
C	3.863728	0.454585	2.866027
H	3.906700	0.315402	3.945693
C	-0.740492	1.760321	0.377676
C	1.694734	0.175806	-4.927224
C	0.731015	0.723145	-2.793523
H	-0.753211	1.329811	1.380064
C	2.808245	-0.076677	2.117050
C	2.288717	-0.961782	-4.355163
H	2.901214	-1.623585	-4.963884
H	2.281748	-0.764046	4.797198
C	2.062424	-1.214850	-3.000247
C	1.675196	-0.818609	2.710518
C	1.532027	-1.080348	4.074951
C	2.589830	-2.387918	-2.269998
H	3.651824	-3.321870	-3.915102
C	0.380553	-1.762442	4.503791
C	3.371223	-3.384718	-2.864661
C	-0.372179	-1.887521	2.223598
H	-1.275031	-1.923400	-2.154682
C	2.642223	-3.502040	-0.219855
C	-0.589809	-2.171589	3.573466
C	-1.632482	-2.253717	-1.178693
H	2.339484	-3.506963	0.827954
C	-1.283021	-2.286141	1.128721
C	3.788178	-4.470241	-2.093202
C	3.413743	-4.536253	-0.749479
H	-1.480492	-2.699313	3.907550
H	4.398520	-5.255989	-2.539617
C	-2.809200	-2.992413	-1.057112
H	3.717040	-5.367019	-0.113266
C	-2.456618	-3.021708	1.325393
H	-3.381512	-3.250336	-1.947340
H	-2.767898	-3.318549	2.325685
C	-3.228539	-3.376764	0.218403
H	-4.146924	-3.948538	0.353352
C	1.897683	0.463039	-6.313362
C	0.195846	-2.041629	5.894104
N	0.045741	-2.269283	7.027650
N	2.063112	0.697177	-7.443423

8.2.3 $[Fe(4'\text{-}SO_2Me\text{-}terpy)_2]^{2+}$

Fe	1.168210	-0.776747	-0.194455
N	1.438113	-0.250522	-2.209836
N	2.162590	-2.505027	-1.095106

N	0.312569	1.230790	-0.369287
N	0.899947	-1.282972	1.826026
N	-0.723771	-1.876592	-0.139950
N	2.923148	0.045152	0.827092
H	-1.144408	4.773786	-0.975171
H	5.858814	1.655396	0.387209
H	5.956910	1.314962	2.884832
H	-0.052030	3.534179	-2.834101
C	-0.739870	3.776353	-0.803357
C	5.056687	1.147263	0.921724
H	-1.303400	3.683974	1.295200
C	-0.125478	3.081506	-1.845950
C	5.106417	0.956533	2.304233
C	-0.829871	3.177503	0.455001
H	0.881835	2.330866	-4.332878
H	3.861261	0.818746	-0.856490
C	3.944507	0.678947	0.222227
C	1.190607	1.349259	-3.977606
C	0.389999	1.804020	-1.601748
C	4.052469	0.298076	2.939224
H	4.077712	0.137209	4.016393
C	-0.286645	1.905031	0.629117
C	1.769449	0.425136	-4.844628
C	1.025695	0.966186	-2.640724
H	-0.324167	1.407596	1.599436
C	2.972203	-0.153076	2.173256
C	2.199305	-0.825593	-4.409236
H	2.666316	-1.524334	-5.101626
H	2.408522	-0.901863	4.835982
C	2.019664	-1.135478	-3.054648
C	1.821974	-0.890529	2.737836
C	1.668692	-1.201029	4.094853
C	2.447994	-2.401108	-2.422489
H	3.339972	-3.327057	-4.169268
C	0.539276	-1.928505	4.464676
C	3.118235	-3.420734	-3.107000
C	-0.192754	-1.994941	2.192763
H	-1.163548	-1.726612	-2.162980
C	2.543622	-3.609501	-0.428322
C	-0.404074	-2.349477	3.531310
C	-1.517214	-2.103140	-1.202508
H	2.289730	-3.649449	0.631817
C	-1.112872	-2.327167	1.084480
C	3.507545	-4.564345	-2.408397
C	3.221040	-4.661298	-1.045073
H	-1.269901	-2.932310	3.841773
H	4.030979	-5.369398	-2.925125
C	-2.727543	-2.789090	-1.102313
H	3.508104	-5.536550	-0.463281
C	-2.310296	-3.029994	1.257332
H	-3.334860	-2.949425	-1.992457
H	-2.608119	-3.390820	2.240635
C	-3.125485	-3.264295	0.149245
H	-4.061646	-3.810915	0.264933
C	-0.494394	-0.939948	6.961379
H	-1.444702	-0.776838	6.441258
H	0.180418	-0.082765	6.856070
C	0.435738	0.475760	-7.393415
H	0.261583	-0.599315	-7.270454
H	-0.349975	1.072934	-6.918015
H	-0.656927	-1.190457	8.016902
H	0.551273	0.742272	-8.451474
S	0.309645	-2.387537	6.230030
O	-0.640551	-3.545500	6.259791
O	1.676893	-2.540558	6.823141
S	2.014338	0.885461	-6.607391
O	2.210821	2.370460	-6.646679
O	3.081052	-0.014859	-7.151500

8.2.4 $[Fe(4'\text{-}SMe\text{-}terpy)_2]^{2+}$

Fe	0.980564	-0.864524	-0.234000
N	1.336583	-0.420168	-2.287282
N	2.182908	-2.525342	-1.004999
N	-0.009265	1.041296	-0.609667
N	0.678433	-1.247792	1.839110
N	-0.881104	-2.011314	-0.102278
N	2.651515	0.084772	0.794530
H	-1.707326	4.425661	-1.483674
H	5.477575	1.873095	0.299890
H	5.562938	1.682298	2.816767
H	-0.447712	3.164864	-3.221219
C	-1.234138	3.475359	-1.236254
C	4.703800	1.342714	0.854808
H	-1.863510	3.462761	0.846168
C	-0.527264	2.768383	-2.209544
C	4.747646	1.234653	2.247596
C	-1.322502	2.946055	0.053981
H	0.651975	1.966784	-4.575076
H	3.568963	0.823488	-0.915967
C	3.639635	0.756327	0.171168
C	1.056524	1.044429	-4.165509
C	0.075323	1.551958	-1.869200
C	3.728229	0.543738	2.903112
H	3.742670	0.449832	3.988646
C	-0.694473	1.730783	0.322808
C	1.801470	0.163216	-4.967849
C	0.842612	0.717672	-2.823589
H	-0.735811	1.287727	1.319395
C	2.692427	-0.023630	2.151688
C	2.311024	-1.020280	-4.390194
H	2.892878	-1.715294	-4.994751
H	2.131581	-0.628661	4.823252
C	2.059802	-1.278586	-3.047003
C	1.566588	-0.781152	2.744459
C	1.404264	-1.014362	4.113184
C	2.539862	-2.478142	-2.316697
H	3.582971	-3.441467	-3.955867
C	0.290677	-1.752066	4.549016
C	3.301894	-3.493592	-2.904824
C	-0.402116	-1.959647	2.244038
H	-1.257883	-2.026437	-2.143264
C	2.571935	-3.577883	-0.261803
C	-0.627853	-2.231385	3.588596
C	-1.621336	-2.361325	-1.170454
H	2.263590	-3.572376	0.784833
C	-1.287038	-2.398937	1.136256

C	3.700745	-4.581816	-2.126874
C	3.329101	-4.627862	-0.781332
H	-1.499115	-2.804126	3.904562
H	4.295096	-5.382630	-2.568333
C	-2.792903	-3.110380	-1.061109
H	3.618876	-5.458028	-0.137765
C	-2.452078	-3.150534	1.322022
H	-3.356989	-3.368784	-1.956631
H	-2.765810	-3.453464	2.319883
C	-3.213762	-3.510701	0.209048
H	-4.125125	-4.095793	0.335414
S	-0.054292	-2.133715	6.235282
C	1.323070	-1.358803	7.155844
H	1.316719	-0.269696	7.029792
H	2.285859	-1.791419	6.860690
S	2.155691	0.428861	-6.674425
C	1.359714	2.034073	-7.043887
H	0.275599	1.979426	-6.887294
H	1.811084	2.839912	-6.454171
H	1.124388	-1.602929	8.206524
H	1.563637	2.206190	-8.107462

8.2.5 $[Fe(4'\text{-}OMe\text{-}terpy)_2]^{2+}$

Fe	1.001240	-0.819833	-0.221897
N	1.311615	-0.365296	-2.281608
N	2.190083	-2.473035	-1.026515
N	-0.009181	1.081174	-0.570594
N	0.732716	-1.217571	1.854875
N	-0.851490	-1.975645	-0.069156
N	2.687207	0.127165	0.788159
H	-1.726643	4.468631	-1.392134
H	5.501606	1.924267	0.262060
H	5.625992	1.715911	2.775602
H	-0.504027	3.216317	-3.162595
C	-1.247804	3.517436	-1.159349
C	4.737278	1.388767	0.825085
H	-1.832777	3.494925	0.935875
C	-0.561547	2.815402	-2.151031
C	4.802516	1.271147	2.215987
C	-1.308434	2.982291	0.129977
H	0.557873	2.025034	-4.548802
H	3.576427	0.877655	-0.931736
C	3.663873	0.804295	0.153772
C	0.976918	1.105853	-4.148055
C	0.049072	1.598057	-1.828891
C	3.794301	0.574057	2.882930
H	3.825714	0.472273	3.967513
C	-0.675231	1.765427	0.379326
C	1.709496	0.225160	-4.963354
C	0.799032	0.769891	-2.803361
H	-0.696767	1.316814	1.374102
C	2.748308	0.010318	2.143410
C	2.240697	-0.957393	-4.406985
H	2.807242	-1.633893	-5.044741
H	2.224408	-0.601293	4.824385
C	2.022337	-1.218182	-3.060525
C	1.630968	-0.752147	2.749158
C	1.491657	-0.986015	4.119981
C	2.523236	-2.417624	-2.344105
H	3.541847	-3.365267	-4.006798
C	0.380461	-1.727109	4.559910
C	3.280476	-3.425415	-2.951014
C	-0.341957	-1.932932	2.271318
H	-1.257106	-1.984760	-2.104744
C	2.598189	-3.527278	-0.295818
C	-0.551302	-2.208602	3.616045
C	-1.605639	-2.324825	-1.128245
H	2.307731	-3.529205	0.755999
C	-1.239508	-2.370243	1.173072
C	3.699755	-4.514980	-2.185933
C	3.352418	-4.569785	-0.834083
H	-1.410193	-2.780287	3.963558
H	4.290813	-5.309993	-2.642101
C	-2.772712	-3.078573	-1.005727
H	3.658405	-5.401572	-0.200144
C	-2.398785	-3.127405	1.372003
H	-3.348204	-3.335323	-1.894508
H	-2.696150	-3.435479	2.373328
C	-3.174751	-3.485897	0.268544
H	-4.082063	-4.075019	0.405109
O	0.123342	-2.024358	5.845915
C	1.039940	-1.545900	6.864203
H	1.072331	-0.447182	6.866538
H	2.044356	-1.962027	6.706078
O	1.954131	0.421866	-6.271053
C	1.438032	1.623821	-6.899642
H	0.340878	1.648827	-6.840645
H	1.870675	2.518598	-6.431954
H	0.629512	-1.910182	7.809884
H	1.756195	1.557427	-7.943741

8.2.6 $[Fe(4'\text{-}N(CH_2CH_2OH)_2\text{-}terpy)_2]^{2+}$

Fe	1.031502	-0.672370	-0.176530
N	1.125073	-0.224486	-2.253301
N	1.396141	-2.610248	-1.214213
N	0.722980	1.524614	-0.351574
N	0.948378	-1.154050	1.899987
N	-1.097744	-1.142859	0.270169
N	3.109666	-0.468493	0.596298
H	0.225356	5.313189	-0.905355
H	6.263686	0.303428	-0.280402
H	6.624802	-0.158221	2.163134
H	0.607627	3.808061	-2.829436
C	0.365402	4.249684	-0.744730
C	5.444266	0.012418	0.366008
H	0.171568	4.335905	1.410443
C	0.577540	3.402954	-1.826298
C	5.639150	-0.244113	1.718939
C	0.334607	3.713604	0.538593
H	0.878420	2.401742	-4.322676
H	3.964436	0.077728	-1.202089
C	4.161057	-0.112527	-0.151776
C	1.023828	1.376259	-4.025239
C	0.752584	2.037771	-1.600857
C	4.551029	-0.613848	2.501001
H	4.690064	-0.815548	3.555432
C	0.519965	2.344973	0.686632
C	1.226754	0.367926	-5.006156
C	0.977276	1.045341	-2.686351

H	0.504699	1.885382	1.669916
C	3.291760	-0.718559	1.911296
C	1.373634	-0.958121	-4.513151
H	1.535780	-1.779632	-5.193096
H	2.968707	-1.365310	4.568923
C	1.319082	-1.206640	-3.155465
C	2.063877	-1.108564	2.655347
C	2.049972	-1.408610	4.004280
C	1.474377	-2.562394	-2.562007
H	1.750439	-3.669661	-4.395973
C	0.835215	-1.781846	4.637042
C	1.688862	-3.715720	-3.316030
C	-0.221225	-1.505814	2.470141
H	-1.803816	-0.812246	-1.641931
C	1.527867	-3.789271	-0.594281
C	-0.318454	-1.822742	3.811087
C	-2.081246	-1.114643	-0.637039
H	1.457648	-3.776364	0.488962
C	-1.381404	-1.511294	1.538660
C	1.825214	-4.937304	-2.666839
C	1.743768	-4.978735	-1.278973
H	-1.278219	-2.088490	4.225551
H	1.993084	-5.842800	-3.239573
C	-3.394242	-1.450946	-0.332205
H	1.844818	-5.908562	-0.731633
C	-2.675686	-1.865090	1.917461
H	-4.156197	-1.412202	-1.101752
H	-2.896244	-2.164823	2.934039
C	-3.693048	-1.834230	0.970810
H	-4.704420	-2.108301	1.250034
N	0.779318	-2.083431	5.960616
N	1.284427	0.643507	-6.332210
C	-0.452490	-2.558768	6.596559
H	-0.170463	-3.187486	7.443518
H	-1.010527	-3.196410	5.908200
C	-1.337357	-1.418082	7.094955
H	-0.779392	-0.799980	7.809826
H	-1.645476	-0.777174	6.259483
C	1.948794	-1.963065	6.834306
H	1.592540	-1.749253	7.844238
H	2.559757	-1.109406	6.533660
C	2.796012	-3.234073	6.859358
H	2.185355	-4.082275	7.193820
H	3.172649	-3.463085	5.854249
C	1.221980	2.009878	-6.871339
H	1.907464	2.052815	-7.721440
H	1.601529	2.717968	-6.133649
C	-0.167836	2.424878	-7.350604
H	-0.550447	1.692070	-8.066008
H	-0.078949	3.386220	-7.870364
C	1.422951	-0.424078	-7.332162
H	0.982961	-0.060448	-8.263637
H	0.831106	-1.292398	-7.034781
C	2.855597	-0.859487	-7.603671
H	3.353175	-1.161130	-6.673930
H	2.822891	-1.729343	-8.272885
O	-1.140711	2.499465	-6.301524
H	-1.032776	3.342330	-5.839614
O	3.561783	0.227326	-8.215740
H	4.481268	-0.045807	-8.343947
O	-2.474060	-2.022083	7.719670
H	-3.059760	-1.318013	8.031815
O	3.875581	-2.993423	7.765465
H	4.425424	-3.788758	7.801929

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