Computing NMR parameters using the GIPAW method (II)

DFT and NMR with Quantum Espresso (QE)

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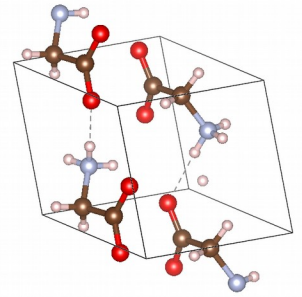
In this tutorial, we pursue the exploration of the GIPAW method by considering first an organic molecular system: Glycine. We will start this example from scratch, i.e., from the crystallographic data given in the cif file. In the second example, we propose you to discover tool facilitating the generation of cif files in the case of disordered solids (i.e., partial occupations in the cif). We have chosen the example of gehnelite (already described in the original publication) but that leads to tractable calculations on a small systems (4 cores).

1. A molecular system: β-glycine

In this exercise, we consider the beta form of Glycine (**06_bGlycine**). Starting from the cif file, you have first to generate the QE input file. Copy/paste a previous scf input file and adapt it for this compounds. To create the atomic coordinates from the cif file, you can use *cif2cell*[1] as follows:



```
cif2cell beta-glycine.cif -p pwscf --pwscf-atomic-units
```

Two structures (cif files) are proposed for this exercise. You can choose to work with one or both. The comparison is interesting to check the influence of the initial structure on the final optimized structure (after DFT optimisation) and related NMR data. Experimental data have been published in *K. Yamada et al. Chemical Letters 37 (2008) 472-473.*

	δ_{11}	δ_{22}	δ_{33}	δ_{iso}	C_Q	η_Q	α	β	γ
β-glycine									
Site-A	470(8)	318(8)	67(8)	285(2)	7.48(8)	0.48(4)	0(4)	90(4)	154(4)
Site-B	468(8)	318(8)	54(8)	280(2)	7.10(8)	0.50(4)	0(4)	90(4)	147(4)
γ-glycine									
Site-A	465(5)	310(5)	65(5)	280(2)	7.3(1)	0.42(4)	0(4)	90(4)	145(4)
Site-B	460(5)	285(5)	71(5)	272(2)	6.7(1)	0.62(4)	0(4)	90(4)	149(4)

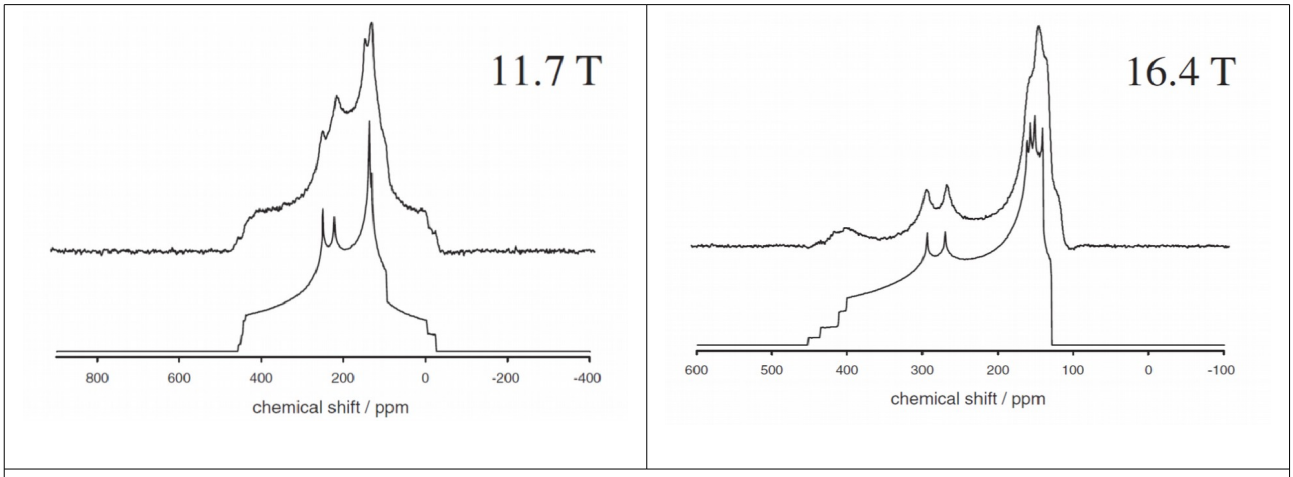
Experimental ^{17}O CSA, EFG tensors and Euler angles from K. Yamada et al. Chemical Letters 37 (2008) 472-473. In parentheses are given the estimated errors.

1 The software is installed on the PC. Your can find documentation at https://sourceforge.net/projects/cif2cell/
Original publication : http://www.sciencedirect.com/science/article/pii/S0010465511000336

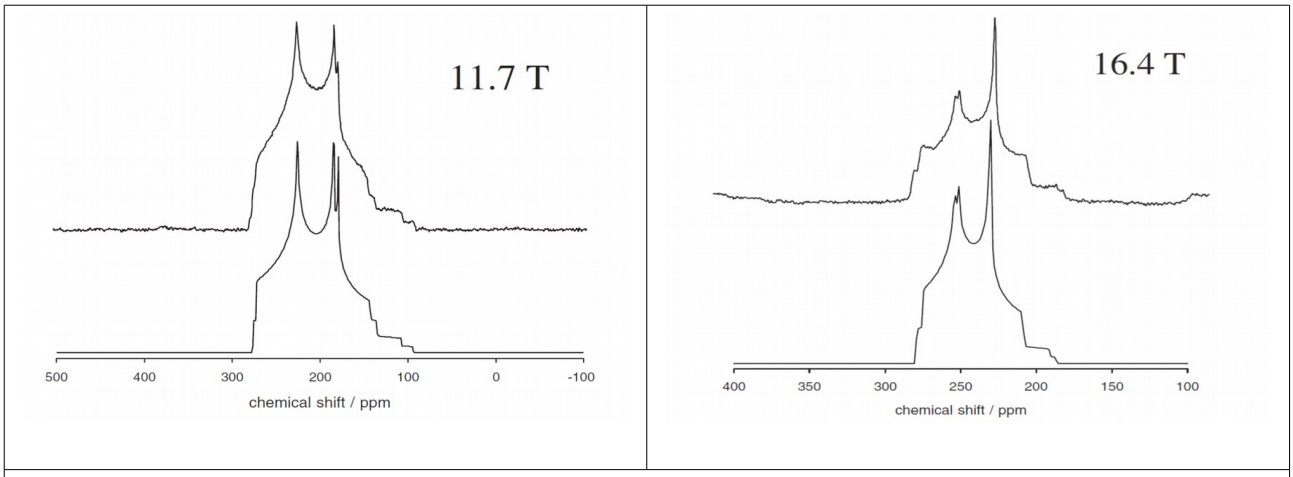
Perform the NMR calculations with the experimental and relaxed structure. Compare the obtained results with the experimental data shown below. A small script is provided to facilitate the calculation (run_nmr.sh) but you must create the xxx-scf.in, efg.in and nmr.in. Then the command line:

```
./run_nmr.sh xxx
```

performs the scf, efg and nmr calculations with xxx-scf.out, xxx-efg.out and xxx-nmr.out as output files, respectively. Similar scripts are provided for relaxation of the structure (input file must be copy/paste from your first calculation, rename them as xxx-relax.in or xxx-vcrelax.in, do not forget to modify the *calculation* field to *'relax'* or *'vc-relax'* and to add the *&ions* and *&cell* section when needed).



*Experimental and simulated ^{17}O **static** NMR spectra (data adapted from from K. Yamada et al. Chemical Letters 37 (2008) 472-473).*



*Experimental and simulated ^{17}O **MAS** NMR spectra (data adapted from from K. Yamada et al. Chemical Letters 37 (2008) 472-473).*

To extract the Euler angles, a small tool is provided *read_nmr_tensor* with reads the NMR tensor (in matrix format) and calculate the Euler angles of their relative orientation (i.e., PAS) with respect to the crystallographic axes as well as the orientations between the tensors. You can use these parameters to make simulation of the NMR spectra and compare directly with the experimental data.[2]

Extra. ***nmr_exp_2002_single***

We have extracted a single molecule from the crystal form. Calculate the NMR parameters. Check the convergence of the NMR parameters by increasing the celldm(1) parameter (box size) so as to minimize the interaction of the molecules with its images. Final number should give the NMR parameters without the environment.

2 Download the binary file (exe) at ftp://ftp.cea.fr/incoming/y2k01/NMRWinterSchool/tools/read_nmr_tensor and ashort tutorial.