Supporting Information

Symmetry-Controlled and Face-Driven Approach for the Assembly of Cerium-based Molecular Polyhedra

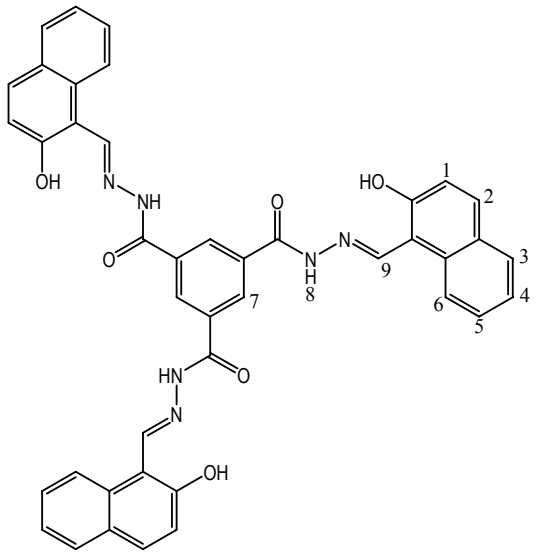
Yang Liu, ZhihuaLin，Cheng He,* Liang Zhao and Chunying Duan

1. Experimental Section.

1.1 Materials and Methods.

All chemicals were of reagent grade quality obtained from commercial sources and used without further purification. ^{1}H NMR spectra were measured on a BRUKER 400M spectrometer. ESI mass spectra were carried out on a HPLC-Q-Tof MS spectrometer using methanol as mobile phase. The elemental analyses of C, H and N were performed on a Vario EL III elemental analyzer.

1.2 Preparation



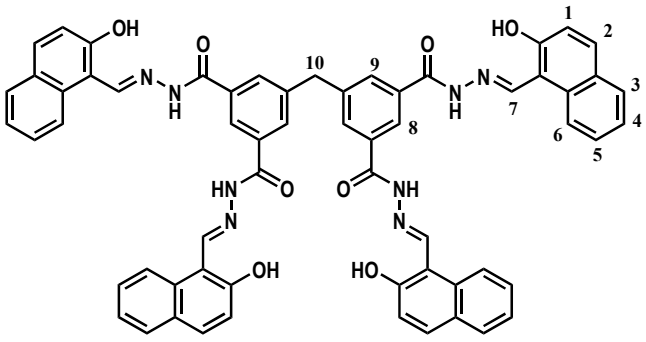
Scheme S1 Chemical structure of **NATB**

NATB: 1, 3, 5-Benzene-tricarbohydrazide (1 mmol, 0.252g) was added to a EtOH solution (70 mL) containing 2-hydroxy-1-naphthaldehyde (3.3 mmol, 0.568 g). After 5 drops of acetic acid was added, the yellow mixture was heated at boiling temperature under magnetic stirring for 24h. During the reaction, a yellow precipitate was formed, which was collected by filtration. Yield: 0.59g, 83%. Anal calc. for ($C_{42}H_{30}N_6O_6 \cdot 2H_2O$): H 4.56, C 67.19, N 11.19%. Found: H 4.38, C 67.38, N 11.02%.

^{1}H NMR (DMSO-d_6, ppm): 12.72(s, 3H$_8$), 12.70(s, 3H$_{OH}$), 9.59(s, 3H$_9$), 8.88(s, 3H$_7$), 8.34(d, 3H$_2$, J = 7.6Hz), 7.98(m, 3H$_3$), 7.92(d, 3H$_6$, J = 8.0Hz), 7.65(dd, 3H$_5$, J = 7.0Hz), 7.44(dd, 3H$_4$, J = 7.6 Hz) , 7.27(dd, 3H$_1$, J = 8.8 Hz).

Ce-**NATB**: A solution of $Ce(NO_3)_3{\cdot}6H_2O$ (13 mg, 0.03mmol) in methanol (6 mL) was layered onto a solution of **NATB** ligand (7.1 mg, 0.01mmol) and KOH (1.7mg, 0.03mmol) in $CH_3OH/CHCl_3$ (v:v = 1:1, 6mL). The solution was left for two weeks at room temperature to give X-ray quality black block crystals. Yield: 53%, based on the crystals that have been collected and then dried in vacuum. Anal calc. for $Ce_4(C_{42}H_{26}N_6O_6)_4$: H 3.08, C 59.29, N 9.88%. Found: H 3.34, C 59.04, N 10.35%. IR (KBr plate): 3430 (*br*), 1648 (*m*), 1611(*s*), 1570(*m*), 1540 (*w*), 1454(*w*), 1421 (*m*), 1381 (*s*), 1335(*m*), 1295 (*w*).

Ce-**NATB**-Cl: A solution of $Ce(NO_3)_3{\cdot}6H_2O$ (13 mg, 0.03mmol) and Bu_4NCl (33.3 mg, 0.12mmol) in methanol (6 mL) was layered onto a solution of **NATB** ligand (7.1 mg, 0.01mmol) and KOH (1.7mg, 0.03mmol) in $CH_3OH/CHCl_3$ (v:v = 1:1, 6mL). The solution was left for two weeks at room temperature to give X-ray quality black block crystals. Yield: 35%, based on the crystals that have been collected and then dried in vacuum. Anal calc. for $HCe_4(C_{42}H_{26}N_6O_6)_4Cl$: H 3.08, C 58.66, N 9.77 %. Found: H 3.94, C 58.83, N 10.05 %. IR (KBr plate) 3413 (*br*), 1617(*s*), 1592 (*m*), 1574(*m*), 1540 (*m*), 1450(*w*), 1426 (*w*), 1383(*s*), 1359(*w*), 1332(*w*), 1295 (*w*).



Scheme S2 Chemical structure of **TBMS**

3,3′,5,5′-Tetracarbohydrizide diphenylmethane A mixture solution of 80% hydrazine hydrate (80 mmol, 5.00g) and 3,3′,5,5′-Tetracarbomethoxy diphenylmethane[1] (1 mmol, 0.42 g) in methanol (30mL) was stirred over 12h. The white precipitate was collected by filtration, washed with methanol and dried in vacuum. Yield: 0.30g, 80%.^{1}H NMR (DMSO-d_6, ppm): 9.74（s,4 H）,8.06 (s, 2 H),7.83 (s, 4 H), 4.59 (s, 8 H), 4.09(s, 2 H).

TBMS: 1,2-Bis(3,5-dicarbohydrazide) ethane (4) (1 mmol, 0.446 g) was added to a methanol solution (50 mL) containing 2-hydroxy-1-naphthaldehyde (4.4 mmol, 0.757 g). After 5 drops of acetic acid was added, the mixture was refluxed for 24h. The white solid was collected by filtration, washed by methanol and dried on vacuum. Yield: 0.72g, 83%. Anal calc. for $C_{61}H_{44}N_8O_8$: H 4.36, C, 72.04, N 11.02 %. Found: C 71.40, H 4.44, N 10.89 %. ^{1}H NMR (DMSO-d_6, ppm): 12.70(s, $4H_{NH}$), 12.42(s, $4H_{OH}$), 9.53(s, $4H_7$), 8.53(s, $2H_8$), 8.27(d, $4H_2$, J = 8.8 Hz), 8.21(s, $4H_9$), 7.95(d, $4H_3$, J = 9.2 Hz), 7.90(d, $4H_6$, J = 8.0 Hz), 7.61 (dd, $4H_5$, J = 7.2 Hz), 7.41 (dd, $4H_4$, J = 7.6 Hz), 7.24(dd, $4H_1$, J = 8.8 Hz), 4.46(s, $2H_{10}$)

Ce-**TBMS:** A solution of $Ce(NO_3)_3{\cdot}6H_2O$ (16.8 mg, 0.04 mmol), **TBMS** (13.6 mg, 0.03mmol) and KOH (6.8 mg, 0.12 mmol) in CH_3OH/DMF (v:v = 1:7, 8 mL) was stirred for 2h. Then the solution was left for two weeks at room temperature to give X-ray quality black block crystals. Yield: 40%, based on the crystals that have been collected and then dried in vacuum. Anal calc. for $Ce_8(C_{61}H_{40}N_8O_8)_6$: H 3.36, C 61.06, N 9.34%. Found: H 4.15, C 60.55, N 10.15 %. IR (KBr plate): 3420 (*br*), 1650 (*m*), 1614 (*s*), 1570(*m*), 1546 (*m*), 1508 (*w*), 1454(*w*), 1426 (*m*), 1384 (*s*), 1331, (*m*), 1295 (*w*).

2. Crystallography:

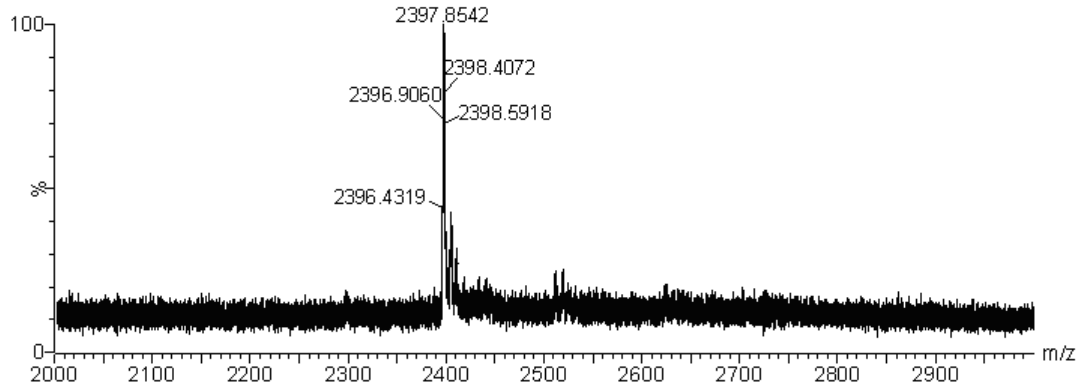
Intensities of the complexes were collected on a Bruker SMART APEX CCD diffractometer with graphite- monochromated Mo-Kα (λ = 0.71073 Å) using the SMART and SAINT programs. The structures were solved by direct methods and refined on F^2 by full-matrix least-squares methods with SHELXTL *version* 5.1. For the structural refinement of the three complexes, except the solvent molecules and the disordered atoms, the other skeleton non-hydrogen atoms were refined anisotropically. Hydrogen atoms within the ligand backbones were fixed geometrically at calculated distances and allowed to ride on the parent non-hydrogen atoms, whereas no hydrogen atoms corresponding to the solvent molecules were added and refined.

For Ce_4(**NATB**)$_4$, to assist the stability of refinements, all the C−O distances in the solvent methanol molecules were fixed to be same, and the thermal parameters on adjacent atoms in the solvent methanol molecules were restrained to be similar

For Ce_4(**NATB**)$_4$**-Cl**, to assist the stability of refinements, several restrains were applied: (1) All the C−O distances in the backbone were fixed as 1.31 Å; (2) Except the Ce atoms, thermal parameters on adjacent atoms in the backbone the solvent molecules were restrained to be similar. (3) The chloride atoms in the two partially occupancy solvent chloroform molecules were disordered into three parts and their site occupied factor (*s. o. f.*) refined as free variables or fixed value, respectively. The disordered chloroform molecules were restrained with the C−O distances being 1.80 Å and every three Cl…Cl distances in one group being same, and the thermal parameters on adjacent atoms in them were restrained to be similar. (4) In the checkcif file, the short D…A distance is due to the partially occupancy of the solvent molecules.

In the structural refinement of **Ce-TBMS**, io assist the stability of refinements, several restrains were applied: (1) The naphthalene rings were disordered into two parts and their site occupied factor (*s. o. f.*) refined as free variables. For all the naphthalene rings, the geometrical constraints of idealized regular polygons were used, the C−C bond distance of the phenyl ring being 1.39 Å and the diagonal C−C distance of the phenyl ring being 2.78 Å; (2) Several solvent DMF molecules were restrained as idealized geometry. Thermal parameters on adjacent atoms in the solvent molecules were restrained to be similar.

3. Figure S1 ESI-MS of **Ce-TBMS** in DMF/CH_3OH in present of 3 equimolar amount of KOH.



4. Table S1 Selective bond distance (Å) and angle (◦) in Ce-**NATB**

Ce(1)- O(1)	2.237(3)	Ce(1)- O(2)	2.447(3)
Ce(1)- N(1)	2.570(4)	O(1)- C(2)	1.309(6)
O(2)- C(12)	1.253(6)	N(2)- C(12)	1.325(6)
O(1)- Ce(1)- O(1A)	82.41(14)	O(1)- Ce(1)- O(2)	128.83(12)
O(1)- Ce(1)- O(2 A)	145.84(12)	O(1)- Ce(1)- O(2 B)	88.10(12)
O(2)- Ce(1)- O(2 A)	72.60(12)	O(1)- Ce(1)- N(1)	67.37(12)
O(1)- Ce(1)- N(1 A)	143.71(13)	O(1)- Ce(1)- N(1 B)	74.39(13)
O(2)- Ce(1)- N(1)	61.66(11)	O(2)- Ce(1)- N(1 A)	71.67(11)
O(2)- Ce(1)- N(1 B)	128.19(12)	N(1)- Ce(1)- N(1 A)	119.40(2)

Symmetry code : A = z, x+1/2, y-1/2 ; B = y-1/2, z+1/2, x

5. Table S2 Selective bond distance (Å) and angle (°) in Ce-**NATB-**Cl

Ce(1)- O(32)	2.116(11)	Ce(1)- O(26)	2.177(11)
Ce(1)- O(6)	2.178(12)	Ce(1)- O(25)	2.347(13)
Ce(1)- O(5)	2.365(12)	Ce(1)- O(31)	2.491(11)
Ce(1)- N(6)	2.573(18)	Ce(1)- N(26)	2.617(17)
Ce(1)- N(32)	2.622(18)	Ce(2)- O(12)	2.126(12)
Ce(2)- O(22)	2.143(13)	Ce(2)- O(11)	2.174(14)
Ce(2)- O(36)	2.203(11)	Ce(2)- O(35)	2.383(13)
Ce(2)- O(21)	2.446(12)	Ce(2)- N(12)	2.53(2)
Ce(2)- N(22)	2.544(16)	Ce(2)- N(36)	2.575(18)
Ce(3)- O(14)	2.136(12)	Ce(3)- O(34)	2.151(13)
Ce(3)- O(4)	2.167(11)	Ce(3)- O(33)	2.359(13)
Ce(3)- O(13)	2.394(13)	Ce(3)- O(3)	2.458(11)
Ce(3)- N(34)	2.572(18)	Ce(3)- N(4)	2.614(17)
Ce(3)- N(14)	2.614(18)	Ce(4)- O(24)	2.054(14)
Ce(4)- O(16)	2.109(14)	Ce(4)- O(2)	2.178(11)
Ce(4)- O(23)	2.306(14)	Ce(4)- O(1)	2.363(12)
Ce(4)- O(15)	2.454(13)	Ce(4)- N(16)	2.453(18)
Ce(4)- N(2)	2.561(18)	Ce(4)- N(24)	2.67(2)
O(1)- C(12)	1.312(9)	O(2)- C(2)	1.320(8)
O(3)- C(19)	1.297(9)	O(4)- C(22)	1.314(8)
O(5)- C(31)	1.322(9)	O(6)- C(34)	1.315(9)
O(11)- C(62)	1.305(9)	O(12)- C(52)	1.319(9)
O(13)- C(69)	1.312(9)	O(14)- C(72)	1.310(8)
O(15)- C(81)	1.308(9)	O(16)- C(84)	1.310(9)
O(21)- C(112)	1.308(9)	O(22)- C(102)	1.318(8)
O(23)- C(119)	1.310(10)	O(24)- C(122)	1.332(9)
O(25)- C(131)	1.307(9)	O(26)- C(134)	1.310(8)
O(31)- C(162)	1.307(9)	O(32)- C(152)	1.315(8)
O(33)- C(169)	1.315(9)	O(34)- C(172)	1.326(9)
O(35)- C(181)	1.310(9)	O(36)- C(184)	1.323(9)
N(1)- C(12)	1.41(2)	N(3)- C(19)	1.23(2)
N(5)- C(31)	1.36(2)	N(11)- C(62)	1.27(2)
N(13)- C(69)	1.31(2)	N(15)- C(81)	1.27(2)
N(21)- C(112)	1.29(2)	N(23)- C(119)	1.36(2)
N(25)- C(131)	1.33(2)	N(31)- C(162)	1.25(2)
N(33)- C(169)	1.26(2)	N(35)- C(181)	1.38(2)
O(32)- Ce(1)- O(26)	86.9(5)	O(32)- Ce(1)- O(6)	81.5(5)
O(26)- Ce(1)- O(6)	85.1(5)	O(32)- Ce(1)- O(25)	87.6(5)
O(26)- Ce(1)- O(25)	129.9(4)	O(6)- Ce(1)- O(25)	142.8(5)
O(32)- Ce(1)- O(5)	146.8(4)	O(26)- Ce(1)- O(5)	84.3(5)
O(6)- Ce(1)- O(5)	129.2(5)	O(25)- Ce(1)- O(5)	74.1(5)

O(32)- Ce(1)- O(31)	127.3(4)	O(26)- Ce(1)- O(31)	143.7(5)
O(6)- Ce(1)- O(31)	88.4(5)	O(25)- Ce(1)- O(31)	70.4(4)
O(5)- Ce(1)- O(31)	72.5(4)	O(32)- Ce(1)- N(6)	148.5(5)
O(26)- Ce(1)- N(6)	83.8(5)	O(6)- Ce(1)- N(6)	67.8(5)
O(25)- Ce(1)- N(6)	121.1(5)	O(5)- Ce(1)- N(6)	61.7(5)
O(31)- Ce(1)- N(6)	60.8(4)	O(32)- Ce(1)- N(26)	80.3(5)
O(26)- Ce(1)- N(26)	67.5(5)	O(6)- Ce(1)- N(26)	147.7(5)
O(25)- Ce(1)- N(26)	62.5(4)	O(5)- Ce(1)- N(26)	66.8(5)
O(31)- Ce(1)- N(26)	123.9(5)	N(6)- Ce(1)- N(26)	122.7(6)
O(32)- Ce(1)- N(32)	65.5(5)	O(26)- Ce(1)- N(32)	147.4(6)
O(6)- Ce(1)- N(32)	74.5(5)	O(25)- Ce(1)- N(32)	68.6(5)
O(5)- Ce(1)- N(32)	128.3(5)	O(31)- Ce(1)- N(32)	62.0(5)
N(6)- Ce(1)- N(32)	110.5(5)	N(26)- Ce(1)- N(32)	120.5(6)
O(12)- Ce(2)- O(22)	84.0(6)	O(12)- Ce(2)- O(11)	126.2(6)
O(22)- Ce(2)- O(11)	148.6(5)	O(12)- Ce(2)- O(36)	85.9(5)
O(22)- Ce(2)- O(36)	86.5(5)	O(11)- Ce(2)- O(36)	87.2(5)
O(12)- Ce(2)- O(35)	140.5(5)	O(22)- Ce(2)- O(35)	82.6(5)
O(11)- Ce(2)- O(35)	78.1(5)	O(36)- Ce(2)- O(35)	129.9(4)
O(12)- Ce(2)- O(21)	86.9(5)	O(22)- Ce(2)- O(21)	124.4(4)
O(11)- Ce(2)- O(21)	71.7(5)	O(36)- Ce(2)- O(21)	147.3(5)
O(35)- Ce(2)- O(21)	70.9(4)	O(12)- Ce(2)- N(12)	66.6(7)
O(22)- Ce(2)- N(12)	149.4(6)	O(11)- Ce(2)- N(12)	59.6(6)
O(36)- Ce(2)- N(12)	83.6(5)	O(35)- Ce(2)- N(12)	125.3(6)
O(21)- Ce(2)- N(12)	64.3(5)	O(12)- Ce(2)- N(22)	73.8(5)
O(22)- Ce(2)- N(22)	64.6(5)	O(11)- Ce(2)- N(22)	127.0(5)
O(36)- Ce(2)- N(22)	145.8(6)	O(35)- Ce(2)- N(22)	66.9(5)
O(21)- Ce(2)- N(22)	60.1(5)	N(12)- Ce(2)- N(22)	111.6(5)
O(12)- Ce(2)- N(36)	149.8(5)	O(22)- Ce(2)- N(36)	80.6(6)
O(11)- Ce(2)- N(36)	68.6(5)	O(36)- Ce(2)- N(36)	67.5(5)
O(35)- Ce(2)- N(36)	62.5(5)	O(21)- Ce(2)- N(36)	123.1(5)
N(12)- Ce(2)- N(36)	121.3(6)	N(22)- Ce(2)- N(36)	121.1(6)
O(14)- Ce(3)- O(34)	85.8(5)	O(14)- Ce(3)- O(4)	85.5(5)
O(34)- Ce(3)- O(4)	83.6(5)	O(14)- Ce(3)- O(33)	85.5(5)
O(34)- Ce(3)- O(33)	129.1(5)	O(4)- Ce(3)- O(33)	145.1(4)
O(14)- Ce(3)- O(13)	128.8(4)	O(34)- Ce(3)- O(13)	142.2(5)
O(4)- Ce(3)- O(13)	84.5(5)	O(33)- Ce(3)- O(13)	75.2(5)
O(14)- Ce(3)- O(3)	145.6(5)	O(34)- Ce(3)- O(3)	89.8(5)
O(4)- Ce(3)- O(3)	127.9(4)	O(33)- Ce(3)- O(3)	71.1(4)
O(13)- Ce(3)- O(3)	69.9(4)	O(14)- Ce(3)- N(34)	84.5(5)
O(34)- Ce(3)- N(34)	67.6(6)	O(4)- Ce(3)- N(34)	150.1(5)
O(33)- Ce(3)- N(34)	61.7(5)	O(13)- Ce(3)- N(34)	123.2(5)
O(3)- Ce(3)- N(34)	62.5(4)	O(14)- Ce(3)- N(4)	147.5(5)
O(34)- Ce(3)- N(4)	74.6(5)	O(4)- Ce(3)- N(4)	67.0(5)
O(33)- Ce(3)- N(4)	127.0(5)	O(13)- Ce(3)- N(4)	67.7(5)

O(3)- Ce(3)- N(4)	61.4(5)	N(34)- Ce(3)- N(4)	110.5(5)
O(14)- Ce(3)- N(14)	66.2(5)	O(34)- Ce(3)- N(14)	146.5(5)
O(4)- Ce(3)- N(14)	76.4(5)	O(33)- Ce(3)- N(14)	69.1(5)
O(13)- Ce(3)- N(14)	62.6(5)	O(3)- Ce(3)- N(14)	123.7(5)
N(34)- Ce(3)- N(14)	124.0(6)	N(4)- Ce(3)- N(14)	119.9(6)
O(24)- Ce(4)- O(16)	81.1(7)	O(24)- Ce(4)- O(2)	87.1(5)
O(16)- Ce(4)- O(2)	86.6(5)	O(24)- Ce(4)- O(23)	128.7(6)
O(16)- Ce(4)- O(23)	148.2(5)	O(2)- Ce(4)- O(23)	84.5(5)
O(24)- Ce(4)- O(1)	143.2(5)	O(16)- Ce(4)- O(1)	88.6(5)
O(2)- Ce(4)- O(1)	127.7(4)	O(23)- Ce(4)- O(1)	73.2(5)
O(24)- Ce(4)- O(15)	87.4(5)	O(16)- Ce(4)- O(15)	126.1(5)
O(2)- Ce(4)- O(15)	145.4(5)	O(23)- Ce(4)- O(15)	72.6(5)
O(1)- Ce(4)- O(15)	70.4(4)	O(24)- Ce(4)- N(16)	75.2(6)
O(16)- Ce(4)- N(16)	66.7(6)	O(2)- Ce(4)- N(16)	149.6(6)
O(23)- Ce(4)- N(16)	125.8(5)	O(1)- Ce(4)- N(16)	68.3(5)
O(15)- Ce(4)- N(16)	59.5(5)	O(24)- Ce(4)- N(2)	149.0(6)
O(16)- Ce(4)- N(2)	81.3(6)	O(2)- Ce(4)- N(2)	66.5(5)
O(23)- Ce(4)- N(2)	67.1(6)	O(1)- Ce(4)- N(2)	61.3(5)
O(15)- Ce(4)- N(2)	123.6(5)	N(16)- Ce(4)- N(2)	120.0(6)
O(24)- Ce(4)- N(24)	63.7(7)	O(16)- Ce(4)- N(24)	144.1(7)
O(2)- Ce(4)- N(24)	85.0(5)	O(23)- Ce(4)- N(24)	65.1(6)
O(1)- Ce(4)- N(24)	123.5(6)	O(15)- Ce(4)- N(24)	62.1(5)
N(16)- Ce(4)- N(24)	108.0(6)	N(2)- Ce(4)- N(24)	125.9(7)

6. Table S3 Selective bond distance (Å) and angle (°) in Ce-**TBMS**

Ce(1)- O(13A)	2.143(7)	Ce(1)- O(11)	2.195(6)
Ce(1)- O(21)	2.196(6)	Ce(1)- O(17A)	2.376(5)
Ce(1)- O(15)	2.422(5)	Ce(1)- O(23)	2.467(5)
Ce(1)- N(21)	2.579(8)	Ce(1)- N(11)	2.587(7)
Ce(1)- N(15A)	2.608(7)	Ce(2)- O(22B)	2.158(6)
Ce(2)- O(12)	2.218(6)	Ce(2)- O(14C)	2.221(7)
Ce(2)- O(16)	2.350(6)	Ce(2)- O(24B)	2.404(6)
Ce(2)- O(18C)	2.469(5)	Ce(2)- N(13)	2.513(7)
Ce(2)- N(23B)	2.614(7)	Ce(2)- N(17C)	2.668(8)
O(11)- C(112)	1.263(8)	O(12)- C(122)	1.288(9)
O(13)- C(132)	1.331(9)	O(14)- C(142)	1.497(12)
N(12)- C(157)	1.296(10)	N(14)- C(158)	1.280(11)
O(15)- C(157)	1.210(10)	N(16)- C(167)	1.284(10)
O(16)- C(158)	1.212(9)	O(23)- C(237)	1.195(9)
O(17)- C(167)	1.249(9)	O(24)- C(238)	1.165(10)
O(18)- C(168)	1.219(10)	N(22)- C(237)	1.390(11)
N(18)- C(168)	1.352(11)	N(24)- C(238)	1.317(11)
O(23)- C(237)	1.195(9)	O(24)- C(238)	1.165(10)
O(13A)- Ce(1)- O(11)	88.4(2)	O(13A)- Ce(1)- O(21)	87.5(2)
O(11)- Ce(1)- O(21)	88.2(2)	O(13A)- Ce(1A)- O(17)	129.3(2)
O(11)- Ce(1A)- O(17)	141.3(2)	O(21)- Ce(1A)- O(17)	85.5(2)
O(13A)- Ce(1)- O(15)	85.7(2)	O(11)- Ce(1)- O(15)	127.9(2)
O(21)- Ce(1)- O(15)	142.9(2)	O(17A)- Ce(1)- O(15)	71.2(2)
O(13A)- Ce(1)- O(23)	142.6(2)	O(11)- Ce(1)- O(23)	83.2 (2)
O(21)- Ce(1)- O(23)	128.4(2)	O(17A)- Ce(1)- O(23)	71.4(2)
O(15)- Ce(1)- O(23)	71.5(2)	O(13A)- Ce(1)- N(21)	151.2(2)
O(11)- Ce(1)- N(21)	79.3(2)	O(21)- Ce(1)- N(21)	66.4(2)
O(17A)- Ce(1)- N(21)	63.3(2)	O(15)- Ce(1)- N(21)	122.4(2)
O(23)- Ce(1)- N(21)	62.0(2)	O(13A)- Ce(1)- N(11)	74.3(2)
O(11)- Ce(1)- N(11)	66.8(2)	O(21)- Ce(1)- N(11)	149.0(2)
O(17A)- Ce(1)- N(11)	125.4(2)	O(15)- Ce(1)- N(11)	61.8(2)
O(23)- Ce(1)- N(11)	68.8(2)	N(21)- Ce(1)- N(11)	122.5(2)
O(22B)- Ce(2)- O(12)	84.2(2)	O(22B)- Ce(2C)- O(14)	81.5(2)
O(12)- Ce(2C)- O(14)	82.3(2)	O(22B)- Ce(2)- O(16)	89.5(2)
O(12)- Ce(2)- O(16)	128.4(2)	O(14C)- Ce(2)- O(16)	147.1(2)
O(12)- Ce(2)- N(13)	67.3(2)	O(22B)- Ce(2)- N(13)	77.0(2)
O(16)- Ce(2)- N(13)	61.3(2)	O(12)- Ce(2)- N(13)	144.1(2)
O(18C)- Ce(2)- N(13)	71.5(2)	O(24B)- Ce(2)- N(13)	128.6(2)

Symmetry Code: A = x+1/2, z+1/2; y+3/2, B = x, 2-y, 1-z; C = -x+1/2, z+3/2, -y-1/2

Reference:

1. *Eur. J. Org. Chem.* **2007**, 3271–3276.