**Weak Intermolecular CH…N Hydrogen Bonding: Determination of 13CH-15N Hydrogen-Bond Mediated J couplings by Solid-State NMR Spectroscopy and First-Principles Calculations**

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1. **Raw files from NMR experiments  
   (recorded by Amy Webber, except for Figure S3 by Emily Corlett)**

**Compound 1**

1H-13C CP MAS, Figure 3b **[102]** (recorded 24/9/2009)

Spin-echo data, Figure 4a **[110]** (recorded 28/9/2009)

**Compound 2**

1H-13C CP MAS **[202]** (recorded 3/10/2009)

Spin-echo data, Figure 4b **[210]** (recorded 26/4/2010)

**Compound 10**

1H-13C CP MAS, Figure S5b **[502]** (recorded 15/12/2009)

Spin-echo data, Figure S6 **[510]** (recorded 23/4/2010)

**Figure S3:** 1H (600 MHz)-13C CP (1.5 ms) MAS (12.5 kHz) NMR spectra of **1** (a) and **2** (b):

1. **[12]** (recorded 07/12/2018)
2. **[9]** (recorded 07/12/2018)
3. **Raw files for the PXRD experiments (recorded by Emily Corlett)**

**Figure S1:** PXRD data of **1** at natural isotopic abundance (top) and 4-[15N] cyano-4’-[13C2] ethynylbiphenyl (middle) recorded with a Panalytical X’Pert Pro MPD diffractometer, λ = 1.5406 Å:

(top) **unlBi\_4-60-2hr17\_1.xrdml** (recorded on 09/01/2019)

(middle) **labBi\_4-60-2hr17\_1.xrdml** (recorded on 09/12/2018)

**Figure S2:** PXRD data of **2** at natural isotopic abundance (top) and [15N3,13C6]-2,4,6-triethynyl-1,3,5-triazine (middle) recorded with a Panalytical X’Pert Pro MPD diffractometer, λ = 1.5406 Å:

(top) **Tri\_unl\_4-60-2hr17\_1.xrdml** (recorded on 29/11/2018)

(middle) **Tri\_lab\_4-55-15hr\_1.xrdml** (recorded on 17/12/2018)

1. **Raw files from DFT calculations (carried out by Miri Zilka)**

.cif files for DFT geometry optimised structures

.magres files for *J* coupling calculations performed using CASTEP