SUPPLEMENTARY INFORMATION

Photoinduced energy transfer across non-covalent bonds in the nanoscale: cyclodextrin hosts with enhanced luminescent properties for guest communication

Jonathan A. Faiz,[†] Lasse E. P. Kyllonen,[†] Pablo Contreras-Carballada,[#] René M. Williams,[#] Luisa De Cola^{#§} and Zoe Pikramenou[†]*

[†]School of Chemistry, University of Birmingham, Edgbaston, B15 2TT, UK.[#]Van't Hoff Institute for Molecular Sciences, Nieuwe Achtergracht 129, NL-1018 WS, Amsterdam, NL. [§]Physikalisches Institut Westfälische Wilhelms Universität Münster, Mendelstraße 7, D-48149 Münster, Germany.

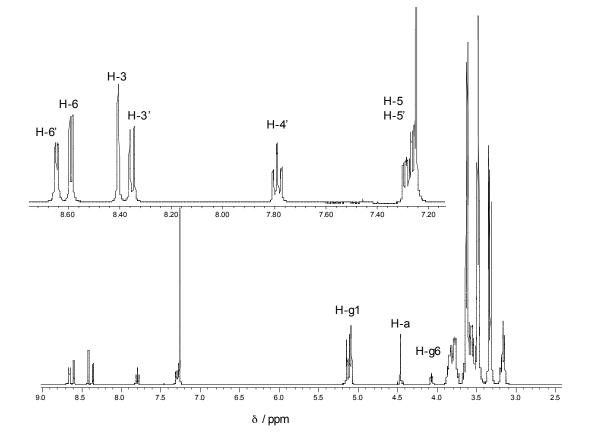


Figure S1. The 500 MHz ¹H NMR spectrum of **1** (CDCl₃).

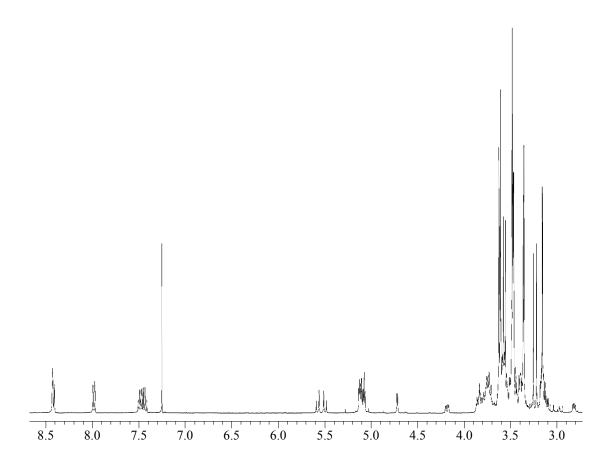


Figure S2. 400 MHz ¹H NMR spectrum of CD-Anth (CDCl₃).

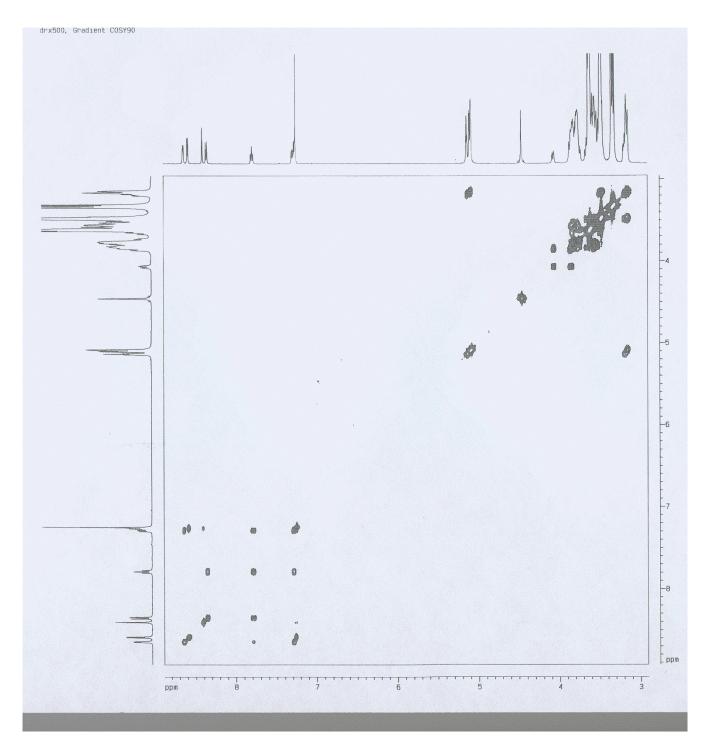


Figure S3. COSY NMR spectrum of 1 (CDCl₃).

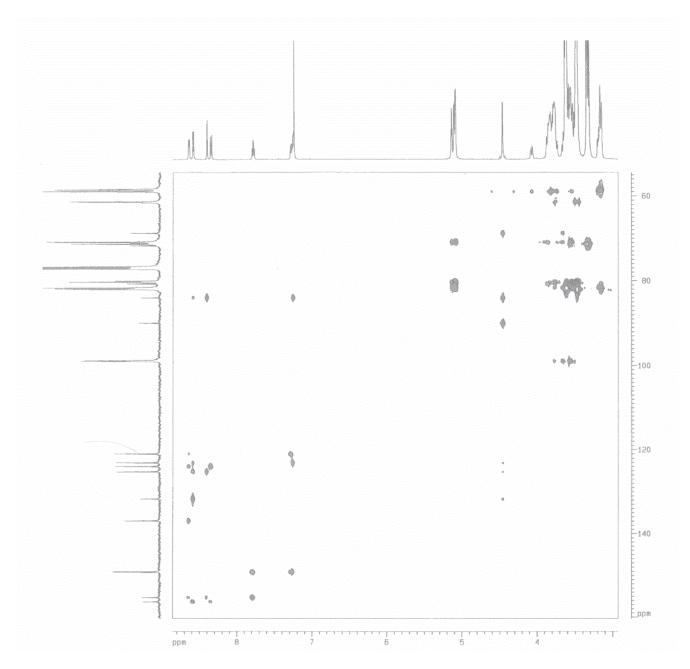


Figure S4. HMBC spectrum of **1** (CDCl₃).

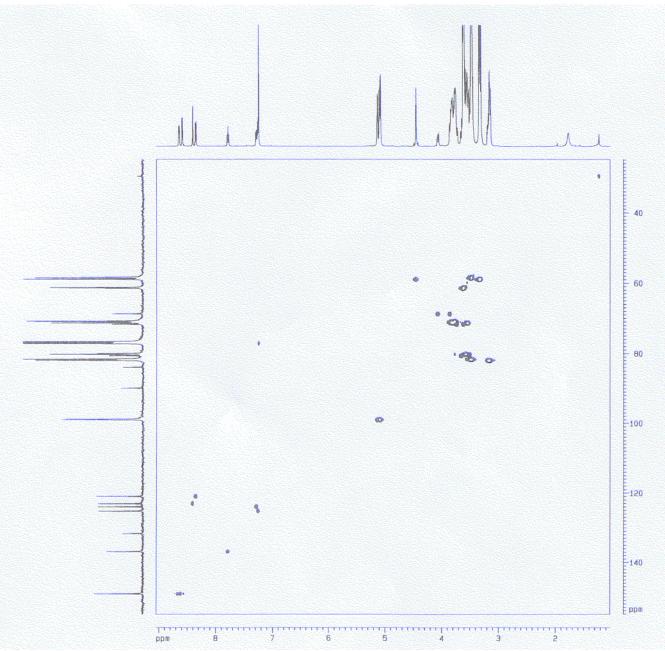


Figure S5. HSQC spectrum of 1 (CDCl₃).

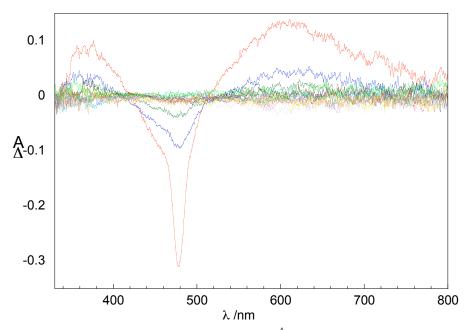


Figure S6 Transient absorption spectrum of **2** (2 x 10⁻⁴ M) and [Ru(biptpy)(tpy)][NO₃]₂ (3 x10⁻⁵ M). (Deaerated H₂O, λ_{exc} = 450 nm, incremental time delay = 5 ns, 20 frames).

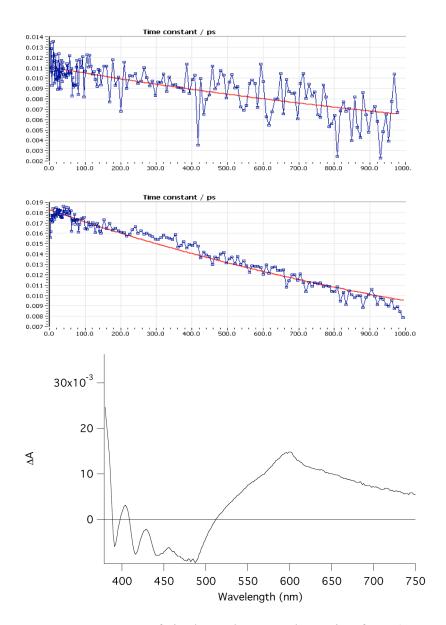
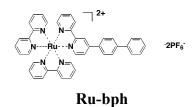


Figure S7. Decay of singlet anthracene absorption for 2 (4×10^{-4} M) in absence (top) and in presence (middle) of [Ru(biptpy)(tpy)](NO₃)₂ (4×10^{-4} M). ($\lambda_{exc} = 360$ nm). The lower image shows a transient absorption spectrum (averaged) of the mixture.

Synthesis of ruthenium complex [Ru(bpy)₂(bpy-bph)](PF₆)₂



Ru(bpy)₂(bpyPhBr) (50 mg, 0.049 mmol), Ph-BOH₂ (15 mg, 0.123 mmol) and cesium carbonate (81 mg, 0.247mmol) were mixed in DMF (15mL) and the solution was degassed with three freeze-pumpthaw cycles. A catalytic amount of Pd(PPh₃)₄ was added (6 mg, 0.005 mmol). The reaction was heated during 20 hours at 105°C. The DMF solution was poured in a solution of water/hexafluorophosphate. The precipitate was filtered over celite and washed with water (5ml) and ether (5ml) and then eluted using acetonitrile. After removal of the solvent in vacuo the isolated solid was purified by column chromatography on silica using magic mixture as an eluent. The organic solvents were evaporated in vacuo and the complex precipitated by addition of a saturated aqueous solution of NH₄PF₆. The precipitate was filtered off, washed with water and diethyl ether. Finally, the solid was dried under high vacuum for 24 h and recovered as an orange solid (48 mg, 94 %).

FAB-MS calculated $[M-2PF_6+H]^+$: 723.1810, observed: 723.1822; ¹H-NMR (300 MHz) (CD₃CN) : 8.18 (1H, d), 8.72 (1H, d), 8.56-8.52 (4H, q), 8.16-8.06 (5H, m), 8.04-7.98 (2H, m), 7.94-7.88 (2H, m), 7.84-7.70 (10H, m), 7.6-7.5 (2H, m), 7.5-7.4 (5H, m); ¹³C-NMR (75-MHz) (CD₃CN) : 158.42, 158.80, 158.51, 153.10, 153.05, 150.36, 144.40, 140.89, 139.22, 135.93, 130.49, 129.63, 129.29, 129.01, 128.42, 126.04, 125.87, 125.68, 123.09

Emission maximum (H₂O, $\lambda_{ex} = 450$ nm): $\lambda_{em} = 620$ nm. Emission quantum yield (H₂O, $\lambda_{ex} = 450$ nm): Φ (air) = 0.031; Φ (Ar) = 0.055. Emission lifetime: (H₂O, $\lambda_{ex} = 450$ nm): τ (air) = 459 ns; τ (Ar) = 736 ns.

For very similar compounds see: Inorg. Chem. 2005, 44, 4706-4718