

## Supplementary Material

### Detailed NMR Analysis of DppzD<sub>2</sub>

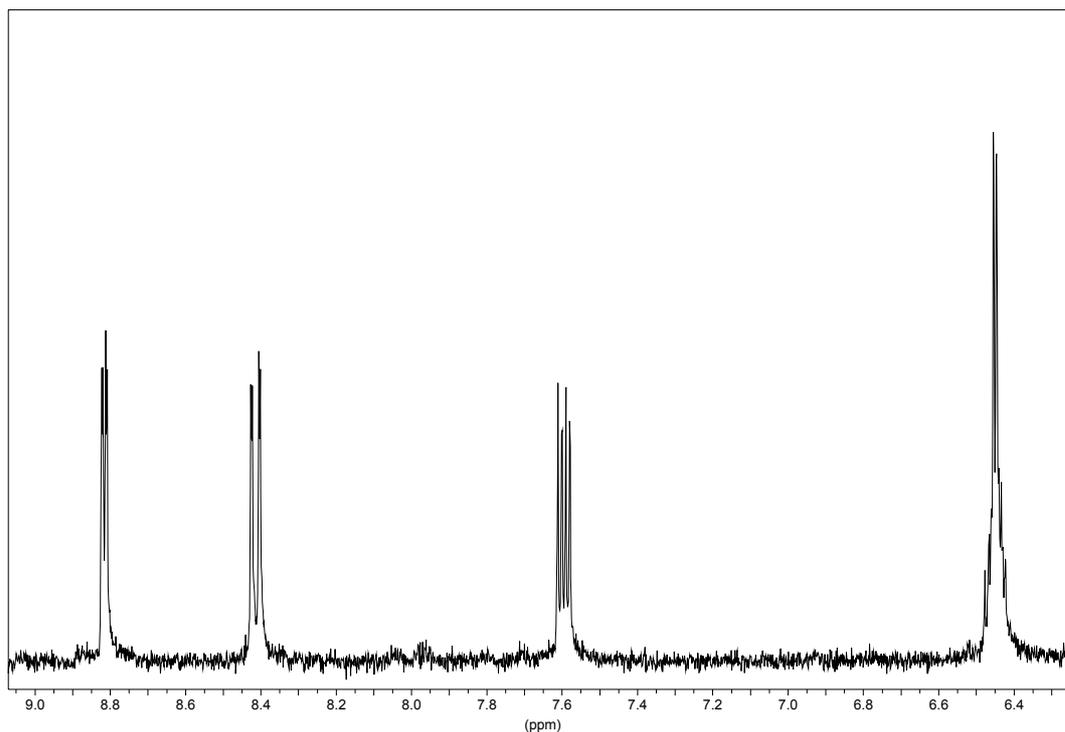
All NMR spectra were carried out on a Bruker DPX400 at 400.13 Hz for <sup>1</sup>H and 100.62Hz for <sup>13</sup>C spectra.

The sample of dppzH<sub>2</sub> was produced by 4 hours of UV ( $\lambda > 330$  nm) irradiation of dppz (c = ca.  $1.9 \times 10^{-3}$  mol dm<sup>-3</sup>) in C<sub>2</sub>D<sub>5</sub>OD.

**Figure 1:** <sup>1</sup>H NMR of dppzD<sub>2</sub> (ca.  $1.9 \times 10^{-3}$  mol dm<sup>-3</sup>) in C<sub>2</sub>D<sub>5</sub>OD.

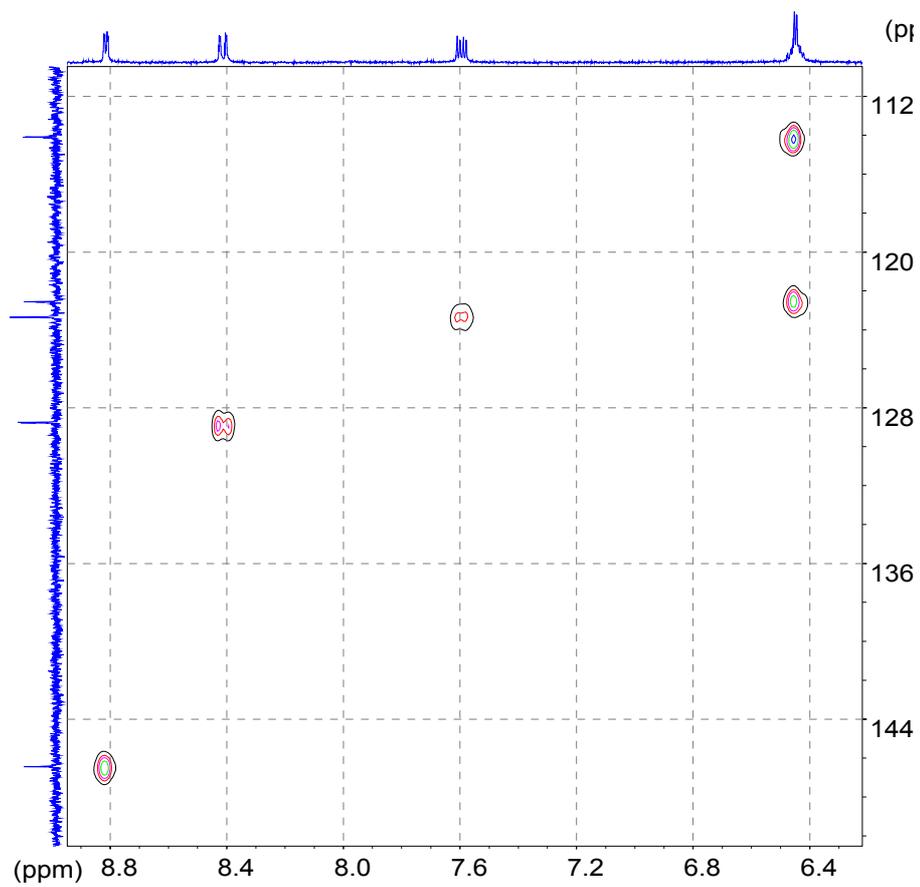
**Figure 2:** <sup>13</sup>C-<sup>1</sup>H COSY (HMQC) of dppzD<sub>2</sub> (ca.  $1.9 \times 10^{-3}$  mol dm<sup>-3</sup>) in C<sub>2</sub>D<sub>5</sub>OD.

**Figure 3:** <sup>13</sup>C NMR spectrum (top) and DEPT 135° spectrum (bottom) of dppzD<sub>2</sub> (ca.  $1.9 \times 10^{-3}$  mol dm<sup>-3</sup>) in C<sub>2</sub>D<sub>5</sub>OD.

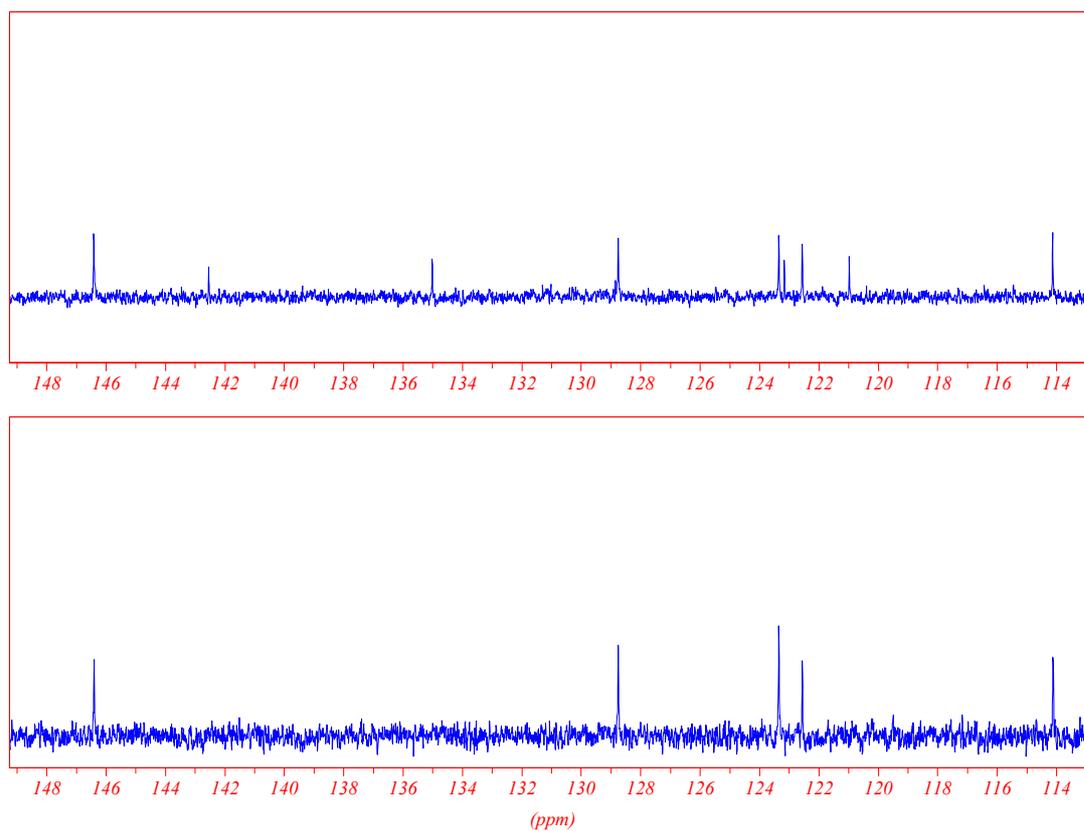


**Figure 1:** NMR spectrum of a solution of dppzH<sub>2</sub> in C<sub>2</sub>D<sub>5</sub>OD (ca. 1.9 x 10<sup>-3</sup> mol dm<sup>-3</sup>)

$\delta_{\text{H}}$  (400.13 MHz, C<sub>2</sub>D<sub>5</sub>OD), 8.81 (1H, d,  $J$  = 4 Hz, H<sub>3</sub>H<sub>6</sub>), 8.41 (1H, d,  $J$  = 8.5 Hz, H<sub>1</sub>H<sub>8</sub>), 7.59 (1H, dd,  $J$  = 8.5, 4 Hz, H<sub>2</sub>H<sub>7</sub>), 6.45 (1H, m,  $J$  = 9 Hz, H<sub>10</sub>H<sub>13</sub>), 6.45 (1H, m,  $J$  = 9 Hz, H<sub>11</sub>H<sub>12</sub>)



**Figure 2:**  $^{13}\text{C}$ - $^1\text{H}$  COSY (HMQC) of  $\text{dppzH}_2$  (*ca.*  $1.9 \times 10^{-3} \text{ mol dm}^{-3}$ ) in  $\text{C}_2\text{D}_5\text{OD}$ .



**Figure 3:** Carbon 13 spectrum (top) and DEPT  $135^\circ$  spectrum (bottom) of  $\text{dppzH}_2$  (*ca.*  $1.9 \times 10^{-3} \text{ mol dm}^{-3}$ ) in  $\text{C}_2\text{D}_5\text{OD}$ .

(100.62 MHz,  $\text{C}_2\text{D}_5\text{OD}$ ) 146.4 ( $\text{C}_3, \text{C}_6$ ), 142.6 (q), 135.0 (q), 128.7 ( $\text{C}_1, \text{C}_8$ ), 123.3 ( $\text{C}_2, \text{C}_7$ ), 123.1 (q), 122.5 ( $\text{C}_{11}, \text{C}_{12}$ ), 121.0 (q), 114.1 ( $\text{C}_{10}, \text{C}_{13}$ ).