

Three 3D Ln^{III}-MOFs based on a nitro-functionalized biphenyltricarboxylate Ligand: syntheses, structures, and magnetic properties

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Table S1 Selected bond lengths [Å] and angles [°] for **1**.

| MOF 1 | | | |
|--------------|------------|--------------|------------|
| Pr1-O2A | 2.373(4) | Pr1-O1 | 2.381(4) |
| Pr1-O4B | 2.423(4) | Pr1-O20 | 2.497(4) |
| Pr1-O12C | 2.529(4) | Pr1-O9 | 2.541(4) |
| Pr1-O19 | 2.576(5) | Pr1-O10 | 2.684(4) |
| Pr1-O11C | 2.698(4) | Pr2-O14D | 2.347(4) |
| Pr2-O17 | 2.475(5) | Pr2-O10 | 2.483(3) |
| Pr2-O11C | 2.483(4) | Pr2-O3B | 2.491(4) |
| Pr2-O5D | 2.528(4) | Pr2-O18 | 2.531(5) |
| Pr2-O6D | 2.533(4) | | |
| O2A-Pr1-O4B | 161.86(15) | O2A-Pr1-O1 | 96.01(15) |
| O1-Pr1-O4B | 78.33(14) | O2A-Pr1-O20 | 89.10(19) |
| O1-Pr1-O20 | 138.8(2) | O4B-Pr1-O20 | 84.29(19) |
| O2A-Pr1-O12C | 75.19(14) | O1-Pr1-O12C | 146.64(16) |
| O4B-Pr1-O12C | 118.73(13) | O20-Pr1-O12C | 74.1(2) |
| O2A-Pr1-O9 | 75.66(15) | O1-Pr1-O9 | 70.43(15) |
| O4B-Pr1-O9 | 117.49(12) | O20-Pr1-O9 | 149.2(2) |

| | | | |
|---------------|------------|---------------|------------|
| O12C-Pr1-O9 | 76.21(15) | O2A-Pr1-O19 | 72.36(18) |
| O1-Pr1-O19 | 72.57(16) | O4B-Pr1-O19 | 89.51(16) |
| O20-Pr1-O19 | 70.21(18) | O12C-Pr1-O19 | 131.34(17) |
| O9-Pr1-O19 | 127.31(15) | O2A-Pr1-O10 | 125.25(15) |
| O1-Pr1-O10 | 70.47(13) | O4B-Pr1-O10 | 69.44(12) |
| O20-Pr1-O10 | 136.14(15) | O12C-Pr1-O10 | 88.23(14) |
| O9-Pr1-O10 | 49.64(11) | O19-Pr1-O10 | 140.32(15) |
| O2A-Pr1-O11C | 123.96(13) | O1-Pr1-O11C | 132.83(12) |
| O4B-Pr1-O11C | 69.79(12) | O20-Pr1-O11C | 71.99(16) |
| O12C-Pr1-O11C | 49.14(12) | O9-Pr1-O11C | 94.33(13) |
| O19-Pr1-O11C | 138.32(14) | O10-Pr1-O11C | 66.27(11) |
| O14D-Pr2-O17 | 86.1(2) | O14D-Pr2-O10 | 93.63(14) |
| O17-Pr2-O10 | 141.95(17) | O14D-Pr2-O11C | 154.52(13) |
| O17-Pr2-O11C | 91.83(18) | O10-Pr2-O11C | 72.65(12) |
| O14D-Pr2-O3B | 83.92(15) | O17-Pr2-O3B | 142.60(18) |
| O10-Pr2-O3B | 74.75(13) | O11C-Pr2-O3B | 111.77(13) |
| O14D-Pr2-O5D | 129.25(13) | O17-Pr2-O5D | 74.8(2) |
| O10-Pr2-O5D | 129.68(13) | O11C-Pr2-O5D | 74.04(13) |
| O3B-Pr2-O5D | 84.03(15) | O14D-Pr2-O18 | 79.40(17) |
| O17-Pr2-O18 | 70.5(2) | O10-Pr2-O18 | 72.06(16) |
| O11C-Pr2-O18 | 75.99(16) | O3B-Pr2-O18 | 141.55(19) |
| O5D-Pr2-O18 | 132.75(19) | O14D-Pr2-O6D | 77.97(14) |
| O17-Pr2-O6D | 70.53(19) | O10-Pr2-O6D | 146.50(15) |
| O11C-Pr2-O6D | 125.12(13) | O3B-Pr2-O6D | 72.15(16) |
| O5D-Pr2-O6D | 51.42(13) | O18-Pr2-O6D | 135.82(17) |

A -x+2,-y+1,-z+3; B -x+2,-y+1,-z+2; C x-y,x-1,-z+3; D x-y,x-1,-z+2.

Table S2 Selected bond lengths [Å] and angles [°] for **2**.

MOF **2**

| | | | |
|-------------|------------|-------------|------------|
| Gd1-O5A | 2.297(3) | Gd1-O9 | 2.355(3) |
| Gd1-O1B | 2.376(3) | Gd1-O6C | 2.399(3) |
| Gd1-O4D | 2.475(3) | Gd1-O2 | 2.483(3) |
| Gd1-O3D | 2.550(3) | Gd1-O3E | 2.604(3) |
| Gd1-O1 | 2.737(3) | | |
| O5A-Gd1-O9 | 95.00(12) | O5A-Gd1-O1B | 87.05(12) |
| O9-Gd1-O1B | 144.37(9) | O5A-Gd1-O6C | 77.08(11) |
| O9-Gd1-O6C | 142.63(10) | O1B-Gd1-O6C | 72.46(9) |
| O5A-Gd1-O4D | 143.05(11) | N2-Gd1-O4D | 79.64(14) |
| O1B-Gd1-O4D | 77.82(14) | O6C-Gd1-O4D | 127.82(12) |
| O5A-Gd1-O2 | 70.81(12) | O9-Gd1-O2 | 79.51(12) |
| O1B-Gd1-O2 | 139.10(11) | O6C-Gd1-O2 | 69.30(12) |
| O4D-Gd1-O2 | 138.90(14) | O5A-Gd1-O3D | 158.02(12) |
| O9-Gd1-O3D | 105.37(10) | O1B-Gd1-O3D | 81.17(9) |
| O6C-Gd1-O3D | 81.73(9) | O4D-Gd1-O3D | 51.63(9) |
| O2-Gd1-O3D | 106.91(10) | O5A-Gd1-O3E | 69.81(9) |
| O9-Gd1-O3E | 79.83(9) | O1B-Gd1-O3E | 67.52(9) |
| O6C-Gd1-O3E | 128.47(10) | O4D-Gd1-O3E | 73.27(11) |
| O2-Gd1-O3E | 129.58(10) | O3D-Gd1-O3E | 121.23(9) |
| O5A-Gd1-O1 | 119.71(10) | O9-Gd1-O1 | 67.44(9) |
| O1B-Gd1-O1 | 140.15(7) | O6C-Gd1-O1 | 84.73(9) |
| O4D-Gd1-O1 | 92.11(11) | O2-Gd1-O1 | 49.07(9) |
| O3D-Gd1-O1 | 63.18(8) | O3E-Gd1-O1 | 146.21(8) |

A -x+2, -y+1, -z+1; B x, -y+3/2, z+1/2; C -x+2, y+1/2, -z-1/2; D -x+1, y+1/2, -z+1/2; E -x+1, y+1/2, -z+1/2.

Table S3 Selected bond lengths [Å] and angles [°] for **3**.

MOF **3**

| | | | |
|---------|----------|---------|----------|
| Dy1-O4A | 2.288(4) | Dy1-O2B | 2.294(5) |
| Dy1-O1 | 2.316(4) | Dy1-O3C | 2.348(4) |

| | | | |
|-------------|------------|-------------|------------|
| Dy1-O10 | 2.378(5) | Dy1-O9 | 2.452(4) |
| Dy1-O6D | 2.457(4) | Dy1-O5D | 2.486(4) |
| O4A-Dy1-O2B | 149.54(17) | O4A-Dy1-O1 | 84.18(18) |
| O2B-Dy1-O1 | 106.54(18) | O4A-Dy1-O3C | 99.47(16) |
| O2B-Dy1-O3C | 85.65(18) | O1-Dy1-O3C | 149.44(18) |
| O4A-Dy1-O10 | 139.43(18) | O2B-Dy1-O10 | 71.01(17) |
| O1-Dy1-O10 | 78.3(2) | O3C-Dy1-O10 | 79.58(17) |
| O4A-Dy1-O9 | 69.10(16) | O2B-Dy1-O9 | 140.03(17) |
| O1-Dy1-O9 | 79.81(17) | O3C-Dy1-O9 | 73.43(18) |
| O10-Dy1-O9 | 71.92(16) | O4A-Dy1-O6D | 80.42(15) |
| O2B-Dy1-O6D | 74.43(17) | O1-Dy1-O6D | 77.73(16) |
| O3C-Dy1-O6D | 132.83(15) | O10-Dy1-O6D | 129.62(15) |
| O9-Dy1-O6D | 143.62(16) | O4A-Dy1-O5D | 74.20(16) |
| O2B-Dy1-O5D | 76.95(16) | O1-Dy1-O5D | 128.08(16) |
| O3C-Dy1-O5D | 81.53(15) | O10-Dy1-O5D | 143.74(18) |
| O9-Dy1-O5D | 130.67(15) | O6D-Dy1-O5D | 52.73(13) |

A -x+1,-y-1,-z+1; B -x+1,-y-1,-z; C x,y-1,z-1; D x-1,y-1,z-1.

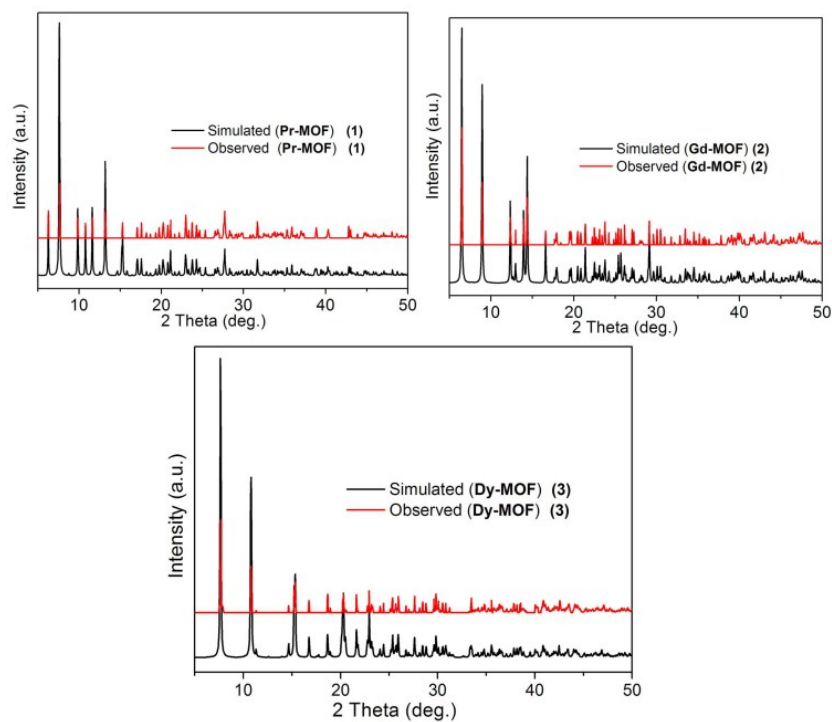


Fig. S1 Powder X-ray diffraction patterns of **1-3**.

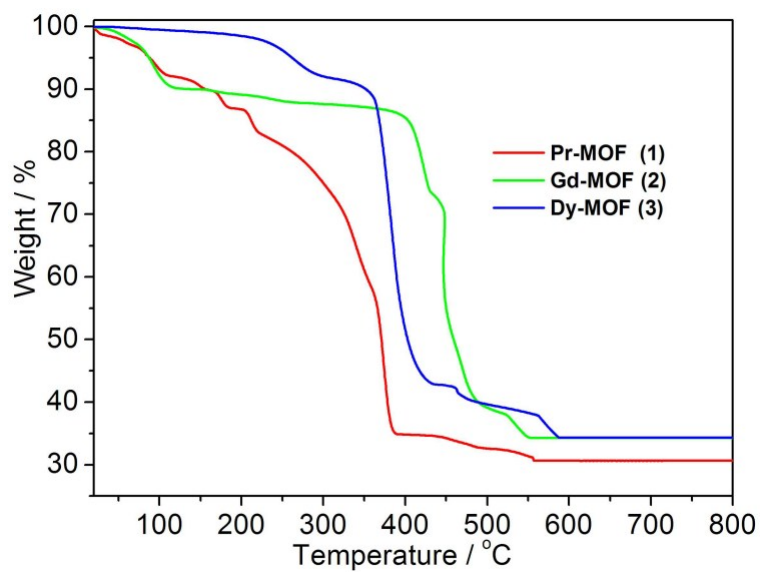


Fig. S2 TGA curve for **1-3**.

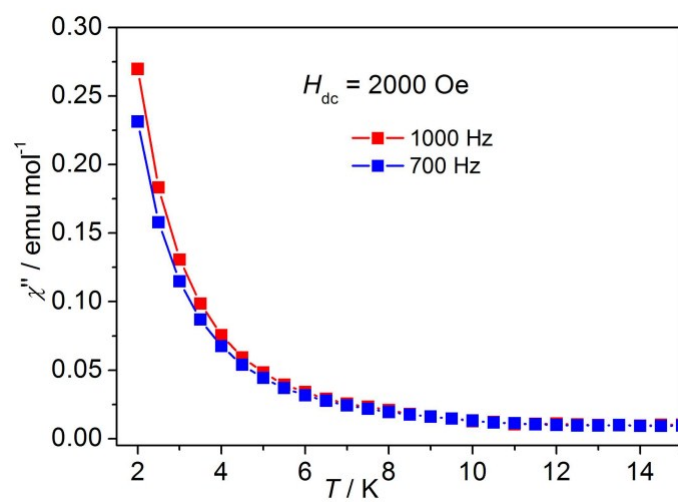


Fig. S3 Temperature-dependent out-of-phase (χ'') ac susceptibilities for Dy-MOF (**3**) under 2000 Oe dc field.