

## Electronic Supplementary Information

### Tetrathioipyridyl-tetrathiafulvalene-based Cd(II) coordination polymers: one ligand, one metal cation, many possibilities

Damien Bechu,<sup>a</sup> Guillaume Rogez,<sup>b</sup> Mir Wais Hosseini<sup>\*a</sup> and Stéphane A. Baudron<sup>\*a</sup>

a. Laboratoire de Tectonique Moléculaire, UMR UdS-CNRS 7140, icFRC

Institut Le Bel, Université de Strasbourg

4 rue Blaise Pascal, CS 90032, F-67081 Strasbourg cedex, France

Fax: (+) 33 3 68 85 13 25. E-mail: [hosseini@unistra.fr](mailto:hosseini@unistra.fr) ; [sbaudron@unistra.fr](mailto:sbaudron@unistra.fr)

b. Institut de Physique et Chimie des Matériaux de Strasbourg, UMR Unistra-CNRS 7504,  
Strasbourg, France

<sup>1</sup>H- and <sup>13</sup>C-NMR spectra were recorded at 25 °C on a Bruker AV500 (500 MHz) spectrometer with the deuterated solvent as the internal reference. NMR chemical shifts and *J* values are given in parts per million (ppm) and in Hertz, respectively. Mass spectrometry was performed at the Service commun d'analyses of the University of Strasbourg.

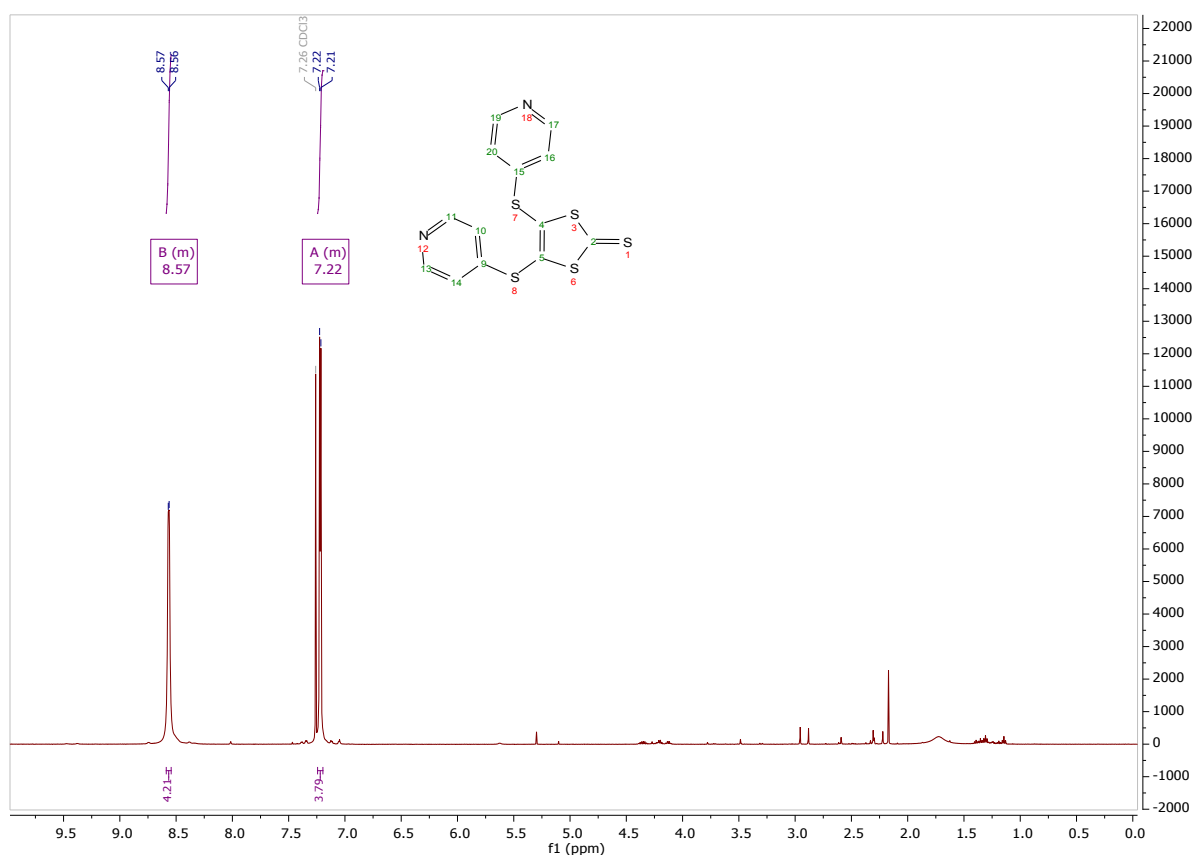
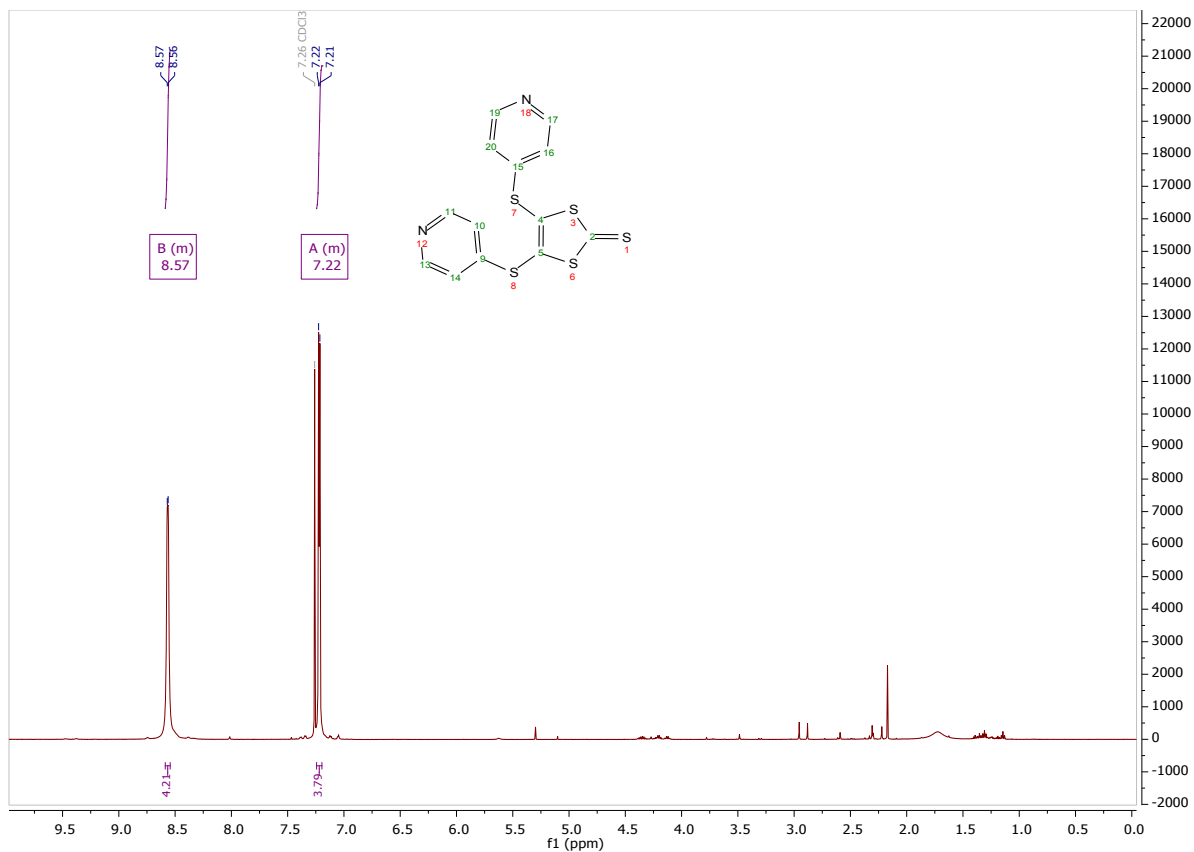
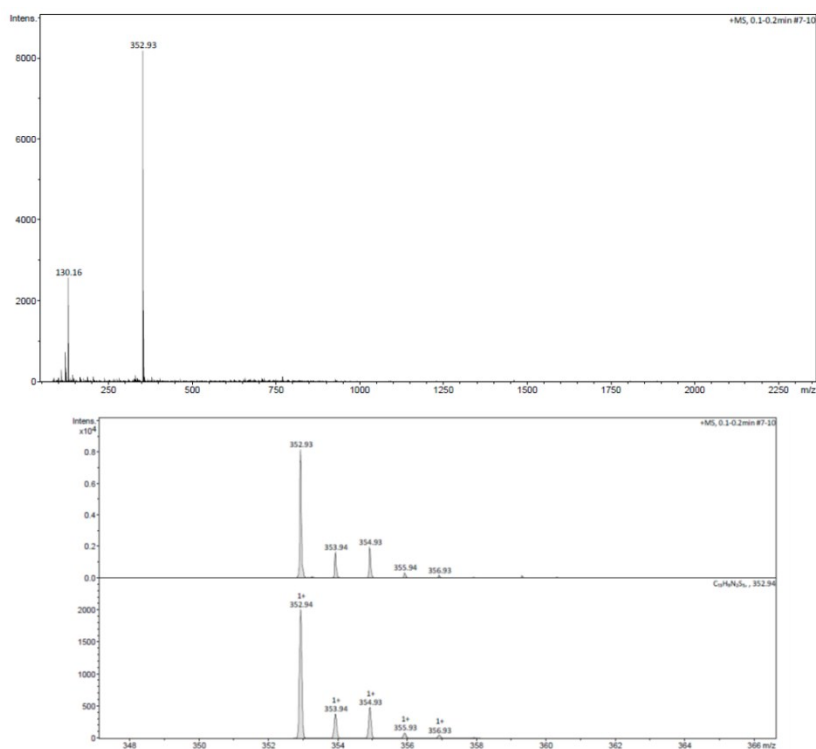


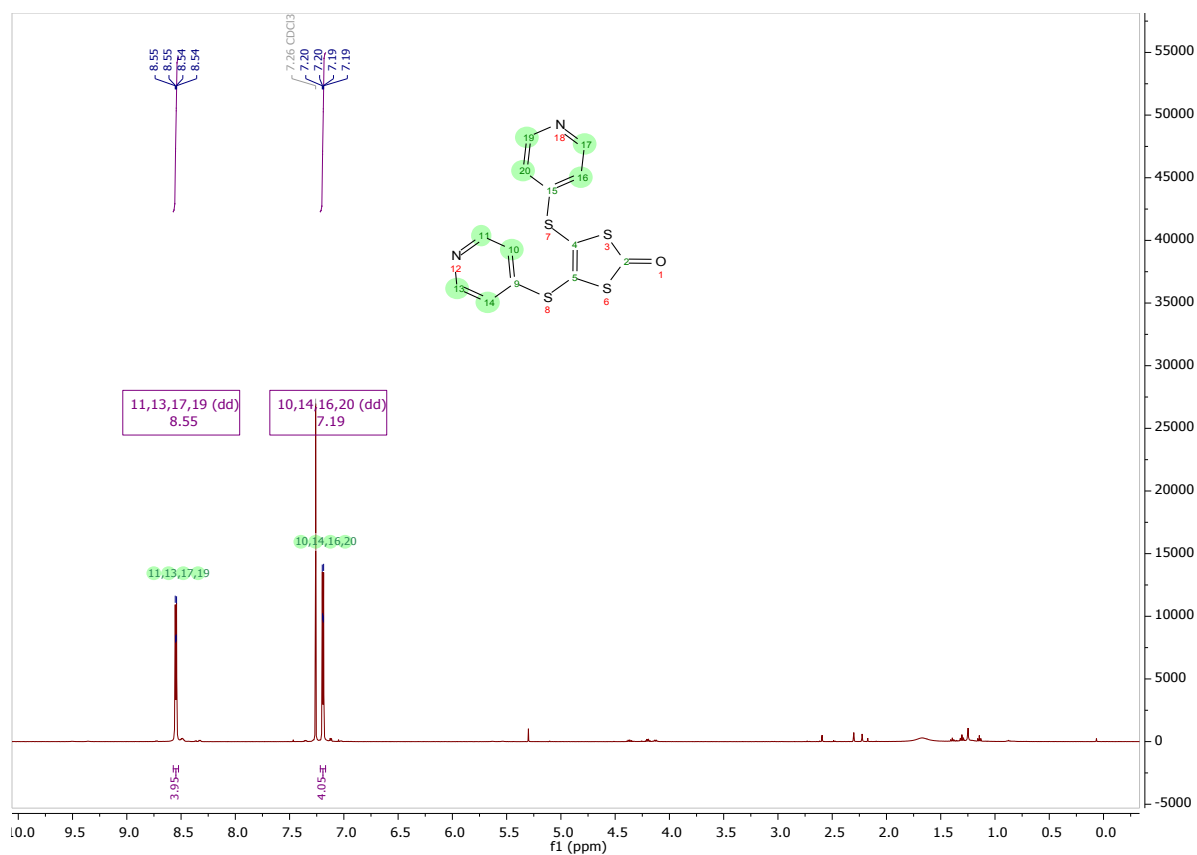
Fig. ESI1 <sup>1</sup>H-NMR spectrum of dithiolthione **2** in CDCl<sub>3</sub>.



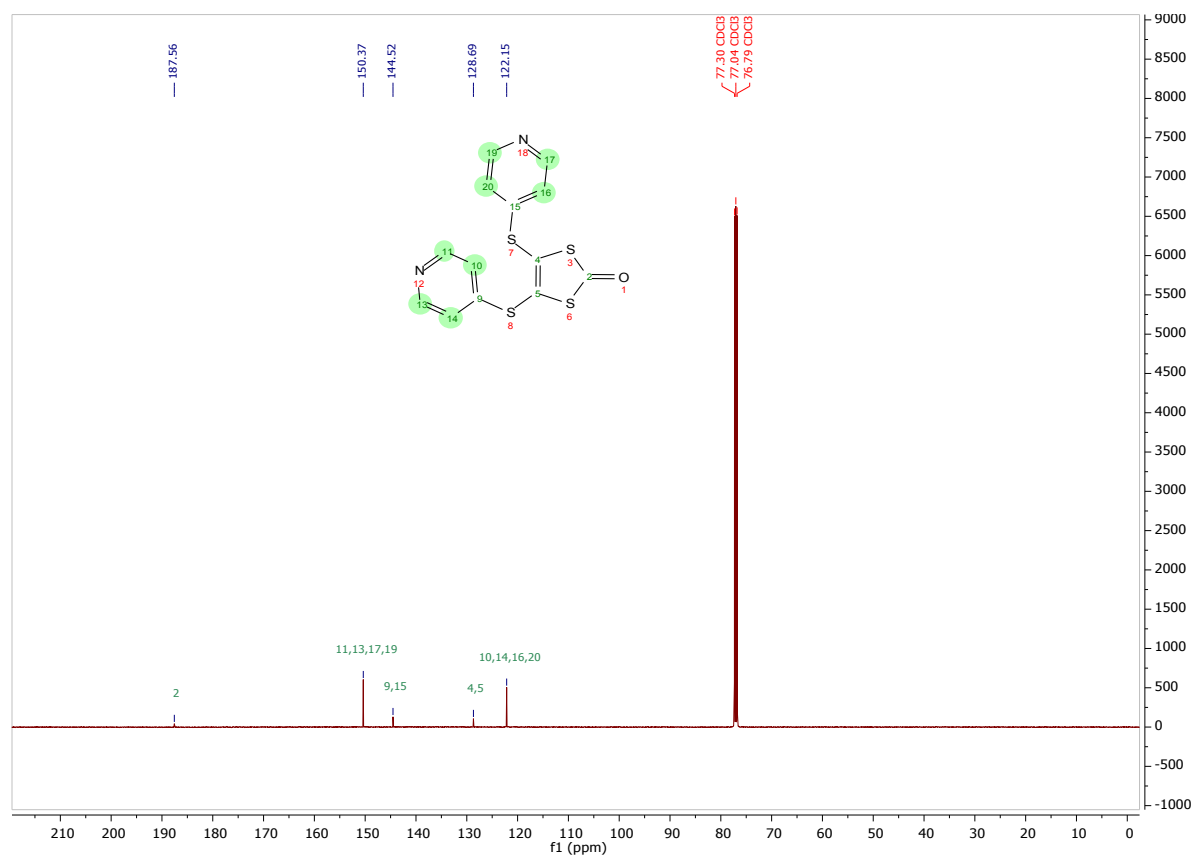
**Fig. ESI2**  $^{13}\text{C}$ -NMR spectrum of dithiolthione **2** in  $\text{CDCl}_3$ .



**Fig. ESI3** HR-MS spectrum of dithiolthione **2**.



**Fig. ESI4** <sup>1</sup>H-NMR spectrum of dithiolone **3** in CDCl<sub>3</sub>.



**Fig. ESI5** <sup>13</sup>C-NMR spectrum of dithiolone **3** in CDCl<sub>3</sub>.

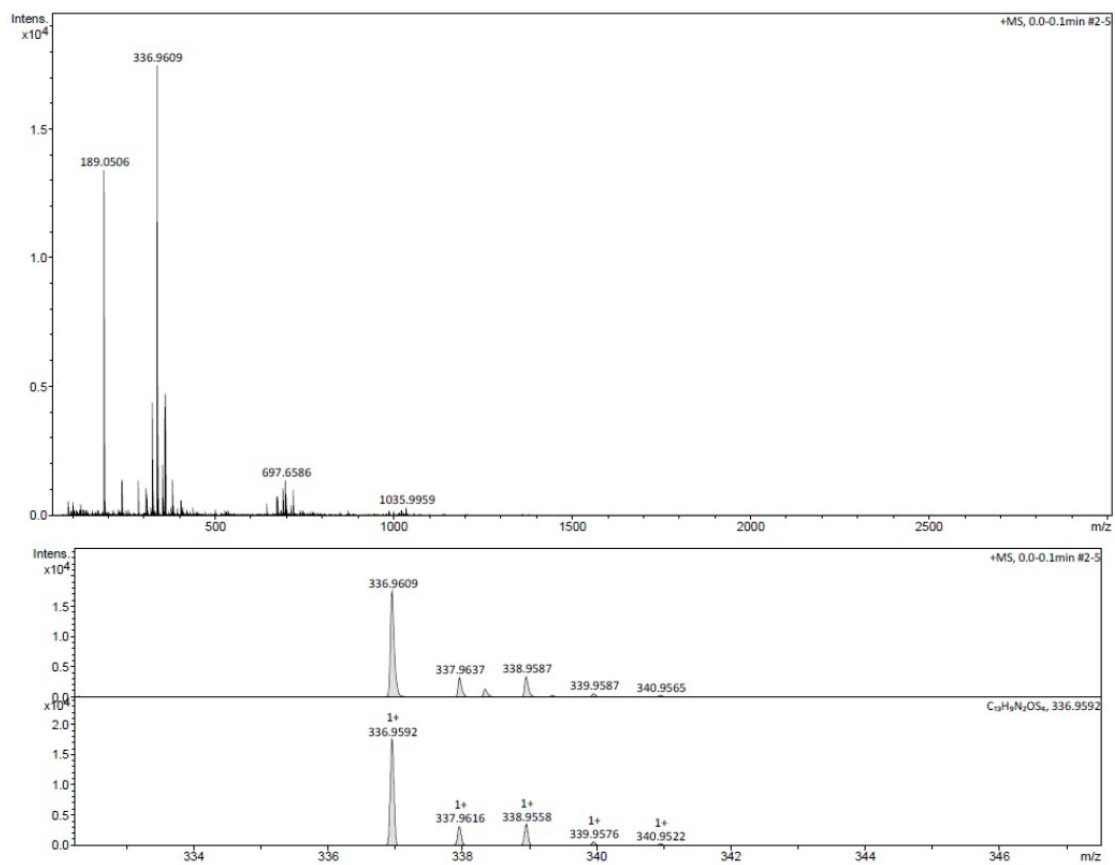


Fig. ESI6 HR-MS spectrum of dithiolone **3**.



Fig. ESI7 <sup>1</sup>H-NMR spectrum of TTF **1** in CD<sub>2</sub>Cl<sub>2</sub>.

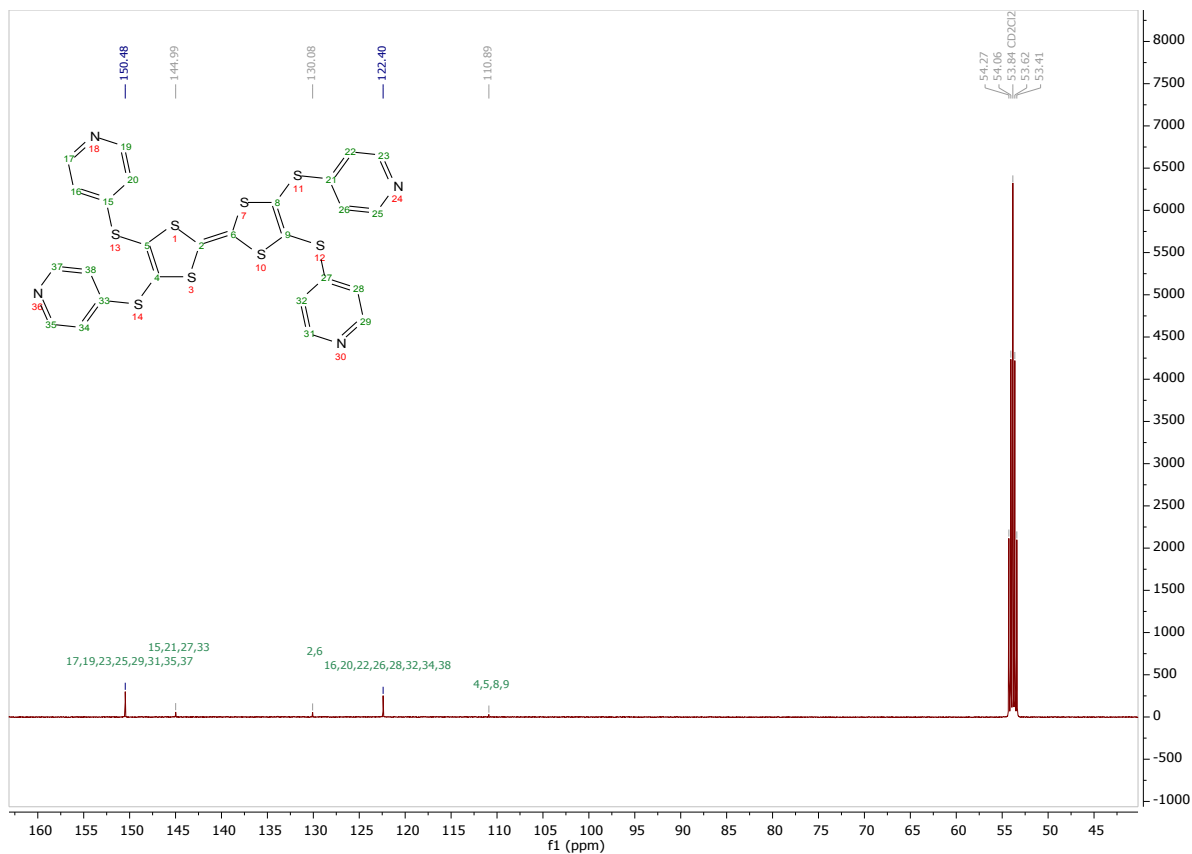


Fig. ESI8  $^{13}\text{C}$ -NMR spectrum of TTF 1 in  $\text{CD}_2\text{Cl}_2$ .

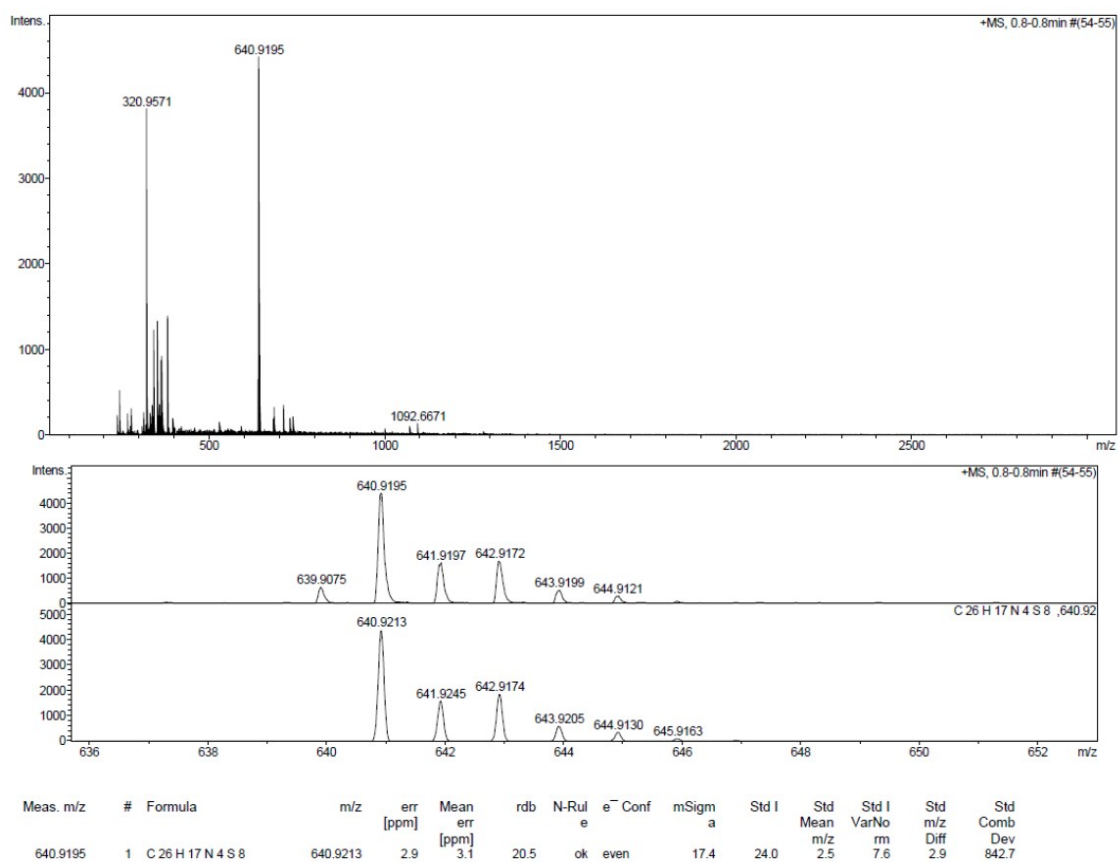
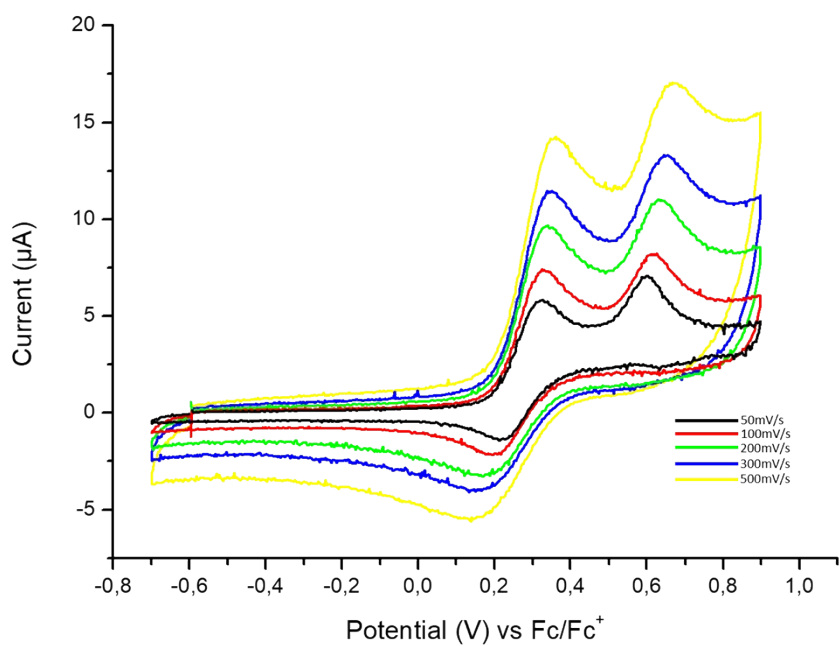
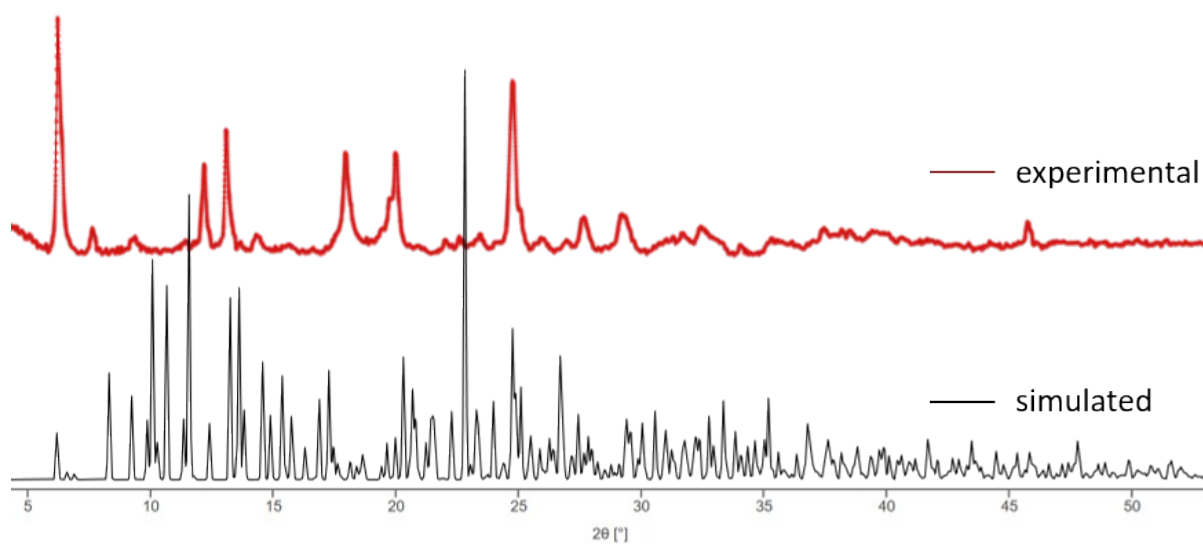


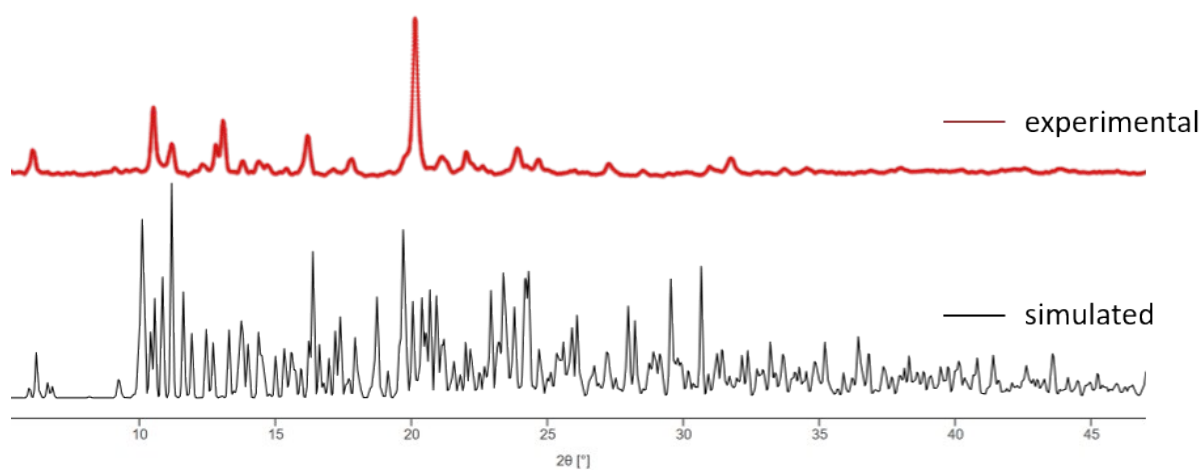
Fig. ESI9 HR-MS spectrum of TTF 1.



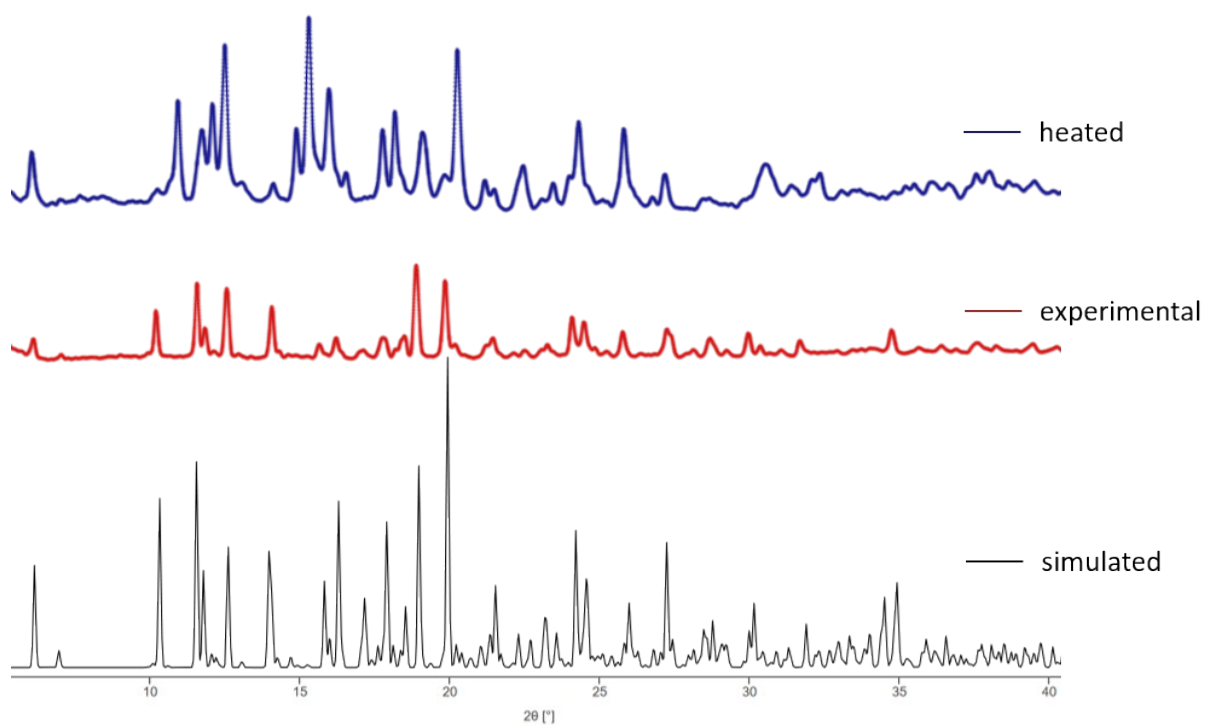
**Fig. ESI10.** Cyclic voltammogram of **1** in CH<sub>2</sub>Cl<sub>2</sub> vs Fc/Fc<sup>+</sup> at various scan speeds.



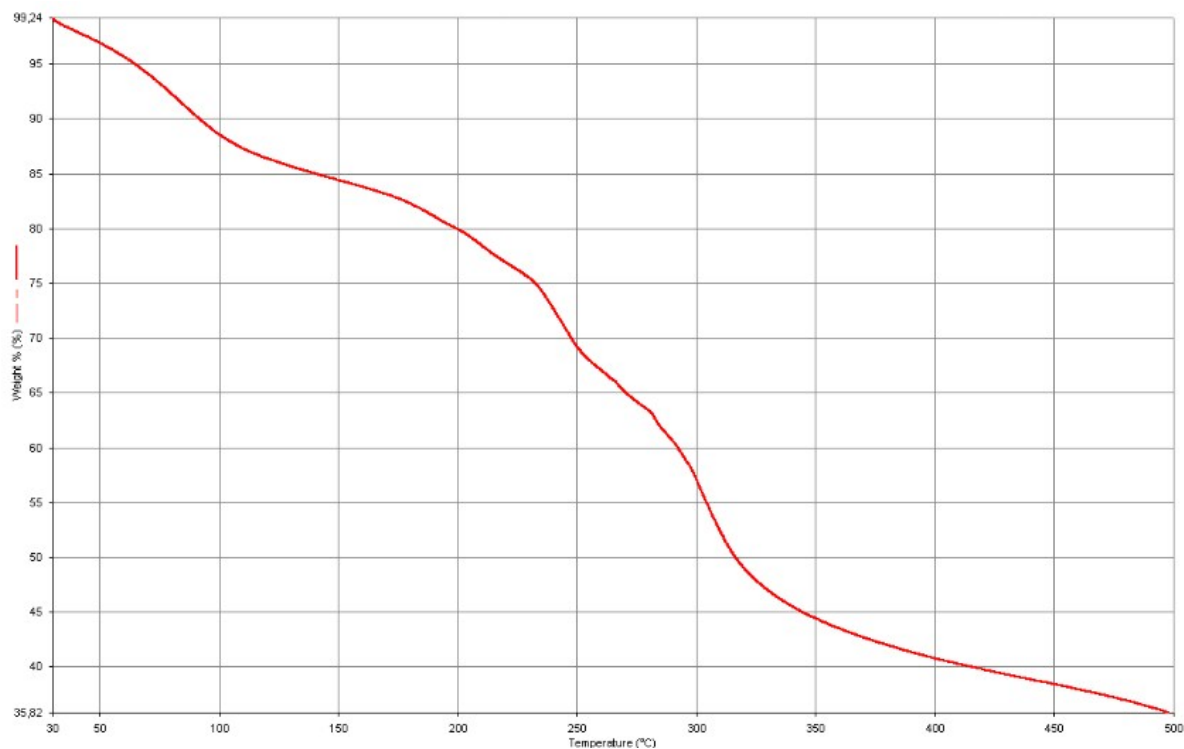
**Fig. ESI11.** Simulated (black) and experimental (red) PRXD pattern for CP **4**.



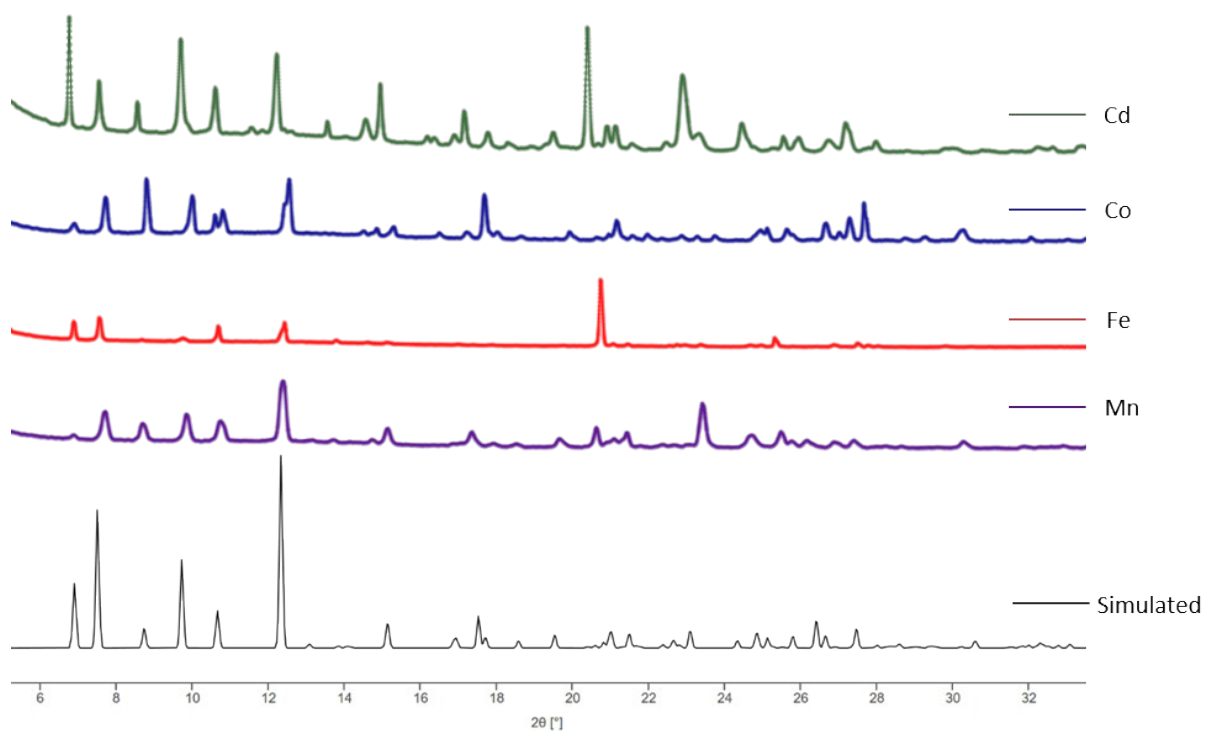
**Fig. ESI12.** Simulated (black) and experimental (red) PRXD pattern for CP 5.



**Fig. ESI13.** Simulated (black), experimental (red) and upon heating at 130°C (blue) PRXD patterns for CP 6.

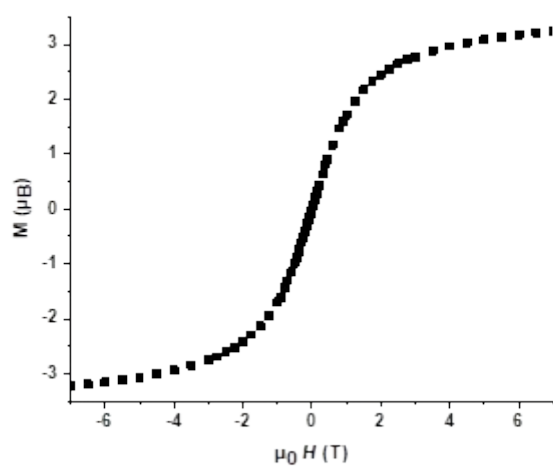
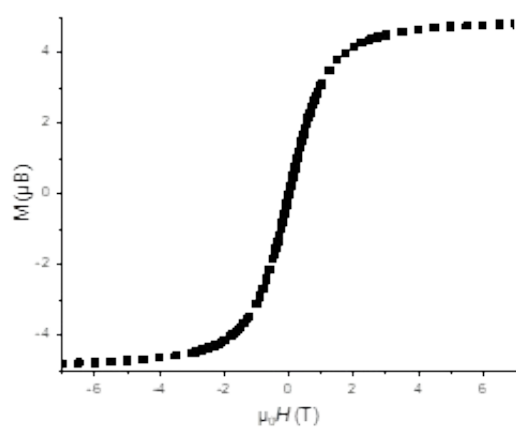


**Fig. ESI14.** TGA for CP 6.



**Fig. ESI15.** Simulated (black) and experimental PRXD patterns for Cd CP 8 (green), Mn CP 9 (purple), Fe CP 10 (red) and Co CP 11 (blue).





**Fig. ESI 16.** Magnetization curves of Mn CP **9** (top) and Fe CP **10** (bottom) at 1.8 K