

This dataset contains:

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

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

Paramagnetic  $^1\text{H}$  NMR spectra of the iron complexes (raw data).

X-ray Crystallographic data:

- Structure of  $\text{L}^1\text{C}_{12}$  (CCDC 2064046).
- Structure of  $\text{L}^2\text{C}_{12}$  (CCDC 2064047).
- Structure of  $\text{L}^2\text{C}_{14}$  (CCDC 2064048).
- Structure of  $[\text{Fe}(\text{L}^2\text{C}_{12})_2][\text{BF}_4]_2$  (CCDC 2064049).
- Preliminary structure solution of  $[\text{Fe}(\text{L}^2\text{C}_{16})_2][\text{BF}_4]_2$  (not deposited to CSD).
- Preliminary structure solution of  $[\text{Fe}(\text{L}^2\text{C}_{18})_2][\text{BF}_4]_2$  (not deposited to CSD).

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

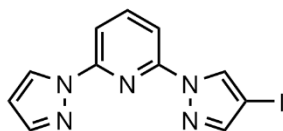
Solution phase magnetic susceptibility measurements (NMR spectra and processed data)

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

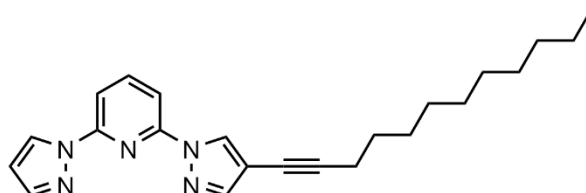
Thermogravimetric analysis (TGA) data.

Differential scanning calorimetry (DSC) data.

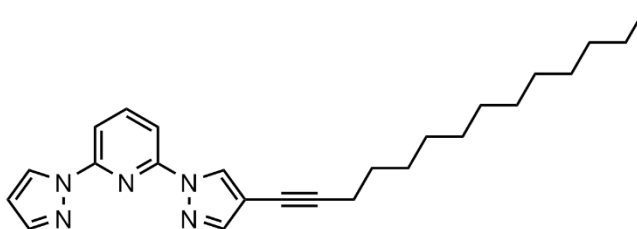
## Ligands employed in this study



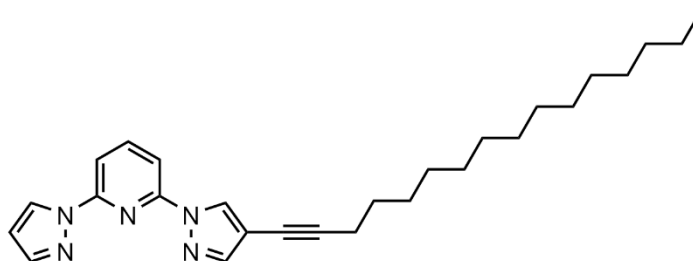
2-(4-Iodopyrazol-1-yl)-6-(pyrazol-1-yl)pyridine  
 $C_{11}H_8IN_5$



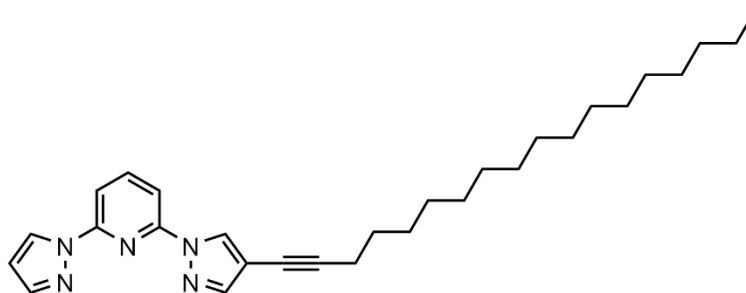
2-(4-{Dodec-1-ynyl}pyrazol-1-yl)-6-(pyrazol-1-yl)pyridine  
 $C_{23}H_{29}N_5$   
 $L^1C_{12}$



2-(4-{Tetradec-1-ynyl}pyrazol-1-yl)-6-(pyrazol-1-yl)pyridine  
 $C_{25}H_{33}N_5$   
 $L^1C_{14}$

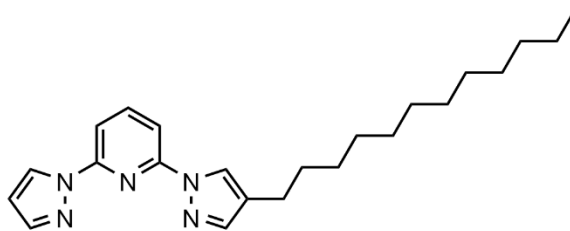


2-(4-{Hexadec-1-ynyl}pyrazol-1-yl)-6-(pyrazol-1-yl)pyridine  
 $C_{27}H_{37}N_5$   
 $L^1C_{16}$



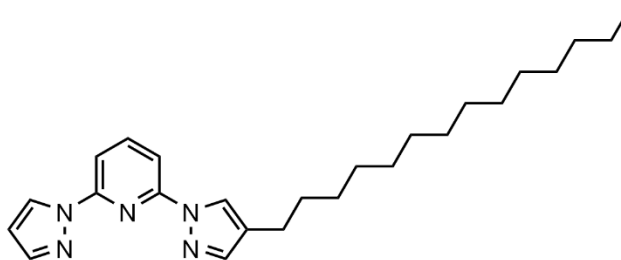
2-(4-{Octadec-1-ynyl}pyrazol-1-yl)-6-(pyrazol-1-yl)pyridine  
 $C_{29}H_{41}N_5$   
 $L^1C_{18}$

## Ligands employed in this study (continued)



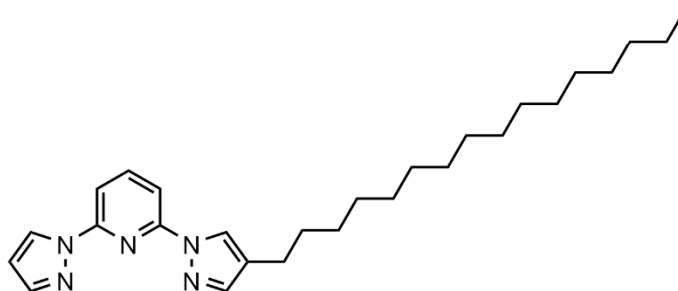
2-(4-{Dodecyl}pyrazol-1-yl)-6-(pyrazol-1-yl)pyridine

$C_{23}H_{33}N_5$   
 $L^2C_{12}$



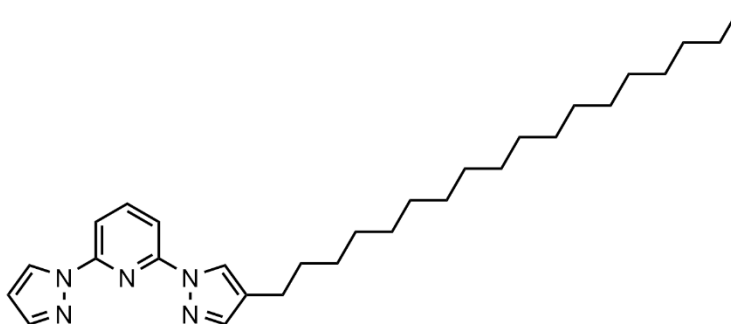
2-(4-{Tetradecyl}pyrazol-1-yl)-6-(pyrazol-1-yl)pyridine

$C_{25}H_{37}N_5$   
 $L^2C_{14}$



2-(4-{Hexadecyl}pyrazol-1-yl)-6-(pyrazol-1-yl)pyridine

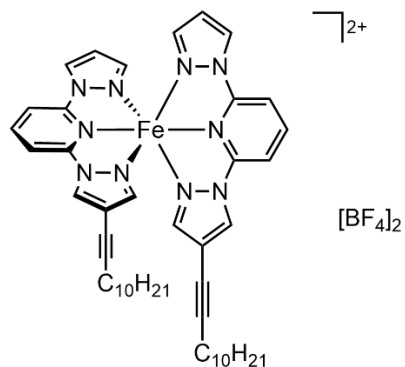
$C_{27}H_{41}N_5$   
 $L^2C_{16}$



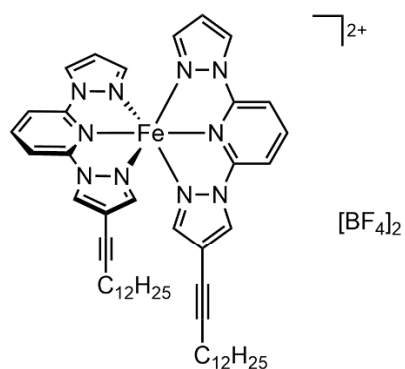
2-(4-{Octadecyl}pyrazol-1-yl)-6-(pyrazol-1-yl)pyridine

$C_{29}H_{45}N_5$   
 $L^2C_{18}$

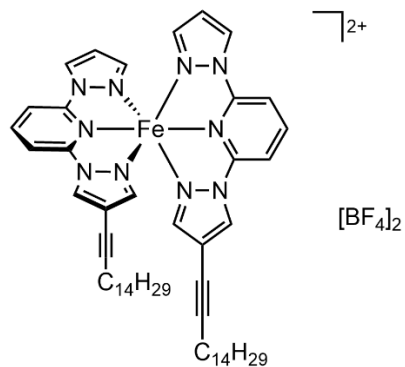
## Iron complexes prepared during this study



Bis[2-(4-(dodec-1-ynyl)pyrazol-1-yl)-6-(pyrazol-1-yl)pyridine]iron(II) di-tetrafluoroborate  
 $C_{46}H_{58}B_2F_8FeN_{10}$   
 $[Fe(L^1C_{12})_2][BF_4]_2$

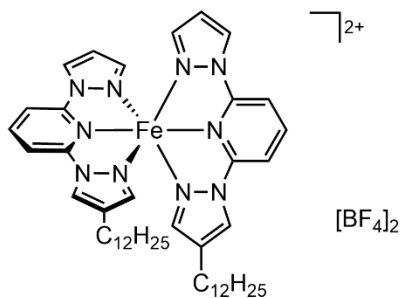


Bis[2-(4-(tetradec-1-ynyl)pyrazol-1-yl)-6-(pyrazol-1-yl)pyridine]iron(II) di-tetrafluoroborate  
 $C_{50}H_{66}B_2F_8FeN_{10}$   
 $[Fe(L^1C_{14})_2][BF_4]_2$

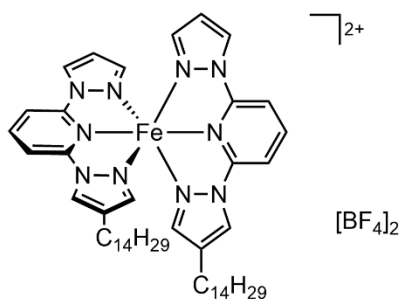
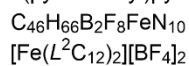


Bis[2-(4-(hexadec-1-ynyl)pyrazol-1-yl)-6-(pyrazol-1-yl)pyridine]iron(II) di-tetrafluoroborate  
 $C_{54}H_{74}B_2F_8FeN_{10}$   
 $[Fe(L^1C_{16})_2][BF_4]_2$

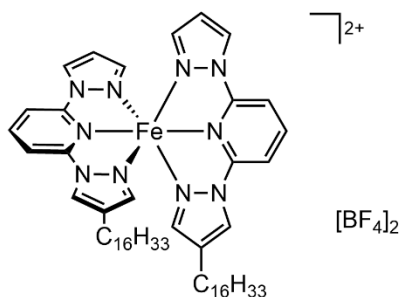
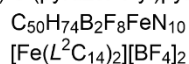
## Iron complexes prepared during this study (continued)



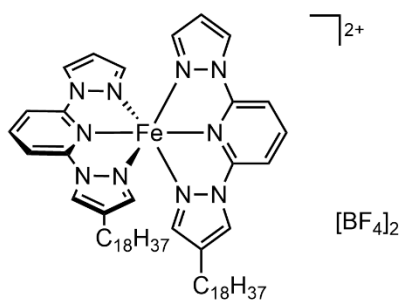
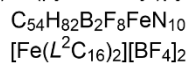
Bis[2-(4-{dodecyl}pyrazol-1-yl)-6-(pyrazol-1-yl)pyridine]iron(II) di-tetrafluoroborate



Bis[2-(4-{tetradecyl}pyrazol-1-yl)-6-(pyrazol-1-yl)pyridine]iron(II) di-tetrafluoroborate



Bis[2-(4-{hexadecyl}pyrazol-1-yl)-6-(pyrazol-1-yl)pyridine]iron(II) di-tetrafluoroborate



Bis[2-(4-{octadecyl}pyrazol-1-yl)-6-(pyrazol-1-yl)pyridine]iron(II) di-tetrafluoroborate

