Supplementary Information

Anion-induced 3d-4f luminescent coordination clusters: structural characters and chemical fixation of CO_2 under mild conditions

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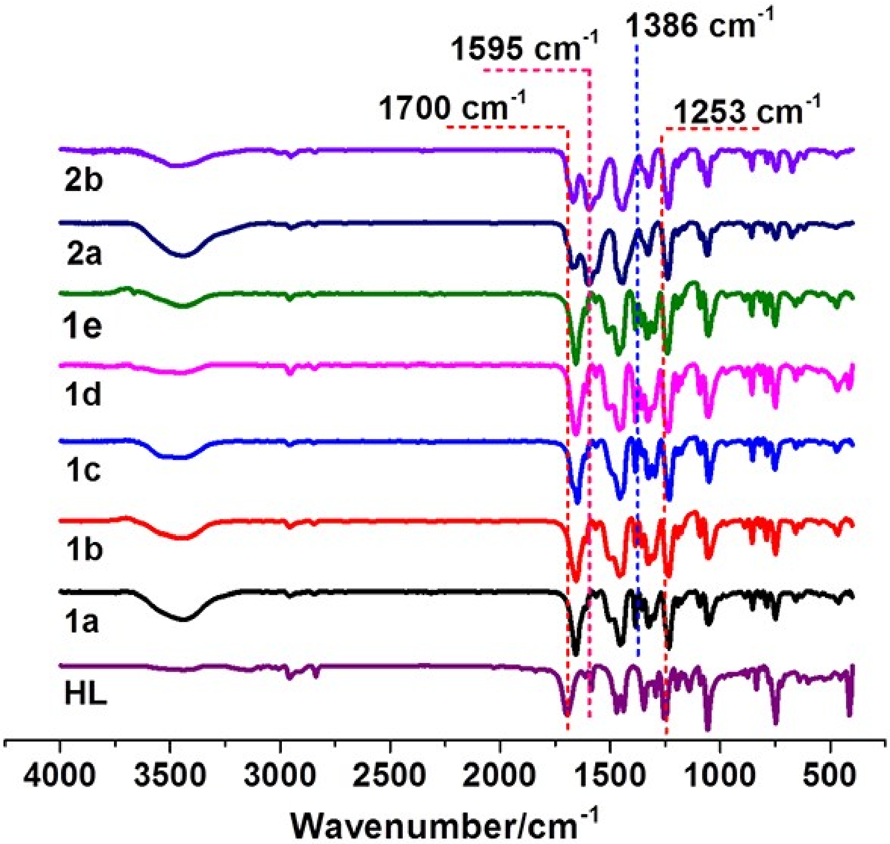


Figure S1 IR spectra of the ligand and complexes in the solid state (KBr disk) at room temperature.

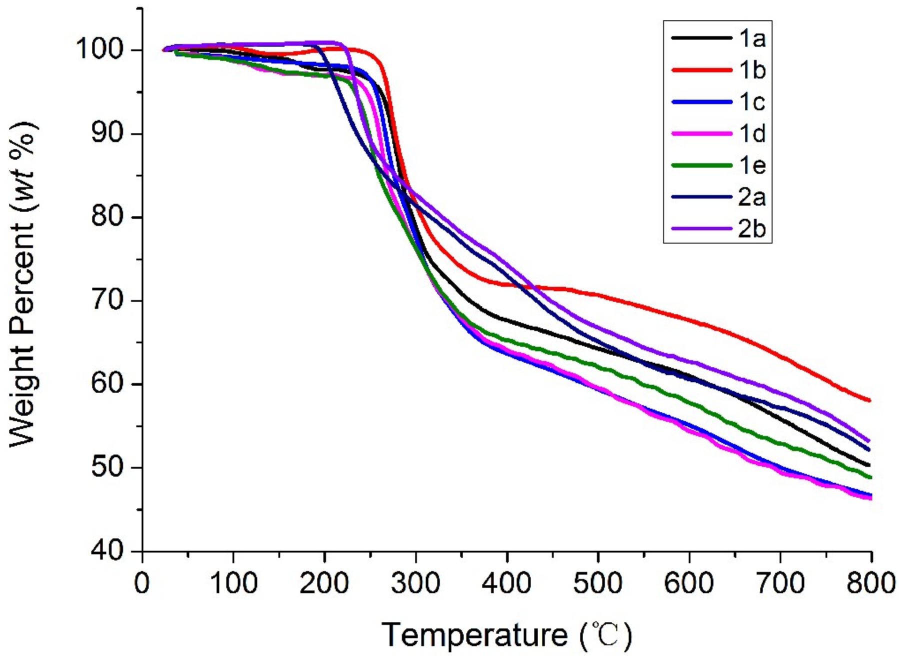


Figure S2 TGA spectra of the complexes.

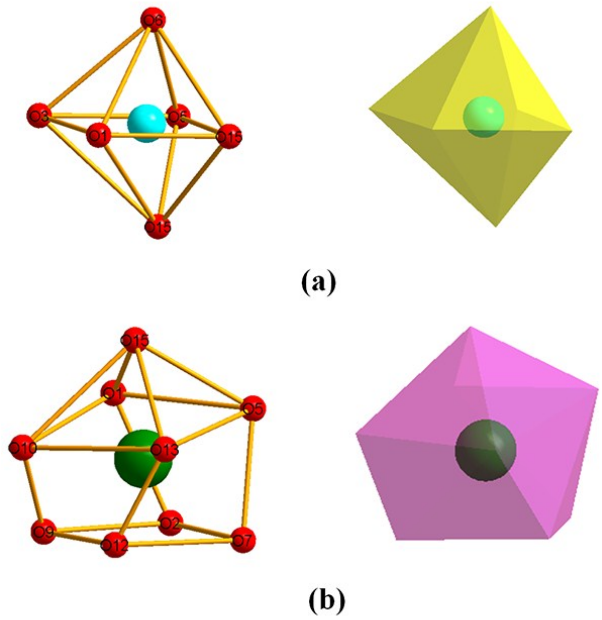


Figure S3. Coordination polyhedra of zinc ion (a) and terbium ion (b) of complex **1b**. Solvent molecule, extra ligands and coordination anions are omitted for clarity.

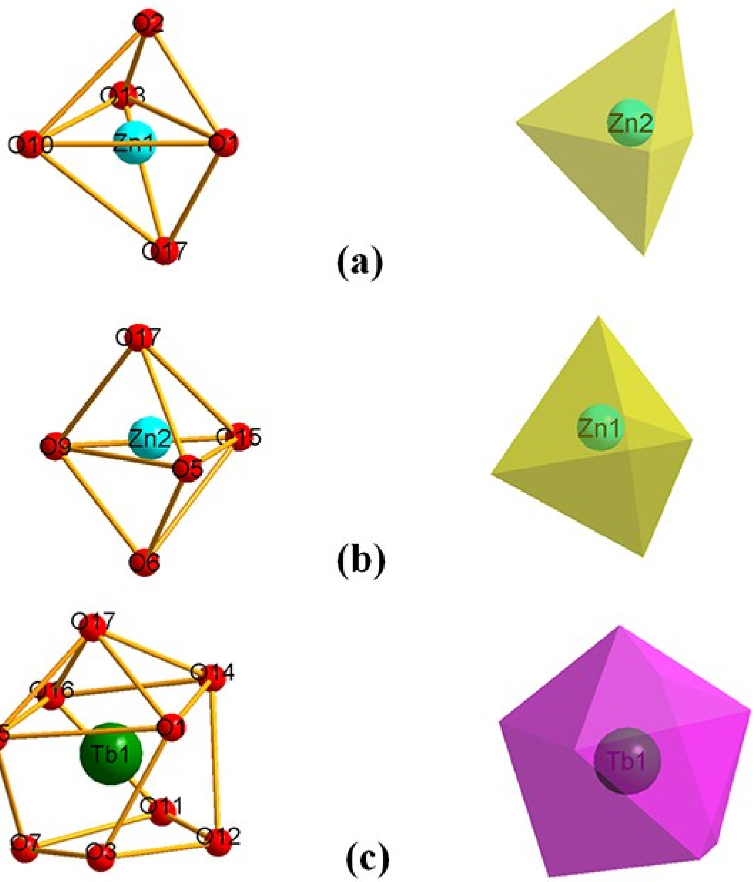


Figure S4. Coordination polyhedra of zinc ion (a)(b) and terbium ion (c) of complex **2a**. Solvent molecule, extra ligands and coordination anions are omitted for clarity.

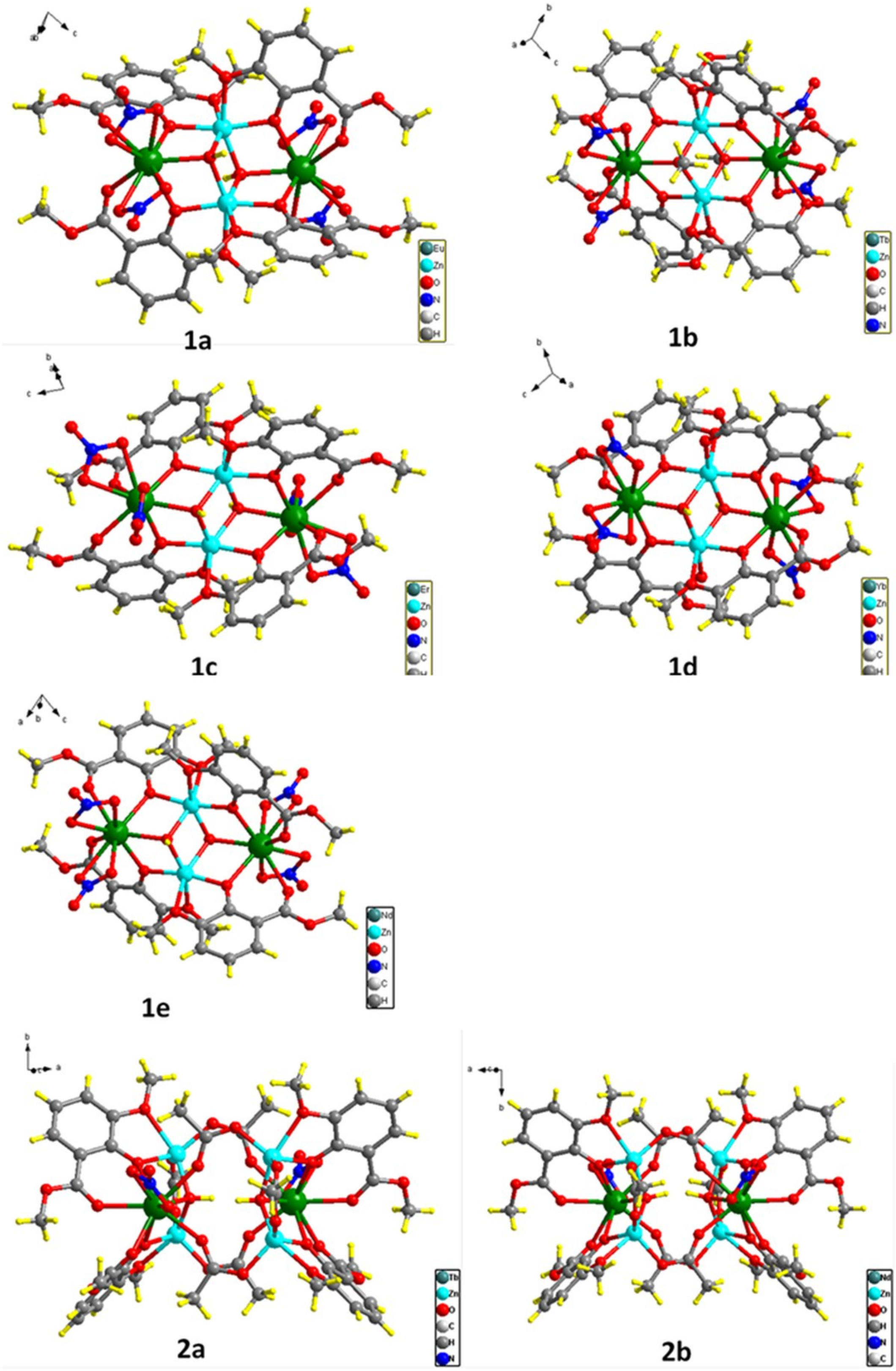


Figure S5. Crystal structures of complexes **1a-1e** and **2a-2b**. Solvent molecules are omitted for clarity.

Table S1 Crystal Data and Structure Refinement Parameters for Complexes **1a-2b.**

	1a (CCDC-1575742)	**1b** (CCDC-1575745)	**1c** (CCDC-1575741)	**1d** (CCDC-1575743)
Formula	$C_{36}H_{38}Eu_2N_4O_{30}Zn_2 \cdot 2(CH_3CN)$	$C_{38}H_{42}N_4O_{30}Tb_2Zn_2 \cdot 2(CH_3CN)$	$C_{36}H_{38}N_4O_{30}Er_2Zn_2 \cdot 4(CH_3CN)$	$C_{36}H_{38}N_4O_{30}Yb_2Zn_2 \cdot 2(CH_3CN)$
Formula Weight	1523.47	1565.44	1636.18	1565.63
Crystal System	Triclinic	Triclinic	Triclinic	Triclinic
Space Group	*P*-1	*P*-1	*P*-1	*P*-1
a (Å)	11.1206 (8)	10.8386 (9)	11.0490 (10)	10.5088 (12)
b (Å)	11.2718 (8)	11.0943 (5)	11.0806 (10)	10.9921 (6)
c (Å)	13.3306 (11)	13.3764 (9)	14.7671 (12)	13.2571 (8)
α (°)	74.493 (7)	111.335 (5)	83.834 (7)	111.997 (5)
β (°)	72.689 (7)	101.544 (7)	68.566 (8)	100.721 (7)
γ (°)	62.178 (7)	102.840 (6)	64.269 (9)	101.715 (7)
Z	1	1	1	1
Volume ($Å^3$)	1394.5 (2)	1389.11 (17)	1513.2 (3)	1331.15 (19)
D_{calcd} (g/cm^3)	1.814	1.871	1.796	1.953
μ (mm^{-1})	3.163	3.464	3.621	4.470
F(000)	752.0	772.0	806.0	766.0
Temperature	293.00(10)	290.83 (10)	293 (2)	293 (2)
Crystal Size (mm)	0.25 × 0.24 × 0.22	0.35 × 0.3 × 0.2	0.23 × 0.22 × 0.21	0.13 × 0.12 × 0.1
Reflections collected	9529	9549	10897	9027
Independent ref.	5469	5447	5961	5228
Data/restraints/ parameters	5469/30/389	5447/30/376	5961/42/417	5228/19/370
R_{int}	0.0302	0.0353	0.0392	0.0474
Final *R* indices [I>2.0σ (*I*)]	R_1 = 0.0374 wR_2 = 0.0914	R_1 = 0.0373 wR_2 = 0.0732	R_1 = 0.0374 wR_2 = 0.0708	R_1 = 0.0408 wR_2 = 0.0674
R indices (all date)	R_1 = 0.0464 wR_2 = 0.0998	R_1 = 0.0495 wR_2 = 0.0817	R_1 = 0.0478 wR_2 = 0.0782	R_1 = 0.0565 wR_2 = 0.0764
GOF	1.063	1.042	1.051	0.987

Table S1 *(Contd.)*

	1e (CCDC-1577169)	**2a** (CCDC-1575744)	**2b** (CCDC-1575746)
Formula	$C_{36}H_{38}N_4Nd_2O_{30}Zn_2 \cdot 2(CH_3CN)$	$C_{48}H_{56}N_2O_{36}Tb_2Zn_4 \cdot 5(CH_3CN)$	$C_{48}H_{56}Nd_2O_{36}Zn_4 \cdot 4(CH_3CN)$
Formula Weight	1508.03	2018.51	1951.12
Crystal System	Triclinic	Monoclinic	Monoclinic
Space Group	*P*-1	*C*2/*c*	*C*2/*c*
a (Å)	11.1988(12)	22.5467 (5)	22.2896 (5)
b (Å)	11.2992(14)	17.8961 (5)	18.4936 (5)
c (Å)	13.3744(14)	19.5235 (5)	19.2391 (4)
α (°)	74.797(10)	90	90
β (°)	72.700(9)	100.736 (2)	99.957 (2)
γ (°)	62.097(12)	90	90
Z	1	4	4

Volume (Å^3)	1412.7(3)	7739.8 (3)	7811.2 (3)
D_{calcd} (g/cm^3)	1.773	1.732	1.659
μ (mm^{-1})	2.739	3.114	2.602
F(000)	746.0	4012.0	3896.0
Temperature	173.00(10)	293.23 (10)	173.00 (10)
Crystal Size (mm)	0.35 × 0.3 × 0.2	0.35 × 0.3 × 0.2	0.35 × 0.3 × 0.2
Reflections collected	9130	15624	15970
Independent ref.	5536	7597	7676
Data/restraints/ parameters	5536/32/389	7597/48/515	7676/62/501
R_{int}	0.0559	0.0342	0.0445
Final *R* indices	R_1 = 0.0586	R_1 = 0.0355	R_1 = 0.0452
[I>2.0σ (*I*)]	wR_2 = 0.1247	wR_2 = 0.0735	wR_2 = 0.1212
R indices (all	R_1 = 0.0895	R_1 = 0.0504	R_1 = 0.0591
date)	wR_2 = 0.1489	wR_2 = 0.0828	wR_2 = 0.1348
GOF	1.036	1.059	1.106

Table S2 Selected Bond Lengths (Å) and Angles (°) for All Complexes.

Complex **1a**					
Eu(1)—Zn(1)	3.4974(7)	Eu(1)—O(6)	2.413(4)	Zn(1)—O(8)	2.221(4)
Eu(1)—(13)	2.542(4)	Eu(1)—O(2)	2.395(4)	Zn(1)—O(1)1	2.034(3)
Eu(1)—O(1)	2.384(3)	Eu(1)—O(10)	2.524(4)	Zn(1)—O(15)1	2.050(3)
Eu(1)—O(15)	2.361(3)	Eu(1)—N(2)	2.931(5)	Zn(1)—O(15)	2.059(4)
Eu(1)—O(5)	2.393(3)	Eu(1)—N(1)	2.910(5)	Zn(1)—O(5)	2.045(3)
Eu(1)—O(12)	2.485(4)	Zn(1)—Zn(1)1	3.0115(11)	Zn(1)—O(4)1	2.185(4)
Eu(1)—O(9)	2.478(4)				
O(13)—Eu(1)—Zn(1)	132.70(8)	O(12)—Eu(1)—O(13)	50.88(12)	Zn(1)^1—Zn(1)—Eu(1)	64.65(2)
O(13)—Eu(1)—N(2)	25.58(12)	O(12)—Eu(1)—O(10)	112.14(14)	O(8)—Zn(1)—Eu(1)^1	99.88(9)
O(13)—Eu(1)—N(1)	63.50(14)	O(12)—Eu(1)—N(2)	25.30(12)	O(8)—Zn(1)—Eu(1)	116.83(9)
O(1)—Eu(1)—Zn(1)	75.33(8)	O(12)—Eu(1)—N(1)	93.67(15)	O(8)—Zn(1)—Zn(1)^1	136.37(10)
O(1)—Eu(1)—O(13)	145.83(12)	O(9)—Eu(1)—Zn(1)	109.26(9)	O(1)^1—Zn(1)—Eu(1)^1	41.15(10)
O(1)—Eu(1)—O(5)	89.38(12)	O(9)—Eu(1)—O(13)	68.40(13)	O(1)^1—Zn(1)—Eu(1)	142.08(11)
O(1)—Eu(1)—O(12)	145.28(12)	O(9)—Eu(1)—O(12)	78.06(14)	O(1)^1—Zn(1)—Zn(1)^1	92.28(10)
O(1)—Eu(1)—O(9)	85.02(13)	O(9)—Eu(1)—O(10)	51.22(13)	O(1)^1—Zn(1)—O(8)	100.72(14)
O(1)—Eu(1)—O(6)	132.29(13)	O(9)—Eu(1)—N(2)	71.99(14)	O(1)^1—Zn(1)—O(15)	101.72(14)
O(1)—Eu(1)—O(2)	70.17(12)	O(9)—Eu(1)—N(1)	25.83(13)	O(1)^1—Zn(1)—O(15)^1	81.64(13)
O(1)—Eu(1)—O(10)	78.22(13)	O(6)—Eu(1)—Zn(1)	100.79(9)	O(1)^1—Zn(1)—O(5)	169.22(14)
O(1)—Eu(1)—N(2)	156.48(13)	O(6)—Eu(1)—O(13)	69.21(13)	O(1)^1—Zn(1)—O(4)^1	76.07(13)
O(1)—Eu(1)—N(1)	83.15(14)	O(6)—Eu(1)—O(12)	77.26(14)	O(15)^1—Zn(1)—Eu(1)	97.52(9)

O(15)—Eu(1)—Zn(1)	34.76(9)	O(6)—Eu(1)—O(9)	137.56(14)	O(15)—Zn(1)—Eu(1)^{1}	97.12(9)
O(15)—Eu(1)—O(13)	120.89(12)	O(6)—Eu(1)—O(10)	109.58(13)	O(15)^{1}—Zn(1)—Eu(1)^{1}	40.60(9)
O(15)—Eu(1)—O(1)	68.45(11)	O(6)—Eu(1)—N(2)	70.92(14)	O(15)—Zn(1)—Eu(1)	40.84(9)
O(15)—Eu(1)—O(5)	69.32(12)	O(6)—Eu(1)—N(1)	124.43(13)	O(15)—Zn(1)—Zn(1)^{1}	42.75(9)
O(15)—Eu(1)—O(12)	77.86(12)	O(2)—Eu(1)—Zn(1)	115.92(10)	O(15)^{1}—Zn(1)—Zn(1)^{1}	42.98(10)
O(15)—Eu(1)—O(9)	74.68(12)	O(2)—Eu(1)—O(13)	103.75(13)	O(15)^{1}—Zn(1)—O(8)	97.76(14)
O(15)—Eu(1)—O(6)	131.60(12)	O(2)—Eu(1)—O(12)	144.41(13)	O(15)—Zn(1)—O(8)	157.56(13)
O(15)—Eu(1)—O(2)	134.65(12)	O(2)—Eu(1)—O(9)	119.20(14)	O(15)^{1}—Zn(1)—O(15)	85.72(14)
O(15)—Eu(1)—O(10)	118.11(13)	O(2)—Eu(1)—O(6)	69.48(14)	O(15)^{1}—Zn(1)—O(4)^{1}	157.70(13)
O(15)—Eu(1)—N(2)	99.82(12)	O(2)—Eu(1)—O(10)	69.39(14)	O(15)—Zn(1)—O(4)^{1}	98.55(14)
O(15)—Eu(1)—N(1)	97.95(13)	O(2)—Eu(1)—N(2)	125.40(13)	O(5)—Zn(1)—Eu(1)	41.65(10)
O(5)—Eu(1)—Zn(1)	34.61(8)	O(2)—Eu(1)—N(1)	94.77(15)	O(5)—Zn(1)—Eu(1)^{1}	148.87(10)
O(5)—Eu(1)—O(13)	124.78(12)	O(10)—Eu(1)—Zn(1)	148.54(10)	O(5)—Zn(1)—Zn(1)^{1}	97.37(10)
O(5)—Eu(1)—O(12)	86.41(13)	O(10)—Eu(1)—O(13)	68.51(13)	O(5)—Zn(1)—O(8)	75.46(13)
O(5)—Eu(1)—O(9)	143.04(12)	O(10)—Eu(1)—N(2)	90.72(14)	O(5)—Zn(1)—O(15)	82.42(13)
O(5)—Eu(1)—O(6)	68.29(12)	O(10)—Eu(1)—N(1)	25.61(13)	O(5)—Zn(1)—O(15)^{1}	108.73(13)
O(5)—Eu(1)—O(2)	92.67(13)	N(2)—Eu(1)—Zn(1)	107.15(10)	O(5)—Zn(1)—O(4)^{1}	93.54(14)
O(5)—Eu(1)—O(10)	160.76(13)	N(1)—Eu(1)—Zn(1)	132.52(10)	O(4)^{1}—Zn(1)—Eu(1)	99.94(10)
O(5)—Eu(1)—N(2)	105.88(13)	N(1)—Eu(1)—N(2)	78.29(15)	O(4)^{1}—Zn(1)—Eu(1)^{1}	117.14(9)
O(5)—Eu(1)—N(1)	166.98(12)	Eu(1)—Zn(1)—Eu(1)^{1}	129.054(17)	O(4)^{1}—Zn(1)—Zn(1)^{1}	137.00(11)
O(12)—Eu(1)—Zn(1)	81.93(9)	Zn(1)^{1}—Zn(1)—Eu(1)^{1}	64.40(2)	O(4)^{1}—Zn(1)—O(8)	86.63(15)
Complex **1b**					
Tb(1)—Zn(1)	3.5033(7)	Tb(1)—O(11)	2.479(4)	Zn(1)—O(7)	2.193(3)
Tb(1)—O(3)	2.518(4)	Tb(1)—N(1)	2.856(5)	Zn(1)—O(5)	2.070(4)
Tb(1)—O(6)^{1}	2.372(4)	Tb(1)—O(14)	2.533(4)	Zn(1)—O(1)	2.055(3)
Tb(1)—O(5)^{1}	2.365(3)	Tb(1)—O(13)	2.472(4)	Zn(1)—O(2)	2.076(4)
Tb(1)—O(1)	2.338(3)	Tb(1)—N(2)	2.929(6)	Zn(1)—O(9)	2.054(3)
Tb(1)—O(9)^{1}	2.356(4)	Zn(1)—Zn(1)^{1}	3.0842(10)	Zn(1)—O(9)^{1}	2.106(3)
Tb(1)—O(10)	2.446(4)				
O(3)—Tb(1)—Zn(1)	96.82(8)	O(9)^{1}—Tb(1)—O(6)^{1}	134.99(12)	Zn(1)^{1}—Zn(1)—Tb(1)^{1}	63.80(2)
O(3)—Tb(1)—N(1)	123.17(15)	O(9)^{1}—Tb(1)—O(5)^{1}	68.83(12)	O(7)—Zn(1)—Tb(1)^{1}	115.43(10)
O(3)—Tb(1)—O(14)	68.78(14)	O(9)^{1}—Tb(1)—O(10)	77.82(13)	O(7)—Zn(1)—Tb(1)	100.76(10)
O(3)—Tb(1)—N(2)	70.52(16)	O(9)^{1}—Tb(1)—O(11)	124.36(14)	O(7)—Zn(1)—Zn(1)^{1}	134.48(11)
O(6)^{1}—Tb(1)—Zn(1)	113.50(9)	O(9)^{1}—Tb(1)—N(1)	102.13(16)	O(5)—Zn(1)—Tb(1)^{1}	40.74(9)
O(6)^{1}—Tb(1)—O(3)	68.63(13)	O(9)^{1}—Tb(1)—O(14)	117.58(15)	O(5)—Zn(1)—Tb(1)	137.52(9)
O(6)^{1}—Tb(1)—O(10)	119.18(14)	O(9)^{1}—Tb(1)—O(13)	73.83(13)	O(5)—Zn(1)—Zn(1)^{1}	88.60(8)
O(6)^{1}—Tb(1)—O(11)	69.92(15)	O(9)^{1}—Tb(1)—N(2)	95.78(16)	O(5)—Zn(1)—O(7)	74.95(13)
O(6)^{1}—Tb(1)—N(1)	95.04(17)	O(10)—Tb(1)—Zn(1)	113.51(11)	O(5)—Zn(1)—O(2)	98.74(15)
O(6)^{1}—Tb(1)—O(14)	107.41(15)	O(10)—Tb(1)—O(3)	137.91(13)	O(5)—Zn(1)—O(9)^{1}	97.06(14)
O(6)^{1}—Tb(1)—O(13)	144.30(14)	O(10)—Tb(1)—O(11)	51.75(16)	O(1)—Zn(1)—Tb(1)	40.01(8)
O(6)^{1}—Tb(1)—N(2)	127.99(17)	O(10)—Tb(1)—N(1)	26.01(16)	O(1)—Zn(1)—Tb(1)^{1}	149.01(9)
O(5)^{1}—Tb(1)—Zn(1)	74.66(8)	O(10)—Tb(1)—O(14)	69.65(14)	O(1)—Zn(1)—Zn(1)^{1}	96.05(9)
O(5)^{1}—Tb(1)—O(3)	130.63(13)	O(10)—Tb(1)—O(13)	82.65(14)	O(1)—Zn(1)—O(7)	95.53(14)
O(5)^{1}—Tb(1)—O(6)^{1}	70.91(13)	O(10)—Tb(1)—N(2)	75.00(15)	O(1)—Zn(1)—O(5)	169.94(14)

O(5)^{1}—Tb(1)—O(10)	86.85(13)	O(11)—Tb(1)—Zn(1)	155.90(12)	O(1)—Zn(1)—O(2)	84.15(15)
O(5)^{1}—Tb(1)—O(11)	84.79(13)	O(11)—Tb(1)—O(3)	106.19(14)	O(1)—Zn(1)—O(9)^{1}	80.80(13)
O(5)^{1}—Tb(1)—N(1)	87.11(13)	O(11)—Tb(1)—N(1)	25.86(16)	O(2)—Zn(1)—Tb(1)^{1}	94.38(11)
O(5)^{1}—Tb(1)—O(14)	152.36(12)	O(11)—Tb(1)—O(14)	69.41(15)	O(2)—Zn(1)—Tb(1)	123.65(13)
O(5)^{1}—Tb(1)—O(13)	142.55(14)	O(11)—Tb(1)—N(2)	92.56(16)	O(2)—Zn(1)—Zn(1)^{1}	135.75(12)
O(5)^{1}—Tb(1)—N(2)	158.56(16)	N(1)—Tb(1)—Zn(1)	137.74(14)	O(2)—Zn(1)—O(7)	89.18(16)
O(1)—Tb(1)—Zn(1)	34.40(9)	N(1)—Tb(1)—N(2)	81.54(15)	O(2)—Zn(1)—O(9)^{1}	163.89(16)
O(1)—Tb(1)—O(3)	64.75(11)	O(14)—Tb(1)—Zn(1)	127.43(11)	O(9)^{1}—Zn(1)—Tb(1)^{1}	95.56(9)
O(1)—Tb(1)—O(6)^{1}	89.33(12)	O(14)—Tb(1)—N(1)	65.37(14)	O(9)^{1}—Zn(1)—Tb(1)	40.87(10)
O(1)—Tb(1)—O(5)^{1}	87.96(11)	O(14)—Tb(1)—N(2)	25.64(14)	O(9)—Zn(1)—Tb(1)	96.74(9)
O(1)—Tb(1)—O(9)^{1}	70.13(11)	O(13)—Tb(1)—Zn(1)	76.89(10)	O(9)—Zn(1)—Tb(1)^{1}	40.36(10)
O(1)—Tb(1)—O(10)	147.21(14)	O(13)—Tb(1)—O(3)	76.40(15)	O(9)—Zn(1)—Zn(1)^{1}	42.80(9)
O(1)—Tb(1)—O(11)	159.24(15)	O(13)—Tb(1)—O(11)	115.04(14)	O(9)^{1}—Zn(1)—Zn(1)^{1}	41.51(8)
O(1)—Tb(1)—N(1)	171.96(16)	O(13)—Tb(1)—N(1)	98.14(15)	O(9)^{1}—Zn(1)—O(7)	97.93(14)
O(1)—Tb(1)—O(14)	119.68(12)	O(13)—Tb(1)—O(14)	50.84(15)	O(9)—Zn(1)—O(7)	155.58(15)
O(1)—Tb(1)—O(13)	82.01(12)	O(13)—Tb(1)—N(2)	25.21(15)	O(9)—Zn(1)—O(5)	80.64(14)
O(1)—Tb(1)—N(2)	101.07(13)	N(2)—Tb(1)—Zn(1)	101.94(13)	O(9)—Zn(1)—O(1)	108.80(14)
O(9)^{1}—Tb(1)—Zn(1)	35.80(8)	Tb(1)—Zn(1)—Tb(1)^{1}	127.820(16)	O(9)—Zn(1)—O(2)	95.20(14)
O(9)^{1}—Tb(1)—O(3)	128.42(11)	Zn(1)^{1}—Zn(1)—Tb(1)	64.01(2)	O(9)—Zn(1)—O(9)^{1}	84.31(13)
Complex **1c**					
Er(1)—Zn(1)	3.4754(6)	Er(1)—O(6)	2.354(4)	Zn(1)—O(15)^{1}	2.041(3)
Er(1)—O(15)	2.339(3)	Er(1)—O(2)	2.378(4)	Zn(1)—O(15)	2.084(3)
Er(1)—O(1)	2.305(3)	Er(1)—O(9)	2.444(3)	Zn(1)—O(1)	2.031(3)
Er(1)—O(5)	2.326(3)	Er(1)—N(1)	2.865(5)	Zn(1)—O(5)^{1}	2.053(3)
Er(1)—O(13)	2.503(3)	Er(1)—N(2)	2.893(4)	Zn(1)—O(3)	2.204(3)
Er(1)—O(10)	2.441(4)	Zn(1)—Zn(1)^{1}	2.9354(11)	Zn(1)—O(7)^{1}	2.194(3)
Er(1)—O(12)	2.442(3)				
O(15)—Er(1)—Zn(1)	35.69(8)	O(10)—Er(1)—O(13)	72.54(13)	Zn(1)^{1}—Zn(1)—Er(1)^{1}	64.25(2)
O(15)—Er(1)—O(13)	149.25(13)	O(10)—Er(1)—O(12)	70.52(13)	O(15)^{1}—Zn(1)—Er(1)	101.09(9)
O(15)—Er(1)—O(10)	76.89(12)	O(10)—Er(1)—O(9)	51.94(14)	O(15)—Zn(1)—Er(1)	40.88(10)
O(15)—Er(1)—O(12)	114.47(13)	O(10)—Er(1)—N(1)	25.97(13)	O(15)^{1}—Zn(1)—Er(1)^{1}	39.23(9)
O(15)—Er(1)—O(6)	130.13(11)	O(10)—Er(1)—N(2)	71.07(13)	O(15)—Zn(1)—Er(1)^{1}	98.43(9)
O(15)—Er(1)—O(2)	128.83(12)	O(12)—Er(1)—Zn(1)	139.98(8)	O(15)^{1}—Zn(1)—Zn(1)^{1}	45.24(9)
O(15)—Er(1)—O(9)	78.36(12)	O(12)—Er(1)—O(13)	51.51(12)	O(15)—Zn(1)—Zn(1)^{1}	44.05(9)
O(15)—Er(1)—N(1)	76.62(12)	O(12)—Er(1)—O(9)	116.88(13)	O(15)^{1}—Zn(1)—O(15)	89.29(13)
O(15)—Er(1)—N(2)	136.27(13)	O(12)—Er(1)—N(1)	93.60(14)	O(15)^{1}—Zn(1)—O(5)^{1}	77.82(13)
O(1)—Er(1)—Zn(1)	34.11(8)	O(12)—Er(1)—N(2)	26.01(12)	O(15)^{1}—Zn(1)—O(3)	93.15(14)
O(1)—Er(1)—O(15)	69.41(12)	O(6)—Er(1)—Zn(1)	104.46(8)	O(15)—Zn(1)—O(3)	153.15(13)
O(1)—Er(1)—O(5)	86.90(11)	O(6)—Er(1)—O(13)	76.91(12)	O(15)—Zn(1)—O(7)^{1}	102.34(13)
O(1)—Er(1)—O(13)	137.15(13)	O(6)—Er(1)—O(10)	144.07(12)	O(15)^{1}—Zn(1)—O(7)^{1}	151.89(13)
O(1)—Er(1)—O(10)	133.97(12)	O(6)—Er(1)—O(12)	75.84(13)	O(1)—Zn(1)—Er(1)	39.53(9)
O(1)—Er(1)—O(12)	152.73(12)	O(6)—Er(1)—O(2)	72.01(12)	O(1)—Zn(1)—Er(1)^{1}	153.82(9)
O(1)—Er(1)—O(6)	81.77(12)	O(6)—Er(1)—O(9)	143.29(13)	O(1)—Zn(1)—Zn(1)^{1}	99.57(10)
O(1)—Er(1)—O(2)	70.39(11)	O(6)—Er(1)—N(1)	153.25(12)	O(1)—Zn(1)—O(15)^{1}	114.69(13)

O(1)—Er(1)—O(9)	90.38(13)	O(6)—Er(1)—N(2)	73.19(13)	O(1)—Zn(1)—O(15)	79.94(13)
O(1)—Er(1)—N(1)	113.16(13)	O(2)—Er(1)—Zn(1)	101.52(8)	O(1)—Zn(1)—O(5)^{1}	167.00(12)
O(1)—Er(1)—N(2)	152.62(13)	O(2)—Er(1)—O(13)	67.81(12)	O(1)—Zn(1)—O(3)	74.76(12)
O(5)—Er(1)—Zn(1)	70.76(7)	O(2)—Er(1)—O(10)	111.97(13)	O(1)—Zn(1)—O(7)^{1}	92.68(13)
O(5)—Er(1)—O(15)	66.90(11)	O(2)—Er(1)—O(12)	115.86(12)	O(5)^{1}—Zn(1)—Er(1)^{1}	38.97(8)
O(5)—Er(1)—O(13)	119.97(11)	O(2)—Er(1)—O(9)	71.57(14)	O(5)^{1}—Zn(1)—Er(1)	137.99(9)
O(5)—Er(1)—O(10)	107.94(13)	O(2)—Er(1)—N(1)	91.60(14)	O(5)^{1}—Zn(1)—Zn(1)^{1}	86.82(9)
O(5)—Er(1)—O(12)	71.58(11)	O(2)—Er(1)—N(2)	91.09(13)	O(5)^{1}—Zn(1)—O(15)	97.38(13)
O(5)—Er(1)—O(6)	71.88(11)	O(9)—Er(1)—Zn(1)	87.19(9)	O(5)^{1}—Zn(1)—O(3)	109.28(12)
O(5)—Er(1)—O(2)	139.52(12)	O(9)—Er(1)—O(13)	85.31(12)	O(5)^{1}—Zn(1)—O(7)^{1}	75.38(12)
O(5)—Er(1)—O(9)	143.78(12)	O(9)—Er(1)—N(1)	25.98(13)	O(3)—Zn(1)—Er(1)^{1}	100.29(8)
O(5)—Er(1)—N(1)	128.60(13)	O(9)—Er(1)—N(2)	103.02(13)	O(3)—Zn(1)—Er(1)	112.70(8)
O(5)—Er(1)—N(2)	95.49(12)	N(1)—Er(1)—Zn(1)	99.36(9)	O(3)—Zn(1)—Zn(1)^{1}	132.21(10)
O(13)—Er(1)—Zn(1)	168.51(9)	N(1)—Er(1)—N(2)	86.52(13)	O(7)^{1}—Zn(1)—Er(1)^{1}	113.02(9)
O(13)—Er(1)—N(1)	77.34(12)	N(2)—Er(1)—Zn(1)	165.86(10)	O(7)^{1}—Zn(1)—Er(1)	104.41(8)
O(13)—Er(1)—N(2)	25.60(12)	Er(1)—Zn(1)—Er(1)^{1}	130.471(17)	O(7)^{1}—Zn(1)—Zn(1)^{1}	139.91(10)
O(10)—Er(1)—Zn(1)	109.27(9)	Zn(1)^{1}—Zn(1)—Er(1)	66.223(18)	O(7)^{1}—Zn(1)—O(3)	87.81(14)
Complex **1d**					
Yb(1)—Zn(1)	3.4470(7)	Yb(1)—O(7)	2.488(4)	Zn(1)—O(15)	2.090(3)
Yb(1)—O(13)	2.406(4)	Yb(1)—O(2)	2.311(4)	Zn(1)—O(15)^{1}	2.047(4)
Yb(1)—O(15)	2.297(4)	Yb(1)—O(9)	2.418(4)	Zn(1)—O(5)	2.043(4)
Yb(1)—O(5)	2.261(3)	Yb(1)—N(2)	2.866(6)	Zn(1)—O(1)^{1}	2.075(4)
Yb(1)—O(1)	2.277(4)	Yb(1)—N(1)	2.803(6)	Zn(1)—O(6)	2.052(4)
Yb(1)—O(12)	2.495(4)	Zn(1)—Zn(1)^{1}	3.0682(13)	Zn(1)—O(3)^{1}	2.187(4)
Yb(1)—O(10)	2.382(4)				
O(13)—Yb(1)—Zn(1)	76.66(11)	O(1)—Yb(1)—N(2)	157.38(15)	Zn(1)^{1}—Zn(1)—Yb(1)^{1}	63.42(2)
O(13)—Yb(1)—O(12)	51.83(16)	O(1)—Yb(1)—N(1)	86.03(15)	O(15)^{1}—Zn(1)—Yb(1)	96.70(11)
O(13)—Yb(1)—O(7)	76.70(15)	O(12)—Yb(1)—Zn(1)	128.15(12)	O(15)—Zn(1)—Yb(1)^{1}	95.49(10)
O(13)—Yb(1)—O(9)	115.79(15)	O(12)—Yb(1)—N(2)	25.96(15)	O(15)^{1}—Zn(1)—Yb(1)^{1}	39.78(11)
O(13)—Yb(1)—N(2)	25.88(15)	O(12)—Yb(1)—N(1)	65.20(16)	O(15)—Zn(1)—Yb(1)	40.38(10)
O(13)—Yb(1)—N(1)	97.57(16)	O(10)—Yb(1)—Zn(1)	112.27(11)	O(15)^{1}—Zn(1)—Zn(1)^{1}	42.66(10)
O(15)—Yb(1)—Zn(1)	36.12(9)	O(10)—Yb(1)—O(13)	81.18(16)	O(15)—Zn(1)—Zn(1)^{1}	41.58(9)
O(15)—Yb(1)—O(13)	72.03(14)	O(10)—Yb(1)—O(12)	69.53(15)	O(15)^{1}—Zn(1)—O(15)	84.25(14)
O(15)—Yb(1)—O(12)	116.81(15)	O(10)—Yb(1)—O(7)	137.18(14)	O(15)^{1}—Zn(1)—O(1)^{1}	78.62(15)
O(15)—Yb(1)—O(10)	76.20(14)	O(10)—Yb(1)—O(9)	52.70(15)	O(15)^{1}—Zn(1)—O(6)	96.46(16)
O(15)—Yb(1)—O(7)	128.61(13)	O(10)—Yb(1)—N(2)	74.01(16)	O(15)^{1}—Zn(1)—O(3)^{1}	153.71(16)
O(15)—Yb(1)—O(2)	136.71(13)	O(10)—Yb(1)—N(1)	26.44(16)	O(15)—Zn(1)—O(3)^{1}	96.36(15)
O(15)—Yb(1)—O(9)	123.45(15)	O(7)—Yb(1)—Zn(1)	97.70(9)	O(5)—Zn(1)—Yb(1)^{1}	150.02(11)
O(15)—Yb(1)—N(2)	94.63(16)	O(7)—Yb(1)—O(12)	67.94(15)	O(5)—Zn(1)—Yb(1)	39.02(10)
O(15)—Yb(1)—N(1)	100.92(17)	O(7)—Yb(1)—N(2)	70.09(15)	O(5)—Zn(1)—Zn(1)^{1}	95.95(11)
O(5)—Yb(1)—Zn(1)	34.67(9)	O(7)—Yb(1)—N(1)	123.03(16)	O(5)—Zn(1)—O(15)^{1}	110.27(15)
O(5)—Yb(1)—O(13)	81.99(14)	O(2)—Yb(1)—Zn(1)	113.43(10)	O(5)—Zn(1)—O(15)	79.21(14)
O(5)—Yb(1)—O(15)	70.64(13)	O(2)—Yb(1)—O(13)	144.08(15)	O(5)—Zn(1)—O(1)^{1}	169.23(14)
O(5)—Yb(1)—O(1)	88.96(13)	O(2)—Yb(1)—O(12)	106.47(15)	O(5)—Zn(1)—O(6)	85.14(16)

O(5)—Yb(1)—O(12)	119.94(14)	O(2)—Yb(1)—O(10)	121.20(16)	O(5)—Zn(1)—O(3)^{1}	95.58(15)
O(5)—Yb(1)—O(10)	146.06(15)	O(2)—Yb(1)—O(7)	67.95(14)	O(1)^{1}—Zn(1)—Yb(1)^{1}	39.44(10)
O(5)—Yb(1)—O(7)	65.40(13)	O(2)—Yb(1)—O(9)	70.45(15)	O(1)^{1}—Zn(1)—Yb(1)	136.25(10)
O(5)—Yb(1)—O(2)	88.86(14)	O(2)—Yb(1)—N(2)	127.30(17)	O(1)^{1}—Zn(1)—Zn(1)^{1}	86.60(11)
O(5)—Yb(1)—O(9)	159.22(14)	O(2)—Yb(1)—N(1)	96.37(17)	O(1)^{1}—Zn(1)—O(15)	96.10(15)
O(5)—Yb(1)—N(2)	101.35(15)	O(9)—Yb(1)—Zn(1)	154.59(12)	O(1)^{1}—Zn(1)—O(3)^{1}	75.17(15)
O(5)—Yb(1)—N(1)	171.31(16)	O(9)—Yb(1)—O(12)	69.85(16)	O(6)—Zn(1)—Yb(1)	123.52(13)
O(1)—Yb(1)—Zn(1)	74.86(10)	O(9)—Yb(1)—O(7)	106.58(15)	O(6)—Zn(1)—Yb(1)^{1}	95.49(12)
O(1)—Yb(1)—O(13)	141.48(15)	O(9)—Yb(1)—N(2)	93.03(17)	O(6)—Zn(1)—Zn(1)^{1}	136.74(13)
O(1)—Yb(1)—O(15)	69.64(13)	O(9)—Yb(1)—N(1)	26.39(15)	O(6)—Zn(1)—O(15)	163.52(17)
O(1)—Yb(1)—O(12)	151.09(15)	N(2)—Yb(1)—Zn(1)	102.36(13)	O(6)—Zn(1)—O(1)^{1}	100.19(16)
O(1)—Yb(1)—O(10)	86.16(14)	N(1)—Yb(1)—Zn(1)	136.75(14)	O(6)—Zn(1)—O(3)^{1}	90.25(17)
O(1)—Yb(1)—O(7)	132.38(13)	N(1)—Yb(1)—N(2)	81.01(17)	O(3)^{1}—Zn(1)—Yb(1)^{1}	114.38(11)
O(1)—Yb(1)—O(2)	72.37(14)	Yb(1)—Zn(1)—Yb(1)^{1}	127.25(2)	O(3)^{1}—Zn(1)—Yb(1)	100.67(11)
O(1)—Yb(1)—O(9)	83.13(15)	Zn(1)^{1}—Zn(1)—Yb(1)	63.83(2)	O(3)^{1}—Zn(1)—Zn(1)^{1}	132.34(11)
Complex **1e**					
Nd(1)—Zn(1)^{1}	3.5274(11)	Nd(1)—O(9)	2.542(6)	Zn(1)—O(5)	2.039(5)
Nd(1)—O(5)	2.432(5)	Nd(1)—O(13)	2.559(6)	Zn(1)—O(15)^{1}	2.066(6)
Nd(1)—O(15)	2.407(5)	Nd(1)—N(1)	2.974(7)	Zn(1)—O(15)	2.056(5)
Nd(1)—O(1)	2.450(5)	Nd(1)—N(2)	2.941(8)	Zn(1)—O(1)^{1}	2.047(5)
Nd(1)—O(2)	2.449(5)	Nd(1)—O(12)	2.517(6)	Zn(1)—O(7)	2.188(5)
Nd(1)—O(6)	2.439(6)	Zn(1)—Zn(1)^{1}	3.0283(17)	Zn(1)—O(3)^{1}	2.230(6)
Nd(1)—O(10)	2.563(6)				
O(5)—Nd(1)—Zn(1)^{1}	75.29(13)	O(2)—Nd(1)—N(2)	124.9(2)	Zn(1)^{1}—Zn(1)—Nd(1)	64.43(3)
O(5)—Nd(1)—O(1)	89.48(18)	O(2)—Nd(1)—O(12)	138.2(2)	O(5)—Zn(1)—Nd(1)	41.75(14)
O(5)—Nd(1)—O(2)	131.1(2)	O(6)—Nd(1)—Zn(1)^{1}	116.25(16)	O(5)—Zn(1)—Nd(1)^{1}	142.68(16)
O(5)—Nd(1)—O(6)	69.38(18)	O(6)—Nd(1)—O(1)	93.8(2)	O(5)—Zn(1)—Zn(1)^{1}	93.13(14)
O(5)—Nd(1)—O(10)	146.77(19)	O(6)—Nd(1)—O(2)	70.0(2)	O(5)—Zn(1)—O(15)^{1}	101.8(2)
O(5)—Nd(1)—O(9)	145.51(19)	O(6)—Nd(1)—O(10)	104.4(2)	O(5)—Zn(1)—O(15)	82.8(2)
O(5)—Nd(1)—O(13)	78.7(2)	O(6)—Nd(1)—O(9)	145.0(2)	O(5)—Zn(1)—O(1)^{1}	167.9(2)
O(5)—Nd(1)—N(1)	157.2(2)	O(6)—Nd(1)—O(13)	69.4(2)	O(5)—Zn(1)—O(7)	75.9(2)
O(5)—Nd(1)—N(2)	84.2(2)	O(6)—Nd(1)—N(1)	126.0(2)	O(5)—Zn(1)—O(3)^{1}	99.6(2)
O(5)—Nd(1)—O(12)	85.8(2)	O(6)—Nd(1)—N(2)	94.3(2)	O(15)—Zn(1)—Nd(1)^{1}	97.23(16)
O(15)—Nd(1)—Zn(1)^{1}	34.65(13)	O(6)—Nd(1)—O(12)	118.4(2)	O(15)^{1}—Zn(1)—Nd(1)^{1}	41.49(14)
O(15)—Nd(1)—O(5)	68.07(17)	O(10)—Nd(1)—Zn(1)^{1}	131.90(13)	O(15)^{1}—Zn(1)—Nd(1)	96.70(14)
O(15)—Nd(1)—O(1)	69.05(17)	O(10)—Nd(1)—N(1)	25.51(19)	O(15)—Zn(1)—Nd(1)	41.15(14)
O(15)—Nd(1)—O(2)	131.16(19)	O(10)—Nd(1)—N(2)	63.4(2)	O(15)—Zn(1)—Zn(1)^{1}	42.84(16)
O(15)—Nd(1)—O(6)	133.88(19)	O(9)—Nd(1)—Zn(1)^{1}	81.89(15)	O(15)^{1}—Zn(1)—Zn(1)^{1}	42.59(14)
O(15)—Nd(1)—O(10)	120.98(18)	O(9)—Nd(1)—O(10)	50.1(2)	O(15)—Zn(1)—O(15)^{1}	85.4(2)
O(15)—Nd(1)—O(9)	78.42(19)	O(9)—Nd(1)—O(13)	111.5(2)	O(15)^{1}—Zn(1)—O(7)	99.0(2)
O(15)—Nd(1)—O(13)	117.63(19)	O(9)—Nd(1)—N(1)	24.65(19)	O(15)—Zn(1)—O(7)	158.7(2)
O(15)—Nd(1)—N(1)	100.01(19)	O(9)—Nd(1)—N(2)	93.1(2)	O(15)—Zn(1)—O(3)^{1}	97.0(2)
O(15)—Nd(1)—N(2)	98.3(2)	O(13)—Nd(1)—Zn(1)^{1}	148.45(14)	O(15)^{1}—Zn(1)—O(3)^{1}	158.6(2)
O(15)—Nd(1)—O(12)	75.3(2)	O(13)—Nd(1)—O(10)	68.9(2)	O(1)^{1}—Zn(1)—Nd(1)^{1}	42.60(15)

O(1)—Nd(1)—Zn(1)^{1}	34.45(11)	O(13)—Nd(1)—N(1)	91.0(2)	O(1)^{1}—Zn(1)—Nd(1)	148.92(15)
O(1)—Nd(1)—O(10)	123.74(18)	O(13)—Nd(1)—N(2)	25.1(2)	O(1)^{1}—Zn(1)—Zn(1)^{1}	98.25(15)
O(1)—Nd(1)—O(9)	85.9(2)	N(1)—Nd(1)—Zn(1)^{1}	106.42(15)	O(1)^{1}—Zn(1)—O(15)^{1}	84.0(2)
O(1)—Nd(1)—O(13)	161.97(19)	N(2)—Nd(1)—Zn(1)^{1}	132.88(16)	O(1)^{1}—Zn(1)—O(15)	108.4(2)
O(1)—Nd(1)—N(1)	104.7(2)	N(2)—Nd(1)—N(1)	78.3(2)	O(1)^{1}—Zn(1)—O(7)	92.8(2)
O(1)—Nd(1)—N(2)	167.30(19)	O(12)—Nd(1)—Zn(1)^{1}	109.66(15)	O(1)^{1}—Zn(1)—O(3)^{1}	75.0(2)
O(1)—Nd(1)—O(12)	143.08(18)	O(12)—Nd(1)—O(10)	68.2(2)	O(7)—Zn(1)—Nd(1)	117.56(15)
O(2)—Nd(1)—Zn(1)^{1}	99.89(14)	O(12)—Nd(1)—O(9)	77.8(2)	O(7)—Zn(1)—Nd(1)^{1}	99.79(17)
O(2)—Nd(1)—O(1)	67.26(18)	O(12)—Nd(1)—O(13)	50.4(2)	O(7)—Zn(1)—Zn(1)^{1}	137.64(18)
O(2)—Nd(1)—O(10)	70.1(2)	O(12)—Nd(1)—N(1)	72.1(2)	O(7)—Zn(1)—O(3)^{1}	86.4(2)
O(2)—Nd(1)—O(9)	77.8(2)	O(12)—Nd(1)—N(2)	25.6(2)	O(3)^{1}—Zn(1)—Nd(1)^{1}	117.32(15)
O(2)—Nd(1)—O(13)	110.7(2)	Nd(1)^{1}—Zn(1)—Nd(1)	129.25(3)	O(3)^{1}—Zn(1)—Nd(1)	99.05(15)
O(2)—Nd(1)—N(1)	71.6(2)	Zn(1)^{1}—Zn(1)—Nd(1)^{1}	64.82(3)	O(3)^{1}—Zn(1)—Zn(1)^{1}	135.92(15)
Complex **2a**					
Tb(1)—Zn(1)	3.4729(6)	Tb(1)—O(7)	2.416(3)	Zn(1)—O(15)	1.956(3)
Tb(1)—Zn(2)	3.4910(5)	Tb(1)—O(12)	2.481(3)	Zn(1)—O(11)	1.971(3)
Tb(1)—O(9)	2.401(3)	Tb(1)—O(13)	2.501(3)	Zn(2)—O(9)	2.000(3)
Tb(1)—O(5)	2.364(3)	Tb(1)—N(1)	2.877(4)	Zn(2)—O(5)	2.036(3)
Tb(1)—O(16)^{1}	2.394(3)	Zn(1)—O(9)	1.991(3)	Zn(2)—O(17)	1.956(3)
Tb(1)—O(1)	2.380(3)	Zn(1)—O(2)	2.257(3)	Zn(2)—O(10)	1.966(3)
Tb(1)—O(18)^{1}	2.350(3)	Zn(1)—O(1)	2.038(3)	Zn(2)—O(6)	2.211(3)
Tb(1)—O(3)	2.437(3)				
Zn(1)—Tb(1)—Zn(2)	57.268(13)	O(1)—Tb(1)—O(12)	129.76(11)	N(1)—Tb(1)—Zn(1)	122.22(10)
O(9)—Tb(1)—Zn(1)	33.78(7)	O(1)—Tb(1)—O(13)	82.05(11)	N(1)—Tb(1)—Zn(2)	172.66(9)
O(9)—Tb(1)—Zn(2)	33.66(7)	O(1)—Tb(1)—N(1)	105.91(12)	O(9)—Zn(1)—Tb(1)	42.10(8)
O(9)—Tb(1)—O(3)	120.66(10)	O(18)^{1}—Tb(1)—Zn(1)	107.49(7)	O(9)—Zn(1)—O(2)	154.26(13)
O(9)—Tb(1)—O(7)	132.30(11)	O(18)^{1}—Tb(1)—Zn(2)	75.96(7)	O(9)—Zn(1)—O(1)	81.20(12)
O(9)—Tb(1)—O(12)	134.84(11)	O(18)^{1}—Tb(1)—O(9)	76.57(10)	O(2)—Zn(1)—Tb(1)	112.55(9)
O(9)—Tb(1)—O(13)	137.23(11)	O(18)^{1}—Tb(1)—O(5)	83.05(10)	O(1)—Zn(1)—Tb(1)	41.81(8)
O(9)—Tb(1)—N(1)	141.54(12)	O(18)^{1}—Tb(1)—O(16)^{1}	80.74(10)	O(1)—Zn(1)—O(2)	73.18(12)
O(5)—Tb(1)—Zn(1)	85.16(7)	O(18)^{1}—Tb(1)—O(1)	142.27(10)	O(15)—Zn(1)—Tb(1)	119.69(9)
O(5)—Tb(1)—Zn(2)	34.34(7)	O(18)^{1}—Tb(1)—O(3)	142.78(11)	O(15)—Zn(1)—O(9)	110.35(12)
O(5)—Tb(1)—O(9)	67.92(10)	O(18)^{1}—Tb(1)—O(7)	77.41(11)	O(15)—Zn(1)—O(2)	85.12(13)
O(5)—Tb(1)—O(16)^{1}	138.19(10)	O(18)^{1}—Tb(1)—O(12)	72.95(11)	O(15)—Zn(1)—O(1)	130.15(13)
O(5)—Tb(1)—O(1)	90.01(10)	O(18)^{1}—Tb(1)—O(13)	123.79(10)	O(15)—Zn(1)—O(11)	103.10(14)
O(5)—Tb(1)—O(3)	75.46(11)	O(18)^{1}—Tb(1)—N(1)	97.90(12)	O(11)—Zn(1)—Tb(1)	132.28(11)
O(5)—Tb(1)—O(7)	69.81(10)	O(3)—Tb(1)—Zn(1)	100.64(8)	O(11)—Zn(1)—O(9)	105.68(14)
O(5)—Tb(1)—O(12)	137.79(11)	O(3)—Tb(1)—Zn(2)	100.45(8)	O(11)—Zn(1)—O(2)	89.83(14)
O(5)—Tb(1)—O(13)	143.15(10)	O(3)—Tb(1)—O(12)	103.63(12)	O(11)—Zn(1)—O(1)	120.67(14)
O(5)—Tb(1)—N(1)	150.13(12)	O(3)—Tb(1)—O(13)	68.12(11)	O(9)—Zn(2)—Tb(1)	41.72(8)
O(16)^{1}—Tb(1)—Zn(1)	63.81(7)	O(3)—Tb(1)—N(1)	86.87(12)	O(9)—Zn(2)—O(5)	82.52(12)
O(16)^{1}—Tb(1)—Zn(2)	104.05(7)	O(7)—Tb(1)—Zn(1)	153.93(7)	O(9)—Zn(2)—O(6)	151.18(12)
O(16)^{1}—Tb(1)—O(9)	70.91(10)	O(7)—Tb(1)—Zn(2)	101.08(8)	O(5)—Zn(2)—Tb(1)	40.90(8)
O(16)^{1}—Tb(1)—O(3)	134.59(11)	O(7)—Tb(1)—O(3)	66.83(11)	O(5)—Zn(2)—O(6)	74.31(11)

O(16)[1]—Tb(1)—O(7)	141.33(10)	O(7)—Tb(1)—O(12)	71.34(11)	O(17)—Zn(2)—Tb(1)	111.28(9)
O(16)[1]—Tb(1)—O(12)	71.93(11)	O(7)—Tb(1)—O(13)	90.39(12)	O(17)—Zn(2)—O(9)	109.54(12)
O(16)[1]—Tb(1)—O(13)	75.87(11)	O(7)—Tb(1)—N(1)	81.21(12)	O(17)—Zn(2)—O(5)	105.42(13)
O(16)[1]—Tb(1)—N(1)	70.64(12)	O(12)—Tb(1)—Zn(1)	134.73(8)	O(17)—Zn(2)—O(10)	113.10(15)
O(1)—Tb(1)—Zn(1)	34.81(7)	O(12)—Tb(1)—Zn(2)	148.90(8)	O(17)—Zn(2)—O(6)	93.21(12)
O(1)—Tb(1)—Zn(2)	77.59(7)	O(12)—Tb(1)—O(13)	51.38(11)	O(10)—Zn(2)—Tb(1)	130.52(11)
O(1)—Tb(1)—O(9)	66.53(10)	O(12)—Tb(1)—N(1)	25.43(11)	O(10)—Zn(2)—O(9)	101.90(13)
O(1)—Tb(1)—O(16)[1]	80.13(10)	O(13)—Tb(1)—Zn(1)	106.47(8)	O(10)—Zn(2)—O(5)	136.66(14)
O(1)—Tb(1)—O(3)	68.57(11)	O(13)—Tb(1)—Zn(2)	159.28(8)	O(10)—Zn(2)—O(6)	84.22(13)
O(1)—Tb(1)—O(7)	134.30(10)	O(13)—Tb(1)—N(1)	26.02(11)	O(6)—Zn(2)—Tb(1)	114.05(8)
Complex **2b**					
Nd(1)—Zn(1)	3.5362(7)	Nd(1)—O(13)	2.563(4)	Zn(1)—O(11)	1.977(4)
Nd(1)—Zn(2)	3.5287(7)	Nd(1)—O(16)[1]	2.417(4)	Zn(1)—O(15)	1.962(4)
Nd(1)—O(1)	2.422(4)	Nd(1)—O(18)[1]	2.455(4)	Zn(2)—O(5)	2.021(4)
Nd(1)—O(3)	2.470(4)	Nd(1)—N(1)	2.947(5)	Zn(2)—O(6)	2.266(4)
Nd(1)—O(5)	2.452(4)	Zn(1)—O(1)	2.032(3)	Zn(2)—O(9)	2.004(4)
Nd(1)—O(7)	2.493(4)	Zn(1)—O(2)	2.217(4)	Zn(2)—O(10)	1.978(4)
Nd(1)—O(9)	2.473(4)	Zn(1)—O(9)	1.998(4)	Zn(2)—O(17)	1.966(4)
Nd(1)—O(12)	2.528(4)				
Zn(2)—Nd(1)—Zn(1)	56.687(15)	O(9)—Nd(1)—Zn(1)	33.23(9)	N(1)—Nd(1)—Zn(1)	172.45(13)
O(1)—Nd(1)—Zn(1)	33.76(8)	O(9)—Nd(1)—Zn(2)	33.52(8)	N(1)—Nd(1)—Zn(2)	122.01(12)
O(1)—Nd(1)—Zn(2)	83.67(8)	O(9)—Nd(1)—O(7)	119.41(13)	O(1)—Zn(1)—Nd(1)	41.48(10)
O(1)—Nd(1)—O(3)	68.26(12)	O(9)—Nd(1)—O(12)	136.76(14)	O(1)—Zn(1)—O(2)	74.73(14)
O(1)—Nd(1)—O(5)	88.86(13)	O(9)—Nd(1)—O(13)	136.03(14)	O(2)—Zn(1)—Nd(1)	114.92(9)
O(1)—Nd(1)—O(7)	76.20(14)	O(9)—Nd(1)—N(1)	141.30(16)	O(9)—Zn(1)—Nd(1)	42.72(10)
O(1)—Nd(1)—O(9)	66.87(12)	O(12)—Nd(1)—Zn(1)	149.95(10)	O(9)—Zn(1)—O(1)	84.03(15)
O(1)—Nd(1)—O(12)	138.33(13)	O(12)—Nd(1)—Zn(2)	136.23(10)	O(9)—Zn(1)—O(2)	151.64(14)
O(1)—Nd(1)—O(13)	144.82(14)	O(12)—Nd(1)—O(13)	50.32(14)	O(11)—Zn(1)—Nd(1)	130.97(13)
O(1)—Nd(1)—O(18)[1]	136.59(12)	O(12)—Nd(1)—N(1)	25.09(14)	O(11)—Zn(1)—O(1)	137.46(18)
O(1)—Nd(1)—N(1)	151.58(15)	O(13)—Nd(1)—Zn(1)	159.12(11)	O(11)—Zn(1)—O(2)	83.65(16)
O(3)—Nd(1)—Zn(1)	99.04(9)	O(13)—Nd(1)—Zn(2)	105.86(11)	O(11)—Zn(1)—O(9)	100.40(16)
O(3)—Nd(1)—Zn(2)	150.75(9)	O(13)—Nd(1)—N(1)	25.36(15)	O(15)—Zn(1)—Nd(1)	111.11(12)
O(3)—Nd(1)—O(7)	67.43(13)	O(16)[1]—Nd(1)—Zn(1)	75.17(9)	O(15)—Zn(1)—O(1)	104.62(15)
O(3)—Nd(1)—O(9)	130.36(12)	O(16)[1]—Nd(1)—Zn(2)	107.65(9)	O(15)—Zn(1)—O(2)	92.87(15)
O(3)—Nd(1)—O(12)	73.00(13)	O(16)[1]—Nd(1)—O(1)	82.31(12)	O(15)—Zn(1)—O(9)	110.79(15)
O(3)—Nd(1)—O(13)	93.43(14)	O(16)[1]—Nd(1)—O(3)	77.47(12)	O(15)—Zn(1)—O(11)	112.76(18)
O(3)—Nd(1)—N(1)	84.23(16)	O(16)[1]—Nd(1)—O(5)	141.41(12)	O(5)—Zn(2)—Nd(1)	42.46(11)
O(5)—Nd(1)—Zn(1)	76.78(9)	O(16)[1]—Nd(1)—O(7)	143.60(13)	O(5)—Zn(2)—O(6)	73.29(15)
O(5)—Nd(1)—Zn(2)	33.81(8)	O(16)[1]—Nd(1)—O(9)	76.63(12)	O(6)—Zn(2)—Nd(1)	113.37(11)
O(5)—Nd(1)—O(3)	133.19(12)	O(16)[1]—Nd(1)—O(12)	74.81(13)	O(9)—Zn(2)—Nd(1)	42.95(10)
O(5)—Nd(1)—O(7)	67.67(13)	O(16)[1]—Nd(1)—O(13)	124.22(14)	O(9)—Zn(2)—O(5)	82.77(15)
O(5)—Nd(1)—O(9)	65.41(12)	O(16)[1]—Nd(1)—O(18)[1]	80.17(13)	O(9)—Zn(2)—O(6)	155.95(15)
O(5)—Nd(1)—O(12)	130.04(13)	O(16)[1]—Nd(1)—N(1)	99.07(15)	O(10)—Zn(2)—Nd(1)	133.01(13)
O(5)—Nd(1)—O(13)	82.46(14)	O(18)[1]—Nd(1)—Zn(1)	103.05(9)	O(10)—Zn(2)—O(5)	122.45(17)

O(5)—Nd(1)—O(18)^{1}	80.93(13)	O(18)^{1}—Nd(1)—Zn(2)	64.70(9)	O(10)—Zn(2)—O(6)	90.42(18)
O(5)—Nd(1)—N(1)	105.98(15)	O(18)^{1}—Nd(1)—O(3)	143.18(13)	O(10)—Zn(2)—O(9)	104.64(17)
O(7)—Nd(1)—Zn(1)	100.49(11)	O(18)^{1}—Nd(1)—O(7)	134.80(14)	O(17)—Zn(2)—Nd(1)	118.43(12)
O(7)—Nd(1)—Zn(2)	98.85(10)	O(18)^{1}—Nd(1)—O(9)	70.55(12)	O(17)—Zn(2)—O(5)	128.35(17)
O(7)—Nd(1)—O(12)	102.72(15)	O(18)^{1}—Nd(1)—O(12)	73.11(14)	O(17)—Zn(2)—O(6)	84.33(16)
O(7)—Nd(1)—O(13)	68.95(15)	O(18)^{1}—Nd(1)—O(13)	75.60(14)	O(17)—Zn(2)—O(9)	109.64(15)
O(7)—Nd(1)—N(1)	87.04(17)	O(18)^{1}—Nd(1)—N(1)	70.82(16)	O(17)—Zn(2)—O(10)	103.14(17)

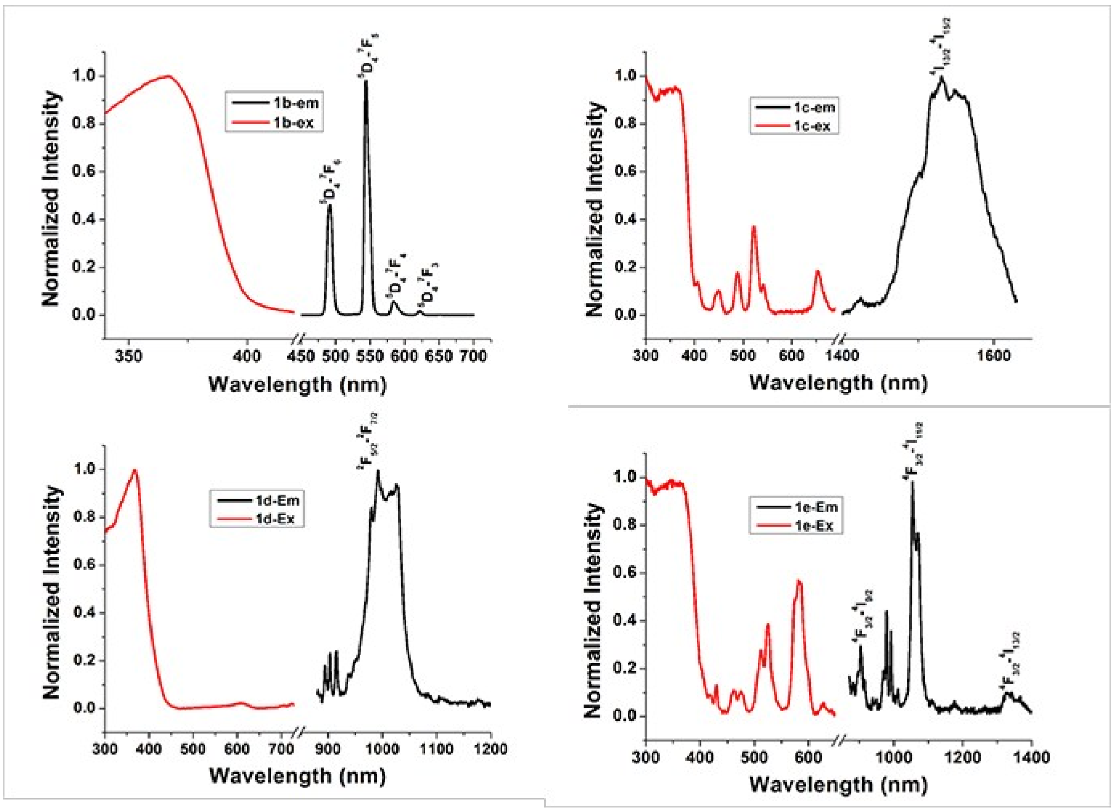


Figure S6. Excitation spectrum and emission of the complexes **1b-1e**.

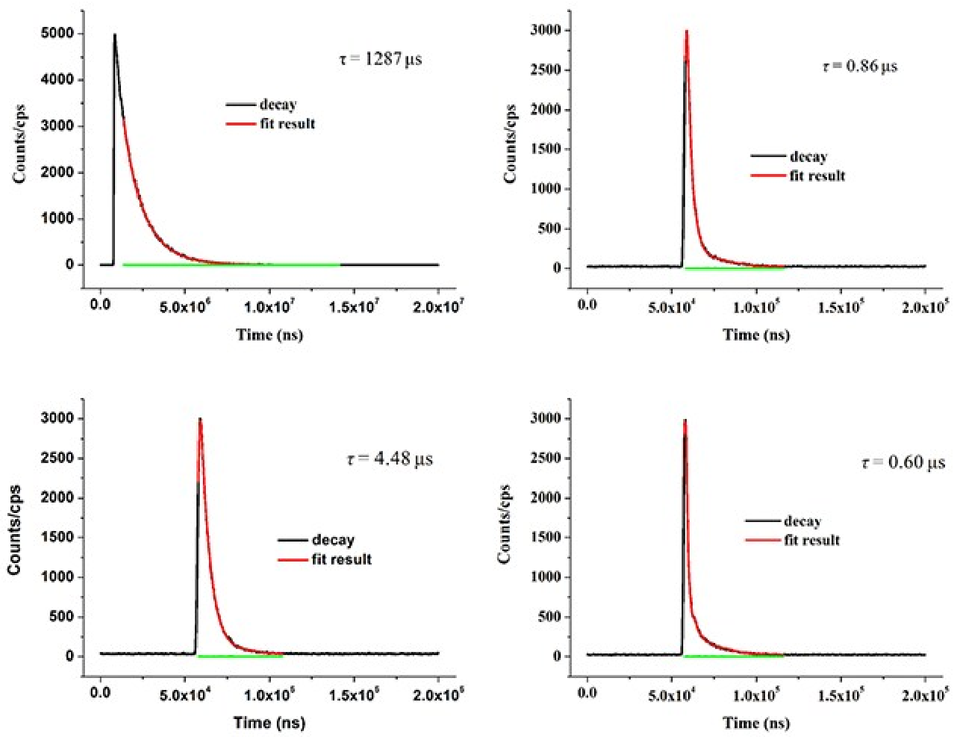


Figure S7. Decay curves of the complex **1b** (Tb^{III}($^5D_4$-$^7F_5$)), complex **1c** (Er^{III}($^4I_{13/2}$-$^4I_{15/2}$)), complex **1d** (Yb^{III}($^2F_{5/2}$-$^2F_{7/2}$)) and complex **1e** (Nd^{III}($^4F_{3/2}$-$^4I_{11/2}$)), respectively.

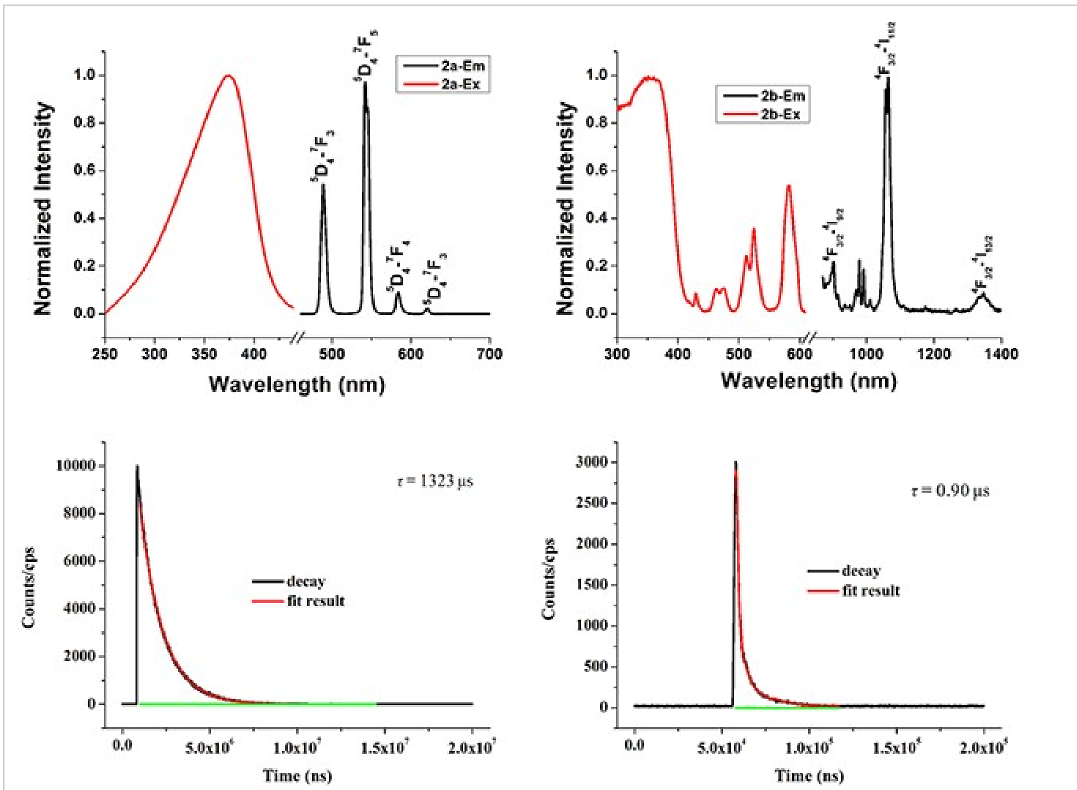


Figure S8. Excitation spectrum and emission of the complexes **2a**, **2b** and their decay curves.

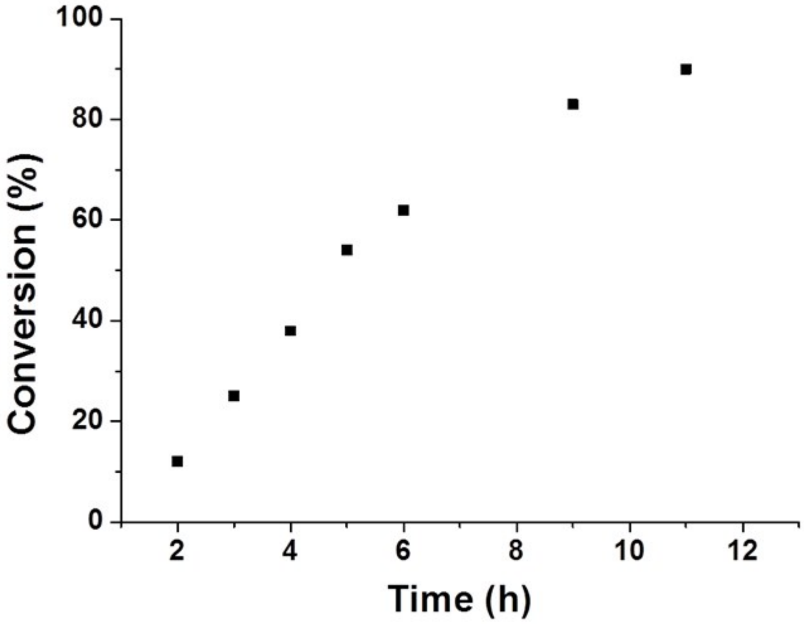


Figure S9. Kinetic curve of catalytic reaction at atmospheric pressure and 120 °C (styrene oxide (10 mmol), 0.01 mol % catalyst **1b**, 0.8 mol % co-catalyst, solvent-free).

Table S3 Cycloaddition of CO_2 and styrene oxide under various pressure [a]

Entry	Cat.	Co-cat.	T (°C)	*P* (MPa)	t (h)	Conversion [b] (%)
1	**1b**	TBAB	120	1	2	97
2	**1b**	TBAB	120	0.8	2	96
3	**1b**	TBAB	120	0.6	2	92
4	**1b**	TBAB	120	0.5	2	91

a. Reaction conditions: styrene oxide (10 mmol), 0.01 mol % catalyst **1b**, 0.8 mol % co-catalyst, solvent-free, 120 °C， 2 h. b. Determined by ^{1}H NMR spectroscopy.

Table S4. Overview of reported Ln-complexes catalysts under mild conditions

Cat. (%)	Co-cat. (%)	Catalyst/Epoxide (Mole ratio)	P_{CO2}	T (°C)	Time (h)	Conversion (%)	TON	TOF (h^{-1})	Ref
$Nd(C_5H_5)_3(THF)$	TBAI (0.8)	(styrene oxide) 1:500	1	85	24	93	465	19	1
Ionic Rare Earth Metal Complexes	-	(styrene oxide) 1:500	1	90	12	93	465	38	2
{[Eu(BTB)(phen)] ·4.5DMF·$2H_2O$}n	TBAB (2.5)	(styrene oxide) 1:286	1	80	12	68	24	2	3
Tb_4 MOF	TBAB (2.5)	(styrene oxide) 1:50	1	60	12	95	48	4	2
1·Gd	TBAB (2.5)	(styrene oxide) 1:133	1	60	12	70	12	1	4
3d-4f MOF	TBAB (2.5)	(styrene oxide) 1:100	1	70	12	77	78	6.5	5
Yb-mesocate	TBAB (0.75)	(styrene oxide) 1:1000	10	120	2.5	95	950	380	6
3d–4f helicates	TBAB (0.75)	(styrene oxide) 1:4000	10	80	6	94	3762	627	7
$[La\{N(SiHMe_2)_2\}_2$-{k^3 -bpzcp}]	TBAB (0.05)	(propylene oxide)	10	70	4	95	236	59	8
Yb-DDPY	TBAB (0.5)	(styrene oxide) 1:400	10	60	12	52	204	17	9
Complex 1b	**TBAB (0.8)**	**(styrene oxide) 1:10000**	**1**	**80**	**14**	**92.6**	**9260**	**661**	**This work**
Complex 2a	**TBAB (0.8)**	**(styrene oxide) 1:10000**	**1**	**80**	**14**	**93.5**	**9350**	**668**	**This work**

Table S5. Overview of reported Mg, Al, Zn, Fe-catalysts under mild conditions

Cat. (%)	Co-cat. (%)	Catalyst/Epoxid e	p_{CO2} (bar	T (°C	Tim e	Conversion(%)	TON	TOF (h^{-1})	Ref
bimetallic Fe-catalyst	[PPN]C l	(styrene oxide) 1:1000	1	80	24	83	830	8	10
Complex 1b	**TBAB (0.8)**	**(styrene oxide) 1:10000**	**1**	**80**	**14**	**92.6**	**9260**	**661**	**This wor**

Complex 2a	**TBAB (0.8)**	**(styrene oxide) 1:10000**	**1**	**80**	**14**	**93.5**	**9350**	**668**	**This wor**
$Zn_4(OCOCF_3)_6O$	TBAI (3.0)	(propylene oxide)	1	25	6	94	94	15.6	11
dimetallic Al-complex	TBAB (2.5)	(styrene oxide) 1:40	1	25	24	98	39.2	-	12
Al-iPOP-2	-	(propylene oxide)	1	25	8	>99	992	124	16
Al-HCP	TBAB (2)	(propylene oxide)	1	25	5	99	396	79.2	17
Complex 1b	**TBAB (3.6)**	**(styrene oxide) 1:800**	**1**	**25**	**48**	**93.5**	**748**	**15.6**	**This wor**
Complex 2a	**TBAB (3.6)**	**(styrene oxide) 1:800**	**1**	**25**	**48**	**95**	**760**	**15.8**	**This wor**
salen Al-complexes	-	(AGE) 1:200	10	100	2.5	96	182.5	76	13
organocatalysts	TBAI (5.0)	(styrene oxide) 1:66	10	50	18	>99	>66	>3.7	14
binary Al-catalysts	TBAB (0.05)	(styrene oxide) 1:1000	10	90	2	13	1300	650	15
Al-iPOP	-	(propylene oxide)	10	40	3	99	990	330	16
Al-HCP	TBAB (2.0)	(propylene oxide)	10	40	1	99	396	396	17
helical bimetallic	TBAB (5.0)	(propylene oxide)	10	r.t.	24	96	19.2	0.8	18
Mg-complex	-	(propylene oxide)	15	120	6	99	19800	3300	19
Salen-Zn	TBAI (0.5)	(styrene oxide) 1:670	10	80	6	89	594	99	20
Zn_3	-	(epichlorohydrin)	10	85	18	80	32.4	1.8	21
Complex 1b	**TBAB (0.8)**	**(propylene oxide)**	**10**	**80**	**8**	**98**	**9800**	**1225**	**This wor**
Complex 2a	**TBAB (0.8)**	**(propylene oxide)**	**10**	**80**	**8**	**>99**	**>9900**	**>1237**	**This wor**

Table S6. Overview of reported catalysts for the conversion of CO_2 to cyclic carbonates under ambient conditions

Cat. (%)	Co-cat. (%)	Catalyst/Epoxide (Mole ratio)	Time (h)	Yields (%)	TON	TOF (h^{-1})	Ref
MMPF-9 (0.125mol % MOF)	TBAB (7.2)	(propylene oxide)	48	87	696	14.5	22
MMCF-2 (0.125mol % MOF)	TBAB (7.2)	(propylene oxide)	48	95	760	15.8	23
HKUST-1 (0.125mol % MOF)	TBAB (7.2)	(propylene oxide)	48	49	392	8.2	23
MOF-505 (0.125mol % MOF)	TBAB (7.2)	(propylene oxide)	48	48	384	8	23
heterometallic helicate	TBAB (7.5)	(styrene oxide) 1:100	48	81	648	13.5	8
MIL-53 (1mol % MOF)	TBAB (6.5)	(propylene oxide)	72	54	-	-	24
MOF-253 (1mol % MOF)	TBAB (6.5)	(propylene oxide)	72	82	-	-	24
MIL-101 (1mol % MOF)	TBAB (6.5)	(propylene oxide)	72	31	-	-	24
UiO-66 (1mol % MOF)	TBAB (6.5)	(propylene oxide)	72	55	-	-	24
Complex 1b	**TBAB (7.2)**	**(styrene oxide) 1:800**	**48**	**>99**	**>792**	**>16.5**	**This work**
Complex 1b	**TBAB (3.6)**	**(styrene oxide) 1:800**	**48**	**93.5**	**748**	**15.6**	**This work**
Complex 2a	**TBAB (7.2)**	**(styrene oxide) 1:800**	**48**	**>99**	**>792**	**>16.5**	**This work**
Complex 2a	**TBAB (3.6)**	**(styrene oxide) 1:800**	**48**	**95**	**760**	**15.8**	**This work**

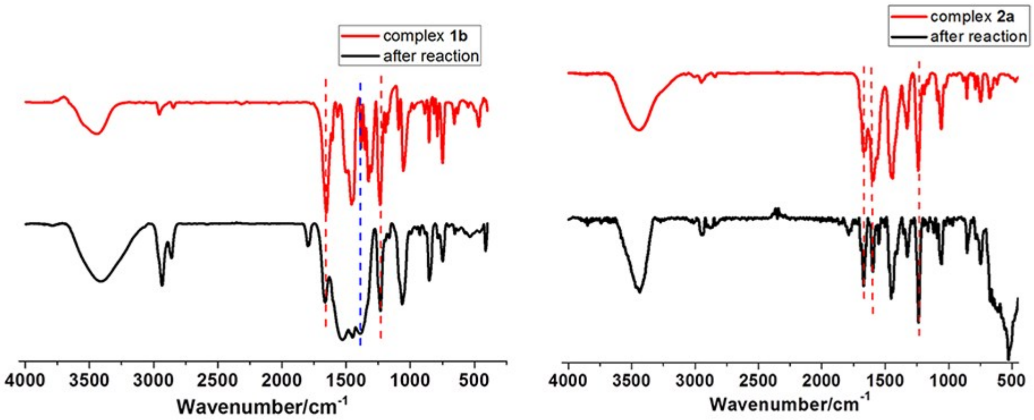


Figure 10. FT-IR spectra of complex **1b** and **2a** before and after the cycloaddition of epoxides with CO_2. The FT-IR peaks are almost no changed, indicates that complexes didn't decomposed during the catalyzed reaction.

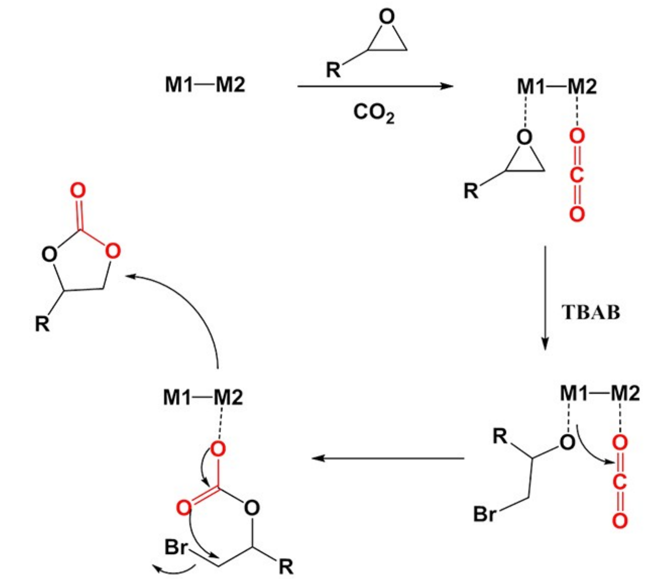
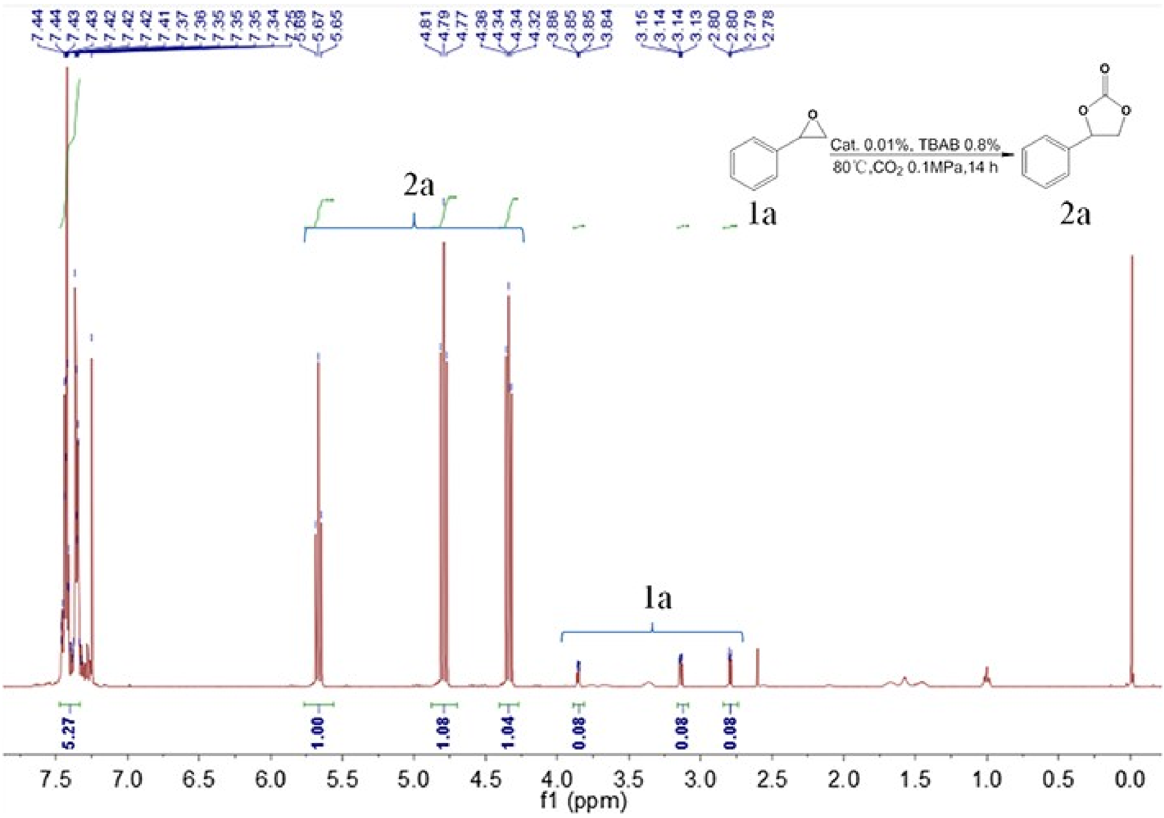
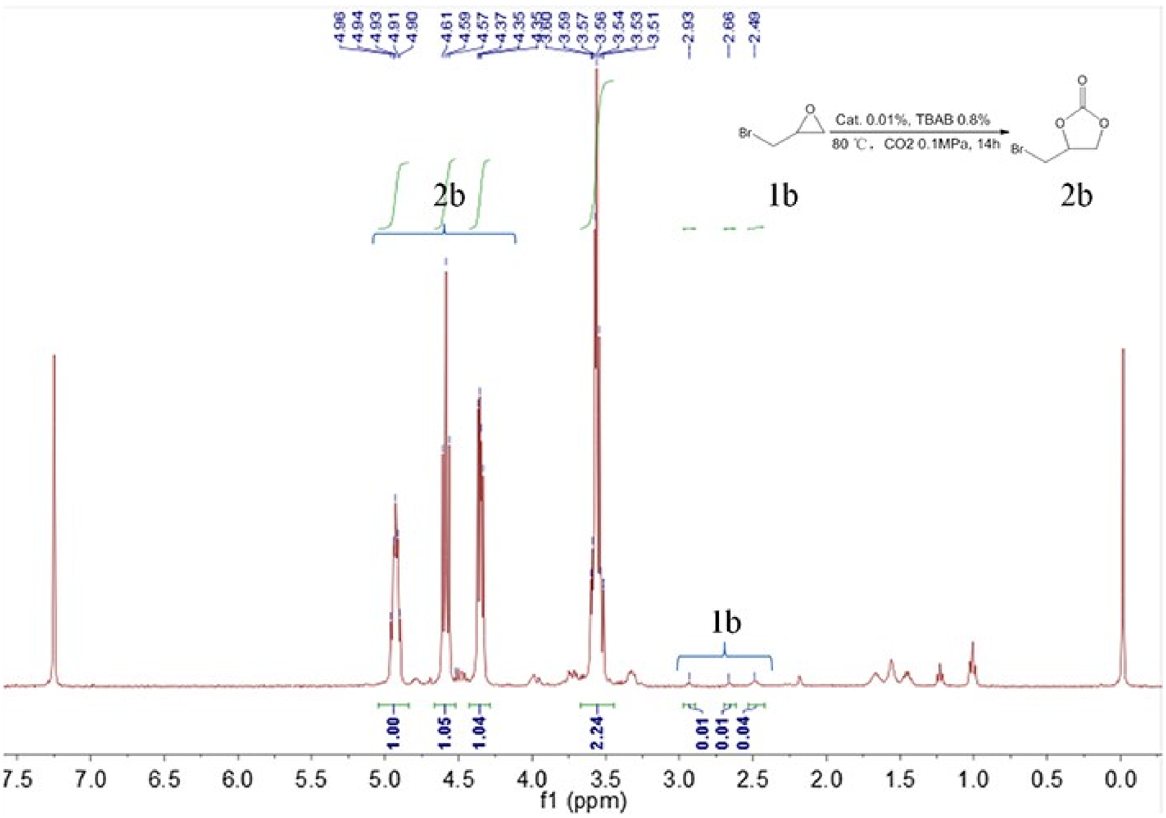
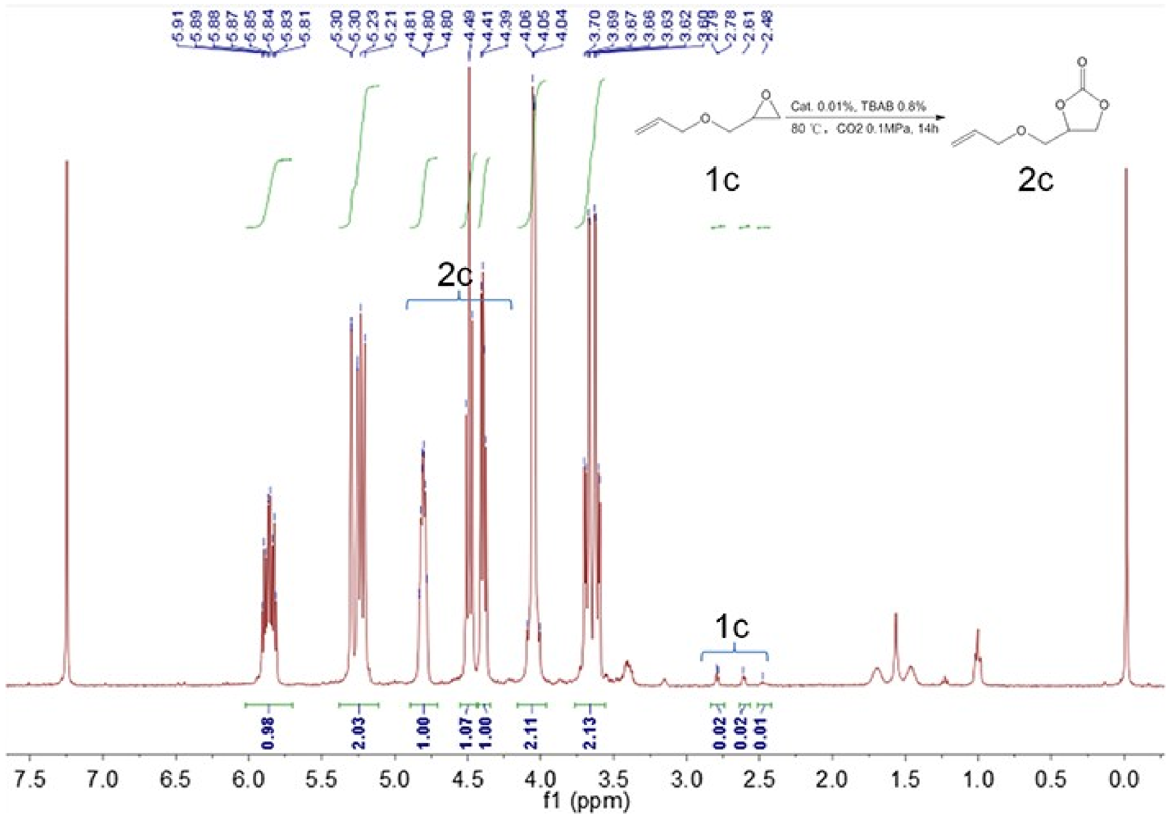
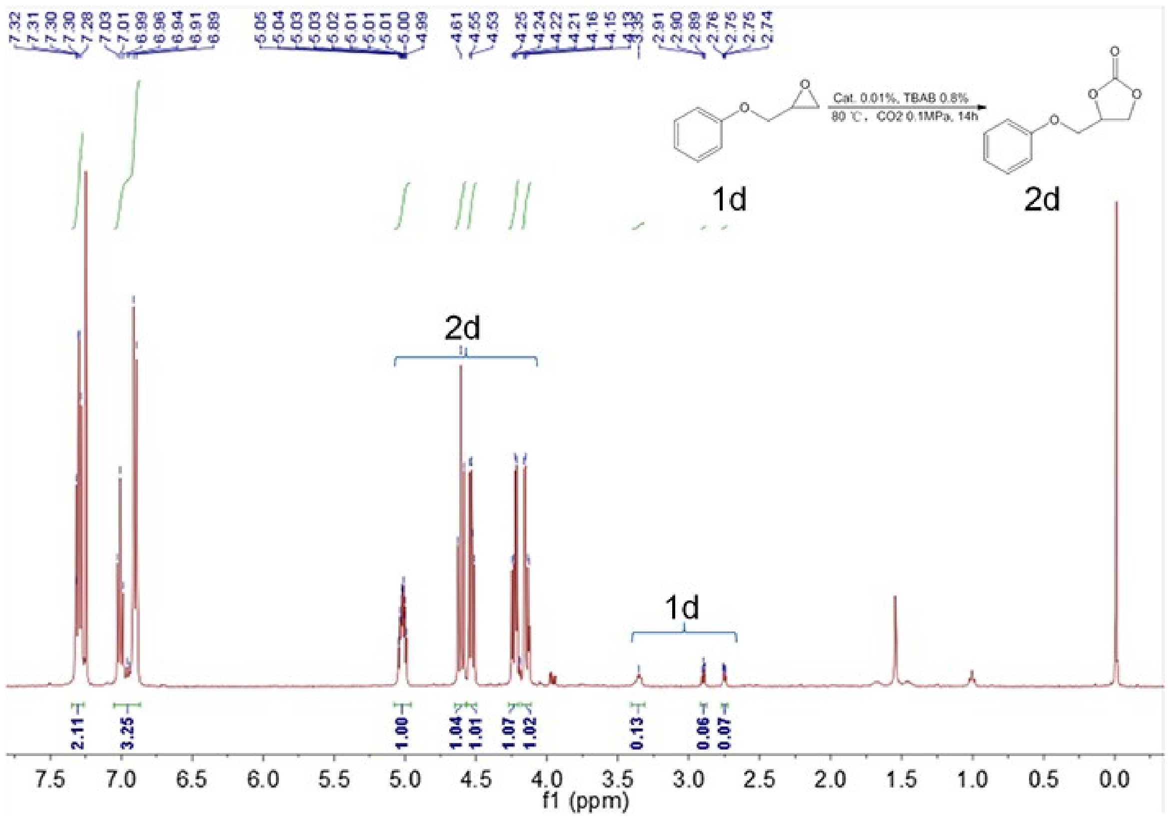


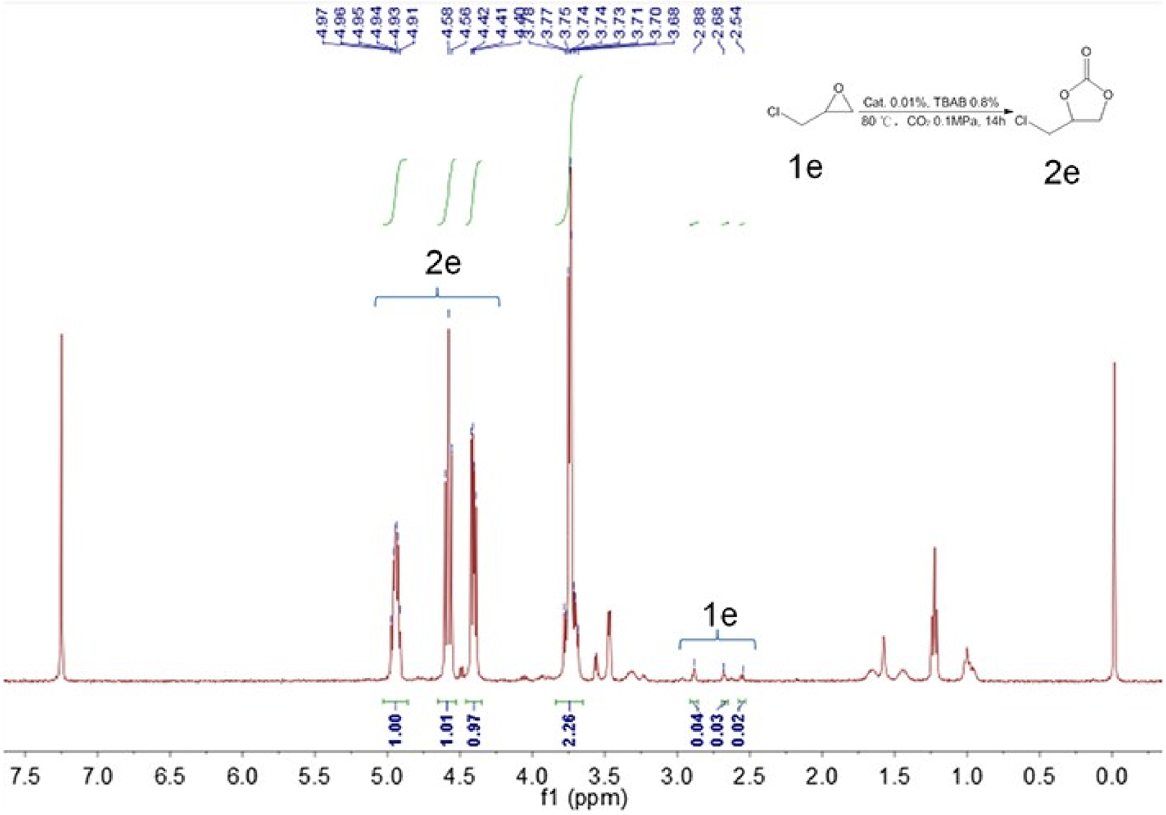
Figure S11. A possible mechanism for the cycloaddition reaction.


7.44 7.44 7.43 7.43 7.42 7.42 7.41 7.37 7.36 7.35 7.35 7.35 7.34 7.25 5.68 5.67 5.65 4.81 4.79 4.77 4.36 4.34 4.34 4.32 3.86 3.85 3.85 3.84 3.15 3.14 3.14 3.13 2.80 2.80 2.79 2.78
Cat. 0.01%, TBAB 0.8%
80℃,CO2 0.1MPa,14 h
1a
2a
2a
1a
5.27
1.00
1.08
1.04
0.08
0.08
0.08
f1 (ppm)

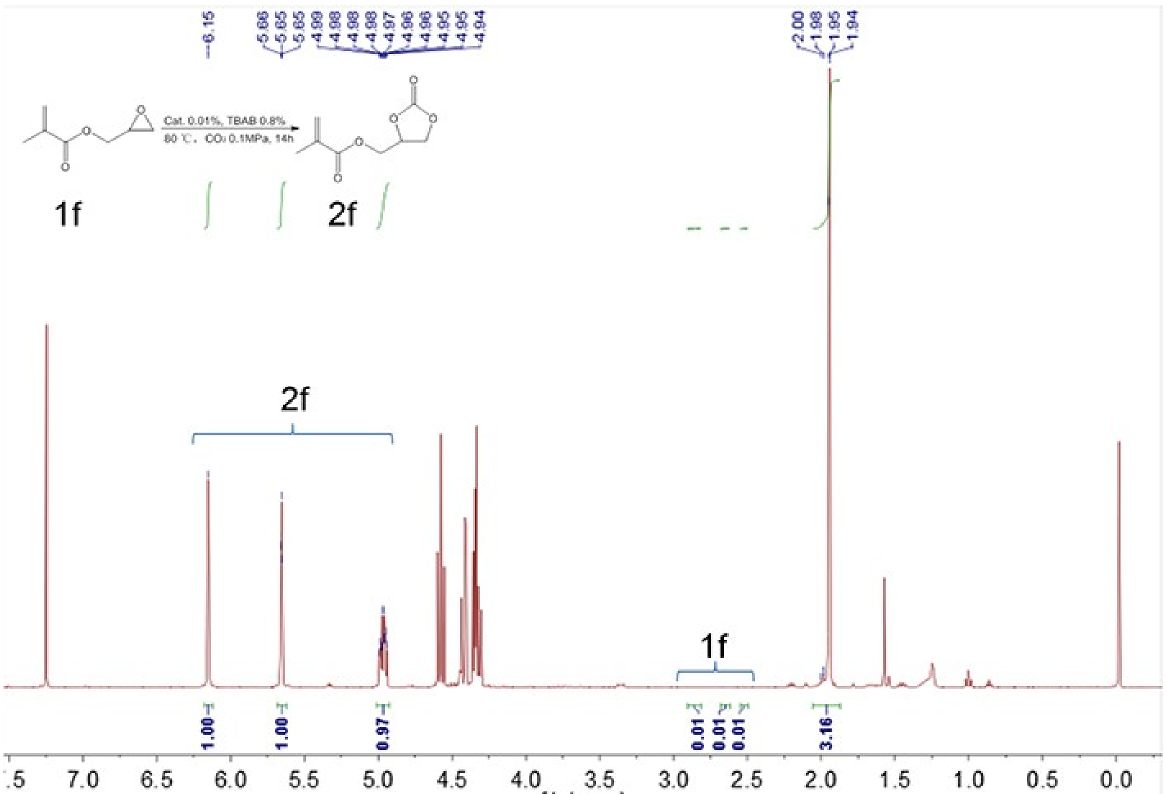

4.96 4.94 4.93 4.91 4.90 4.61 4.59 4.57 4.37 4.35 3.60 3.59 3.57 3.56 3.54 3.53 3.51 2.93 2.66 2.49
Cat. 0.01%, TBAB 0.8%
80 ℃， CO2 0.1MPa, 14h
Br
Br
1b
2b
2b
1b
1.00
1.05
1.04
2.24
0.01
0.01
0.04
f1 (ppm)


Cat. 0.01%, TBAB 0.8%
80 ℃, CO2 0.1MPa, 14h
1c
2c
f1 (ppm)

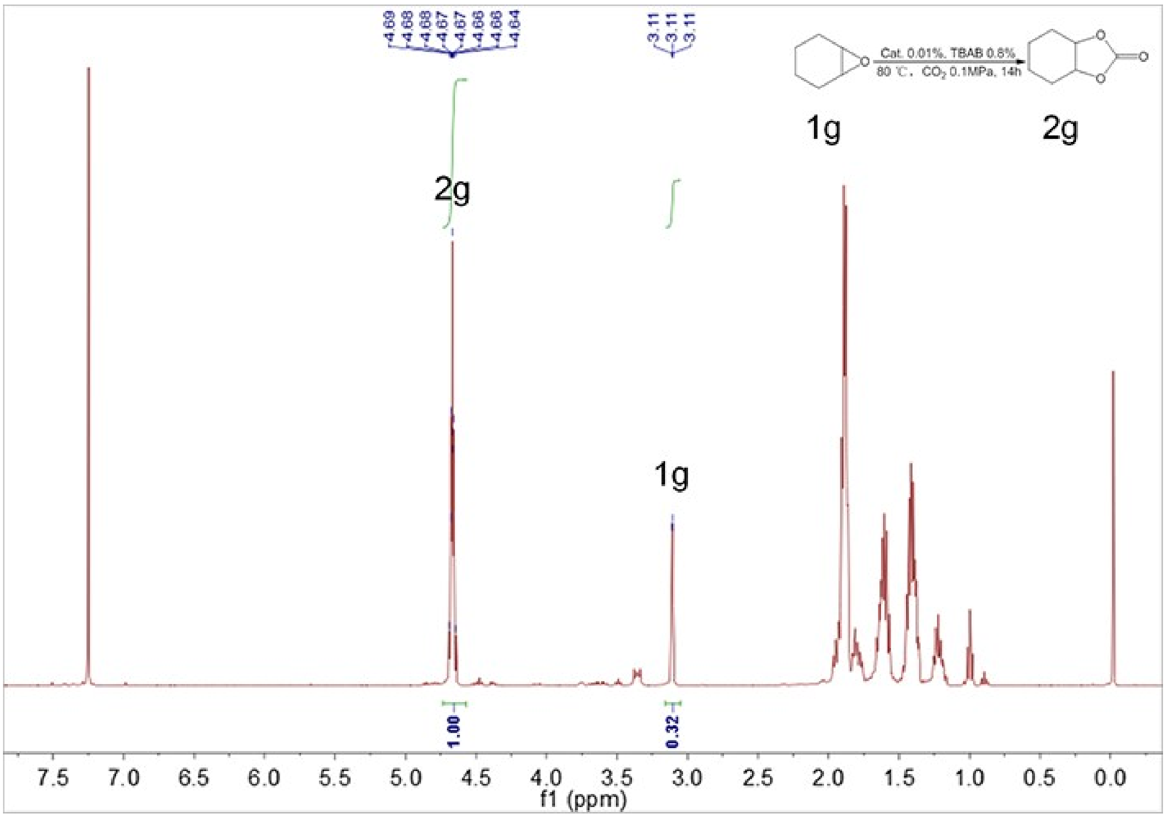

Cat. 0.01%, TBAB 0.8%
80 ℃, CO2 0.1MPa, 14h
1d
2d
f1 (ppm)



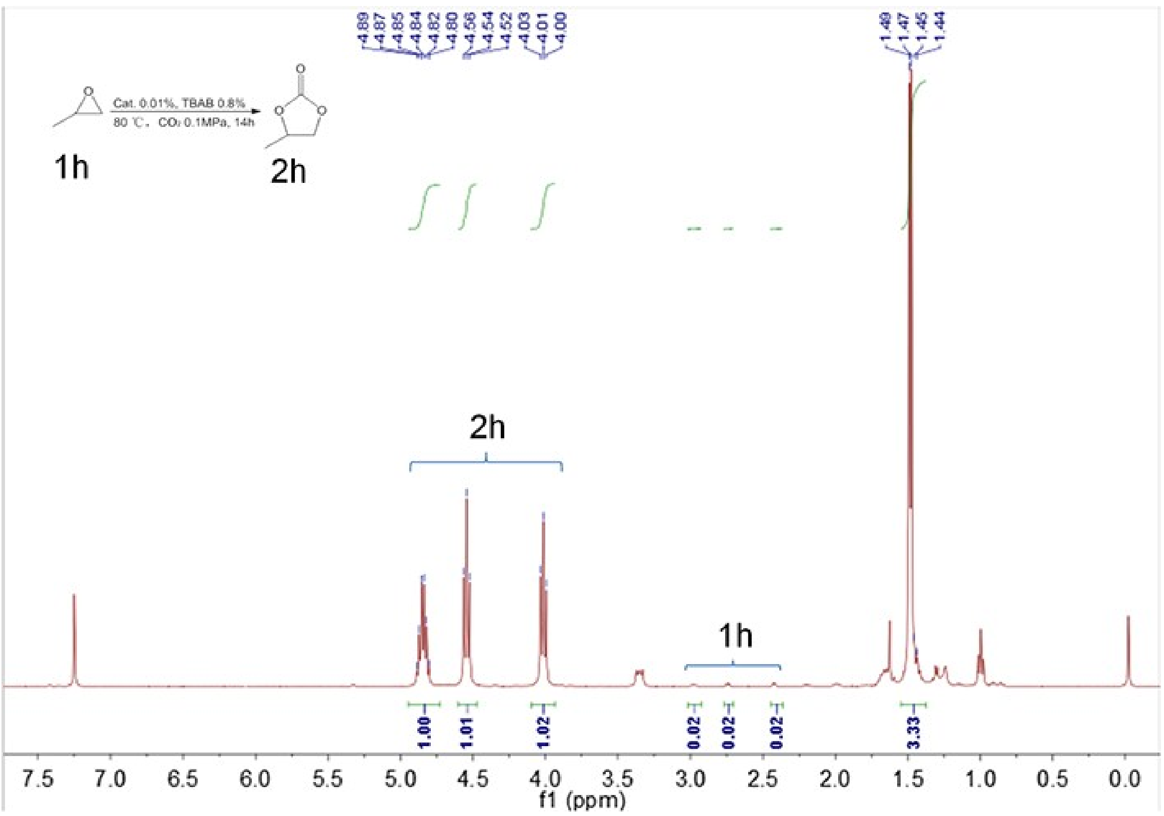
Cat. 0.01%, TBAB 0.8%
80 ℃, CO₂ 0.1MPa, 14h
1e
2e
f1 (ppm)



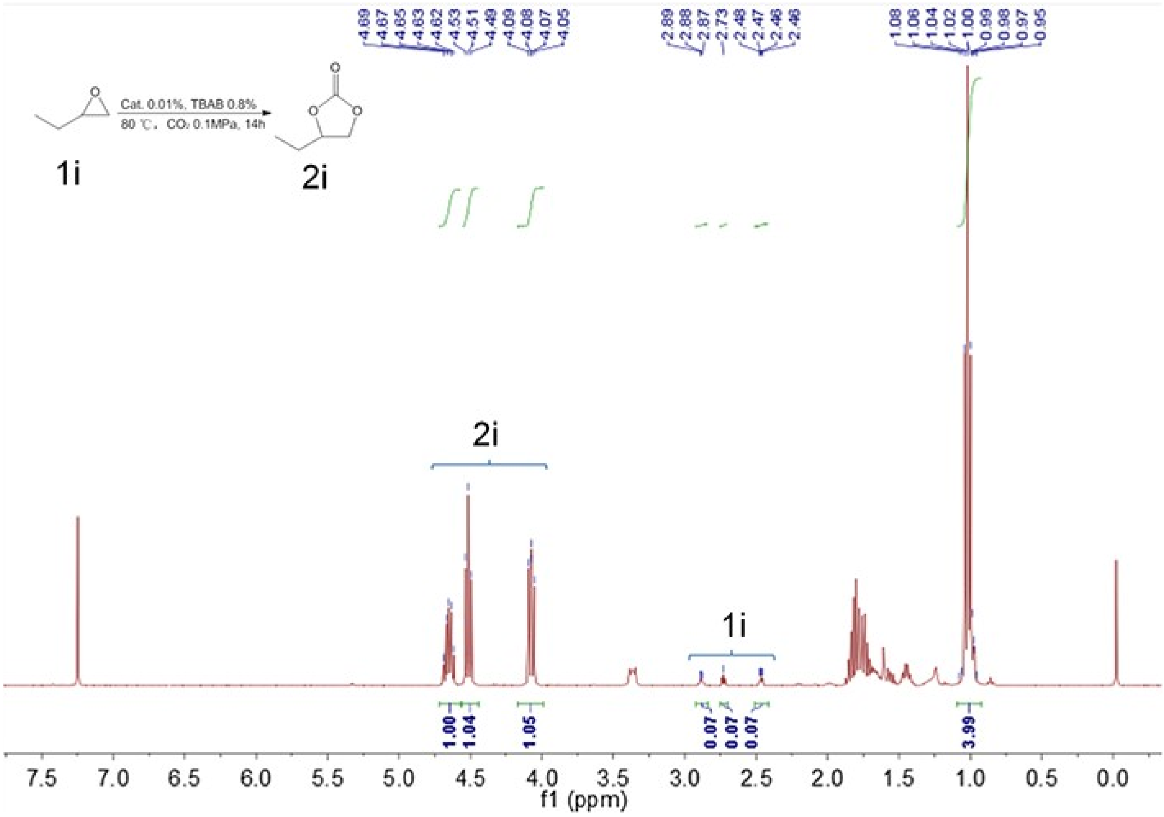
Cat. 0.01%, TBAB 0.8%
80 ℃, CO₂ 0.1MPa, 14h
1f
2f
f1 (ppm)



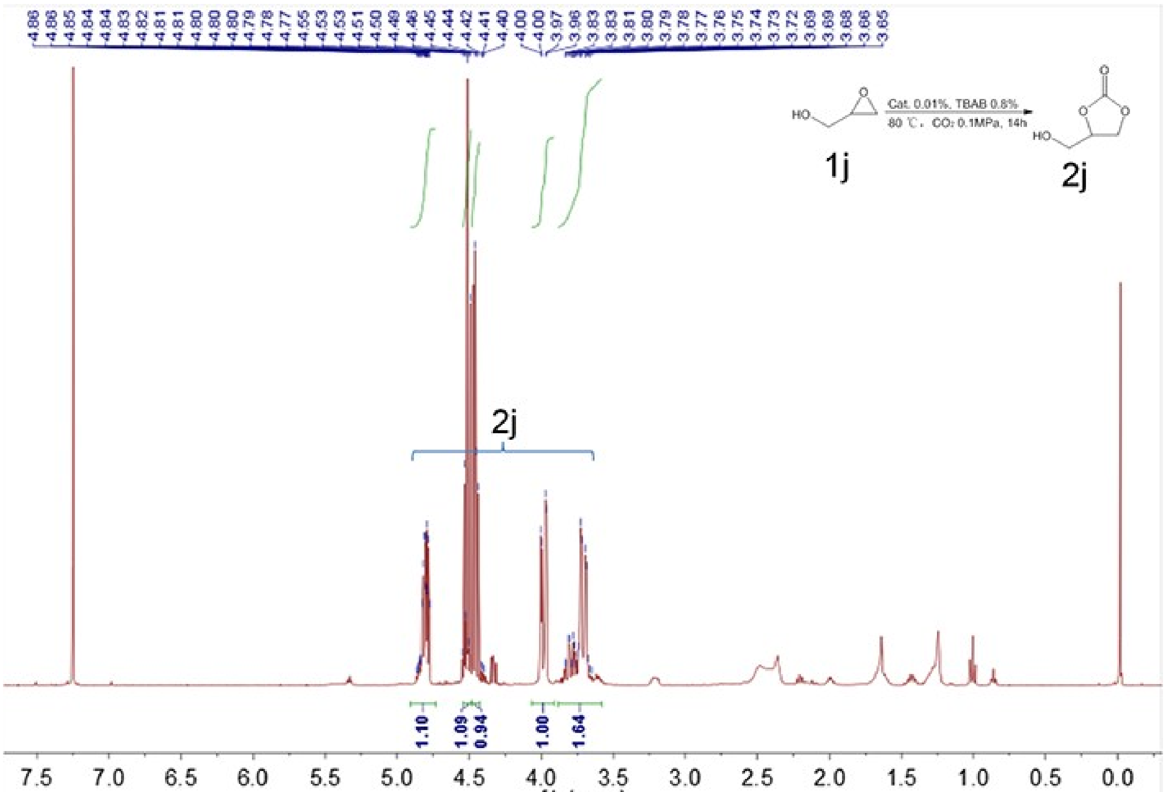
Cat. 0.01%, TBAB 0.8%
80 ℃, CO2 0.1MPa, 14h
1g
2g
1.00
0.32
f1 (ppm)



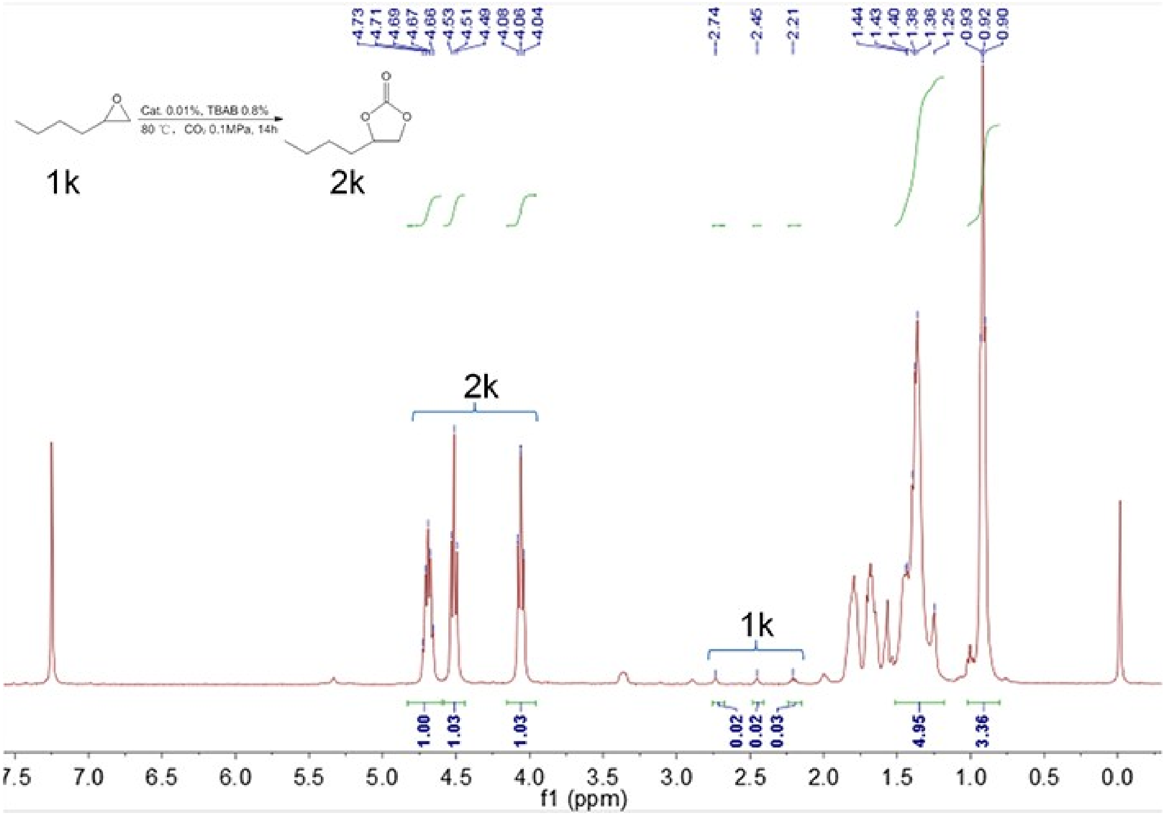
Cat. 0.01%, TBAB 0.8%
80 ℃, CO2 0.1MPa, 14h
1h
2h
1.00
1.01
1.02
0.02
0.02
0.02
3.33
f1 (ppm)



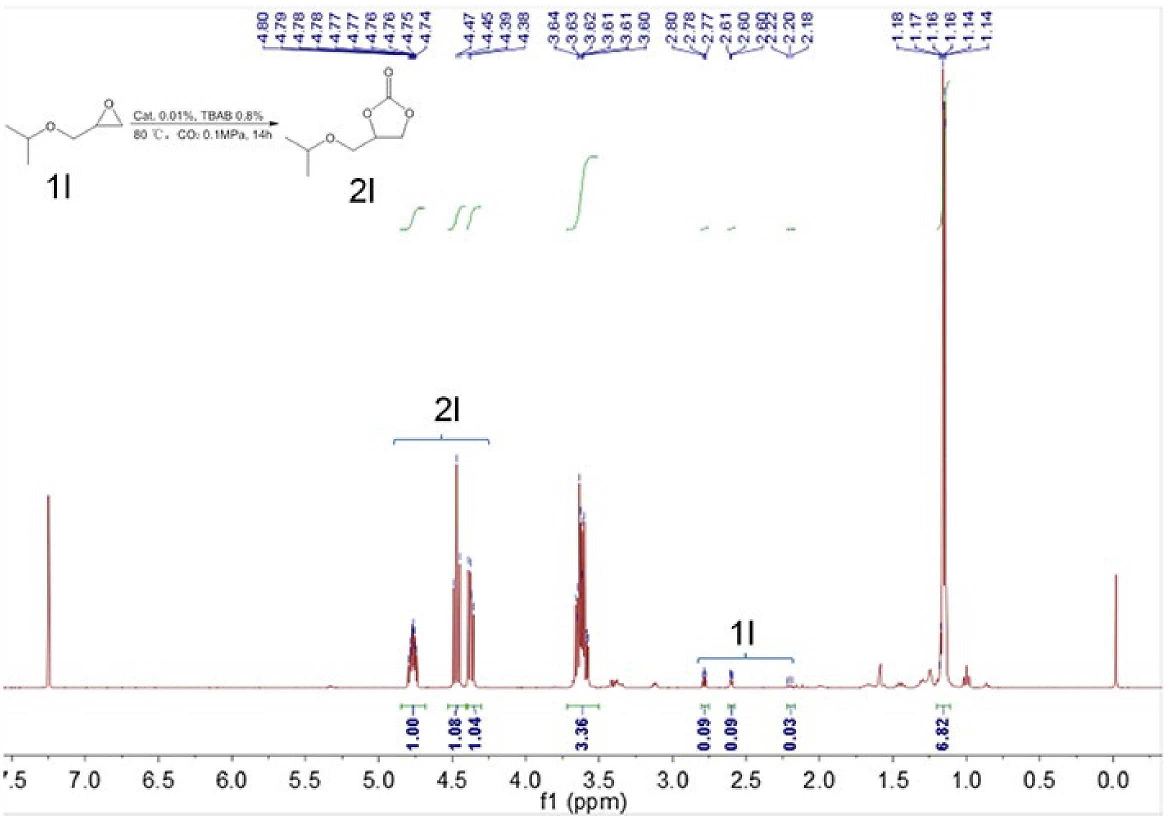
Cat. 0.01%, TBAB 0.8%
80 ℃，CO2 0.1MPa, 14h
1i
2i
2i
1i
f1 (ppm)



HO
Cat. 0.01%, TBAB 0.8%
80 ℃，CO2 0.1MPa, 14h
HO
1j
2j
2j
f1 (ppm)



Cat. 0.01%, TBAB 0.8%
80 ℃, CO2 0.1MPa, 14h
1k
2k
4.73 4.71 4.69 4.67 4.66 4.53 4.51 4.49 4.08 4.06 4.04
2.74 2.45 2.21
1.44 1.43 1.40 1.38 1.36 1.25 0.93 0.92 0.90
2k
1k
1.00 1.03 1.03 0.02 0.02 0.03 4.95 3.36
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



Cat. 0.01%, TBAB 0.8%
80 ℃, CO2 0.1MPa, 14h
1l
2l
4.80 4.79 4.78 4.77 4.77 4.76 4.76 4.75 4.74
4.47 4.45 4.39 4.38
3.64 3.63 3.62 3.61 3.61 3.60
2.80 2.78 2.77 2.61 2.60 2.60 2.22 2.20 2.18
1.18 1.17 1.16 1.16 1.14 1.14
2l
1l
1.00 1.08 1.04 3.36 0.09 0.09 0.03 6.82
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

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