**Probing intermolecular interactions in a diethylcarbamazine citrate salt by fast MAS 1H solid-state NMR spectroscopy and GIPAW calculations**

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In the following, the names of all raw data files from the solid-state NMR measurements and different calculations are presented:

1. **Raw files for the solid-state NMR experiments as recorded by Tiago Venâncio.**

**Figure 1a: 13C CP MAS (5 kHz, 500 MHz):** 13C\_CPMAS\_Fig1a (recorded on 07.11.2016)

**Figure 1b: 1H single pulse (60 kHz, 600 MHz):** 1H\_singlepulse\_Fig1b (recorded on 28.05.2016)

**Figure 1c: 15N CP MAS (5 kHz, 500 MHz):** 15N\_CPMAS\_Fig1c (recorded on 26.11.2016)

**Figure 2a: 1H-1H-DQ-SQ\_BABA (60 kHz, 600 MHz):** DQ-SQ\_BABA\_Fig2a (recorded on 28.05.2016)

**Figures 2b, 3: 1H-13C HETCOR (12.5 kHz, 500 MHz, p15 = 200 µs):** 1H-13C-HETCOR\_Figs2b\_3 (recorded on 02.05.2016)

**Figure 2c:** **14N-1H-HMQC (60 kHz, 600 MHz, l6=4):** 14N-1H\_HMQC\_Fig2c (recorded on 28.05.2016)

1. **For the calculations, the initial CIF file, the CIF file after geometry optimization and the magres-file for the full crystal structure. All calculations were run by Tiago Venâncio.**

original\_DECCIT\_PXRD.cif (as determined by single-crystal X-ray diffraction)

DECCIT-conformer1\_PXRD.cif (as determined by single-crystal X-ray diffraction)

DECCIT-conformer1\_NMR\_opt.cif

DECCIT-conformer1\_NMR.magres