

## Synthesis and investigation of fullerene-based acceptor materials

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### *Selected spectral data*

**1a** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ= 2.9 (t, 2H), 3.26 (t, 2H), 3.71 (s, 3H), 7.51 (t, 1H), 7.58 (t, 2H), 7.95 (d, 2H) ppm.

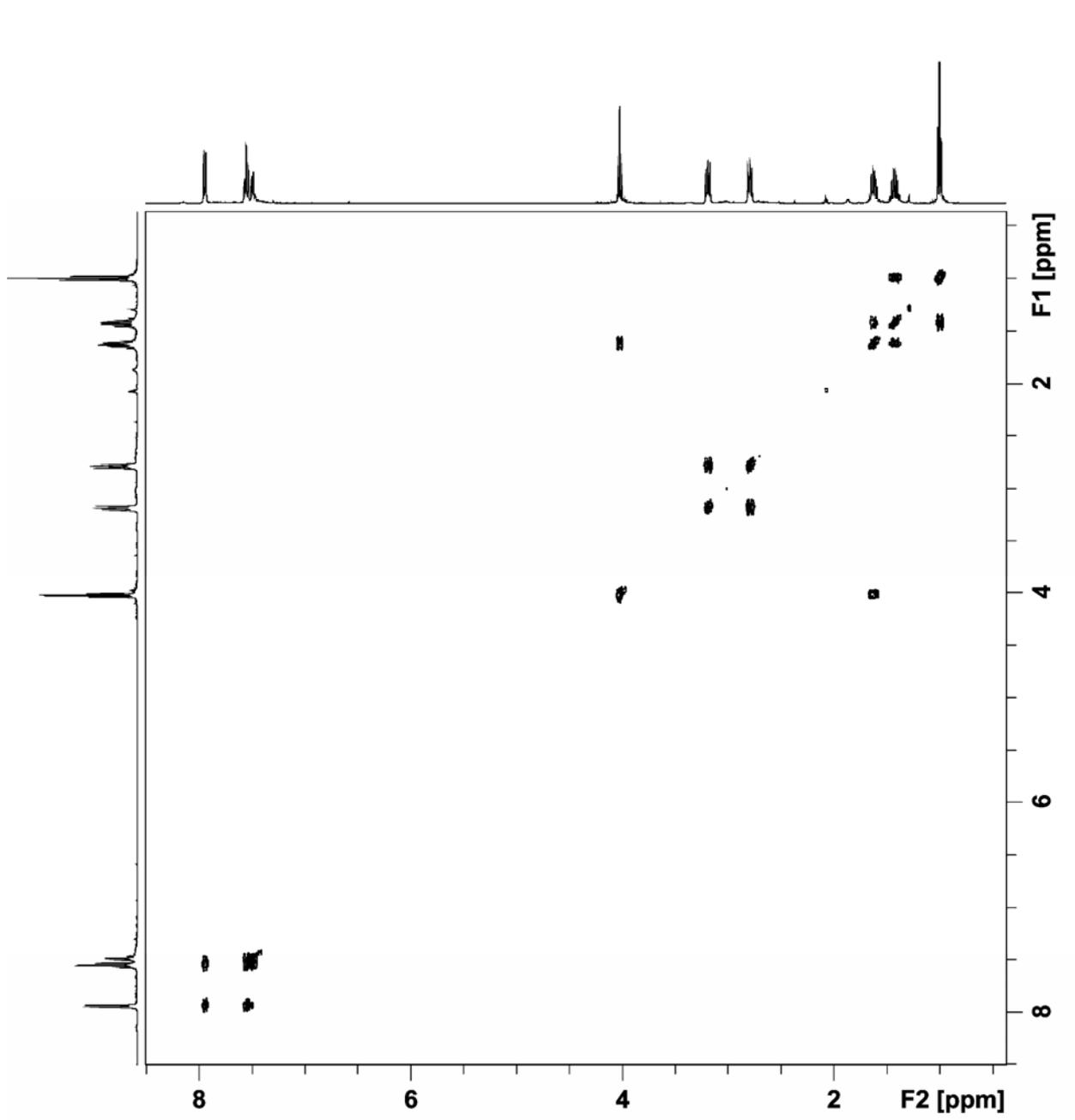
**1b** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): 1.30 (t, 3H), 2.88 (t, 2H), 3.26 (t, 2H), 4.15 (t, 2H), 7.51 (t, 1H), 7.58 (t, 2H), 7.95 (d, 2H) ppm. <sup>13</sup>C NMR (150 MHz, CS<sub>2</sub>-acetone-d<sup>6</sup> 10:1): δ= 14.49, 29.78, 31.51, 50.79, 60.27, 79.4, 125.33, 127.37, 128.19, 128.32, 128.48, 128.91, 130.4, 132.03, 136.1, 137.18, 137.66, 138.15, 140.73, 140.98, 141.95, 142.07, 142.16, 142.89, 142.93, 142.98, 143.01, 143.68, 144.06, 144.42, 144.59, 144.69, 144.74, 144.92, 144.99, 145.1, 145.69, 147.3, 148.35, 170.44 ppm.

**1c** <sup>1</sup>H NMR (600 MHz, CS<sub>2</sub>-acetone-d<sup>6</sup> 10:1): δ= 1.39 (d, 6H), 2.88 (t, 2H), 3.31 (t, 2H), 5.06 (m, 1H), 7.61 (t, 1H), 7.67 (t, 2H), 8.05 (d, 2H) ppm. <sup>13</sup>C NMR (150 MHz, CS<sub>2</sub>-acetone-d<sup>6</sup> 10:1): δ= 21.87, 29.68, 31.72, 50.8, 79.4, 128.29, 128.47, 132.01, 136.09, 137.61, 138.13, 140.68, 140.95, 141.91, 142.04, 142.14, 142.83, 142.87, 142.94, 143.64, 144.02, 144.38, 144.56, 144.65, 144.72, 144.91, 144.95, 145.05, 145.67, 147.3, 148.34, 170.03 ppm.

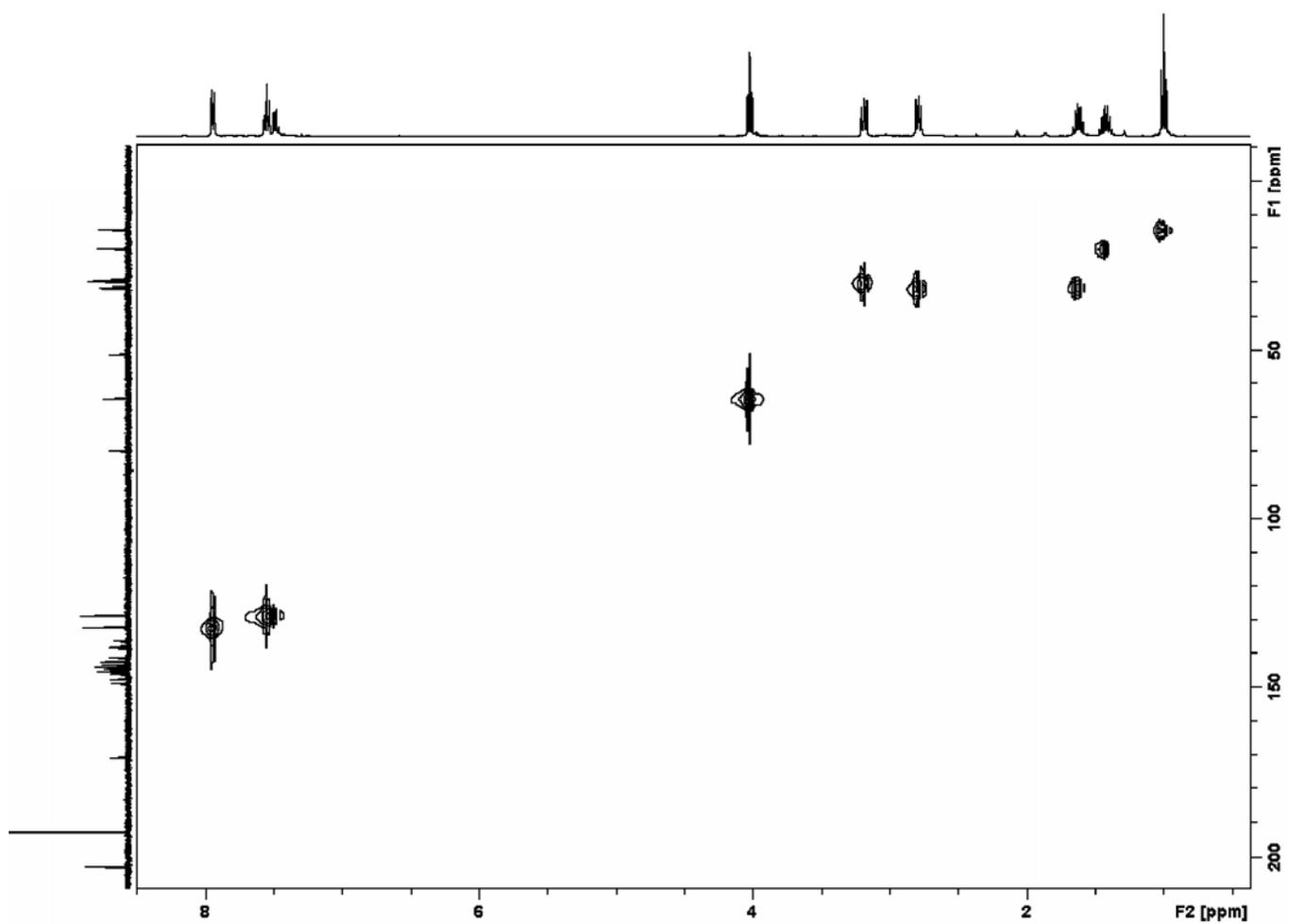
**1d** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ= 0.98 (t, 3H), 1.69 (m, 2H), 2.88 (t, 2H), 3.26 (t, 2H), 4.06 (t, 2H), 7.52 (t, 1H), 7.58 (t, 2H), 7.97 (d, 2H) ppm. <sup>13</sup>C NMR (100 MHz, CS<sub>2</sub>-acetone-d<sup>6</sup> 10:1): δ= 11.68, 23.43, 30.61, 32.31, 51.63, 66.75, 80.22, 129.17, 129.33, 132.85, 136.89, 138.48, 138.96, 141.54, 141.79, 142.76, 142.88, 142.98, 143.69, 143.72, 143.75, 143.8, 143.84, 144.49, 144.88, 145.24, 145.41, 145.51, 145.56, 145.75, 145.81, 145.91, 146.52, 148.12, 149.17, 171.35 ppm.

**1e** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ= 0.95 (t, 3H), 1.39 (m, 2H), 1.63 (m, 2H), 2.87 (t, 2H), 3.24 (t, 2H), 4.08 (t, 2H), 7.49 (t, 1H), 7.56 (t, 2H), 7.94 (d, 2H) ppm. <sup>13</sup>C NMR (150 MHz, CS<sub>2</sub>-C<sub>6</sub>D<sub>12</sub> 10:1): δ= 14.36, 19.95, 29.93, 31.27, 31.7, 51.13, 64.38, 79.67, 128.57, 128.72, 132.25, 136.2, 137.79, 138.29, 140.85, 141.1, 142.11, 142.24, 142.33, 143.03, 143.08, 143.14, 143.19, 143.84, 144.21, 144.55, 144.74, 144.85, 144.92, 145.15, 145.19, 145.25, 145.95, 147.62, 148.65, 170.88 ppm.

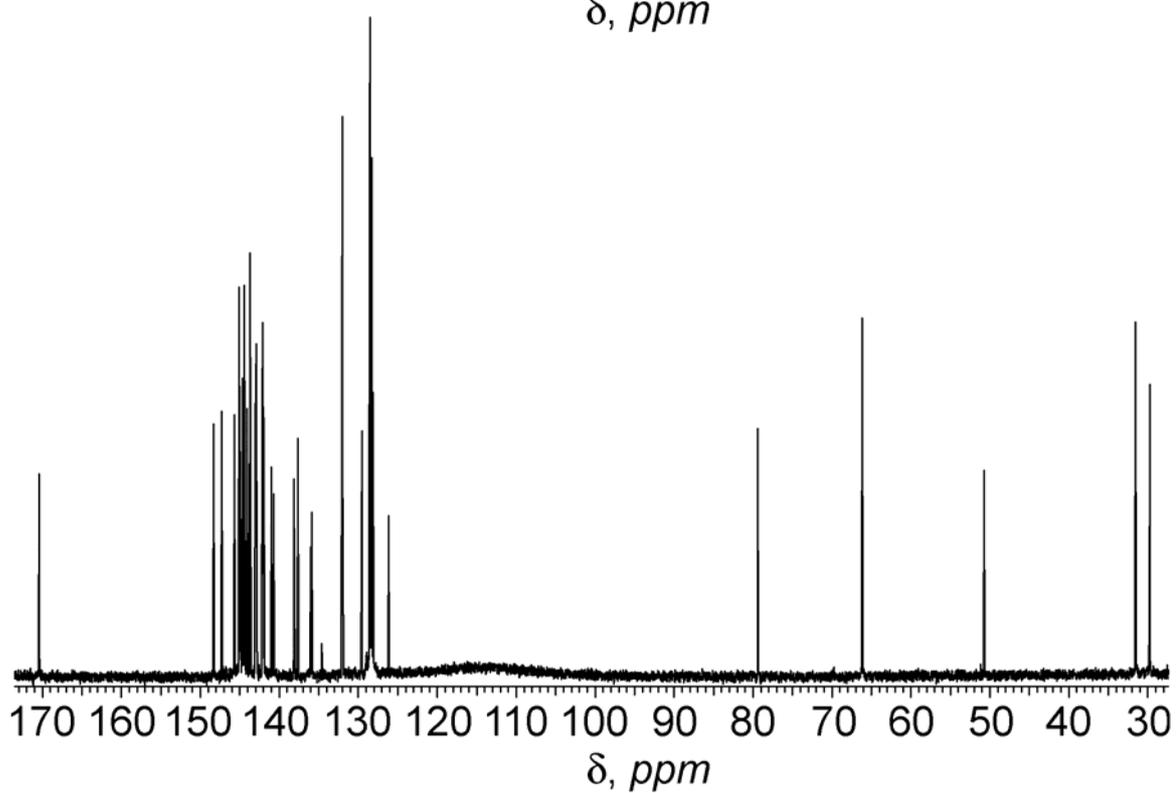
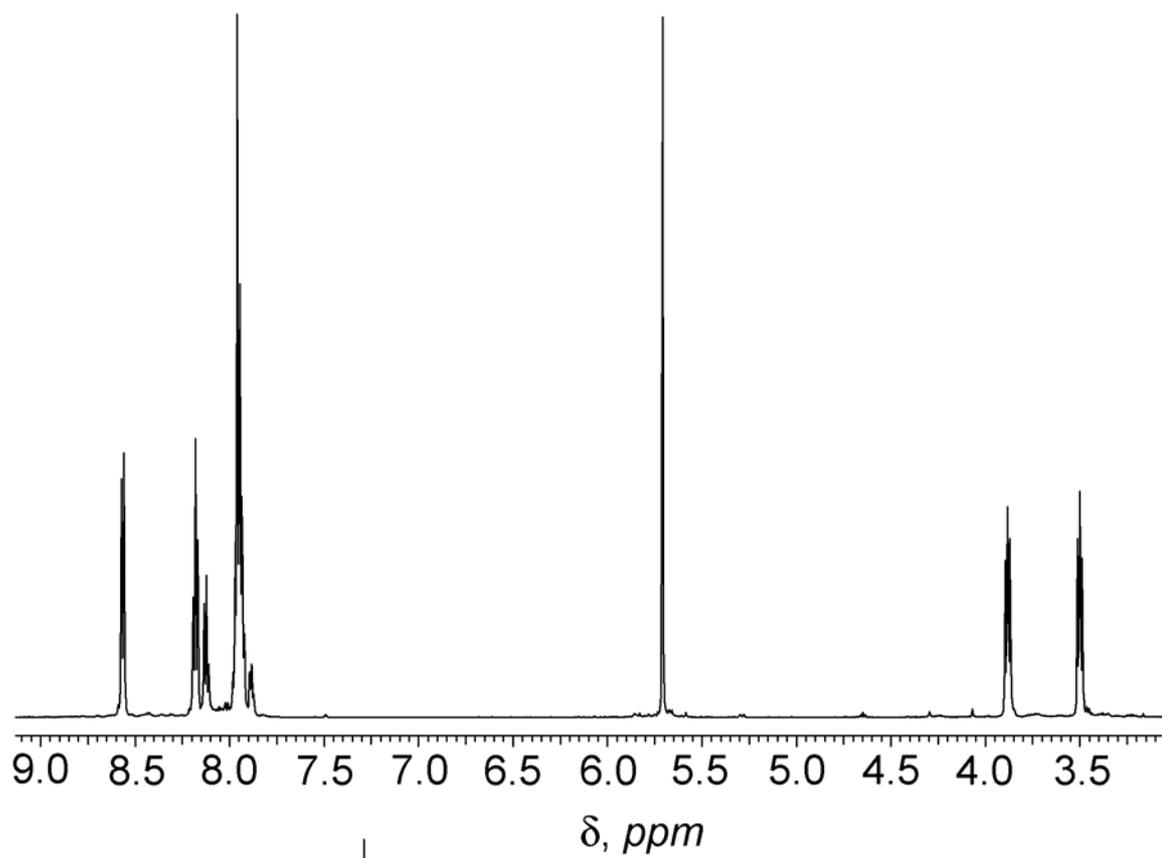
**1f** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ= 3.5 (t, 2H), 3.88 (t, 2H), 5.71 (s, 2H), 7.96 (m, 5H), 8.12 (t, 1H), 8.18 (t, 2H), 8.56 (d, 2H) ppm. <sup>13</sup>C NMR (150 MHz, CS<sub>2</sub>-C<sub>6</sub>D<sub>12</sub> 10:1): δ= 29.75, 31.55, 50.74, 66.19, 79.37, 126.18, 128.14, 128.29, 128.36, 128.48, 128.53, 128.56, 129.54, 132.01, 135.85, 135.99, 137.66, 138.14, 140.71, 140.98, 141.94, 142.06, 142.16, 142.87, 142.93, 142.98, 143.01, 143.67, 144.06, 144.42, 144.59, 144.69, 144.73, 144.92, 144.99, 145.1, 145.69, 147.27, 148.31, 170.41 ppm.



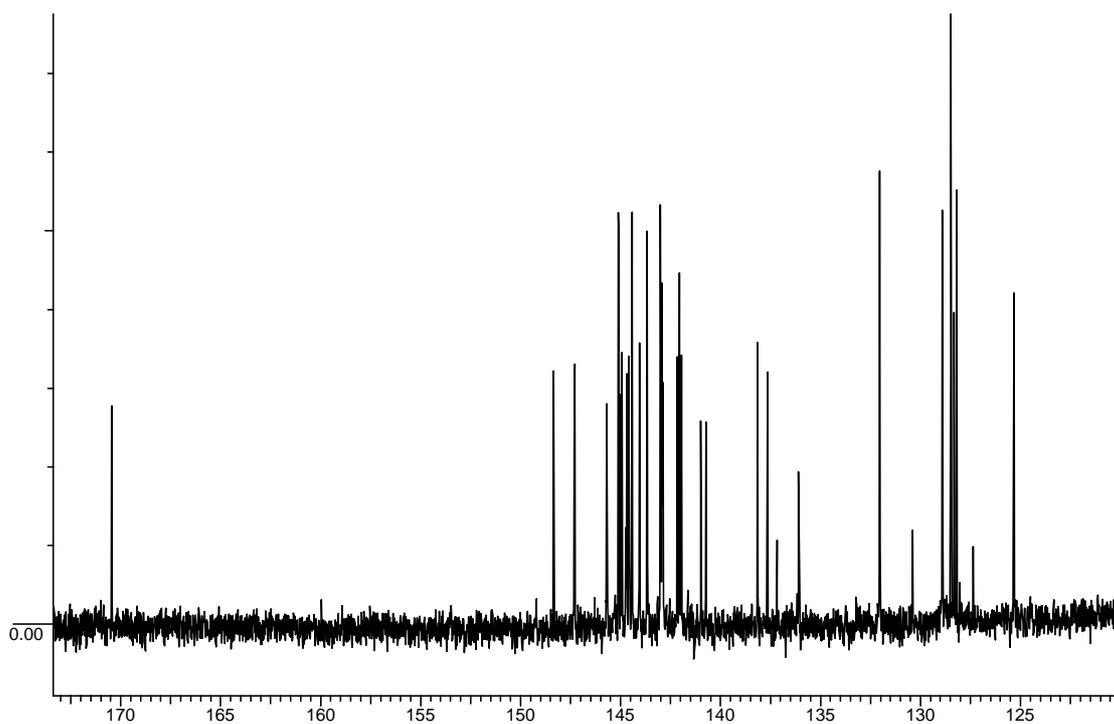
H-H COSY 2D NMR spectrum of **1e**.



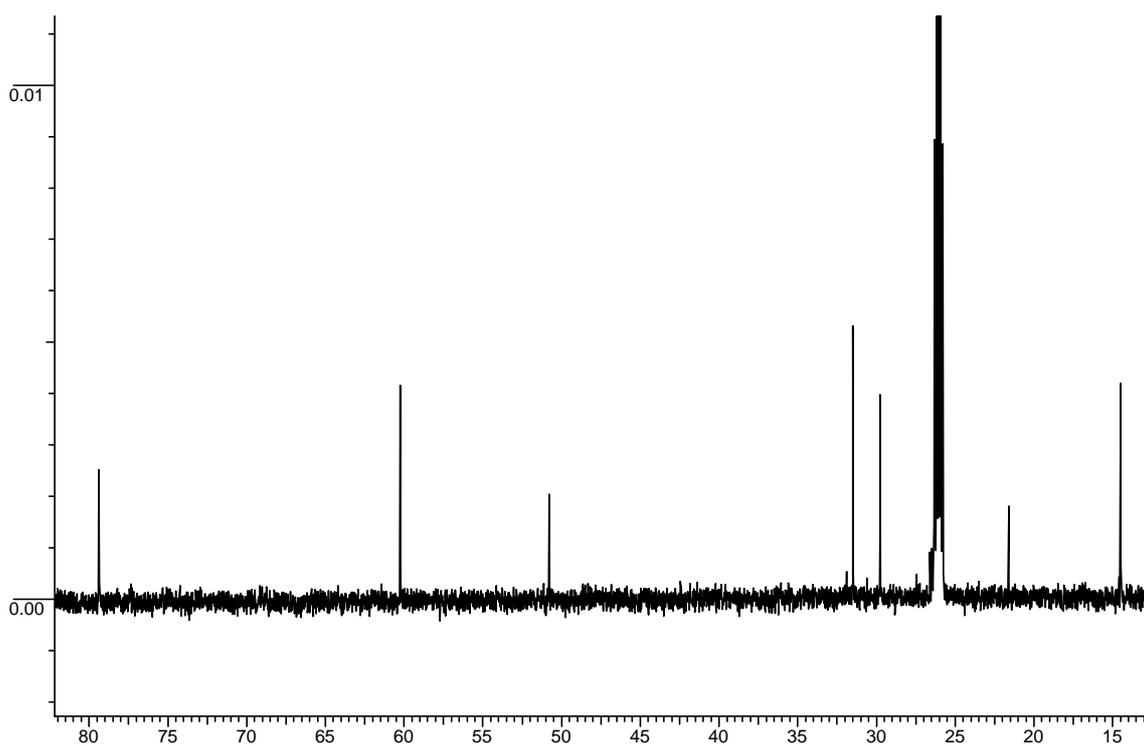
H-C HSQC 2D NMR spectrum of **1e**.



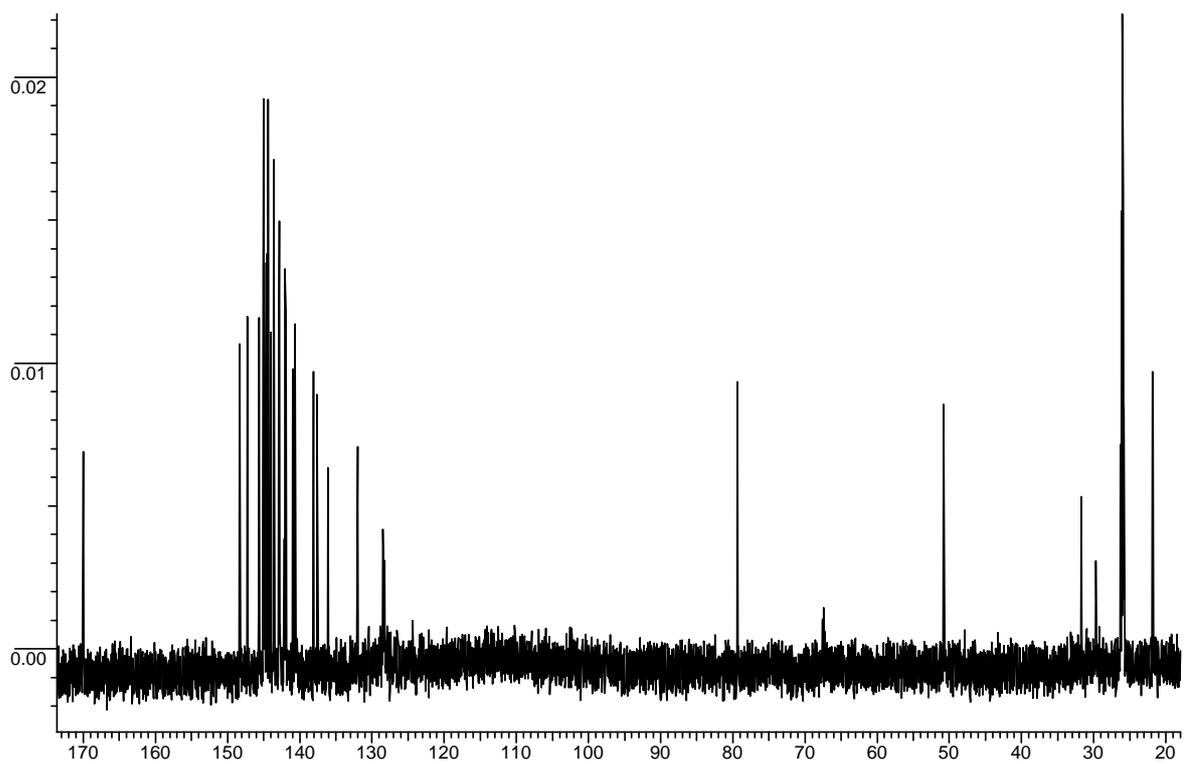
The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of **1a**.



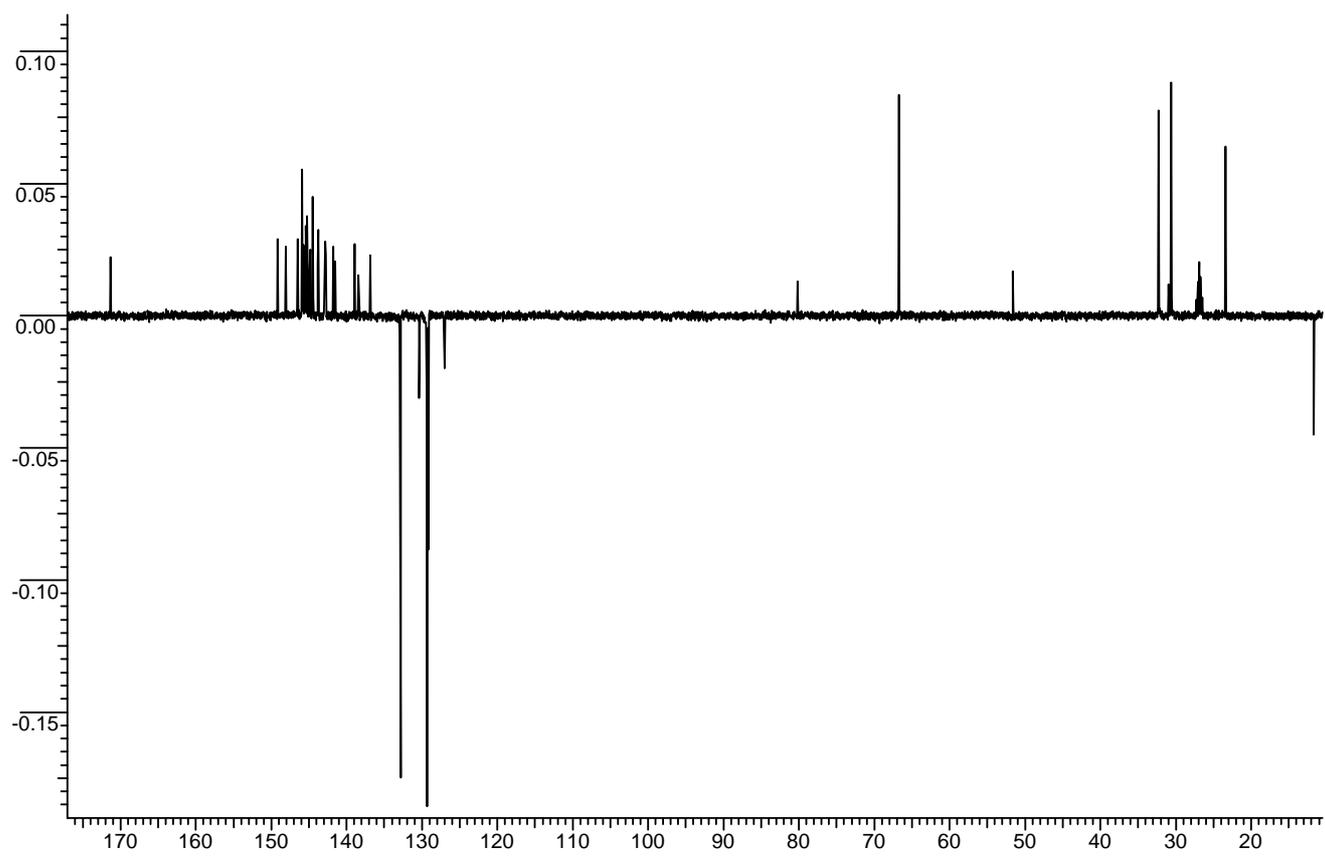
Low field part of the  $^{13}\text{C}$  NMR spectrum of **1b**



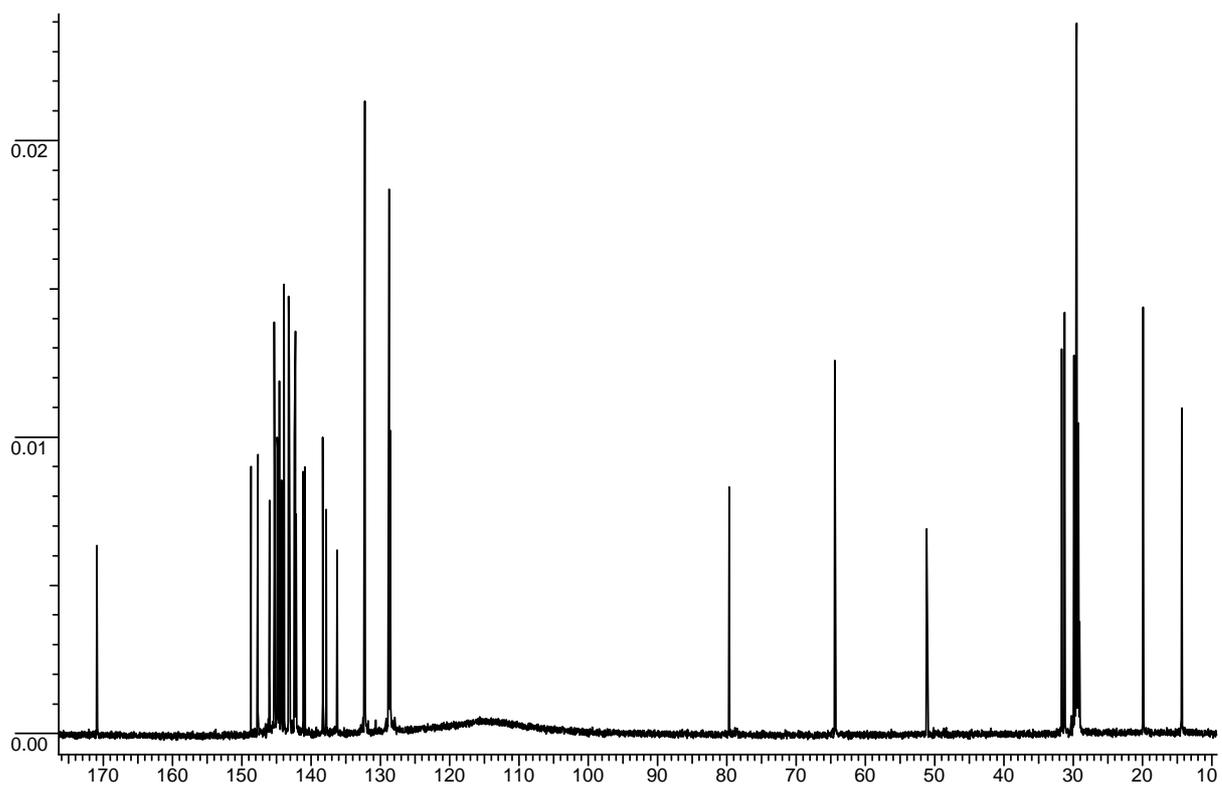
High field part of the  $^{13}\text{C}$  NMR spectrum of **1b**.



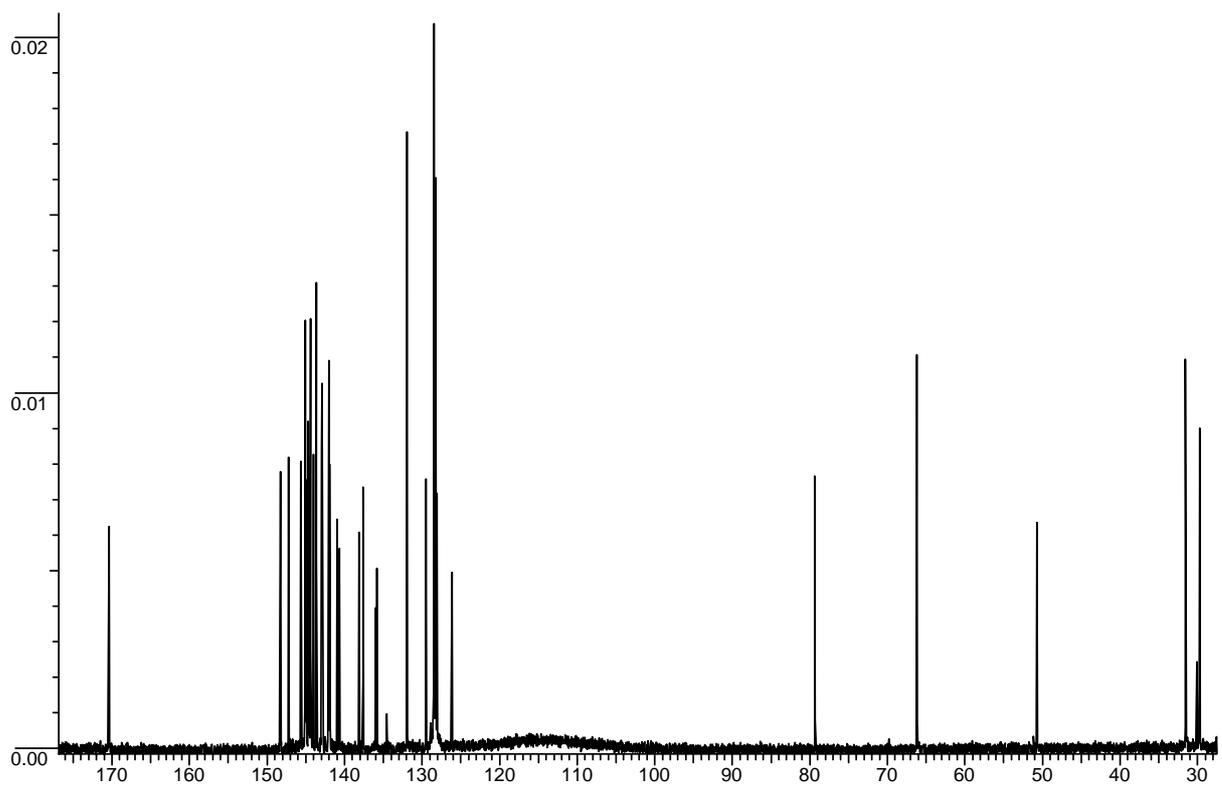
The  $^{13}\text{C}$  NMR spectrum of **1c**.



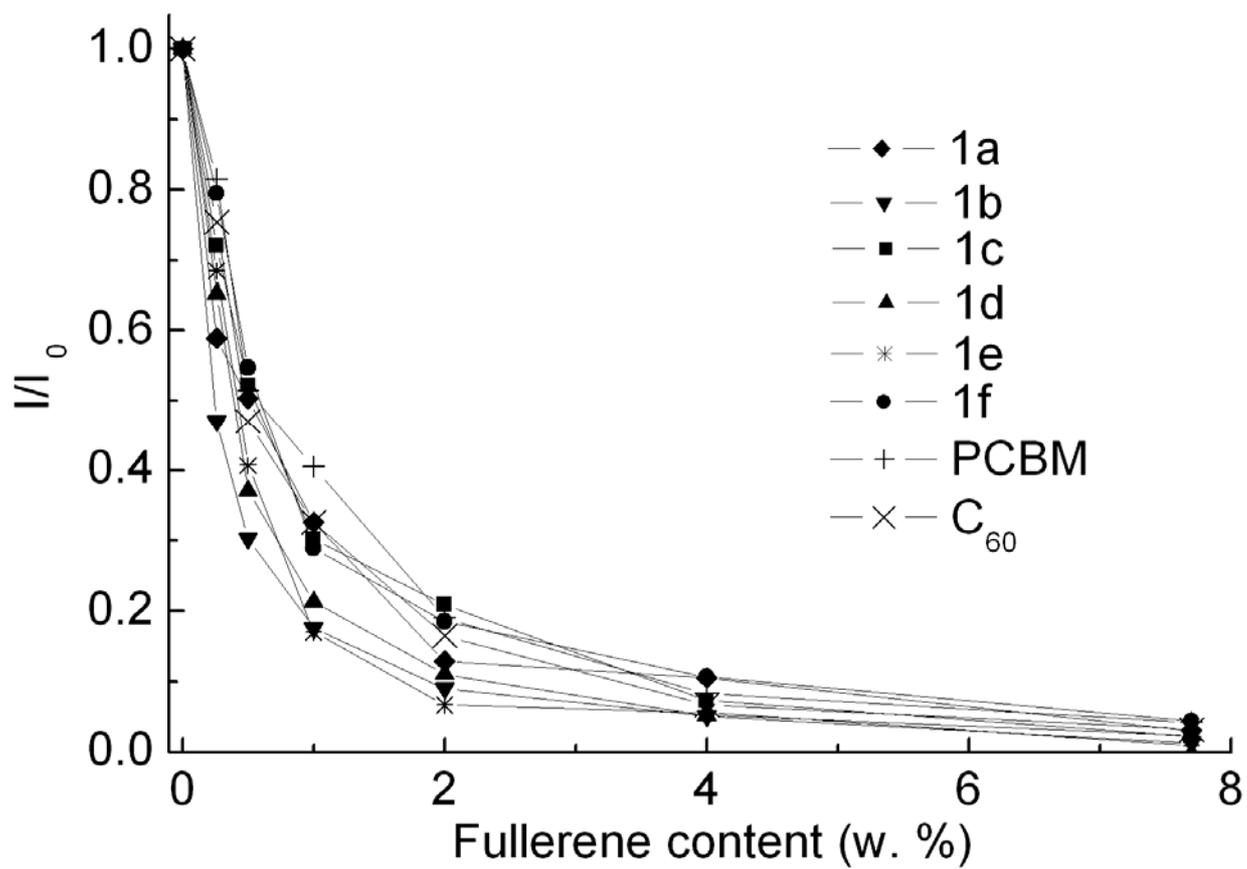
The  $^{13}\text{C}$  NMR spectrum of **1d**.



The  $^{13}\text{C}$  NMR spectrum of **1e**.



The  $^{13}\text{C}$  NMR spectrum of **1f**.



The quenching rates of the MDMO-PPV photoluminescence (585 nm band) for different fullerene compounds.