Supplementary Material (ESI) for Chemical Communications

SUPPORTING INFORMATION

A three-dimensional lanthanide-organic radical open-framework.

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Figure SI1. X-ray powder diffractograms recorded for [Tb(PTMTC)DMF_3] (**1**) in desolvatation-resolvatation process

Figure SI2. Thermogravimetric analyses curve of [Tb(PTMTC)$(DMF)_3$] (**1**).

Figure SI3. Ortep view of the asymmetric unit of **1**

Table SI4. Final coordinates and equivalent isotropic displacement parameters of the non-hydrogen atoms of **1**.

Table SI5. Hydrogen Atom Positions and Isotropic Displacement Parameters of **1**.

Table SI6. Bond Distances (Angstrom) of **1**.

Table SI7. Bond Angles (Degrees) of **1**.

Figure SI8. Ortep view of the asymmetric unit of **2**

Table SI9. Final coordinates and equivalent isotropic displacement parameters of the non-hydrogen atoms of **2**.

Table SI10. Hydrogen Atom Positions and Isotropic Displacement Parameters of **2**.

Table SI11. Bond Distances (Angstrom) of **2**.

Table S12. Bond Angles (Degrees) of **2**.

Elemental analysis for (1) and (2)

Figure SI1. X-ray powder diffractograms recorded for [Tb(PTMTC)DMF_3] in desolvatation-resolvation process

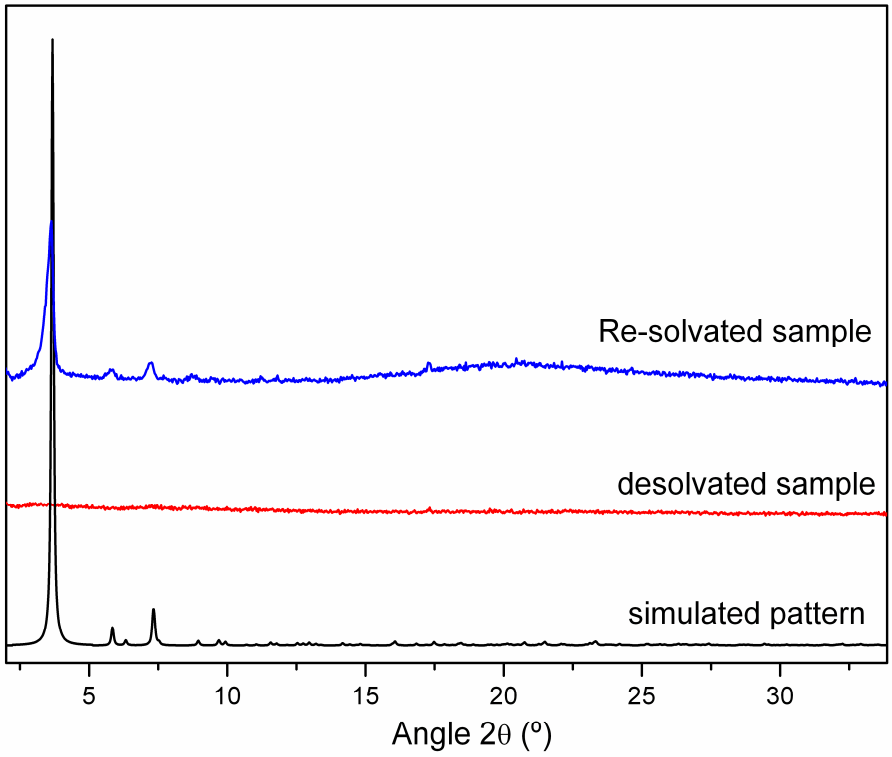

Figure SI2. Thermogravimetric analyses curve of [Tb(PTMTC)(DMF)$_3$] (**1**).

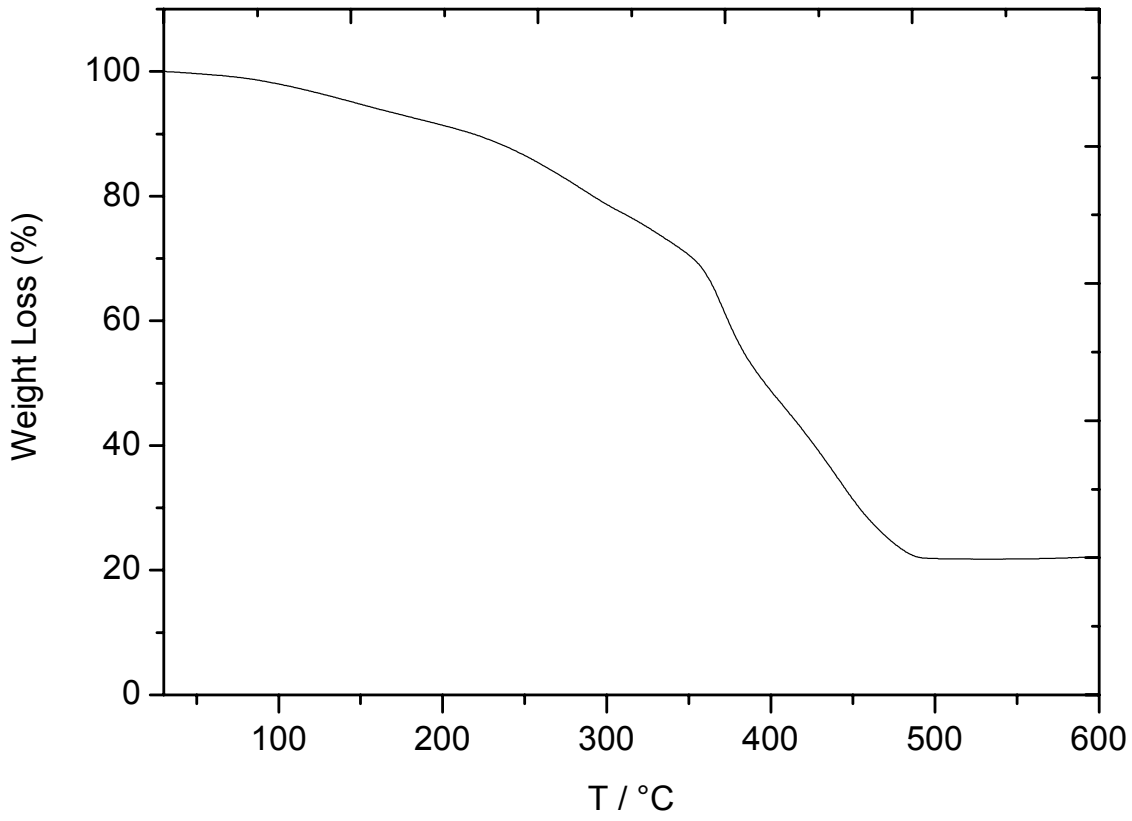

Figure SI3. Ortep view of the asymmetric unit of **1**

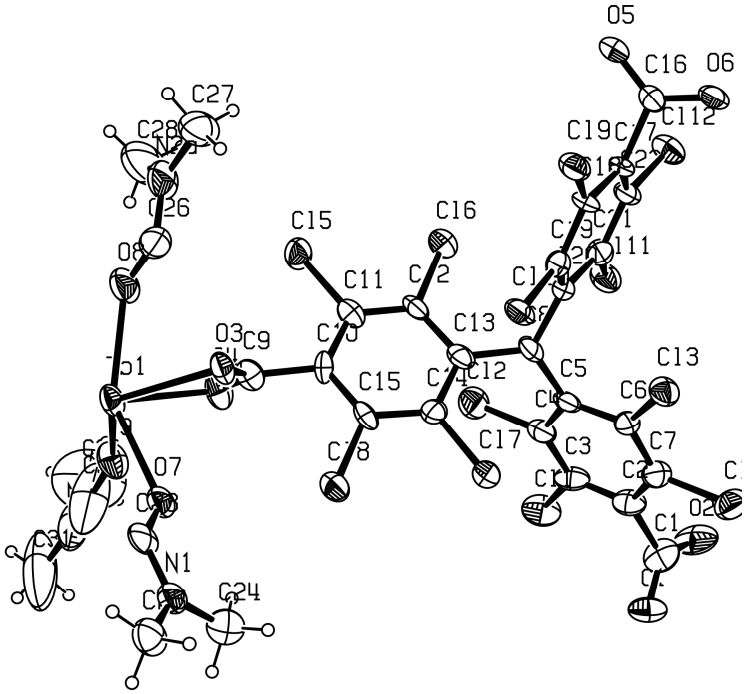

Table SI4. Final coordinates and equivalent isotropic displacement parameters of the non-hydrogen atoms of **1**.

Atom	x	y	z	U(eq) [Ang^2]
Tb1	0.80028(1)	0.16082(1)	0.25487(1)	0.0603(2)
Cl1	1.15409(10)	0.03809(9)	0.24304(5)	0.0902(11)
Cl2	1.05539(8)	0.02616(9)	0.21507(5)	0.0803(9)
Cl3	1.12326(7)	0.11427(7)	0.12019(4)	0.0627(8)
Cl4	1.22187(7)	0.12247(8)	0.14893(5)	0.0800(9)
Cl5	0.86995(7)	0.03411(7)	0.19123(5)	0.0723(8)
Cl6	0.96032(7)	-0.00137(7)	0.16019(5)	0.0705(8)
Cl7	1.04658(7)	0.16873(7)	0.18288(4)	0.0619(8)
Cl8	0.95622(7)	0.20113(7)	0.21497(4)	0.0679(8)
Cl9	0.96514(7)	0.09576(7)	0.05690(4)	0.0609(8)
Cl10	0.99255(7)	0.13721(7)	0.11534(4)	0.0604(8)
Cl11	1.08476(8)	-0.02857(8)	0.14035(4)	0.0724(9)
Cl12	1.06481(8)	-0.06393(7)	0.07897(4)	0.0719(9)
O1	1.2380(2)	0.1230(2)	0.22270(13)	0.082(3)
O2	1.2588(3)	0.0518(3)	0.20557(16)	0.107(3)
O3	0.8476(2)	0.1613(2)	0.20901(11)	0.059(2)
O4	0.8694(2)	0.11345(19)	0.24291(14)	0.072(2)
O5	0.9672(2)	-0.0203(2)	0.03836(10)	0.066(2)
O6	1.0378(2)	0.00646(18)	0.02319(12)	0.060(2)
O7	0.8605(2)	0.2198(2)	0.26072(10)	0.065(2)
O8	0.7676(2)	0.1031(2)	0.22432(17)	0.089(3)
O9	0.8352(2)	0.1366(2)	0.29679(15)	0.081(3)
N1	0.8897(3)	0.2962(3)	0.26364(14)	0.066(3)
N2A	0.7511(3)	0.0586(4)	0.1849(2)	0.100(4)
N3	0.8443(3)	0.1355(6)	0.3427(3)	0.151(7)
C1	1.2312(4)	0.0853(5)	0.2087(2)	0.082(4)
C2	1.1827(3)	0.0805(3)	0.1947(2)	0.064(4)
C3	1.1443(4)	0.0594(3)	0.20895(18)	0.064(3)
C4	1.1007(3)	0.0555(3)	0.1966(2)	0.062(4)
C5	1.0918(3)	0.0722(3)	0.16837(17)	0.051(3)
C6	1.1304(3)	0.0914(3)	0.15372(16)	0.051(3)
C7	1.1748(3)	0.0958(3)	0.1672(2)	0.064(3)
C8	1.0433(3)	0.0693(3)	0.15560(17)	0.072(4)
C9	0.8750(3)	0.1305(3)	0.2189(2)	0.058(4)
C10	0.9180(3)	0.1155(3)	0.20166(16)	0.052(3)
C11	0.9202(3)	0.0713(3)	0.18851(17)	0.056(3)
C12	0.9594(3)	0.0565(3)	0.17406(15)	0.052(3)
C13	1.0012(3)	0.0852(3)	0.17190(15)	0.053(3)
C14	0.9987(3)	0.1297(3)	0.18557(16)	0.053(3)
C15	0.9572(3)	0.1443(3)	0.19967(14)	0.049(3)
C16	1.0064(4)	0.0001(3)	0.04173(18)	0.057(4)
C17	1.0177(3)	0.0183(3)	0.07129(17)	0.052(3)
C18	1.0001(3)	0.0622(3)	0.07990(16)	0.051(3)
C19	1.0097(3)	0.0803(3)	0.10657(19)	0.053(3)
C20	1.0360(3)	0.0528(3)	0.12653(17)	0.054(3)
C21	1.0539(3)	0.0076(3)	0.11707(18)	0.056(3)
C22	1.0443(3)	-0.0090(3)	0.09016(19)	0.051(3)
C23	0.8548(4)	0.2648(5)	0.25961(16)	0.070(4)
C24	0.9382(4)	0.2818(4)	0.2711(2)	0.099(5)
C25	0.8797(4)	0.3463(3)	0.26060(19)	0.084(4)
C26	0.7666(3)	0.0977(4)	0.1983(3)	0.088(5)

C27	0.7501(4)	0.0548(4)	0.1543(2)	0.107(5)
C28	0.7412(6)	0.0136(5)	0.2014(3)	0.167(8)
C29	0.8375(5)	0.1470(11)	0.3175(4)	0.282(17)
C30	0.8455(12)	0.0790(7)	0.3443(6)	0.34(2)
C31	0.8442(7)	0.1458(13)	0.3717(6)	0.60(5)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table SI5. Hydrogen Atom Positions and Isotropic Displacement Parameters of **1**.

Atom	x	y	z	U(iso) [Ang^2]
H24A	0.94770	0.29750	0.28840	0.1480
H24B	0.95970	0.29070	0.25600	0.1480
H24C	0.93920	0.24770	0.27370	0.1480
H25A	0.89940	0.35950	0.24580	0.1270
H25B	0.88650	0.36250	0.27820	0.1270
H25C	0.84660	0.35070	0.25580	0.1270
H27A	0.76700	0.02640	0.14850	0.1610
H27B	0.76530	0.08240	0.14610	0.1610
H27C	0.71750	0.05300	0.14790	0.1610
H28A	0.70790	0.00550	0.19970	0.2500
H28B	0.74900	0.01860	0.22110	0.2500
H28C	0.76030	-0.01200	0.19390	0.2500
H30D	0.84010	0.06590	0.32570	0.5080
H30E	0.82090	0.06800	0.35700	0.5080
H30F	0.87620	0.06880	0.35120	0.5080
H31D	0.83530	0.17870	0.37460	0.8980
H31E	0.87560	0.14040	0.37940	0.8980
H31F	0.82160	0.12540	0.38120	0.8980

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table SI6. Bond Distances (Angstrom) of **1**.

Tb1	-O3	2.526(5)	O9	-C29	1.02(2)
Tb1	-O4	2.406(6)	N1	-C23	1.324(15)
Tb1	-O7	2.370(6)	N1	-C24	1.455(14)
Tb1	-O8	2.342(7)	N1	-C25	1.434(12)
Tb1	-O9	2.298(7)	N2A	-C26	1.332(16)
Tb1	-O5_a	2.377(5)	N2A	-C27	1.441(13)
Tb1	-O1_f	2.291(6)	N2A	-C28	1.502(18)
Tb1	-O6_n	2.300(5)	N3	-C29	1.24(2)
Cl1	-C3	1.729(9)	N3	-C30	1.58(3)
Cl2	-C4	1.739(9)	N3	-C31	1.39(3)
Cl3	-C6	1.710(8)	C1	-C2	1.511(14)
Cl4	-C7	1.737(9)	C2	-C3	1.394(13)
Cl5	-C11	1.750(9)	C2	-C7	1.378(13)
Cl6	-C12	1.742(8)	C3	-C4	1.353(14)
Cl7	-C14	1.729(9)	C4	-C5	1.427(12)
Cl8	-C15	1.742(8)	C5	-C6	1.386(12)
Cl9	-C18	1.731(8)	C5	-C8	1.483(12)
Cl10	-C19	1.710(9)	C6	-C7	1.397(12)
Cl11	-C21	1.719(9)	C8	-C13	1.471(12)
Cl12	-C22	1.719(9)	C8	-C20	1.455(11)
O1	-C1	1.255(14)	C9	-C10	1.507(12)
O2	-C1	1.221(15)	C10	-C11	1.381(12)
O3	-C9	1.241(10)	C10	-C15	1.361(12)
O4	-C9	1.233(11)	C11	-C12	1.352(12)
O5	-C16	1.244(12)	C12	-C13	1.419(12)
O6	-C16	1.248(11)	C13	-C14	1.400(12)
O7	-C23	1.268(15)	C14	-C15	1.395(11)
O8	-C26	1.231(16)	C16	-C17	1.511(12)
C17	-C18	1.381(12)	C27	-H27A	0.9600
C17	-C22	1.385(12)	C27	-H27B	0.9600
C18	-C19	1.376(12)	C27	-H27C	0.9600
C19	-C20	1.417(12)	C28	-H28A	0.9600
C20	-C21	1.428(12)	C28	-H28B	0.9600
C21	-C22	1.372(12)	C28	-H28C	0.9600
C24	-H24A	0.9600	C30	-H30D	0.9600
C24	-H24B	0.9600	C30	-H30E	0.9600
C24	-H24C	0.9600	C30	-H30F	0.9600
C25	-H25A	0.9600	C31	-H31D	0.9600
C25	-H25B	0.9600	C31	-H31E	0.9600
C25	-H25C	0.9600	C31	-H31F	0.9600

Table SI7. Bond Angles (Degrees) of **1**.

O3	-Tb1	-O4	52.0(2)	O1_f	-Tb1	-O9	78.1(2)
O3	-Tb1	-O7	73.97(17)	O6_n	-Tb1	-O9	154.1(2)
O3	-Tb1	-O8	71.7(2)	O5_a	-Tb1	-C9	149.0(2)
O3	-Tb1	-O9	120.63(19)	O1_f	-Tb1	-C9	134.4(2)
O3	-Tb1	-C9	26.2(2)	O6_n	-Tb1	-C9	103.8(2)
O3	-Tb1	-O5_a	138.10(18)	O1_f	-Tb1	-O5_a	74.6(2)
O1_f	-Tb1	-O3	142.31(19)	O5_a	-Tb1	-O6_n	77.19(19)
O3	-Tb1	-O6_n	77.69(18)	O1_f	-Tb1	-O6_n	98.45(19)
O4	-Tb1	-O7	80.78(19)	Tb1_g	-O1	-C1	137.9(6)
O4	-Tb1	-O8	78.0(2)	Tb1	-O3	-C9	90.0(5)
O4	-Tb1	-O9	72.4(2)	Tb1	-O4	-C9	95.9(5)
O4	-Tb1	-C9	25.9(2)	Tb1_c	-O5	-C16	145.9(5)
O4	-Tb1	-O5_a	143.2(2)	Tb1_h	-O6	-C16	156.0(5)
O1_f	-Tb1	-O4	117.57(19)	Tb1	-O7	-C23	126.5(6)
O4	-Tb1	-O6_n	129.5(2)	Tb1	-O8	-C26	134.5(6)
O7	-Tb1	-O8	145.6(2)	Tb1	-O9	-C29	139.6(15)
O7	-Tb1	-O9	78.71(18)	C23	-N1	-C24	122.4(9)
O7	-Tb1	-C9	75.7(2)	C23	-N1	-C25	119.2(9)
O5_a	-Tb1	-O7	73.32(18)	C24	-N1	-C25	118.3(8)
O1_f	-Tb1	-O7	143.68(19)	C26	-N2A	-C27	122.5(10)
O6_n	-Tb1	-O7	90.59(18)	C26	-N2A	-C28	120.1(10)
O8	-Tb1	-O9	119.2(2)	C27	-N2A	-C28	116.7(10)
O8	-Tb1	-C9	73.4(2)	C29	-N3	-C30	108(2)
O5_a	-Tb1	-O8	136.3(2)	C29	-N3	-C31	152(2)
O1_f	-Tb1	-O8	70.7(2)	C30	-N3	-C31	99(2)
O6_n	-Tb1	-O8	82.6(2)	O1	-C1	-O2	127.6(10)
O9	-Tb1	-C9	96.4(2)	O1	-C1	-C2	116.0(10)
O5_a	-Tb1	-O9	77.17(19)	O2	-C1	-C2	116.5(10)
C1	-C2	-C3	121.2(8)	C9	-C10	-C15	120.9(7)
C1	-C2	-C7	121.6(8)	C11	-C10	-C15	117.5(8)
C3	-C2	-C7	117.2(8)	Cl5	-C11	-C10	117.5(6)
Cl1	-C3	-C2	117.9(8)	Cl5	-C11	-C12	120.3(7)
Cl1	-C3	-C4	120.7(8)	C10	-C11	-C12	122.2(8)
C2	-C3	-C4	121.4(8)	Cl6	-C12	-C11	118.9(7)
Cl2	-C4	-C3	118.6(7)	Cl6	-C12	-C13	119.0(6)
Cl2	-C4	-C5	119.4(6)	C11	-C12	-C13	121.9(8)
C3	-C4	-C5	121.9(8)	C8	-C13	-C12	121.6(7)
C4	-C5	-C6	116.9(7)	C8	-C13	-C14	123.1(8)
C4	-C5	-C8	121.1(7)	C12	-C13	-C14	115.3(7)
C6	-C5	-C8	122.0(7)	Cl7	-C14	-C13	119.2(6)
Cl3	-C6	-C5	120.7(6)	Cl7	-C14	-C15	119.5(6)
Cl3	-C6	-C7	119.2(6)	C13	-C14	-C15	121.2(8)
C5	-C6	-C7	119.9(7)	Cl8	-C15	-C10	119.8(6)
Cl4	-C7	-C2	118.3(7)	Cl8	-C15	-C14	118.3(6)
Cl4	-C7	-C6	119.0(7)	C10	-C15	-C14	121.9(8)
C2	-C7	-C6	122.6(8)	O5	-C16	-O6	126.5(8)
C5	-C8	-C13	120.2(7)	O5	-C16	-C17	117.0(8)
C5	-C8	-C20	121.6(7)	O6	-C16	-C17	116.5(8)
C13	-C8	-C20	118.1(7)	C16	-C17	-C18	119.5(7)
Tb1	-C9	-O3	63.8(4)	C16	-C17	-C22	121.0(8)
Tb1	-C9	-O4	58.3(4)	C18	-C17	-C22	119.5(7)
Tb1	-C9	-C10	175.0(6)	Cl9	-C18	-C17	119.9(6)
O3	-C9	-O4	122.1(8)	Cl9	-C18	-C19	118.6(6)
O3	-C9	-C10	118.9(8)	C17	-C18	-C19	121.5(8)
O4	-C9	-C10	119.0(7)	Cl10	-C19	-C18	120.4(7)
C9	-C10	-C11	121.6(7)	Cl10	-C19	-C20	119.3(7)

C18	-C19	-C20	120.2(8)	N2A	-C27	-H27A	109.00
C8	-C20	-C19	121.4(8)	N2A	-C27	-H27B	109.00
C8	-C20	-C21	121.5(7)	N2A	-C27	-H27C	110.00
C19	-C20	-C21	117.1(7)	H27A	-C27	-H27B	109.00
Cl11	-C21	-C20	119.8(6)	H27A	-C27	-H27C	109.00
Cl11	-C21	-C22	119.0(6)	H27B	-C27	-H27C	110.00
C20	-C21	-C22	121.1(8)	N2A	-C28	-H28A	109.00
Cl12	-C22	-C17	118.3(7)	N2A	-C28	-H28B	109.00
Cl12	-C22	-C21	121.2(7)	N2A	-C28	-H28C	109.00
C17	-C22	-C21	120.5(8)	H28A	-C28	-H28B	110.00
O7	-C23	-N1	123.9(10)	H28A	-C28	-H28C	109.00
O8	-C26	-N2A	125.2(11)	H28B	-C28	-H28C	110.00
O9	-C29	-N3	148(3)	N3	-C30	-H30D	110.00
N1	-C24	-H24A	110.00	N3	-C30	-H30E	110.00
N1	-C24	-H24B	109.00	N3	-C30	-H30F	109.00
N1	-C24	-H24C	109.00	H30D	-C30	-H30E	109.00
H24A	-C24	-H24B	109.00	H30D	-C30	-H30F	110.00
H24A	-C24	-H24C	110.00	H30E	-C30	-H30F	110.00
H24B	-C24	-H24C	109.00	N3	-C31	-H31D	110.00
N1	-C25	-H25A	110.00	N3	-C31	-H31E	110.00
N1	-C25	-H25B	110.00	N3	-C31	-H31F	109.00
N1	-C25	-H25C	110.00	H31D	-C31	-H31E	109.00
H25A	-C25	-H25B	109.00	H31D	-C31	-H31F	109.00
H25A	-C25	-H25C	109.00	H31E	-C31	-H31F	109.00
H25B	-C25	-H25C	109.00				

Translation of Symmetry Code to Equiv.Pos

```
a =[  2545.00 ]  = 3/4-y,-3/4+x,1/4+z
b =[  3664.00 ]  = 3/2-x,1-y,-1/2+z
c =[  4554.00 ]  = 3/4+y,3/4-x,-1/4+z
d =[  5765.00 ]  = 2-x,1-y,-z
e =[  6564.00 ]  = 1/4+y,7/4-x,-1/4-z
f =[  7455.00 ]  = -1/2+x,y,1/2-z
g =[  7555.00 ]  = 1/2+x,y,1/2-z
h =[  8645.00 ]  = 5/4-y,-3/4+x,1/4-z
i =[  9554.00 ]  = 1/2+x,1/2+y,-1/2+z
j =[ 10644.00 ]  = 5/4-y,-1/4+x,-1/4+z
k =[ 11755.00 ]  = 2-x,1/2-y,z
l =[ 12564.00 ]  = 1/4+y,5/4-x,-3/4+z
m =[ 13655.00 ]  = 3/2-x,1/2-y,1/2-z
n =[ 14565.00 ]  = 3/4+y,5/4-x,1/4-z
o =[ 15555.00 ]  = x,1/2+y,-z
p =[ 16544.00 ]  = 3/4-y,-1/4+x,-1/4-z
q =[  5755.00 ]  = 2-x,-y,-z
```

Figure SI8. Ortep view of the asymmetric unit of **2**

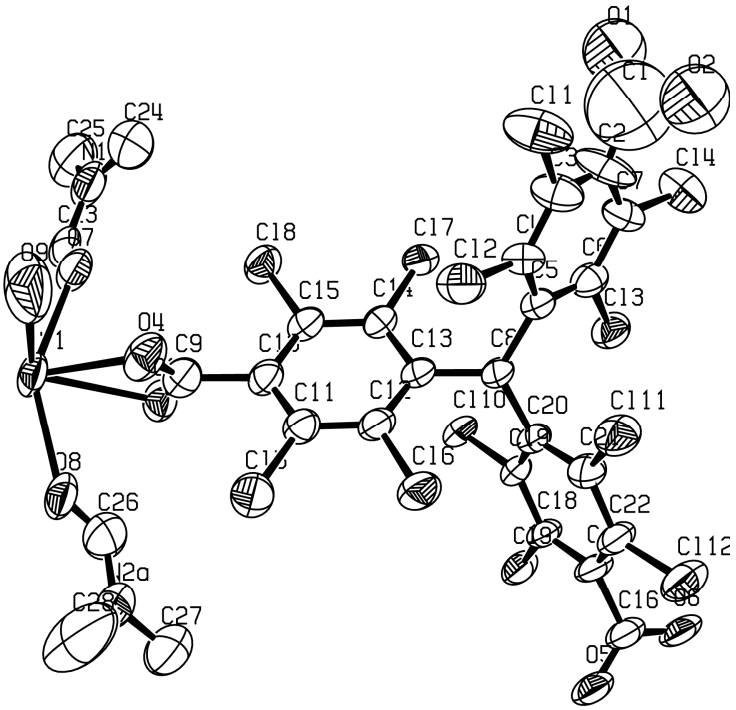

Table SI9. Final coordinates and equivalent isotropic displacement parameters of the non-hydrogen atoms of **2**.

Atom	x	y	z	U(eq) [Ang^2]
Tb1	0.79547(2)	0.16387(2)	0.25416(1)	0.1434(4)
Cl1	1.15424(18)	0.04925(18)	0.24659(10)	0.222(3)
Cl2	1.05925(13)	0.03083(13)	0.21908(8)	0.1637(17)
Cl3	1.11937(11)	0.11727(12)	0.12228(6)	0.1393(13)
Cl4	1.21430(13)	0.13292(16)	0.15099(10)	0.184(2)
Cl5	0.87107(13)	0.03974(12)	0.19454(9)	0.1683(16)
Cl6	0.95896(12)	0.00313(11)	0.16463(8)	0.1560(16)
Cl7	1.04419(9)	0.16999(11)	0.18561(6)	0.1265(11)
Cl8	0.95628(12)	0.20219(10)	0.21749(7)	0.1443(14)
Cl9	0.96993(11)	0.09915(10)	0.05821(6)	0.1349(11)
Cl10	0.99451(10)	0.13807(10)	0.11746(6)	0.1353(12)
Cl11	1.08138(14)	-0.02597(14)	0.14283(7)	0.1690(16)
Cl12	1.05979(15)	-0.06048(12)	0.08157(8)	0.1753(19)
O1	1.2281(6)	0.1295(6)	0.2258(3)	0.334(14)
O2	1.2493(9)	0.0811(10)	0.2038(6)	0.400(14)
O3	0.8476(3)	0.1641(3)	0.20856(19)	0.140(4)
O4	0.8658(4)	0.1215(3)	0.2445(2)	0.170(5)
O5	0.9662(4)	-0.0157(3)	0.04072(17)	0.151(4)
O6	1.0354(4)	0.0090(3)	0.0243(2)	0.160(4)
O7	0.8539(4)	0.2188(4)	0.2628(2)	0.159(4)
O8	0.7658(4)	0.1069(4)	0.2213(2)	0.191(5)
O9	0.8375(5)	0.1296(5)	0.2976(3)	0.355(15)
N1	0.8906(7)	0.2900(6)	0.2685(3)	0.190(8)
N2A	0.7510(6)	0.0635(7)	0.1811(5)	0.257(10)
C1	1.2143(7)	0.1033(9)	0.2110(6)	0.68(7)
C2	1.1781(5)	0.0934(4)	0.1980(5)	0.212(10)
C3	1.1425(5)	0.0684(5)	0.2119(3)	0.155(6)
C4	1.1000(4)	0.0610(4)	0.1993(3)	0.120(5)
C5	1.0903(4)	0.0758(4)	0.1719(2)	0.110(4)
C6	1.1269(5)	0.0969(4)	0.1576(2)	0.115(5)
C7	1.1709(4)	0.1051(4)	0.1702(3)	0.132(5)
C8	1.0424(4)	0.0697(7)	0.1595(3)	0.218(11)
C9	0.8732(5)	0.1365(4)	0.2211(3)	0.125(6)
C10	0.9177(4)	0.1188(4)	0.2043(2)	0.113(4)
C11	0.9198(4)	0.0749(4)	0.1926(2)	0.114(4)
C12	0.9600(5)	0.0600(4)	0.1782(2)	0.115(5)
C13	1.0004(4)	0.0871(4)	0.17517(19)	0.109(4)
C14	0.9986(4)	0.1318(4)	0.1879(2)	0.106(4)
C15	0.9579(4)	0.1472(3)	0.2024(2)	0.109(4)
C16	1.0051(6)	0.0041(5)	0.0435(3)	0.133(6)
C17	1.0150(4)	0.0214(4)	0.0730(2)	0.120(5)
C18	1.0006(3)	0.0644(4)	0.0820(2)	0.110(4)
C19	1.0111(4)	0.0812(4)	0.1092(2)	0.112(4)
C20	1.0353(4)	0.0546(4)	0.1290(2)	0.115(4)
C21	1.0511(4)	0.0115(5)	0.1200(2)	0.135(5)
C22	1.0400(4)	-0.0050(4)	0.0916(2)	0.132(5)
C23	0.8537(6)	0.2596(9)	0.2612(3)	0.172(8)
C24	0.9327(9)	0.2682(11)	0.2780(6)	0.307(18)
C25	0.8871(8)	0.3426(8)	0.2662(5)	0.263(14)
C26	0.7698(7)	0.1019(8)	0.1957(6)	0.238(13)
C27	0.7571(9)	0.0603(9)	0.1498(5)	0.290(16)
C28	0.7287(19)	0.0269(16)	0.1941(8)	0.69(5)

U(eq) = 1/3 of the trace of the orthogonalized U Tenso

Table SI10. Hydrogen Atom Positions and Isotropic Displacement Parameters of **2**.

Atom	x	y	z	U(iso) [Ang^2]
H8	1.03920	0.03780	0.16700	0.2640
H9	0.83940	0.15220	0.30970	2.0000
H9A	0.81920	0.12810	0.31120	0.5350
H24A	0.93910	0.27760	0.29730	0.4580
H24B	0.95820	0.27760	0.26580	0.4580
H24C	0.92920	0.23470	0.27720	0.4580
H25A	0.85540	0.35120	0.26150	0.3910
H25B	0.90790	0.35350	0.25150	0.3910
H25C	0.89570	0.35650	0.28420	0.3910
H27A	0.77420	0.08720	0.14310	0.4370
H27B	0.72690	0.05920	0.14070	0.4370
H27C	0.77430	0.03230	0.14520	0.4370
H28A	0.71870	0.00470	0.17990	1.0370
H28B	0.70190	0.03840	0.20440	1.0370
H28C	0.74990	0.01190	0.20720	1.0370

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table SI11. Bond Distances (Angstrom) of **2**.

Tb1	-O3	2.595(9)	O9	-H9A	0.8200
Tb1	-O4	2.382(11)	O9	-H9	0.8600
Tb1	-O7	2.320(11)	N1	-C25	1.51(3)
Tb1	-O8	2.388(11)	N1	-C23	1.40(3)
Tb1	-O9	2.549(14)	N1	-C24	1.42(3)
Tb1	-O5_a	2.420(10)	N2A	-C27	1.47(3)
Tb1	-O1_f	2.349(17)	N2A	-C26	1.40(3)
Tb1	-O6_n	2.221(10)	N2A	-C28	1.36(5)
Cl1	-C3	1.741(15)	C1	-C2	1.23(3)
Cl2	-C4	1.714(13)	C2	-C3	1.40(2)
Cl3	-C6	1.761(10)	C2	-C7	1.36(3)
Cl4	-C7	1.721(13)	C3	-C4	1.362(19)
Cl5	-C11	1.714(12)	C4	-C5	1.375(17)
Cl6	-C12	1.740(12)	C5	-C6	1.376(17)
Cl7	-C14	1.698(12)	C5	-C8	1.492(16)
Cl8	-C15	1.718(9)	C6	-C7	1.404(18)
Cl9	-C18	1.725(10)	C8	-C13	1.487(17)
Cl10	-C19	1.731(12)	C8	-C20	1.501(17)
Cl11	-C21	1.738(12)	C9	-C10	1.574(18)
Cl12	-C22	1.742(12)	C10	-C15	1.405(16)
O1	-C1	1.09(3)	C10	-C11	1.366(16)
O2	-C1	1.23(3)	C11	-C12	1.394(17)
O3	-C9	1.222(16)	C12	-C13	1.393(18)
O4	-C9	1.192(17)	C13	-C14	1.406(16)
O5	-C16	1.25(2)	C14	-C15	1.412(15)
O6	-C16	1.252(19)	C16	-C17	1.490(17)
O7	-C23	1.17(3)	C17	-C22	1.352(15)
O8	-C26	1.21(3)	C17	-C18	1.358(16)
C18	-C19	1.389(14)	C25	-H25B	0.9600
C19	-C20	1.380(15)	C25	-H25C	0.9600
C20	-C21	1.374(18)	C27	-H27A	0.9600
C21	-C22	1.442(14)	C27	-H27B	0.9600
C8	-H8	0.9800	C27	-H27C	0.9600
C24	-H24A	0.9600	C28	-H28A	0.9600
C24	-H24B	0.9600	C28	-H28B	0.9600
C24	-H24C	0.9600	C28	-H28C	0.9600
C25	-H25A	0.9600			

Table S12. Bond Angles (Degrees) of **2**.

O3	-Tb1	-O4	50.6(3)	O1_f	-Tb1	-O9	84.7(5)
O3	-Tb1	-O7	74.4(3)	O6_n	-Tb1	-O9	160.9(4)
O3	-Tb1	-O8	71.2(3)	O5_a	-Tb1	-C9	146.6(3)
O3	-Tb1	-O9	112.6(4)	O1_f	-Tb1	-C9	138.3(5)
O3	-Tb1	-C9	25.7(3)	O6_n	-Tb1	-C9	102.8(4)
O3	-Tb1	-O5_a	141.0(3)	O1_f	-Tb1	-O5_a	71.9(5)
O1_f	-Tb1	-O3	142.7(4)	O5_a	-Tb1	-O6_n	81.8(3)
O3	-Tb1	-O6_n	77.0(3)	O1_f	-Tb1	-O6_n	97.3(5)
O4	-Tb1	-O7	76.8(4)	Tb1_g	-O1	-C1	146.3(17)
O4	-Tb1	-O8	80.3(4)	Tb1	-O3	-C9	87.0(8)
O4	-Tb1	-O9	64.0(4)	Tb1	-O4	-C9	98.1(9)
O4	-Tb1	-C9	24.8(3)	Tb1_c	-O5	-C16	141.0(8)
O4	-Tb1	-O5_a	137.8(3)	Tb1_h	-O6	-C16	158.3(9)
O1_f	-Tb1	-O4	123.5(5)	Tb1	-O7	-C23	131.2(11)
O4	-Tb1	-O6_n	127.6(3)	Tb1	-O8	-C26	133.0(13)
O7	-Tb1	-O8	145.5(4)	Tb1	-O9	-H9A	110.00
O7	-Tb1	-O9	77.5(4)	H9	-O9	-H9A	65.00
O7	-Tb1	-C9	73.6(4)	Tb1	-O9	-H9	105.00
O5_a	-Tb1	-O7	73.3(3)	C24	-N1	-C25	121(2)
O1_f	-Tb1	-O7	143.0(4)	C23	-N1	-C25	123.2(18)
O6_n	-Tb1	-O7	90.0(4)	C23	-N1	-C24	116.0(19)
O8	-Tb1	-O9	114.6(4)	C26	-N2A	-C27	119(2)
O8	-Tb1	-C9	74.8(4)	C26	-N2A	-C28	124(3)
O5_a	-Tb1	-O8	138.4(3)	C27	-N2A	-C28	117(2)
O1_f	-Tb1	-O8	71.5(4)	O1	-C1	-O2	104(2)
O6_n	-Tb1	-O8	83.8(4)	O1	-C1	-C2	141(2)
O9	-Tb1	-C9	87.7(4)	O2	-C1	-C2	115(3)
O5_a	-Tb1	-O9	80.8(4)	C1	-C2	-C7	122.9(19)
C1	-C2	-C3	120(2)	C11	-C10	-C15	117.8(10)
C3	-C2	-C7	117.4(14)	C10	-C11	-C12	120.5(11)
Cl1	-C3	-C2	116.9(12)	Cl5	-C11	-C10	118.6(9)
Cl1	-C3	-C4	121.6(11)	Cl5	-C11	-C12	120.9(9)
C2	-C3	-C4	121.5(14)	Cl6	-C12	-C11	116.4(10)
Cl2	-C4	-C5	121.3(9)	Cl6	-C12	-C13	119.6(9)
Cl2	-C4	-C3	116.5(11)	C11	-C12	-C13	124.0(10)
C3	-C4	-C5	122.2(12)	C8	-C13	-C12	122.0(11)
C6	-C5	-C8	123.7(10)	C12	-C13	-C14	115.4(10)
C4	-C5	-C8	120.6(11)	C8	-C13	-C14	122.6(12)
C4	-C5	-C6	115.7(10)	C13	-C14	-C15	120.9(10)
Cl3	-C6	-C5	120.4(10)	Cl7	-C14	-C13	121.7(9)
Cl3	-C6	-C7	116.5(9)	Cl7	-C14	-C15	117.3(8)
C5	-C6	-C7	123.1(10)	Cl8	-C15	-C10	118.5(8)
C2	-C7	-C6	119.7(11)	Cl8	-C15	-C14	120.1(8)
Cl4	-C7	-C2	120.2(10)	C10	-C15	-C14	121.4(9)
Cl4	-C7	-C6	120.0(10)	O5	-C16	-O6	126.0(13)
C5	-C8	-C13	120.4(12)	O5	-C16	-C17	114.4(12)
C5	-C8	-C20	121.6(10)	O6	-C16	-C17	119.6(13)
C13	-C8	-C20	117.0(10)	C16	-C17	-C22	120.6(11)
Tb1	-C9	-O3	67.3(7)	C16	-C17	-C18	121.8(10)
O3	-C9	-C10	116.6(11)	C18	-C17	-C22	117.5(9)
O4	-C9	-C10	119.0(11)	Cl9	-C18	-C17	118.1(7)
Tb1	-C9	-O4	57.1(8)	Cl9	-C18	-C19	120.0(9)
Tb1	-C9	-C10	176.1(8)	C17	-C18	-C19	121.9(10)
O3	-C9	-O4	124.4(13)	C18	-C19	-C20	122.0(10)
C9	-C10	-C11	121.9(10)	Cl10	-C19	-C20	120.1(8)

C9	-C10	-C15	120.2(9)	Cl10	-C19	-C18	117.9(8)
C8	-C20	-C19	123.1(11)	H24B	-C24	-H24C	109.00
C8	-C20	-C21	120.1(11)	N1	-C25	-H25A	109.00
C19	-C20	-C21	116.7(9)	N1	-C25	-H25B	109.00
Cl11	-C21	-C20	121.6(8)	N1	-C25	-H25C	109.00
Cl11	-C21	-C22	118.2(10)	H25A	-C25	-H25B	110.00
C20	-C21	-C22	120.1(10)	H25A	-C25	-H25C	110.00
Cl12	-C22	-C21	118.2(9)	H25B	-C25	-H25C	110.00
Cl12	-C22	-C17	120.2(8)	N2A	-C27	-H27A	109.00
C17	-C22	-C21	121.7(11)	N2A	-C27	-H27B	110.00
O7	-C23	-N1	126.6(17)	N2A	-C27	-H27C	109.00
O8	-C26	-N2A	123(2)	H27A	-C27	-H27B	110.00
C5	-C8	-H8	93.00	H27A	-C27	-H27C	109.00
C13	-C8	-H8	93.00	H27B	-C27	-H27C	109.00
C20	-C8	-H8	93.00	N2A	-C28	-H28A	110.00
N1	-C24	-H24A	109.00	N2A	-C28	-H28B	109.00
N1	-C24	-H24B	109.00	N2A	-C28	-H28C	109.00
N1	-C24	-H24C	110.00	H28A	-C28	-H28B	110.00
H24A	-C24	-H24B	110.00	H28A	-C28	-H28C	109.00
H24A	-C24	-H24C	110.00	H28B	-C28	-H28C	109.00

Translation of Symmetry Code to Equiv.Pos

```
a =[  2545.00 ]  = 3/4-y,-3/4+x,1/4+z
b =[  3664.00 ]  = 3/2-x,1-y,-1/2+z
c =[  4554.00 ]  = 3/4+y,3/4-x,-1/4+z
d =[  5765.00 ]  = 2-x,1-y,-z
e =[  6564.00 ]  = 1/4+y,7/4-x,-1/4-z
f =[  7455.00 ]  = -1/2+x,y,1/2-z
g =[  7555.00 ]  = 1/2+x,y,1/2-z
h =[  8645.00 ]  = 5/4-y,-3/4+x,1/4-z
i =[  9554.00 ]  = 1/2+x,1/2+y,-1/2+z
j =[ 10644.00 ]  = 5/4-y,-1/4+x,-1/4+z
k =[ 11755.00 ]  = 2-x,1/2-y,z
l =[ 12564.00 ]  = 1/4+y,5/4-x,-3/4+z
m =[ 13655.00 ]  = 3/2-x,1/2-y,1/2-z
n =[ 14565.00 ]  = 3/4+y,5/4-x,1/4-z
o =[ 15555.00 ]  = x,1/2+y,-z
p =[ 16544.00 ]  = 3/4-y,-1/4+x,-1/4-z
q =[  5755.00 ]  = 2-x,-y,-z
```

Elemental analyses:

Elemental analyses were realized on the evacuated samples of **1** and **2** used to perform magnetic measurements. The formulations and the corresponding formula found for both **1** and **2** are in good agreement with the formula determined thanks to X-ray diffraction. The corresponding molecular weights have been used to treat the magnetic data.

Compound **1**:

Crystal structure formula: $[Tb(PTMTC)(DMF)_3]$
Calculated values for $C_{31}H_{21}N_3Cl_{12}O_9Tb_1$: C 31.99%, H 1.82%, N 3.60%
Found values: C 28.06-28.19%, H 1.06-1.27%, N 1.95%
Formulation deduced from elemental analysis: $C_{28}H_{24}N_2Cl_{12}O_{13}Tb_1$
Elemental analyses formula: Tb PTMTC $(DMF)_2$ $(H_2O)_5$

Compound **2**:

Crystal structure formula: $[Tb(\alpha H\text{-}PTMTC)(DMF)_2H_2O]$
Calculated values for $C_{28}H_{17}N_2Cl_{12}O_9Tb_1$: C 30.30%, H 1.54%, N 2.52%
Found values: C 30.65-30.72%, H 2.15-2.29%, N 3.92-4.00%
Formulation deduced from elemental analysis: $C_{31}H_{26}N_3Cl_{12}O_{11}Tb_1$
Elemental analyses formula: Tb (αH-PTMTC) $(DMF)_3$ $(H_2O)_2$