

**Title:** Data to support study of The Influence of Counterions on an Iron(II) Complex Exhibiting a Spin-Transition with Wide Thermal Hysteresis

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**Organisation(s):** 1. University of Leeds. 2. University of Oslo. 3. University of Manchester.

**Rights-holder(s):** Malcolm A. Halcrow

**Publication Year:** 2022

**Description:** A diiron(II) complex has been crystallised in three different helicate conformations, which differ in the torsions of the butane-1,4-diyl ligand linker groups. The crystals exhibit a range of spin state properties, including stepwise spin-crossover of the two iron atoms. A related ligand with a rigid pyrid-2,6-diyl spacer forms more a distorted, high-spin diiron(II) helicate structure.

**Cite as:** Roberts, Thomas D., Pask, Christopher M., Capel Berdiell, Izar, Tuna, Floriana and Halcrow, Malcolm A. (2022). Data to support study of The Influence of Counterions on an Iron(II) Complex Exhibiting a Spin-Transition with Wide Thermal Hysteresis. University of Leeds. [Dataset] <https://doi.org/10.5518/1233>

**Related publication:** Roberts, Thomas D., Pask, Christopher M., Capel Berdiell, Izar, Tuna, Floriana and Halcrow, Malcolm A. (2022). Data to support study of The Influence of Counterions on an Iron(II) Complex Exhibiting a Spin-Transition with Wide Thermal Hysteresis. *Journal of Materials Chemistry C*, doi: 10.1039/d2tc03654a

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## 2. TERMS OF USE

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## 3. PROJECT AND FUNDING INFORMATION

Title: DTP studentship to Thomas Roberts

Dates: 2011-2015

Funding organisation: EPSRC

Grant no.:

Title: Brotherton Scholarship to Thomas Roberts

Dates: 2011-2014

Funding organisation: University of Leeds

Title: TomoCAT

Dates:

Funding organisation: Research Council of Norway

Grant no.: 301619

## 4. CONTENTS

The dataset contains data for this study:

Elemental microanalyses (*microanalysis.zip*).

X-ray powder diffraction data (measured and simulated – *XRPD.zip*).

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

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

- Structure of **2[ClO<sub>4</sub>]<sub>2</sub>·2H<sub>2</sub>O** at 120 K (CCDC 2195223).
- Structure of **2[ClO<sub>4</sub>]<sub>2</sub>**, phase B at 350 K (CCDC 2195224).
- Structure of **2[ClO<sub>4</sub>]<sub>2</sub>**, phase B at 300 K (CCDC 2195225).
- Structure of **2[ClO<sub>4</sub>]<sub>2</sub>**, phase B at 250 K (CCDC 2195226).
- Structure of **2[ClO<sub>4</sub>]<sub>2</sub>**, phase B at 200 K (CCDC 2195227).
- Structure of **2[ClO<sub>4</sub>]<sub>2</sub>**, phase C at 120 K (CCDC 2195228).

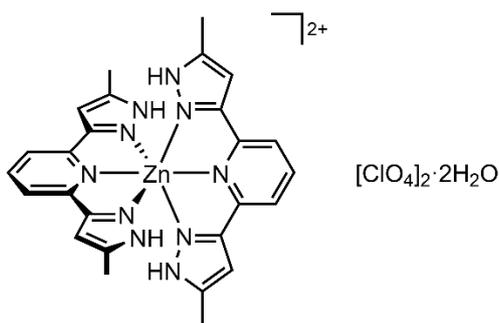
Differential scanning calorimetry data (*DSC.zip*)

Thermogravimetric analyses (*TGA.zip*)

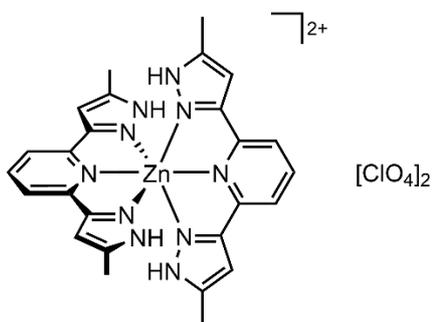
## 5. METHODS

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

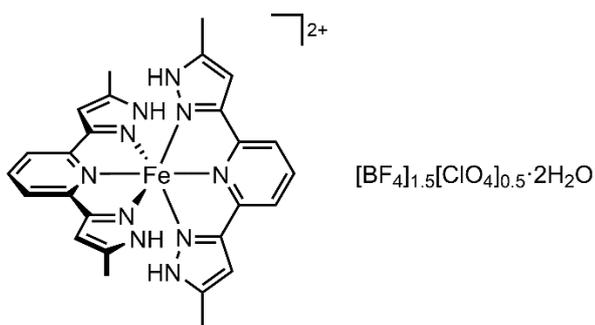
## Compounds referred to in this dataset



*Bis*-(2,6-*bis*[5-methyl-1*H*-pyrazol-3-yl]pyridine)zinc(II) diperchlorate dihydrate  
 $[ZnL_2][ClO_4]_2 \cdot 2H_2O$   
 $C_{26}H_{30}Cl_2N_{10}O_{10}Zn$   
**2b**·2H<sub>2</sub>O

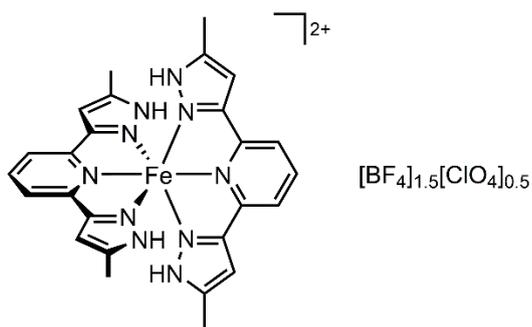


*Bis*-(2,6-*bis*[5-methyl-1*H*-pyrazol-3-yl]pyridine)zinc(II) diperchlorate  
 $[ZnL_2][ClO_4]_2$   
 $C_{26}H_{26}Cl_2N_{10}O_8Zn$   
**2b**

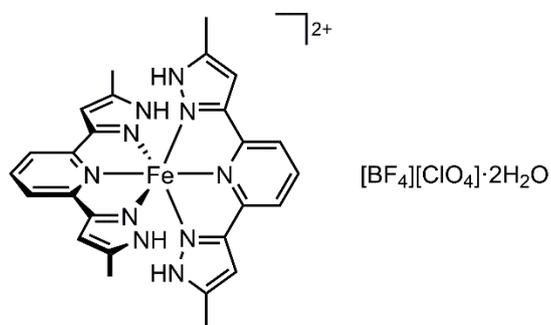


*Bis*-(2,6-*bis*[5-methyl-1*H*-pyrazol-3-yl]pyridine)iron(II) sesqui(tetrafluoroborate) hemi(perchlorate) dihydrate  
 $[FeL_2][BF_4]_{1.5}[ClO_4]_{0.5} \cdot 2H_2O$   
 $C_{26}H_{30}B_{1.5}Cl_{0.5}F_6FeN_{10}O_4$   
**1c**·2H<sub>2</sub>O

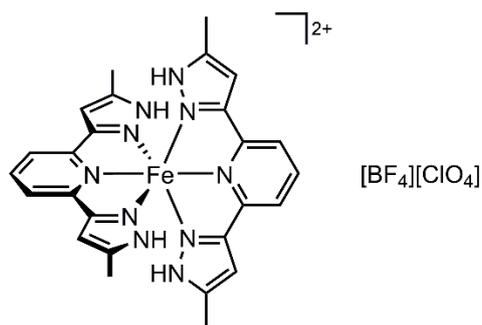
Compounds referred to in this dataset (continued)



*Bis*-(2,6-*bis*[5-methyl-1*H*-pyrazol-3-yl]pyridine)iron(II) sesqui(tetrafluoroborate) hemi(perchlorate)  
 [FeL<sub>2</sub>][BF<sub>4</sub>]<sub>1.5</sub>[ClO<sub>4</sub>]<sub>0.5</sub>  
 C<sub>26</sub>H<sub>26</sub>B<sub>1.5</sub>Cl<sub>0.5</sub>F<sub>6</sub>FeN<sub>10</sub>O<sub>2</sub>  
**1c**



*Bis*-(2,6-*bis*[5-methyl-1*H*-pyrazol-3-yl]pyridine)iron(II) tetrafluoroborate perchlorate dihydrate  
 [FeL<sub>2</sub>][BF<sub>4</sub>][ClO<sub>4</sub>]·2H<sub>2</sub>O  
 C<sub>26</sub>H<sub>30</sub>BClF<sub>4</sub>FeN<sub>10</sub>O<sub>6</sub>  
**1d**·2H<sub>2</sub>O



*Bis*-(2,6-*bis*[5-methyl-1*H*-pyrazol-3-yl]pyridine)iron(II) tetrafluoroborate perchlorate  
 [FeL<sub>2</sub>][BF<sub>4</sub>][ClO<sub>4</sub>]  
 C<sub>26</sub>H<sub>26</sub>BClF<sub>4</sub>FeN<sub>10</sub>O<sub>4</sub>  
**1d**