# The magnetic spy: probing local magnetic properties with solid-state NMR

Ridvan Ince*[1] and Gwendal Kervern[1]

[1]Cristallographie, Résonance Magnétique et Modélisations (CRM2) – Université de Lorraine, Centre National de la Recherche Scientifique : UMR7036 – Université de Lorraine - Faculté des Sciences, boulevard des Aiguillettes, BP 70239, 54506 Vandoeuvre-les-Nancy Cedex, France

## Résumé

Acquisition of information on the magnetic properties at the molecular scale - namely the local magnetic susceptibility - is important because it will leads to faster developments of advanced technological applications based on local magnetic properties such as new methods for information storage [1], contrast agents for MRI [2], spintronics [3], etc...
Polarized Neutron Diffraction [4], SQUID-based magnetometry [5], muon spin rotation [6], Electron Paramagnetic Resonance [7] give a precise insight on local magnetic susceptibility. These methods however require heavy equipment as well as relatively large crystalline samples which may be difficult to obtain.

We implemented a model that has been tested and proven efficient in predicting paramagnetic SS-NMR spectra of microcrystalline powders [8]. This model calculates the effect of the hyperfine interaction on the NMR spectra. To this end, we need the crystallographic structure of the molecule. With the structure, the program will generate the position of all paramagnetic atoms on a given radius (50 Å) and set an initial rank-2 magnetic susceptibility tensor. This tensor is the only free parameter of this model and it affects the shape of the theoretical spectrum. From there, the program calculates the hyperfine interaction between all the paramagnetic atoms and one NMR observable nucleus and repeats this for each observable nucleus in the asymmetric unit cell. In the end, the program uses an optimization function to find the best agreement between the experimental and theoretical spectra, giving us an orientation of the local magnetic susceptibility tensor.

This model was compared to experimental data on a series of isostructural lanthanide oxalate metal-organic frameworks. We will present and discuss our results on lanthanum, praseodymium and cerium oxalates.

. Matsumoto, T. *et al. Nat. Commun.* **5**, 3865 (2014).

. Na, H. B. *et al. Adv. Mater.* **21**, 2133–2148 (2009).

. Manyala, N. *et al. Nat. Mater.* **3**, 255–262 (2004).

. Ridier, K. *et al. Chem. - Eur. J.* **22**, 724–735 (2016).

---

*Intervenant

. Moro, F. *et al.* *J. Magn. Magn. Mater.* **361**, 188–196 (2014).

. Gygax, F. N. *et al.* *Phys. B Condens. Matter* **326**, 359–363 (2003).

. Žilić, D. *et al.* *J. Magn. Reson.* **207**, 34–41 (2010).

. Kervern, G. *et al.* *Angew. Chem.* **121**, 3128–3132 (2009).