Supplementary Material (ESI) for Dalton Transactions

Supporting Information

First Example of Pt···Pt Interaction in Platinum(II) Complexes Bearing Bulky Tri-*tert*-butyl-2,2':6',2"-Terpyridine Pendants *via* Conformational Control of the Calix[4]arene Moiety

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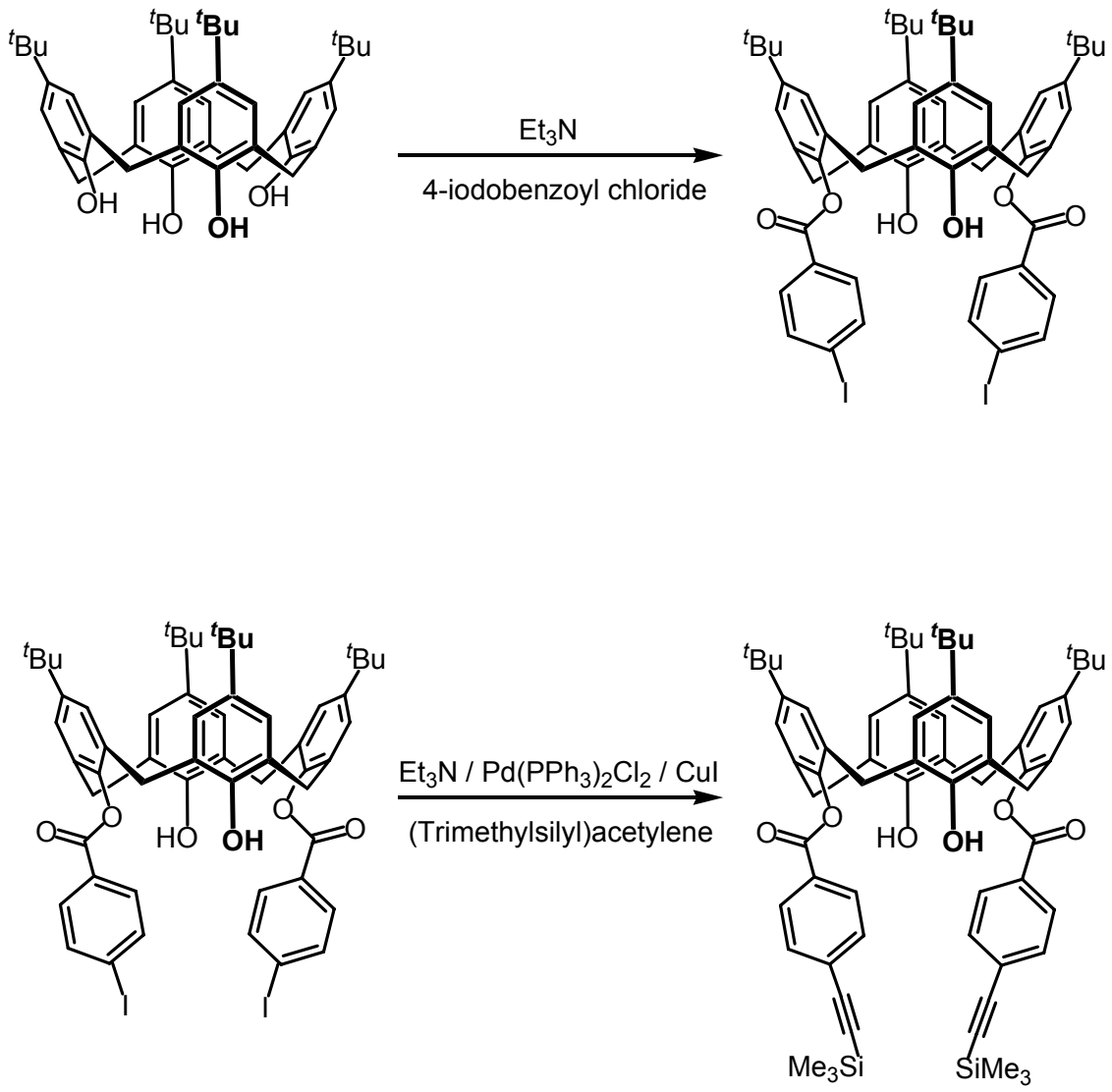
Fig. S1 Synthetic route of **L**



L

Characterisation of 25,27-di(iodobenzoyl)-26,28-dihydroxy-*p*-tert-butylcalix[4]arene

^{1}H NMR (400 MHz, $CDCl_3$, 298 K, relative to $SiMe_3$)/ppm: δ 1.00 (s, 18H, -^{t}Bu), 1.17 (s, 18H, -^{t}Bu), 3.50 (d, 4H, J = 14.1 Hz, -CH_2-), 3.89 (d, 4H, J = 14.1 Hz, -CH_2-), 5.05 (s, 2H, -OH), 6.91 (s, 4H, -C_6H_2), 7.01 (s, 4H, -C_6H_2), 7.88 (d, 4H, J = 8.3 Hz, -C_6H_4), 8.02 (d, 4H, J = 8.3 Hz, -C_6H_4). Positive-ion FAB-MS: m/z 1108 $[M]^+$. Anal. Calc. for $C_{58}H_{62}I_2O_6$•1/2 C_6H_{14}: C, 63.60; H, 6.04. Found: C, 63.51; H, 6.08.

Characterisation of L

^{1}H NMR (400 MHz, $CDCl_3$, 298 K, relative to $SiMe_3$)/ppm: δ 0.32 (s, 18H, -$SiMe_3$), 1.00 (s, 18H, -^{t}Bu), 1.23 (s, 18H, -^{t}Bu), 3.45 (d, 4H, J = 14.1 Hz, -CH_2-), 3.93 (d, 4H, J = 14.1 Hz, -CH_2-), 5.03 (s, 2H, -OH), 6.86 (s, 4H, -C_6H_2), 7.04 (s, 4H, -C_6H_2), 7.60 (d, 4H, J = 8.3 Hz, -C_6H_4), 8.27 (d, 4H, J = 8.3 Hz, -C_6H_4). IR (KBr disc, ν/cm^{-1}): 2160 (m), ν(C≡C); 1746 (s), ν(C=O). Positive-ion FAB-MS: m/z 905 $[M - 2SiMe_3]^+$. Anal. Calc. for $C_{68}H_{80}O_6Si_2$: C, 77.82; H, 7.68. Found: C, 77.72; H, 7.47.

Characterisation of Complex 1

^{1}H NMR (400 MHz, CD_3CN, 298 K, relative to $SiMe_3$)/ppm: δ 1.02 (s, 18H, -^{t}Bu), 1.20 (s, 18H, -^{t}Bu), 1.37 (s, 36H, -^{t}Bu), 1.43 (s, 18H, - -^{t}Bu), 3.45 (d, 4H, J = 14.0 Hz, -CH_2-), 4.00 (d, 4H, J = 14.0 Hz, -CH_2-), 5.73 (s, 2H, -OH), 6.95 (s, 4H, -C_6H_2), 7.07 (s, 4H, -C_6H_2), 7.60 (dd, 4H, J = 2.0 and 6.0 Hz, -trpy), 7.72 (d, 4H, J = 8.4 Hz, -C_6H_4), 8.35 (m, 8H, -trpy), 8.42 (d, 4H, J = 8.4 Hz, -C_6H_4), 9.10 (d, 4H, J = 6 Hz, -trpy). IR (KBr disc, ν/cm^{-1}): 2117 (m), ν(C≡C); 1736 (s), ν(C=O). Positive-ion FAB-MS: m/z 2097 $[M–2OTf]^+$. Anal. Calc. for $C_{118}H_{132}O_{12}Pt_2N_6S_2F_6$: C, 59.18; H, 5.56; N, 3.51. Found: C, 58.99; H, 5.58; N, 3.73.

Characterisation of Complex 2

^{1}H NMR (400 MHz, CD_3CN, 298 K, relative to $SiMe_3$)/ ppm: δ 1.18 (s, 18H, -^{t}Bu), 1.27 (s, 18H, -^{t}Bu), 3.59 (d, 4H, J = 13.8 Hz, -CH_2-), 4.08 (d, 4H, J = 13.8 Hz, -CH_2-), 6.25 (s, 2H, -OH), 7.28 (s, 4H, -C_6H_2), 7.30 (s, 4H, -C_6H_2), 7.57 (d, 4H, J = 8.2 Hz, -C_6H_4), 7.61 (m, 4H, -trpy), 7.80 (d, 8H, J = 8.0 Hz, -trpy), 8.16 – 8.33(m, 6H, -trpy) 8.49 (d, 4H, J = 8.2 Hz, -C_6H_4), 8.84 (d, 4H, J = 6 Hz, -trpy). IR (KBr disc, ν/cm^{-1}): 2120 (m), ν(C≡C); 1731 (s), ν(C=O). Positive-ion FAB-MS: m/z 1760 $[M–2OTf]^+$. Anal. Calc. for $C_{94}H_{86}O_{12}Pt_2N_6S_2F_6$•$CHCl_3$: C, 52.37; H, 4.03; N, 3.86. Found: C, 52.29; H, 4.14; N, 4.09.

Fig S2. UV-vis absorption spectra of complex **1** (—) and **2** (—) in acetonitrile solution at 298 K.

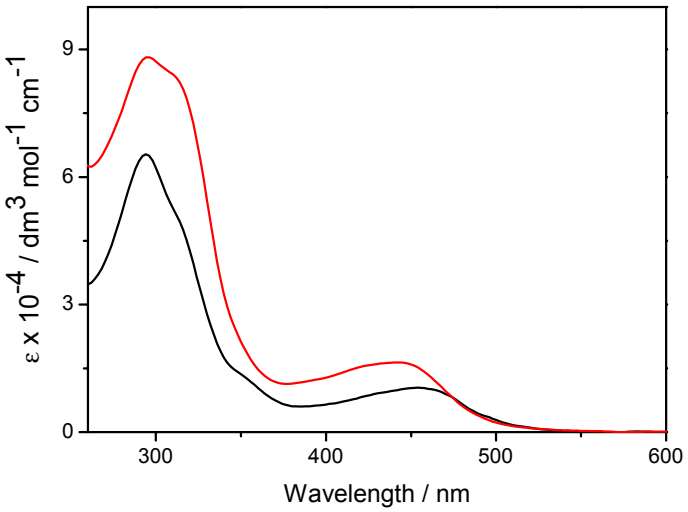


Fig S3. Normalized emission spectra of the powder form of **1** at 298 K (—) and 77 K (—) and the crystalline form at 298 K (—) and 77 K (—) in the solid state.