## A Cd(II) Coordination Polymer based on mixed ligands: Synthesis, Crystal Structure, and Properties

Shuai-Shuai Han, Zi-Wei He, Lei Li and Shui-Sheng Chen\*



Scheme 1: The synthesis method of 1-(4-(1H-imidazol-5-yl) phenyl)-1H-1,2,4-triazole

## 1. Synthesis of 4-(1H-1,2,4-triazol-1-yl)benzaldehyde (I)

10 mmol of 4-fluorobenzaldehyde and potassium carbonate anhydrous (2.76 g, 20 mmol) were dissolved in 30 mL of dimethyl sulfoxide and reacted at 130 °C for 24 h. Then, solvent was poured into water and the resulting residue was filtered. The crude products were recrystallized from hexanes to get 4-(1H-1,2,4-triazol-1-yl)benzaldehyde (I, yield of 86%).

2. Synthesis of N-(dimethylsulfamoyl)-p-fluorobenzaldimine (II)

10 mmol of 4-(1H-1,2,4-triazol-1-yl)benzaldehyde and 1.24 g (10 mmol) of *N*,*N*-dimethylsulfamide were dissolved in 50 mL of benzene and refluxed for 10 h. Then, solvent was removed under reduced pressure to get residue, then, the residue was dissolved in ethyl acetate and filtered. After removing ethyl acetate under reduced pressure, the crude products were recrystallized from hexanes to get N-(dimethylsulfamoyl)-p-fluorobenzaldimine (II, yield of 72%).

 Synthesis of 5-(4-(1H-1,2,4-triazol-1-yl)phenyl)-N,N-dimethyl-1H-imidazole-1-sulfonamide (III)

A mixure of (dimethylsulfamoyl)-p-fluorobenzaldimine (2.30g, 10mmol) and TosMIC (2.0 g, 10 mmol), K<sub>2</sub>CO<sub>3</sub> (3.0 g, 20 mmol) in MeOH (30 mL) was refluxed for 1 h. After cooling, 100 mL water was pour into the reaction mixture, then the mixture was poured in 100 mL of water and extracted with ethyl acetate (2 x 100 mL) to get 5-(4-(1H-1,2,4-triazol-1-yl)phenyl)-N,N-dimethyl-1H-imidazole-1-sulfonamide (III, yield of 65%).

4. The synthesis of 1-(4-(1H-imidazol-5-yl) phenyl)-1H-1,2,4-triazole (L)

The compound of L can easily be got by the reaction of III (3018 g, 10 mmol) by 5 h of reflux with 40 % HBr. After the reaction finished, yellow solid was washed with acetone to get purpose compound of 1-(4-(1H-imidazol-5-yl)phenyl)-1H-1,2,4-triazole (L, yield of 91%). IR(KBr): 3118(s), 1564(w), 1523(s), 1401(vs), 1276(m), 1227(w), 1148(m), 1065(m), 984(m), 969(m), 937(m), 839(m), 772(w), 672(m), 618(m), 527(w) cm<sup>-1</sup>. <sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 400 MHz): ( $\delta$  = 9.30 (s, 1H), 8.24 (s, 1H), 7.95 (d, 2H), 7.85 (d, 2H), 7.77 (s, 1H), 7.71 (s, 1H).



Figure S1. The IR spectra for L ligand.



Figure S2. The <sup>1</sup>H NMR for L molecule.