Electronic Supplementary Material (ESI) for New Journal of Chemistry.

This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2015

Electronic Supplementary Information

Manuscript ID: NJ-ART-08-2015-002032 (submitted to *New Journal of Chemistry*)

Title: A novel cationic iridium(III) complex as red phosphor applied in warm white light-emitting diodes

Authors: Guoyun Meng, Zeyu Chen, Huaijun Tang,* Yong Liu, Liying Wei and Zhengliang Wang*

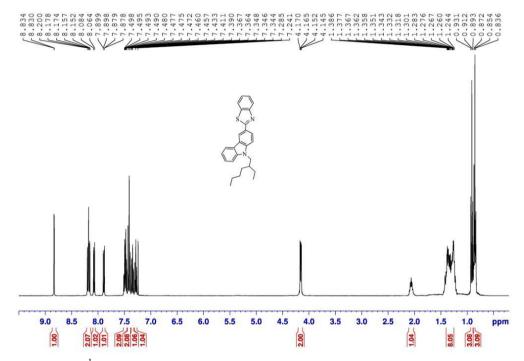


Figure S1. ¹H NMR spectra of 2-(9-(2-ethylhexyl)-9H-carbazol-3-yl)benzo[d]thiazole (compound 3)

¹H NMR (400MHz, CDCl₃, ppm), δ: 8.83 (d, 1H, ${}^{3}J$ = 1.6 Hz, ArH), δ: 8.15–8.20 (m, 2H, ArH), δ: 8.07 (d, 1H, ${}^{3}J$ = 8.0 Hz, ArH), δ: 7.89 (dd, 1H, ${}^{3}J$ = 8.0 Hz, ${}^{4}J$ = 0.4 Hz, ArH), δ: 7.24–7.50 (m, 6H, ArH), δ: 4.16 (dd, 2H, ${}^{3}J$ = 7.6 Hz, ${}^{4}J$ = 2.0 Hz, ${}^{4}J$ = 3.5 Hz, -N-CH₂-), δ: 2.01–2.11 (m, 1H, -CH<), δ: 1.26–1.39 (m, 8H, alkyl–H), δ: 0.91 (t, 3H, ${}^{3}J$ = 5.7 Hz, -CH₃), δ: 0.86 (t, 3H, ${}^{3}J$ = 4.4 Hz, -CH₃).

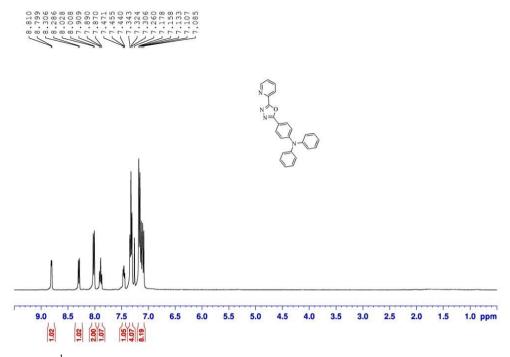


Figure S2. ¹H NMR spectra of N,N-diphenyl-4-(5-(pyridin-2-yl)-1,3,4-oxadiazol-2-yl)aniline (compound **8**)

¹H NMR (400MHz, CDCl₃, ppm), δ: 8.80 (d, 1H, ${}^{3}J$ = 4.4 Hz, pyridine–H), δ: 8.30 (d, 1H, ${}^{3}J$ = 8.0 Hz, ArH), δ: 8.02 (d, 2H, ${}^{3}J$ = 8.0 Hz, ArH), δ: 7.89(t, 1H, ${}^{3}J$ = 8.0 Hz, ArH), δ: 7.46 (t, 1H, ${}^{3}J$ = 6.4 Hz, ArH), δ: 7.32 (t, 4H, ${}^{3}J$ = 7.6 Hz, ArH), δ: 7.09-7.18 (m, 8H, ArH).

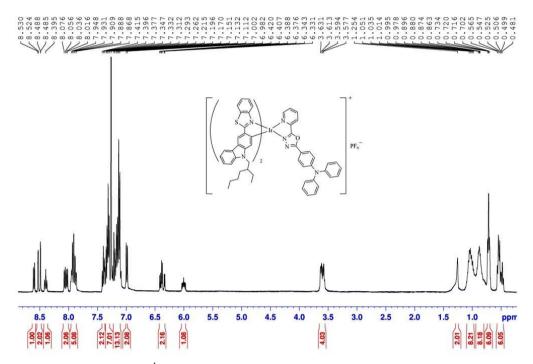


Figure S3. ¹H NMR spectra of the cationic iridium(III) complex

¹H NMR (400MHz, CDCl₃, ppm), δ: 8.60 (d, 1H, ${}^{3}J$ = 7.6 Hz, ArH), δ: 8.53 (s, 1H, ArH), 8.49 (s, 1H, ArH), δ: 8.40 (t, 1H, ${}^{3}J$ = 8.0 Hz, ArH), δ: 8.05 (q, 2H, ${}^{3}J$ = 8.0 Hz, ArH), δ: 7.87–7.95 (m, 5H, ArH), δ: 7.40 (t, 2H, ${}^{3}J$ = 7.6 Hz, ArH), δ: 7.29–7.35 (m, 7H, ArH), δ: 7.11–7.22 (m, 13H, ArH), δ: 6.99 (d, 2H, ${}^{3}J$ = 8.0 Hz, ArH), δ: 6.33–6.42 (m, 2H, ArH), δ: 6.01 (m, 1H, ArH), δ: 3.60 (dd, 4H, ${}^{3}J$ = 14.4 Hz, ${}^{4}J$ = 6.8 Hz, -N–CH₂–), δ: 1.25 (s, 2H, –CH<), δ: 0.86–1.05 (m, 16H, alkyl–H), δ: 0.72 (t, 6H, ${}^{3}J$ = 5.6 Hz, –CH₃), δ: 0.46-0.57 (m, 6H, –CH₃)

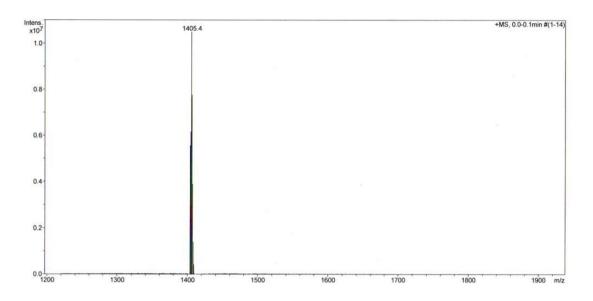


Figure S4. MS spectra of the cationic iridium(III) complex

ESI-MS(m/Z): 1405.4 $[M-PF_6]^+$