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

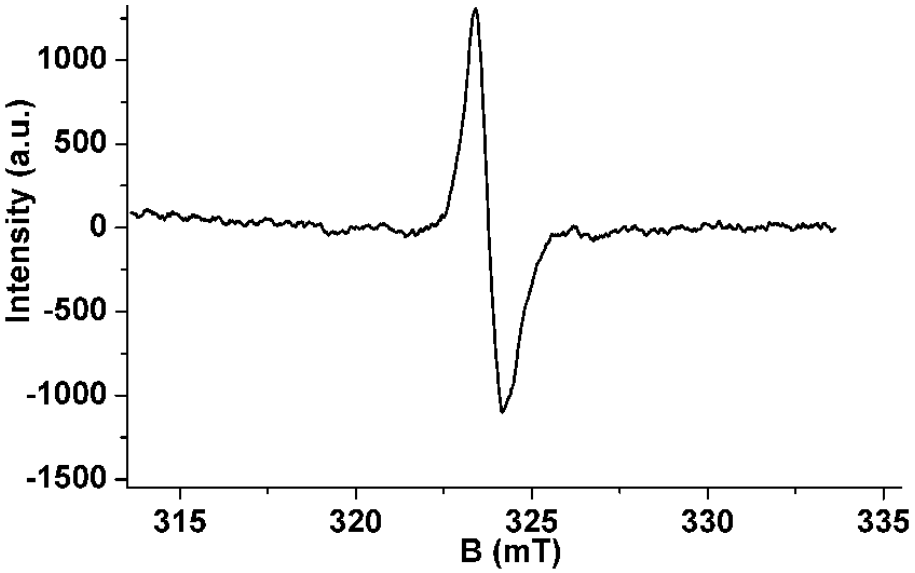

Fig. S1 Solid-state EPR spectrum of 2-(imidazo[1,2-*a*]pyridin-2-yl)-2-oxoacetic acid radical at room temperature.

Fig. S2 The dihedral angle between the plane of coplanar Cl^-, H_2O and MeOH, and the plane of carboxycarbonyl substituted imidazo[1,2-*a*]pyridinium unit in **1**, showing they are almost coplanar.

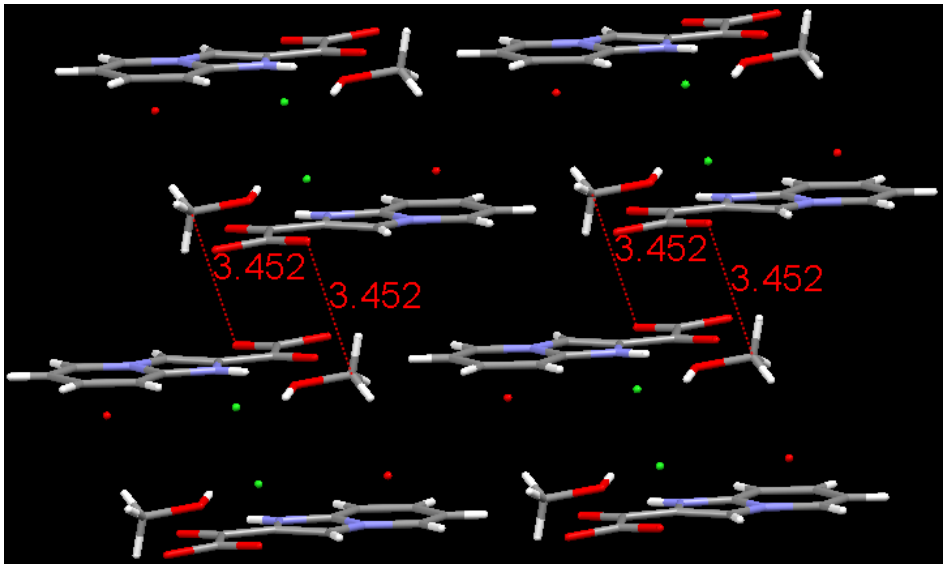

Fig. S3 The 2D supramolecular network of **1** assembled by hydrogen bonding interactions (red dashed lines).

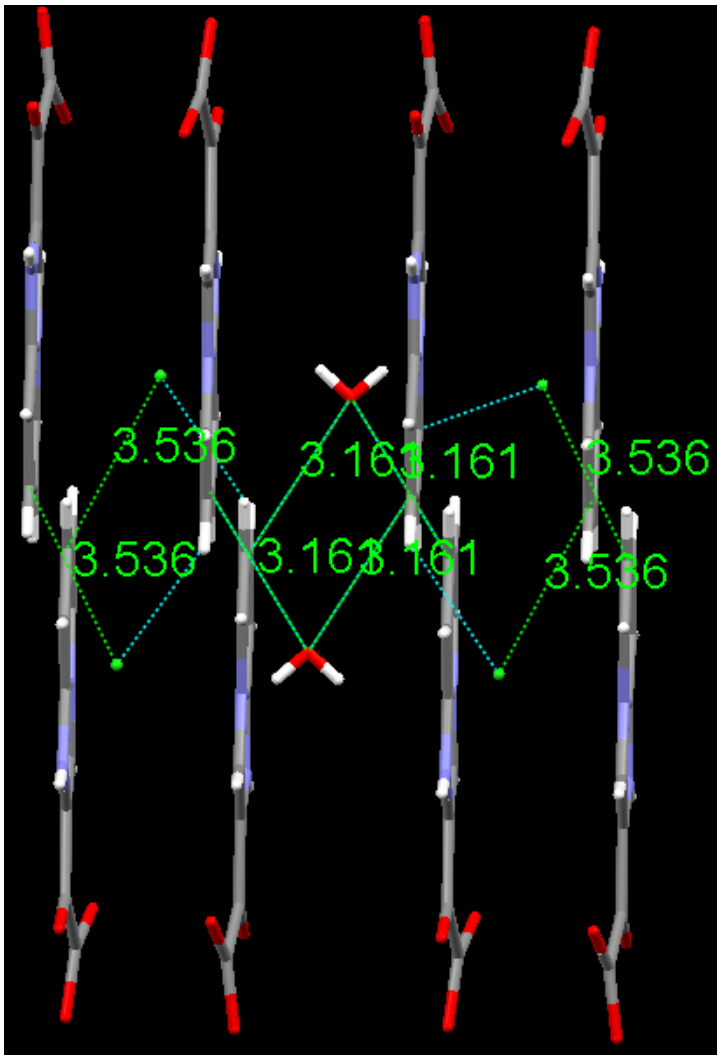

Fig. S4 The 2D supramolecular network of **2** assembled by hydrogen bonding interactions (green dashed lines).

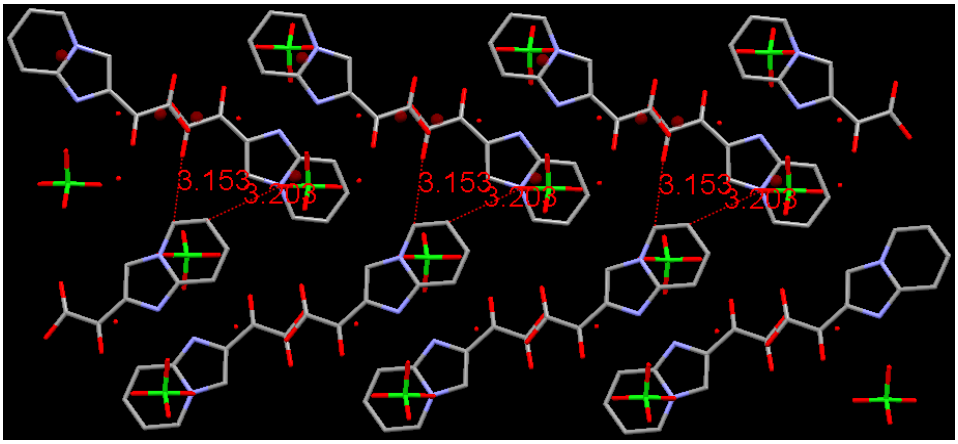

Fig. S5 2D supramolecular network of **3** via hydrogen bonds, giving rise to short intermolecular C···O' contacts between carboxylic acid-oxygen or perchlorate-oxygen atom and imidazo[1,2-*a*]pyridine-carbon atoms.

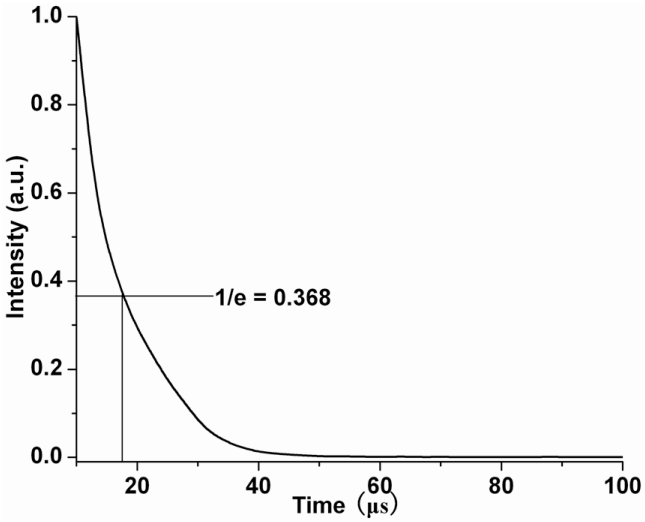

Fig. S6 The decay lifetime curve of **3** in the dilute H_2O solution. The lifetime (τ) is defined as the time in which the emission intensity decays to 1/e of the initial intensity (I_o), where e is the natural log constant and is equal to 2.718. ($I = I_o e^{-(t/\tau)} \Rightarrow \tau = t \Rightarrow I = (1/e)\ I_o$).[S1]

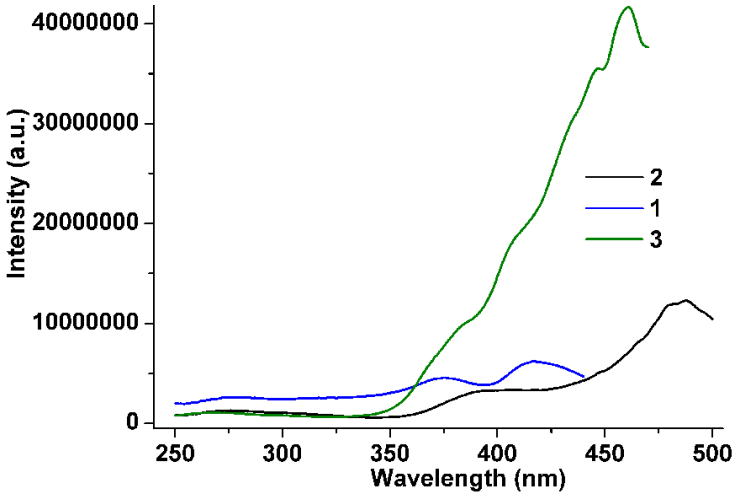

Fig. S7 Solid excitation spectra of **1–3** at room temperature.

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 %).

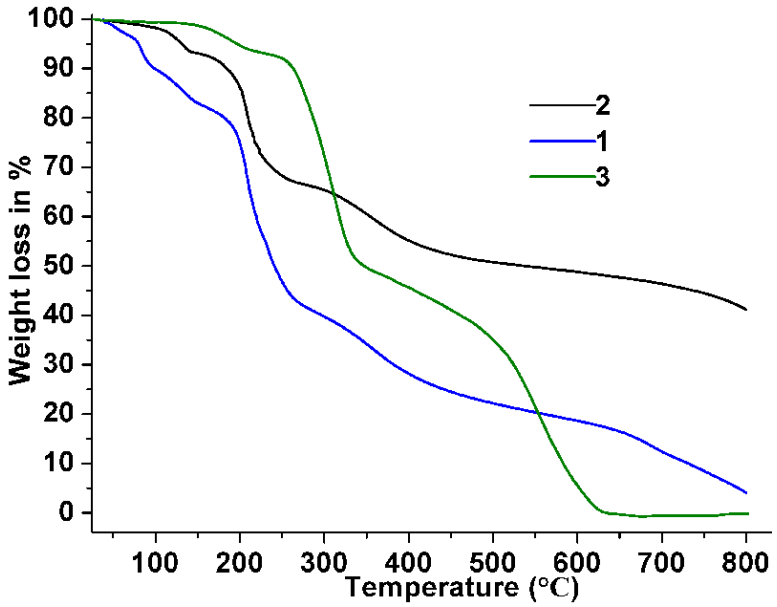

Fig. S8 TGA curves of **1–3**.

References:

S1 K. C. Stylianou, R. Heck, S.Y. Chong, J. Bacsa, J. T. A. Jones, Y. Z. Khimyak, D. Bradshaw and M. J. Rosseinsky, *J. Am. Chem. Soc.*, 2010, **132**, 4119−4130.