

# **CHEMISTRY**

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### Supporting Information

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#### **Luminescence Responsive Charge Transfer Intercluster Crystals**

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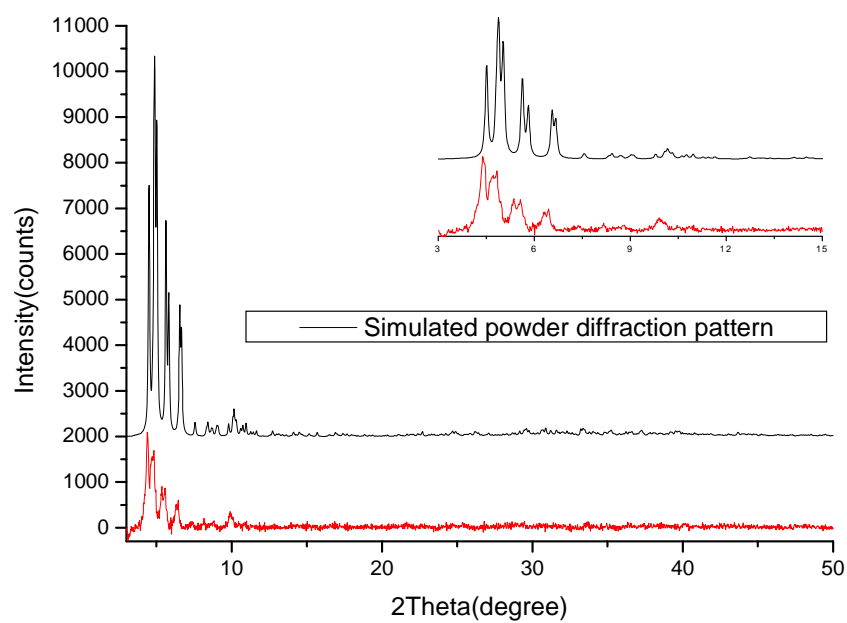
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## I. Physical measurements

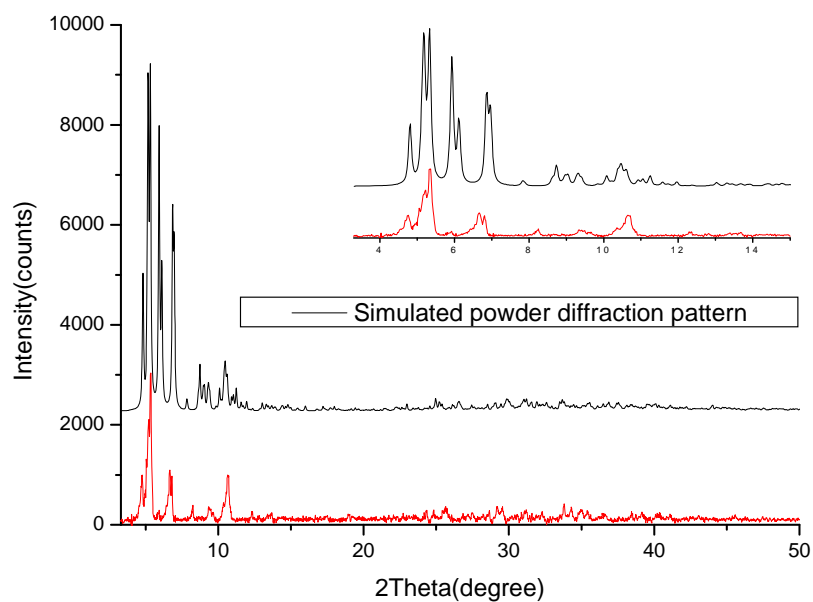
The C, H, N microanalyses were carried out with a CE instruments EA 1110 elemental analyzer. The FT-IR spectra were recorded from KBr pellets in the range 4000-400  $\text{cm}^{-1}$  with a Nicolet AVATAR FT-IR330 spectrometer. Luminescence were measured on a Hitachi F-7000 spectrometer. Lifetime was measured on Horiba Jobin Yvon Fluoromax-4P-Tcspc spectrometer. UV-vis diffuse reflectance spectra were recorded on a Varian Cary5000 UV-VIS-NIR Spectrophotometer with  $\text{BaSO}_4$  as the reference. X-ray powder diffractometry study of the complex was performed on a Panalytical X-Pert pro diffractometer with  $\text{Cu K}\alpha$  radiation.

## X-ray experimental

Intensity data of compounds **1** and **2** were collected on an Oxford Gemini S Ultra system ( $\text{Mo K}\alpha$ ). Absorption corrections were applied by using the program CrysAlis (multi-scan). The structures were solved by direct methods, and non-hydrogen atoms except solvent molecules and counteranions were refined anisotropically by least-squares on  $F^2$  using the SHELXTL program. The hydrogen atoms of *tert*-butyl groups were generated geometrically, while no attempt was made to locate H atoms of  $\text{H}_2\text{O}$  molecules.



**Figure S1.** X-ray powder diffraction pattern of **2**



**Figure S2.** X-ray powder diffraction pattern of **3**

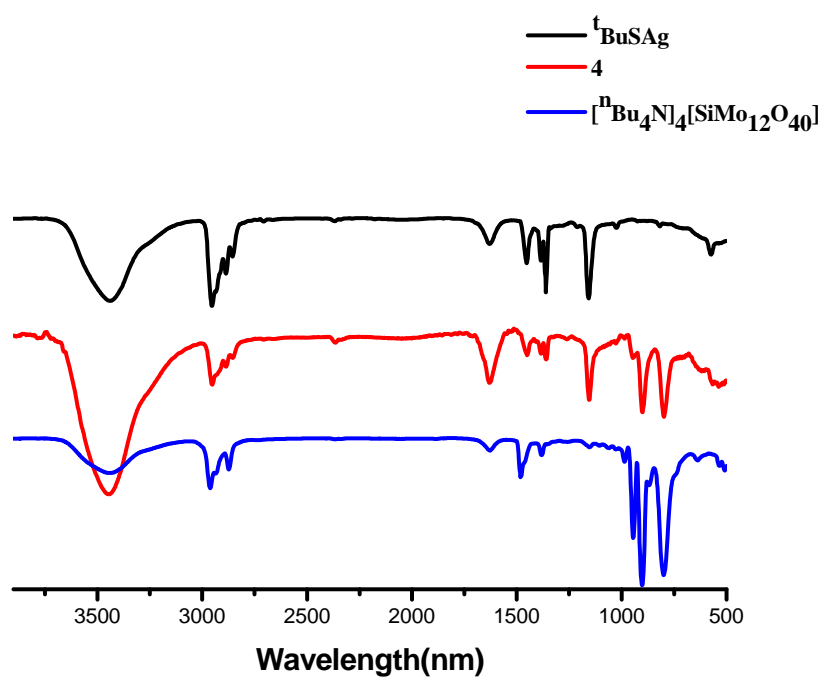


Figure S3. IR Specture of 4

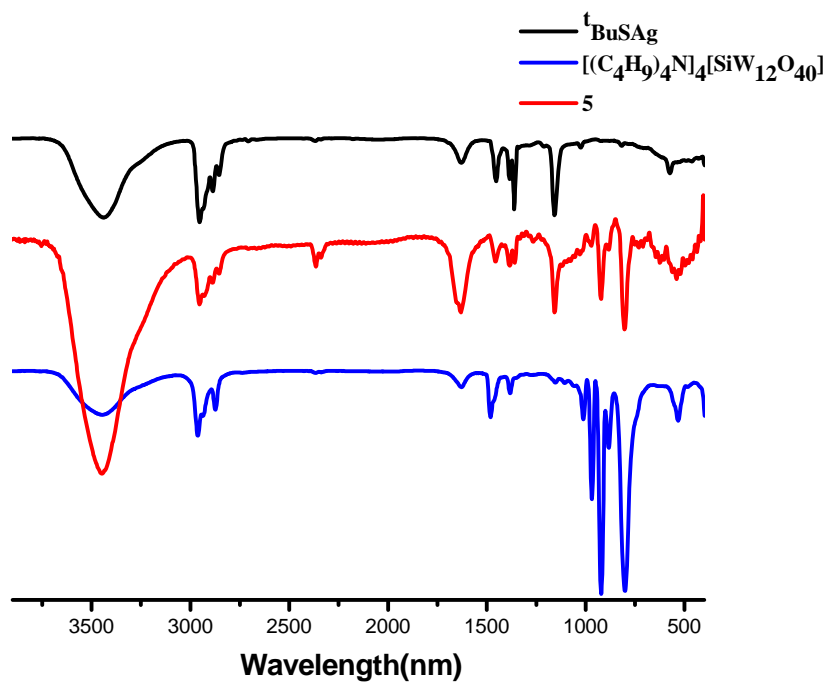
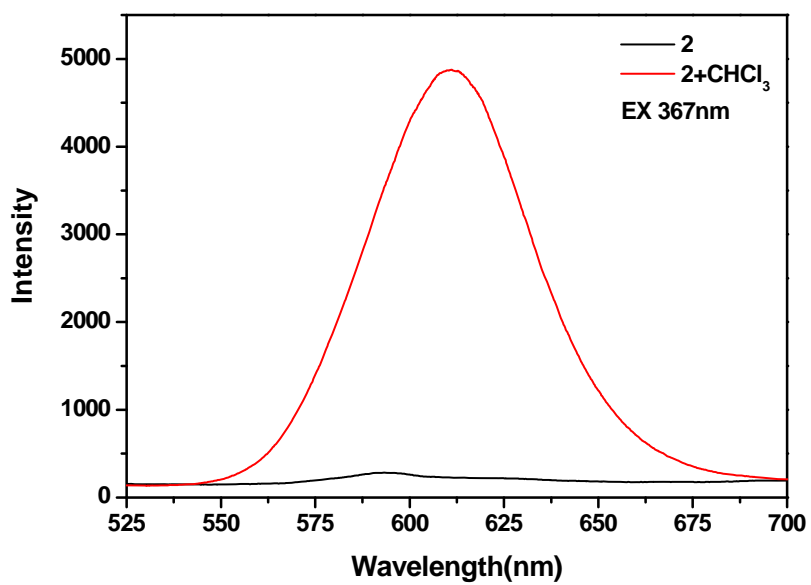
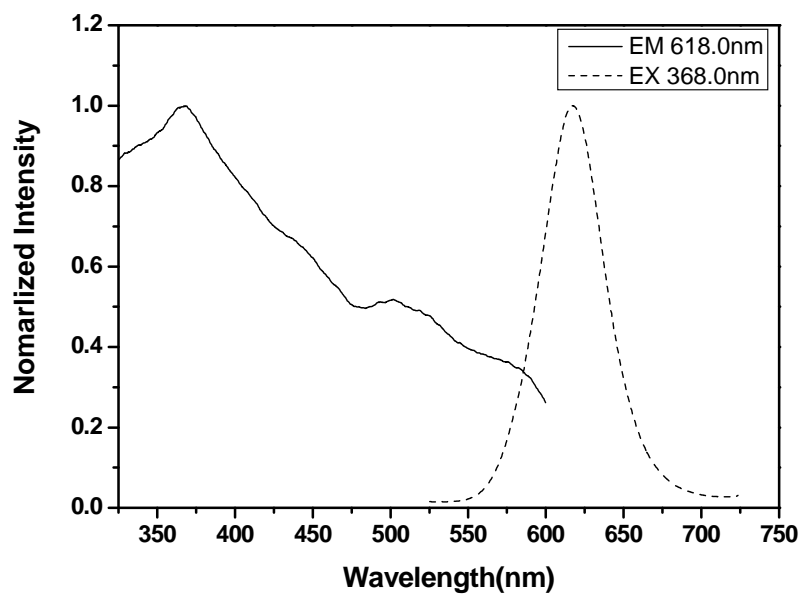


Figure S4. IR Specture of 5

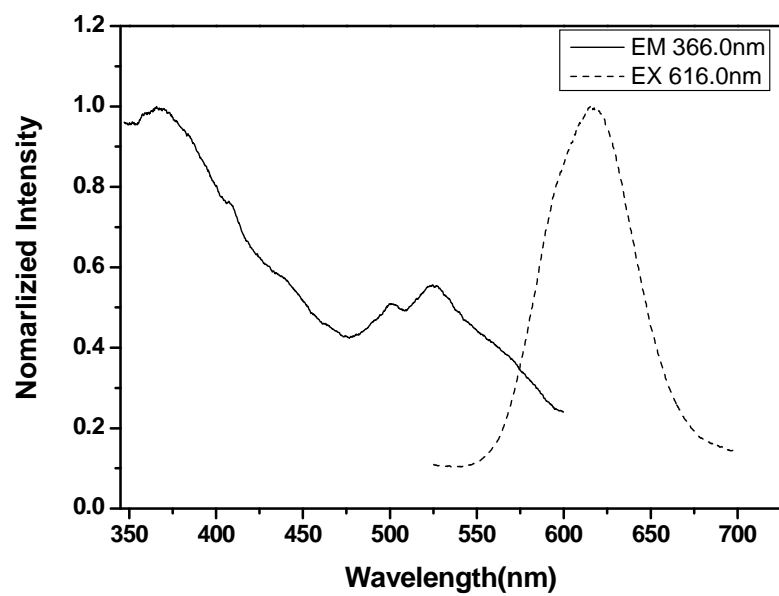


**Figure S3.** Emission spectra of **2** and **2** with  $\text{CHCl}_3$  in the solid state.

Excitation at 367 nm.



**Figure S4.** Excitation and emission spectra of **3** in the solid state



**Figure S7.** Excitation and emission spectra of **5** in the solid state