**Single-crystal X-ray diffraction and NMR crystallography of a 1:1 co-crystal of dithianon and pyrimethanil**

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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 Harriet Pearce, Emily K. Corlett and Ann-Christin Pöppler.

**Figure 3a: 1H (60 kHz, 600 MHz):** DI\_PM\_60kHz\_1H\_600 (recorded on 06.05.2016)

**Figure 2: 13C CP MAS (12.5 kHz, 600 MHz):** DI\_PM\_12\_5kHz\_13C\_600 (recorded on 11.08.2015)

**Figure 3c, 4a:** 1H-13C HETCOR (12.5 kHz, 500 MHz, p15 = 100 µs): DI\_PM\_12\_5kHz\_HETCOR\_100 (recorded on 18.05.2016)

**Figure 4b:** 1H-13C HETCOR (12.5 kHz, 500 MHz, p15 = 500 µs): DI\_PM\_12\_5kHz\_HETCOR\_500 (recorded on 03.09.2016)

**Figure 4c:** 1H-13C HETCOR (12.5 kHz, 500 MHz, p15 = 1000 µs): DI\_PM\_12\_5kHz\_HETCOR\_1000 (recorded on 11.07.2017)

**Figure 3b:** DI\_PM\_60kHz\_BABA\_700 (recorded on 07.06.2016)

**2. For the calculations, the initial CIF file, the CIF file after geometry optimization and the magres-files for the full crystal structure and the single molecule are given. All calculations were run by Harriet Pearce and analyzed together with Emily K. Corlett and Ann-Christin Pöppler.**

DI\_PM\_original.cif (as determined by single-crystal X-ray diffraction)

DI\_PM\_700\_out.cif

DI\_PM\_700\_NMR.magres

DI\_NMR.magres

PM\_NMR.magres