Title: Data to support study of Spin-Crossover in a New Iron(II)/Di(pyrazolyl)pyridine Complex with a Terpyridine Embrace Lattice.

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

Publication Year: 2022

Description: $[FeL_2]X_2$ (L = 2,6-di{4-fluoropyrazol-1-yl}pyridine) exhibit hysteretic spin-transitions at $T_{½}$ = 164 (X = BF_4) and 148 K (X = ClO_4). The perchlorate salt shows efficient TIESST below 120 K, and was characterized in its thermally trapped high-spin form, as well as in its thermodynamic high- and low-spin states.

Cite as: Michaels, Evridiki, Capel Berdiell, Izar, Babu Vasili, Hari, Pask, Christopher M., Howard, Mark J., Cespedes, Oscar and Halcrow, Malcolm A. (2022): Data to support study of Spin-Crossover in a New Iron(II)/Di(pyrazolyl)pyridine Complex with a Terpyridine Embrace Lattice. [Dataset] https://doi.org/10.5518/1229

Related publication: Michaels, Evridiki, Capel Berdiell, Izar, Babu Vasili, Hari, Pask, Christopher M., Howard, Mark J., Cespedes, Oscar and Halcrow, Malcolm A. (2022). Spin-Crossover in a New Iron(II)/Di(pyrazolyl)pyridine Complex with a Terpyridine Embrace Lattice. Thermally Induced Excited Spin State Trapping and Clarification of a Structure–Function Correlation. *Crystal Growth and Design*, doi: 10.1021/acs.cgd.2c00980

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2. TERMS OF USE

3. PROJECT AND FUNDING INFORMATION

Title: TomoCAT
Dates:
Funding organisation: Research Council of Norway
Grant no.: 301619

This work was also funded by the University of Leeds.

4. CONTENTS

The dataset contains data for this study:

Elemental microanalyses (*microanalysis.zip*).

Electrospray mass spectrum of the new ligand *L* (*ESMS.zip*).

^{1}H, ^{13}C and ^{19}F NMR spectra of *L*, and a paramagnetic ^{1}H NMR spectrum of the complex (raw and processed data – *NMR*.zip).

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

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

Evans method solution magnetic susceptibility data (raw NMR spectra and processed data – *Evans*.zip).

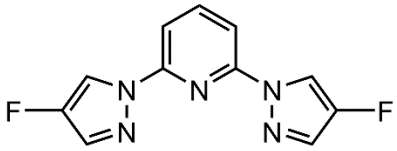
X-ray Crystallographic data (*crystal*.zip):

- Structure of **1[BF_4]$_2$** phase 1 at 300 K (CCDC 2193311).
- Structure of **1[BF_4]$_2$** phase 2 at 280 K (high-spin; preliminary structure solution).
- Structure of **1[BF_4]$_2$** phase 2 at 220 K (high-spin; preliminary structure solution).
- Structure of **1[BF_4]$_2$** phase 2 at 120 K (low-spin; preliminary structure solution).
- Structure of **1[ClO_4]$_2$** at 250 K (high-spin; CCDC 2193312).
- Structure of **1[ClO_4]$_2$** at 180 K (high-spin; CCDC 2193313).
- Structure of **1[ClO_4]$_2$** at 100 K (high-spin; CCDC 2193314).
- Structure of **1[ClO_4]$_2$** at 145 K (low-spin; CCDC 2193315).

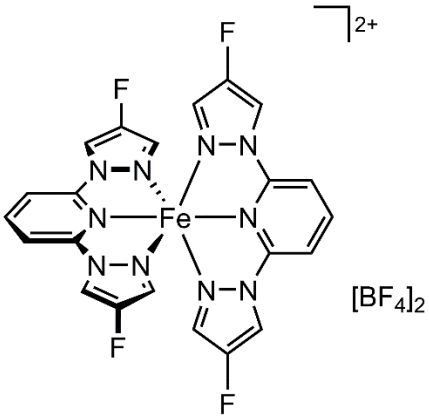
5. METHODS

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

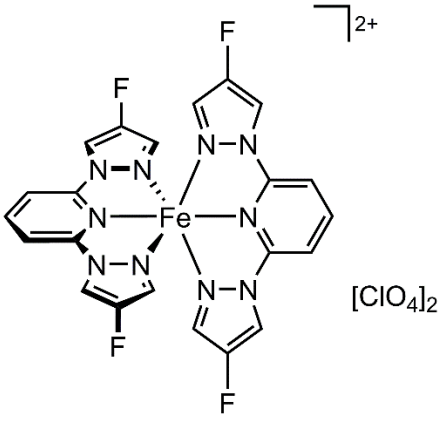
Compounds referred to in this dataset



L
2,6-Di(4-fluoropyrazol-1-yl)pyridine
$C_{11}H_7F_2N_5$



$[FeL_2][BF_4]_2$
1[BF_4]$_2$
Bis[di(4-fluoropyrazol-1-yl)pyridine]iron(II) di(tetrafluoroborate)
$C_{22}H_{14}B_2F_{12}FeN_{10}$



$[FeL_2][ClO_4]_2$
1[ClO_4]$_2$
Bis[di(4-fluoropyrazol-1-yl)pyridine]iron(II) diperchlorate
$C_{22}H_{14}Cl_2F_4FeN_{10}O_8$