

Supporting information for DT-ART-04-2011-010631

# Synthesis, Characterization, and Single-Molecule Metamagnetism of New Co(II) Polynuclear Complexes of Pyridine-2-ylmethanol

Roberto Pattacini,<sup>a</sup> Peili Teo,<sup>a,b</sup> Jun Zhang,<sup>a,b</sup> Yanhua Lan,<sup>c</sup> Annie K. Powell,<sup>c</sup> Joscha Nehr Korn,<sup>d</sup> Oliver Waldmann,<sup>d</sup> T. S. Andy Hor,<sup>b</sup> and Pierre Braunstein<sup>a</sup>

<sup>a</sup> *Laboratoire de Chimie de Coordination, UMR 7177 CNRS/Université de Strasbourg, Institut Le Bel 4, Rue Blaise Pascal, CS90032, F-67081 Strasbourg Cedex, France. Fax: +33 368851322; Tel: 33 368851308; E-mail: braunstein@unistra.fr*

<sup>b</sup> *Department of Chemistry, National University of Singapore, 3, Science Drive 3, Singapore, 117543, Singapore.*

<sup>c</sup> *Institute of Inorganic Chemistry, Karlsruhe Institute of Technology (KIT), Engesserstrasse 15, D-76131 Karlsruhe, Germany.*

<sup>d</sup> *Physikalisches Institut, Universität Freiburg, Hermann-Herder-Strasse 3, D-79104 Freiburg, Germany.*

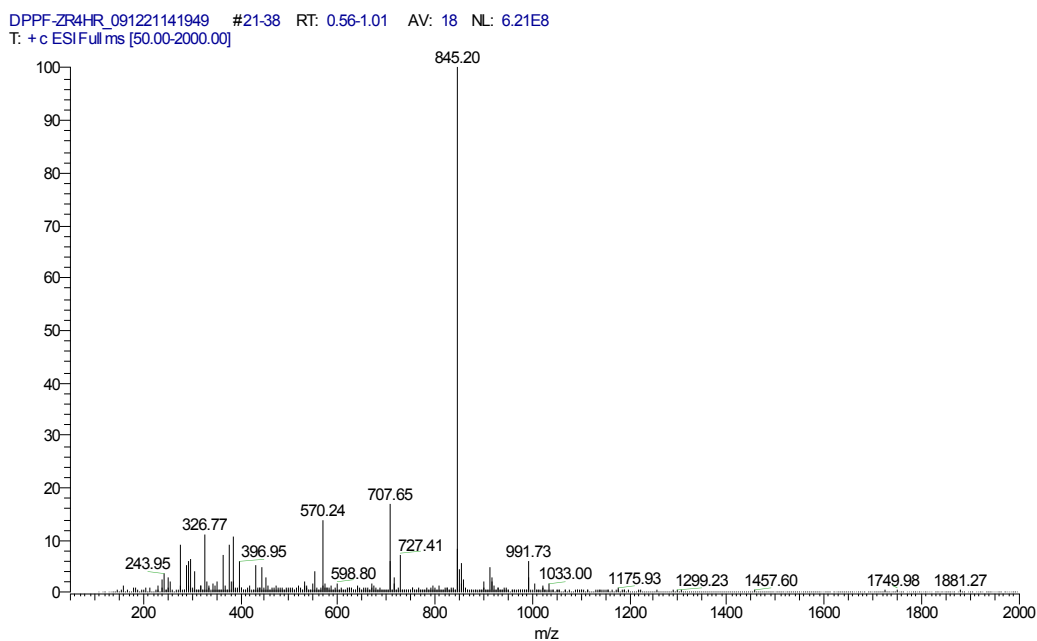
## Content

mass spectroscopy data (Figures S1-S4)

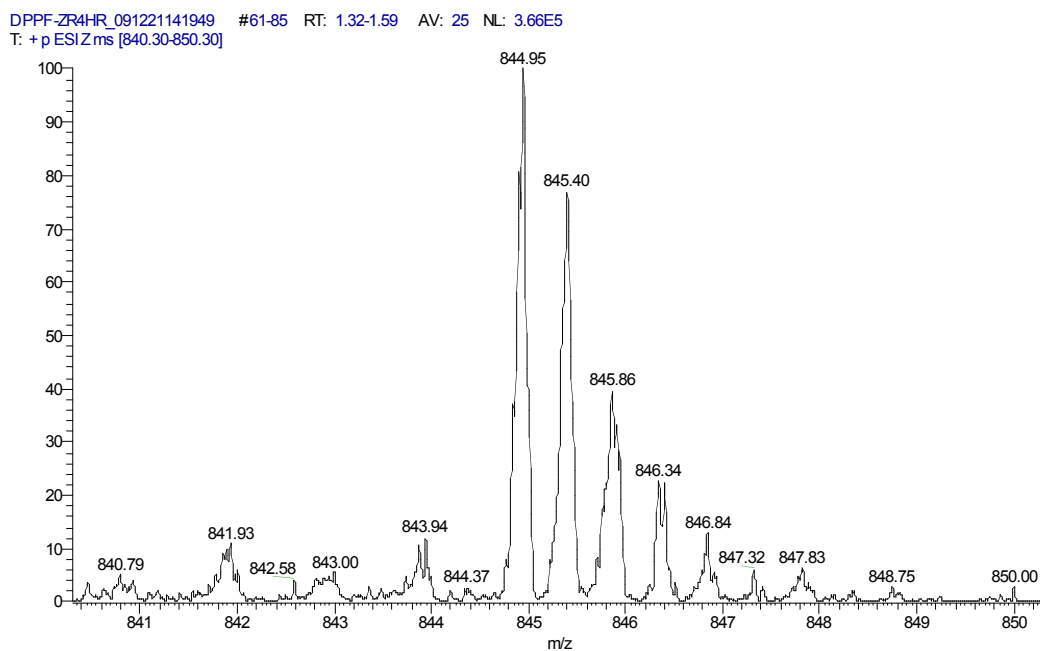
infrared spectra (Figures S5-S10)

crystallographic data

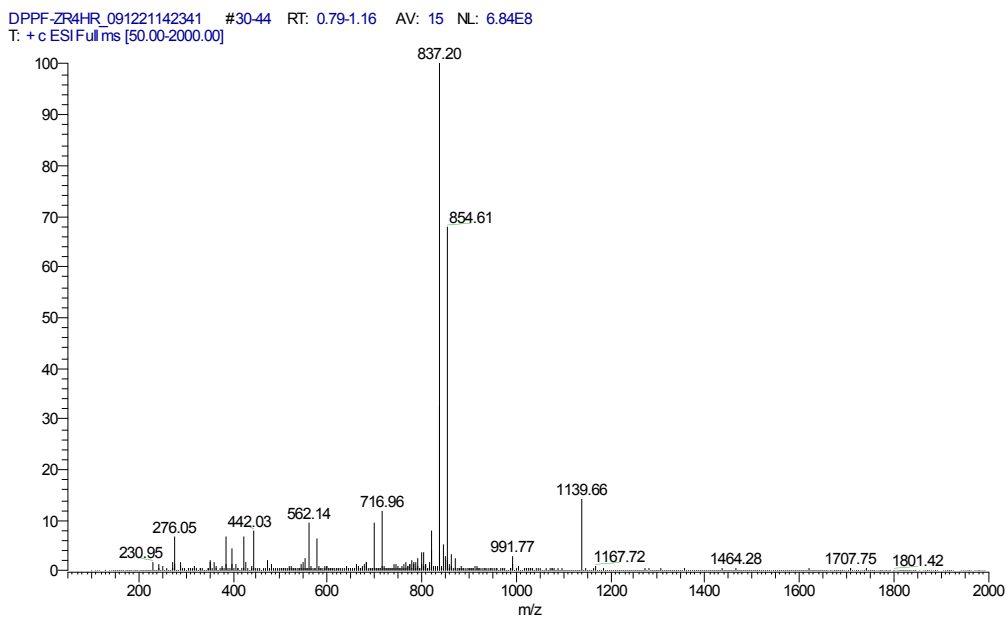
magnetic data (Figures S11-S13)



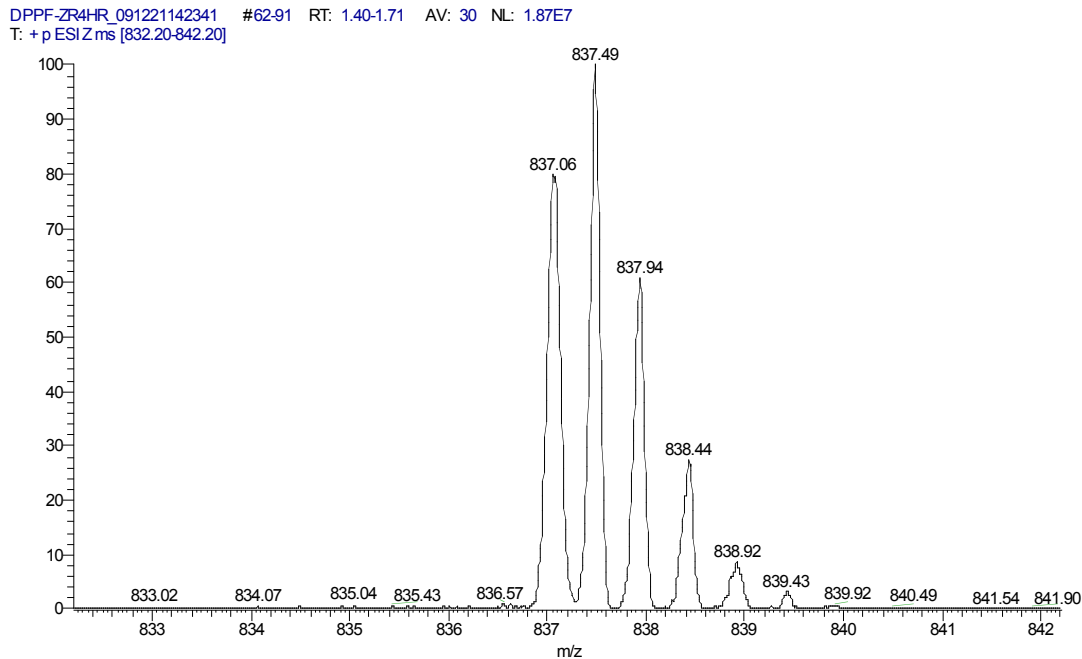
**Figure S-1:** ESI-MS spectrum of a solution containing  $[\text{CaCo}_6\text{L}_{12}]^{2+}$  (see main text). Calculated  $m/z$  (doubly charged): 845.2.



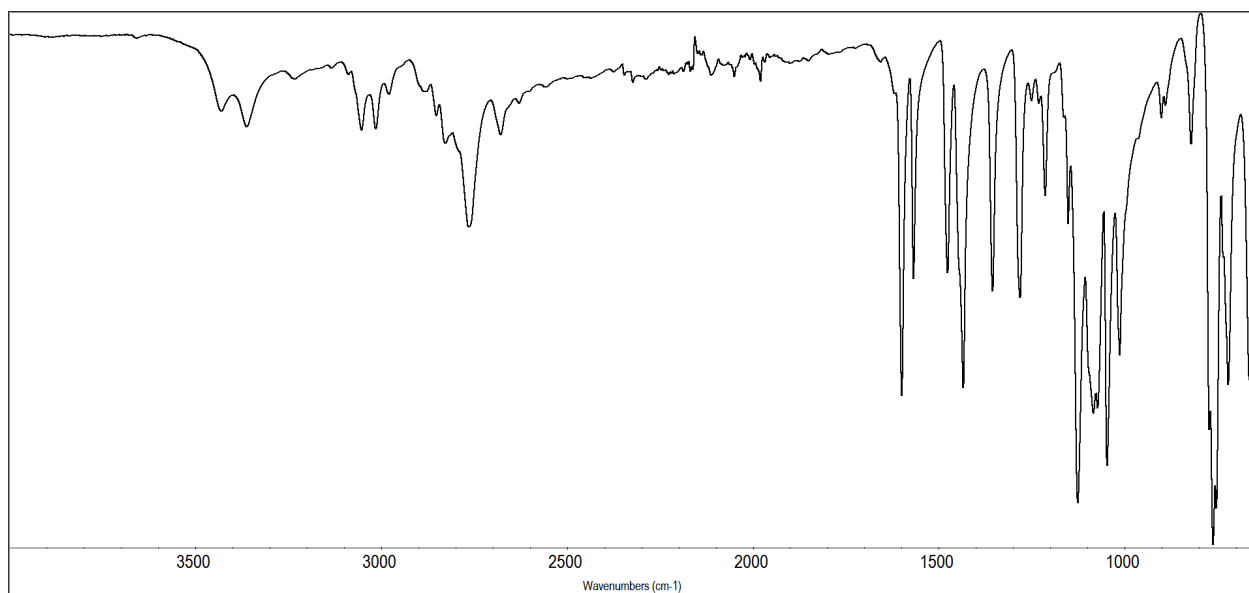
**Figure S-2:** Zoom of the ESI-MS spectrum (Figure S-1) of a solution containing  $[\text{CaCo}_6\text{L}_{12}]^{2+}$  (see main text). Calculated  $m/z$  (doubly charged): 845.2.



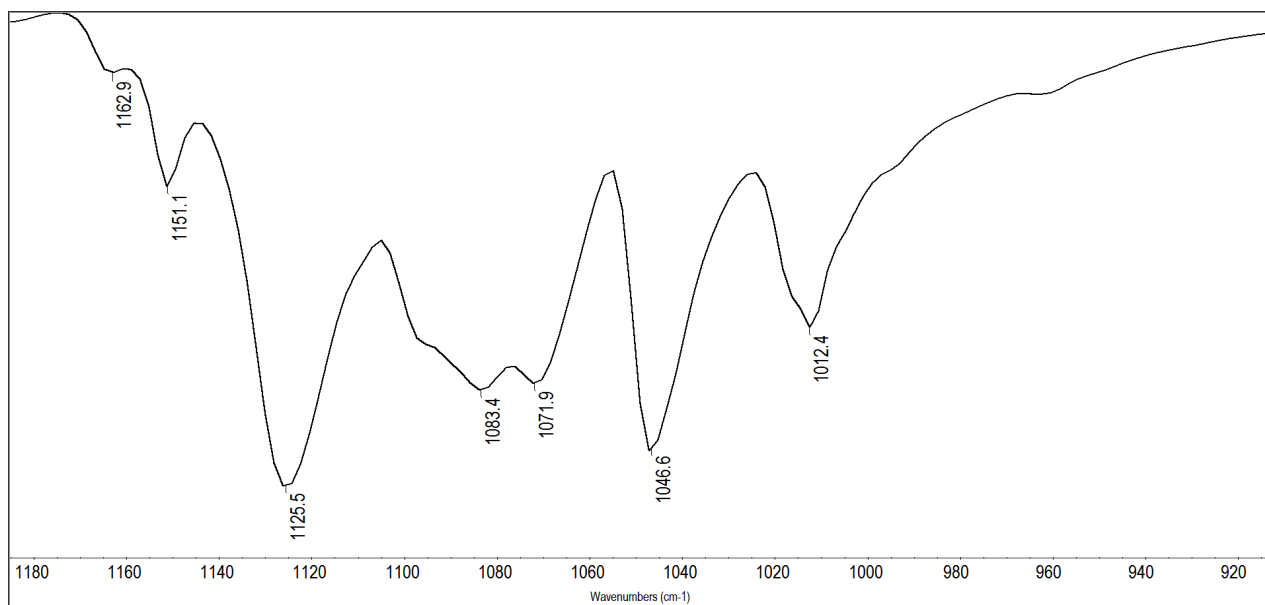
**Figure S-3:** ESI-MS spectrum of a solution containing  $[\text{Co}_6\text{MgL}_{12}]^{2+}$  (see main text). Calculated  $m/z$  (doubly charged): 837.2.



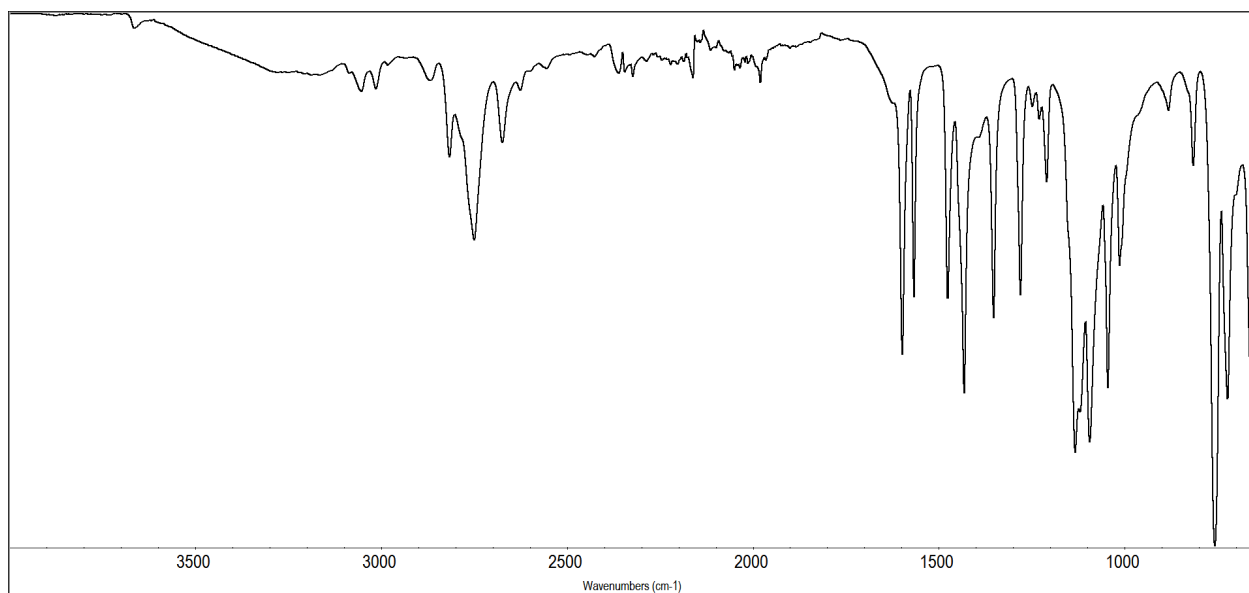
**Figure S-4:** Zoom of the ESI-MS spectrum (Figure S-1) of a solution containing  $[\text{Co}_6\text{MgL}_{12}]^{2+}$  (see main text). Calculated  $m/z$  (doubly charged): 837.2.



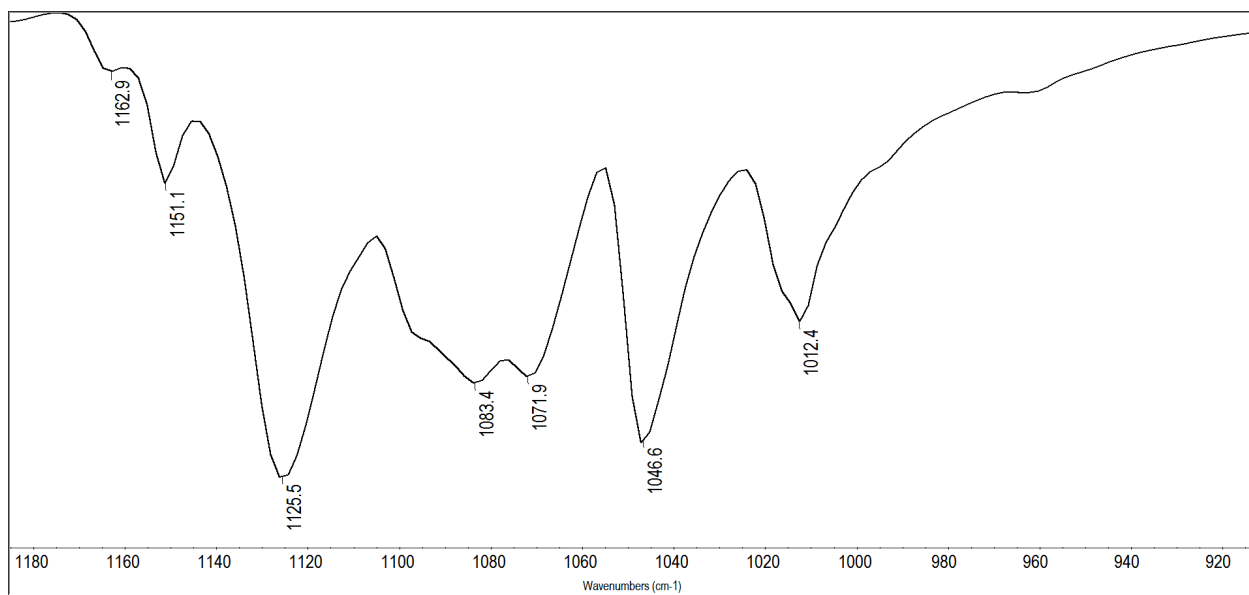
**Figure S-5:** FTIR spectrum of solid **1** (crystals).



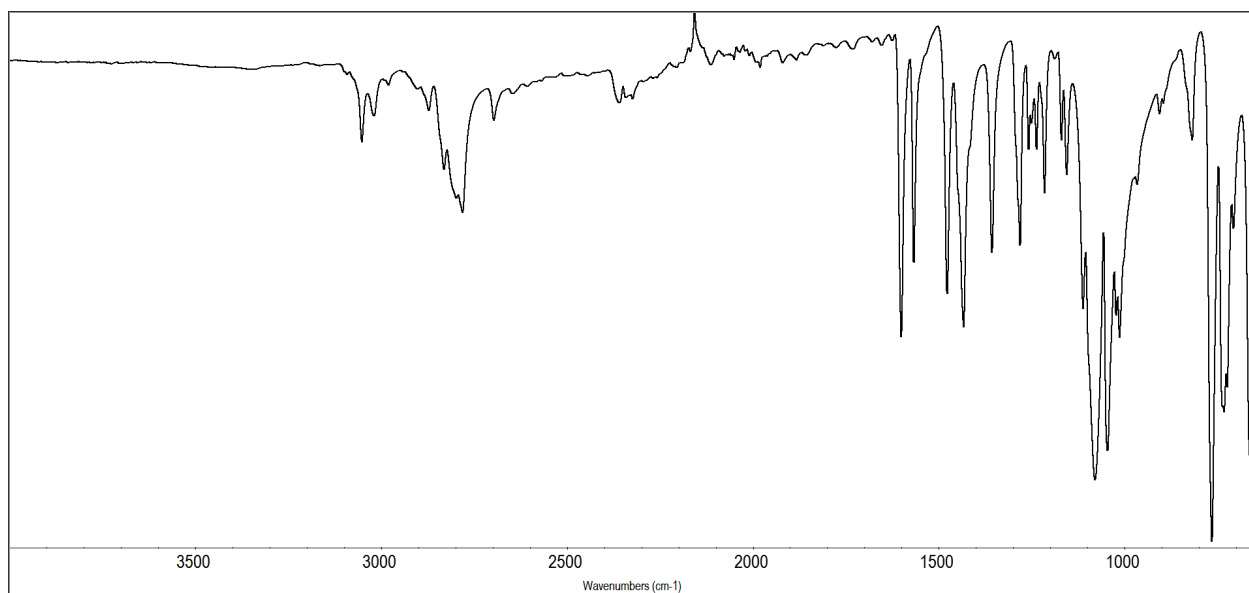
**Figure S-6:** Zoom of FTIR spectrum of solid **1** (crystals), showing the diagnostic C-O pattern.



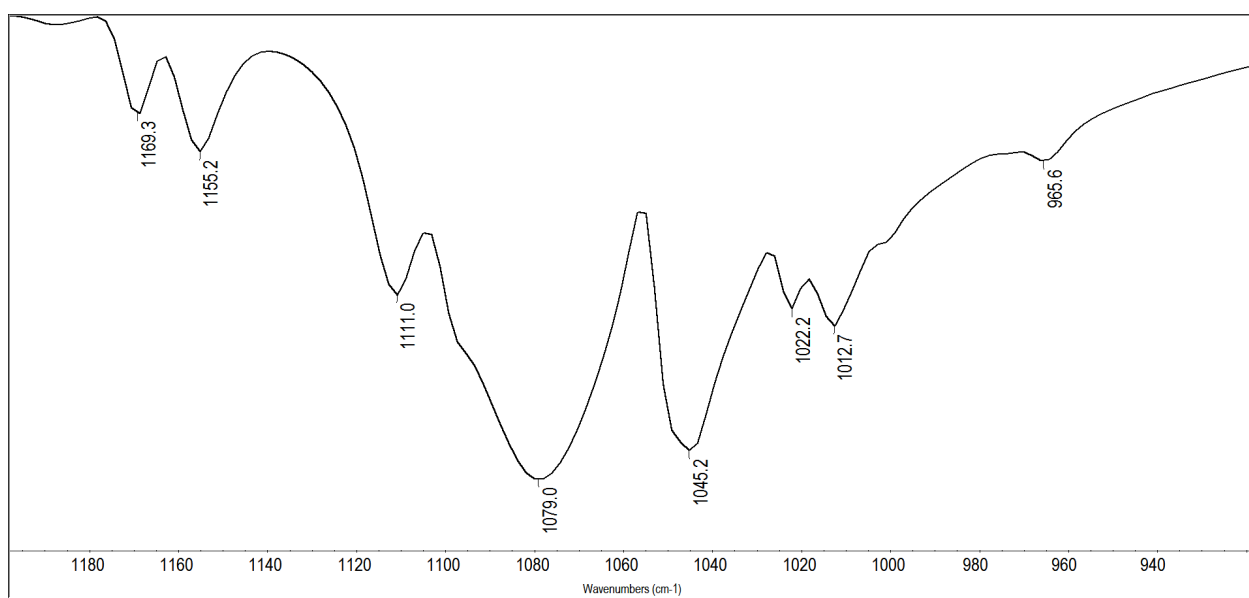
**Figure S-7:** FTIR spectrum of solid **2** (crystals).



**Figure S-8:** Zoom of FTIR spectrum of solid **2** (crystals), showing the diagnostic C-O pattern.



**Figure S-9:** FTIR spectrum of solid **3** (crystals).

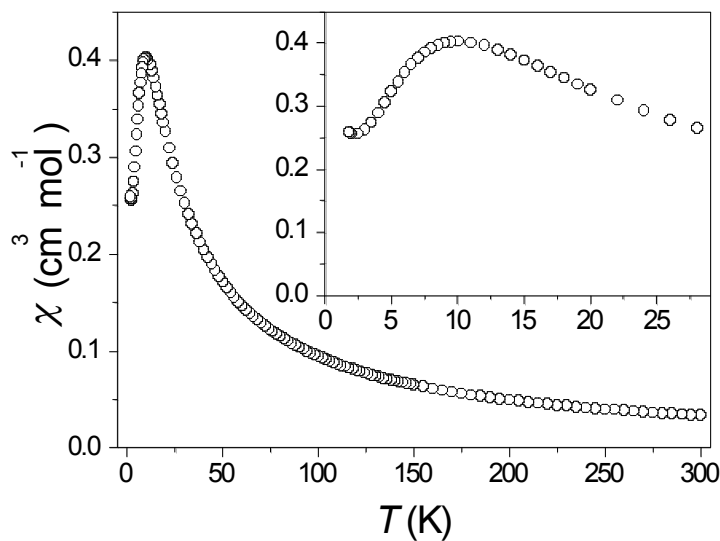


**Figure S-10:** Zoom of FTIR spectrum of solid **3** (crystals), showing the diagnostic C-O pattern.

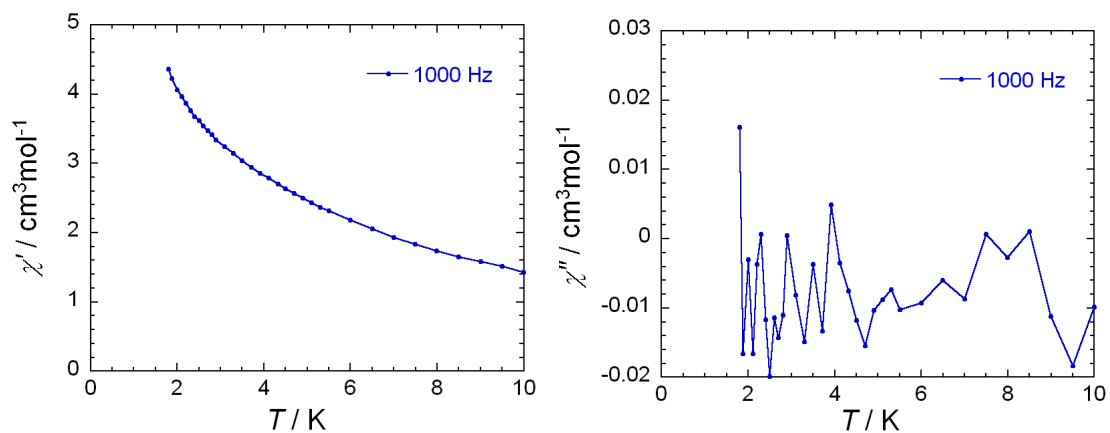
### Details on the X-ray refinement of structures **1** and **3**

The dichloromethane molecule in **2** was found disordered in two positions with equal occupancy factors. In **3**, the dichloromethane molecule was found disordered by symmetry over two positions around the symmetry centre. This molecule was refined with constrained anisotropic parameters.

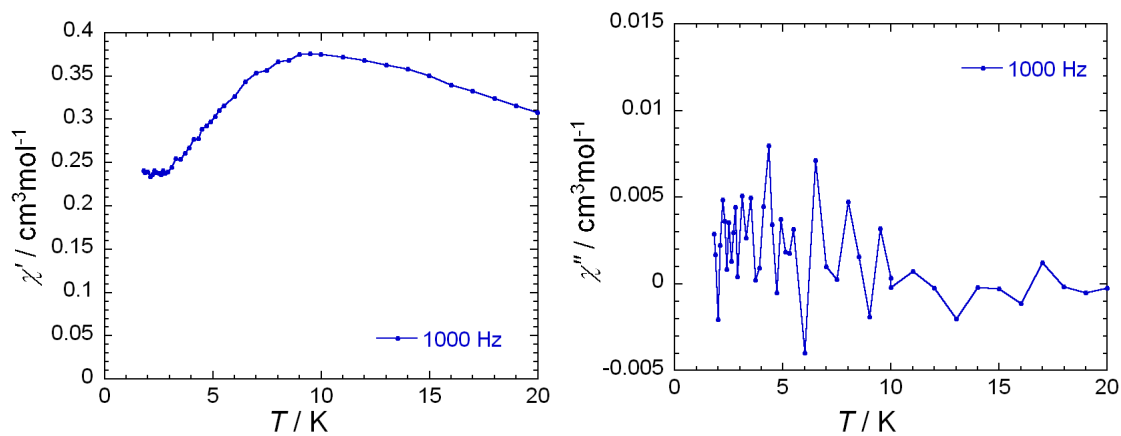
### Variation of the magnetic susceptibility of **3** as a function of the temperature



**Figure S-11:** Plot of  $\chi$  vs. temperature of **3**. The inset shows a magnified view of  $\chi$  at low temperatures.



**Figure S-12.** Plots of the in-phase ( $\chi'$ , left) and out-of-phase ( $\chi''$ , right) ac susceptibility signals vs temperature for complex **1** under 1000 Hz in the absence of dc field.



**Figure S-13.** Plots of the in-phase ( $\chi'$ , left) and out-of-phase ( $\chi''$ , right) ac susceptibility signals vs temperature for complex **3** under 1000 Hz in the absence of dc field.