

This dataset contains:

Analytical characterisation of the $[\text{Fe}(\text{3-bpp})_2][\text{NCS}]_2$ and $[\text{Fe}(\text{3-bpp})_2][\text{NCSe}]_2$ (CHN microanalysis).

X-ray Crystallographic data from $[\text{Fe}(\text{3-bpp})_2][\text{NCS}]_2$ at three temperatures:

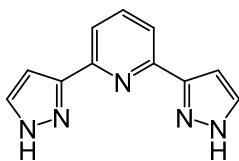
- $T = 270 \text{ K}$ (CCDC 1903939)
- $T = 230 \text{ K}$ (CCDC 1903940)
- $T = 120 \text{ K}$ (CCDC 1903941).

Solid state magnetic susceptibility data (raw and plotted data).

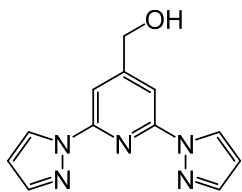
Solution phase (Evans method) magnetic susceptibility data (plotted data).

Simulated powder diffraction pattern for $[\text{Fe}(\text{3-bpp})_2][\text{NCS}]_2$ at room temperature.

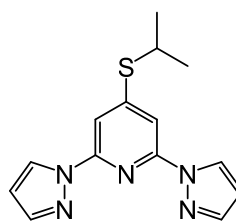
Ligands referred to in this dataset



2,6-Di(1*H*-pyrazol-3-yl)pyridine
3-bpp
 $\text{C}_{11}\text{H}_9\text{N}_5$

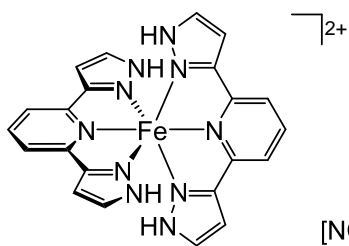


4-Hydroxymethyl-2,6-di(pyrazol-1-yl)pyridine
 $\text{bpp}^{\text{CH}_2\text{OH},\text{H}}$
 $\text{C}_{12}\text{H}_{11}\text{N}_5\text{O}$

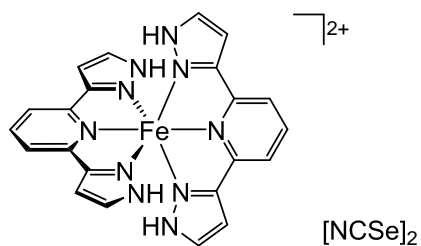


4-Isopropylsulfanyl-2,6-di(pyrazol-1-yl)pyridine
 $\text{bpp}^{\text{SiPr},\text{H}}$
 $\text{C}_{14}\text{H}_{15}\text{N}_5\text{S}$

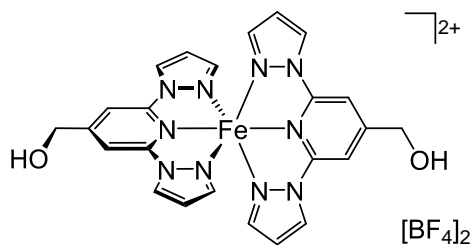
Complexes referred to in this dataset



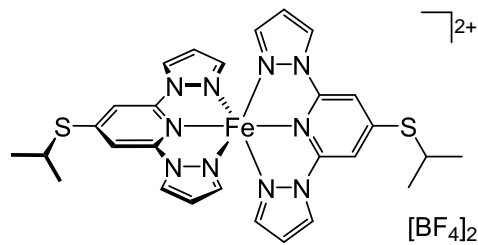
Bis[2,6-di(pyrazol-3-yl)pyridine]iron(II)
di(thiocyanate)
[Fe(3-bpp)₂][NCS]₂
C₂₄H₁₈FeN₁₂S₂



Bis[2,6-di(pyrazol-3-yl)pyridine]iron(II)
di(thiocyanate)
[Fe(3-bpp)₂][NCSe]₂
C₂₄H₁₈FeN₁₂Se₂



Bis[4-(hydroxymethyl)-2,6-di(pyrazol-1-yl)-
pyridine]iron(II) ditetrafluoroborate
[Fe(bpp^{CH₂OH,H})₂][BF₄]₂
C₂₄H₂₂B₂F₈FeN₁₀O₂



Bis[4-(isopropylsulfanyl)-2,6-di(pyrazol-1-yl)-
pyridine]iron(II) ditetrafluoroborate
[Fe(bpp^{SiPr,H})₂][BF₄]₂
C₂₈H₃₀B₂F₈FeN₁₀S₂