**Improving confidence in crystal structure solutions using NMR crystallography: the case of -piroxicam**

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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 Andrew Tatton.

**Figure 3a: 13C CPMAS (10 kHz, 400 MHz):** piroxicam\_13C\_CPMAS\_10k\_i/ii (recorded on 14/08/2017)

**Figure 4a: 1Honepulse (65 kHz, 400 MHz):** piroxicam\_1H\_zg\_65k (recorded on 19/06/2017)

**Figure 4d: 13C-1H HETCOR (10 kHz, 400 MHz):** piroxicam\_13C\_HETCOR\_10k (recorded on 13/06/2017)

**Figure 5a: 15N CPMAS (10 kHz, 500 MHz):** piroxicam\_15N\_CPMAS\_10k\_i/ii (recorded on 15/06/17 and 27/07/2017)

**Figure 6a: 1H-14N HMQC (60 kHz, 700 MHz,  = 266.7 s):** piroxicam\_14N\_HMQC\_267\_60k (recorded on 24/07/17)

**Figure 6b: 1H-14N HMQC (60 kHz, 700 MHz,  = 533.3 s):** piroxicam\_14N\_HMQC\_533\_60k (recorded on 25/07/17)

**Figure 7a: 1H DQ-BABA (60 kHz, 400 MHz):** piroxicam\_1H\_BABA\_60k (recorded on 16/08/17)

**2. Outputted CASTEP files as recorded by Andrew Tatton.**

For the calculations, the initial CIF file, the CIF file after geometry optimisation were protons only are permitted to relax, and the CIF file after geometry optimisation allowing all atoms to relax are given using both starting structures. The magres-files for the full crystal structure calculated from an all atom relaxation during geometry optimisation, proton only relaxation during geometry optimization, and the single molecule are given.

BIYSEH03.cif (as determined by powder X-ray diffraction)

BIYSEH13.cif (as determined by single crystal X-ray diffraction)

BIYSEH03\_allatom.cif

BIYSEH03\_Honly.cif

BIYSEH13\_allatom.cif

BIYSEH03\_Honly.cif

BIYSEH03\_allatom.magres

BIYSEH03\_Honly.magres

BIYSEH03\_singlemol.magres

BIYSEH13\_allatom.magres

BIYSEH13\_Honly.magres

BIYSEH13\_singlemol.amgres