This dataset contains:

Analytical characterisation of the new complexes (CHN microanalysis).

Thermogravimetric analyses.

X-ray Crystallographic data:

- Structure of **1Cu**·$2H_2O$ at 150 K (CCDC 1973396)
- Structure of **1Cu** phase B at 350 K (CCDC 1973398)
- Structure of **1Cu** phase B at 300 K (CCDC 1973393)
- Structure of **1Cu** phase C' at 250 K (CCDC 1973394)
- Structure of **1Cu** phase C' at 200 K (CCDC 1973395)
- Structure of **1Cu** phase C' at 150 K (CCDC 1973397)
- Structure of **1Zn**·$2H_2O$ at 150 K (CCDC 1973389)
- Structure of **1Zn** phase B at 305 K (CCDC 1973390)
- Structure of **1Zn** phase C at 285 K (CCDC 1973391)
- Structure of **1Zn** phase C at 240 K (CCDC 1973392)
- Structure of **1Zn** phase C at 150 K (CCDC 1973368).

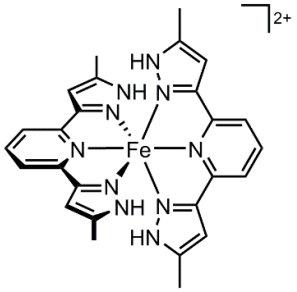
X-ray powder diffraction data collected with Cu-K_α and synchrotron radiation (measured and simulated).

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

Differential Scanning Calorimetry (DSC) data.

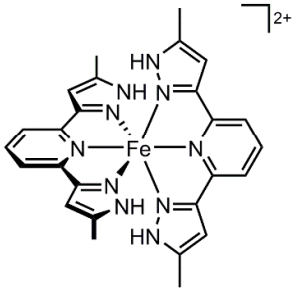
X-band and Q-band EPR spectra (measured and simulated).

Compounds prepared during this study



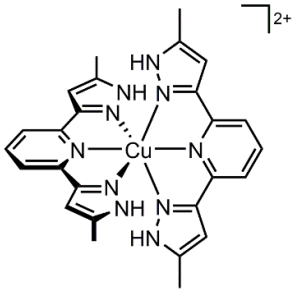
$[BF_4]_2 \cdot 2H_2O$

Bis-(2,6-*bis*[5-methyl-1*H*-pyrazol-3-yl]pyridine)iron(II) ditetrafluoroborate dihydrate
$[FeL_2][BF_4]_2 \cdot 2H_2O$
$C_{26}H_{30}B_2F_8FeN_{10}O_2$
1Fe$\cdot 2H_2O$



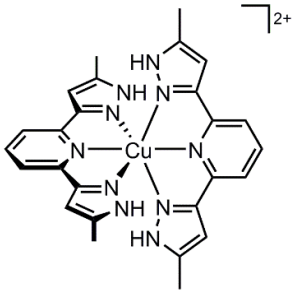
$[BF_4]_2$

Bis-(2,6-*bis*[5-methyl-1*H*-pyrazol-3-yl]pyridine)iron(II) ditetrafluoroborate
$[FeL_2][BF_4]_2$
$C_{26}H_{26}B_2F_8FeN_{10}$
1Fe



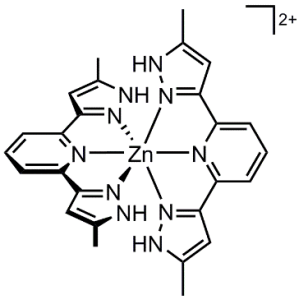
$[BF_4]_2 \cdot 2H_2O$

Bis-(2,6-*bis*[5-methyl-1*H*-pyrazol-3-yl]pyridine)copper(II) ditetrafluoroborate dihydrate
$[CuL_2][BF_4]_2 \cdot 2H_2O$
$C_{26}H_{30}B_2CuF_8N_{10}O_2$
1Cu$\cdot 2H_2O$



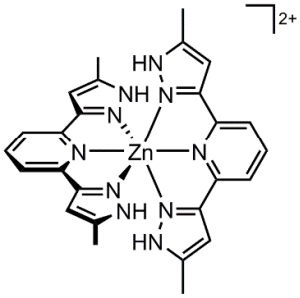
$[BF_4]_2$

Bis-(2,6-*bis*[5-methyl-1*H*-pyrazol-3-yl]pyridine)copper(II) ditetrafluoroborate
$[CuL_2][BF_4]_2$
$C_{26}H_{26}B_2CuF_8N_{10}$
1Cu



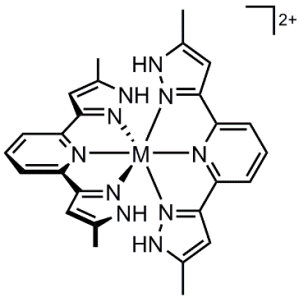
$[BF_4]_2 \cdot 2H_2O$

Bis-(2,6-*bis*[5-methyl-1*H*-pyrazol-3-yl]pyridine)zinc(II) ditetrafluoroborate dihydrate
$[ZnL_2][BF_4]_2 \cdot 2H_2O$
$C_{26}H_{30}B_2F_8N_{10}O_2Zn$
1Zn$\cdot 2H_2O$



$[BF_4]_2$

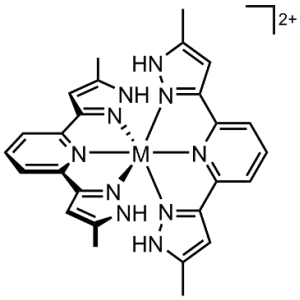
Bis-(2,6-*bis*[5-methyl-1*H*-pyrazol-3-yl]pyridine)zinc(II) ditetrafluoroborate
$[ZnL_2][BF_4]_2$
$C_{26}H_{26}B_2F_8N_{10}Zn$
1Zn



$[BF_4]_2 \cdot 2H_2O$

M = Fe_xCu_{1-x} (x = 0.97)

Bis-(2,6-*bis*[5-methyl-1*H*-pyrazol-3-yl]pyridine)iron,copper(II) ditetrafluoroborate dihydrate solid solution
$[Fe_{0.97}Cu_{0.03}L_2][BF_4]_2 \cdot 2H_2O$
$C_{26}H_{30}B_2Cu_{0.03}F_8Fe_{0.97}N_{10}O_2$
1Fe,Cu$\cdot 2H_2O$



$[BF_4]_2$

M = Fe_xCu_{1-x} (x = 0.97)

Bis-(2,6-*bis*[5-methyl-1*H*-pyrazol-3-yl]pyridine)iron,copper(II) ditetrafluoroborate solid solution
$[Fe_{0.97}Cu_{0.03}L_2][BF_4]_2$
$C_{26}H_{26}B_2Cu_{0.03}F_8Fe_{0.97}N_{10}$
1Fe,Cu