Supporting Information for

Effect of Bulky Groups in Ruthenium Heteroleptic Sensitizers on Dye Sensitized Solar Cell Performance

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Experimental Details

\(^1\)H-NMR and \(^{13}\)C-NMR spectra of compound 1

\(^1\)H-NMR and \(^{13}\)C-NMR spectra of compound 2

\(^1\)H-NMR and \(^{13}\)C-NMR spectra of compound 3

\(^1\)H-NMR and \(^{13}\)C-NMR spectra of compound 4

\(^1\)H-NMR and UV-Vis spectra of Ru(II) complex TT204

FT-IR spectra of Ru(II) complex TT204

MALDI-TOF spectra of Ru(II) complex TT204

\(^1\)H-NMR and UV-Vis spectra of Ru(II) complex TT205

\(^{13}\)C-NMR spectrum of Ru(II) complex TT205

MALDI-TOF spectrum of Ru(II) complex TT205

TT204 and TT205 NMR spectra assignment
EXPERIMENTAL DETAILS

Chemicals employed all over this work were purchased from Aldrich Chemical Co. and used as received without further purification. Dry solvents were purchased from SDS in *anhydrous grade* and further dried over activated molecular sieves. The monitoring of the reactions was carried out by TLC, employing aluminum sheets coated with silica gel 60 *F*₂₅₄ (normal phase) or with LiChroprep RP-18 *F*₂₅₄-*S* (reverse phase), both purchased from Merck. Purification of compounds was performed by flash column chromatography using silica gel Merck-60 (230-400 mesh, 0.040-0.063 mm) or Aldrich Sephadex LH-20. EI-MS spectra were determined on a VG AutoSpec instrument, MALDI-TOF MS and HRMS spectra were recorded with a Bruker Reflex III spectrometer. NMR spectra were recorded with a Bruker AC-300 instrument with a laser beam operating at 337 nm. Dithranol (1,8,9-anthracenetriol) and PEGNa1000 poly(ethyleneglycol)-1000 were used as matrix and internal reference, respectively. The logarithm of the absorption coefficient (*ε*) is indicated in brackets for each maximum. FT-IR spectra were recorded on a Bruker Vector 22 spectrophotometer from solid samples embedded in pressed disks of KBr.
Figure S1: $^1$H-NMR and $^{13}$C-NMR spectra of compound 1
Figure S2: $^1$H-NMR and $^{13}$C-NMR spectra of compound 2
Figure S3: $^1$H-NMR and $^{13}$C-NMR spectra of compound 3
Figure S4: $^1$H-NMR and $^{13}$C-NMR spectra of compound 4
Figure S5: $^1$H-NMR and UV-vis spectra of TT204
Figure S6: FT-IR and MALDI-TOF spectra of TT204.
Figure S7: FiMALDI-TOF spectra of TT204
Figure S8: $^1$H-NMR and UV-vis spectra of TT205
Figure S8: $^{13}$C-NMR spectrum of TT205

Figure S9: MALDI-TOF spectra of TT205
Ru complex TT204. $^1$H-RMN (300 MHz, CDCl$_3$), δ (ppm): 9.58 (d, $J = 5.7$ Hz, 1H, H-6), 9.18 (s (br), 1H, H-3), 9.07 (d, $J = 5.7$ Hz, 1H, H-6”), 9.0 (s (br), 1H, H-3’), 8.83 (s (br), 1H, H-8), 8.68 (s (br), 1H, H-8”), 8.41 (d, $J = 5.7$ Hz, 1H, H-5), 8.15 (m, 2H, H-5”), 7.63 (d, $J = 6.1$ Hz, 1H, H-10), 7.2-6.9 (m, 4H, H-11’, H-10’, H-14, H-14’), 1.8-1.5 (m, 12H, C-CH$_2$-CH$_2$-CH$_3$, C’-CH$_2$’-CH$_2’$-CH$_3’$), 1.3-1.0 (m, 12H, C-CH$_2$-CH$_2$-CH$_3$, C’-CH$_2$’-CH$_2’$-CH$_3’$), 1.0-0.8 (m, 27H, CH$_3$, CH$_3’$).

Ru complex TT205. $^1$H-RMN (300 MHz, CDCl$_3$), δ (ppm): 9.52 (d, $J = 5.9$ Hz, 1H, H-6), 9.12 (m, 2H, H-6’, H-3), 8.90 (s, 1H, H-3’), 8.78 (s, 1H, H-8), 8.70 (s, 1H, H-8’), 8.39 (d, $J = 5.7$ Hz, 1H, H-5), 8.10 (s, 1H, H-13), 8.03 (s, 1H, H-5”) 7.96 (m, 2H, H-13”), 7.68 (s (br), 1H, H-10), 7.30 (d, $J = 6.2$ Hz, 1H, H-11”), 7.19 (s (br), 1H, H-10”), 7.13 (s (br), 1H, H-14), 7.04 (s (br), 1H, H-14”), 1.57 (m, 4H, C(CH$_3$)$_2$-CH$_2$-(CH$_2$)$_2$-CH$_3$, C(CH$_3$)$_2$-CH$_2$’-(CH$_2$)$_2’$-CH$_3’$), 1.50 (s, 6H, C(CH$_3$)$_2$-CH$_2$-(CH$_2$)$_2$-CH$_3$, C(CH$_3$)$_2$-CH$_2$’-(CH$_2$)$_2’$-CH$_3’$), 1.48 (s, 6H, C’(CH$_3$)$_2’$-CH$_2$’-(CH$_2$)$_2’$-CH$_3’$), 1.5-1.0 (m, 8H, C(CH$_3$)$_2$-CH$_2$-(CH$_2$)$_2$-CH$_3$, C(CH$_3$)$_2$-CH$_2$’-(CH$_2$)$_2’$-CH$_3’$), 0.74 (t, $J = 7.1$ Hz, 3H, C(CH$_3$)$_2$-CH$_2$-(CH$_2$)$_2$-CH$_3$), 0.70 (t, $J = 7.1$ Hz, 3H, C(CH$_3$)$_2$’-CH$_2’$-(CH$_2$)$_2’$-CH$_3’$). $^{13}$C-RMN (75.5 MHz, CDCl$_3$), δ (ppm): 165.8 (C-17), 165.4 (C-17’), 160.75 (C-2), 160.71 (C-2’), 159.5 (C-7), 158.6 (C-7’), 158.1 (C-11), 157.2 (C-11’), 153.7 (C-6), 153.0,153.08 (C-4, C-4’), 152.5 (C-6’), 152.0 (C-9, C-9’), 142.3 (C-12), 141.5 (C-12’), 136.5 (C-15), 135.9 (C-15’), 135.1 (C-17), 134.2 (C-17’), 129.2, 129.1 (C13, C13’), 126.6 (C-5), 125.6 (C-10), 125.3 (C-14, C-14”), 122.3 (C-5’), 123.2 (C-3’), 122.8 (C-8), 121.8 (C10’), 119.0 (C-3’), 118.8 (C-8’), 45.2, 45.0 (C(CH$_3$)$_2$-
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\[ \text{CH}_2-(\text{CH}_2)_2-\text{CH}_3, \ C(\text{CH}_3)_2'-\text{CH}_2'-\text{(CH}_2)_2'-\text{CH}_3'), \ 38.3, \ 38.2 \ (C(\text{CH}_3)_2-\text{CH}_2-(\text{CH}_2)_2-\text{CH}_3, \ C(\text{CH}_3)_2'-\text{CH}_2'-\text{(CH}_2)_2'-\text{CH}_3'), \ 30.2, \ 30.0 \ (C(\text{CH}_3)_2-\text{CH}_2-(\text{CH}_2)_2-\text{CH}_3, \ C'(\text{CH}_3)_2'-\text{CH}_2'-\text{(CH}_2)_2'-\text{CH}_3'), \ 27.1, \ 26.9, \ 23.1, \ 23.0 \ C(\text{CH}_3)_2-\text{CH}_2-(\text{CH}_3)_2-\text{CH}_3, \ C(\text{CH}_3)_2'-\text{CH}_2'-\text{(CH}_2)_2'-\text{CH}_3'), \ 14.4, \ 14.3 \ (C(\text{CH}_3)_2-\text{CH}_2-(\text{CH}_2)_2-\text{CH}_3, \ C(\text{CH}_3)_2'-\text{CH}_2'-\text{(CH}_2)_2'-\text{CH}_3'). \]