Two dimethylphenyl imidazole dicarboxylate-based lanthanide metal–organic frameworks for luminescence sensing of benzaldehyde

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Supporting information

IR characterization

The IR spectra display characteristic absorption bands for carboxylate, imidazolyl units, phenyl units. Compounds **1** and **2** show absorption bands in the range of 3400-3500 cm⁻¹, which may be attributed to $v_{\text{N-H}}$ or $v_{\text{O-H}}$ stretching frequencies of the imidazole ring or carboxylate group, respectively. The coordination of the carboxylate can be seen from the absorption bands in the frequency range 1381-1633 cm⁻¹ in **1** and **2** due to vas(COO-) and vs(COO-) vibrations respectively. The strong bands in the range of 2919-3154 cm⁻¹ and broad absorption bands in the range of 1633-1548 cm⁻¹ in complexes **1** and **2** imply the C=N and C=C stetching bands of imidazole ring in H3DMPhIDC. The characteristic IR band of the phenyl ring at 733-879 cm⁻¹ is due to δ =C-H vibrations. In conclusion, the infrared spectral data of the complexes **1** and **2** are consistent with crystal structure analysis.

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Figure S1. Powder X-ray diffraction patterns of (a) simulated from the crystal data of **1** (b) as-synthesized **1**, and the diffraction patterns of **1** obtained after the introduction of various solvents: (c) ethanol, (d) benzaldehyde.



Figure S2. Powder X-ray diffraction patterns of (a) simulated from the crystal data of **2**. (b) as-synthesized **2**, and the diffraction patterns of **2** obtained after the introduction of various solvents: (c) ethanol, (d) benzaldehyde.



Figure S3. (a) Emission spectrum of 1 in solid state excited at 345 nm. (b) Emission spectrum of 2 in solid state excited at 332 nm.



(b)

Figure S4. (a) Emissive response spectra of 1 for *m*-methylbenzaldehyde in acetone solution with different *m*-methylbenzaldehyde volume concentrations (insert is graph of the fluorescent intensity of 1 acetone as a function of *m*-methylbenzaldehyde content). (b) Emissive response spectra of 2 for *m*-methylbenzaldehyde in acetone solution with different *m*-methylbenzaldehyde volume concentrations (insert is graph of the fluorescent intensity of 2 for *m*-methylbenzaldehyde in acetone solution with different *m*-methylbenzaldehyde volume concentrations (insert is graph of the fluorescent intensity of 2 acetone as a function of *m*-methylbenzaldehyde content).