Electronic Supplementary Material (ESI) for CrystEngComm.

A water-stable 3D Eu-MOF based on a metallacyclodimeric secondary building unit for sensitive fluorescent detection of acetone molecule

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Contents

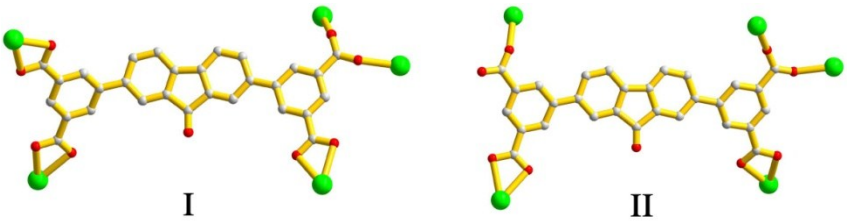

Fig. S1 Coordination modes of the two ligands in compound **2**.

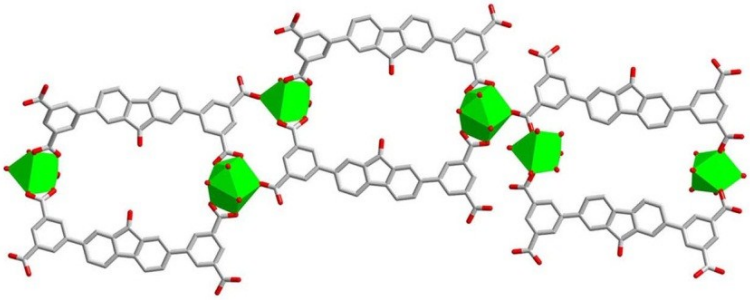

Fig. S2 2D layer network constructed from the 1D chain in **2**.

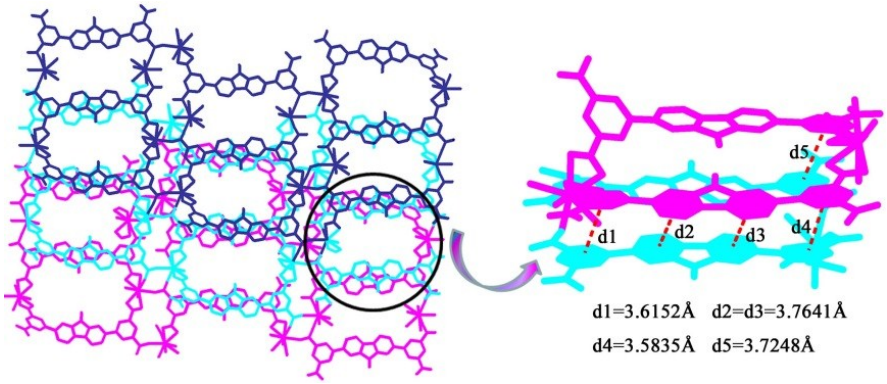

Fig. S3 The modes of the partial π···π stacking interactions of partially overlapping aromatic rings in complex **2**.

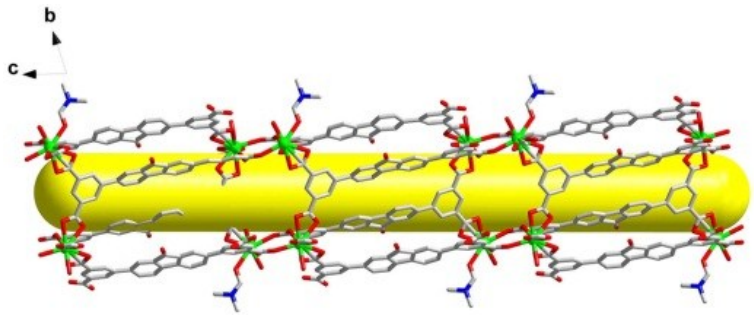

Fig. S4 1D microporous tetragonal channel viewed along the *c* axis in **2**.

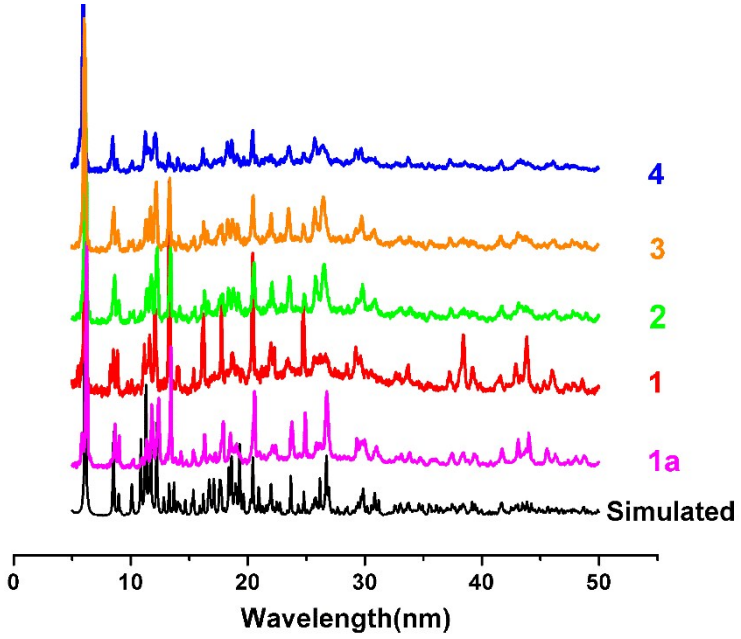

Fig. S5 PXRD patterns of compounds **1-4.**

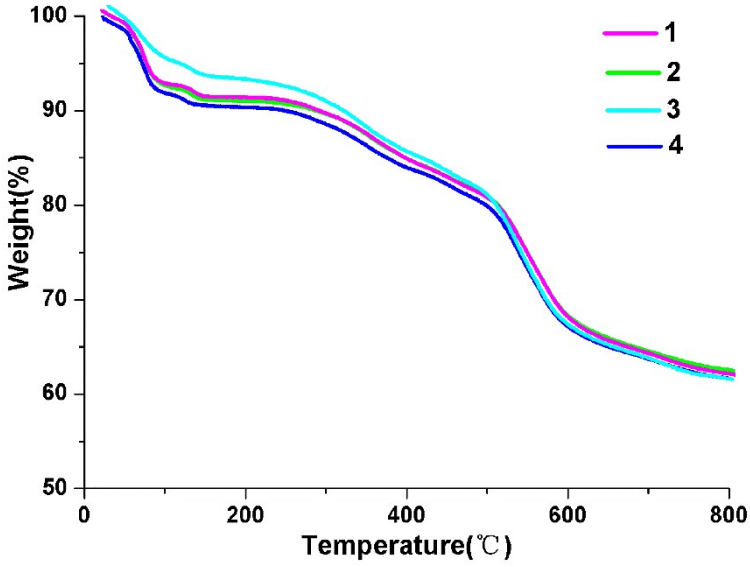

Fig. S6 TGA curves of compounds **1-4.**

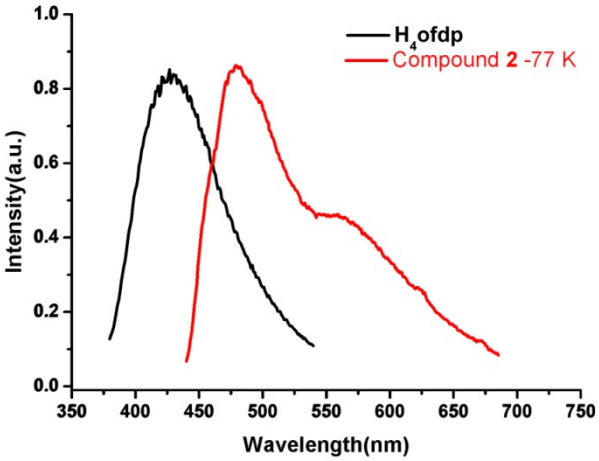

Fig. S7 Room-temperature emission spectra of ligand H_4ofdp and phosphorescence spectrum of compound $[Me_2NH_2]_2[(Gd)_2(ofdp)_2(DMF)(H_2O)]\cdot 7H_2O\cdot DMF$ **(2)** at 77 K.

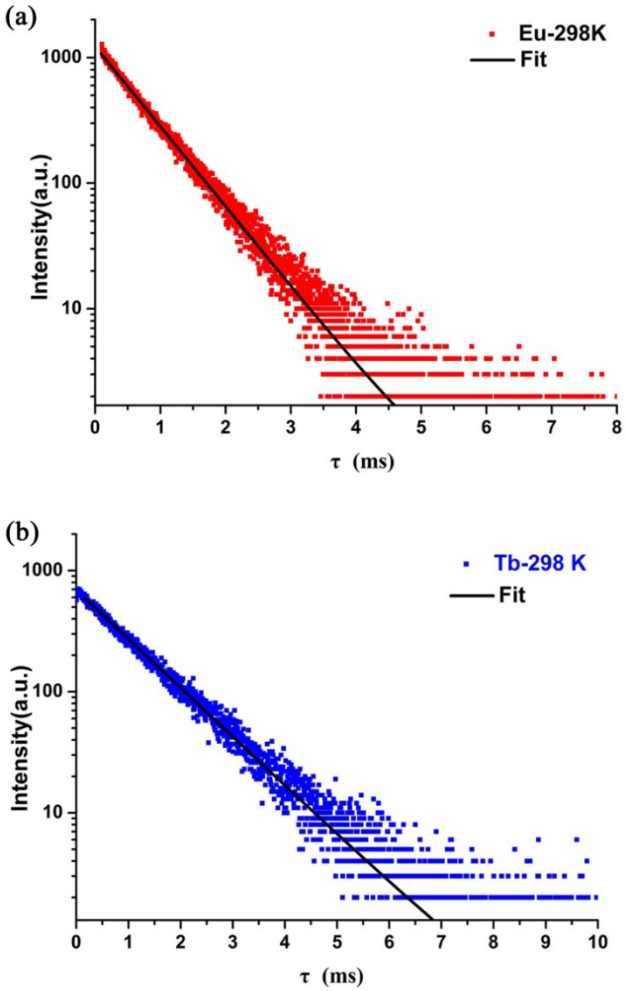

Fig. S8 The luminescence decay curves excited at 340 nm for Eu^{3+} in **1** and Tb^{3+} in **3** at 298 K (Scattering points: the experimental data; Solid lines: the fitting results.).

Table S1. The comparison of limit of detection for acetone between compound **1** and

several selected Ln-MOFs.

Ln-MOFs	Limit of detection for acetone (vol %)	Ref.
Compound **1**	7.4 %	**this work**
$Eu(BTC)(H_2O)\cdot 1.5H_2O$	3.75 %	21a
$Eu(FBPT)(H_2O)(DMF)$	5 %	15a
$\{[Tb(FDA)_{1.5}(DMF)]\cdot DMF\}_n$	14 %	21b
$Yb(BPT)(H_2O)\cdot(DMF)_{1.5}\cdot(H_2O)$	5 %	22b
$[Eu_4(BPT)_4(DMF)_2(H_2O)_8]$	5 %	23b
Eu^{3+}@MIL-124	2 mg/2 ml	21c

Table S2. Selected bond lengths (Å) and bond angles (°) for **1**, **2, 3** and **4**.

Bond	Dist.	Bond	Dist.
Eu1—O12^{i}	2.314 (3)	Eu2—O13^{iv}	2.253 (3)
Eu1—O5^{ii}	2.368 (3)	Eu2—O4^{v}	2.287 (3)
Eu1—O1	2.375 (3)	Eu2—O14^{vi}	2.312 (3)
Eu1—O17	2.453 (3)	Eu2—O18	2.382 (3)
Eu1—O3	2.460 (3)	Eu2—O9	2.437 (3)
Eu1—O7^{iii}	2.467 (3)	Eu2—O8	2.443 (4)
Eu1—O16	2.474 (3)	Eu2—O11	2.453 (3)
Eu1—O2	2.477 (3)	Eu2—O10	2.482 (4)
Eu1—O6^{iii}	2.486 (3)		
Angle	(º)	Angle	(º)
O12^{i}—Eu1—O5^{ii}	78.30 (10)	O7^{iii}—Eu1—O16	108.12 (10)
O12^{i}—Eu1—O1	82.77 (11)	O12^{i}—Eu1—O2	72.94 (10)
O5^{ii}—Eu1—O1	139.35 (10)	O5^{ii}—Eu1—O2	130.15 (10)
O12^{i}—Eu1—O17	138.26 (11)	O1—Eu1—O2	75.87 (11)
O5^{ii}—Eu1—O17	95.39 (10)	O17—Eu1—O2	132.74 (10)
O1—Eu1—O17	75.66 (10)	O3—Eu1—O2	53.00 (9)
O12^{i}—Eu1—O3	124.15 (10)	O7^{iii}—Eu1—O2	106.04 (10)
O5^{ii}—Eu1—O3	146.78 (10)	O16—Eu1—O2	143.86 (10)
O1—Eu1—O3	72.46 (11)	O12i—Eu1—O6^{iii}	94.00 (11)
O17—Eu1—O3	82.67 (9)	O5^{ii}—Eu1—O6^{iii}	72.17 (10)
O12^{i}—Eu1—O7^{iii}	142.40 (11)	O1—Eu1—O6^{iii}	145.35 (11)
O5^{ii}—Eu1—O7^{iii}	74.58 (10)	O17—Eu1—O6^{iii}	123.63 (9)
O1—Eu1—O7^{iii}	134.32 (10)	O3—Eu1—O6^{iii}	81.36 (11)
O17—Eu1—O7^{iii}	70.54 (10)	O7^{iii}—Eu1—O6^{iii}	53.09 (9)
O3—Eu1—O7^{iii}	73.55 (10)	O16—Eu1—O6^{iii}	142.49 (11)

O12^{i}—Eu1—O16	86.85 (10)	O2—Eu1—O6^{iii}	70.26 (11)
O13^{iv}—Eu2—O4^{v}	79.21 (11)	O9—Eu2—O8	53.01 (10)
O13^{iv}—Eu2—O14^{vi}	99.10 (13)	O13^{iv}—Eu2—O11	152.73 (11)
O4^{v}—Eu2—O14^{vi}	87.36 (11)	O4^{v}—Eu2—O11	128.03 (11)
O13^{iv}—Eu2—O18	77.70 (12)	O14^{vi}—Eu2—O11	82.94 (11)
O4^{v}—Eu2—O18	146.65 (13)	O18—Eu2—O11	76.95 (12)
O14^{vi}—Eu2—O18	73.00 (12)	O9—Eu2—O11	73.89 (10)
O13^{iv}—Eu2—O9	89.11 (11)	O8—Eu2—O11	98.09 (15)
O4^{v}—Eu2—O9	130.61 (11)	O13^{iv}—Eu2—O10	154.13 (10)
O14^{vi}—Eu2—O9	142.03 (10)	O4^{v}—Eu2—O10	75.02 (11)
O18—Eu2—O9	72.73 (11)	O14^{vi}—Eu2—O10	77.63 (13)
O13^{iv}—Eu2—O8	87.84 (16)	O18—Eu2—O10	124.28 (11)
O4^{v}—Eu2—O8	78.51 (12)	O9—Eu2—O10	109.40 (12)
O14^{vi}—Eu2—O8	162.85 (12)	O8—Eu2—O10	89.26 (15)
O18—Eu2—O8	124.01 (11)	O11—Eu2—O10	53.02 (10)

Bond	Dist.	Bond	Dist.
Gd1—O7^{i}	2.357 (6)	Gd2—O6^{iv}	2.274 (7)
Gd1—O15^{ii}	2.404 (6)	Gd2—O4^{v}	2.319 (7)
Gd1—O19	2.415 (6)	Gd2—O16^{vi}	2.357 (6)
Gd1—O17	2.453 (7)	Gd2—O20	2.426 (8)
Gd1—O2	2.485 (6)	Gd2—O9	2.432 (6)
Gd1—O12^{iii}	2.494 (8)	Gd2—O11	2.439 (8)
Gd1—O1	2.497 (6)	Gd2—O10	2.485 (7)
Gd1—O18	2.509 (6)	Gd2—O8	2.492 (8)
Gd1—O13^{iii}	2.509 (7)		
Angle	(º)	Angle	(º)
O7^{i}—Gd1—O15^{ii}	78.4 (2)	O17—Gd1—O1	129.3 (2)
O7^{i}—Gd1—O19	82.2 (2)	O2—Gd1—O1	52.5 (2)
O15^{ii}—Gd1—O19	140.7 (2)	O12^{iii}—Gd1—O1	143.0 (2)
O7^{i}—Gd1—O17	123.3 (2)	O7^{i}—Gd1—O18	72.8 (2)
O15^{ii}—Gd1—O17	146.2 (2)	O15^{ii}—Gd1—O18	128.4 (2)
O19—Gd1—O17	72.2 (2)	O19—Gd1—O18	76.0 (2)
O7^{i}—Gd1—O2	136.9 (2)	O17—Gd1—O18	52.5 (2)
O15^{ii}—Gd1—O2	96.3 (2)	O2—Gd1—O18	133.6 (2)
O19—Gd1—O2	75.5 (2)	O12^{iii}—Gd1—O18	70.3 (3)
O17—Gd1—O2	84.0 (2)	O1—Gd1—O18	143.9 (2)
O7^{i}—Gd1—O12^{iii}	97.6 (2)	O7^{i}—Gd1—O13^{iii}	144.5 (2)
O15^{ii}—Gd1—O12^{iii}	72.4 (2)	O15^{ii}—Gd1—O13^{iii}	74.9 (2)
O19—Gd1—O12^{iii}	144.6 (2)	O19—Gd1—O13^{iii}	132.9 (2)
O17—Gd1—O12^{iii}	78.8 (3)	O17—Gd1—O13^{iii}	73.7 (2)
O2—Gd1—O12^{iii}	121.7 (2)	O2—Gd1—O13^{iii}	69.6 (2)
O7^{i}—Gd1—O1	85.9 (2)	O12^{iii}—Gd1—O13^{iii}	52.2 (2)

O15^{ii}—Gd1—O1	72.4 (2)	O1—Gd1—O13^{iii}	107.3 (2)
O19—Gd1—O1	72.4 (2)	O18—Gd1—O13^{iii}	106.9 (2)
O6^{iv}—Gd2—O4^{v}	97.0 (3)	O4^{v}—Gd2—O11	164.5 (3)
O6^{iv}—Gd2—O16^{vi}	78.6 (3)	O16^{vi}—Gd2—O11	77.3 (2)
O4^{v}—Gd2—O16^{vi}	90.2 (2)	O20—Gd2—O11	123.0 (3)
O6^{iv}—Gd2—O20	77.6 (3)	O9—Gd2—O11	94.7 (3)
O4^{v}—Gd2—O20	72.3 (3)	O6^{iv}—Gd2—O10	88.3 (2)
O16^{vi}—Gd2—O20	148.2 (3)	O4^{v}—Gd2—O10	140.8 (2)
O6^{iv}—Gd2—O9	153.6 (3)	O16^{vi}—Gd2—O10	128.8 (2)
O4^{v}—Gd2—O9	85.7 (3)	O20—Gd2—O10	71.0 (2)
O16^{vi}—Gd2—O9	127.8 (3)	O9—Gd2—O10	73.7 (2)
O20—Gd2—O9	78.3 (3)	O11—Gd2—O10	53.1 (2)
O6^{iv}—Gd2—O11	89.5 (3)	O6^{iv}—Gd2—O8	153.6 (3)
O6^{iv}—Gd2—O4^{v}	97.0 (3)	O4^{v}—Gd2—O11	164.5 (3)
O6^{iv}—Gd2—O16^{vi}	78.6 (3)	O16^{vi}—Gd2—O11	77.3 (2)
O4^{v}—Gd2—O16^{vi}	90.2 (2)	O20—Gd2—O11	123.0 (3)

Bond	Dist.	Bond	Dist.
Tb1—O12^{i}	2.312 (2)	Tb2—O13^{iv}	2.257 (3)
Tb1—O1	2.373 (3)	Tb2—O4^{v}	2.302 (2)
Tb1—O5^{ii}	2.382 (3)	Tb2—O14^{vi}	2.305 (3)
Tb1—O3	2.433 (3)	Tb2—O18	2.390 (3)
Tb1—O17	2.460 (2)	Tb2—O11	2.423 (3)
Tb1—O16	2.480 (2)	Tb2—O8	2.428 (3)
Tb1—O6^{iii}	2.490 (3)	Tb2—O9	2.466 (2)
Tb1—O7^{iii}	2.490 (3)	Tb2—O10	2.486 (3)
Tb1—O2	2.503 (3)		
Angle	(º)	Angle	(º)
O12^{i}—Tb1—O1	82.10 (10)	O3—Tb1—O6^{iii}	73.28 (9)
O12^{i}—Tb1—O5^{ii}	77.94 (9)	O17—Tb1—O6^{iii}	69.64 (8)
O1—Tb1—O5^{ii}	140.03 (9)	O16—Tb1—O6^{iii}	107.30 (8)
O12^{i}—Tb1—O3	123.71 (9)	O12^{i}—Tb1—O7^{iii}	97.32 (9)
O1—Tb1—O3	73.09 (10)	O1—Tb1—O7^{iii}	144.37 (9)
O5^{ii}—Tb1—O3	146.04 (10)	O5^{ii}—Tb1—O7^{iii}	72.98 (9)
O12^{i}—Tb1—O17	136.99 (9)	O3—Tb1—O7^{iii}	78.07 (10)
O1—Tb1—O17	75.44 (9)	O17—Tb1—O7^{iii}	122.08 (8)
O5^{ii}—Tb1—O17	96.48 (8)	O16—Tb1—O7^{iii}	143.37 (9)
O3—Tb1—O17	84.03 (8)	O6^{iii}—Tb1—O7^{iii}	52.49 (8)
O12^{i}—Tb1—O16	85.83 (9)	O12^{i}—Tb1—O2	72.61 (9)
O1—Tb1—O16	72.26 (9)	O1—Tb1—O2	76.17 (10)
O5^{ii}—Tb1—O16	72.06 (9)	O5^{ii}—Tb1—O2	128.26 (9)
O3—Tb1—O16	129.71 (9)	O3—Tb1—O2	52.91 (8)
O17—Tb1—O16	52.64 (8)	O17—Tb1—O2	133.69 (9)

O12^{i}—Tb1—O6^{iii}	144.32 (10)	O16—Tb1—O2	143.81 (9)
O1—Tb1—O6^{iii}	133.26 (9)	O6^{iii}—Tb1—O2	107.09 (9)
O5^{ii}—Tb1—O6^{iii}	75.14 (9)	O7^{iii}—Tb1—O2	69.83 (10)
O13^{iv}—Tb2—O4^{v}	78.50 (10)	O11—Tb2—O8	96.27 (11)
O13^{iv}—Tb2—O14^{vi}	97.31 (11)	O13^{iv}—Tb2—O9	89.06 (9)
O4^{v}—Tb2—O14^{vi}	89.14 (10)	O4^{v}—Tb2—O9	129.66 (9)
O13^{iv}—Tb2—O18	78.02 (10)	O14^{vi}—Tb2—O9	141.08 (9)
O4^{v}—Tb2—O18	147.97 (11)	O18—Tb2—O9	71.26 (9)
O14^{vi}—Tb2—O18	72.65 (10)	O11—Tb2—O9	73.78 (9)
O13^{iv}—Tb2—O11	153.57 (9)	O8—Tb2—O9	53.24 (9)
O4^{v}—Tb2—O11	127.92 (10)	O13^{iv}—Tb2—O10	152.71 (9)
O14^{vi}—Tb2—O11	84.71 (10)	O4^{v}—Tb2—O10	74.82 (9)
O18—Tb2—O11	77.49 (10)	O14^{vi}—Tb2—O10	76.80 (11)
O13^{iv}—Tb2—O8	88.89 (11)	O18—Tb2—O10	123.73 (10)
O4^{v}—Tb2—O8	77.69 (10)	O11—Tb2—O10	53.41 (9)
O14^{vi}—Tb2—O8	164.06 (10)	O8—Tb2—O10	90.97 (11)
O18—Tb2—O8	123.15 (9)	O9—Tb2—O10	112.43 (10)

Bond	Dist.	Bond	Dist.
Dy1—O12^{i}	2.315 (3)	Dy2—O13^{iv}	2.253 (4)
Dy1—O5^{ii}	2.377 (3)	Dy2—O14^{v}	2.302 (4)
Dy1—O1	2.382 (4)	Dy2—O4^{vi}	2.309 (3)
Dy1—O3	2.447 (3)	Dy2—O18	2.399 (4)
Dy1—O17	2.455 (3)	Dy2—O8	2.419 (4)
Dy1—O16	2.477 (3)	Dy2—O11	2.428 (3)
Dy1—O7^{iii}	2.483 (4)	Dy2—O9	2.462 (3)
Dy1—O2	2.499 (3)	Dy2—O10	2.488 (4)
Dy1—O6^{iii}	2.504 (4)		
Angle	(º)	Angle	(º)
O12^{i}—Dy1—O5^{ii}	77.77 (12)	O3—Dy1—O7^{iii}	78.11 (13)
O12^{i}—Dy1—O1	82.24 (13)	O17—Dy1—O7^{iii}	121.80 (11)
O5^{ii}—Dy1—O1	140.08 (11)	O16—Dy1—O7^{iii}	143.18 (12)
O12^{i}—Dy1—O3	123.90 (12)	O12^{i}—Dy1—O2	72.88 (12)
O5^{ii}—Dy1—O3	146.03 (12)	O5^{ii}—Dy1—O2	128.28 (12)
O1—Dy1—O3	73.05 (13)	O1—Dy1—O2	76.18 (13)
O12^{i}—Dy1—O17	137.09 (12)	O3—Dy1—O2	52.82 (11)
O5^{ii}—Dy1—O17	96.56 (11)	O17—Dy1—O2	133.53 (12)
O1—Dy1—O17	75.47 (12)	O16—Dy1—O2	143.86 (12)
O3—Dy1—O17	83.88 (11)	O7^{iii}—Dy1—O2	69.94 (13)
O12^{i}—Dy1—O16	85.58 (12)	O12^{i}—Dy1—O6^{iii}	144.23 (13)
O5^{ii}—Dy1—O16	71.97 (11)	O5^{ii}—Dy1—O6^{iii}	75.00 (11)
O1—Dy1—O16	72.34 (12)	O1—Dy1—O6^{iii}	133.26 (12)
O3—Dy1—O16	129.86 (12)	O3—Dy1—O6^{iii}	73.44 (12)

O17—Dy1—O16	52.97 (10)	O17—Dy1—O6^{iii}	69.40 (11)
O12^{i}—Dy1—O7^{iii}	97.44 (13)	O16—Dy1—O6^{iii}	107.18 (11)
O5^{ii}—Dy1—O7^{iii}	72.88 (12)	O7^{iii}—Dy1—O6^{iii}	52.46 (11)
O1—Dy1—O7^{iii}	144.48 (12)	O2—Dy1—O6iii	107.20 (11)
O13^{iv}—Dy2—O14^{v}	97.13 (14)	O8—Dy2—O11	96.49 (14)
O13^{iv}—Dy2—O4^{vi}	78.29 (13)	O13^{iv}—Dy2—O9	89.13 (12)
O14^{v}—Dy2—O4^{vi}	89.46 (13)	O14^{v}—Dy2—O9	141.09 (12)
O13^{iv}—Dy2—O18	77.93 (14)	O4^{vi}—Dy2—O9	129.32 (12)
O14^{v}—Dy2—O18	72.58 (14)	O18—Dy2—O9	71.32 (12)
O4^{vi}—Dy2—O18	147.96 (14)	O8—Dy2—O9	53.31 (11)
O13^{iv}—Dy2—O8	88.77 (15)	O11—Dy2—O9	73.77 (11)
O14^{v}—Dy2—O8	164.11 (14)	O13^{iv}—Dy2—O10	152.64 (12)
O4^{vi}—Dy2—O8	77.26 (13)	O14^{v}—Dy2—O10	76.79 (15)
O18—Dy2—O8	123.21 (12)	O4^{vi}—Dy2—O10	75.03 (12)
O13^{iv}—Dy2—O11	153.56 (12)	O18—Dy2—O10	123.75 (13)
O14^{v}—Dy2—O11	84.79 (13)	O8—Dy2—O10	91.19 (15)
O4^{vi}—Dy2—O11	128.14 (13)	O11—Dy2—O10	53.46 (12)
O18—Dy2—O11	77.54 (14)	O9—Dy2—O10	112.52 (13)