This dataset contains:

Analytical characterisation of the new ligands and the complexes (CHN microanalysis)

^{1}H and ^{13}C NMR spectra of the new organic ligands (raw data and plotted spectra).

Paramagnetic ^{1}H NMR spectra of the iron complexes (raw data and plotted spectra).

Electrospray mass spectra (plotted spectra).

X-ray Crystallographic data:

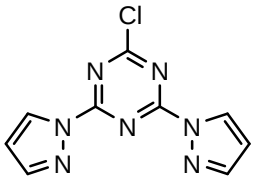
- Structure of L^{1} (CCDC 1504278).
- Structure of L^{3} (CCDC 1504279).
- Structure of $L^{4}\cdot CH_2Cl_2$ (CCDC 1504280).
- Structure of L^{5} (CCDC 1546568).
- Structure of L^{6} (CCDC 1504281).
- Structure of L^{8} (CCDC 1504282).
- Structure of α-$[Fe(L^{2})][BF_4]_2$ (CCDC 1504283).
- Structure of β-$[Fe(L^{2})][BF_4]_2$ (CCDC 1504284).
- Unit cell determination of $[Fe(L^{2})][ClO_4]_2$.
- Structure of $[Fe(L^{3})_2][BF_4]_2\cdot 2CH_2Cl_2$ (CCDC 1504285).
- Structure of $[Fe(L^{4})_2][BF_4]_2\cdot 1.55CH_3CN\cdot 0.45CH_2Cl_2$ (CCDC 1504286).
- Structure of $[Fe(L^{5})_2][BF_4]_2\cdot {}^{1}/_{2}CH_3CN$ (CCDC 1504287).
- Structure of $[Fe(L^{6})_2][BF_4]_2\cdot {}^{1}/_{2}CH_2Cl_2$ (CCDC 1504288).
- Structure of $[Fe(L^{6})_2][BF_4]_2\cdot n CH_2Cl_2$ ($n \approx 0.57$; CCDC 1534692).
- Structure of $[Fe(L^{7})_2][BF_4]_2$ (CCDC 1502196).
- Structure of $[Fe(L^{8})_2][BF_4]_2$ (CCDC 1504289).

X-ray powder diffraction data (measured and simulated).

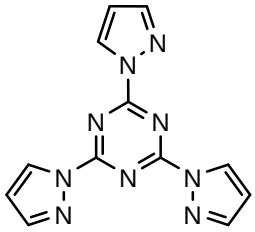
Solid state magnetic susceptibility measurements (raw and processed data).

Solution magnetic susceptibility data.

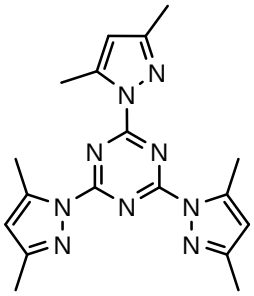
Ligands prepared during this study



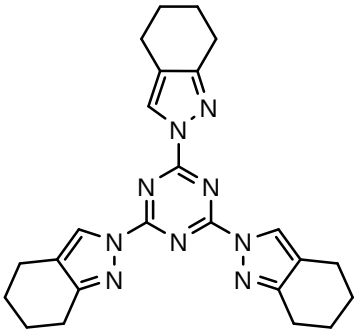
2,4-Di(pyrazol-1-yl)-6-chloro-1,3,5-triazine
$C_9H_6ClN_7$
L^1



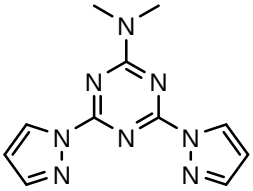
2,4,6-Tri(pyrazol-1-yl)-1,3,5-triazine
$C_{12}H_9N_9$
L^2



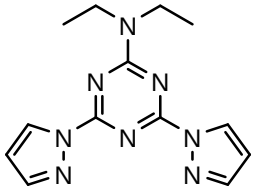
2,4,6-Tri(3,5-dimethylpyrazol-1-yl)-1,3,5-triazine
$C_{18}H_{21}N_9$
L^3



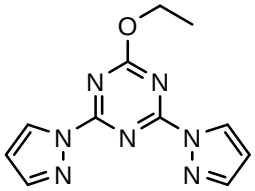
2,4,6-Tri(4,5,6,7-tetrahydroindazol-2-yl)-1,3,5-triazine
$C_{24}H_{27}N_9$
L^4



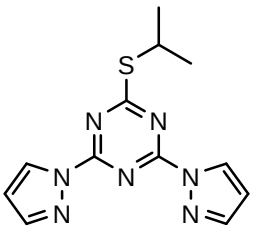
2,4-Di(pyrazol-1-yl)-6-(dimethylamino)-1,3,5-triazine
$C_{11}H_{12}N_8$
L^5



2,4-Di(pyrazol-1-yl)-6-(diethylamino)-1,3,5-triazine
$C_{13}H_{16}N_8$
L^6

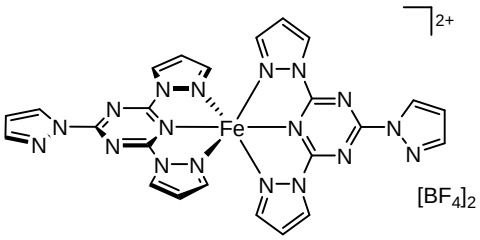


2,4-Di(pyrazol-1-yl)-6-ethoxy-1,3,5-triazine
$C_{11}H_{11}N_7O$
L^7

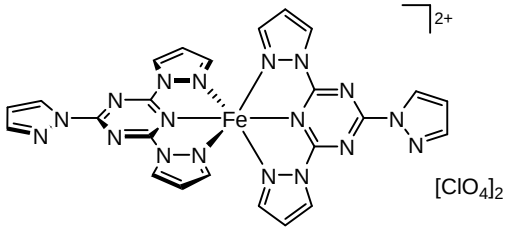


2,4-Di(pyrazol-1-yl)-6-(*iso*propylsulfanyl)-1,3,5-triazine
$C_{12}H_{13}N_7S$
L^8

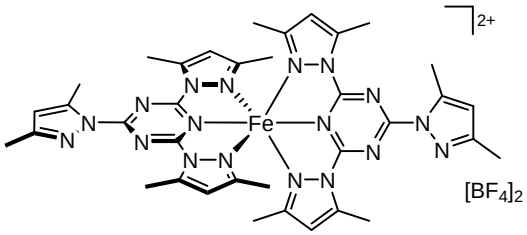
Complexes prepared during this study



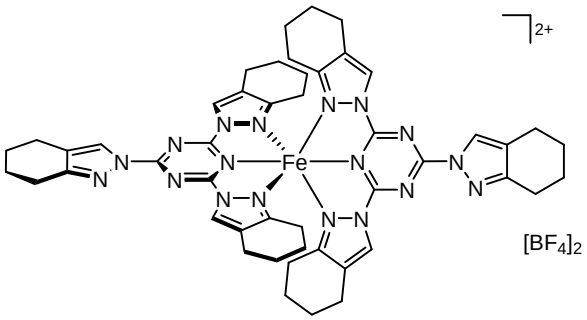
Bis-[2,4,6-tri(pyrazol-1-yl)-1,3,5-triazine]iron(II)
di-tetrafluoroborate
$C_{24}H_{18}B_2F_8FeN_{18}$
$[Fe(L^2)_2][BF_4]_2$



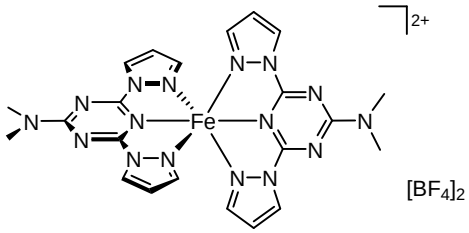
Bis-[2,4,6-tri(pyrazol-1-yl)-1,3,5-triazine]iron(II) diperchlorate
$C_{24}H_{18}Cl_2FeN_{18}O_8$
$[Fe(L^2)_2][ClO_4]_2$



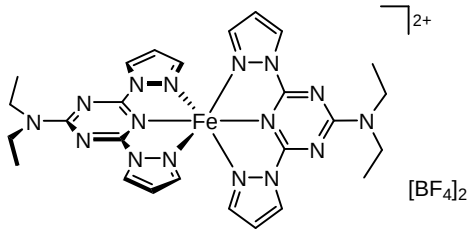
Bis-[2,4,6-tri(3,5-dimethylpyrazol-1-yl)-1,3,5-triazine]iron(II)
di-tetrafluoroborate
$C_{36}H_{42}B_2F_8FeN_{18}$
$[Fe(L^3)_2][BF_4]_2$



Bis-[2,4,6-tri(4,5,6,7-tetrahydroindazol-2-yl)-1,3,5-triazine]iron(II)
di-tetrafluoroborate
$C_{48}H_{54}B_2F_8FeN_{18}$
$[Fe(L^4)_2][BF_4]_2$

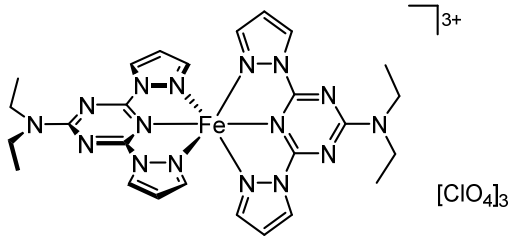


Bis-[2,4-di(pyrazol-1-yl)-6-(dimethylamino)-1,3,5-triazine]iron(II)
di-tetrafluoroborate
$C_{22}H_{24}B_2F_8FeN_{16}$
$[Fe(L^5)_2][BF_4]_2$

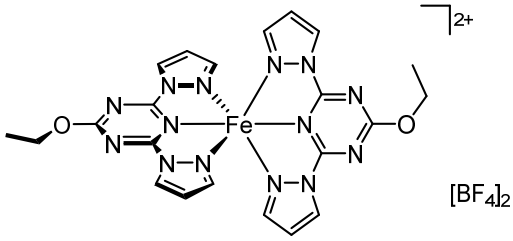


Bis-[2,4-di(pyrazol-1-yl)-6-(diethylamino)-1,3,5-triazine]iron(II)
di-tetrafluoroborate
$C_{26}H_{32}B_2F_8FeN_{16}$
$[Fe(L^6)_2][BF_4]_2$

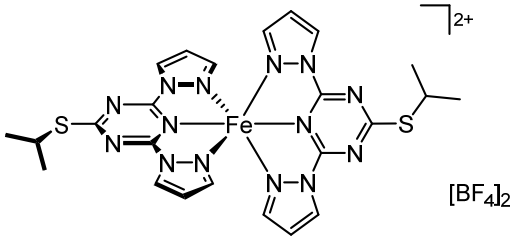
Complexes prepared during this study (continued)



Bis-[2,4-di(pyrazol-1-yl)-6-(diethylamino)-1,3,5-triazine]iron(III)
triperchlorate
$C_{26}H_{32}Cl_3FeN_{16}O_{12}$
$[Fe(L^6)_2][ClO_4]_3$

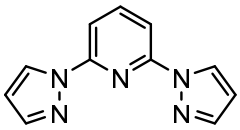


Bis-[2,4-di(pyrazol-1-yl)-6-ethoxy-1,3,5-triazine]iron(II)
di-tetrafluoroborate
$C_{22}H_{22}B_2F_8FeN_{14}O_2$
$[Fe(L^7)_2][BF_4]_2$

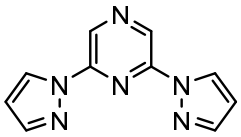


Bis-[2,4-di(pyrazol-1-yl)-6-(*iso*propylsulfanyl)-1,3,5-triazine]iron(II)
di-tetrafluoroborate
$C_{24}H_{26}B_2F_8FeN_{14}S_2$
$[Fe(L^8)_2][BF_4]_2$

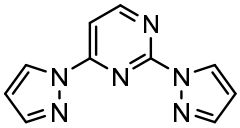
Ligands and complexes studied computationally



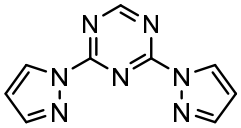
2,6-Di(pyrazol-1-yl)pyridine
$C_{11}H_9N_5$
bpp



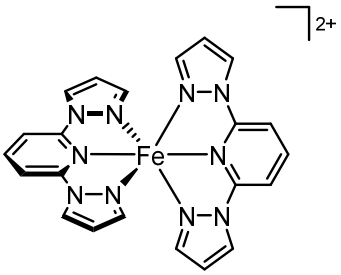
2,6-Di(pyrazol-1-yl)pyrazine
$C_{10}H_8N_6$
bpyz



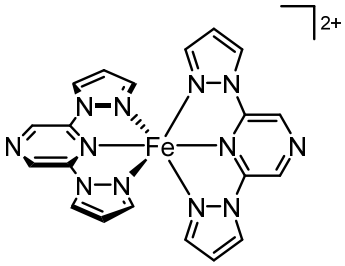
2,6-Di(pyrazol-1-yl)pyrimidine
$C_{10}H_8N_6$
bpym



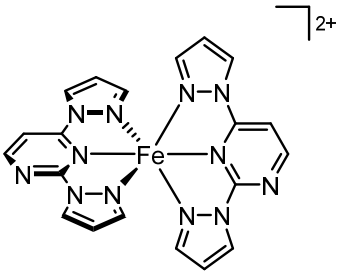
2,4-Di(pyrazol-1-yl)-1,3,5-triazine
$C_9H_7N_7$
bpt



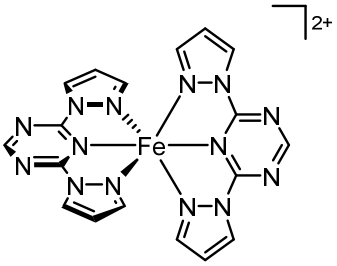
Bis-[2,6-di(pyrazol-1-yl)-pyridine]iron(II)
$[C_{22}H_{18}FeN_{10}]^{2+}$
$[Fe(bpp)_2]^{2+}$



Bis-[2,6-di(pyrazol-1-yl)-pyrazine]iron(II)
$[C_{20}H_{16}FeN_{12}]^{2+}$
$[Fe(bpyz)_2]^{2+}$

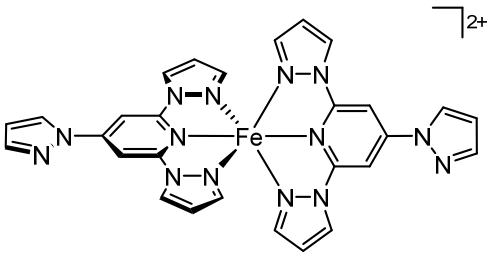


Bis-[2,6-di(pyrazol-1-yl)-pyrimidine]iron(II)
$[C_{20}H_{16}FeN_{12}]^{2+}$
$[Fe(bpym)_2]^{2+}$

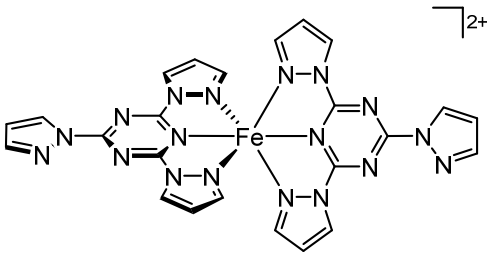


Bis-[2,4-di(pyrazol-1-yl)-1,3,5-triazine]iron(II)
$[C_{18}H_{14}FeN_{14}]^{2+}$
$[Fe(bpt)_2]^{2+}$

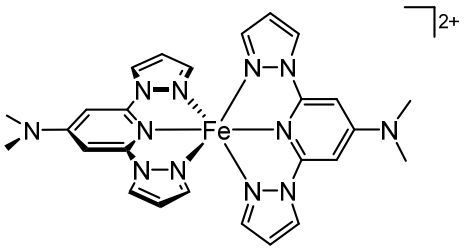
Ligands and complexes studied computationally (continued)



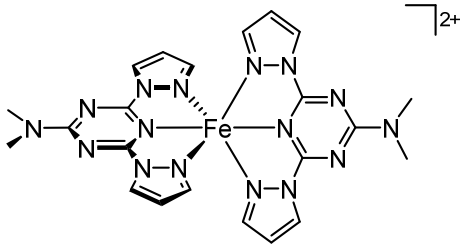
Bis-[2,4,6-tri(pyrazol-1-yl)-pyridine]iron(II)
$[C_{28}H_{22}FeN_{14}]^{2+}$
$[Fe(tpp)_2]^{2+}$



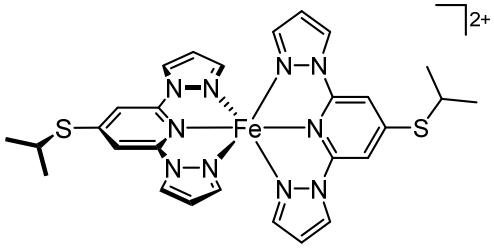
Bis-[2,4,6-tri(pyrazol-1-yl)-1,3,5-triazine]iron(II)
$[C_{24}H_{18}B_2F_8FeN_{18}]^{2+}$
$[Fe(L^2)_2]^{2+}$



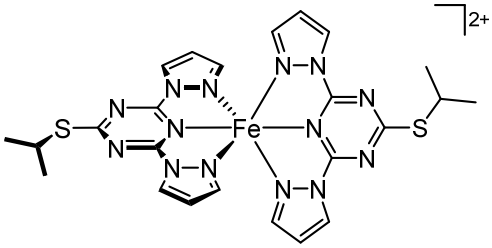
Bis-[2,6-di(pyrazol-1-yl)-4-dimethylaminopyridine]-iron(II)
$[C_{28}H_{22}FeN_{14}]^{2+}$
$[Fe(bpp^{NMe2})_2]^{2+}$



Bis-[2,4-di(pyrazol-1-yl)-6-(dimethylamino)-1,3,5-triazine]-iron(II)
$[C_{22}H_{24}B_2F_8FeN_{16}]^{2+}$
$[Fe(L^5)_2]^{2+}$



Bis-[2,6-di(pyrazol-1-yl)-4-(*iso*propylsulfanyl)pyridine]-iron(II)
$[C_{28}H_{30}FeN_{10}S_2]^{2+}$
$[Fe(bpp^{SiPr})_2]^{2+}$



Bis-[2,4-di(pyrazol-1-yl)-6-(*iso*propylsulfanyl)-1,3,5-triazine]-iron(II)
$[C_{24}H_{26}FeN_{14}S_2]^{2+}$
$[Fe(L^8)_2]^{2+}$