

Title: Data to support study of The Impact of Whole-Molecule Disorder on Spin-Crossover in a Family of Isomorphous Molecular Crystals

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Rights-holder(s): Malcolm A. Halcrow

Publication Year: 2025

Description: Seven iron(II) complex salts, of 2,6-di(pyrazol-1-yl)pyridines bearing a substituent at one pyrazolyl C4 position, are isomorphous but show a variety of spin-crossover behaviours. Crystal structures show disorder of the two ligand substituents around the four pyrazolyl groups in the molecules, which can lead to resolvable whole-molecule disorder as shown. Unusual discontinuities in the more abrupt spin-transitions may arise from heterogeneous lattice sites within the *cooperative* SCO material.

Cite as: Sephton, Holly E., Watson, Rhiannon L., Shahid, Namrah, Vasili, Hari Babu, Baker, Daniel L., Saha, Dipankar, Capel Berdiell, Izar, Pask, Christopher M., Cespedes, Oscar and Halcrow, Malcolm A. (2025): Data to support study of The Impact of Whole-Molecule Disorder on Spin-Crossover in a Family of Isomorphous Molecular Crystals. [Dataset] <https://doi.org/10.5518/1625>

Related publication: Sephton, Holly E., Watson, Rhiannon L., Shahid, Namrah, Vasili, Hari Babu, Baker, Daniel L., Saha, Dipankar, Capel Berdiell, Izar, Pask, Christopher M., Cespedes, Oscar and Halcrow, Malcolm A. (2025): The Impact of Whole-Molecule Disorder on Spin-Crossover in a Family of Isomorphous Molecular Crystals *Chemical Science*, doi: 10.1039/d5sc00090d

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2 PROJECT AND FUNDING INFORMATION

Title: University of Leeds DTP studentship

Dates: 2016-17

Funding organisation: EPSRC

Grant no.: EP/N509681/1

Title: Metallo-Supramolecular and Functional Complexes

Dates: 2021-2023

Funding organisation: Diamond Light Source

Grant no.: CY26879

Title: Norwegian Centre for X-ray Diffraction, Scattering and Imaging (RECX)

Dates: 2011-2018

Funding organisation: Research Council of Norway

Grant no.: 208896

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3. TERMS OF USE

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4. CONTENTS

The dataset contains data for this study:

Elemental microanalyses (*microanalysis.zip*).

^1H , ^{13}C and ^{19}F NMR spectra of the organic ligands L^{R} , and paramagnetic ^1H NMR spectra of the complexes (raw and processed data – *NMR.zip*).

Electrospray mass spectra of the L^{R} ligands (plotted spectra – *ESMS.zip*)

Room temperature X-ray powder diffraction data (measured and simulated – *XRPD_RT.zip*).

Variable temperature X-ray powder diffraction data (*Origin* files containing measured data – *XRPD_VT.zip*).

Solid state magnetic susceptibility measurements (raw and processed data – *SQUID.zip*).

Differential scanning calorimetry data – (*DSC.zip*).

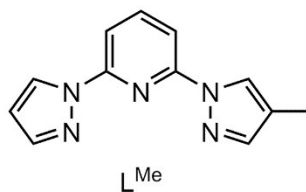
X-ray crystallographic data (*crystal.zip*):

- Structure of **1**[ClO_4]₂ at 100 K (CCDC 2411009).
- Structure of **1**[ClO_4]₂ at 180 K (CCDC 2411010).
- Structure of **1**[ClO_4]₂ at 220 K (CCDC 2411011).
- Structure of **1**[ClO_4]₂ at 300 K (CCDC 2411012).
- Unit cell determination of **2**[BF_4]₂ at 100 K.
- Structure of **3**[BF_4]₂ at 100 K (CCDC 2411013).
- Unit cell determination of **3**[BF_4]₂ at 300 K.
- Unit cell determination of $[\text{Fe}(\text{L}^{\text{Cl}})_2][\text{BF}_4]_2$ at 200 K.

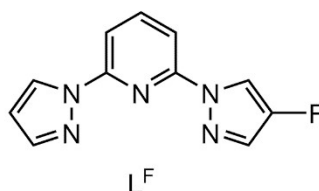
5. METHODS

Full details are provided in the related publication, listed above.

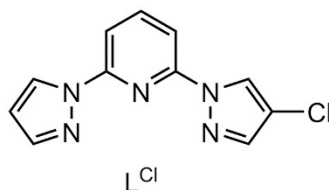
Compounds referred to in this dataset



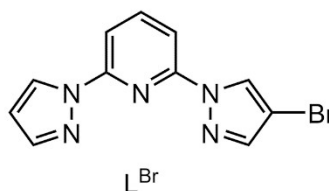
2-(Pyrazol-1-yl)-6-(4-methylpyrazol-1-yl)pyridine
 $C_{12}H_{11}N_5$



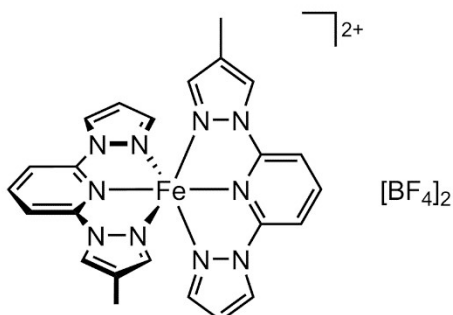
2-(Pyrazol-1-yl)-6-(4-fluoropyrazol-1-yl)pyridine
 $C_{11}H_8FN_5$



2-(Pyrazol-1-yl)-6-(4-chloropyrazol-1-yl)pyridine
 $C_{11}H_8ClN_5$



2-(Pyrazol-1-yl)-6-(4-bromopyrazol-1-yl)pyridine
 $C_{11}H_8BrN_5$



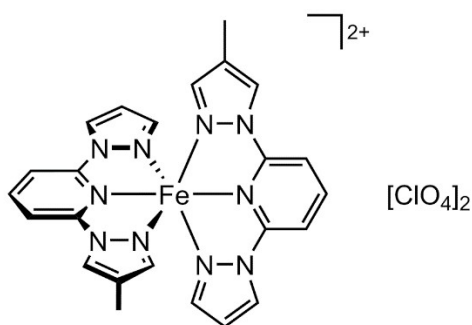
1[BF₄]₂

$[Fe(L^{\text{Me}})_2][BF_4]_2$

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

$C_{24}H_{22}B_2F_8FeN_{10}$

Compounds referred to in this dataset (continued)

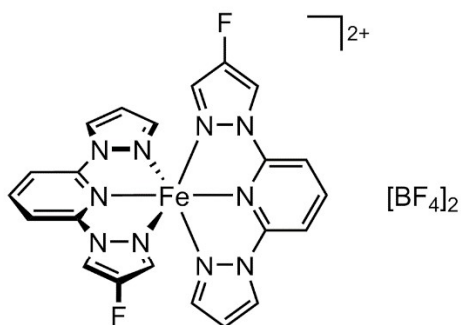


1[ClO₄]₂

[Fe(L^{Me})₂][ClO₄]₂

Bis[2-(pyrazol-1-yl)-6-(4-methylpyrazol-1-yl)pyridine]iron(II) diperchlorate

C₂₄H₂₂Cl₂FeN₁₀O₈

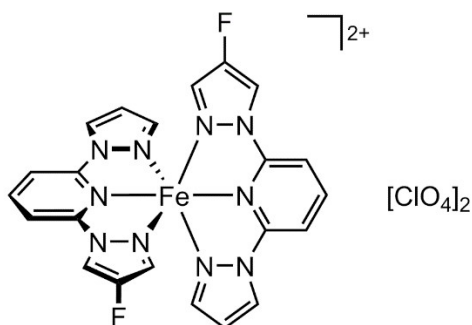


2[BF₄]₂

[Fe(L^F)₂][BF₄]₂

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

C₂₂H₁₆B₂F₁₀FeN₁₀



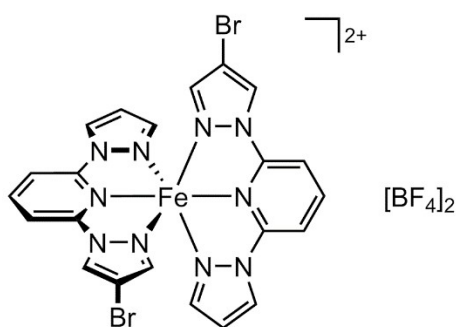
2[ClO₄]₂

[Fe(L^F)₂][ClO₄]₂

Bis[2-(pyrazol-1-yl)-6-(4-fluoropyrazol-1-yl)pyridine]iron(II) diperchlorate

C₂₂H₁₆Cl₂F₂FeN₁₀O₈

Compounds referred to in this dataset (continued)

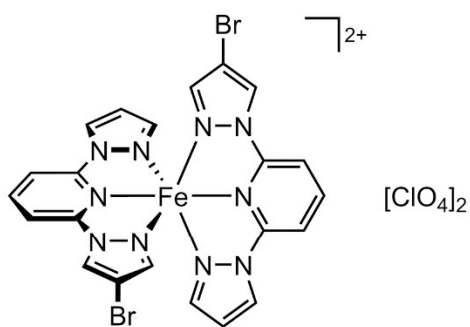


3[BF₄]₂

$[\text{Fe}(\text{L}^{\text{Br}})_2][\text{BF}_4]_2$

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

$\text{C}_{22}\text{H}_{16}\text{B}_2\text{Br}_2\text{F}_8\text{FeN}_{10}$

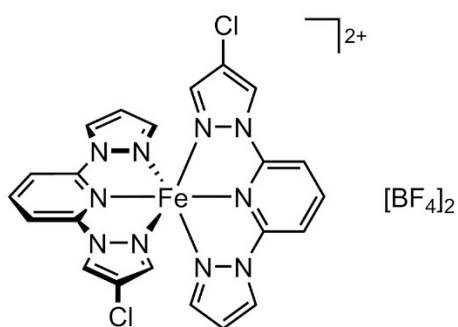


3[ClO₄]₂

$[\text{Fe}(\text{L}^{\text{Br}})_2][\text{ClO}_4]_2$

Bis[2-(pyrazol-1-yl)-6-(4-bromopyrazol-1-yl)pyridine]iron(II) diperchlorate

$\text{C}_{22}\text{H}_{16}\text{Br}_2\text{Cl}_2\text{FeN}_{10}\text{O}_8$



$[\text{Fe}(\text{L}^{\text{Cl}})_2][\text{BF}_4]_2$

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

$\text{C}_{22}\text{H}_{16}\text{B}_2\text{Cl}_2\text{F}_8\text{FeN}_{10}$