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Data Article

# Structural data of thermostable 3D Ln-MOFs that based on flexible ligand of 1,3-adamantanediacetic acid

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ABSTRACT

In this data article, we present the structural and PARD data of the Ln-MOFs. Detailed structure, luminescence and sensing properties were discussed in our previous study (Zeng et al., in press) [1] The data includes the SBU structure patterns of these Ln-MOFs, thermostability of Ln-MOFs in water and also detailed structure information listed in Tables 1–8.



**Specifications Table** [Please fill in right-hand column of the table below.]

| | |
|---|---|
| Subject area | *Chemistry* |
| More specific subject area | *Single crystal data of lanthanide complexes* |
| Type of data | *Table, figure* |
| How data was acquired | *Crystallography open data base and crystallographic tool – Diamond: Crystallographic Information File Code: 1562078–1562085.cif* |
| Data format | *Analyzed* |
| Experimental factors | *Single crystal X-ray diffraction data was collected on a Bruker SMART 1000 CCD at 293(2) K, with Mo-Ka radiation (0.71073Å) at room temperature. The* |

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| | |
|---|---|
| | *structure was refined by full-matrix least-squares methods with SHELXL-97 module. The eight structures are isostructural, they crystallize in monoclinic space group C2/c (no. 15).* |
| Experimental features | *Needle like colorless single crystal.* |
| Data source location | *Jiangxi Normal University, Nanchang, China.* |
| Data accessibility | *The data are with this article.* |
| Related research article | *K. Zheng, Z.-Q. Liu, Y. Huang, F. Chen, C.-H. Zeng, S. Zhong, et al., Highly Luminescent Ln-MOFs Based on 1,3-Adamantanediacetic Acid as Bifunctional Sensor, Sensors and Actuators B: Chemical, in press.* |

**Value of the data**

- This data would be valuable for further studies of lanthanide complexes that based on flexible ligand.
- This data would be valuable for the further studies of lanthanide complexes that coordinated by phen.
- This data provide a new way to synthesize thermostable lanthanide complexes.

## 1. Data

The crystal structures of isostructural **1a**-**1h** have the same chemical formula of $[Ln(ADA)_{1.5}(phen)]_n$ ($Ln^{3+}$ = $Eu^{3+}$ **1a**, $Gd^{3+}$ **1b**, $Tb^{3+}$ **1c**, $La^{3+}$ **1d**, $Ce^{3+}$ **1e**, $Pr^{3+}$ **1f**, $Nd^{3+}$ **1g**, $Y^{3+}$ **1h**, 1,10-phenanthroline = phen) [1]. *Since they are isostructural data, as an example, the crystal structure of **1a** is described in somewhat greater detail.* As shown in Fig. 1, two crystallographically independent $Eu^{3+}$ are bridged by two carboxyl and two O, each dinuclear second building unit (SBU) contains two $Eu^{3+}$, two phen and three fully deprotonated ADA, forming a electroneutral unit. Two phen arranged at two ends of the dinuclear cluster (Fig. 2). The coordination environment of the nine-coordinated $Eu^{3+}$ center consists seven O and two N. Detailed information about selected bond lengths and angles for **1a**–**1h** are listed in Tables 1–8, they show that the bond lengths and angles are in the normal value as our previous reports [2–9]. PXRD patterns of **1a** that incubation in $H_2O$ for 24 h competes well with the simulated single crystal data and the as synthesized sample, confirming **1a** has high stability in water and also has high stability while sensing (Fig. 3).

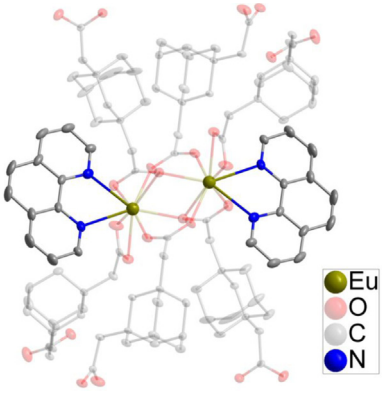


**Fig. 1.** The SBU structure shows the coordination environment of the metal ions, two chelated phen arranged at two ends of the dinuclear cluster.

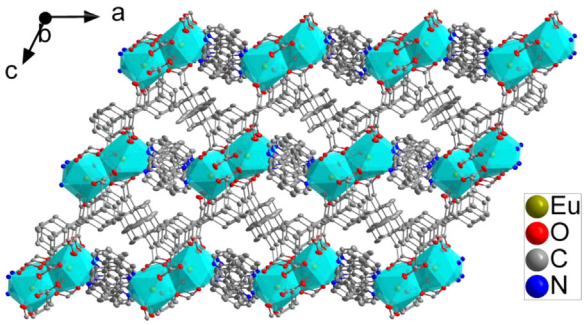


**Fig. 2.** The 3D Ln-MOFs structure of **1a** view from the ob direction.

**Table 1**
Selected bond lengths and bond angles of **1a**.

| | | | |
|---|---|---|---|
| Eu(1)-O(1) | 2.3751(14) | Eu(1)-N(2) | 2.5961(16) |
| Eu(1)-O(2) | 2.3779(13) | Eu(1)-N(1) | 2.6563(16) |
| Eu(1)-O(4) | 2.3802(14) | Eu(1)-O(4)#1 | 2.7171(15) |
| Eu(1)-O(8) | 2.4397(14) | Eu(1)-C(14) | 2.8253(19) |
| Eu(1)-O(7) | 2.4749(14) | Eu(1)-C(15) | 2.9887(19) |
| Eu(1)-O(3) | 2.4859(14) | Eu(1)-Eu(1)#1 | 3.9681(2) |
| O(1)-Eu(1)-O(2) | 136.90(5) | O(1)-Eu(1)-O(4)#1 | 76.74(5) |
| O(1)-Eu(1)-O(4) | 73.03(5) | O(2)-Eu(1)-O(4)#1 | 97.21(5) |
| O(2)-Eu(1)-O(4) | 75.65(5) | O(4)-Eu(1)-O(4)#1 | 165.75(5) |
| O(1)-Eu(1)-O(8) | 127.43(5) | O(8)-Eu(1)-O(4)#1 | 87.00(5) |
| O(2)-Eu(1)-O(8) | 75.10(5) | O(7)-Eu(1)-O(4)#1 | 71.15(5) |
| O(4)-Eu(1)-O(8) | 81.74(5) | O(3)-Eu(1)-O(4)#1 | 101.67(5) |
| O(1)-Eu(1)-O(7) | 83.91(5) | N(2)-Eu(1)-O(4)#1 | 143.89(5) |
| O(2)-Eu(1)-O(7) | 128.06(5) | N(1)-Eu(1)-O(4)#1 | 157.58(5) |
| O(4)-Eu(1)-O(7) | 95.22(5) | O(1)-Eu(1)-C(14) | 24.14(5) |
| O(8)-Eu(1)-O(7) | 52.96(5) | O(2)-Eu(1)-C(14) | 89.84(5) |
| O(1)-Eu(1)-O(3) | 102.46(5) | O(4)-Eu(1)-C(14) | 80.90(5) |
| O(2)-Eu(1)-O(3) | 71.88(5) | O(8)-Eu(1)-C(14) | 25.13(5) |
| O(4)-Eu(1)-O(3) | 123.75(5) | O(7)-Eu(1)-C(14) | 165.57(5) |
| O(8)-Eu(1)-O(3) | 129.69(5) | O(3)-Eu(1)-C(14) | 72.15(5) |
| O(7)-Eu(1)-O(3) | 140.83(5) | N(2)-Eu(1)-C(14) | 72.95(4) |
| O(1)-Eu(1)-N(2) | 135.35(5) | N(1)-Eu(1)-C(14) | 77.96(5) |
| O(2)-Eu(1)-N(2) | 82.69(5) | O(4)#1-Eu(1)-C(14) | 145.45(5) |
| O(4)-Eu(1)-N(2) | 150.43(5) | O(1)-Eu(1)-C(15) | 156.06(5) |
| O(8)-Eu(1)-N(2) | 73.32(5) | O(2)-Eu(1)-C(15) | 49.26(4) |
| O(7)-Eu(1)-N(2) | 82.42(5) | O(4)-Eu(1)-C(15) | 114.73(5) |
| O(3)-Eu(1)-N(2) | 65.81(5) | O(8)-Eu(1)-C(15) | 95.79(5) |
| O(1)-Eu(1)-N(1) | 73.00(5) | O(7)-Eu(1)-C(15) | 106.22(6) |
| O(2)-Eu(1)-N(1) | 135.22(5) | O(3)-Eu(1)-C(15) | 101.45(5) |
| O(4)-Eu(1)-N(1) | 145.73(5) | N(2)-Eu(1)-C(15) | 87.99(5) |
| O(8)-Eu(1)-N(1) | 116.30(5) | N(1)-Eu(1)-C(15) | 26.35(5) |
| O(7)-Eu(1)-N(1) | 76.85(5) | O(4)#1-Eu(1)-C(15) | 26.61(5) |
| O(3)-Eu(1)-N(1) | 68.60(5) | C(14)-Eu(1)-C(15) | 142.43(5) |
| N(2)-Eu(1)-N(1) | 62.54(5) | | |

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2, -y+3/2, -z; #2 -x, y, -z-1/2; #3 -x+1/2, y+1/2, -z+1/2; #4 -x+1/2, y-1/2, -z+1/2.

**Table 2**
Selected bond lengths and bond angles of **1b**.

| | | | |
|---|---|---|---|
| Gd(1)-O(2)#1 | 2.451(3) | Gd(1)-N(1) | 2.675(3) |
| Gd(1)-O(1) | 2.455(3) | Gd(1)-N(2) | 2.732(3) |
| Gd(1)-O(6)#1 | 2.463(3) | Gd(1)-O(6) | 2.751(3) |
| Gd(1)-O(4)#2 | 2.506(3) | Gd(1)-C(14)#2 | 2.900(3) |
| Gd(1)-O(3)#2 | 2.554(3) | Gd(1)-C(15) | 3.041(3) |
| Gd(1)-O(5) | 2.567(3) | Gd(1)-Gd(1)#1 | 4.0419(4) |
| O(2)#1-Gd(1)-O(1) | 136.41(9) | N(1)-Gd(1)-C(14)#2 | 76.19(9) |
| O(2)#1-Gd(1)-O(6)#1 | 74.81(9) | N(2)-Gd(1)-C(14)#2 | 97.41(10) |
| O(1)-Gd(1)-O(6)#1 | 72.69(9) | O(6)-Gd(1)-C(14)#2 | 167.91(9) |
| O(2)#1-Gd(1)-O(4)#2 | 75.64(9) | O(2)#1-Gd(1)-C(15) | 70.67(9) |
| O(1)-Gd(1)-O(4)#2 | 127.59(10) | O(1)-Gd(1)-C(15) | 88.25(10) |
| O(6)#1-Gd(1)-O(4)#2 | 83.65(9) | O(6)#1-Gd(1)-C(15) | 101.55(9) |
| O(2)#1-Gd(1)-O(3)#2 | 127.00(9) | O(4)#2-Gd(1)-C(15) | 142.99(9) |
| O(1)-Gd(1)-O(3)#2 | 85.20(9) | O(3)#2-Gd(1)-C(15) | 157.89(9) |
| O(6)#1-Gd(1)-O(3)#2 | 96.61(10) | O(5)-Gd(1)-C(15) | 23.77(9) |
| O(4)#2-Gd(1)-O(3)#2 | 51.36(9) | O(2)#1-Gd(1)-O(6) | 72.66(8) |
| O(2)#1-Gd(1)-O(5) | 71.06(9) | O(1)-Gd(1)-O(6) | 73.03(9) |
| O(1)-Gd(1)-O(5) | 104.02(10) | O(6)#1-Gd(1)-O(6) | 78.49(9) |
| O(6)#1-Gd(1)-O(5) | 122.94(9) | O(4)#2-Gd(1)-O(6) | 146.69(9) |
| O(4)#2-Gd(1)-O(5) | 127.86(9) | O(3)#2-Gd(1)-O(6) | 158.18(9) |
| O(3)#2-Gd(1)-O(5) | 140.43(9) | O(5)-Gd(1)-O(6) | 48.43(8) |
| O(2)#1-Gd(1)-N(1) | 84.53(10) | N(1)-Gd(1)-O(6) | 112.97(8) |
| O(1)-Gd(1)-N(1) | 133.98(10) | N(2)-Gd(1)-O(6) | 94.09(8) |
| O(6)#1-Gd(1)-N(1) | 152.34(9) | O(2)#1-Gd(1)-C(14)#2 | 101.34(10) |
| O(4)#2-Gd(1)-N(1) | 73.40(9) | O(1)-Gd(1)-C(14)#2 | 106.80(10) |
| O(3)#2-Gd(1)-N(1) | 81.15(10) | O(6)#1-Gd(1)-C(14)#2 | 89.86(9) |
| O(5)-Gd(1)-N(1) | 64.63(9) | O(4)#2-Gd(1)-C(14)#2 | 25.70(10) |
| O(2)#1-Gd(1)-N(2) | 135.25(10) | O(3)#2-Gd(1)-C(14)#2 | 25.66(10) |
| O(1)-Gd(1)-N(2) | 73.11(10) | O(5)-Gd(1)-C(14)#2 | 140.48(9) |
| O(6)#1-Gd(1)-N(2) | 145.69(10) | N(1)-Gd(1)-C(15) | 88.38(9) |
| O(4)#2-Gd(1)-N(2) | 115.87(9) | N(2)-Gd(1)-C(15) | 79.98(9) |
| O(3)#2-Gd(1)-N(2) | 77.91(10) | O(6)-Gd(1)-C(15 | 24.68(9) |
| O(5)-Gd(1)-N(2) | 68.67(9) | C(14)#2-Gd(1)-C(15) | 163.41(10) |
| N(1)-Gd(1)-N(2) | 61.12(10) | | |

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y, -z+1; #2 ×+1/2, -y+1/2, z+1/2; #3 -x+1, y, -z+1/2; #4 ×-1/2, -y+1/2, z-1/2.

**Table 3**
Selected bond lengths and bond angles of **1c**.

| | | | |
|---|---|---|---|
| Tb(1)-O(6) | 2.3454(17) | Tb(1)-N(1) | 2.5730(18) |
| Tb(1)-O(2) | 2.3457(16) | Tb(1)-N(2) | 2.6375(18) |
| Tb(1)-O(1) | 2.3561(15) | Tb(1)-O(6)#2 | 2.775(2) |
| Tb(1)-O(3)#1 | 2.4232(15) | Tb(1)-C(14)#1 | 2.803(2) |
| Tb(1)-O(4)#1 | 2.4499(16) | Tb(1)-C(15) | 3.004(2) |
| Tb(1)-O(5) | 2.4514(16) | Tb(1)-Tb(1)#2 | 3.9815(2) |
| O(6)-Tb(1)-O(2) | 73.26(6) | O(5)-Tb(1)-N(2) | 68.73(6) |
| O(6)-Tb(1)-O(1) | 76.26(6) | N(1)-Tb(1)-N(2) | 63.11(6) |
| O(2)-Tb(1)-O(1) | 136.15(5) | N(1)-Tb(1)-C(14)#1 | 77.04(6) |
| O(6)-Tb(1)-O(3)#1 | 81.08(6) | N(2)-Tb(1)-C(14)#1 | 97.21(6) |
| O(2)-Tb(1)-O(3)#1 | 128.82(6) | O(6)#2-Tb(1)-C(14)#1 | 164.94(6) |
| O(1)-Tb(1)-O(3)#1 | 75.06(5) | O(6)-Tb(1)-C(15) | 101.89(6) |
| O(6)-Tb(1)-O(4)#1 | 94.30(7) | O(2)-Tb(1)-C(15) | 85.32(6) |
| O(2)-Tb(1)-O(4)#1 | 84.85(6) | O(1)-Tb(1)-C(15) | 70.95(5) |
| O(1)-Tb(1)-O(4)#1 | 128.48(5) | O(3)#1-Tb(1)-C(15) | 143.93(6) |
| O(3)#1-Tb(1)-O(4)#1 | 53.41(5) | O(4)#1-Tb(1)-C(15) | 157.75(6) |
| O(6)-Tb(1)-O(5) | 124.00(6) | O(5)-Tb(1)-C(15) | 23.83(5) |
| O(2)-Tb(1)-O(5) | 100.16(6) | O(6)-Tb(1)-O(6)#2 | 78.25(6) |
| O(1)-Tb(1)-O(5) | 72.18(6) | O(2)-Tb(1)-O(6)#2 | 71.34(6) |
| O(3)#1-Tb(1)-O(5) | 130.71(6) | O(1)-Tb(1)-O(6)#2 | 72.17(5) |
| O(4)#1-Tb(1)-O(5) | 141.35(6) | O(3)#1-Tb(1)-O(6)#2 | 144.49(5) |

**Table 3** (*continued*)

| | | | |
|---|---|---|---|
| O(6)-Tb(1)-N(1) | 149.90(6) | O(4)#1-Tb(1)-O(6)#2 | 156.17(5) |
| O(2)-Tb(1)-N(1) | 135.76(6) | O(5)-Tb(1)-O(6)#2 | 48.61(5) |
| O(1)-Tb(1)-N(1) | 82.12(6) | N(1)-Tb(1)-O(6)#2 | 114.75(5) |
| O(3)#1-Tb(1)-N(1) | 73.21(6) | N(2)-Tb(1)-O(6)#2 | 96.65(5) |
| O(4)#1-Tb(1)-N(1) | 82.92(6) | O(6)-Tb(1)-C(14)#1 | 86.99(6) |
| O(5)-Tb(1)-N(1) | 66.72(5) | O(2)-Tb(1)-C(14)#1 | 107.40(6) |
| O(6)-Tb(1)-N(2) | 145.39(6) | O(1)-Tb(1)-C(14)#1 | 101.62(6) |
| O(2)-Tb(1)-N(2) | 72.71(6) | O(3)#1-Tb(1)-C(14)#1 | 26.56(6) |
| O(1)-Tb(1)-N(2) | 135.27(6) | O(4)#1-Tb(1)-C(14)#1 | 26.86(6) |
| O(3)#1-Tb(1)-N(2) | 116.39(6) | O(5)-Tb(1)-C(14)#1 | 143.70(6) |
| O(4)#1-Tb(1)-N(2) | 76.57(6) | | |

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2, y+1/2, -z+1/2; #2 -x+1/2, -y+1/2, -z; #3 -x, y, -z-1/2; #4 -x+1/2, y-1/2, -z+1/2.

**Table 4**
Selected bond lengths and bond angles of **1d**.

| | | | |
|---|---|---|---|
| La(1)-O(3) | 2.4706(13) | La(1)-N(1) | 2.6995(16) |
| La(1)-O(4)#1 | 2.4786(14) | La(1)-N(2) | 2.7534(16) |
| La(1)-O(5) | 2.4866(13) | La(1)-O(5)#1 | 2.7712(13) |
| La(1)-O(2) | 2.5295(13) | La(1)-C(1) | 2.9250(18) |
| La(1)-O(1) | 2.5790(14) | La(1)-C(15)#1 | 3.0650(18) |
| La(1)-O(6)#1 | 2.5869(13) | La(1)-La(1)#1 | 4.0771(2) |
| O(3)-La(1)-O(4)#1 | 135.96(4) | N(1)-La(1)-C(1) | 76.01(5) |
| O(3)-La(1)-O(5) | 74.67(5) | N(2)-La(1)-C(1) | 97.56(5) |
| O(4)#1-La(1)-O(5) | 72.44(5) | O(5)#1-La(1)-C(1) | 168.33(5) |
| O(3)-La(1)-O(2) | 75.84(5) | O(3)-La(1)-C(15)#1 | 70.48(5) |
| O(4)#1-La(1)-O(2) | 128.06(5) | O(4)#1-La(1)-C(15)#1 | 88.19(5) |
| O(5)-La(1)-O(2) | 84.42(4) | O(5)-La(1)-C(15)#1 | 101.37(5) |
| O(3)-La(1)-O(1) | 126.80(4) | O(2)-La(1)-C(15)#1 | 142.69(5) |
| O(4)#1-La(1)-O(1) | 85.97(5) | O(1)-La(1)-C(15)#1 | 157.86(5) |
| O(5)-La(1)-O(1) | 97.18(5) | O(6)#1-La(1)-C(15)#1 | 23.55(4) |
| O(2)-La(1)-O(1) | 50.96(5) | O(3)-La(1)-O(5)#1 | 72.35(4) |
| O(3)-La(1)-O(6)#1 | 70.99(5) | O(4)#1-La(1)-O(5)#1 | 73.02(5) |
| O(4)#1-La(1)-O(6)#1 | 103.85(5) | O(5)-La(1)-O(5)#1 | 78.45(4) |
| O(5)-La(1)-O(6)#1 | 122.60(4) | O(2)-La(1)-O(5)#1 | 146.84(4) |
| O(2)-La(1)-O(6)#1 | 127.53(5) | O(1)-La(1)-O(5)#1 | 158.92(4) |
| O(1)-La(1)-O(6)#1 | 140.21(5) | O(6)#1-La(1)-O(5)#1 | 48.05(4) |
| O(3)-La(1)-N(1) | 85.16(5) | N(1)-La(1)-O(5)#1 | 112.44(4) |
| O(4)#1-La(1)-N(1) | 133.54(5) | N(2)-La(1)-O(5)#1 | 93.75(4) |
| O(5)-La(1)-N(1) | 153.15(5) | O(3)-La(1)-C(1) | 101.23(5) |
| O(2)-La(1)-N(1) | 73.42(5) | O(4)#1-La(1)-C(1) | 107.49(5) |
| O(1)-La(1)-N(1) | 80.71(5) | O(5)-La(1)-C(1) | 90.52(5) |
| O(6)#1-La(1)-N(1) | 64.45(4) | O(2)-La(1)-C(1) | 25.40(5) |
| O(3)-La(1)-N(2) | 135.03(5) | O(1)-La(1)-C(1) | 25.56(5) |
| O(4)#1-La(1)-N(2) | 73.37(5) | O(6)#1-La(1)-C(1) | 140.04(5) |
| O(5)-La(1)-N(2) | 145.73(5) | N(1)-La(1)-C(15)#1 | 87.99(5) |
| O(2)-La(1)-N(2) | 115.65(5) | N(2)-La(1)-C(15)#1 | 79.68(5) |
| O(1)-La(1)-N(2) | 78.19(5) | | |

Symmetry transformations used to generate equivalent atoms: #1 -x+3/2, -y+3/2, -z+1; #2 -x+3/2, y+1/2, -z+3/2; #3 -x+2, y, -z+3/2; #4 -x+3/2, y-1/2, -z+3/2.

**Table 5**
Selected bond lengths and bond angles of **1e**.

| | | | |
|---|---|---|---|
| Ce(1)-O(1) | 2.4498(14) | Ce(1)-N(1) | 2.6756(17) |
| Ce(1)-O(2)#1 | 2.4536(15) | Ce(1)-N(2) | 2.7296(17) |
| Ce(1)-O(6)#1 | 2.4653(14) | Ce(1)-O(6) | 2.7514(14) |
| Ce(1)-O(3)#2 | 2.5054(14) | Ce(1)-C(14)#2 | 2.9004(19) |
| Ce(1)-O(4)#2 | 2.5545(15)2. | Ce(1)-C(15) | 3.0425(19) |
| Ce(1)-O(5) | 5674(14) | Ce(1)-Ce(1)#1 | 4.0437(2) |
| O(1)-Ce(1)-O(2)#1 | 136.41(5) | O(1)-Ce(1)-O(6) | 76.15(5) |
| O(1)-Ce(1)-O(6)#1 | 74.85(5) | O(2)#1-Ce(1)-O(6) | 97.46(6) |
| O(2)#1-Ce(1)-O(6)#1 | 72.59(5) | O(6)#1-Ce(1)-O(6) | 167.96(5) |
| O(1)-Ce(1)-O(3)#2 | 75.48(5) | O(3)#2-Ce(1)-O(6) | 70.78(5) |
| O(2)#1-Ce(1)-O(3)#2 | 127.72(5) | O(4)#2-Ce(1)-O(6) | 88.20(5) |
| O(6)#1-Ce(1)-O(3)#2 | 83.75(5) | O(5)-Ce(1)-O(6) | 101.56(5) |
| O(1)-Ce(1)-O(4)#2 | 126.91(5) | N(1)-Ce(1)-O(6) | 142.91(5) |
| O(2)#1-Ce(1)-O(4)#2 | 85.32(5) | N(2)-Ce(1)-O(6) | 157.77(5) |
| O(6)#1-Ce(1)-O(4)#2 | 96.74(5) | O(1)-Ce(1)-C(14)#2 | 72.76(4) |
| O(3)#2-Ce(1)-O(4)#2 | 51.43(5) | O(2)#1-Ce(1)-C(14)#2 | 72.98(5) |
| O(1)-Ce(1)-O(5) | 71.15(5) | O(6)#1-Ce(1)-C(14)#2 | 78.51(5) |
| O(2)#1-Ce(1)-O(5) | 103.97(5) | O(3)#2-Ce(1)-C(14)#2 | 146.67(5) |
| O(6)#1-Ce(1)-O(5) | 122.94(5) | O(4)#2-Ce(1)-C(14)#2 | 158.25(5) |
| O(3)#2-Ce(1)-O(5) | 127.78(5) | O(5)-Ce(1)-C(14)#2 | 48.39(4) |
| O(4)#2-Ce(1)-O(5) | 140.29(5) | N(1)-Ce(1)-C(14)#2 | 112.91(5) |
| O(1)-Ce(1)-N(1) | 84.57(5) | N(2)-Ce(1)-C(14)#2 | 94.04(5) |
| O(2)#1-Ce(1)-N(1) | 133.93(5) | O(6)-Ce(1)-C(14)#2 | 101.17(6) |
| O(6)#1-Ce(1)-N(1) | 152.49(5) | O(1)-Ce(1)-C(15) | 106.94(6) |
| O(3)#2-Ce(1)-N(1) | 73.40(5) | O(2)#1-Ce(1)-C(15) | 89.93(5) |
| O(4)#2-Ce(1)-N(1) | 81.03(5) | O(6)#1-Ce(1)-C(15) | 25.70(6) |
| O(5)-Ce(1)-N(1) | 64.60(5) | O(3)#2-Ce(1)-C(15) | 25.73(6) |
| O(1)-Ce(1)-N(2) | 135.09(5) | O(4)#2-Ce(1)-C(15) | 140.41(5) |
| O(2)#1-Ce(1)-N(2) | 73.33(5) | O(5)-Ce(1)-C(15) | 23.74(5) |
| O(6)#1-Ce(1)-N(2) | 145.83(5) | | |

Symmetry transformations used to generate equivalent atoms: #1 -x+3/2, -y+3/2, -z+1; #2 -x+3/2, y+1/2, -z+3/2; #3 -x+2, y, -z+3/2; #4 -x+3/2, y-1/2, -z+3/2.

**Table 6**
Selected bond lengths and bond angles of **1f**.

| | | | |
|---|---|---|---|
| Pr(1)-O(4)#1 | 2.4320(14) | Pr(1)-N(2) | 2.6541(17) |
| Pr(1)-O(3)#2 | 2.4372(15) | Pr(1)-N(1) | 2.7111(18) |
| Pr(1)-O(5) | 2.4470(15) | Pr(1)-O(5)#3 | 2.7383(15) |
| Pr(1)-O(1) | 2.4905(15) | Pr(1)-C(1) | 2.883(2) |
| Pr(1)-O(2) | 2.5366(15) | Pr(1)-C(15)#3 | 3.029(2) |
| Pr(1)-O(6)#3 | 2.5482(15) | Pr(1)-Pr(1)#3 | 4.0220(2) |
| O(4)#1-Pr(1)-O(3)#2 | 136.70(5) | O(4)#1-Pr(1)-O(5)#3 | 72.92(5) |
| O(4)#1-Pr(1)-O(5) | 75.03(5) | O(3)#2-Pr(1)-O(5)#3 | 72.90(5) |
| O(3)#2-Pr(1)-O(5) | 72.75(5) | O(5)-Pr(1)-O(5)#3 | 78.42(5) |
| O(4)#1-Pr(1)-O(1) | 75.39(5) | O(1)-Pr(1)-O(5)#3 | 146.48(5) |
| O(3)#2-Pr(1)-O(1) | 127.39(6) | O(2)-Pr(1)-O(5)#3 | 157.62(5) |
| O(5)-Pr(1)-O(1) | 83.16(5) | O(6)#3-Pr(1)-O(5)#3 | 48.71(4) |
| O(4)#1-Pr(1)-O(2) | 127.15(5) | N(2)-Pr(1)-O(5)#3 | 113.45(5) |
| O(3)#2-Pr(1)-O(2) | 84.74(5) | N(1)-Pr(1)-O(5)#3 | 94.40(5) |
| O(5)-Pr(1)-O(2) | 96.29(6) | O(4)#1-Pr(1)-C(1) | 101.18(6) |
| O(1)-Pr(1)-O(2) | 51.76(5) | O(3)#2-Pr(1)-C(1) | 106.59(6) |
| O(4)#1-Pr(1)-O(6)#3 | 71.35(5) | O(5)-Pr(1)-C(1) | 89.43(5) |
| O(3)#2-Pr(1)-O(6)#3 | 103.83(5) | O(1)-Pr(1)-C(1) | 25.79(6) |
| O(5)-Pr(1)-O(6)#3 | 123.24(5) | O(2)-Pr(1)-C(1) | 25.97(6) |
| O(1)-Pr(1)-O(6)#3 | 128.26(5) | O(6)#3-Pr(1)-C(1) | 140.79(5) |
| O(2)-Pr(1)-O(6)#3 | 140.42(5) | N(2)-Pr(1)-C(1) | 76.22(5) |
| O(4)#1-Pr(1)-N(2) | 84.20(5) | N(1)-Pr(1)-C(1) | 97.41(6) |
| O(3)#2-Pr(1)-N(2) | 134.16(6) | O(5)#3-Pr(1)-C(1) | 167.47(5) |
| O(5)-Pr(1)-N(2) | 152.00(5) | O(4)#1-Pr(1)-C(15)#3 | 70.91(5) |

**Table 6** (*continued*)

| | | | |
|---|---|---|---|
| O(1)-Pr(1)-N(2) | 73.44(5) | O(3)#2-Pr(1)-C(15)#3 | 88.11(5) |
| O(2)-Pr(1)-N(2) | 81.33(6) | O(5)-Pr(1)-C(15)#3 | 101.63(5) |
| O(6)#3-Pr(1)-N(2) | 64.86(5) | O(1)-Pr(1)-C(15)#3 | 143.22(5) |
| O(4)#1-Pr(1)-N(1) | 135.14(6) | O(2)-Pr(1)-C(15)#3 | 157.77(5) |
| O(3)#2-Pr(1)-N(1) | 73.21(6) | O(6)#3-Pr(1)-C(15)#3 | 23.91(5) |
| O(5)-Pr(1)-N(1) | 145.82(5) | N(2)-Pr(1)-C(15)#3 | 88.75(5) |
| O(1)-Pr(1)-N(1) | 115.98(5) | N(1)-Pr(1)-C(15)#3 | 80.10(5) |
| O(2)-Pr(1)-N(1) | 77.69(5) | O(5)#3-Pr(1)-C(15)#3 | 24.82(5) |
| O(6)#3-Pr(1)-N(1) | 68.50(5) | C(1)-Pr(1)-C(15)#3 | 163.82(6) |
| N(2)-Pr(1)-N(1) | 61.21(6) | | |

Symmetry transformations used to generate equivalent atoms: #1 -x+3/2, y-1/2, -z+3/2; #2 ×, -y+1, z-1/2; #3 -x+3/2, -y+1/2, -z+1; #4 -x+2, y, -z+3/2; #5 -x+3/2, y+1/2, -z+3/2; #6 ×, -y+1, z+1/2.

**Table 7**
Selected bond lengths and bond angles of **1 g**.

| | | | |
|---|---|---|---|
| Nd(1)-O(1) | 2.4192(14) | Nd(1)-N(2) | 2.6360(18) |
| Nd(1)-O(2)#1 | 2.4211(15) | Nd(1)-N(1) | 2.6923(18) |
| Nd(1)-O(5)#1 | 2.4298(15) | Nd(1)-O(5) | 2.7278(16) |
| Nd(1)-O(4)#2 | 2.4757(15) | Nd(1)-C(14)#2 | 2.871(2) |
| Nd(1)-O(3)#2 | 2.5194(15) | Nd(1)-C(15) | 3.015(2) |
| Nd(1)-O(6) | 2.5307(15) | Nd(1)-Nd(1)#1 | 4.0061(2) |
| O(1)-Nd(1)-O(2)#1 | 136.86(5) | O(1)-Nd(1)-O(5) | 73.02(5) |
| O(1)-Nd(1)-O(5)#1 | 75.10(5) | O(2)#1-Nd(1)-O(5) | 72.83(5) |
| O(2)#1-Nd(1)-O(5)#1 | 72.81(5) | O(5)#1-Nd(1)-O(5) | 78.23(5) |
| O(1)-Nd(1)-O(4)#2 | 75.31(5) | O(4)#2-Nd(1)-O(5) | 146.28(5) |
| O(2)#1-Nd(1)-O(4)#2 | 127.15(6) | O(3)#2-Nd(1)-O(5) | 157.21(5) |
| O(5)#1-Nd(1)-O(4)#2 | 82.78(5) | O(6)-Nd(1)-O(5) | 48.93(4) |
| O(1)-Nd(1)-O(3)#2 | 127.35(5) | N(2)-Nd(1)-O(5) | 113.94(5) |
| O(2)#1-Nd(1)-O(3)#2 | 84.40(5) | N(1)-Nd(1)-O(5) | 94.77(5) |
| O(5)#1-Nd(1)-O(3)#2 | 96.20(6) | O(1)-Nd(1)-C(14)#2 | 101.24(6) |
| O(4)#2-Nd(1)-O(3)#2 | 52.04(5) | O(2)#1-Nd(1)-C(14)#2 | 106.31(6) |
| O(1)-Nd(1)-O(6) | 71.44(5) | O(5)#1-Nd(1)-C(14)#2 | 89.20(6) |
| O(2)#1-Nd(1)-O(6) | 103.77(6) | O(4)#2-Nd(1)-C(14)#2 | 25.93(6) |
| O(5)#1-Nd(1)-O(6) | 123.29(5) | O(3)#2-Nd(1)-C(14)#2 | 26.11(6) |
| O(4)#2-Nd(1)-O(6) | 128.59(5) | O(6)-Nd(1)-C(14)#2 | 141.10(5) |
| O(3)#2-Nd(1)-O(6) | 140.45(5) | N(2)-Nd(1)-C(14)#2 | 55.64(10) |
| O(1)-Nd(1)-N(2) | 83.74(6) | N(1)-Nd(1)-C(14)#2 | 167.12(5) |
| O(2)#1-Nd(1)-N(2) | 134.62(6) | O(5)-Nd(1)-C(14)#2 | 70.98(5) |
| O(5)#1-Nd(1)-N(2) | 151.41(5) | O(1)-Nd(1)-C(15) | 76.15(6) |
| O(4)#2-Nd(1)-N(2) | 73.29(5) | O(2)#1-Nd(1)-C(15) | 88.08(6) |
| O(3)#2-Nd(1)-N(2) | 81.43(6) | O(5)#1-Nd(1)-C(15) | 101.62(5) |
| O(6)-Nd(1)-N(2) | 65.18(5) | O(4)#2-Nd(1)-C(15) | 143.40(5) |
| O(1)-Nd(1)-N(1) | 135.31(6) | O(3)#2-Nd(1)-C(15) | 157.66(5) |
| O(2)#1-Nd(1)-N(1) | 73.11(6) | O(6)-Nd(1)-C(15) | 23.95(5) |
| O(5)#1-Nd(1)-N(1) | 145.76(6) | N(2)-Nd(1)-C(15) | 89.09(6) |
| O(4)#2-Nd(1)-N(1) | 116.07(5) | N(1)-Nd(1)-C(15) | 80.37(5) |
| O(3)#2-Nd(1)-N(1) | 77.32(6) | O(5)-Nd(1)-C(15) | 24.99(5) |
| O(6)-Nd(1)-N(1) | 68.69(5) | C(14)#2-Nd(1)-C(15) | 164.16(6) |
| N(2)-Nd(1)-N(1) | 61.78(6) | | |

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2, -y+3/2, -z; #2 -x+1/2, y+1/2, -z+1/2; #3 -x+1/2, y-1/2, -z+1/2; #4 -x, y, -z-1/2.

## 2. Experimental design, materials, and methods

Ln-MOFs **1a-1h** were synthesized with similar procedure. 100 mg (0.396 mmol) $H_2ADA$ and 20 mL $H_2O$ were mixed in a 50 mL beaker, and adjusted to pH = 6 with 0.1 M NaOH solution. The ligand solution mixed with 20 mL water solution which contains 0.26 mmol $Ln(NO_3)_3{\cdot}6H_2O$. Then, 48 mg phen EtOH solution (20 mL) was added to the upward mixed solution, the reaction mixture was

**Table 8**
Selected bond lengths and bond angles of **1 h**.

| | | | |
|---|---|---|---|
| Y(1)-O(5) | 2.2662(15) | Y(1)-O(1) | 2.4080(13) |
| Y(1)-O(4)#1 | 2.2983(13) | Y(1)-N(2) | 2.5418(15) |
| Y(1)-O(3)#2 | 2.3225(13) | Y(1)-N(1) | 2.6141(15) |
| Y(1)-O(6)#3 | 2.3602(15) | Y(1)-C(1) | 2.7670(18) |
| Y(1)-O(2) | 2.4016(13) | | |
| O(5)-Y(1)-O(4)#1 | 73.25(5) | O(6)#3-Y(1)-N(2) | 70.45(5) |
| O(5)-Y(1)-O(3)#2 | 79.97(6) | O(2)-Y(1)-N(2) | 73.35(5) |
| O(4)#1-Y(1)-O(3)#2 | 130.88(5) | O(1)-Y(1)-N(2) | 83.54(5) |
| O(5)-Y(1)-O(6)#3 | 125.93(7) | O(5)-Y(1)-N(1) | 142.54(6) |
| O(4)#1-Y(1)-O(6)#3 | 90.33(6) | O(4)#1-Y(1)-N(1) | 72.57(5) |
| O(3)#2-Y(1)-O(6)#3 | 73.14(5) | O(3)#2-Y(1)-N(1) | 135.37(5) |
| O(5)-Y(1)-O(2) | 78.70(6) | O(6)#3-Y(1)-N(1) | 69.05(5) |
| O(4)#1-Y(1)-O(2) | 135.32(5) | O(2)-Y(1)-N(1) | 116.96(5) |
| O(3)#2-Y(1)-O(2) | 75.26(5) | O(1)-Y(1)-N(1) | 76.57(5) |
| O(6)#3-Y(1)-O(2) | 134.34(6) | N(2)-Y(1)-N(1) | 63.56(5) |
| O(5)-Y(1)-O(1) | 89.23(7) | O(5)-Y(1)-C(1) | 82.20(7) |
| O(4)#1-Y(1)-O(1) | 91.05(5) | O(4)#1-Y(1)-C(1) | 113.73(6) |
| O(3)#2-Y(1)-O(1) | 129.40(4) | O(3)#2-Y(1)-C(1) | 102.17(5) |
| O(6)#3-Y(1)-O(1) | 143.43(5) | O(6)#3-Y(1)-C(1) | 148.48(6) |
| O(2)-Y(1)-O(1) | 54.13(5) | O(2)-Y(1)-C(1) | 26.93(5) |
| O(5)-Y(1)-N(2) | 149.86(6) | O(1)-Y(1)-C(1) | 27.24(5) |
| O(4)#1-Y(1)-N(2) | 135.87(5) | N(2)-Y(1)-C(1) | 78.05(5) |
| O(3)#2-Y(1)-N(2) | 82.21(5) | N(1)-Y(1)-C(1) | 97.93(5) |

Symmetry transformations used to generate equivalent atoms: #1 ×, -y+2, z-1/2; #2 -x+3/2, y-1/2, -z+3/2; #3 -x+3/2, -y+3/2, -z+1; #4 -x+3/2, y+1/2, -z+3/2; #5 ×, -y+2, z+1/2; #6 -x+2, y, -z+3/2.

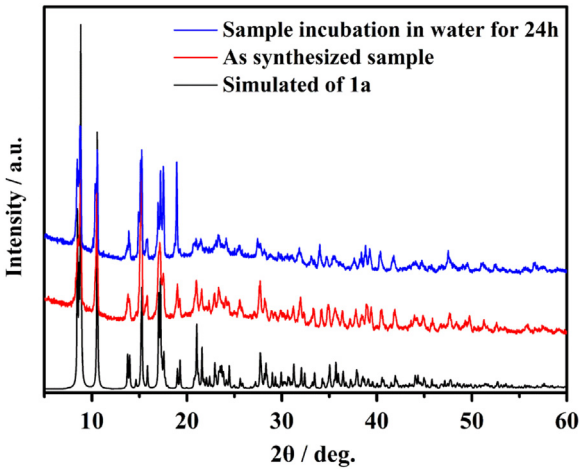


**Fig. 3.** PXRD patterns comparison of single crystal data **1a**, as synthesized **1a** and bulk sample **1a** immersed in water for 24 h, they compete with each other very well, confirming **1a** is highly stable that incubated in aqueous solution for 24 h.

transferred to a bottle and sealed, reacted at 60 °C for three days. After cooling to room temperature in the oven, colorless crystals suitable for X-ray single crystal test were obtained by filtration, they were washed with 5 mL EtOH three times and air-dried.

Single crystal X-ray diffraction data was collected on a Bruker SMART 1000 CCD, with Mo-Ka radiation (Wavelength = 0.71073 Å) at room temperature. The structure was refined by full-matrix least-squares methods with SHELXL-97 module. Phase purity of bulk sample was determined by PXRD, using a DMAX2200VPC diffractometer, at 30 kV and 30 mA.

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## Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2018.01.094.

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