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

**Ann-Christin Poepplera†, Emily K. Corlettab, Harriet Pearceab, Mark P. Seymourc, Matthew Reidcd, Mark G. Montgomeryc and Steven P. Browna\***

aDepartment of Physics, University of Warwick, Coventry, Warwickshire, CV47AL, UK  
bDepartment of Chemistry, University of Warwick, Coventry, Warwickshire, CV47AL, UK  
cInternational Research Centre, Syngenta, Jealott's Hill, Bracknall, Berkshire, RG426EY, UK  
dAfton Chemical, London Road, Bracknell, Berkshire, RG122UW, UK

**†** A.-C. Pöppler is now located at the University of Würzburg, Department of Organic Chemistry, 97074 Wurzburg, Germany.

Correspondence email: S.P.Brown@warwick.ac.uk

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