**The use of variable temperature 13C solid-state MAS NMR and GIPAW DFT calculations to explore the dynamics of diethylcarbamazine citrate**

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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 1:** 1H (500 MHz)-13C HETCOR MAS NMR spectra of diethylcarbamazine citrate recorded using FSLG 1H decoupling and CP contact times of:

**(a)** 50 μs (12.5 kHz): **Fig1-CPHETCOR-DEC [1]** - (recorded on 02.05.2016) and

**(b)** 2000 μs (10.0 kHz): **Fig1-CPHETCOR-DEC [2]** - (recorded on 27.09.2016)

**Figures 2 and 4:** 1H (500 MHz)-13C CP MAS (5 kHz) spectra for diethylcarbamazine citrate at different temperatures from 0 to -40 oC: **Fig2-CPMAS-TempVar\_LowTemp** (recorded on 07/11/2016).

**[5]** 0 oC

**[6]** -5 oC

**[7]** -10 oC

**[8]** -15 oC

**[9]** -20 oC

**[10]** -25 oC

**[11]** -30 oC

**[12]** -35 oC

**[14]** - 40 oC

**Figure 3:** 1H (500 MHz)-13C CP MAS (5 kHz) spectra for diethylcarbamazine citrate at different temperatures from 0 to +50 oC: **Fig3-CPMAS-TempVar\_HighTemp** (recorded on 22/10/2016).

**[1]** 0 oC

**[2]** +10 oC

**[3]** +20 oC

**[4]** +30 oC

**[5]** +40 oC

**[6]** +50 oC

**[100]** +5 oC

**[200]** +15 oC

**[300]** +25 oC

**[400]** +35 oC

**[500]** +55 oC

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 and Tomasz Pawlak.**

original\_DECCIT293K\_PXRD.cif (as determined by single-crystal X-ray diffraction)

DECCIT293K-conformer1\_PXRD.cif (as determined by single-crystal X-ray diffraction)

DECCIT293K-conformer2\_PXRD.cif (as determined by single-crystal X-ray diffraction)

DECCIT293K -conformer1\_NMR\_opt.cif

DECCIT293K -conformer1\_NMR.magres

DECCIT293K -conformer2\_NMR\_opt.cif

DECCIT293K-conformer2\_NMR.magres

original\_DECCIT235K\_PXRD.cif (as determined by single-crystal X-ray diffraction)

DECCIT235K-conformer1\_PXRD.cif (as determined by single-crystal X-ray diffraction)

DECCIT235K-conformer2\_PXRD.cif (as determined by single-crystal X-ray diffraction)

DECCIT235K-conformer1\_NMR\_opt.cif

DECCIT235K-conformer1\_NMR.magres

DECCIT235K-conformer2\_NMR\_opt.cif

DECCIT235K-conformer2\_NMR.magres

original\_DECCIT150K\_PXRD.cif (as determined by single-crystal X-ray diffraction)

DECCIT150K\_NMR\_opt.cif

DECCIT150K\_NMR.magres

original\_DECCIT100K\_PXRD.cif (as determined by single-crystal X-ray diffraction)

DECCIT100K\_NMR\_opt.cif

DECCIT100K\_NMR.magres

DECCIT-conformer-1-plusC1-C4from-conformer2\_NMR\_opt.cif

DECCIT-conformer-1-plusC1-C4from-conformer2.magres

DECCIT-conformer-2-plusC1-C4from-conformer1\_NMR\_opt.cif

DECCIT-conformer-2-plusC1-C4from-conformer1.magres