Electronic Supplementary Material (ESI) for CrystEngComm

Supplementary Materials

The multifunctional roles of the ionic liquid [Bmim][BF_4] in the creation of cadmium metal-organic frameworks

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Physical Measurements

All chemicals employed in this study were analytical reagents and commercially available without further purification. The purity of all samples has been confirmed by XRD patterns before physical measurements. The infrared spectra were taken on a PerKin-Elmer spectrum one FT-IR spectrometer in the 4000-400 cm^{-1} region by using KBr pellets. Powder X-ray diffraction patterns were recorded on a Rigaku Dmax/2500 diffractometer using Cu$K\alpha$ radiation or a PANalytical X'Pert PRO diffractometer using Cu$K\alpha$ radiation. a Rigaku SCXmini CCD diffractometer for compound **4** with graphite-monochromated Mo$K\alpha$ radiation (□λ □= 0.71073 Å) at room temperature. The structures were solved by direct methods and refined by full-matrix least-squares on F^2 using the SHELX97 program package. Thermogravimetric analyses (TGA) were carried out on a METTLER TGA/SDTA851e thermal analyzer on the pure polycrystalline samples from room temperature to ~500 °C in a ramp rate of 10 °C/min in a dynamic N_2 atmosphere. Photoluminescence analyses were recorded on a Perkin-Elmer LS 55 luminescence spectrometer with an R928 red-sensitive photomultiplier without correction. C, H, N elemantal analyses were performed on a German Elementary Vario EL III instrument.

Experiment detail of compound 4

$Cd_3F_2(C_2O_4)(ina)_2$ (**4**): $Cd(NO_3)_2{\cdot}4H_2O$ (1.5 mmol, 0.450 g) and isonicotinate (0.5 mmol, 0.123 g) in *ca.* 1.0 g $BmimBF_4$ were mixed in a 20 mL stainless steel reactor with a Teflon liner, the sample was heated at 160 °C for 6 days and then cooled to room temperature. Yellow lathe crystals of **4** and indefinite yellow powder was obtained by filtration. The crystalline products were selected by hand. Anal. calc. for $Cd_3F_2C_{14}H_8N_2O_8$: C, 23.77%; H, 1.14%; N, 3.96%. Found: C, 23.33%; H, 1.21%; N, 3.77%.

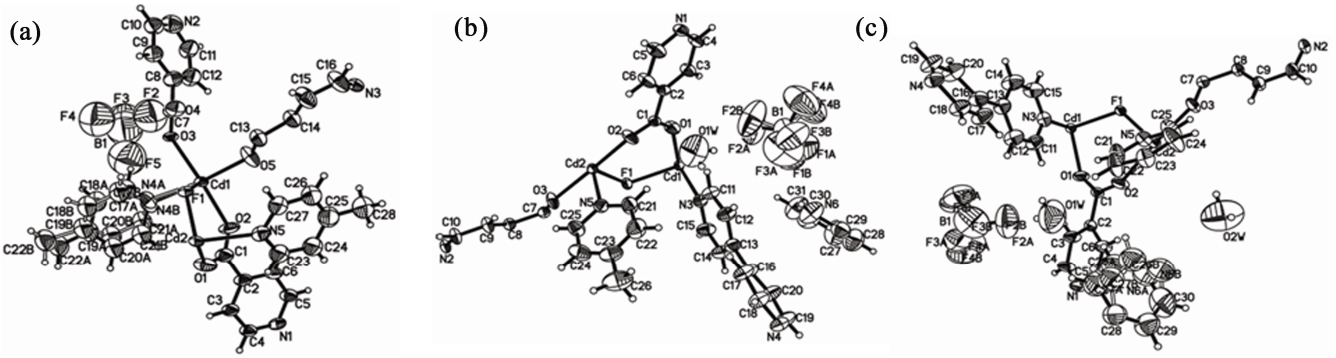

Fig. S1 *ORTEP* plots showing the crystallographically asymmetric units of compounds **1** (a), **2** (b) and **3** (c); thermal ellipsoids are given at the 50% probability level.

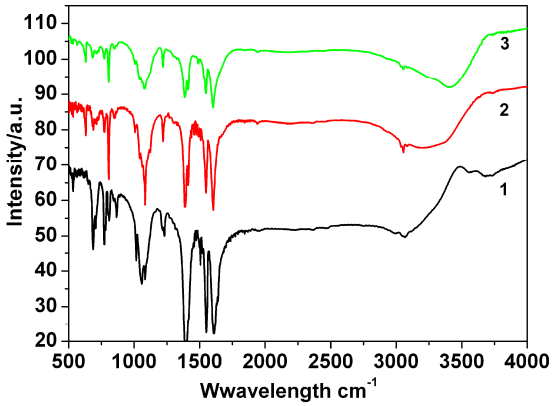

Fig. S2 FT-IR spectra of compounds **1**, **2,** and **3**.

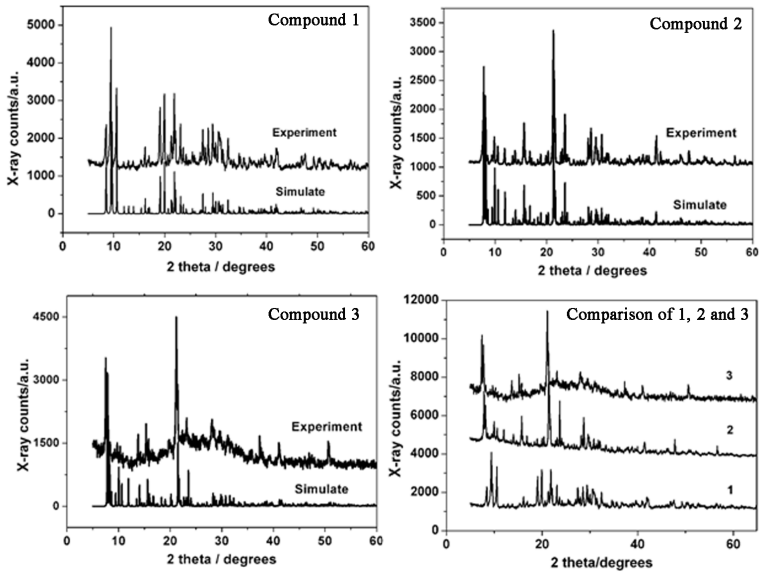

Fig. S3 The PXRD patterns of compounds **1-3** are in good agreement with their simulated PXRD patterns calculated from the single crystal X-ray data.