Electronic supplementary information (ESI) for DT-ART-11-2012-032869

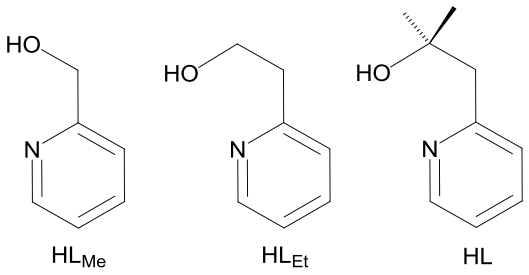
Synthesis of Cubane-type Ni(II) Complexes from Pyridyl-Alcohols Ligands; their Single-Molecule Magnet Behaviour

Sophie Hameury,[a] Laure Kayser,[a] Roberto Pattacini,[a] Guillaume Rogez,[b] Wolfgang Wernsdorfer,[c] and Pierre Braunstein [a]

 This document contains the IR spectra of complexes **1-5**

 Details of the fitting procedures for the $\chi T = f(T)$ magnetic data

 CCDC 912356 - 912360 contain the supplementary crystallographic data for this paper that can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif



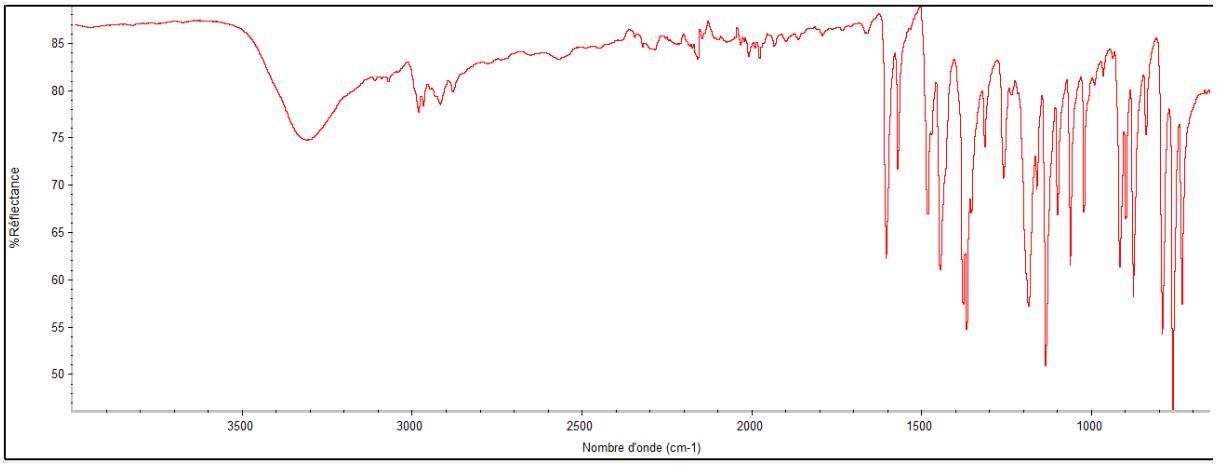
---

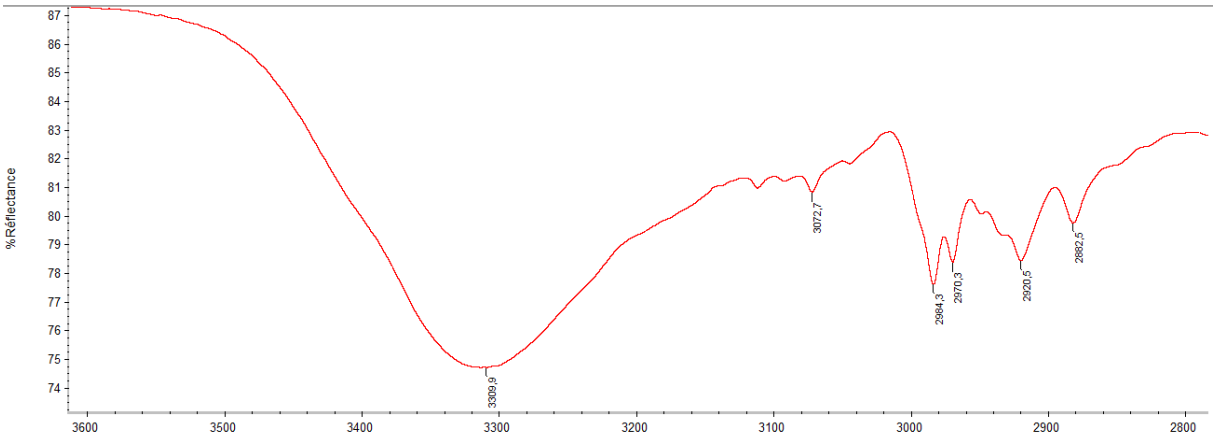
[a] *Laboratoire de Chimie de Coordination, UMR 7177 CNRS/Université de Strasbourg, Institut Le Bel 4, Rue Blaise Pascal, CS90032, 67081 Strasbourg Cedex, France. Fax: +33 368851322; Tel: 33 368851308; E-mail: braunstein@unistra.fr*

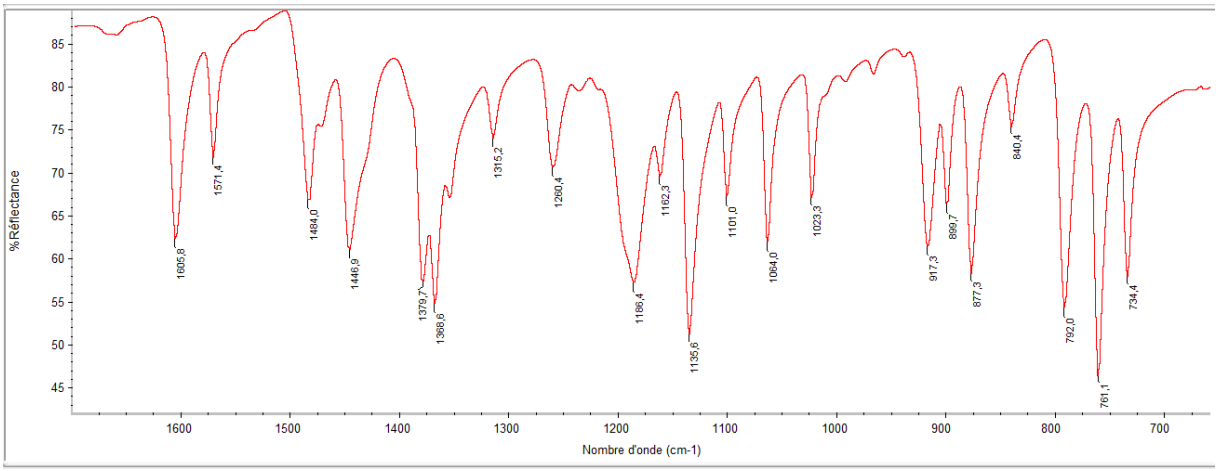
[b] *Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504 CNRS-Université de Strasbourg, 23 rue du Loess, BP43, 67034 Strasbourg Cedex, France. E-mail: Guillaume.Rogez@ipcms.unistra.fr*

[c] *Institut Néel, CNRS, BP 166, 25 rue des Martyrs, 38042 Grenoble Cedex 9, France. E-mail: wolfgang.wernsdorfer@grenoble.cnrs.fr*

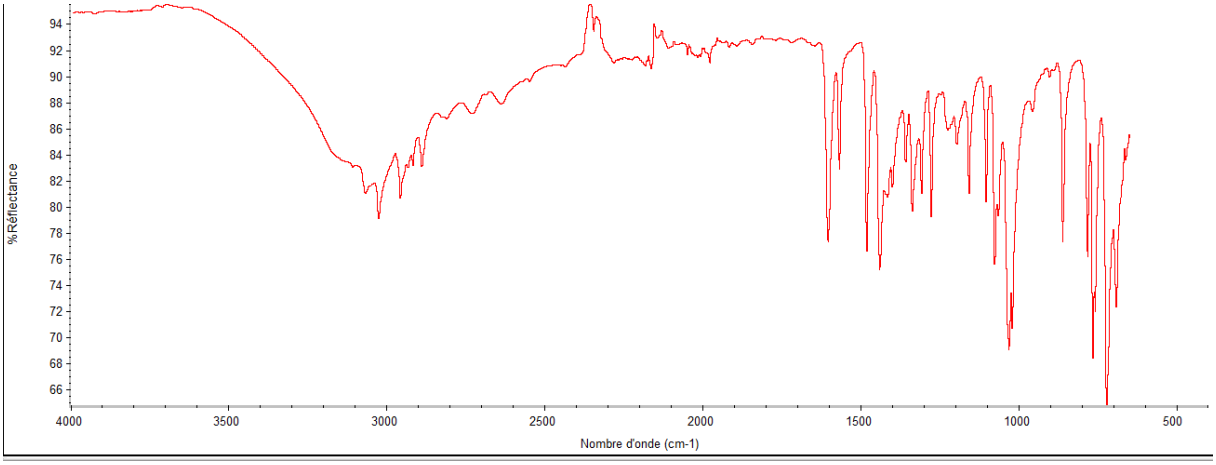
$[NiCl_2(HL)_2]$ (1)

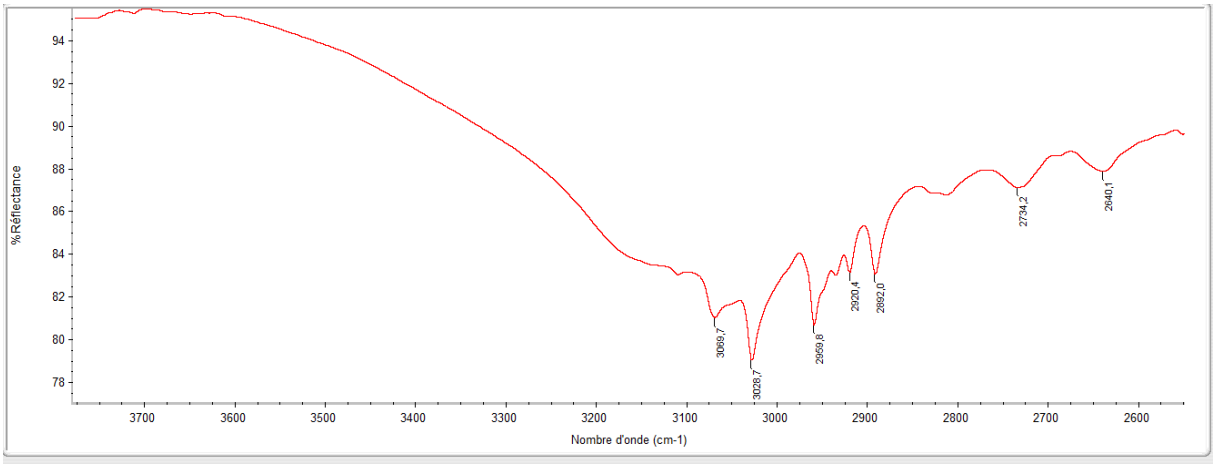


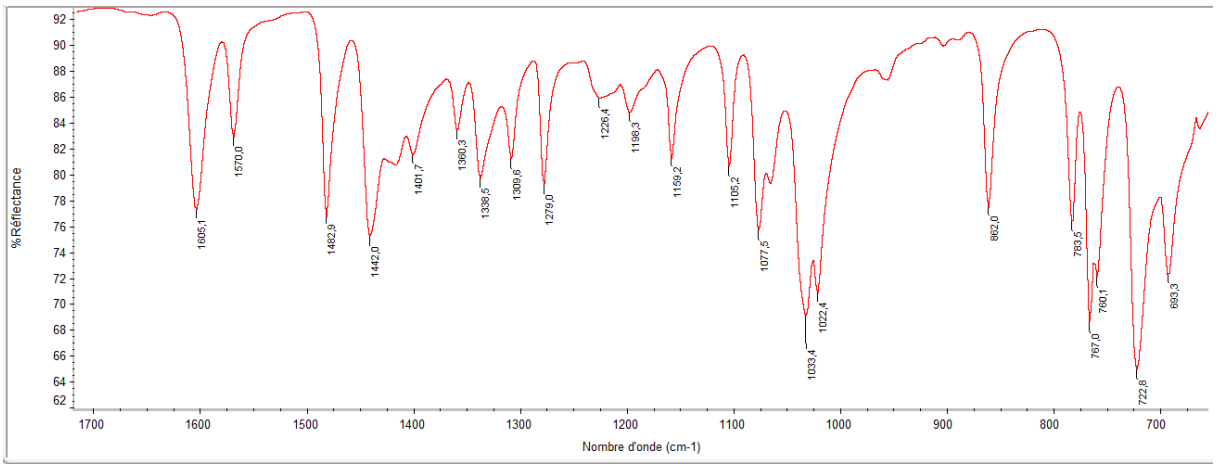




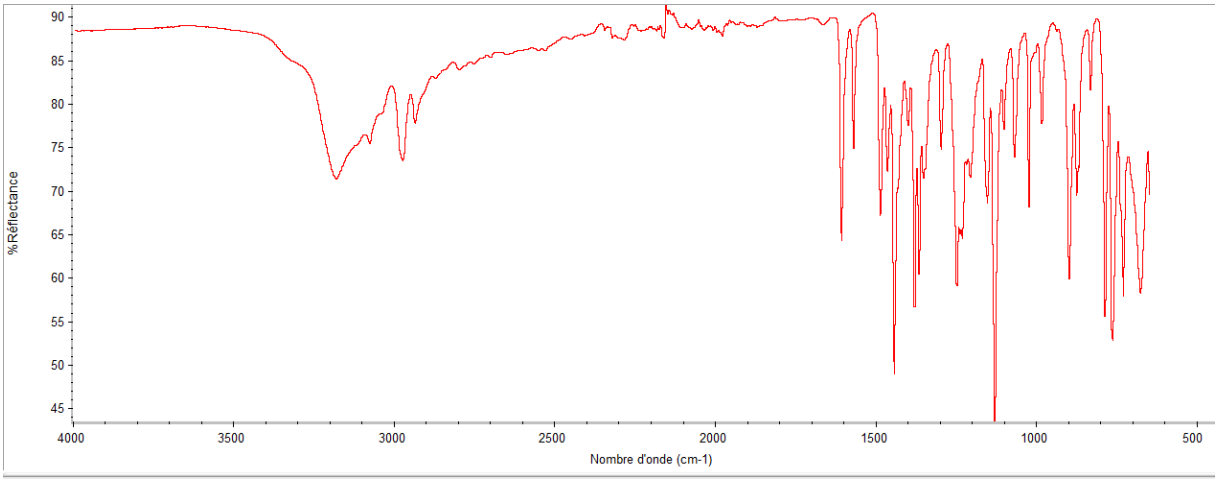
$[Ni(\mu\text{-}Cl)(HL_{Et})_2]_2Cl_2$ (2)

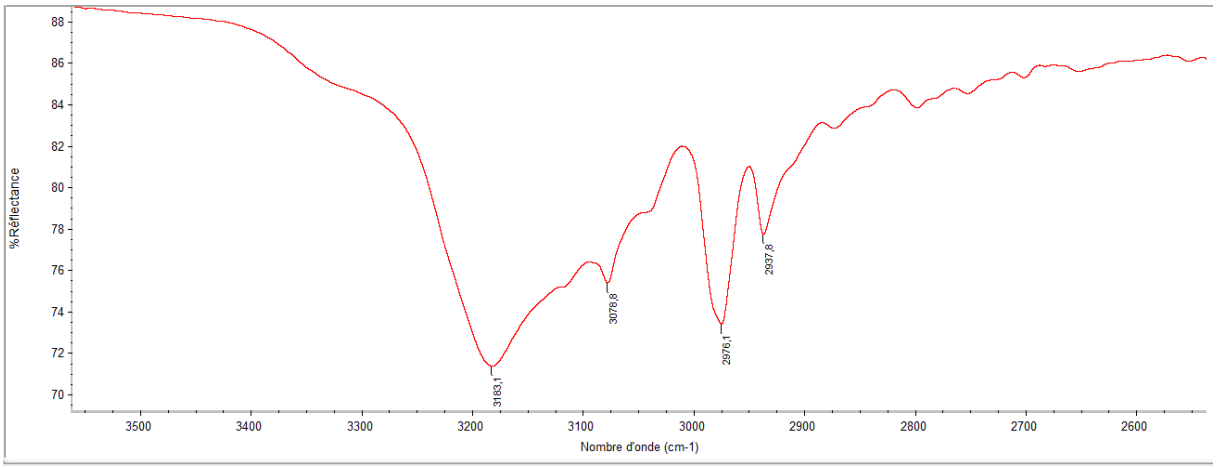


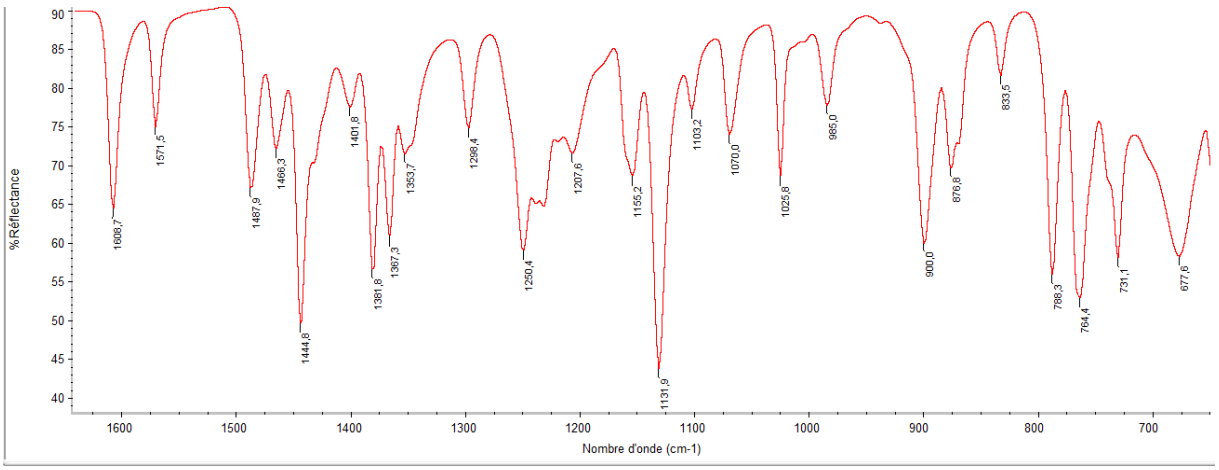




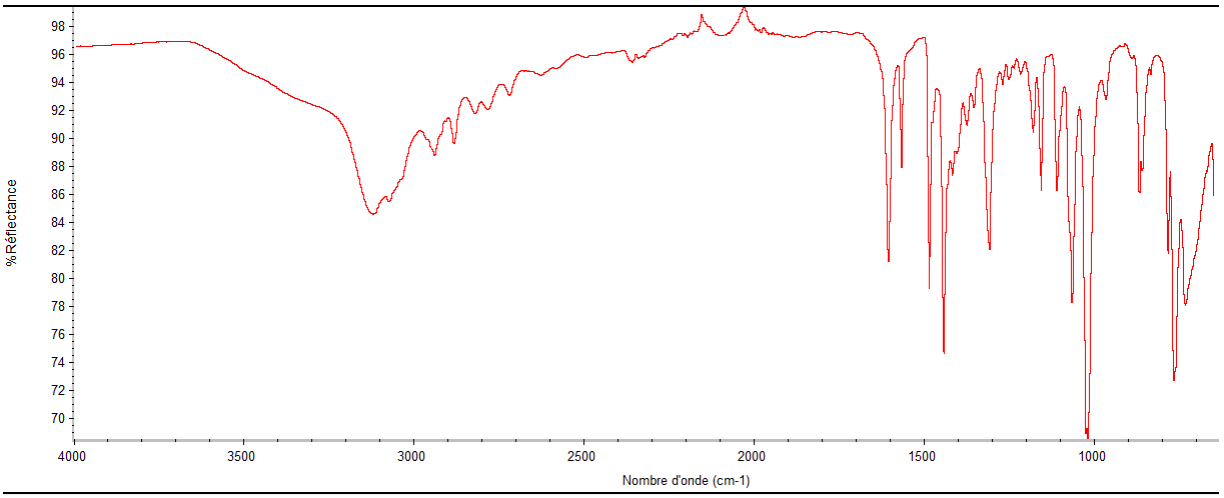
$[Ni(\mu_3\text{-}Cl)(Cl)(HL)]_4$ (3)

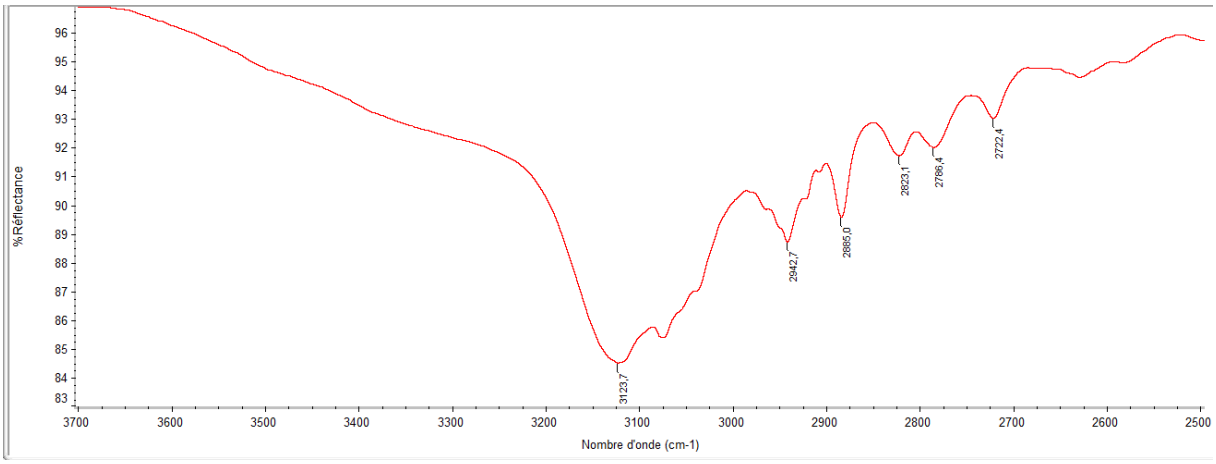


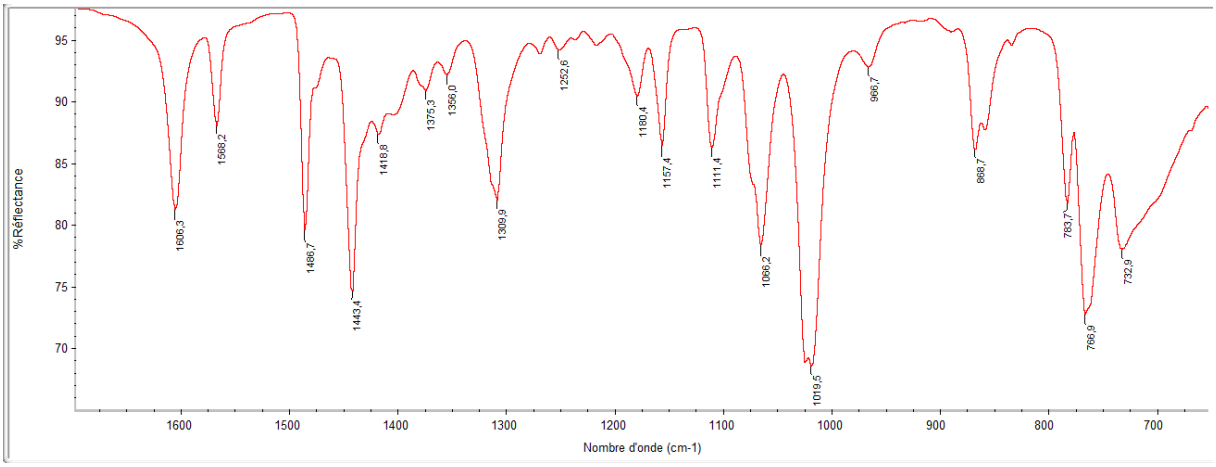




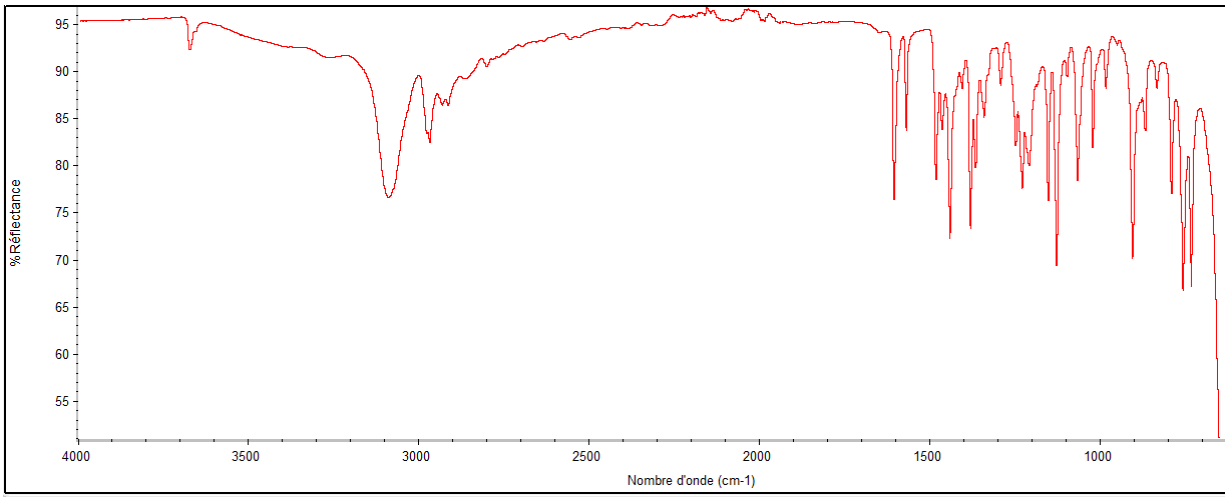
$[Ni(\mu_3\text{-}Cl)(Cl)(HL_{Et})]_4$ (4)

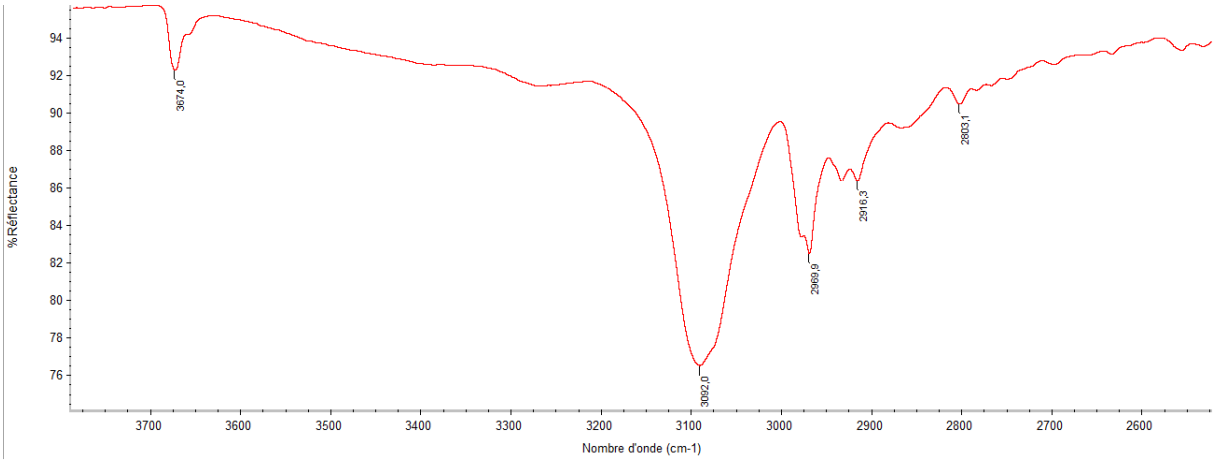


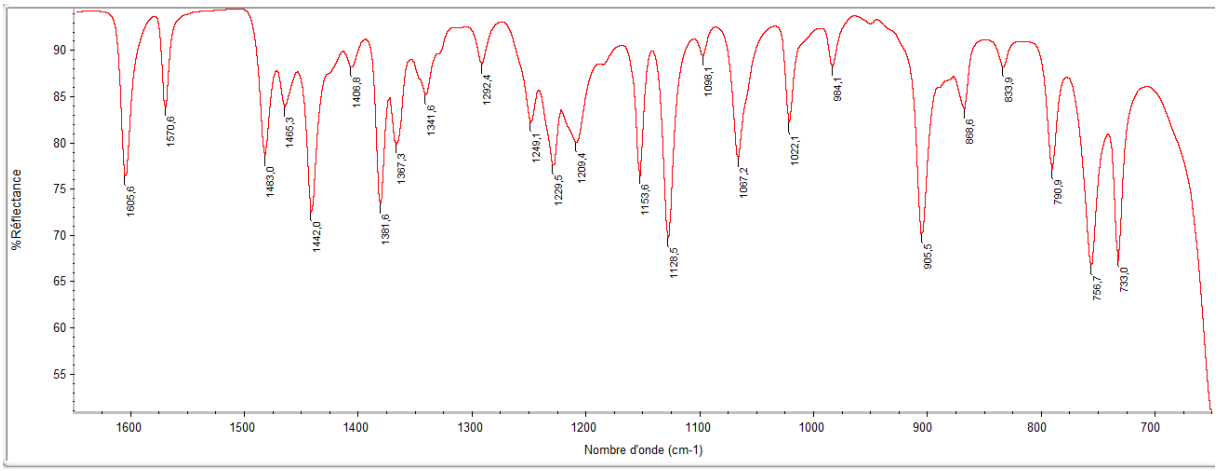




[NiCl(μ$_3$-OH)(HL)]$_4$ (5)







Magnetic data.

The fitting procedure for the χT = f(T) data is rather classical (see O. Kahn, *Molecular Magnetism*, Wiley-VCH, 1993). First, the eigen values of the spin Hamiltonian corresponding to the spin topology defined are calculated and then introduced in the van Vleck equation. This affords a χT = f(T, J, g) relationship. This parameterized equation is introduced into a minimization procedure and, after a fit using the least squares method, the best parameters to reproduce experimental data are obtained. The axial zero field splitting parameter (D) is introduced only on the ground state (S = 4) and intermolecular interactions (zJ) are introduced *via* the mean field approach.