Electronic Supplementary Information

The anion-π interactions in new electron-deficient π systems: the relevance to solid phosphorescent colors

Guo-Ping Yong,* Yi-Man Zhang and Wen-Long She

Department of Chemistry, University of Science and Technology of China, Hefei 230026, P. R. China

E-mail: gpyong@ustc.edu.cn

Fig. S1 Solid-state EPR spectrum of 2-(imidazo[1,2-a]pyridin-2-yl)-2-oxoacetic acid radical at room temperature.

Fig. S2 The dihedral angle between the plane of coplanar Cl−, H2O and MeOH, and the plane of carboxycarbonyl substituted imidazo[1,2-a]pyridinium unit in 1, showing they are almost coplanar.
**Fig. S3** The 2D supramolecular network of 1 assembled by hydrogen bonding interactions (red dashed lines).

**Fig. S4** The 2D supramolecular network of 2 assembled by hydrogen bonding interactions (green dashed lines).
Fig. S5 2D supramolecular network of 3 via hydrogen bonds, giving rise to short intermolecular C···O' contacts between carboxylic acid-oxygen or perchlorate-oxygen atom and imidazo[1,2-α]pyridine-carbon atoms.

Fig. S6 The decay lifetime curve of 3 in the dilute H₂O solution. The lifetime (τ) is defined as the time in which the emission intensity decays to 1/e of the initial intensity (I₀), where e is the natural log constant and is equal to 2.718. (I = I₀e⁻(t/τ) => τ = t => I = (1/e) I₀).

Fig. S7 Solid excitation spectra of 1–3 at room temperature.
Thermogravimetric analyses (TGA) of 1–3 were performed in N$_2$ at a heating rate of 10 °C min$^{-1}$ on crystalline sample, as shown in Fig. S8. The TG curve of 1 displays a continuous weight loss: the weight loss of 17.6 % was completed at about 157°C, ascribed to the loss of one guest water molecule and one guest methanol molecule (calc. 18.8 %). Compared to 1, 2 exhibits higher thermal stability, and the first weight loss ends at about 143 °C (6.8 %), corresponding to the loss of one guest water molecule (calc. 7.3 %). 3 displays the first weight loss starts at ca. 85 °C and ends at 121 °C (5.1 %), corresponding to the loss of one water molecule (calc. 5.8 %).

**Fig. S8** TGA curves of 1–3.

**References:**