

Figure S1. The  $\pi$ - $\pi$  stacking make the traps intercross each other in the form of (4, 4) lattice along the  $c$  direction in compound **2**.

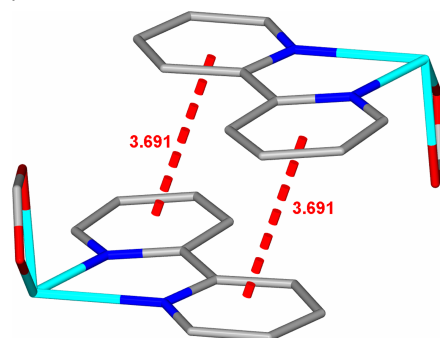
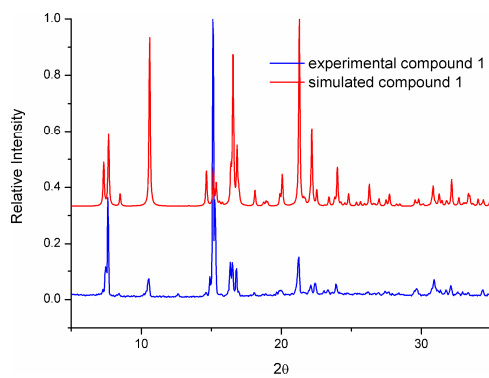
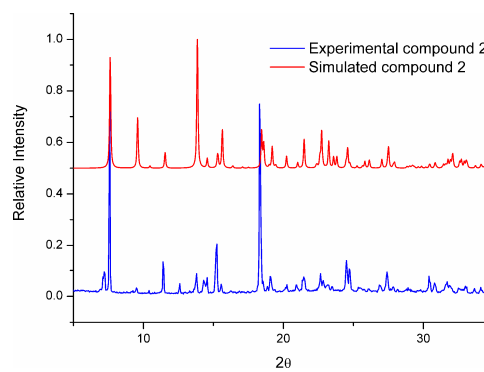


Figure S2. The  $\pi$ - $\pi$  stacking between the 2, 2'-bipy molecule in compound **4**.



(1)



(2)

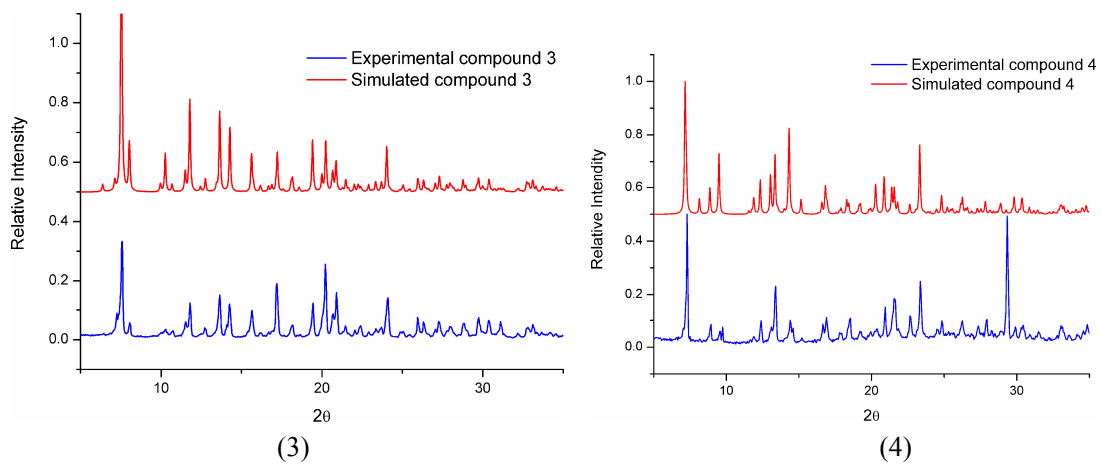


Figure S3. X-ray powder diffraction (XPD) patterns of compounds **1-4**.