

# Supporting Information

for

## **Tuning the interactions between electron spins in fullerene-based triad systems**

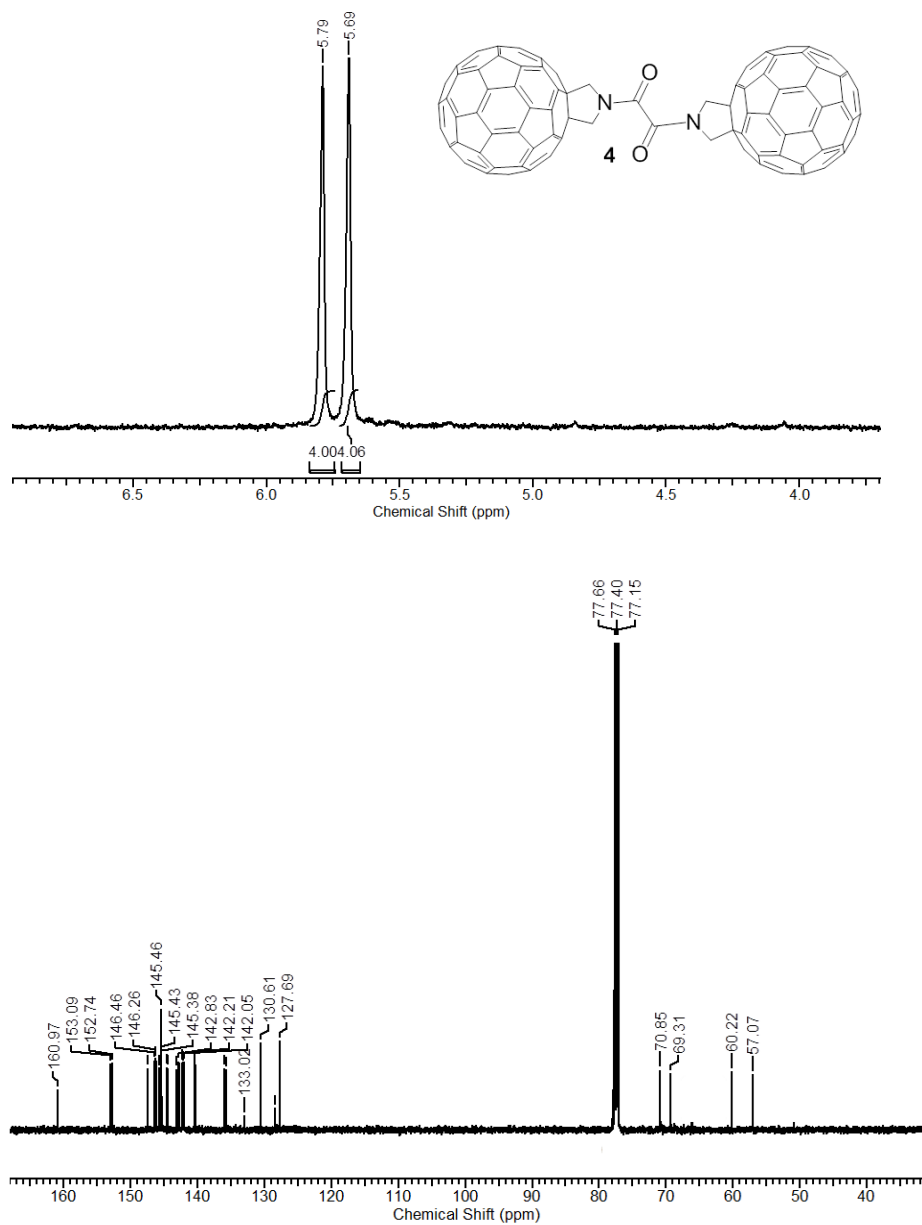
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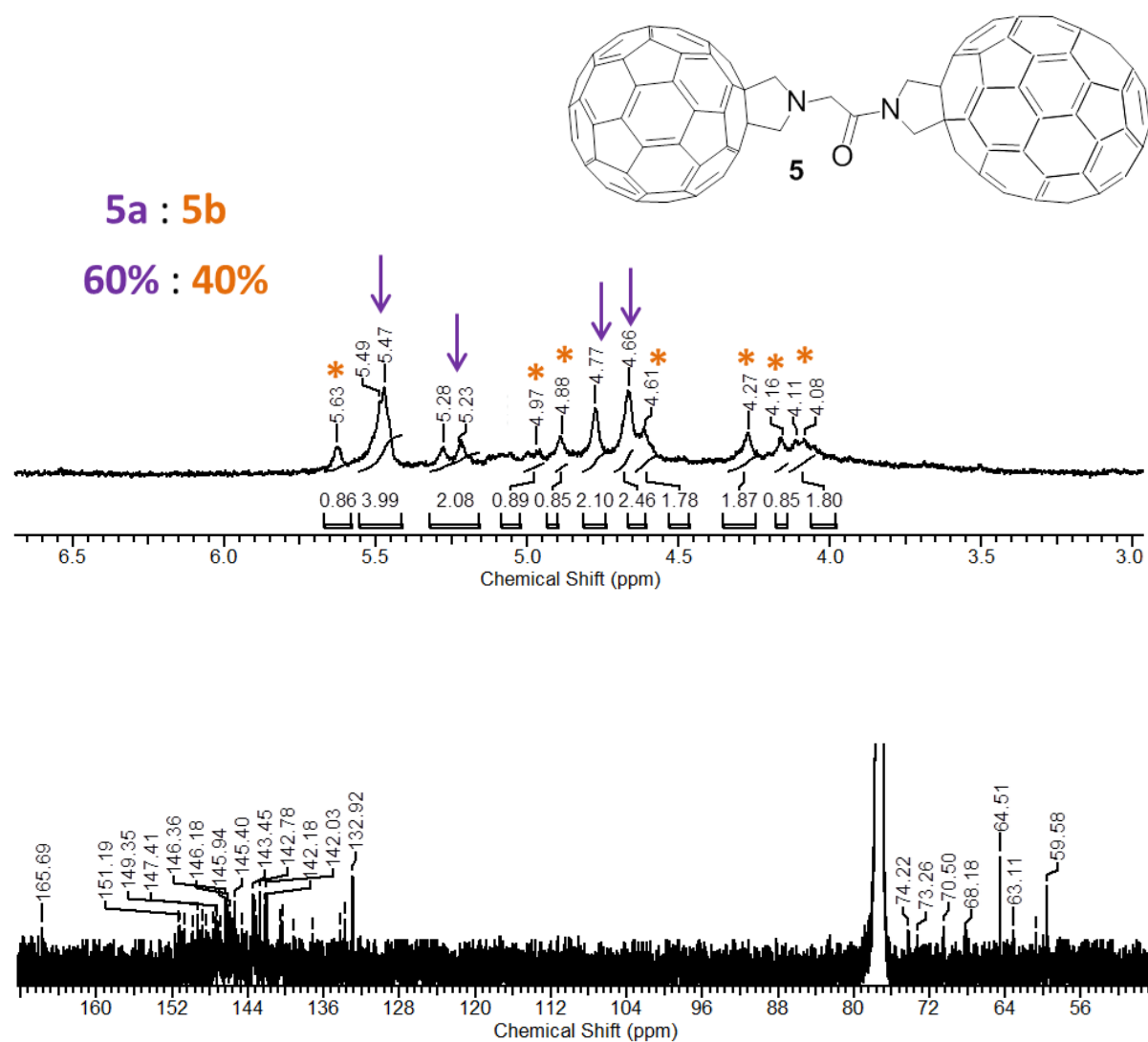
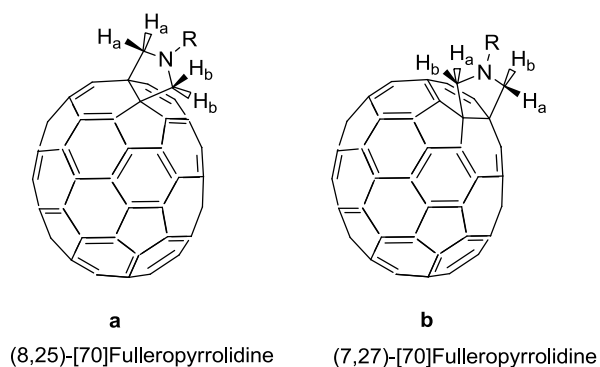
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## **Additional spectra**

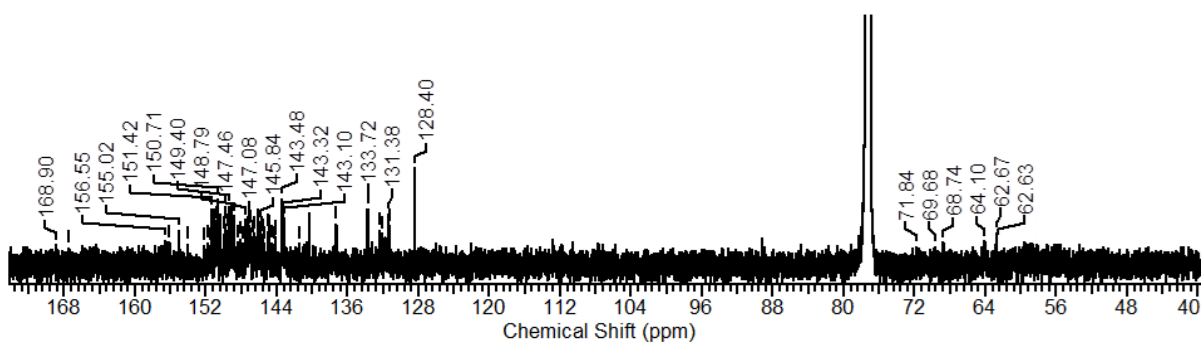
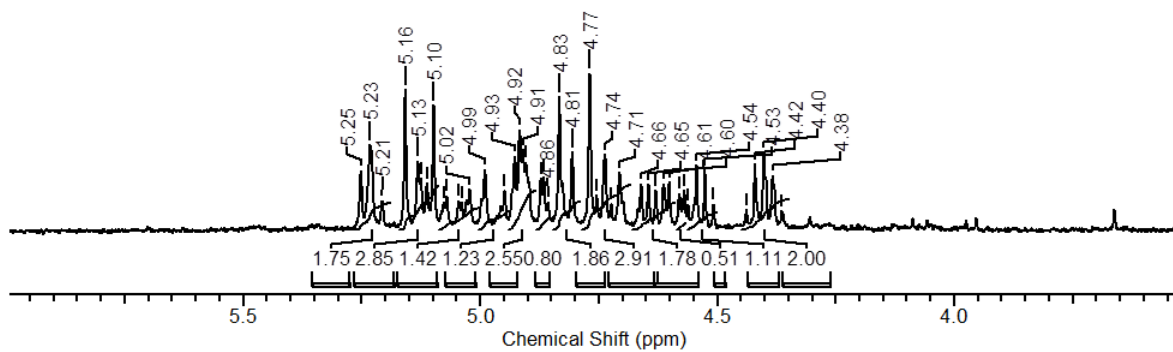
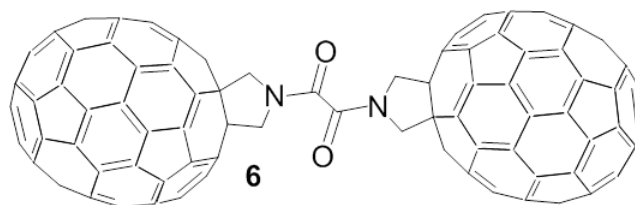


**Figure S1:**  $^1\text{H}$  (top) and  $^{13}\text{C}$  (bottom) NMR spectra of triad **4**. Spectra were recorded in a 1:1 mixture of  $\text{CS}_2$  and  $\text{CDCl}_3$ .

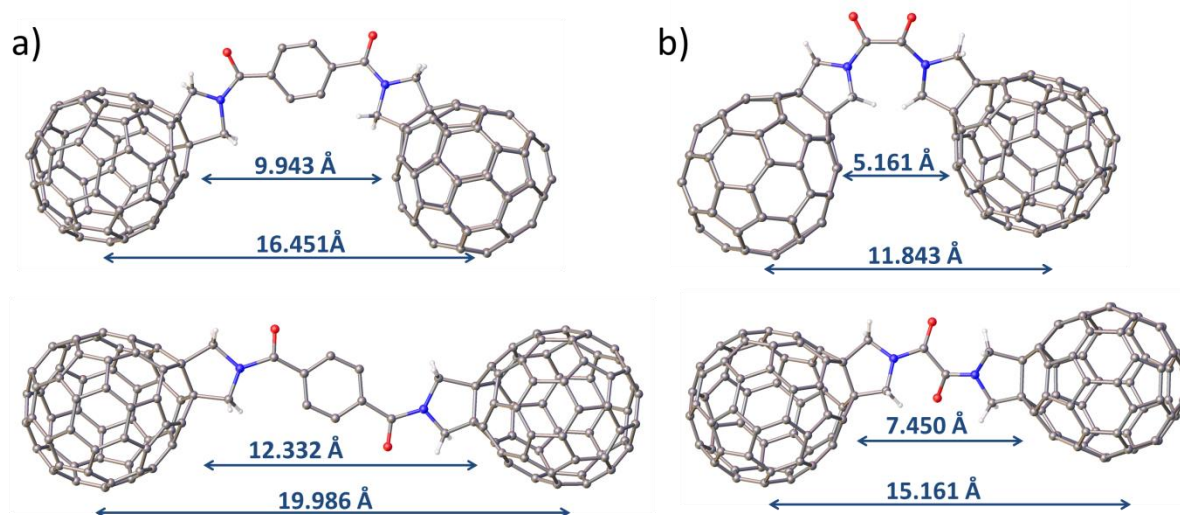


**Figure S2:** Views of (8,25) (**a**) and (7,22) (**b**) regioisomers of functionalised C<sub>70</sub> (top) and <sup>1</sup>H NMR (middle) and <sup>13</sup>C NMR (bottom) spectra of triad **5**. The spectra were recorded in a mixture of CS<sub>2</sub> and CDCl<sub>3</sub>.

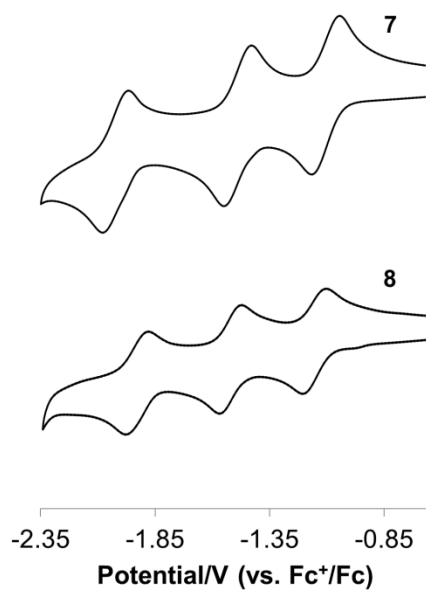
6aa : 6bb : 6ab



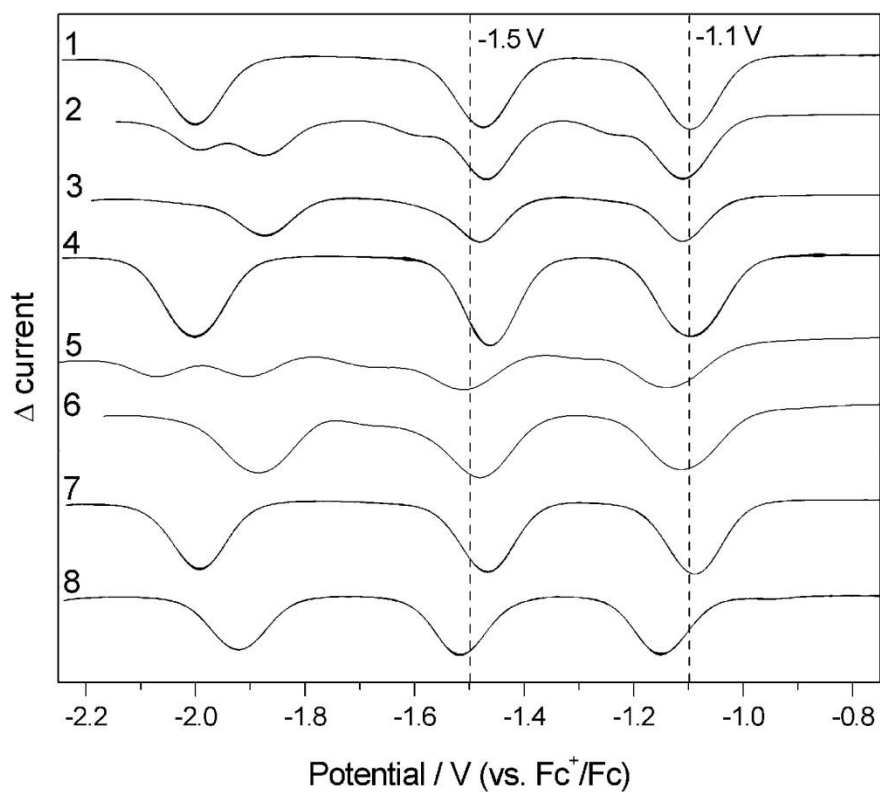
**Figure S3:**  $^1\text{H}$  NMR (top) and  $^{13}\text{C}$  NMR (bottom) spectra of triad **6**. The spectra were recorded in a mixture of  $\text{CS}_2$  and  $\text{CDCl}_3$ .



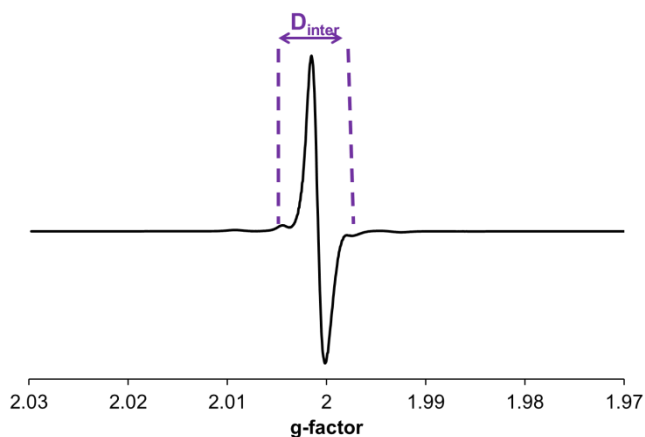
**Figure S4:** Views of shortest (top) and longest (bottom) possible conformations of fullerene dimers **1** (a) and **4** (b) showing the shortest distances between the fullerene cages and the centre-to-centre distances.



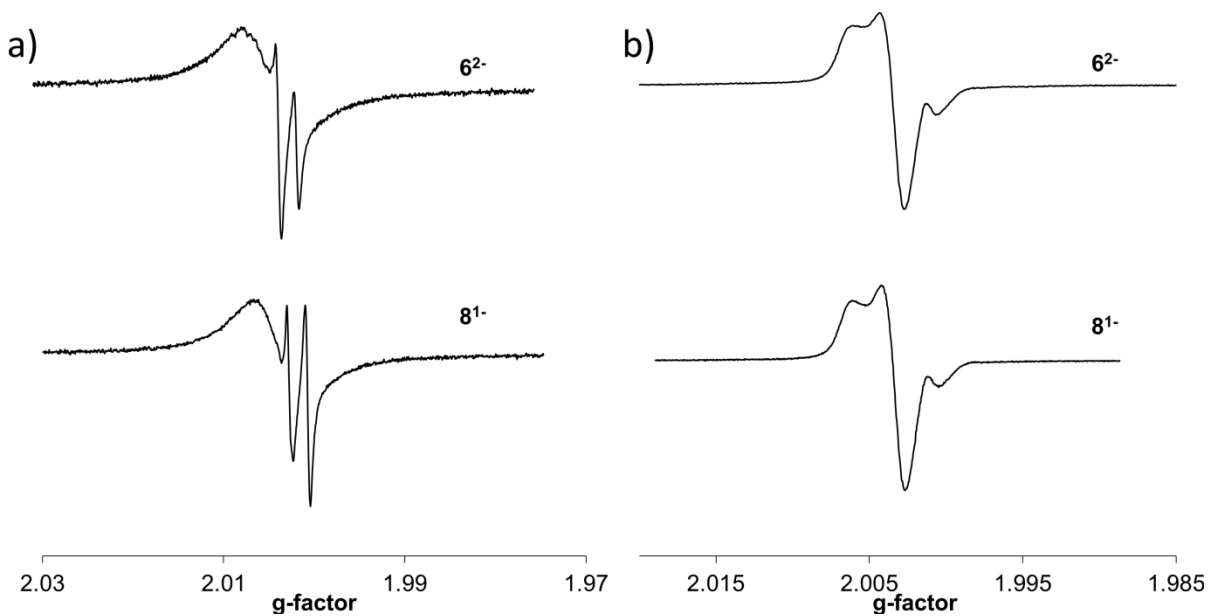
**Figure S5:** Cyclic voltammograms of **7** (top) and **8** (bottom). Scans were recorded as 0.5 mM solutions in *o*-dichlorobenzene containing 0.2 M [*n*-Bu<sub>4</sub>N][BF<sub>4</sub>] as the supporting electrolyte at a scan rate of 100 mV.



**Figure S6:** Square wave voltammograms of **1–8**. Scans were recorded as 0.5 mM solutions in *o*-dichlorobenzene containing 0.2 M [*n*-Bu<sub>4</sub>N][BF<sub>4</sub>] as the supporting electrolyte.



**Figure S7:** Frozen solution EPR spectrum of  $7^{1-}$  recorded at 77 K showing the central feature corresponding to the  $C_{60}^-$  and features with  $D = 9$  G corresponding to the intermolecular, or “powder” triplet. Additional small features are noted in the spectrum. The origin of these features is unclear but may result from an unidentified triplet ( $D = 26$  G).



**Figure S8:** Fluid solution EPR spectra recorded at room temperature (a) and frozen solution EPR spectra recorded at 77 K (b) for  $6^{2-}$  and  $8^{1-}$ .