

Supplementary Materials: Effects of Introducing Methoxy Groups into the Ancillary Ligands in Bis(diimine) Copper(I) Dyes for Dye-Sensitized Solar Cells

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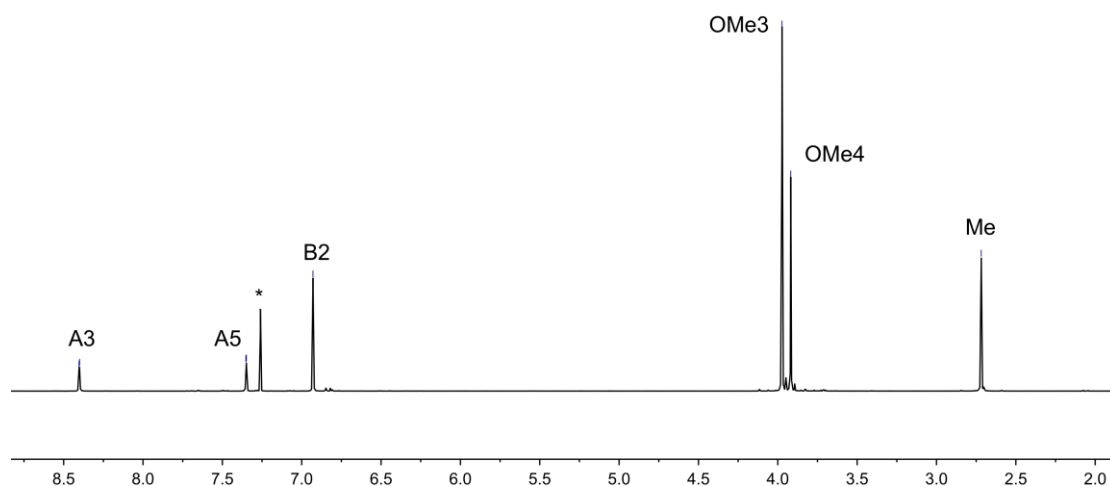


Figure S1. 500 MHz ^1H NMR spectrum of **4** (CDCl_3). * = residual CHCl_3 . Chemical shifts in δ/ppm . See Scheme 1 for labelling.

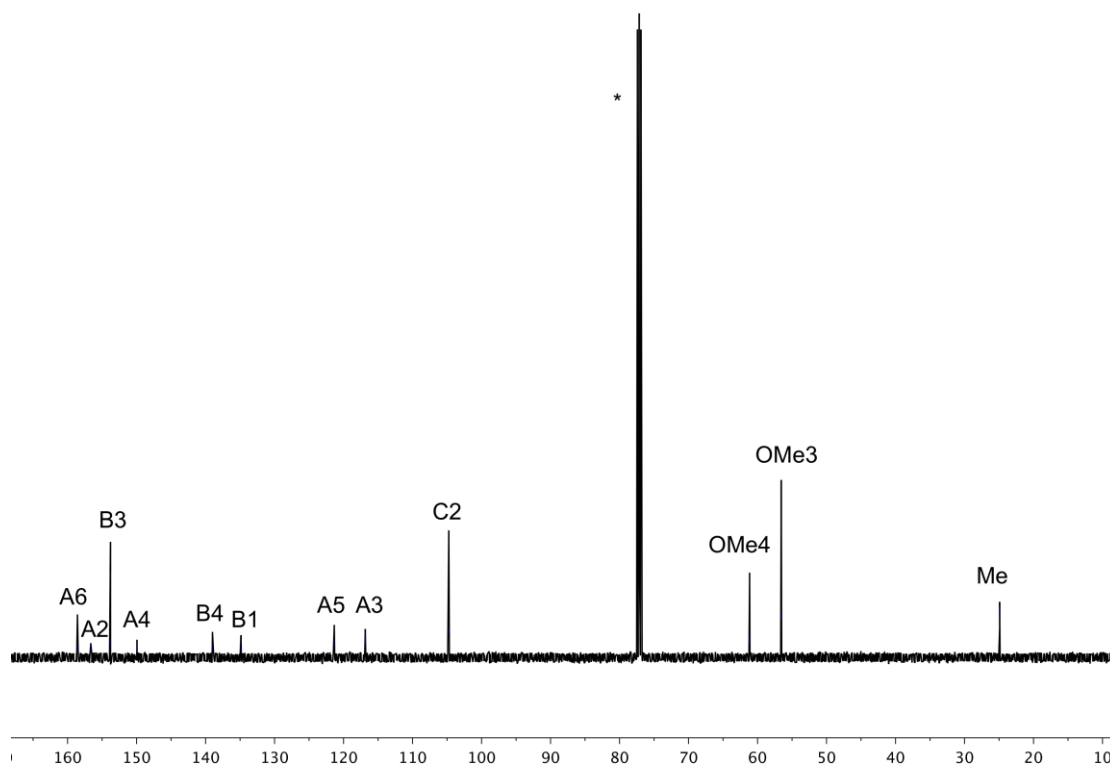


Figure S2. 126 MHz ^{13}C NMR spectrum of **4** (CDCl_3^*). Chemical shifts in δ/ppm . See Scheme 1 for labelling.

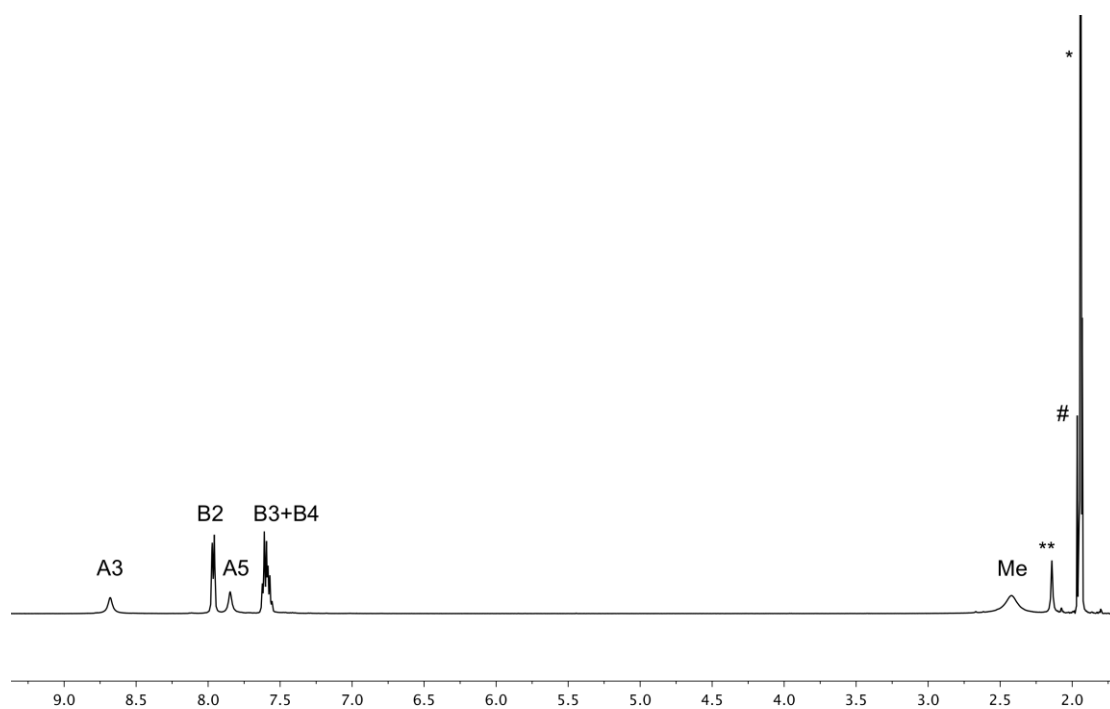


Figure S3. 500 MHz ^1H NMR spectrum of $[\text{Cu}(\mathbf{1})_2][\text{PF}_6]$ (CD_3CN). * = residual CHD_2CN ; # = CH_3CN ; ** = H_2O). Chemical shifts in δ/ppm . See Scheme 1 for labelling.

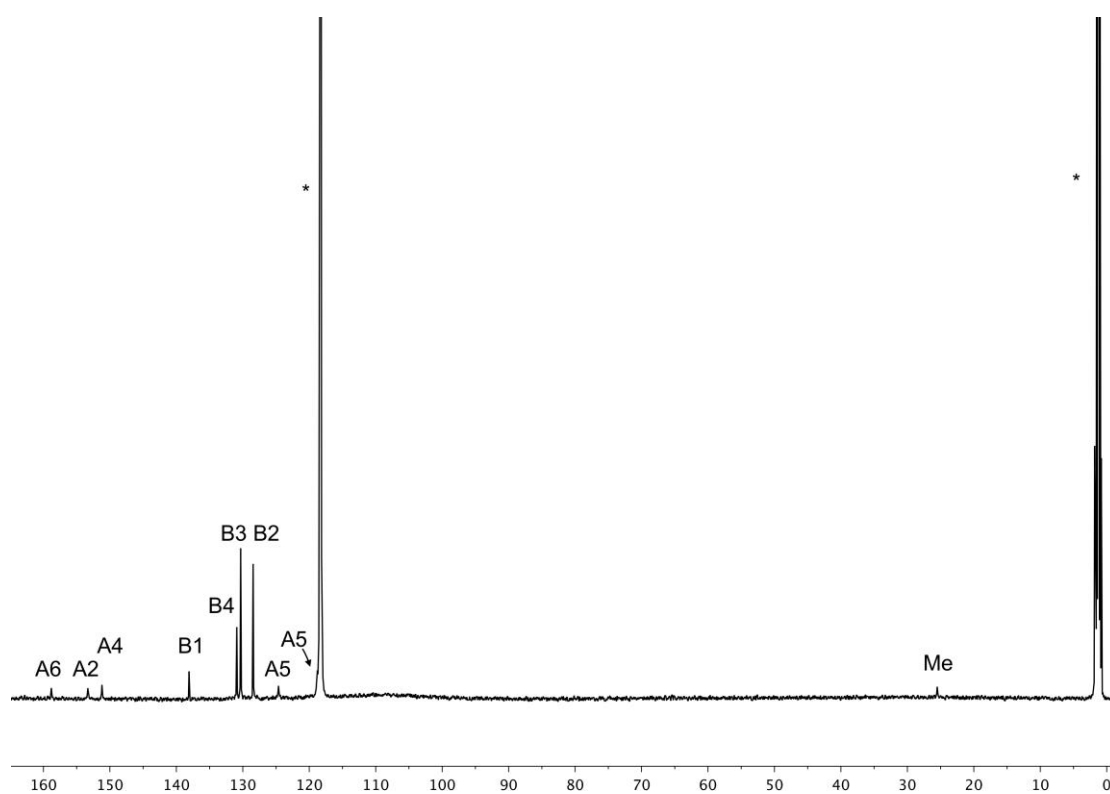


Figure S4. 126 MHz ^{13}C NMR spectrum of $[\text{Cu}(\mathbf{1})_2][\text{PF}_6]$ (CD_3CN^*). Chemical shifts in δ/ppm . See Scheme 1 for labelling.

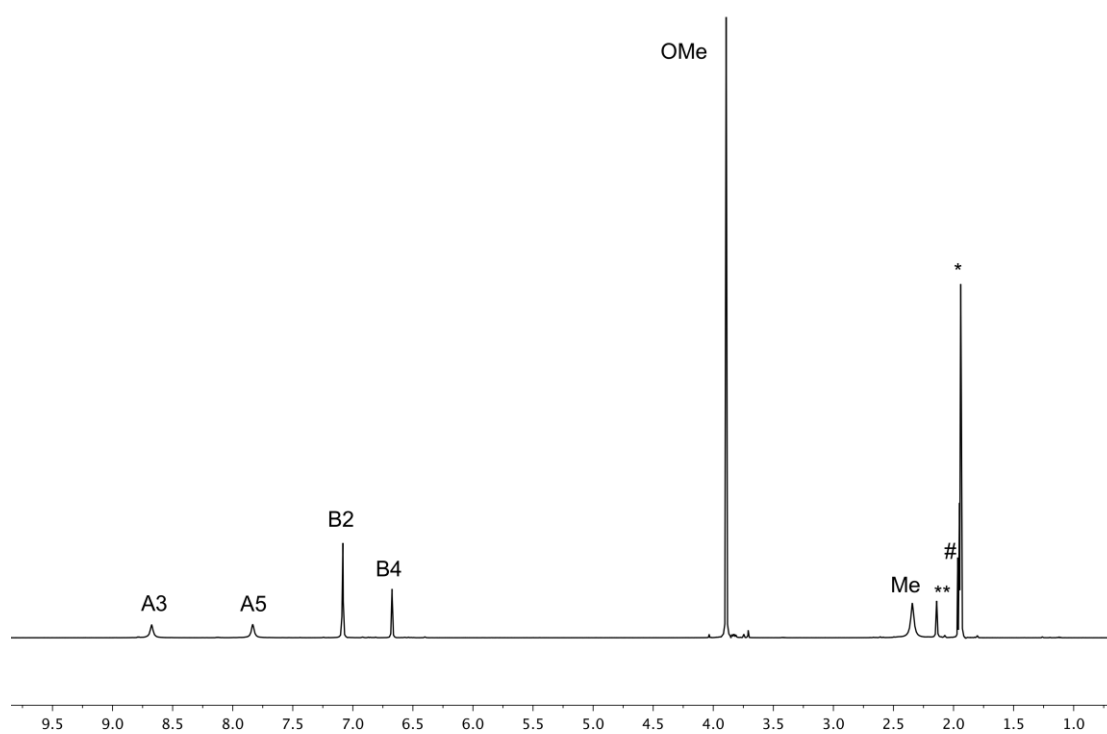


Figure S5. 500 MHz ^1H NMR spectrum of $[\text{Cu}(\mathbf{3})_2][\text{PF}_6]$ (CD_3CN). * = residual CHD_2CN ; # = CH_3CN ; ** = H_2O). Chemical shifts in δ/ppm . See Scheme 1 for labelling.

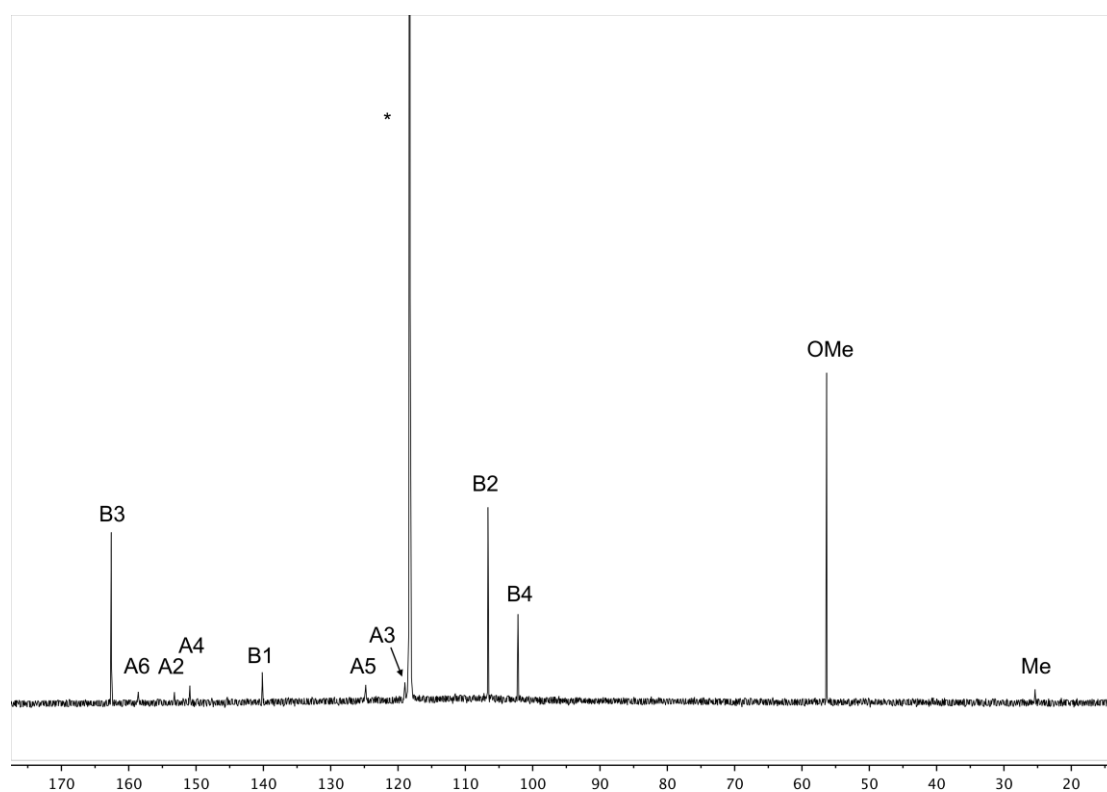


Figure S6. 126 MHz ^{13}C NMR spectrum of $[\text{Cu}(\mathbf{3})_2][\text{PF}_6]$ (CD_3CN^*). Chemical shifts in δ/ppm . See Scheme 1 for labelling.

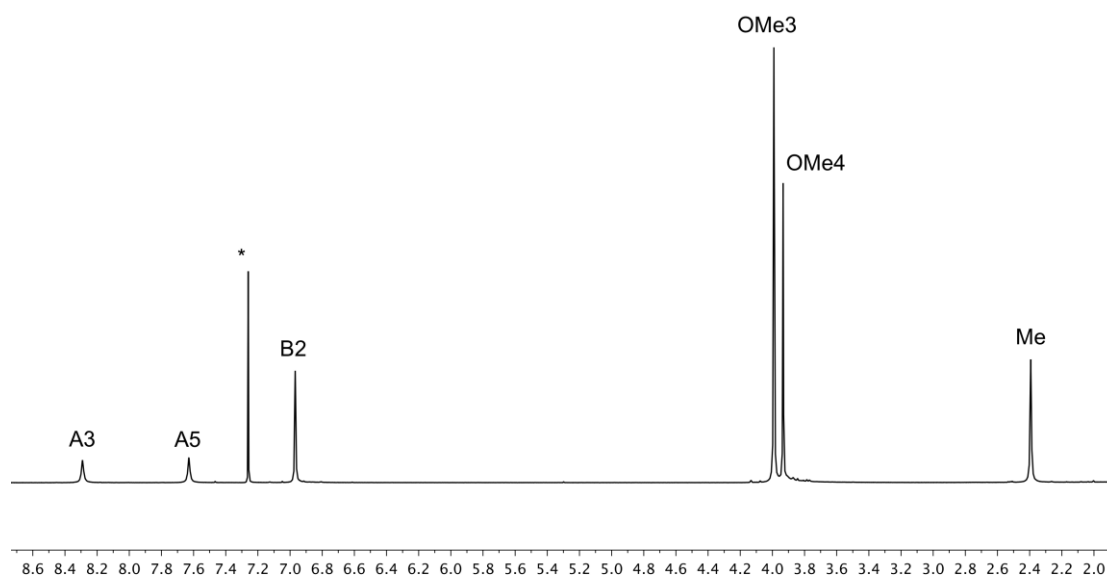


Figure S7. 500 MHz ^1H NMR spectrum of $[\text{Cu}(\mathbf{4})_2][\text{PF}_6]$ (CDCl_3). * = residual CHCl_3 . Chemical shifts in δ/ppm . See Scheme 1 for labelling.

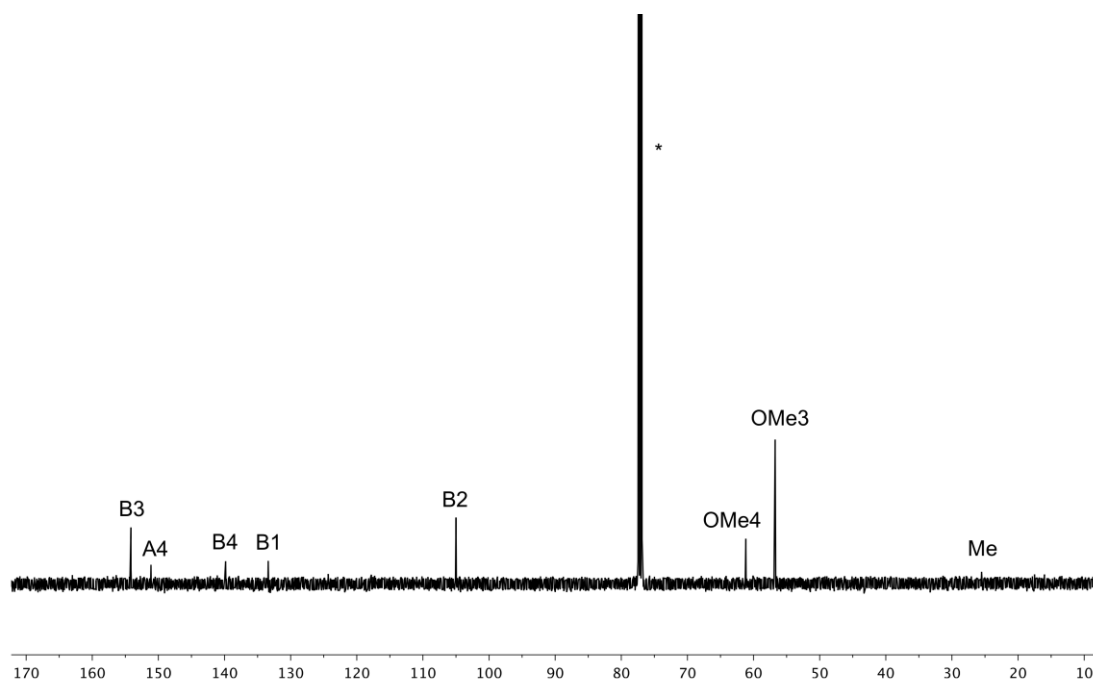


Figure S8. 126 MHz ^{13}C NMR spectrum of $[\text{Cu}(\mathbf{4})_2][\text{PF}_6]$ (CDCl_3^*). Chemical shifts in δ/ppm . See Scheme 1 for labelling. See also Figure S9.



Figure S9. (a) ESI mass spectrum of $[\text{Cu}(4)_2][\text{PF}_6]$; the base peak arises from the $[\text{M} - \text{PF}_6]^+$ ion. (b) Calculated isotope pattern for the base peak.