Electronic Supplementary Material (ESI) for Dalton Transactions

Electronic Supplementary Information for

First Application of the HETPHEN Concept to New Heteroleptic Bis(diimine) Copper(I) Complexes as Sensitisers in Dye Sensitized Solar Cells

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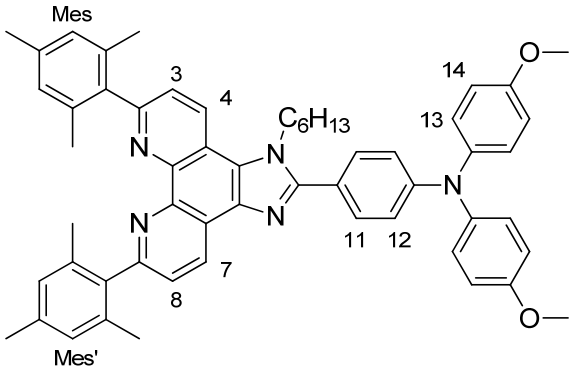
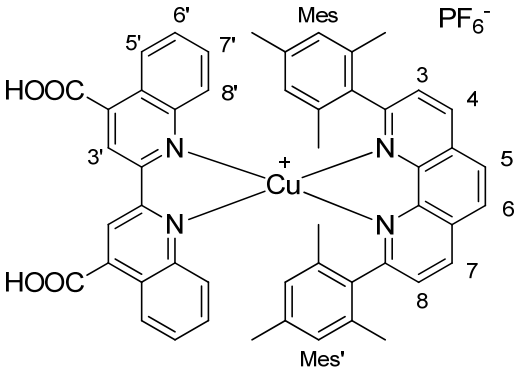
Hydrogen nuclei numbering for ^{1}H-NMR spectra assignment:

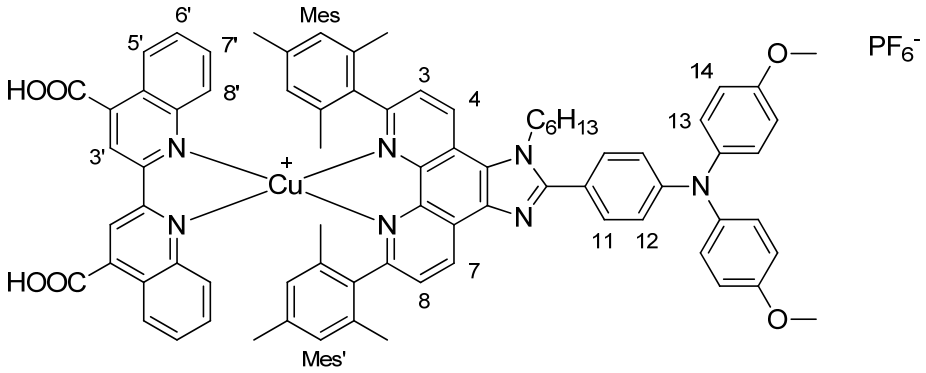
L1



C1



C2



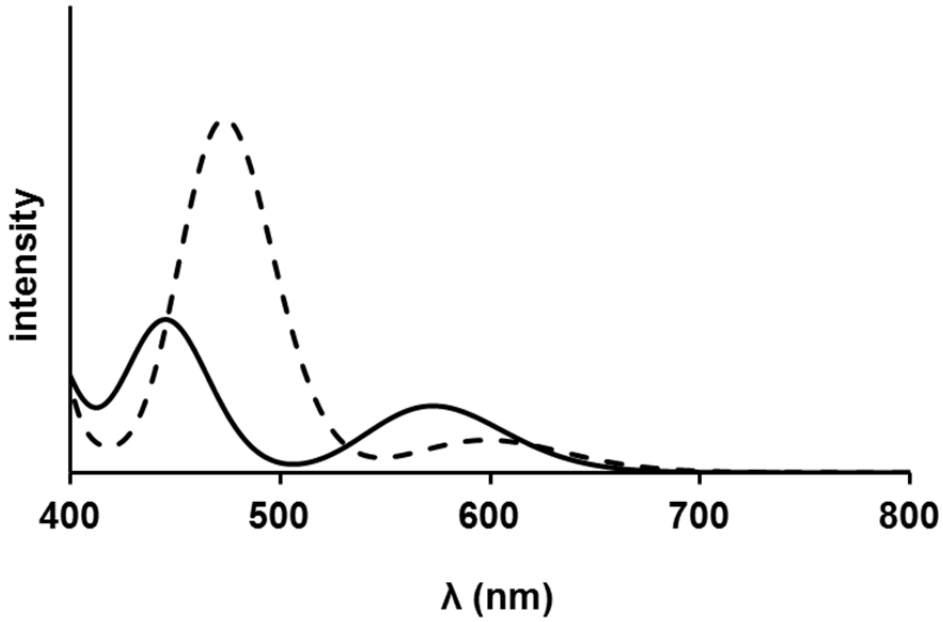


Figure S1. Simulated spectra for complexes **C1** (plain line) and **C2** (dashed line).

Complex	State	ΔE (nm)	F
C1	$MLCT_L$	562	0.03
	$MLCT_L/MLCT_{phen}$	440	0.06
	$MLCT_L/MLCT_{phen}$	372	0.04
	$MLCT_L$	369	0.03
	$MLCT_L/IL_L$	342	0.08
	$LLCT_L/MLCT_L$	334	0.07
	$IL_L/LLCT_L$	315	0.09
	$IL_L/LLCT_L/MLCT_L$	311	0.03
	$MLCT_{phen}/IL_{phen}$	308	0.13
	$IL_{phen}/MLCT_L$	306	0.04
C2	$MLCT_L$	472	0.16
	$IL_{phen}/MLCT_{phen}$	395	0.17
	IL_{phen}	361	0.70
	$LLCT_L/IL_L$	341	0.08
	$MLCT_{phen}/LLCT_L$	337	0.07
	$MLCT_{phen}/MLCT_L$	327	0.10
	$MLCT_{phen}/LLCT_L/IL_L$	327	0.15
	$LLCT_L/IL_L$	321	0.05
	$IL_{phen}/MLCT_{phen}$	319	0.63
	$MLCT_{phen}$	305	0.03

Table S1. Calculated UV-Visible transitions for complexes **C1** and **C2**. “L” denotes the anchoring $dcbqH_2$ ligand, while “phen” denotes the mesityl bearing phenanthroline ligand.

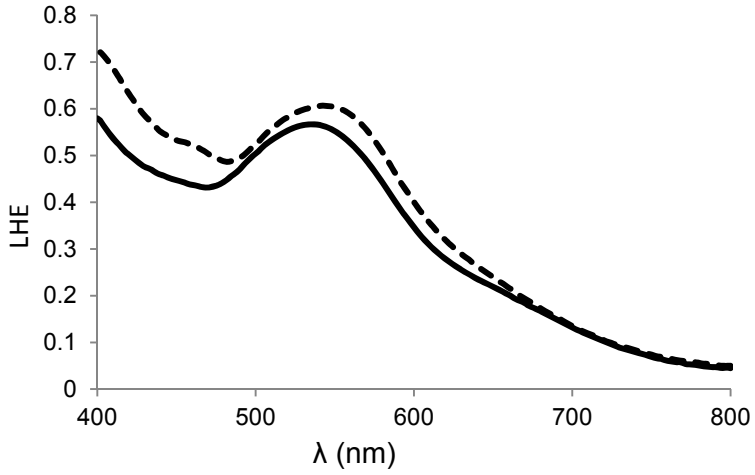


Figure S2. LHE of TiO_2 photo-electrodes sensitized by **C1** (plain line) and **C2** (dashed line).

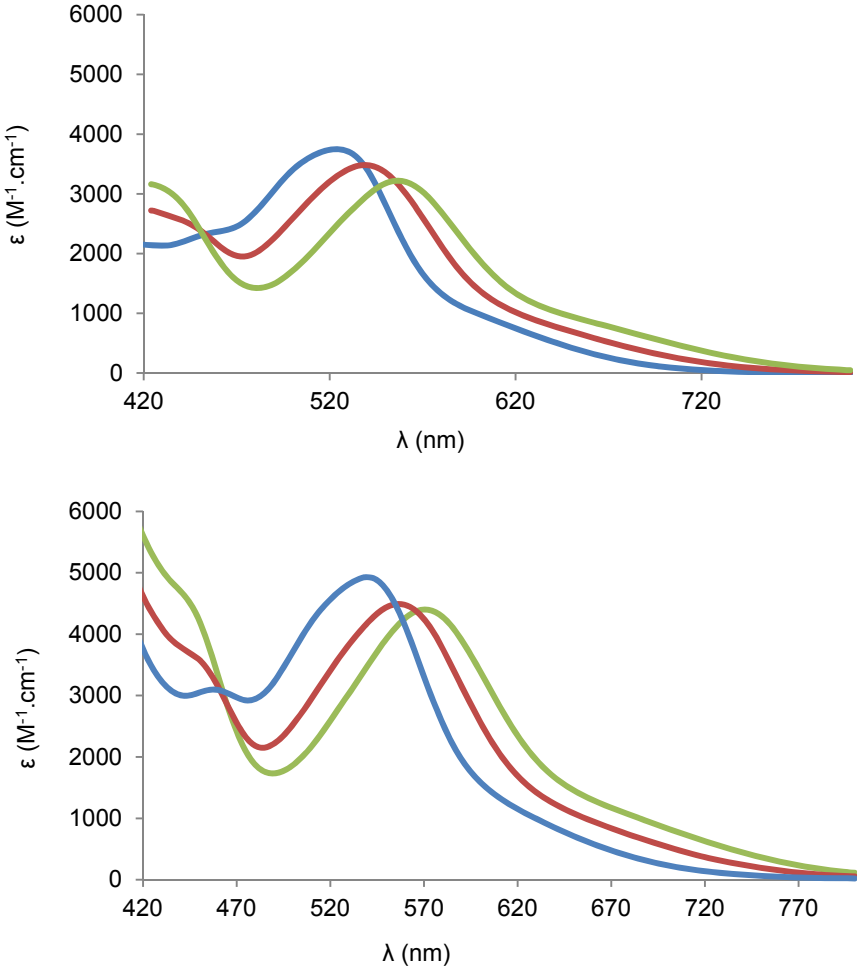


Figure S3. Evolution of the electronic absorption spectra of **C1** in methanol and **C2** with the protonation state of $dcbqH_2$: **Cn** (green), **Cn**$_{-H}$ (red) and **Cn**$_{-2H}$ (blue) with n = 1 or 2.

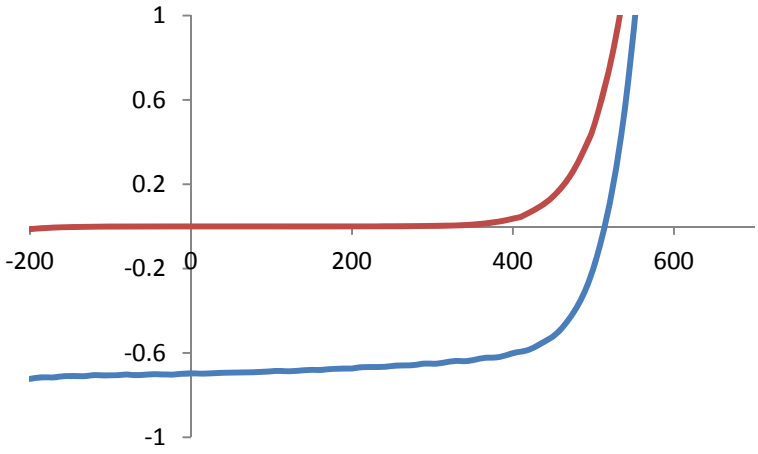


Figure S4. J vs. V characteristic of DSSC where TiO_2 is sensitized by **C1**$_{-H}$, and the electrolyte composition is: 0.25 M tert-butylpyridine. Parameters are: Jsc = 0.70 mA/cm^2, Voc = 515 mV, FF = 68.3% and η = 0.25%