

The dataset contains:

Analytical characterisation of the complexes (CHN microanalysis)

X-ray Crystallographic data:

- Structures of **1** at two temperatures (CCDC 1532884 and 1532885).
- Structure of (*R*)-**2** (CCDC 1532886).
- Structures of (*R*)-**3**·MeNO<sub>2</sub> at sixteen temperatures (CCDC 1519275–1519290).
- Structures of (*RS*)-**3**·3MeCN at two temperatures (CCDC 1532887 and 1532888).
- Structure of (*R*)-**4**·½MeCN (CCDC 1532889).
- Structure of (*RS*)-**4** (CCDC 1532890).

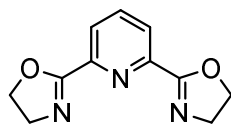
X-ray powder diffraction data (measured and simulated)

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

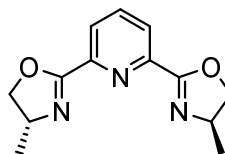
Paramagnetic <sup>1</sup>H NMR spectra (raw data and plotted spectra).

Solution magnetic susceptibility measurements (spectra, calculated XmT values and *SIGMAPLOT* fits to derive thermodynamic parameters).

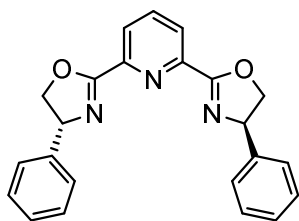
## Ligands referred to in this study



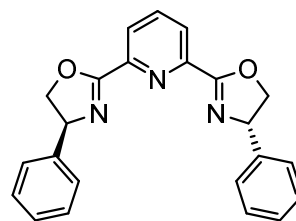
2,6-Bis(4,5-dihydrooxazol-2-yl)pyridine  
 $C_{11}H_{11}N_3O_2$   
 $L^H$  (PyBox)



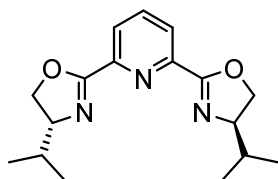
2,6-Bis((*R*)-4-methyl-4,5-dihydrooxazol-2-yl)pyridine  
 $C_{13}H_{15}N_3O_2$   
(*R*)- $L^{Me}$



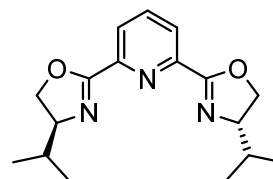
2,6-Bis(4-(*R*)-phenyl-4,5-dihydrooxazol-2-yl)pyridine  
 $C_{23}H_{19}N_3O_2$   
(*R*)- $L^{Ph}$



2,6-Bis(4-(*S*)-phenyl-4,5-dihydrooxazol-2-yl)pyridine  
 $C_{23}H_{19}N_3O_2$   
(*S*)- $L^{Ph}$

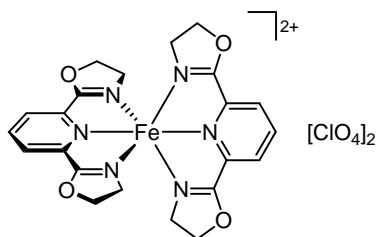


2,6-Bis(4-(*R*)-isopropyl-4,5-dihydrooxazol-2-yl)pyridine  
 $C_{17}H_{23}N_3O_2$   
(*R*)- $L^{iPr}$

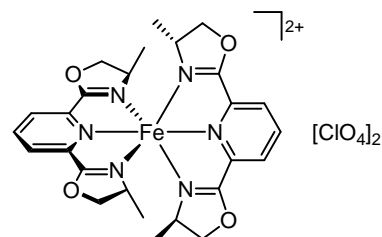


2,6-Bis(4-(*S*)-isopropyl-4,5-dihydrooxazol-2-yl)pyridine  
 $C_{17}H_{23}N_3O_2$   
(*S*)- $L^{iPr}$

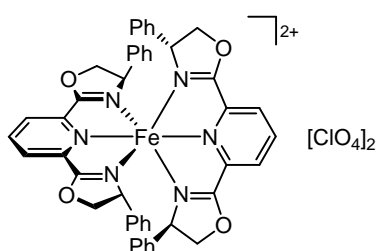
## Complexes referred to in this study



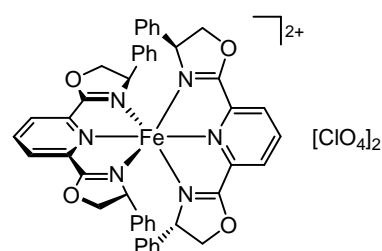
Bis[2,6-bis(4,5-dihydrooxazol-2-yl)pyridine]iron(II) diperchlorate  
 $C_{22}H_{22}Cl_2FeN_6O_{12}$   
 Compound 1



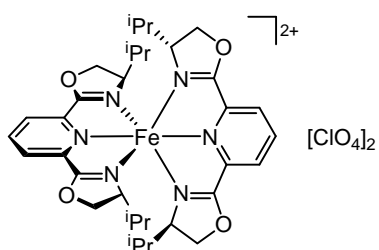
Bis[2,6-bis((*R*)-4-methyl-4,5-dihydrooxazol-2-yl)pyridine]iron(II) diperchlorate  
 $C_{26}H_{30}Cl_2FeN_6O_{12}$   
 Compound (*R*)-2



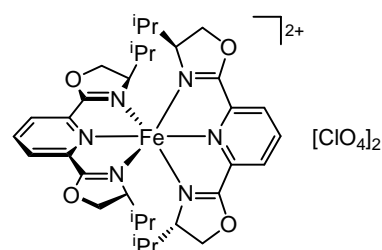
Bis[2,6-bis((*R*)-4-phenyl-4,5-dihydrooxazol-2-yl)pyridine]iron(II) diperchlorate  
 $C_{46}H_{38}Cl_2FeN_6O_{12}$   
 Compound (*R*)-3



[2,6-Bis((*R*)-4-phenyl-4,5-dihydrooxazol-2-yl)pyridine]-[2,6-bis((*S*)-4-phenyl-4,5-dihydrooxazol-2-yl)pyridine]iron(II) diperchlorate  
 $C_{46}H_{38}Cl_2FeN_6O_{12}$   
 Compound (*RS*)-3



Bis[2,6-bis((*R*)-4-*isopropyl*-4,5-dihydrooxazol-2-yl)pyridine]iron(II) diperchlorate  
 $C_{34}H_{46}Cl_2FeN_6O_{12}$   
 Compound (*R*)-4



[2,6-Bis((*R*)-4-*isopropyl*-4,5-dihydrooxazol-2-yl)pyridine]-[2,6-bis((*S*)-4-*isopropyl*-4,5-dihydrooxazol-2-yl)pyridine]iron(II) diperchlorate  
 $C_{34}H_{46}Cl_2FeN_6O_{12}$   
 Compound (*RS*)-4