Effect of pH on the photophysical properties of two new carboxylic-substituted iridium (III) complexes

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**Figure S1.** UV-vis absorption (normalized) and emission (excited at 400nm) spectra of: (a, ■), DMSO solution of (TPAQCE)$_2$Irpic; (b, ●), solution (a) in presence of 10 equiv of aqueous NaOH; (c, ▽), DMSO solution of (TPAQCOOH)$_2$Irpic.

**Figure S2.** UV-vis absorption (normalized) and emission spectra of: (a, ■), ethanol solution of (TPAQCE)$_2$Irpic; (b, ●), solution (a) in presence aqueous NaOH, (c, ▲), solution (b) in presence of HCl; (d, ▽), ethanol solution of (TPAQCOOH)$_2$Irpic; (e, ◇), solution (d) in presence of HCl. Excited at 400nm.

**Figure S3.** Aromatic part of the $^1$H NMR in DMSO-$d_6$ (from top to bottom): (TPAQCE)$_2$Irpic; (TPAQCE)$_2$Irpic containing 10 equiv of NaOH; and (TPAQCOOH)$_2$Irpic.
Figure S4. Aromatic part of the $^1$H NMR in DMSO-$d_6$: (TPAQCE)$_2$Irpic containing 10 equiv of NaOH.

Figure S5. Aromatic part of the $^1$H NMR in DMSO-$d_6$: (TPAQCE)$_2$Irpic (1) and gradual addition of HCl (ca. 2%-3% in methanol / DMSO-$d_6$) (2-6); The six new peaks are marked with *.
Figure S6. Aromatic part of the $^1$H NMR in DMSO-$d_6$: (TPAQCE)$_2$Irpic (1); addition of ca. 20-30 equiv of HCl (ca. 2-3% in methanol / DMSO-$d_6$) to the (TPAQCE)$_2$Irpic solution for 2h (2); addition of ca. 20-30 equiv of HCl (ca. 2-3% in methanol / DMSO-$d_6$) to the (TPAQCE)$_2$Irpic solution for 48h (3). The six new peaks appeared by addition HCl to the solution of (TPAQCE)$_2$Irpic are marked with *.

Figure S7. Aromatic part of the $^1$H NMR in DMSO-$d_6$: (TPAQC(OOH))$_2$Irpic (1); addition of ca. 20-30 equiv of HCl (ca. 2-3% in methanol / DMSO-$d_6$) to the (TPAQC(OOH))$_2$Irpic solution for 2h (2); addition of ca. 20-30 equiv of HCl (ca. 2-3% in methanol / DMSO-$d_6$) to the (TPAQC(OOH))$_2$Irpic solution for 48h (3).
**Figure S8.** Aromatic part of the $^1$H NMR in DMSO-$d_6$: (TPAQCE)$_2$Irpic (1); (TPAQCE)$_2$Irpic containing 10 equiv of NaOH (2); gradual addition of HCl to the solution of (TPAQCE)$_2$Irpic containing 10 equiv of NaOH (3-7).

**Figure S9.** Aromatic part of the $^1$H NMR in DMSO-$d_6$: (TPAQCE)$_2$Irpic (1); (TPAQCE)$_2$Irpic containing aqueous NaOH (10 equiv, in D$_2$O) (2); addition of HCl (ca. 2-3% in methanol / DMSO-$d_6$) to the (TPAQCE)$_2$Irpic solution containing NaOH (3); (TPAQCOOH)$_2$Irpic containing HCl (20-30% in methanol) (4); (TPAQCOOH)$_2$Irpic (5). The five new peaks appeared by addition HCl to the solution of (TPAQCOOH)$_2$Irpic are marked with *.
**Figure S10.** Change in absorption spectra of (TPAQCOOH)$_2$Irpic ($c = 1.34 \times 10^{-4}$ M) in DMSO upon the repeated addition of HCl (0.2 M) and aqueous NaOH (0.2 M). (a) = (TPAQCOOH)$_2$Irpic before the addition of HCl; (b): (a) + HCl; (c): (b) + NaOH; (d): (c) + HCl; (e): (d) + NaOH; (f): (e) + HCl; (g): (f) + NaOH. Inset: Change in absorbance at 546nm of (TPAQCOOH)$_2$Irpic caused by the repeated addition of HCl (5μL) and NaOH (5μL).

**Figure S11.** Change in emission spectra of (TPAQCOOH)$_2$Irpic ($c = 1.34 \times 10^{-4}$ M) in DMSO (excited at 400nm) upon the repeated addition of HCl (0.2 M) and aqueous NaOH (0.2 M). (a) = (TPAQCOOH)$_2$Irpic before the addition of HCl; (b): (a) + HCl; (c): (b) + NaOH; (d): (c) + HCl; (e): (d) + NaOH; (f): (e) + HCl; (g): (f) + NaOH. Inset: Change in emission intensity at 598nm of (TPAQCOOH)$_2$Irpic caused by the repeated addition of HCl (5μL) and NaOH (5μL).
**Figure S13.** A plot of emission intensity of (TPAQCOOH)$_2$Irpic at 625nm vs pH (6.50 – 8.00) in aqueous buffer solutions. The red solid curve is fitting line of experimental data with relative coefficient $R = 0.985$.

**Figure S14.** pH-Dependent changes in molar absorption coefficients (424 nm) and emission intensity (625 nm) of the probe (TPAQCOOH)$_2$Irpic in aqueous PBS buffers and the corresponding error bars were provided.

**Figure 15.** pH-Dependence of the absorption spectra of (TPAQCOOH)$_2$Irpic in ethanol:H$_2$O = 3:7 (containing 0.1 M NaCl) at concentration of 5.0 $\times 10^{-5}$ M.
Figure 16. pH-Dependence of the emission spectra of \((\text{TPAQCOOH})_2\text{Irpic}\) in ethanol:H\(_2\)O = 3:7 (containing 0.1 M NaCl) at concentration of 5.0 \(\times\) 10\(^{-5}\) M.

Figure S17. \(^1\)H NMR of TPAQCE in CDCl\(_3\)
Figure S18. $^{13}$C NMR of TPAQCE in DMSO-$d_6$.

Figure S19. MADIL-TOF MS of TPAQCE.

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Figure S20. IR spectrum of TPAQCE

Figure S21. $^1$H NMR of (TPAQCE)$_2$Irpic in DMSO-$d_6$
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Figure S23. IR spectrum of (TPAQCE)$_2$Irpic
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Figure S25. MADIL-TOF MS of (TPAQCOOH)$_2$Irpic

Figure S26. IR spectrum of (TPAQCOOH)$_2$Irpic