

The dataset contains data for this study:

Elemental microanalyses.

X-ray Crystallographic data:

- Structure of **1**[BF<sub>4</sub>]<sub>2</sub>·2CH<sub>3</sub>CN at 120 K (CCDC 2078647).
- Structure of **1**[BF<sub>4</sub>]<sub>2</sub>·CH<sub>3</sub>CN at 200 K (CCDC 2078648).
- Structure of **1**[BF<sub>4</sub>]<sub>2</sub>·CH<sub>3</sub>CN at 125 K (CCDC 2078649).
- Variable temperature unit cell data for **1**[BF<sub>4</sub>]<sub>2</sub>·CH<sub>3</sub>CN.
- Structure of **1**[ClO<sub>4</sub>]<sub>2</sub>·CH<sub>3</sub>CN at 200 K (CCDC 2078650).
- Structure of **1**[ClO<sub>4</sub>]<sub>2</sub>·CH<sub>3</sub>CN at 160 K (CCDC 2078651).
- Variable temperature unit cell data for **1**[ClO<sub>4</sub>]<sub>2</sub>·CH<sub>3</sub>CN.
- Structure of **1**[BF<sub>4</sub>]<sub>2</sub>·C<sub>2</sub>H<sub>5</sub>CN at 200 K (CCDC 2078652).
- Structure of **1**[BF<sub>4</sub>]<sub>2</sub>·C<sub>2</sub>H<sub>5</sub>CN at 187 K (CCDC 2078653).
- Structure of **1**[BF<sub>4</sub>]<sub>2</sub>·C<sub>2</sub>H<sub>5</sub>CN at 160 K (CCDC 2078654).
- Variable temperature unit cell data for **1**[BF<sub>4</sub>]<sub>2</sub>·C<sub>2</sub>H<sub>5</sub>CN.
- Structure of **1**[ClO<sub>4</sub>]<sub>2</sub>·C<sub>2</sub>H<sub>5</sub>CN, phase 1 at 240 K (CCDC 2078655).
- Structure of **1**[ClO<sub>4</sub>]<sub>2</sub>·C<sub>2</sub>H<sub>5</sub>CN, phase 2 at 170 K (CCDC 2078656).
- Structure of **1**[ClO<sub>4</sub>]<sub>2</sub>·C<sub>2</sub>H<sub>5</sub>CN, phase 1 at 120 K (CCDC 2078657).
- Variable temperature unit cell data for **1**[ClO<sub>4</sub>]<sub>2</sub>·C<sub>2</sub>H<sub>5</sub>CN.
- Structure of **1**[BF<sub>4</sub>]<sub>0.9</sub>[ClO<sub>4</sub>]<sub>1.1</sub>·C<sub>2</sub>H<sub>5</sub>CN, phase 1 at 240 K (CCDC 2078658).
- Structure of **1**[BF<sub>4</sub>]<sub>0.9</sub>[ClO<sub>4</sub>]<sub>1.1</sub>·C<sub>2</sub>H<sub>5</sub>CN, phase 2 at 170 K (CCDC 2078659).
- Structure of **1**[BF<sub>4</sub>]<sub>0.9</sub>[ClO<sub>4</sub>]<sub>1.1</sub>·C<sub>2</sub>H<sub>5</sub>CN, phase 1 at 120 K (CCDC 2078660).
- Variable temperature unit cell data for **1**[BF<sub>4</sub>]<sub>0.9</sub>[ClO<sub>4</sub>]<sub>1.1</sub>·C<sub>2</sub>H<sub>5</sub>CN.
- Structure of **1**[BF<sub>4</sub>]<sub>2</sub>·2CH<sub>3</sub>NO<sub>2</sub> at 120 K (CCDC 2078661).
- Structure of **1**[ClO<sub>4</sub>]<sub>2</sub>·2CH<sub>3</sub>NO<sub>2</sub> at 120 K (CCDC 2078662).
- Structure of **1**[BF<sub>4</sub>]<sub>2</sub>·CH<sub>3</sub>OH at 120 K (CCDC 2078663).
- Structure of **1**[ClO<sub>4</sub>]<sub>2</sub>·½C<sub>2</sub>H<sub>5</sub>OH at 120 K (CCDC 2078664).

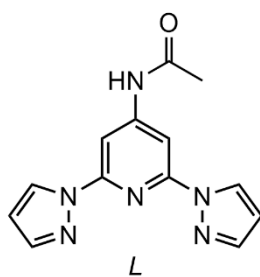
X-ray powder diffraction data (measured and simulated).

Thermogravimetric analyses (raw and plotted data).

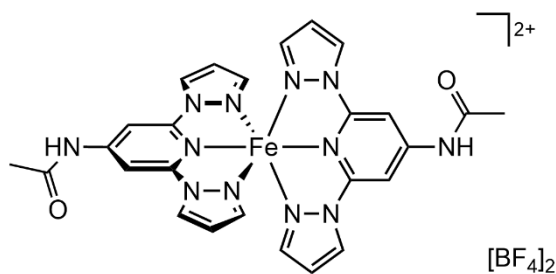
Solid state magnetic susceptibility measurements (raw and processed data).

Solution magnetic susceptibility measurements by Evans method (NMR spectra and processed data).

## Compounds referred to in this dataset

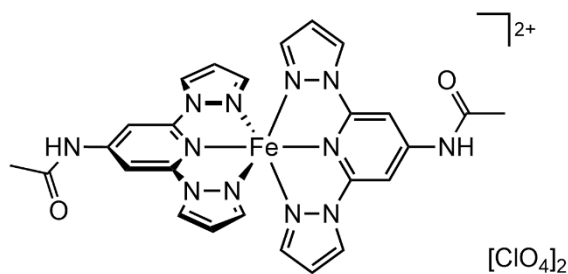


*N*-(2,6-di{pyrazol-1-yl}pyrid-4-yl)acetamide  
 $C_{13}H_{12}N_6O$



$[FeL_2][BF_4]_2$   
**1[BF<sub>4</sub>]<sub>2</sub>**

Bis[*N*-(2,6-di{pyrazol-1-yl}pyrid-4-yl)acetamide]iron(II)  
di(tetrafluoroborate)  
 $C_{26}H_{24}B_2F_8FeN_{12}O_2$



$[FeL_2][ClO_4]_2$   
**1[ClO<sub>4</sub>]<sub>2</sub>**

Bis[*N*-(2,6-di{pyrazol-1-yl}pyrid-4-yl)acetamide]iron(II)  
diperchlorate  
 $C_{26}H_{24}Cl_2FeN_{12}O_{10}$