

Supporting Information

Tuning the Interactions between Electron Spins in Fullerene-Based Triad Systems

Maria A. Lebedeva,^a Thomas W. Chamberlain,^a E. Stephen Davies,^a Bradley E. Thomas,^a Martin Schröder^a and Andrei N. Khlobystov*^{a,b}

^aSchool of Chemistry, University of Nottingham, Nottingham, NG7 2RD, UK

^bNottingham Nanoscience & Nanotechnology Centre, University of Nottingham, University Park, Nottingham, NG7 2RD, UK

1. ^1H and ^{13}C NMR spectra of fullerene dimers **4-6**.

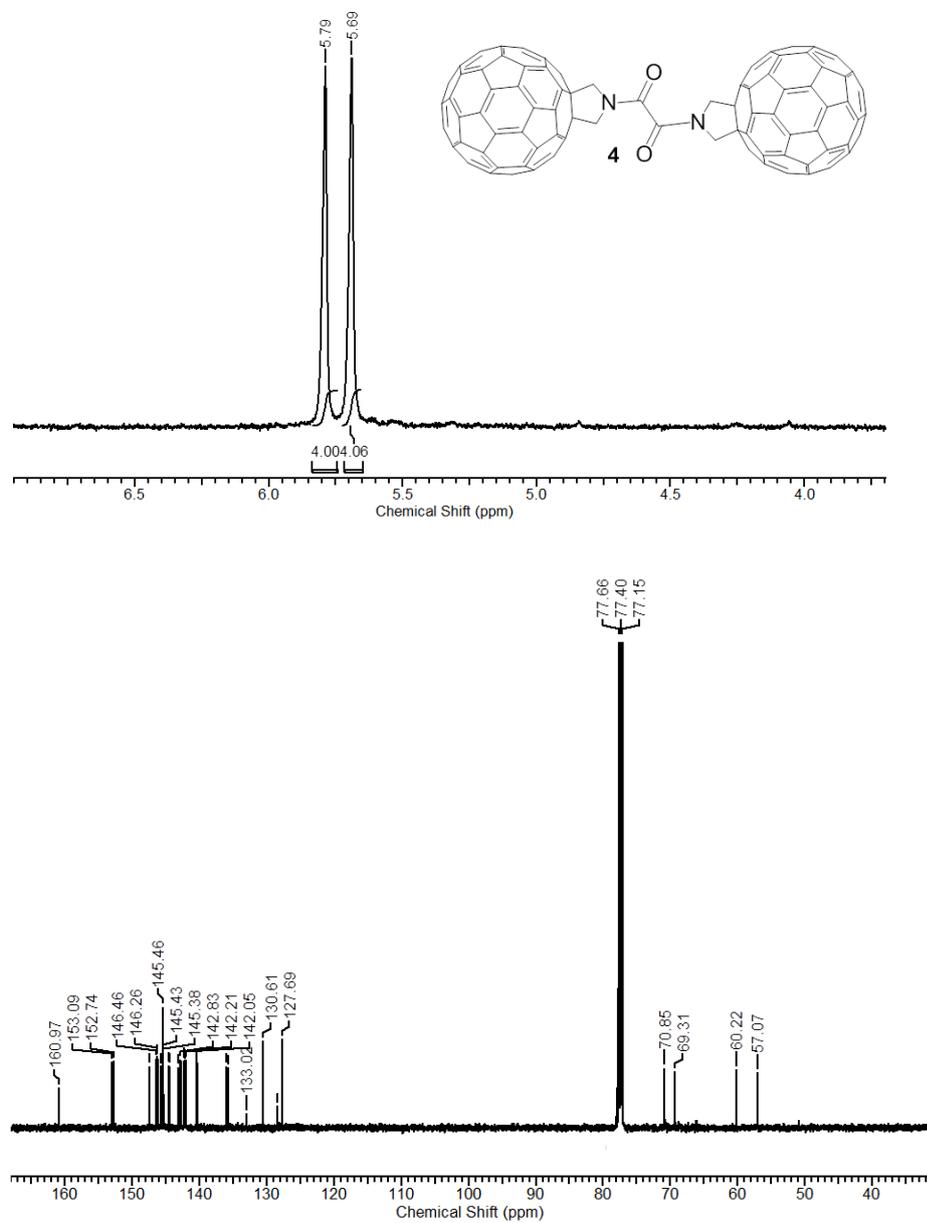


Figure S1. ^1H (top) and ^{13}C (bottom) NMR spectra of triad **4**. Spectra were recorded in a 1:1 mixture of CS_2 and CDCl_3 .

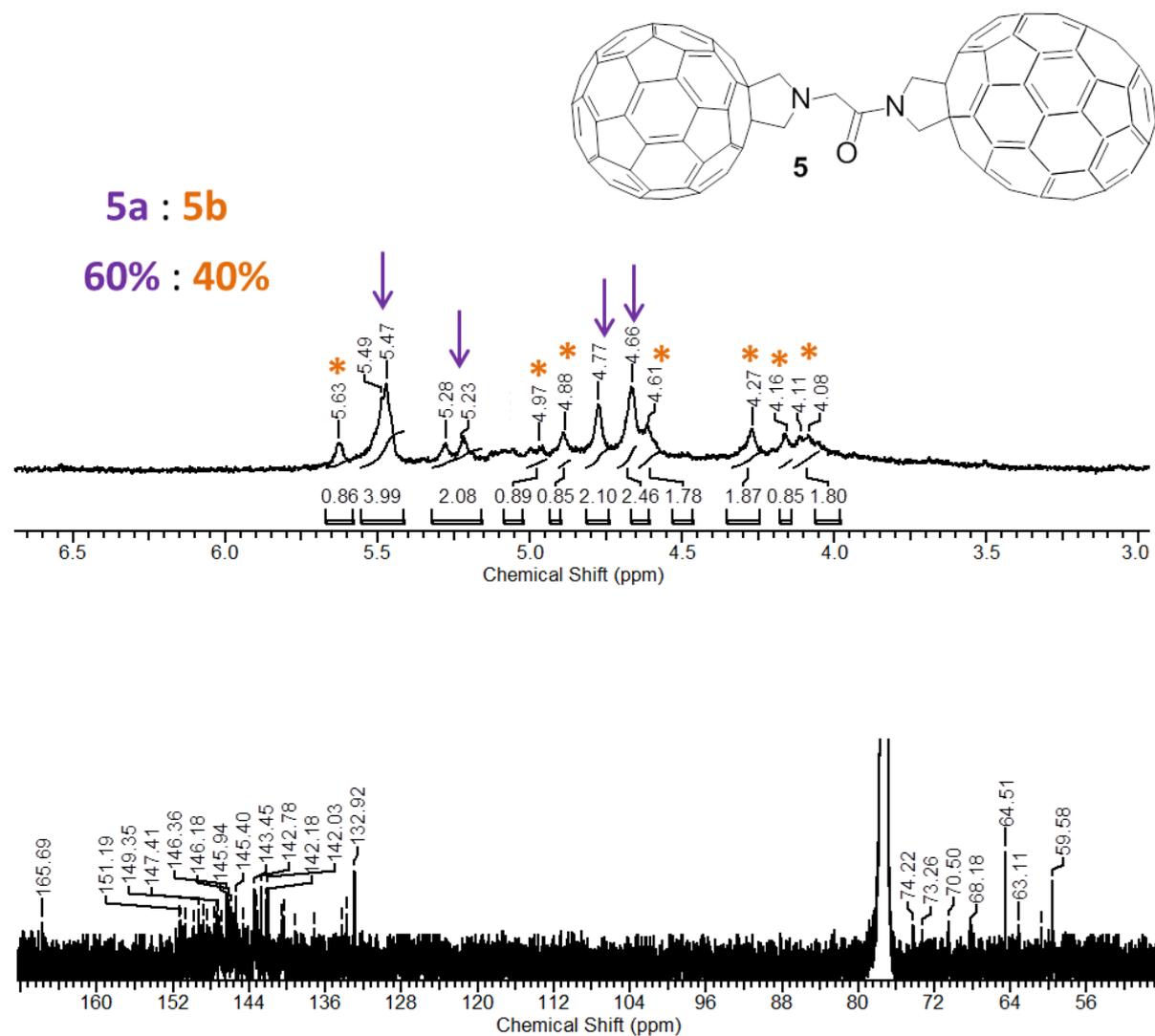
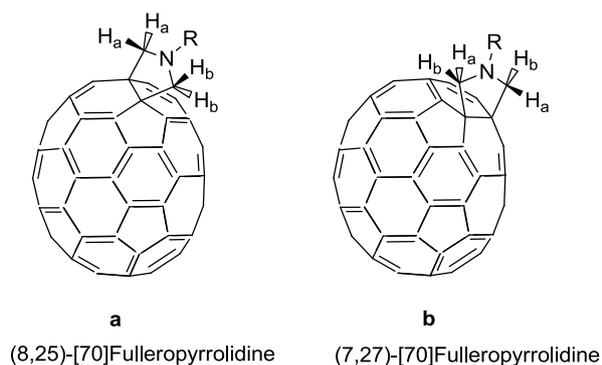


Figure S2. Views of (8,25) (**a**) and (7,22) (**b**) regio isomers of functionalised C₇₀ (top) and ¹H NMR (middle) and ¹³C NMR (bottom) spectra of triad **5**. The spectra were recorded in a mixture of CS₂ and CDCl₃.

6aa : **6bb** : **6ab**

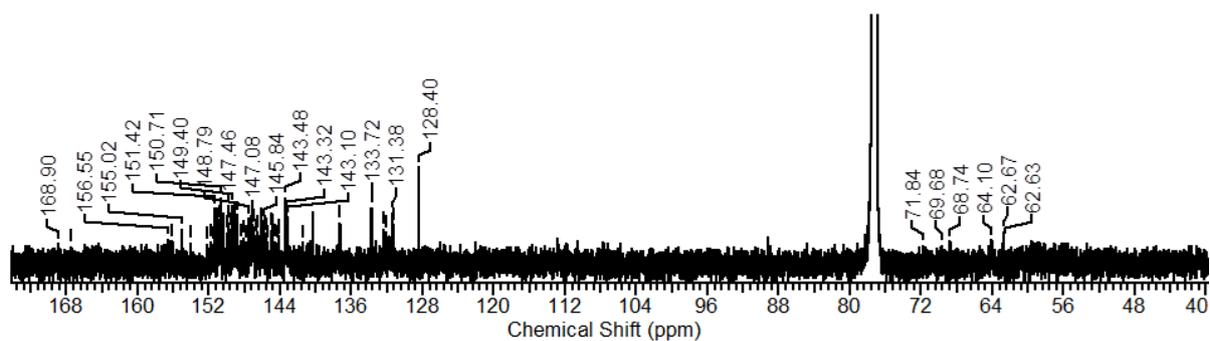
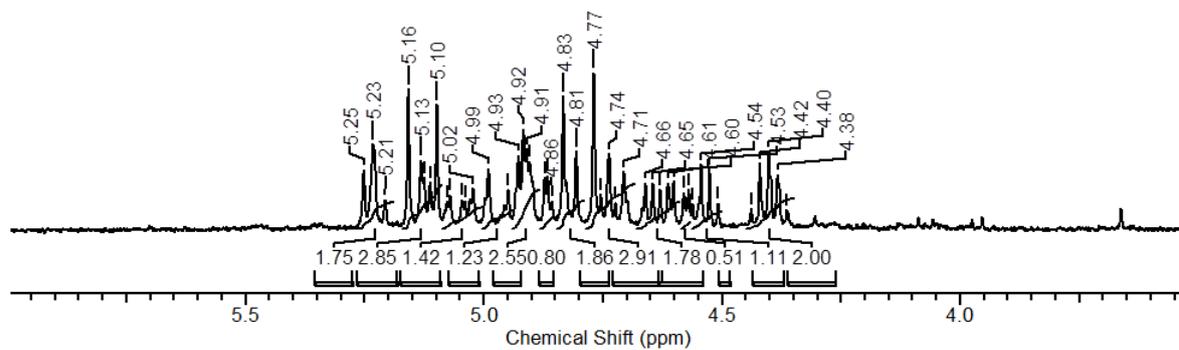
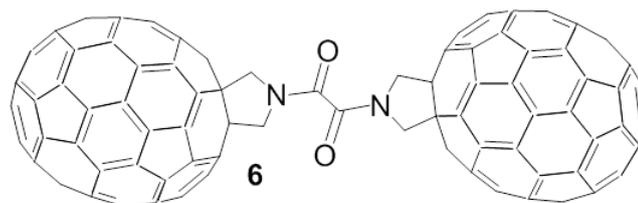


Figure S3. ¹H NMR (top) and ¹³C NMR (bottom) spectra of triad **6**. The spectra were recorded in a mixture of CS₂ and CDCl₃.

2. Geometry of fullerene dimers **1** and **4**.

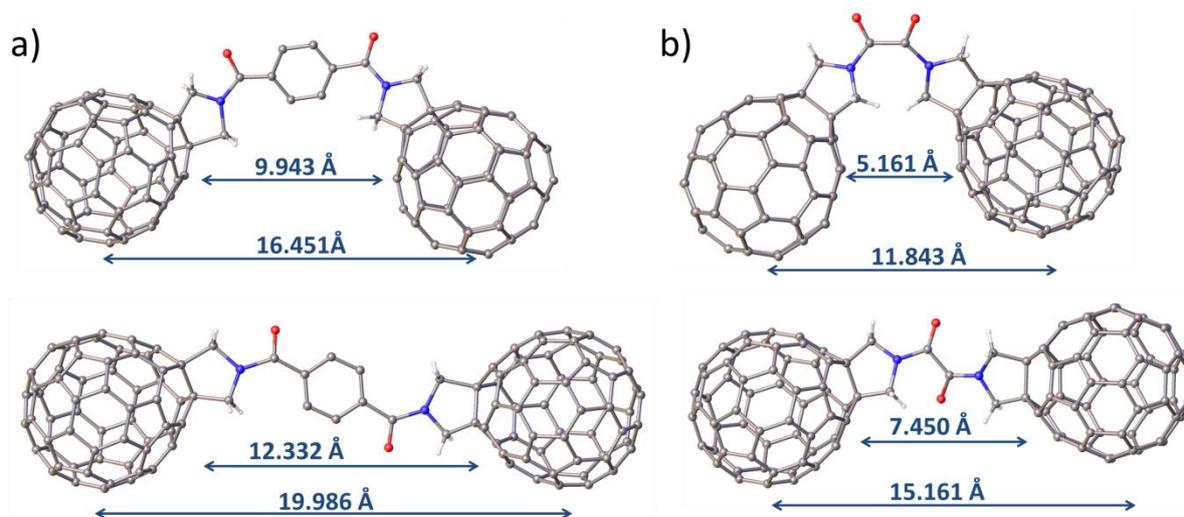


Figure S4. Views of shortest (top) and longest (bottom) possible conformations of fullerene dimers **1** (a) and **4** (b) showing the shortest distances between the fullerene cages and the centre-to-centre distances.

3. Cyclic voltammetry of **7** and **8**.

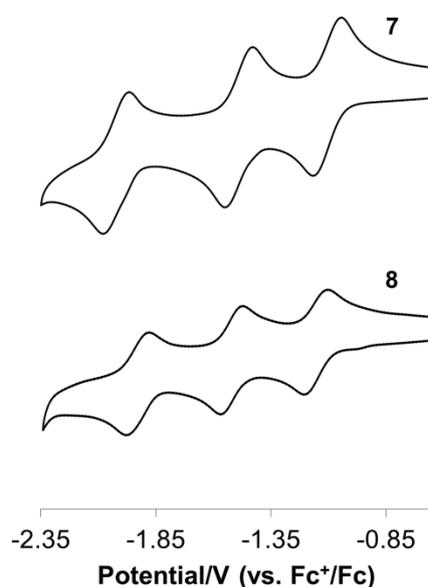


Figure S5. Cyclic voltammograms of **7** (top) and **8** (bottom). Scans were recorded as 0.5 mM solutions in *o*-dichlorobenzene containing 0.2 M [nBu₄N][BF₄] as the supporting electrolyte at a scan rate of 100 mV.

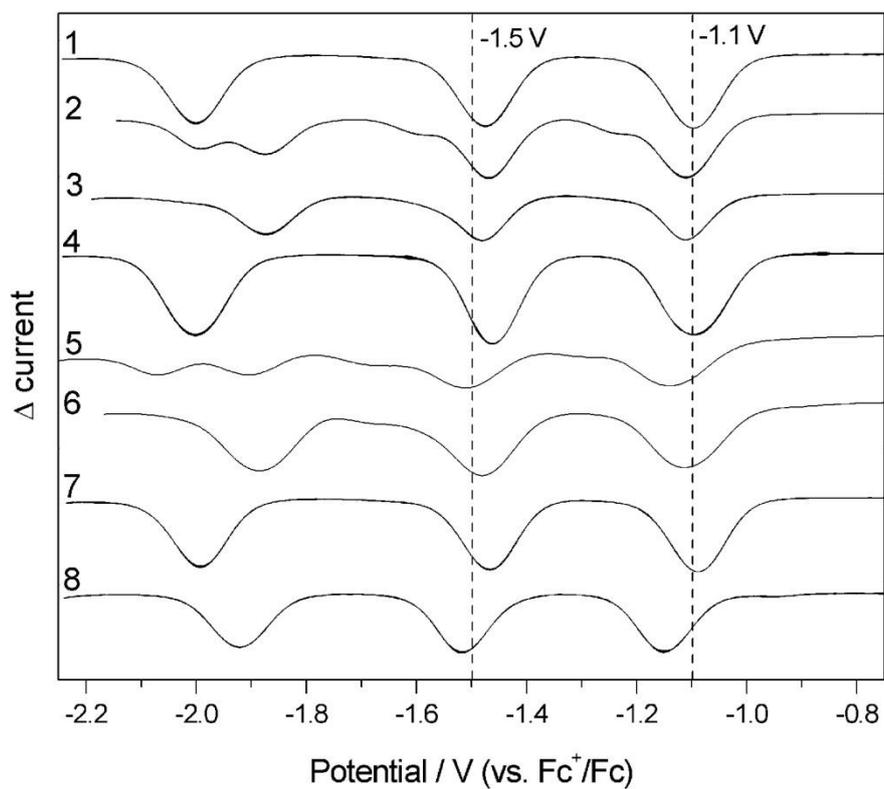


Figure S6. Square wave voltammograms of **1** - **8**. Scans were recorded as 0.5 mM solutions in *o*-dichlorobenzene containing 0.2 M [ⁿBu₄N][BF₄] as the supporting electrolyte.

4. EPR spectra for compound 7^{1-} .

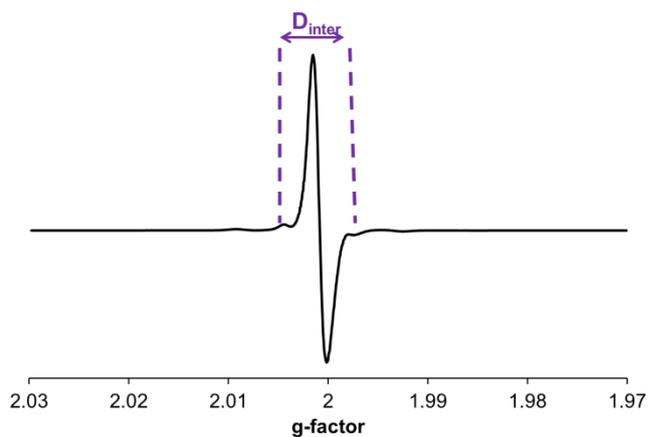


Figure S7. Frozen solution EPR spectrum of 7^{1-} recorded at 77 K showing the central feature corresponding to the C_{60}^- and features with $D = 9$ G corresponding to the intermolecular, or “powder” triplet. Additional small features are noted in the spectrum. The origin of these features is unclear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

5. EPR spectra for C_{70} containing triad **6** and precursor **8**.

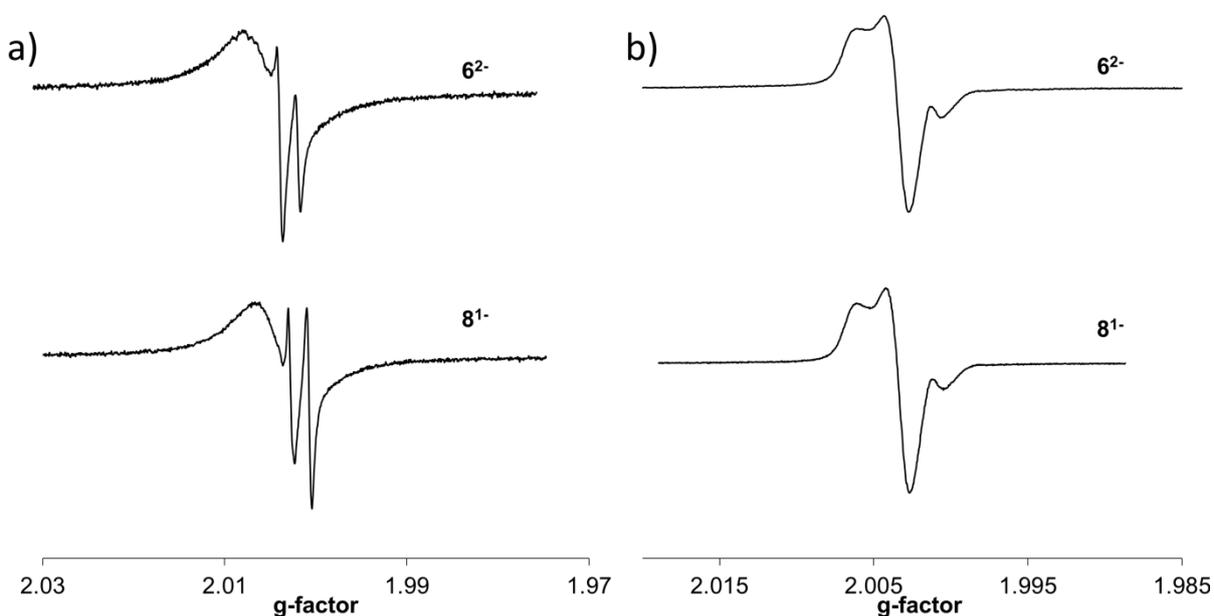


Figure S8. Fluid solution EPR spectra recorded at room temperature (a) and frozen solution EPR spectra recorded at 77 K (b) for 6^{2-} and 8^{1-} .