Supplementary Materials: Luminescence and Magnetic Properties of Two Three-dimensional Terbium and Dysprosium MOFs Based on Azobenzene-4,4'-Dicarboxylic Linker

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1. Bond Distances and Angles

| Bond | Bond distances (Å) | Bond | Bond angles (°) | Bond | Bond angles (°) |
|---------|--------------------|-------------|-----------------|-------------|-----------------|
| Tb1–O1B | 2.307(4) | O1B-Tb1-O1A | 148.16(14) | O2W-Tb1-O4A | 126.79(12) |
| Tb1–O1A | 2.317(3) | O1B-Tb1-O2A | 88.23(13) | O1B-Tb1-O3W | 78.28(12) |
| Tb1–O2A | 2.358(3) | O1A-Tb1-O2A | 98.34(12) | O1A-Tb1-O3W | 73.60(13) |
| Tb1–O2B | 2.372(4) | O1B-Tb1-O2B | 108.51(13) | O2A-Tb1-O3W | 74.68(12) |
| Tb1–O2W | 2.386(4) | O1A-Tb1-O2B | 84.99(13) | O2B-Tb1-O3W | 140.56(12) |
| Tb1–O4A | 2.407(3) | O2A-Tb1-O2B | 142.37(13) | O2W-Tb1-O3W | 139.35(12) |
| Tb1–O3W | 2.467(4) | O1B-Tb1-O2W | 72.84(13) | O4A-Tb1-O3W | 71.57(12) |
| Tb1–O1C | 2.497(4) | O1A-Tb1-O2W | 138.99(13) | O1B-Tb1-O1C | 143.11(13) |
| | | O2A-Tb1-O2W | 76.40(13) | O1A-Tb1-O1C | 68.11(13) |
| | | O2B-Tb1-O2W | 76.90(13) | O2A-Tb1-O1C | 75.40(13) |
| | | O1B-Tb1-O4A | 77.20(12) | O2B-Tb1-O1C | 71.20(12) |
| | | O1A-Tb1-O4A | 79.96(12) | O2W-Tb1-O1C | 71.27(13) |
| | | O2A-Tb1-O4A | 145.26(13) | O4A-Tb1-O1C | 132.86(12) |
| | | O2B-Tb1-O4A | 72.34(13) | O3W-Tb1-O1C | 126.44(12) |

| Table S1. Selected bond distances | s (Å |) and angles | (°) 1 |
|-----------------------------------|------|--------------|-------|
| Table 51. Selected Dond distances | 5 (Л |) and angles | |

2. LeBail Refinement

Compound **2** is isostructural to **1**. We realized a LeBail refinement (Figure S4) with TOPAS software to establish the purity and the unit cell of the powders pertaining to this material.





Figure S1. Lebail Refinement for **2**: *a* = 9.93, *b* = 11.67, *c* = 16.70, *α* = 106.37, *β* = 100.98, *γ* = 100.53, *V* = 1765.77, *sample displacement* = -0.151 mm.

3. Pore Size Distribution



Figure S2. Pore size distribution.

4. Magnetic Properties



Figure S3. Curie-Weiss fit of the χ_{M^1} *vs. T* curves of compounds **1** (top) and **2** (bottom).

5. TGA Spectra



Figure S4. TGA spectra of MOFs 1 (green) and 2 (blue).

6. UV Spectra

Steady-state measurements were performed using a Hewlett Packard diode array spectrophotometer (model 8453; Nortwalk, CT, USA) interfaced to a Pentium MMX 200 microcomputer via an HP IB interface board for absorption measurement.



Figure S5. UV spectra of compounds 1 (dark blue) and 2 (sky-blue).



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