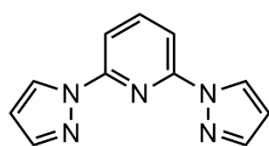


The dataset contains data for this study:

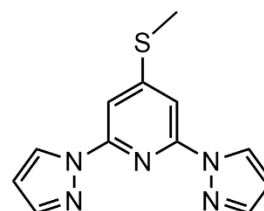
Solution magnetic susceptibility measurements by Evans method (NMR spectra and processed data).

Density functional calculations (*SPARTAN 18*).

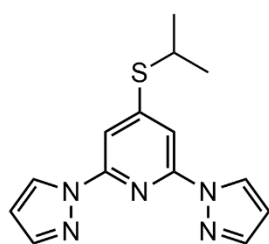
Compounds referred to in this dataset



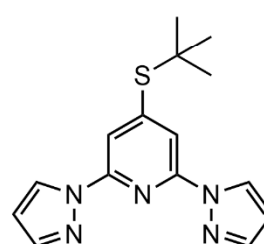
bpp
2,6-Di(pyrazol-1-yl)pyridine
 $C_{11}H_9N_5$



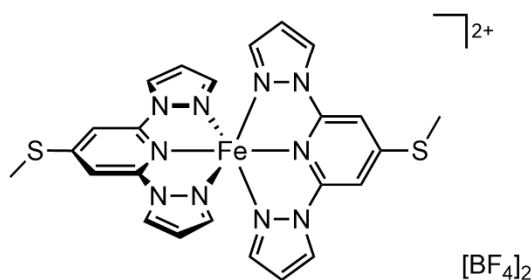
bpp^{SMe}
4-(Methylsulfanyl)-2,6-di(pyrazol-1-yl)pyridine
 $C_{12}H_{11}N_5S$



bpp^{SPr}
4-(*Iso*-propylsulfanyl)-2,6-di(pyrazol-1-yl)pyridine
 $C_{14}H_{15}N_5S$

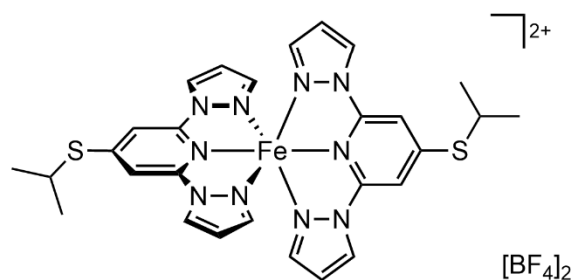


bpp^{StBu}
4-(*Tert*-butylsulfanyl)-2,6-di(pyrazol-1-yl)pyridine
 $C_{15}H_{17}N_5S$



$[Fe(bpp^{SMe})_2][BF_4]_2$
1 $[BF_4]_2$

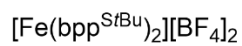
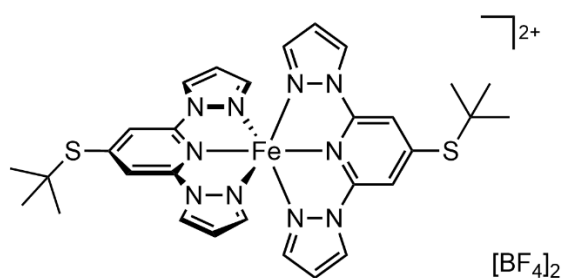
Bis[4-(methylsulfanyl)-2,6-di(pyrazol-1-yl)pyridine]-
iron(II) di(tetrafluoroborate)
 $C_{24}H_{22}B_2F_8FeN_{10}S_2$



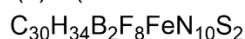
$[Fe(bpp^{SPr})_2][BF_4]_2$
2 $[BF_4]_2$

Bis[4-(*iso*-propylsulfanyl)-2,6-di(pyrazol-1-yl)pyridine]-
iron(II) di(tetrafluoroborate)
 $C_{28}H_{30}B_2F_8FeN_{10}S_2$

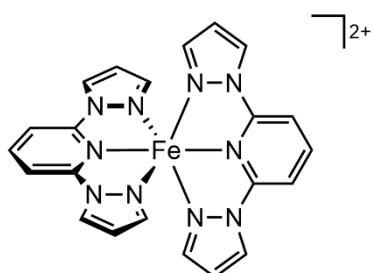
Compounds referred to in this dataset (continued)



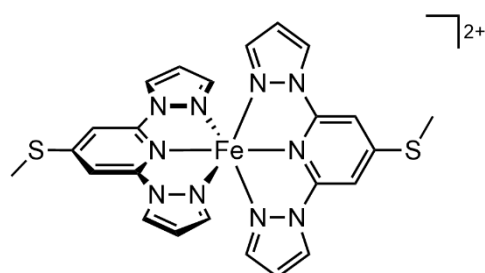
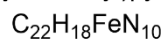
Bis[4-(*tert*-butylsulfanyl)-2,6-di(pyrazol-1-yl)pyridine]-
iron(II) di(tetrafluoroborate)



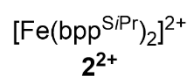
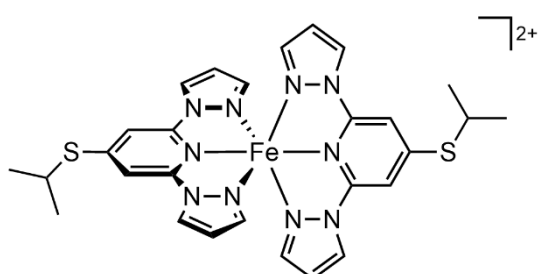
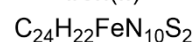
Compounds referred to in the DFT calculations



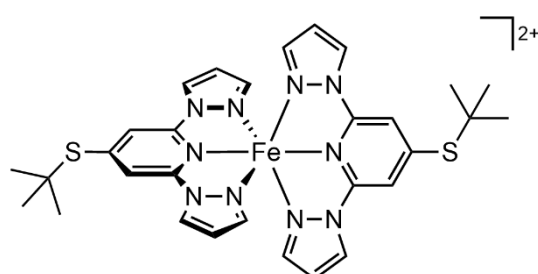
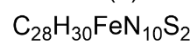
Bis[2,6-di(pyrazol-1-yl)pyridine]iron(II)



Bis[4-(methylsulfanyl)-2,6-di(pyrazol-1-yl)pyridine]-
iron(II)



Bis[4-(*iso*-propylsulfanyl)-2,6-di(pyrazol-1-yl)pyridine]-
iron(II)



Bis[4-(*tert*-butylsulfanyl)-2,6-di(pyrazol-1-yl)pyridine]-
iron(II)

