Four anionic Ln-MOF for remarkable separations for C2H2–CH4 / CO2–CH4 and highly sensitive sensing of nitrobenzene

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S1 Materials

All starting materials and regents were purchased from commercial suppliers and used without further purification. 3-(3,5-dicarboxylphenyl)-5-(4-carboxylphenyl)-1,2,4-triazole; $HO(NO_3)_3 \cdot 6H_2O$; $Dy(NO_3)_3 \cdot 6H_2O$; $Tb(NO_3)_3 \cdot 6H_2O$; $Gd(NO_3)_3 \cdot 6H_2O$; DMF; H_2O; HNO_3.

S2 General Experimental Section

Powder X-ray Diffraction (PXRD)

Powder XRD patterns were obtained using a Bruker D8 Advance X-ray diffractometer with (λ (CuKα) = 1.5405 Å) radiation.

Thermogravimetric Analyses (TGA)

They were carried out on a TA Instruments STA499 F5 thermobalance with a 100 $mL \cdot min^{-1}$ flow of nitrogen; the temperature was ramped from 20 °C to 800 °C at a rate of 5 $°C \cdot min^{-1}$.

Single-crystal X-ray diffraction (SCXRD)

A suitable crystal of $[Gd_3L_3(HCOO)] \cdot Me_2NH_2^+ \cdot 7DMF$ **(1);** $[Tb_3L_3(HCOO)] \cdot Me_2NH_2^+ \cdot 7DMF$ **(2);** $[Ho_3L_3(HCOO)] \cdot Me_2NH_2^+ \cdot 7DMF$ **(3);** $[Dy_3L_3(HCOO)] \cdot Me_2NH_2^+ \cdot 7DMF$ **(4)** were mounted in a Hampton cryoloop with Paratone® N oil cryoprotectant. Intensity data collections were carried out at T =296(2) K with a Bruker D8 VENTURE diffractometer equipped with a PHOTON

100 CMOS bidimensional detector using a high brilliance IμS microfocus X-ray Mo Ka monochromatized radiation (λ = 0.71073 Å). The structures were solved by intrinsic phasing methods and refined by full-matrix least squares using the SHELX-TL package.[1] Single crystal X-ray analysis shows that: 1-4 are heterogeneous homocrystalline structures, monoclinic crystal system, *C2/m* space group. In the process of structural refinement, it was found that the two positions of the benzoate (C24-C29, C31, O9 and O10) of one of the ligands L^{3-} were statistically distributed, and the occupancy ratio was 0.5:0.5. Crystallographic data and structural refinement parameters of 1-4 are listed in Table 1-4. Further details about of the crystal structure determinations may be obtained free of charge via the Internet at https://www.ccdc.cam.ac.uk/. CCDC 2063236-2063239. Crystallographic data for single-crystal X-ray diffraction studies are summarized in Table S1.

S3. Synthesis and Experimental Section

Synthesis of $[Gd_3L_3(HCOO)]\cdot Me_2NH_2^+\cdot 7DMF$ (1)

H_3L (5.0 mg, 0.014 mmol), $Gd(NO_3)_3\cdot 6H_2O$（15 mg, 0.033 mmol）, 1.5 mL DMF, 0.3 mL H_2O, 30 μL 68% HNO_3, then the mixture was sealed in a 20 mL Teflon-lined bomb, put it in the programed raising and cooling oven (first heat up to 160°C for 4 h, keep 160°C constant temperature for 3 days, then cool down for 3 days to 35°C). The reaction kettle was taken out, washed with DMF, and the colorless bulk single crystal 10 was synthesized. Yield: 65% (based on H_3L), chemical formula: $C_{75}H_{82}N_{17}O_{27}Gd_3$. Elemental analysis calcd for 1 (%): C, 42.38; H, 3.89; N, 11.21. Found (%): C, 42.36; H, 3.91; N, 11.23. Main infrared spectrum peak position (KBr, cm^{-1}): 3425, 1654, 1576, 1415, 1099, 1021, 859, 788, 665, 516.

Synthesis of $[Tb_3L_3(HCOO)]\cdot Me_2NH_2^+\cdot 7DMF$ (2)

$Tb(NO_3)_3\cdot 6H_2O$ was used to replace $Gd(NO_3)_3\cdot 6H_2O$, and 2 was obtained by using the synthesis method of 1. Yield: 76% (based on H_3L), chemical formula: $C_{75}H_{82}N_{17}O_{27}Tb_3$. Elemental analysis calcd for 2 (%): C, 42.28; H, 3.88; N, 11.18. Found (%): C, 42.25; H, 3.80; N, 11.20. Main infrared spectrum peak position (KBr, cm^{-1}): 3425, 1654, 1557, 1402, 1092, 1021, 859, 794, 658, 516.

Synthesis of $[Ho_3L_3(HCOO)]\cdot Me_2NH_2^+\cdot 7DMF$ (3)

$Ho(NO_3)_3\cdot 6H_2O$ was used to replace $Gd(NO_3)_3\cdot 6H_2O$, and 3 was obtained by using the synthesis method of 1. Yield: 58% (based on H_3L), chemical formula: $C_{75}H_{82}N_{17}O_{27}Ho_3$. Elemental analysis calcd for 3 (%): C, 41.93; H, 3.85; N, 11.09. Found (%):C, 41.69; H, 3.91; N, 11.23. Main infrared spectrum peak position (KBr, cm^{-1}): 3425, 1654, 1538, 1402, 1105, 1021, 859, 795, 665, 516.

Synthesis of $[Dy_3L_3(HCOO)]\cdot Me_2NH_2^+\cdot 7DMF$ (4)

$Dy(NO_3)_3\cdot 6H_2O$ was used to replace $Gd(NO_3)_3\cdot 6H_2O$, and 4 was obtained by using the synthesis method of 1. Yield: 76% (based on H_3L), chemical formula: ： $C_{75}H_{82}N_{17}O_{27}Dy_3$. Elemental analysis calcd for 4 (%): C, 42.07; H, 3.86; N, 11.12 Found (%): C, 41.90; H, 3.92; N, 11.23. Main infrared spectrum peak position (KBr, cm^{-1}): 3425, 1654, 1545, 1408, 1099, 1021, 859, 795, 665, 516.

S4. Crystal data and structure refinement

Table S1. Crystal data and structure refinement for compounds 1-4.

Compound	H_3LGd	H_3LTb	H_3LHo	H_3LDy
Empirical formula	$C_{52}H_{25}Gd_3N_9O_{20}$	$C_{52}H_{25}Tb_3N_9O_{20}$	$C_{52}H_{25}Ho_3N_9O_{20}$	$C_{52}H_{25}Dy_3N_9O_{20}$
Formula weight	1567.56	1572.60	1590.60	1583.31
Temperature/K	296(2)	296(2)	296(2)	296(2)
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	*C2/m*	*C2/m*	*C2/m*	*C2/m*
a/Å	19.2170(13)	19.173(3)	19.0512(16)	19.120(5)
b/Å	28.514(2)	28.476(3)	28.4046(16)	28.411(5)
c/Å	15.3668(11)	15.403(2)	15.4074(10)	15.383(4)
α/°	90.00	90.00	90.00	90.00
β/°	100.677(4)	100.962(11)	101.195(5)	100.982(18)

γ/°	90.00	90.00	90.00	90.00
Volume/Å^3	8274.6(10)	8255.7(19)	8178.9(10)	8203(3)
Z	4	4	4	4
ρcalcg/cm^3	1.258	1.265	1.292	1.282
μ/mm^{-1}	2.467	2.632	2.965	2.795
F(000)	4236.0	4248.0	4272.0	4260.0
Crystal size/mm3	0.21 × 0.14 × 0.10	0.23 × 0.12 × 0.11	0.20 × 0.13 × 0.12	0.22 × 0.12 × 0.10
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection / °	2.7 to 55.38	2.6 to 49.98	2.6 to 55.4	2.6 to 50
Index ranges	-25 ≤ h ≤ 25, -37 ≤ k ≤ 37, -20 ≤ l ≤ 20	-22 ≤ h ≤ 22, -33 ≤ k ≤ 33, -18 ≤ l ≤ 18	-24 ≤ h ≤ 24, -36 ≤ k ≤ 36, -20 ≤ l ≤ 20	-22 ≤ h ≤ 22, -33 ≤ k ≤ 33, -18 ≤ l ≤ 18
Reflections collected	110232	121194	133145	110073
Independent reflections	9793 [Rint = 0.0905, Rsigma = N/A]	7432 [Rint = 0.2065, Rsigma = N/A]	9693 [Rint = 0.1420, Rsigma = N/A]	7396 [Rint = 0.1524, Rsigma = N/A]
Data/restraints/parameters	9793/41/360	7432/120/348	9693/78/360	7396/125/360
Goodness-of-fit on F^2	1.046	1.047	1.039	1.283
Final R indexes [I>=2σ (I)]	R1 = 0.0533, wR2 = 0.1359	R1 = 0.0966, wR2 = 0.2632	R1 = 0.0823, wR2 = 0.2078	R1 = 0.0986, wR2 = 0.2263
Final R indexes [all data]	R1 = 0.0736, wR2 = 0.1441	R1 = 0.1208, wR2 = 0.2860	R1 = 0.1099, wR2 = 0.2267	R1 = 0.1184, wR2 = 0.2392
Largest diff. peak/ hole / e Å^{-3}	3.41/-2.58	3.77/-3.37	2.64/-3.78	4.10/-1.58

S5 Powder X-ray diffraction (PXRD)

As shown in Figure S1, from the theoretical simulation and experimental PXRD spectra of 1-4, it can be seen that the main peak positions of the four MOFs are the same, and the individual small peaks are different, mainly due to the influence of the solvent molecules in the MOFs. It shows that the experimentally synthesized crystal is a pure phase substance and can be used for the determination of other properties

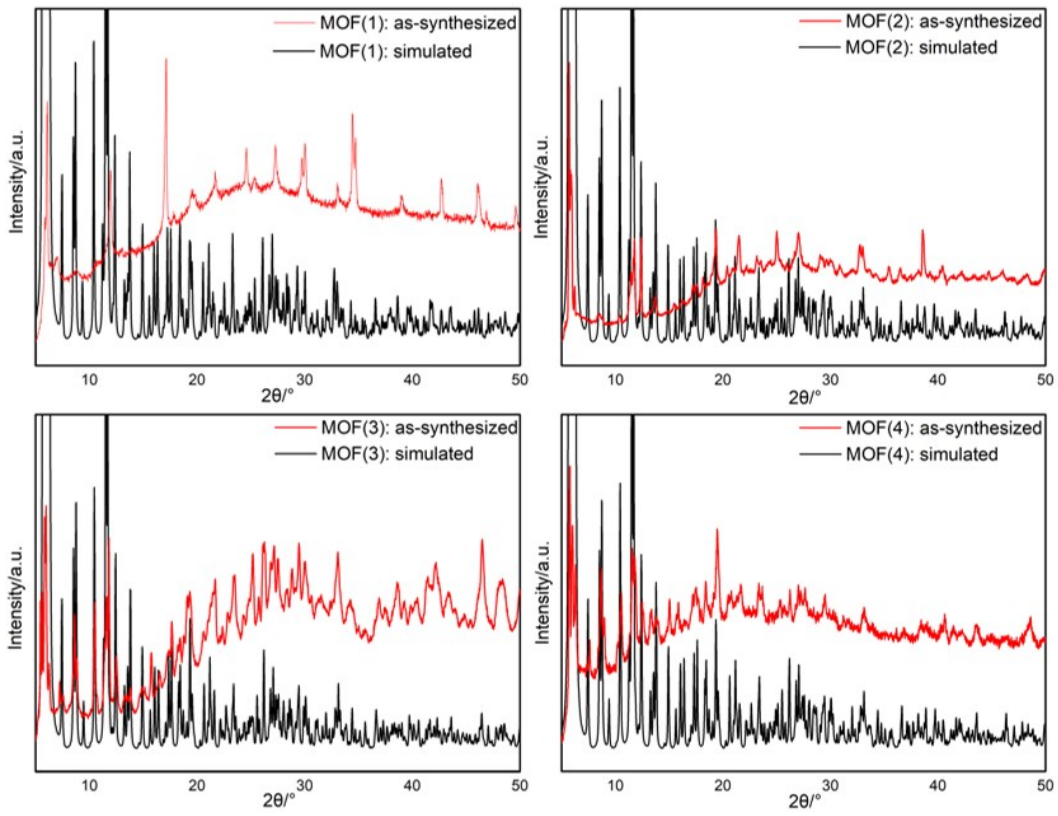

Figure S1 Experimental and simulated PXRD patterns.

S6 Thermogravimetric analyses (TGA)

As shown in Figure S2, from the thermogravimetric curve of 1-4, it can be seen that their TG curves are very similar, which indicates that they have similar thermal stability. Take 1 as an example for analysis. The thermogravimetric curve of 1 shows that the first significant weight loss occurred in the temperature range of 30-301°C, with a total loss of 25.3%. In this interval, seven DMF molecules and one counterion were lost (theoretical value 25.7%). As the temperature slowly increased, the ligand L^{3-} began to decompose, and the 1-4 skeleton opened and slowly collapsed.

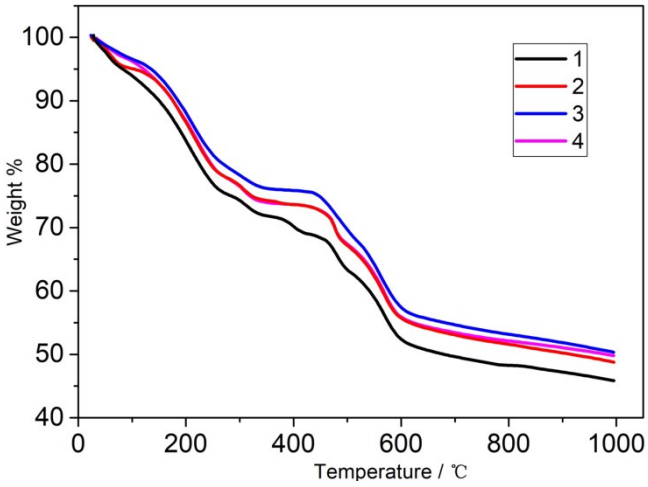

Figure S2 Thermogravimetric curve of 1-4

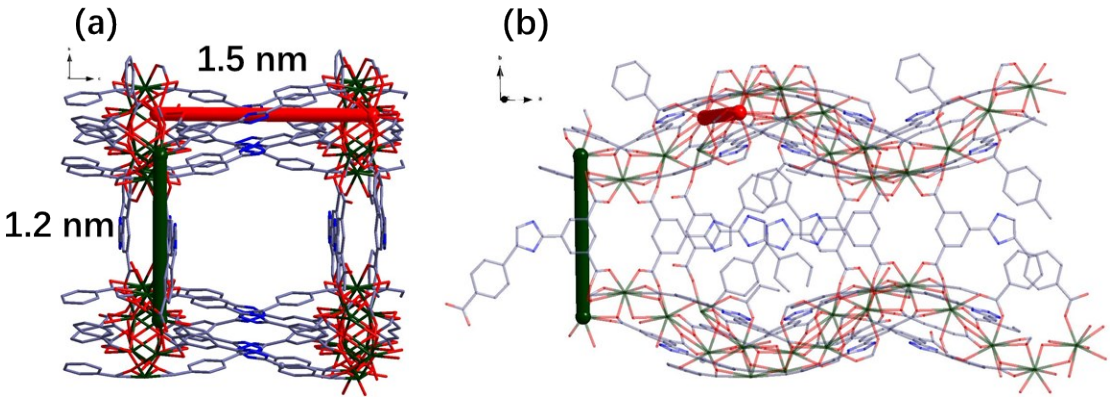

Figure S3 The estimated aperture of one-dimensional tunnels viewed by two directions.

S7 Reference

1 Sheldrick, G. M. *Acta Cryst. A* **2008**, 64, 112.

S8 Tables for bond lengths

Table 1. Bond lengths (Å) for compound 1

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Gd1	O8	2.281(4)	N5	N511	1.240(14)
Gd1	O81	2.281(4)	N5	C2311	1.240(14)
Gd1	O32	2.363(3)	N5	C24	1.748(8)
Gd1	O33	2.363(3)	C1	C6	1.380(8)
Gd1	O64	2.425(4)	C1	C2	1.402(6)
Gd1	O65	2.425(4)	C1	C15	1.498(6)
Gd1	O55	2.560(3)	C2	C3	1.392(7)
Gd1	O54	2.560(3)	C3	C4	1.396(8)

Gd1	C175	2.860(5)	C3	C16	1.493(7)
Gd1	C174	2.860(5)	C4	C5	1.391(7)
Gd1	Gd2	4.0088(4)	C5	C6	1.385(8)
Gd1	Gd21	4.0088(4)	C5	C7	1.478(9)
Gd2	O11	2.278(6)	C8	C9	1.474(9)
Gd2	O122	2.355(5)	C9	C14	1.386(9)
Gd2	O106	2.362(10)	C9	C10	1.403(9)
Gd2	O7	2.370(4)	C10	C11	1.367(8)
Gd2	O22	2.383(4)	C11	C12	1.392(8)
Gd2	O1	2.444(4)	C12	C13	1.371(8)
Gd2	O55	2.478(4)	C12	C17	1.511(7)
Gd2	O33	2.534(3)	C13	C14	1.376(8)
Gd2	O97	2.550(9)	C16	Gd28	2.892(5)
Gd2	O43	2.557(4)	C17	Gd19	2.860(5)
Gd2	O2	2.610(3)	C18	C19	1.385(6)
Gd2	C163	2.892(5)	C18	C1911	1.385(6)
O1	C15	1.263(6)	C19	C20	1.391(7)
O2	C15	1.266(6)	C19	C30	1.525(6)
O2	Gd22	2.383(4)	C20	C21	1.386(7)
O3	C16	1.293(7)	C21	C2011	1.386(7)
O3	Gd12	2.363(3)	C21	C22	1.495(13)
O3	Gd28	2.534(3)	C22	N411	1.315(9)
O4	C16	1.226(6)	C24	C25	1.4016
O4	Gd28	2.557(4)	C24	C29	1.4018
O5	C17	1.256(7)	C25	C26	1.4008
O5	Gd29	2.478(4)	C26	C27	1.4016

O5	Gd19	2.560(3)	C27	C28	1.402
O6	C17	1.275(7)	C27	C31	1.411
O6	Gd19	2.425(4)	C27	C3210	1.5366
O7	C30	1.247(6)	C28	C29	1.4014
O8	C30	1.263(6)	C31	C3210	0.3224
O9	O1110	0.330(9)	C31	O1210	1.0988
O9	C3210	0.956(9)	C31	O1110	1.5682
O9	C31	1.251(9)	O11	O97	0.330(12)
O9	Gd210	2.550(9)	O11	C32	1.264
O10	O1210	0.254(11)	O11	C317	1.5682
O10	C31	1.235(9)	C32	C317	0.3224
O10	C3210	1.438(9)	C32	O97	0.956(15)
O10	Gd26	2.362(10)	C32	O12	1.271
N1	C8	1.314(9)	C32	O107	1.438(15)
N1	C7	1.337(8)	C32	C277	1.5366
N2	C7	1.323(9)	O12	O107	0.254(18)
N2	N3	1.365(8)	O12	C317	1.0988
N3	C8	1.307(9)	O12	Gd22	2.355(8)
N4	C22	1.315(9)			

Table 2. Bond lengths (Å) for compound 2

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Tb1	O8	2.275(9)	N5	N511	1.313(19)
Tb1	O81	2.275(9)	N5	C2311	1.313(19)
Tb1	O32	2.354(9)	N5	C24	1.733(18)
Tb1	O33	2.354(9)	C1	C2	1.387(17)

Tb1	O64	2.414(10)	C1	C6	1.396(19)
Tb1	O65	2.414(10)	C1	C15	1.482(16)
Tb1	O54	2.565(9)	C2	C3	1.374(17)
Tb1	O55	2.565(9)	C3	C4	1.395(19)
Tb1	C174	2.869(13)	C3	C16	1.491(18)
Tb1	C175	2.869(13)	C4	C5	1.37(2)
Tb1	Tb21	4.0016(8)	C5	C6	1.36(2)
Tb1	Tb2	4.0016(8)	C5	C7	1.48(2)
Tb2	O122	2.317(11)	C8	C9	1.50(2)
Tb2	O11	2.320(15)	C9	C10	1.39(2)
Tb2	O106	2.33(2)	C9	C14	1.38(2)
Tb2	O7	2.335(9)	C10	C11	1.41(2)
Tb2	O22	2.346(9)	C11	C12	1.38(2)
Tb2	O1	2.428(9)	C12	C13	1.412(19)
Tb2	O55	2.496(9)	C12	C17	1.473(19)
Tb2	O33	2.519(9)	C13	C14	1.38(2)
Tb2	O97	2.53(2)	C16	Tb28	2.904(13)
Tb2	O43	2.561(10)	C17	Tb19	2.869(13)
Tb2	O2	2.609(8)	C18	C19	1.389(16)
Tb2	C163	2.904(13)	C18	C1911	1.389(16)
O1	C15	1.278(16)	C19	C20	1.362(17)
O2	C15	1.295(15)	C19	C30	1.552(16)
O2	Tb22	2.346(9)	C20	C21	1.402(16)
O3	C16	1.292(15)	C21	C2011	1.402(16)
O3	Tb12	2.354(9)	C21	C22	1.46(4)
O3	Tb28	2.519(9)	C22	N411	1.34(2)

O4	C16	1.253(16)	C24	C29	1.402(2)
O4	Tb28	2.561(10)	C24	C25	1.404(2)
O5	C17	1.250(14)	C25	C26	1.402(2)
O5	Tb29	2.496(9)	C26	C27	1.402(2)
O5	Tb19	2.565(9)	C27	C28	1.405(2)
O6	C17	1.260(15)	C27	C31	1.412(2)
O6	Tb19	2.414(10)	C27	C3210	1.504(2)
O7	C30	1.247(14)	C28	C29	1.403(2)
O8	C30	1.245(14)	C31	C3210	0.2595
O9	O1110	0.270(19)	C31	O1210	1.1470(18)
O9	C3210	1.051(16)	C31	O1110	1.479(2)
O9	C31	1.244(15)	O11	O97	0.27(3)
O9	Tb210	2.53(2)	O11	C32	1.2665(19)
O10	O1210	0.16(2)	O11	C317	1.479(2)
O10	C31	1.231(16)	C32	C317	0.2595
O10	C3210	1.366(16)	C32	O97	1.05(3)
O10	Tb26	2.33(2)	C32	O12	1.2705(19)
N1	C8	1.32(2)	C32	O107	1.37(3)
N1	C7	1.33(2)	C32	C277	1.504(2)
N2	C7	1.33(2)	O12	O107	0.16(4)
N2	N3	1.348(19)	O12	C317	1.1470(17)
N3	C8	1.32(2)	O12	Tb22	2.317(19)
N4	C22	1.34(2)			

Table 3. Bond lengths (Å) for compound 3

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ho1	O81	2.247(7)	N5	C2311	1.288(18)

Ho1	O8	2.247(7)	N5	N511	1.288(18)
Ho1	O32	2.333(6)	N5	C24	1.711(14)
Ho1	O33	2.333(6)	C1	C2	1.385(12)
Ho1	O64	2.396(7)	C1	C6	1.393(12)
Ho1	O65	2.396(7)	C1	C15	1.495(12)
Ho1	O54	2.541(6)	C2	C3	1.390(12)
Ho1	O55	2.541(6)	C3	C4	1.405(13)
Ho1	C174	2.843(10)	C3	C16	1.470(13)
Ho1	C175	2.843(10)	C4	C5	1.399(14)
Ho1	Ho2	3.9660(5)	C5	C6	1.380(13)
Ho1	Ho21	3.9660(5)	C5	C7	1.438(14)
Ho2	O106	2.272(18)	C8	C9	1.476(16)
Ho2	O7	2.322(6)	C9	C10	1.353(15)
Ho2	O123	2.334(8)	C9	C14	1.392(16)
Ho2	O11	2.349(11)	C10	C11	1.413(14)
Ho2	O23	2.350(6)	C11	C12	1.413(15)
Ho2	O1	2.402(6)	C12	C13	1.385(14)
Ho2	O54	2.457(6)	C12	C17	1.474(13)
Ho2	O32	2.491(6)	C13	C14	1.381(15)
Ho2	O97	2.502(16)	C16	Ho28	2.861(10)
Ho2	O42	2.540(7)	C17	Ho19	2.843(10)
Ho2	O2	2.583(6)	C18	C1911	1.394(11)
Ho2	C162	2.861(10)	C18	C19	1.394(11)
O1	C15	1.270(11)	C19	C20	1.367(13)
O2	C15	1.264(11)	C19	C30	1.525(11)
O2	Ho23	2.350(6)	C20	C21	1.400(12)

O3	C16	1.299(11)	C21	C2011	1.400(12)
O3	Ho13	2.333(6)	C21	C22	1.46(3)
O3	Ho28	2.491(6)	C22	N411	1.334(18)
O4	C16	1.232(12)	C24	C29	1.3941(16)
O4	Ho28	2.540(7)	C24	C25	1.4022(16)
O5	C17	1.252(10)	C25	C26	1.3972(16)
O5	Ho29	2.457(6)	C26	C27	1.3941(16)
O5	Ho19	2.541(6)	C27	C28	1.4025(16)
O6	C17	1.266(12)	C27	C31	1.4062(16)
O6	Ho19	2.396(7)	C27	C3210	1.4709(16)
O7	C30	1.225(10)	C28	C29	1.3979(16)
O8	C30	1.275(10)	C31	C3210	0.2938
O9	O1110	0.276(15)	C31	O1210	1.0868(12)
O9	C3210	1.048(13)	C31	O1110	1.5038(17)
O9	C31	1.265(13)	O11	O97	0.28(2)
O9	Ho210	2.502(16)	O11	C32	1.2644(14)
O10	O1210	0.161(16)	O11	C317	1.5038(17)
O10	C31	1.224(13)	C32	C317	0.2938
O10	C3210	1.404(13)	C32	O97	1.05(2)
O10	Ho26	2.272(18)	C32	O12	1.2637(14)
N1	C8	1.326(15)	C32	O107	1.40(2)
N1	C7	1.326(16)	C32	C277	1.4709(17)
N2	C7	1.352(15)	O12	O107	0.16(3)
N2	N3	1.351(14)	O12	C317	1.0868(12)
N3	C8	1.314(18)	O12	Ho23	2.334(14)
N4	C22	1.334(18)			

Table 4. Bond lengths (Å) for compound 4

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Dy1	O8	2.251(8)	N5	C2311	1.300(18)
Dy1	O81	2.251(8)	N5	N511	1.300(18)
Dy1	O32	2.342(8)	N5	C24	1.705(15)
Dy1	O33	2.342(8)	C1	C2	1.402(15)
Dy1	O64	2.393(8)	C1	C6	1.370(17)
Dy1	O65	2.393(9)	C1	C15	1.462(16)
Dy1	O54	2.552(8)	C2	C3	1.369(16)
Dy1	O55	2.552(8)	C3	C4	1.402(18)
Dy1	C174	2.874(10)	C3	C16	1.487(16)
Dy1	C175	2.874(10)	C4	C5	1.394(17)
Dy1	Dy2	3.9800(10)	C5	C6	1.375(18)
Dy1	Dy21	3.9800(10)	C5	C7	1.45(2)
Dy2	O122	2.317(10)	C8	C9	1.46(2)
Dy2	O106	2.30(2)	C9	C14	1.398(19)
Dy2	O11	2.325(14)	C9	C10	1.37(2)
Dy2	O7	2.328(8)	C10	C11	1.382(18)
Dy2	O22	2.340(8)	C11	C12	1.401(17)
Dy2	O1	2.395(9)	C12	C13	1.398(18)
Dy2	O54	2.466(8)	C12	C17	1.465(17)
Dy2	O33	2.505(7)	C13	C14	1.357(18)
Dy2	O97	2.514(18)	C16	Dy28	2.889(12)
Dy2	O43	2.547(10)	C17	Dy19	2.874(10)
Dy2	O2	2.597(7)	C18	C1911	1.385(14)
Dy2	C163	2.889(12)	C18	C19	1.385(14)

O1	C15	1.292(14)	C19	C20	1.396(15)
O2	C15	1.273(14)	C19	C30	1.530(14)
O2	Dy22	2.340(8)	C20	C21	1.377(14)
O3	C16	1.307(14)	C21	C2011	1.377(14)
O3	Dy12	2.342(8)	C21	C22	1.49(3)
O3	Dy28	2.505(7)	C22	N411	1.342(18)
O4	C16	1.232(15)	C24	C29	1.3966(19)
O4	Dy28	2.547(10)	C24	C25	1.3999(19)
O5	C17	1.259(13)	C25	C26	1.3976(19)
O5	Dy29	2.466(8)	C26	C27	1.3966(19)
O5	Dy19	2.552(7)	C27	C28	1.4003(19)
O6	C17	1.273(14)	C27	C31	1.4072(19)
O6	Dy19	2.393(8)	C27	C3210	1.513(2)
O7	C30	1.222(12)	C28	C29	1.3980(19)
O8	C30	1.278(13)	C31	C3210	0.2912
O9	O1110	0.274(17)	C31	O1210	1.1301(16)
O9	C3210	1.038(15)	C31	O1110	1.501(2)
O9	C31	1.257(15)	O11	O97	0.27(3)
O9	Dy210	2.514(18)	O11	C32	1.2626(17)
O10	O1210	0.14(2)	O11	C317	1.501(2)
O10	C31	1.228(15)	C32	C317	0.2912
O10	C3210	1.374(15)	C32	O97	1.04(3)
O10	Dy26	2.30(2)	C32	O12	1.2660(17)
N1	C8	1.32(2)	C32	O107	1.37(3)
N1	C7	1.337(19)	C32	C277	1.513(2)
N2	C7	1.34(2)	O12	O107	0.14(4)

N2	N3	1.363(19)	O12	C317	1.1301(15)
N3	C8	1.30(2)	O12	Dy22	2.317(17)
N4	C22	1.342(18)			