Supporting Information

Lanthanides (III) (Er/Ho) coordination polymers for photocatalytic CO_2 cycloaddition reaction

Reem H. Alzard,[a] Lamia A. Siddig,[a] Abdalla S. Abdelhamid,[a] Alejandro Perez Paz,[a] Ha L. Nguyen,[b,c] K. Sethupathi,[d] P. K. Sreejith,[d] and Ahmed Alzamly[a*]

[a]Department of Chemistry, UAE University, P.O. Box 15551, Al-Ain, UAE

[b]Department of Chemistry, University of California Berkeley; Kavli Energy Nanoscience Institute at UC Berkeley; and Berkeley Global Science Institute, Berkeley, California 94720, United States

[c]Joint UAEU−UC Berkeley Laboratories for Materials Innovations, United Arab Emirates University, Al-Ain 15551, United Arab Emirates

[d]Low temperature Physics Laboratory, Department of Physics, Indian Institute of Technology Madras, Chennai 600036, India

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Section 1: Characterization of Ln-CPs

Powder X-ray Diffraction (PXRD) for Ln-CPs prepared at different ratios

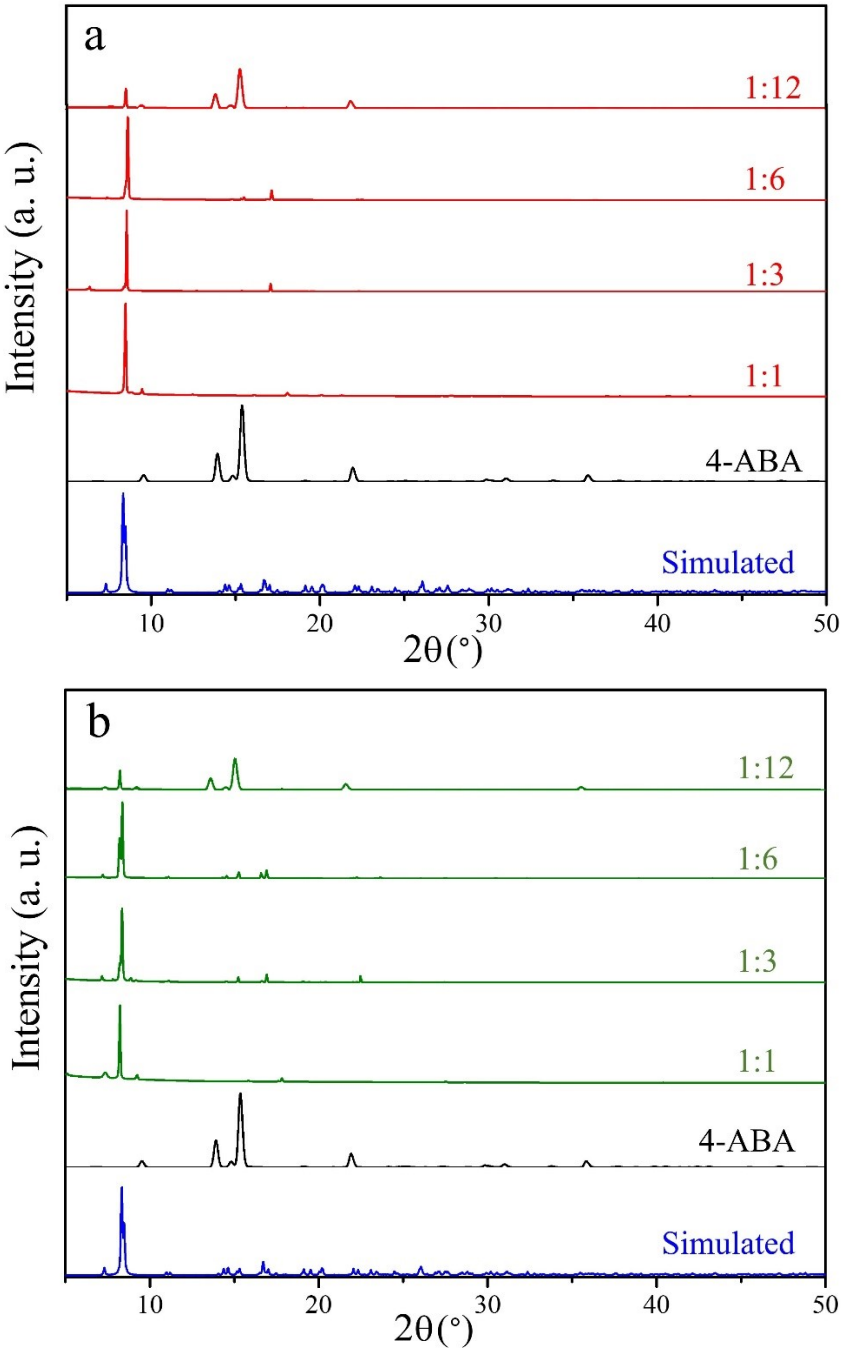

Figure S1. PXRD patterns of (a) Ho-CP and (b) Er-CP prepared at different ratios compared to the simulated pattern and 4-ABA starting material.

Energy-dispersive X-ray spectroscopy (EDX)

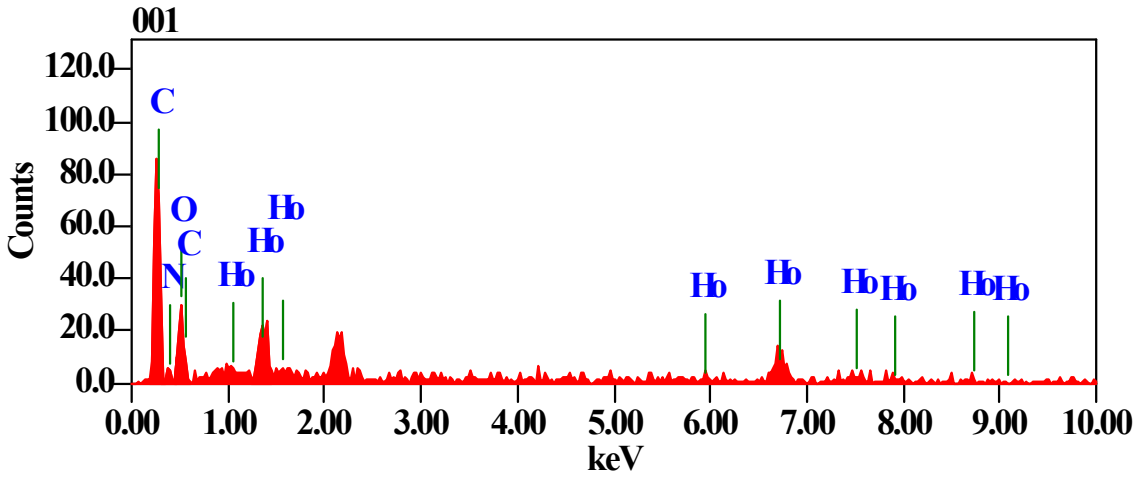

Figure S2. EDX spectrum of Ho-CP indicating the presence of Ho, N, O, and C atoms in the sample.

Table S1. Average weight and atomic percentages of Ho-CP based on EDX analysis.

Element	**Weight %**	**Atom %**
C	44.05	64.14
O	15.97	17.50
N	12.37	15.47
Ho	27.6	2.93

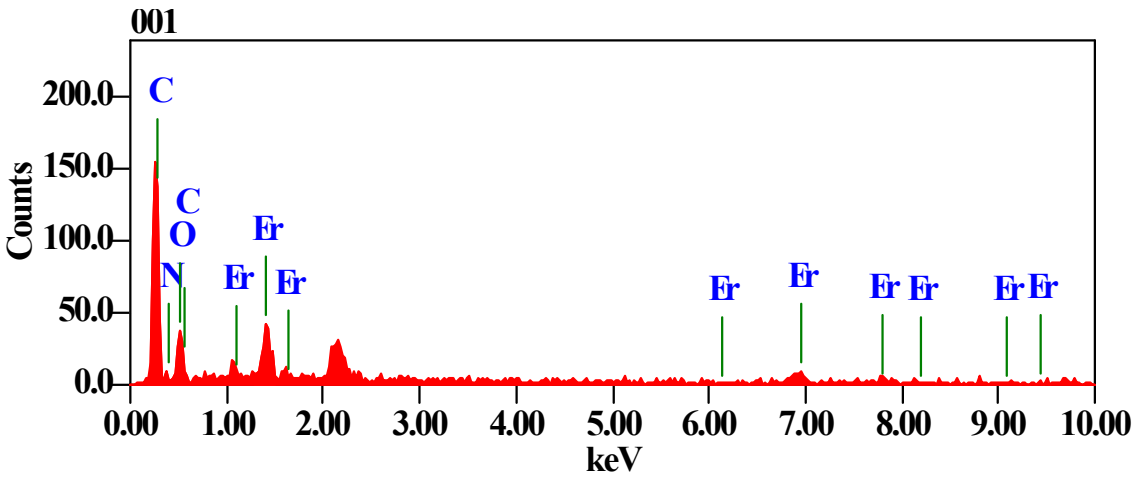

Figure S3. EDX spectrum of Er-CP indicating the presence of Er, N, O, and C atoms in the sample.

Table S2. Average weight and atomic percentages of Er-CP based on EDX analysis.

Element	Weight %	Atom %
C	44.83	66.71
O	14.97	13.39
N	10.50	16.72
Er	29.3	3.17

Thermogravimetric analysis of Ln-CPs

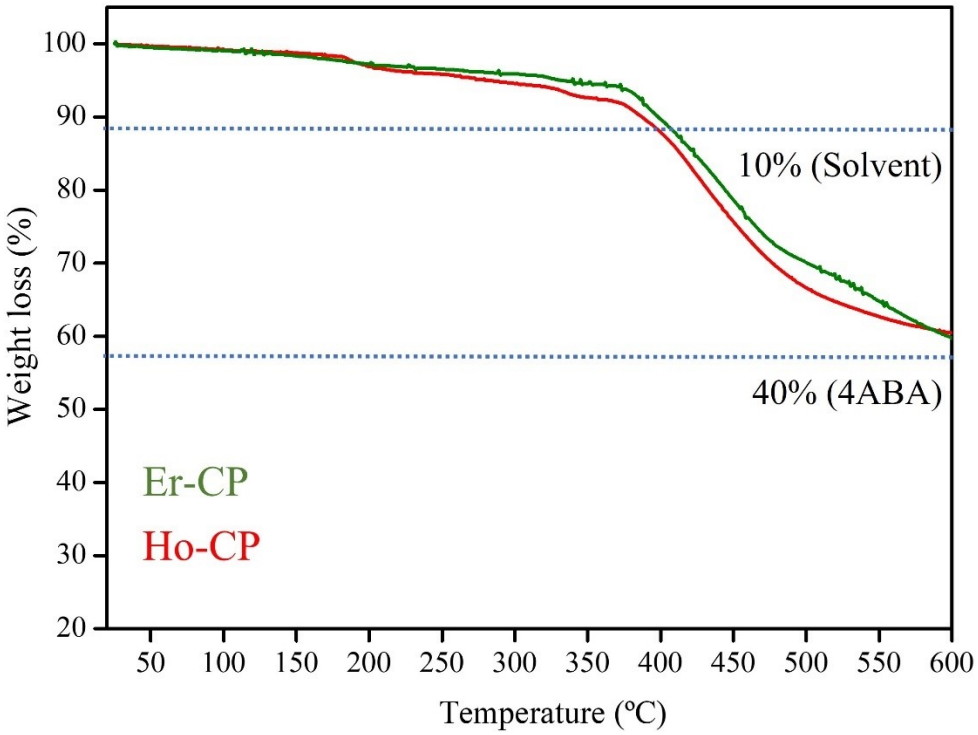

Figure S4. Thermogravimetric analysis of Ln-CPs. The blue lines indicate percentages corresponding to the solvent and organic linker losses.

Chemical stability of Ln-CPs in different solvents

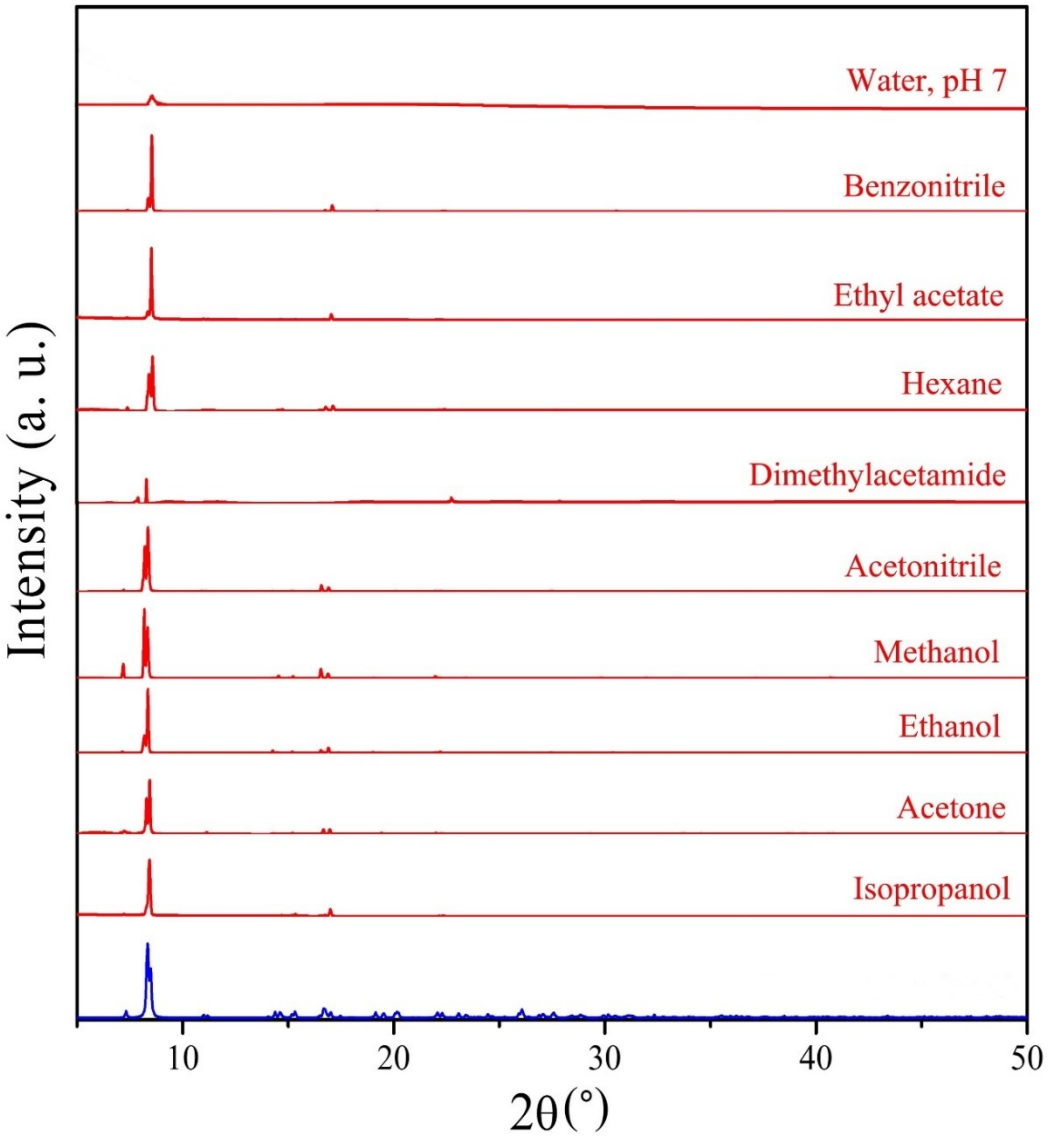

Figure S5. Powder X-ray diffraction patterns of Ho-CP (1:6 ratio) after being immersed in various solvents for 24 hours.

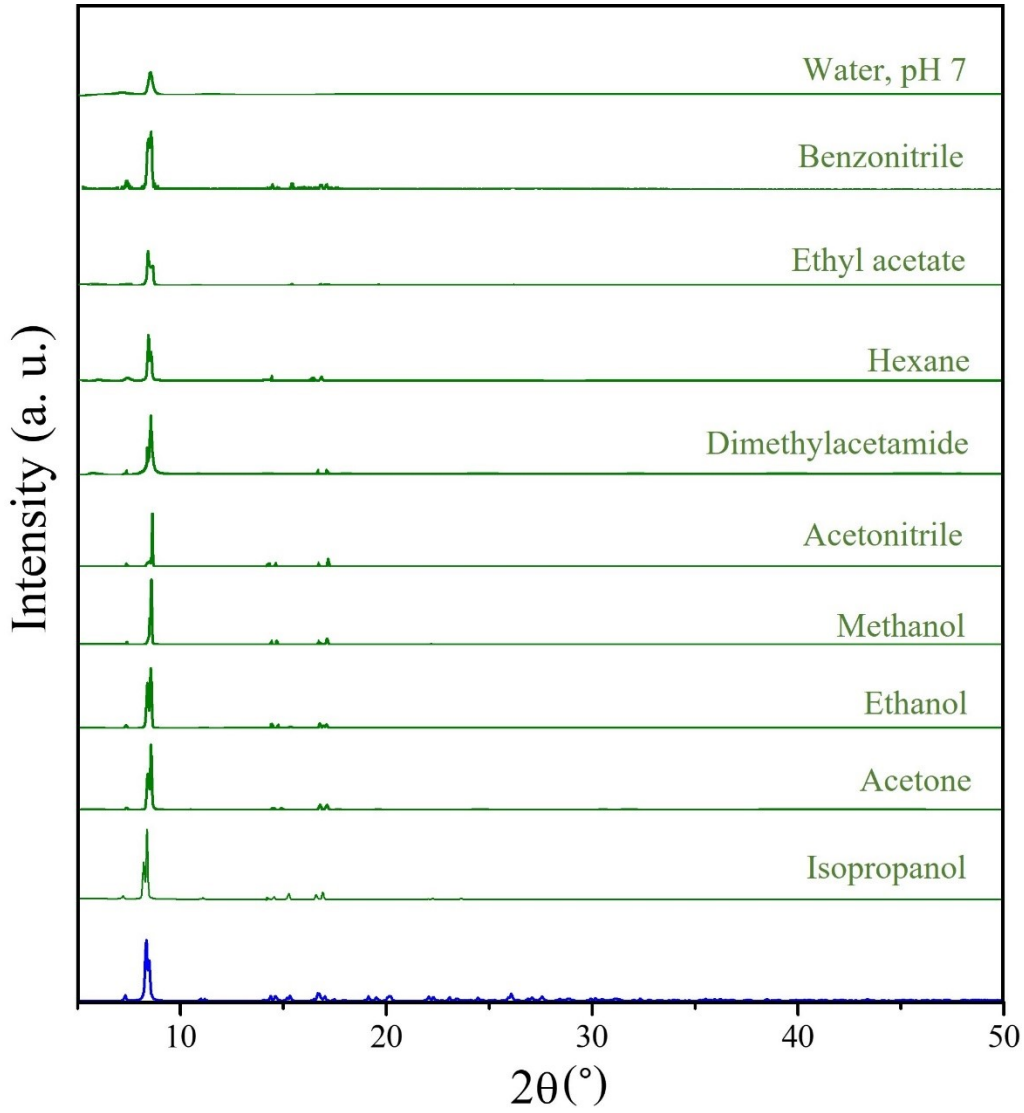

Figure S6. Powder X-ray diffraction patterns of Er-CP (1:6 ratio) after being immersed in various solvents for 24 hours.

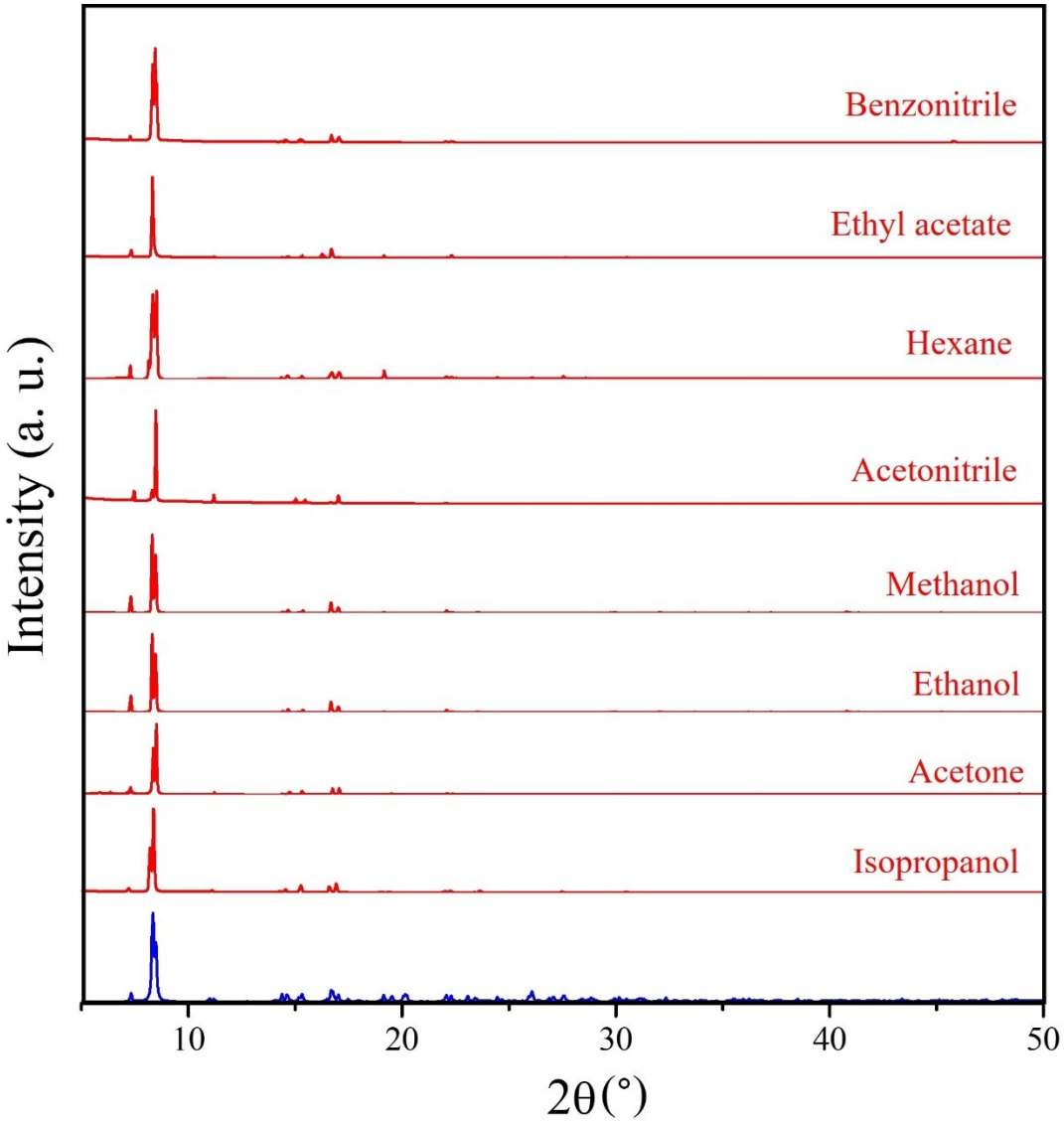

Figure S7. Powder X-ray diffraction patterns of Ho-CP (1:6 ratio) after being immersed in various solvents for 1 week. Patterns of the sample in H_2O and dimethylacetamide were not included as sample was destructed and no diffraction peaks appeared.

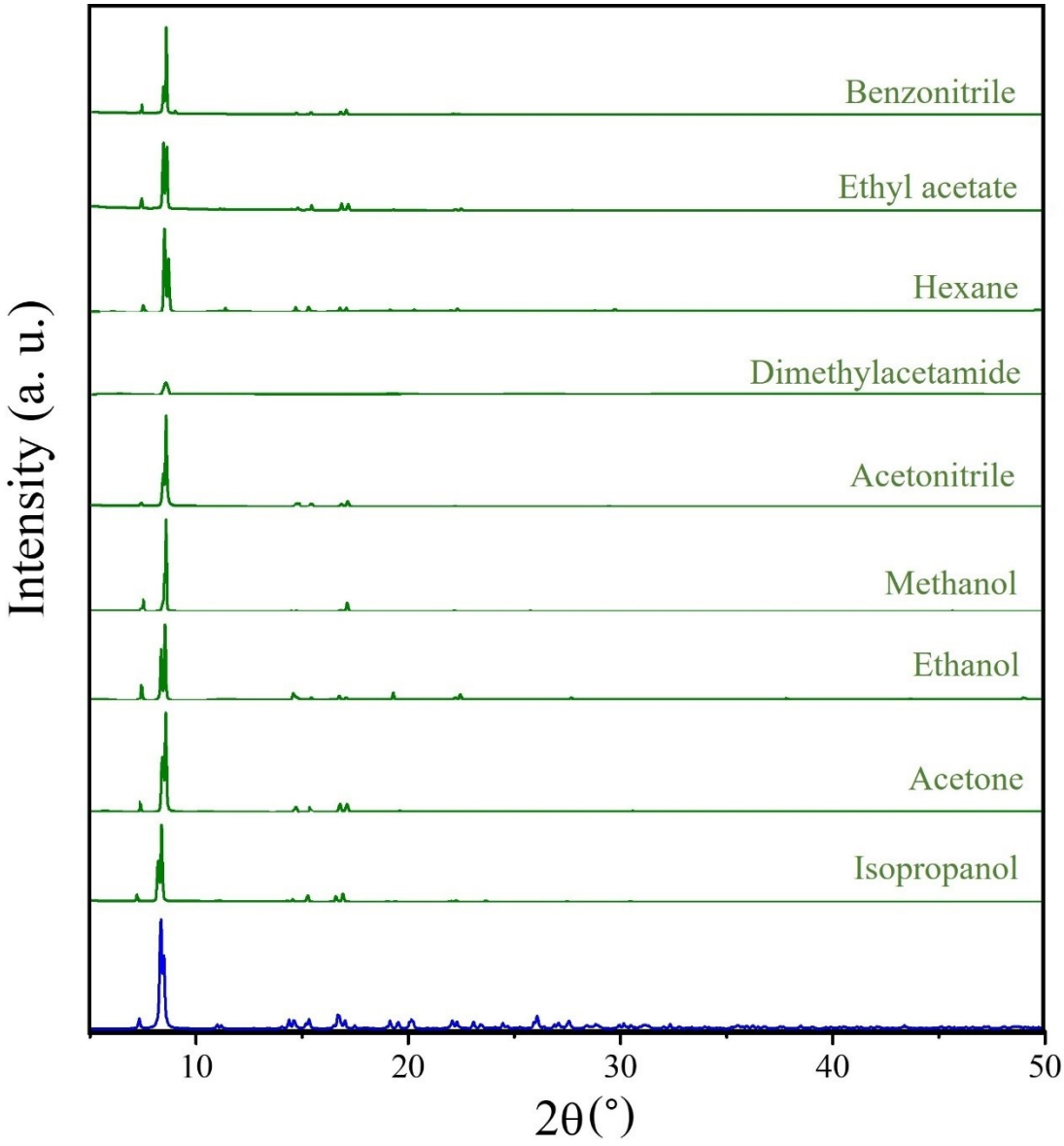

Figure S8. Powder X-ray diffraction patterns of Er-CP (1:6 ratio) after being immersed in various solvents for 1 week. Patterns of the sample in H_2O was not included as the sample was destructed and no diffraction peaks appeared.

UV−Vis Diffuse-reflectance data of Ln-CPs

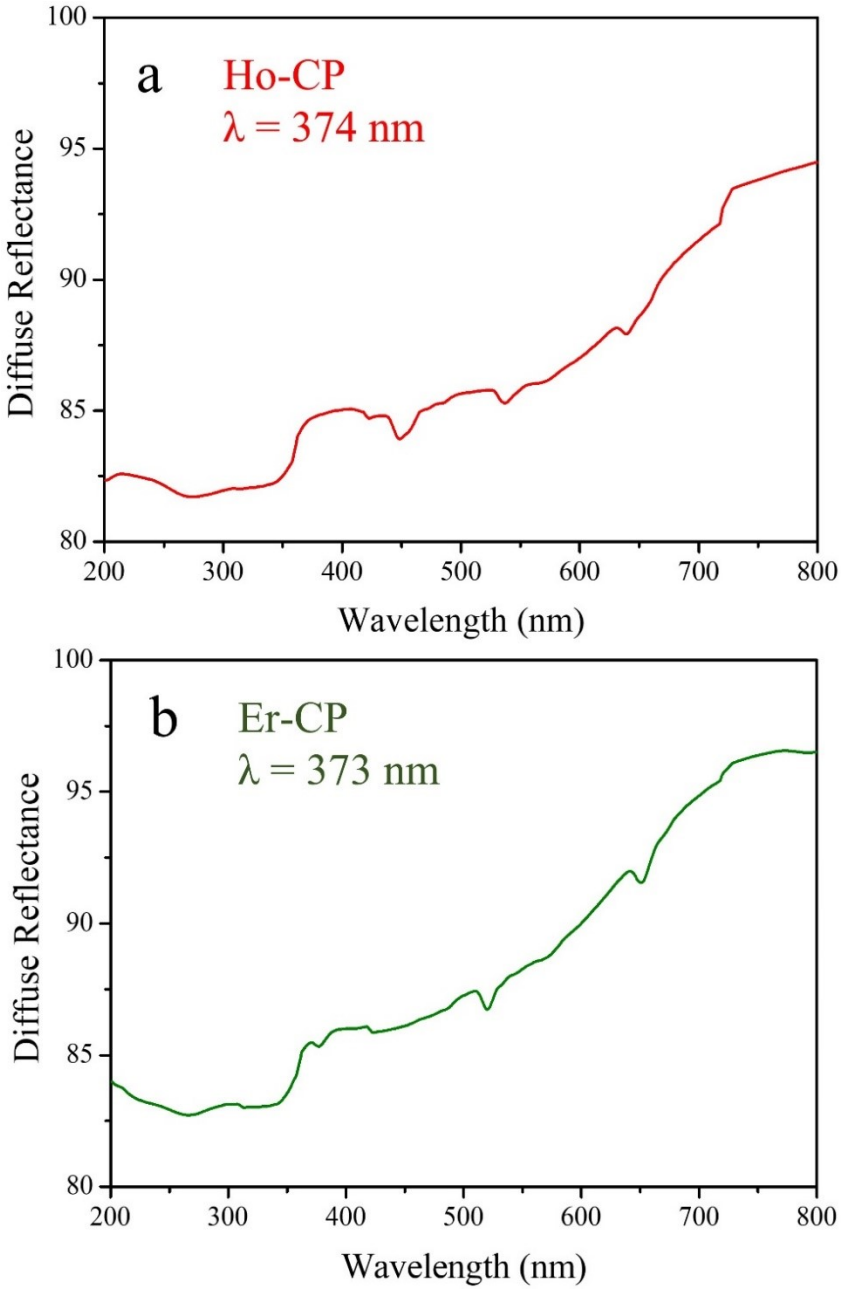

Figure S9. UV−Vis DRS spectra of Ho-CP (a) and Er-CP (b) under air atmosphere and room temperature conditions.

Section 2: Crystallographic details

Crystal details of Er-CP

Table S3. Crystal data and structure refinement for Er-CP.

Identification code	Er-CP, Deposition Number 2180346
Empirical formula	$C_{42}H_{36}Er_2N_6O_{12}$
Formula weight	1151.29
Temperature/K	297.00(10)
Crystal system	triclinic
Space group	*P*-1
a/Å	7.87907(16)
b/Å	12.1676(3)
c/Å	21.2187(5)
α/°	88.844(2)
β/°	89.7102(18)
γ/°	83.4768(18)
Volume/Å^3	2020.63(8)
Z	2
ρ_{calc}g/cm^3	1.892
μ/mm^{-1}	8.105
F(000)	1124.0
Crystal size/mm^3	0.143 × 0.061 × 0.036
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.314 to 155.324
Index ranges	$-8 \le h \le 9$, $-15 \le k \le 15$, $-26 \le l \le 25$
Reflections collected	37964
Independent reflections	8148 [R_{int} = 0.0514, R_{sigma} = 0.0372]
Data/restraints/parameters	8148/0/566
Goodness-of-fit on F^2	1.104
Final R indexes [I>=2σ (I)]	R_1 = 0.0366, wR_2 = 0.0982
Final R indexes [all data]	R_1 = 0.0403, wR_2 = 0.1003
Largest diff. peak/hole / e Å^{-3}	1.10/-1.07

Table S4. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Er-CP. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Er1	3565.1(3)	6546.8(2)	2655.0(2)	30.80(9)
Er2	-1534.0(3)	7284.3(2)	2321.6(2)	30.82(9)

O11	1269(3)	6267(2)	2029.1(13)	35.6(6)
O21	4216(4)	7403(3)	1739.4(14)	43.6(7)
O31	5336(4)	5022(2)	2443.3(15)	42.1(7)
O40	4570(4)	6733(3)	3685.1(15)	48.2(8)
O20	6471(4)	8347(3)	1746.9(15)	42.2(7)
O51	1925(4)	5510(2)	3261.2(15)	40.9(7)
O10	-288(4)	7197(3)	1307.0(15)	43.8(7)
O	6032(3)	7526(2)	2960.7(13)	36.7(6)
O50	-754(4)	6324(3)	3199.1(16)	49.5(8)
O30	7531(4)	5725(2)	1997.3(18)	49.3(8)
O61	1941(5)	8083(3)	2868(2)	62.0(10)
O60	-548(4)	8923(3)	2562.9(17)	49.6(8)
C13	4151(5)	9016(3)	1097(2)	34.3(8)
C7	2166(6)	5258(4)	-136(2)	47.2(11)
C18	4680(6)	10066(4)	1027(2)	47.0(11)
N32	9553(7)	638(4)	1407(2)	63.8(12)
C3	1768(5)	5750(3)	951(2)	35.2(8)
C8	1407(6)	5957(4)	316(2)	41.2(9)
C17	3915(6)	10834(4)	605(3)	52.5(12)
C59	950(6)	8959(3)	2766(2)	42.0(10)
C14	2871(5)	8744(3)	696(2)	38.7(9)
C24	6600(6)	2881(4)	2049(2)	44.9(10)
C16	2658(6)	10566(4)	197(2)	44.6(10)
C4	2918(5)	4841(4)	1119(2)	39.5(9)
C19	4998(5)	8207(3)	1558(2)	37.0(9)
C23	7487(5)	3795(3)	1958(2)	36.0(8)
C6	3283(6)	4334(4)	28(2)	44.9(11)
C5	3676(6)	4138(4)	665(2)	45.3(10)
C37	6358(6)	8642(4)	5120(2)	49.2(11)
C39	5612(5)	7425(4)	3547(2)	36.8(9)
C48	1051(6)	4269(4)	4319(2)	42.5(10)
C53	1579(5)	10024(3)	2901(2)	37.2(9)
C58	3335(6)	10086(4)	2936(2)	46.6(10)
C43	-159(5)	4812(4)	3912(2)	39.7(9)
C54	476(6)	10981(4)	2997(2)	45.1(10)
N42	7900(7)	10147(4)	5419(2)	66.2(13)
C49	369(5)	5595(4)	3424(2)	37.5(9)
C33	6222(5)	8126(4)	4028(2)	39.0(9)
N52	-1537(7)	2733(4)	5393(2)	61.3(12)
C9	888(5)	6454(3)	1442(2)	34.6(8)
C27	9794(7)	2596(4)	1497(3)	53.9(12)

C44	-1871(6)	4640(5)	4003(3)	52.2(12)
N	3941(6)	3586(4)	-421(2)	58.6(11)
N62	3522(7)	13007(4)	3264(3)	72.7(15)
C26	8899(7)	1682(4)	1594(2)	47.7(11)
C25	7292(7)	1844(4)	1880(3)	50.1(11)
C29	6738(5)	4915(3)	2151(2)	35.8(9)
N22	1884(6)	11336(4)	-219(2)	63.2(13)
C57	3957(6)	11072(4)	3055(3)	51.4(12)
C36	7320(6)	9495(4)	4965(2)	48.1(11)
C35	7715(7)	9663(4)	4328(3)	53.1(12)
C28	9103(6)	3634(4)	1681(2)	46.8(11)
C34	7168(6)	8996(4)	3870(2)	46.0(10)
C38	5814(6)	7978(4)	4662(2)	47.2(11)
C47	587(6)	3593(4)	4800(2)	46.9(11)
C15	2165(6)	9499(4)	245(2)	44.9(10)
C45	-2338(6)	3957(5)	4483(3)	54.1(12)
C46	-1109(7)	3428(4)	4892(2)	48.6(11)
C56	2855(7)	12039(4)	3146(2)	49.8(11)
C55	1095(7)	11967(4)	3124(3)	51.9(12)

Table S5. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Er-CP. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	$\mathbf{U_{11}}$	$\mathbf{U_{22}}$	$\mathbf{U_{33}}$	$\mathbf{U_{23}}$	$\mathbf{U_{13}}$	$\mathbf{U_{12}}$
Er1	26.67(13)	32.12(13)	33.99(15)	-2.01(9)	0.39(9)	-4.74(9)
Er2	26.86(14)	31.34(13)	34.52(15)	-0.63(9)	1.51(9)	-4.60(9)
O11	31.5(14)	47.5(16)	28.7(14)	-3.4(12)	-1.5(11)	-7.9(12)
O21	48.2(17)	47.9(17)	36.8(16)	8.9(13)	-4.1(13)	-16.3(14)
O31	36.4(15)	38.5(15)	50.1(18)	-6.3(13)	7.5(13)	1.9(12)
O40	47.9(17)	64(2)	36.4(17)	-3.8(15)	-2.4(14)	-21.6(15)
O20	30.7(14)	49.1(17)	45.7(18)	6.8(14)	-6.2(12)	-1.2(12)
O51	35.0(15)	45.1(16)	43.3(17)	9.2(13)	3.9(13)	-9.2(12)
O10	40.3(16)	50.4(17)	38.9(17)	-0.1(13)	6.6(13)	2.2(13)
O	31.0(14)	46.0(15)	33.3(15)	-7.0(12)	3.4(11)	-4.0(12)
O50	47.6(18)	53.9(18)	43.6(18)	14.7(15)	6.7(14)	5.7(14)
O30	49.6(18)	31.0(14)	69(2)	-10.2(14)	3.4(16)	-12.9(13)
O61	67(2)	30.2(15)	86(3)	-8.5(16)	16(2)	4.9(15)
O60	54.4(19)	44.3(17)	54(2)	-5.5(15)	0.9(16)	-19.6(14)
C13	28.3(19)	39(2)	35(2)	1.9(16)	-2.8(16)	-2.0(15)

C7	46(2)	61(3)	36(2)	-9(2)	2.0(19)	-14(2)
C18	44(2)	41(2)	58(3)	1(2)	-14(2)	-9.9(18)
N32	90(3)	42(2)	56(3)	-5(2)	12(2)	8(2)
C3	29.0(19)	43(2)	35(2)	-4.2(17)	2.7(16)	-11.1(16)
C8	40(2)	50(2)	34(2)	-1.3(18)	-0.7(18)	-8.3(18)
C17	53(3)	37(2)	69(3)	5(2)	-5(2)	-12(2)
C59	52(3)	34(2)	41(2)	-8.4(18)	9(2)	-10.1(18)
C14	33(2)	38(2)	46(2)	-0.7(18)	-0.3(18)	-6.9(16)
C24	40(2)	45(2)	51(3)	-10(2)	8(2)	-9.7(18)
C16	35(2)	50(2)	46(3)	10(2)	3.9(19)	0.9(18)
C4	39(2)	41(2)	39(2)	-5.7(18)	2.3(18)	-9.7(17)
C19	34(2)	40(2)	37(2)	-0.9(17)	1.0(17)	-6.3(16)
C23	36(2)	32.6(19)	39(2)	-1.5(16)	3.6(17)	-4.0(15)
C6	44(2)	50(2)	45(3)	-18(2)	13(2)	-21(2)
C5	41(2)	41(2)	55(3)	-8(2)	3(2)	-6.2(18)
C37	49(3)	64(3)	34(2)	-10(2)	-2.5(19)	-4(2)
C39	29.8(19)	47(2)	34(2)	-3.0(17)	-3.1(16)	-1.4(16)
C48	34(2)	48(2)	44(2)	0.5(19)	1.2(18)	0.2(17)
C53	41(2)	32.4(19)	39(2)	-2.5(17)	-0.6(18)	-7.1(16)
C58	46(2)	38(2)	55(3)	-2(2)	4(2)	-3.9(18)
C43	38(2)	40(2)	41(2)	3.6(18)	2.8(18)	-6.4(17)
C54	44(2)	40(2)	51(3)	-4(2)	-2(2)	-1.2(18)
N42	77(3)	67(3)	57(3)	-16(2)	-9(2)	-16(2)
C49	34(2)	42(2)	37(2)	0.5(17)	0.6(17)	-5.9(16)
C33	31(2)	46(2)	39(2)	-6.2(18)	-1.1(17)	-1.4(17)
N52	71(3)	63(3)	51(3)	13(2)	11(2)	-15(2)
C9	27.9(18)	39(2)	38(2)	-2.3(17)	5.4(16)	-9.0(15)
C27	48(3)	48(3)	63(3)	4(2)	20(2)	5(2)
C44	37(2)	63(3)	56(3)	10(2)	-2(2)	-6(2)
N	66(3)	60(3)	53(3)	-19(2)	15(2)	-18(2)
N62	96(4)	50(2)	78(4)	-21(2)	25(3)	-32(2)
C26	63(3)	39(2)	39(2)	-3.0(19)	5(2)	6(2)
C25	59(3)	36(2)	57(3)	-5(2)	2(2)	-12(2)
C29	38(2)	32.2(19)	37(2)	-5.2(16)	-6.9(17)	-0.1(16)
N22	48(2)	72(3)	68(3)	29(2)	-3(2)	-3(2)
C57	46(3)	52(3)	59(3)	-9(2)	7(2)	-16(2)
C36	45(2)	55(3)	44(3)	-13(2)	-11(2)	1(2)
C35	54(3)	56(3)	53(3)	-9(2)	-2(2)	-18(2)
C28	40(2)	40(2)	61(3)	4(2)	13(2)	-5.3(18)
C34	45(2)	55(3)	40(2)	-8(2)	3.3(19)	-11(2)
C38	41(2)	60(3)	41(3)	-3(2)	1.4(19)	-11(2)

C47	46(2)	45(2)	48(3)	7(2)	2(2)	4.5(19)
C15	37(2)	54(3)	43(3)	4(2)	-4.9(19)	-6.9(19)
C45	39(2)	64(3)	60(3)	13(3)	4(2)	-13(2)
C46	56(3)	45(2)	45(3)	3(2)	6(2)	-10(2)
C56	64(3)	43(2)	44(3)	-8(2)	11(2)	-15(2)
C55	60(3)	33(2)	61(3)	-6(2)	6(2)	1(2)

Table S6. Bond Lengths for Er-CP.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Er1	O11	2.310(3)	C59	C53	1.473(6)
Er1	O21	2.270(3)	C14	C15	1.387(6)
Er1	O31	2.243(3)	C24	C23	1.389(6)
Er1	O40	2.352(3)	C24	C25	1.371(6)
Er1	O51	2.281(3)	C16	N22	1.368(6)
Er1	O	2.488(3)	C16	C15	1.398(7)
Er1	O61	2.196(3)	C4	C5	1.388(6)
Er2	O11	2.489(3)	C23	C29	1.487(5)
Er2	O20[1]	2.264(3)	C23	C28	1.395(6)
Er2	O10	2.361(3)	C6	C5	1.397(7)
Er2	O[1]	2.337(3)	C6	N	1.388(6)
Er2	O50	2.230(3)	C37	C36	1.386(8)
Er2	O30[1]	2.234(3)	C37	C38	1.376(7)
Er2	O60	2.288(3)	C39	C33	1.461(6)
O11	C9	1.294(5)	C48	C43	1.390(6)
O21	C19	1.266(5)	C48	C47	1.372(7)
O31	C29	1.258(5)	C53	C58	1.397(6)
O40	C39	1.271(5)	C53	C54	1.390(6)
O20	C19	1.261(5)	C58	C57	1.375(7)
O51	C49	1.266(5)	C43	C49	1.483(6)
O10	C9	1.248(5)	C43	C44	1.400(6)
O	C39	1.293(5)	C54	C55	1.378(7)
O50	C49	1.266(5)	N42	C36	1.373(7)
O30	C29	1.263(5)	C33	C34	1.397(7)
O61	C59	1.263(6)	C33	C38	1.394(7)
O60	C59	1.264(6)	N52	C46	1.408(6)
C13	C18	1.394(6)	C27	C26	1.394(7)
C13	C14	1.396(6)	C27	C28	1.380(7)
C13	C19	1.480(6)	C44	C45	1.376(7)

C7	C8	1.382(6)	N62	C56	1.371(6)
C7	C6	1.387(7)	C26	C25	1.396(7)
C18	C17	1.371(7)	C57	C56	1.397(7)
N32	C26	1.381(6)	C36	C35	1.402(7)
C3	C8	1.390(6)	C35	C34	1.379(7)
C3	C4	1.390(6)	C47	C46	1.385(7)
C3	C9	1.481(6)	C45	C46	1.397(7)
C17	C16	1.389(7)	C56	C55	1.400(7)

[1]-1+X,+Y,+Z

Table S7. Bond Angles for Er-CP.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O11	Er1	O40	146.59(10)	C15	C14	C13	120.6(4)
O11	Er1	O	153.88(10)	C25	C24	C23	121.3(4)
O21	Er1	O11	78.30(10)	C17	C16	C15	117.7(4)
O21	Er1	O40	130.43(11)	N22	C16	C17	120.9(5)
O21	Er1	O51	152.91(11)	N22	C16	C15	121.3(5)
O21	Er1	O	77.44(10)	C5	C4	C3	120.9(4)
O31	Er1	O11	100.23(11)	O21	C19	C13	118.5(4)
O31	Er1	O21	92.70(12)	O20	C19	O21	123.2(4)
O31	Er1	O40	95.42(12)	O20	C19	C13	118.2(4)
O31	Er1	O51	89.92(11)	C24	C23	C29	121.0(4)
O31	Er1	O	90.46(10)	C24	C23	C28	118.2(4)
O40	Er1	O	53.73(10)	C28	C23	C29	120.8(4)
O51	Er1	O11	74.70(10)	C7	C6	C5	118.4(4)
O51	Er1	O40	76.00(11)	C7	C6	N	121.4(5)
O51	Er1	O	129.52(10)	N	C6	C5	120.1(5)
O61	Er1	O11	82.14(13)	C4	C5	C6	120.2(4)
O61	Er1	O21	86.31(14)	C38	C37	C36	121.0(5)
O61	Er1	O31	177.19(13)	O40	C39	Er1	56.6(2)
O61	Er1	O40	83.27(15)	O40	C39	O	117.4(4)
O61	Er1	O51	92.16(13)	O40	C39	C33	121.0(4)
O61	Er1	O	86.76(13)	O	C39	Er1	62.7(2)
O20[1]	Er2	O11	131.94(10)	O	C39	C33	121.5(4)
O20[1]	Er2	O10	78.51(11)	C33	C39	Er1	162.6(3)
O20[1]	Er2	O[1]	74.26(11)	C47	C48	C43	121.3(4)
O20[1]	Er2	O60	85.05(12)	C58	C53	C59	119.7(4)
O10	Er2	O11	53.44(10)	C54	C53	C59	122.1(4)
O[1]	Er2	O11	151.54(10)	C54	C53	C58	118.3(4)
O[1]	Er2	O10	149.71(10)	C57	C58	C53	120.9(4)

O50	Er2	O11	76.91(10)	C48	C43	C49	119.9(4)
O50	Er2	O20[1]	150.45(11)	C48	C43	C44	118.0(4)
O50	Er2	O10	129.78(11)	C44	C43	C49	122.0(4)
O50	Er2	O[1]	76.21(11)	C55	C54	C53	121.0(4)
O50	Er2	O30[1]	85.57(14)	O51	C49	O50	123.5(4)
O50	Er2	O60	98.93(13)	O51	C49	C43	118.1(4)
O30[1]	Er2	O11	81.60(11)	O50	C49	C43	118.4(4)
O30[1]	Er2	O20[1]	92.13(12)	C34	C33	C39	121.5(4)
O30[1]	Er2	O10	80.77(12)	C38	C33	C39	120.9(4)
O30[1]	Er2	O[1]	87.19(11)	C38	C33	C34	117.5(4)
O30[1]	Er2	O60	174.99(13)	O11	C9	Er2	63.3(2)
O60	Er2	O11	97.20(11)	O11	C9	C3	119.9(4)
O60	Er2	O10	94.59(12)	O10	C9	Er2	57.5(2)
O60	Er2	O[1]	96.00(11)	O10	C9	O11	118.4(4)
Er1	O11	Er2	116.36(11)	O10	C9	C3	121.6(4)
C9	O11	Er1	134.7(2)	C3	C9	Er2	161.3(3)
C9	O11	Er2	89.0(2)	C28	C27	C26	120.5(4)
C19	O21	Er1	138.7(3)	C45	C44	C43	120.9(5)
C29	O31	Er1	130.3(3)	N32	C26	C27	121.6(5)
C39	O40	Er1	96.6(3)	N32	C26	C25	119.9(5)
C19	O20	Er2[2]	133.2(3)	C27	C26	C25	118.4(4)
C49	O51	Er1	135.0(3)	C24	C25	C26	120.6(4)
C9	O10	Er2	96.0(3)	O31	C29	O30	122.9(4)
Er2[2]	O	Er1	117.09(11)	O31	C29	C23	119.4(4)
C39	O	Er1	89.7(2)	O30	C29	C23	117.7(4)
C39	O	Er2[2]	139.3(3)	C58	C57	C56	121.1(5)
C49	O50	Er2	142.9(3)	C37	C36	C35	118.0(4)
C29	O30	Er2[2]	145.5(3)	N42	C36	C37	121.4(5)
C59	O61	Er1	158.1(4)	N42	C36	C35	120.6(5)
C59	O60	Er2	121.7(3)	C34	C35	C36	120.9(5)
C18	C13	C14	117.6(4)	C27	C28	C23	120.9(4)
C18	C13	C19	120.5(4)	C35	C34	C33	121.0(5)
C14	C13	C19	121.8(4)	C37	C38	C33	121.6(5)
C8	C7	C6	121.5(4)	C48	C47	C46	120.7(4)
C17	C18	C13	121.8(4)	C14	C15	C16	121.2(4)
C8	C3	C4	118.8(4)	C44	C45	C46	120.4(4)
C8	C3	C9	120.7(4)	C47	C46	N52	119.1(5)
C4	C3	C9	120.4(4)	C47	C46	C45	118.7(4)
C7	C8	C3	120.2(4)	C45	C46	N52	122.1(5)
C18	C17	C16	121.0(4)	N62	C56	C57	119.5(5)
O61	C59	O60	121.1(4)	N62	C56	C55	122.7(5)

O61	C59	C53	118.1(4)	C57	C56	C55	117.8(4)
O60	C59	C53	120.9(4)	C54	C55	C56	120.9(4)

[1]-1+X,+Y,+Z; [2]1+X,+Y,+Z

Table S8. Hydrogen Bonds for Er-CP.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N32	H32B	O60[1]	0.86	2.37	3.195(6)	161.3
N52	H52B	O40[2]	0.86	2.28	3.100(6)	158.8

[1]1+X,-1+Y,+Z; [2]-X,1-Y,1-Z

Table S9. Torsion Angles for Er-CP.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Er1	O11	C9	Er2	-127.4(3)	C14	C13	C18	C17	3.7(7)
Er1	O11	C9	O10	-110.1(4)	C14	C13	C19	O21	-23.2(6)
Er1	O11	C9	C3	73.6(5)	C14	C13	C19	O20	156.2(4)
Er1	O21	C19	O20	48.6(7)	C24	C23	C29	O31	5.3(6)
Er1	O21	C19	C13	-132.0(4)	C24	C23	C29	O30	-172.9(4)
Er1	O31	C29	O30	10.9(6)	C24	C23	C28	C27	0.5(8)
Er1	O31	C29	C23	-167.2(3)	C4	C3	C8	C7	0.8(6)
Er1	O40	C39	O	-16.6(4)	C4	C3	C9	Er2	-90.5(10)
Er1	O40	C39	C33	159.6(3)	C4	C3	C9	O11	4.4(6)
Er1	O51	C49	O50	8.0(7)	C4	C3	C9	O10	-171.7(4)
Er1	O51	C49	C43	-170.9(3)	C19	C13	C18	C17	-179.8(5)
Er1	O	C39	O40	15.6(4)	C19	C13	C14	C15	-176.5(4)
Er1	O	C39	C33	-160.6(4)	C23	C24	C25	C26	-1.8(8)
Er1	O61	C59	O60	66.4(11)	C6	C7	C8	C3	0.8(7)
Er1	O61	C59	C53	-114.7(9)	C37	C36	C35	C34	-0.3(8)
Er1	C39	C33	C34	-93.8(11)	C39	C33	C34	C35	179.0(4)
Er1	C39	C33	C38	83.3(11)	C39	C33	C38	C37	-179.0(4)
Er2	O11	C9	O10	17.3(4)	C48	C43	C49	O51	21.0(6)
Er2	O11	C9	C3	-159.0(3)	C48	C43	C49	O50	-158.0(4)
Er2[1]	O20	C19	O21	9.4(7)	C48	C43	C44	C45	0.2(8)
Er2[1]	O20	C19	C13	-170.0(3)	C48	C47	C46	N52	-179.7(5)
Er2	O10	C9	O11	-18.3(4)	C48	C47	C46	C45	0.5(8)
Er2	O10	C9	C3	157.9(3)	C53	C58	C57	C56	0.3(8)
Er2[1]	O	C39	Er1	-133.8(4)	C53	C54	C55	C56	1.3(8)
Er2[1]	O	C39	O40	-118.3(4)	C58	C53	C54	C55	0.1(7)

Er2[1]	O	C39	C33	65.5(6)	C58	C57	C56	N62	179.9(5)
Er2	O50	C49	O51	34.7(8)	C58	C57	C56	C55	1.1(8)
Er2	O50	C49	C43	-146.4(4)	C43	C48	C47	C46	0.3(8)
Er2[1]	O30	C29	O31	46.7(7)	C43	C44	C45	C46	0.6(9)
Er2[1]	O30	C29	C23	-135.2(4)	C54	C53	C58	C57	-1.0(7)
Er2	O60	C59	O61	-3.0(6)	N42	C36	C35	C34	178.6(5)
Er2	O60	C59	C53	178.2(3)	C49	C43	C44	C45	-176.2(5)
O40	C39	C33	C34	-170.7(4)	C9	C3	C8	C7	-176.5(4)
O40	C39	C33	C38	6.5(6)	C9	C3	C4	C5	176.3(4)
O	C39	C33	C34	5.4(6)	C27	C26	C25	C24	1.3(8)
O	C39	C33	C38	-177.4(4)	C44	C43	C49	O51	-162.7(5)
O61	C59	C53	C58	20.5(7)	C44	C43	C49	O50	18.4(7)
O61	C59	C53	C54	-159.2(5)	C44	C45	C46	N52	179.3(5)
O60	C59	C53	C58	-160.6(4)	C44	C45	C46	C47	-0.9(8)
O60	C59	C53	C54	19.7(7)	N	C6	C5	C4	-175.2(4)
C13	C18	C17	C16	-4.7(8)	N62	C56	C55	C54	179.3(5)
C13	C14	C15	C16	-2.8(7)	C26	C27	C28	C23	-1.0(8)
C7	C6	C5	C4	1.9(6)	C25	C24	C23	C29	-179.1(4)
C18	C13	C14	C15	0.1(7)	C25	C24	C23	C28	0.9(7)
C18	C13	C19	O21	160.3(4)	C29	C23	C28	C27	-179.6(5)
C18	C13	C19	O20	-20.2(6)	N22	C16	C15	C14	-175.7(5)
C18	C17	C16	N22	179.4(5)	C57	C56	C55	C54	-1.9(8)
C18	C17	C16	C15	1.9(8)	C36	C37	C38	C33	0.8(8)
N32	C26	C25	C24	-177.7(5)	C36	C35	C34	C33	-0.8(8)
C3	C4	C5	C6	-0.4(6)	C28	C23	C29	O31	-174.7(4)
C8	C7	C6	C5	-2.1(7)	C28	C23	C29	O30	7.2(6)
C8	C7	C6	N	174.9(4)	C28	C27	C26	N32	179.0(5)
C8	C3	C4	C5	-1.0(6)	C28	C27	C26	C25	0.0(8)
C8	C3	C9	Er2	86.7(10)	C34	C33	C38	C37	-1.8(7)
C8	C3	C9	O11	-178.4(4)	C38	C37	C36	N42	-178.5(5)
C8	C3	C9	O10	5.4(6)	C38	C37	C36	C35	0.3(7)
C17	C16	C15	C14	1.8(7)	C38	C33	C34	C35	1.8(7)
C59	C53	C58	C57	179.3(5)	C47	C48	C43	C49	175.9(4)
C59	C53	C54	C55	179.9(5)	C47	C48	C43	C44	-0.6(7)

[1]1+X,+Y,+Z

Table S10. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Er-CP.

Atom	***x***	***y***	***z***	**U(eq)**
H7	1922.99	5411.75	-558.75	57

H18	5576	10251.83	1271.96	56
H32A	10648.45	616.07	1381.43	77
H32B	9296.28	147.76	1678.74	77
H8	650.81	6566.49	194.84	49
H17	4241.73	11544.59	592	63
H14	2489.03	8049.39	731.25	46
H24	5513.97	2975.06	2227.79	54
H4	3183.43	4700.65	1541.92	47
H5	4447.45	3535.71	784.9	54
H37	6075.59	8517.28	5539.34	59
H48	2196.27	4365.59	4263.75	51
H58	4093.21	9452.17	2879.56	56
H54	-697.22	10955.18	2975.71	54
H42A	7885.41	10825.21	5284.55	79
H42B	7246.29	10139.22	5748.75	79
H52A	-703.39	2631.75	5657.11	74
H52B	-2436.7	3035.51	5583.39	74
H27	10865.84	2505.71	1307.51	65
H44	-2702.83	4992.39	3736.21	63
HA	3837.11	3887.68	-791.25	70
HB	5008.97	3417.62	-337.66	70
H62A	2849.22	13555.45	3106.99	87
H62B	3569.26	13076.17	3668.8	87
H25	6686.16	1241.86	1956.84	60
H22A	2603.3	11784.81	-331.52	76
H22B	1569.41	11002.41	-544.73	76
H57	5130.91	11095.68	3074.45	62
H35	8354.56	10231.89	4211.9	64
H28	9721.97	4233.86	1618.59	56
H34	7432.37	9128.21	3449.43	55
H38	5159.05	7417.49	4778.65	57
H47	1419.67	3241.77	5067.13	56
H15	1348.56	9291.7	-30.37	54
H45	-3480	3847.06	4534.78	65
H55	333.77	12594.1	3195.48	62

Crystal details of Ho-CP

Table S11. Crystal data and structure refinement for Ho-CP.

Identification code	Ho-CP, Deposition number 2180441
Empirical formula	$C_{42}H_{36}Ho_2N_6O_{12}$
Formula weight	1146.63
Temperature/K	297(2)
Crystal system	triclinic
Space group	*P*-1
a/Å	7.88458(12)
b/Å	12.1481(2)
c/Å	21.2468(3)
α/°	88.9472(13)
β/°	89.6458(12)
γ/°	83.3501(13)
Volume/Å^3	2021.02(5)
Z	2
ρ_{calc}g/cm^3	1.884
μ/mm^{-1}	7.708
F(000)	1120.0
Crystal size/mm^3	0.107 × 0.077 × 0.043
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.328 to 155.224
Index ranges	-9 ≤ h ≤ 8, -15 ≤ k ≤ 14, -26 ≤ l ≤ 24
Reflections collected	22328
Independent reflections	7819 [R_{int} = 0.0338, R_{sigma} = 0.0358]
Data/restraints/parameters	7819/0/570
Goodness-of-fit on F^2	1.060
Final R indexes [I>=2σ (I)]	R_1 = 0.0282, wR_2 = 0.0702
Final R indexes [all data]	R_1 = 0.0327, wR_2 = 0.0721
Largest diff. peak/hole / e Å^{-3}	0.43/-0.54

Table S12. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Ho-CP. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Ho1	6540.8(2)	2705.4(2)	2675.1(2)	27.87(7)
Ho2	1457.3(2)	3448.2(2)	2344.4(2)	28.05(7)
O11	5608(3)	1030(2)	2439.7(11)	50.7(6)
O21	5769(3)	3687(2)	1799.4(10)	47.9(5)
O31	3743(2)	3750.8(17)	2978.6(8)	32.6(4)

O41	806(3)	2592.0(19)	3259.7(10)	40.9(5)
O51	8994(2)	2465.5(18)	2033.3(9)	34.3(4)
N32	1054(4)	6412(3)	5423.8(15)	58.1(8)
O50	457(3)	3246(2)	1313.5(10)	48.2(6)
O61	-326(3)	4978.8(18)	2556.2(10)	41.2(5)
O30	5289(3)	2794.4(19)	3691.4(9)	40.2(5)
O10	3133(4)	1916(2)	2142.5(15)	66.6(7)
O20	3087(2)	4493.2(18)	1735.6(10)	39.0(5)
C49	-591(3)	2565(3)	1449.6(13)	34.3(6)
C27	1330(4)	5859(3)	4339.2(16)	43.1(7)
O40	8547(2)	1646.6(19)	3253.6(10)	39.8(5)
N62	-4579(5)	9359(3)	3596.0(16)	63.7(9)
C53	-2484(3)	6196(2)	3039.0(14)	34.6(6)
C25	2850(4)	4736(3)	5137.7(14)	46.0(8)
C46	-2319(4)	504(3)	33.3(16)	45.9(7)
C36	2350(4)	-561(3)	4807.8(15)	41.6(7)
C14	6867(4)	5359(3)	987.8(17)	47.4(8)
C58	-1595(4)	7119(3)	2953.5(15)	40.5(7)
C57	-2307(5)	8159(3)	3120.2(16)	47.8(8)
N42	3115(4)	-1337(3)	5224.2(16)	63.0(9)
C47	-2708(5)	330(3)	667.5(17)	51.9(8)
C13	5165(4)	5191(3)	1085.9(13)	35.4(6)
C18	3953(4)	5734(3)	681.0(15)	40.9(7)
C28	2087(4)	5164(3)	3888.8(14)	37.0(6)
C48	-2157(4)	1001(3)	1125.7(15)	43.2(7)
C17	4412(4)	6408(3)	198.8(16)	45.4(7)
C16	6105(5)	6575(3)	101.5(16)	46.8(7)
C33	858(3)	978(2)	3905.5(13)	31.8(6)
C44	-797(4)	2019(3)	336.3(14)	44.1(7)
C24	3599(4)	4040(3)	4685.3(13)	38.5(6)
C55	-4792(5)	7398(3)	3504.4(18)	52.1(8)
C38	337(4)	-67(3)	3976.3(16)	45.6(8)
C15	7329(4)	6048(3)	510.3(18)	54.5(9)
C39	23(3)	1787(3)	3441.0(13)	33.4(6)
C37	1096(4)	-833(3)	4398.5(18)	49.4(8)
N12	1463(5)	-2995(3)	1725(2)	69.9(10)
C7	1053(4)	-1064(3)	1949.0(17)	49.7(8)
C3	3454(4)	-32(2)	2100.8(13)	35.8(6)
C4	4531(4)	-996(3)	2002.1(15)	42.0(7)
C5	3889(5)	-1973(3)	1871.4(17)	49.0(8)
N52	-2913(5)	-132(3)	-421.8(16)	63.9(9)

C23	3242(3)	4250(2)	4048.5(13)	32.3(6)
O60	7495(3)	4270.2(18)	3000.9(12)	47.3(5)
N22	6521(4)	7271(3)	-392.1(15)	59.5(8)
C8	1695(4)	-80(3)	2070.5(16)	43.5(7)
C43	-1212(3)	1868(3)	969.3(13)	36.6(6)
C29	4114(3)	3552(2)	3562.5(12)	31.4(6)
C35	2841(4)	507(3)	4757.1(14)	41.4(7)
C54	-4090(4)	6366(3)	3315.6(16)	45.0(7)
C6	2139(5)	-2028(3)	1855.5(16)	47.0(8)
C26	1716(4)	5664(3)	4976.4(15)	41.3(7)
C56	-3917(5)	8317(3)	3408.0(15)	45.3(7)
C34	2143(3)	1252(3)	4302.9(14)	35.1(6)
C19	4639(4)	4415(3)	1576.8(13)	34.4(6)
C59	-1733(3)	5093(2)	2849.6(13)	34.2(6)
C9	4103(4)	1024(3)	2239.2(14)	41.3(7)
C45	-1350(4)	1356(3)	-120.3(15)	48.5(8)

Table S13. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Ho-CP. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	$\mathbf{U_{11}}$	$\mathbf{U_{22}}$	$\mathbf{U_{33}}$	$\mathbf{U_{23}}$	$\mathbf{U_{13}}$	$\mathbf{U_{12}}$
Ho1	24.91(10)	28.95(11)	29.57(11)	1.68(8)	1.26(7)	-2.77(8)
Ho2	25.09(10)	30.03(12)	29.12(11)	-0.02(8)	0.33(7)	-3.59(8)
O11	60.0(14)	47.5(14)	49.3(13)	-6.6(11)	2.5(11)	-25.0(12)
O21	44.3(11)	53.8(14)	41.0(11)	19.1(10)	5.6(9)	10.7(10)
O31	27.6(8)	44.1(12)	26.9(9)	-2.8(8)	1.0(7)	-7.5(8)
O41	44.0(11)	44.0(12)	36.0(10)	11.3(9)	-4.3(9)	-12.2(10)
O51	30.1(9)	43.3(12)	29.1(9)	-4.2(8)	1.4(7)	-2.1(8)
N32	65.3(18)	60(2)	52.3(17)	-20.4(15)	18.1(15)	-16.8(16)
O50	52.1(12)	65.6(16)	31.6(10)	-0.7(10)	-1.1(9)	-26.6(12)
O61	36.6(10)	37.5(12)	48.0(12)	-5.6(9)	5.5(9)	2.3(9)
O30	40.0(10)	46.5(13)	32.0(10)	2.6(9)	5.2(8)	3.4(9)
O10	77.5(17)	28.9(13)	90(2)	-7.1(13)	24.8(15)	7.0(12)
O20	32.1(9)	43.0(12)	42.2(11)	12.0(9)	1.7(8)	-7.9(9)
C49	30.0(12)	42.7(17)	30.2(13)	-1.3(12)	-0.7(11)	-3.6(12)
C27	41.1(15)	40.4(18)	48.2(17)	-7.5(14)	6.1(13)	-5.4(13)
O40	30.7(9)	46.9(13)	41.3(11)	11.9(9)	-7.1(8)	-3.3(9)
N62	91(2)	39.2(17)	55.9(18)	-2.9(14)	11.4(17)	14.1(16)
C53	34.5(13)	31.4(15)	38.2(14)	-2.1(12)	0.5(11)	-5.5(11)
C25	49.0(17)	61(2)	30.4(14)	-8.3(14)	4.3(13)	-15.2(16)

C46	43.6(16)	52(2)	41.9(16)	-10.6(14)	-9.1(13)	-0.4(14)
C36	33.0(14)	45.9(18)	43.1(16)	13.5(14)	5.0(12)	5.0(13)
C14	35.0(15)	54(2)	52.8(19)	13.5(16)	-2.0(14)	-6.4(14)
C58	38.3(14)	37.7(17)	46.3(17)	-4.4(13)	5.1(13)	-7.9(13)
C57	58.4(19)	35.4(17)	51.0(18)	-5.6(14)	5.0(15)	-11.1(15)
N42	51.5(16)	70(2)	64(2)	34.2(18)	-2.0(15)	-0.2(16)
C47	56.5(19)	55(2)	47.0(18)	-8.7(16)	-2.2(15)	-17.5(17)
C13	36.7(14)	35.5(16)	33.5(14)	2.2(12)	4.7(11)	-2.4(12)
C18	35.7(14)	42.4(17)	42.5(16)	5.8(13)	4.3(12)	2.6(13)
C28	36.5(14)	40.7(17)	34.6(14)	-3.4(12)	1.0(11)	-8.1(12)
C48	43.3(16)	53(2)	34.1(15)	-3.9(13)	1.4(13)	-8.8(14)
C17	48.4(17)	42.2(18)	43.3(17)	7.6(14)	2.0(14)	2.7(14)
C16	57.2(18)	41.7(18)	42.1(16)	6.3(14)	6.7(14)	-10.0(15)
C33	28.3(12)	33.8(15)	32.6(13)	2.5(11)	0.1(10)	-1.9(11)
C44	42.3(15)	55(2)	35.9(15)	-0.5(14)	-1.0(13)	-9.8(15)
C24	36.0(14)	48.0(18)	32.2(14)	-3.8(12)	0.3(12)	-6.9(13)
C55	52.0(18)	43.4(19)	57(2)	3.5(16)	21.9(16)	7.1(15)
C38	45.6(16)	39.0(17)	53.4(18)	3.5(14)	-15.4(14)	-10.1(14)
C15	41.4(16)	66(2)	58(2)	14.6(18)	3.9(15)	-16.6(17)
C39	32.3(13)	37.4(16)	30.1(13)	0.0(11)	2.7(11)	-3.1(12)
C37	52.2(18)	32.7(17)	64(2)	8.0(15)	-5.0(16)	-8.4(14)
N12	80(2)	46(2)	89(3)	-15.1(18)	24(2)	-28.2(19)
C7	44.4(16)	49(2)	57(2)	-3.3(16)	5.8(15)	-11.9(15)
C3	43.1(15)	29.5(15)	34.5(14)	-2.8(11)	3.0(12)	-2.4(12)
C4	42.3(15)	37.8(17)	44.9(17)	-2.6(13)	-2.7(13)	0.4(13)
C5	54.1(18)	31.7(16)	60(2)	-5.7(15)	8.5(16)	1.6(14)
N52	79(2)	65(2)	49.4(17)	-14.7(16)	-8.7(17)	-14.0(18)
C23	28.3(12)	39.2(16)	31.0(13)	-3.6(11)	2.9(10)	-10.7(11)
O60	48.0(12)	29.2(11)	66.1(15)	-6.9(10)	4.1(11)	-9.9(10)
N22	69.9(19)	56(2)	52.7(17)	16.8(15)	8.1(15)	-12.2(16)
C8	42.9(16)	34.8(16)	51.9(18)	-2.6(14)	4.0(14)	-0.9(13)
C43	30.2(13)	47.6(18)	31.7(14)	-5.2(12)	-2.5(11)	-2.3(12)
C29	25.3(11)	40.3(16)	30.3(13)	0.7(11)	2.3(10)	-11.1(11)
C35	29.8(13)	54(2)	39.9(16)	4.8(14)	-5.5(12)	-4.3(13)
C54	40.7(15)	36.9(17)	57.4(19)	5.0(14)	11.1(14)	-5.7(13)
C6	62(2)	37.8(18)	43.2(17)	-8.8(13)	10.7(15)	-13.3(16)
C26	41.3(15)	44.1(18)	41.8(16)	-13.6(13)	13.6(13)	-17.3(14)
C56	62.7(19)	33.8(16)	36.3(15)	-2.1(12)	5.2(14)	7.1(14)
C34	32.3(13)	34.7(15)	38.8(15)	2.3(12)	-0.1(11)	-6.4(11)
C19	35.8(13)	34.8(15)	32.8(13)	2.1(11)	-0.5(11)	-4.6(12)
C59	31.7(13)	33.9(15)	37.3(14)	-4.9(12)	-2.9(11)	-4.1(11)

C9	53.9(18)	35.0(16)	36.6(15)	-5.7(12)	12.9(13)	-11.6(14)
C45	50.3(17)	62(2)	32.5(15)	-7.0(15)	-0.1(13)	-2.7(16)

Table S14. Bond Lengths for Ho-CP.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ho1	O11	2.307(2)	C46	C45	1.389(5)
Ho1	O21	2.240(2)	C36	N42	1.370(4)
Ho1	O31	2.502(2)	C36	C37	1.392(5)
Ho1	O51	2.3534(19)	C36	C35	1.399(5)
Ho1	O30	2.368(2)	C14	C13	1.394(4)
Ho1	O40	2.2722(19)	C14	C15	1.377(5)
Ho1	O60	2.246(2)	C58	C57	1.373(5)
Ho2	O31	2.3238(16)	C57	C56	1.400(5)
Ho2	O41	2.273(2)	C47	C48	1.385(5)
Ho2	O51[1]	2.4928(18)	C13	C18	1.390(4)
Ho2	O50	2.359(2)	C13	C19	1.483(4)
Ho2	O61	2.248(2)	C18	C17	1.372(4)
Ho2	O10	2.202(3)	C28	C23	1.391(4)
Ho2	O20	2.2873(19)	C48	C43	1.393(4)
O11	C9	1.265(4)	C17	C16	1.387(5)
O21	C19	1.267(4)	C16	C15	1.393(5)
O31	C29	1.289(3)	C16	N22	1.397(4)
O41	C39	1.268(3)	C33	C38	1.384(4)
O51	C49[2]	1.288(3)	C33	C39	1.482(4)
N32	C26	1.385(4)	C33	C34	1.396(4)
O50	C49	1.264(4)	C44	C43	1.396(4)
O61	C59	1.264(4)	C44	C45	1.377(5)
O30	C29	1.255(4)	C24	C23	1.397(4)
O10	C9	1.266(4)	C55	C54	1.376(5)
O20	C19	1.261(4)	C55	C56	1.390(5)
C49	C43	1.460(4)	C38	C37	1.370(5)
C27	C28	1.376(5)	N12	C6	1.378(4)
C27	C26	1.399(5)	C7	C8	1.380(5)
O40	C39[2]	1.263(3)	C7	C6	1.385(5)
N62	C56	1.377(5)	C3	C4	1.383(4)
C53	C58	1.398(4)	C3	C8	1.397(4)
C53	C54	1.388(4)	C3	C9	1.471(4)
C53	C59	1.463(4)	C4	C5	1.377(5)

C25	C24	1.377(5)	C5	C6	1.390(5)
C25	C26	1.394(5)	C23	C29	1.465(4)
C46	C47	1.398(5)	O60	C59[2]	1.265(4)
C46	N52	1.367(4)	C35	C34	1.383(4)

[1]-1+X,+Y,+Z; [2]1+X,+Y,+Z

Table S15. Bond Angles for Ho-CP.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O11	Ho1	O31	99.03(8)	N42	C36	C37	120.5(3)
O11	Ho1	O51	95.54(8)	N42	C36	C35	121.8(3)
O11	Ho1	O30	94.61(8)	C37	C36	C35	117.6(3)
O21	Ho1	O11	100.47(9)	C15	C14	C13	121.1(3)
O21	Ho1	O31	77.05(7)	C57	C58	C53	121.2(3)
O21	Ho1	O51	76.13(7)	C58	C57	C56	120.8(3)
O21	Ho1	O30	129.66(8)	C48	C47	C46	120.6(3)
O21	Ho1	O40	150.40(8)	C14	C13	C19	122.4(3)
O21	Ho1	O60	85.08(9)	C18	C13	C14	117.7(3)
O51	Ho1	O31	151.35(7)	C18	C13	C19	119.9(3)
O51	Ho1	O30	149.64(7)	C17	C18	C13	121.3(3)
O30	Ho1	O31	53.15(6)	C27	C28	C23	121.6(3)
O40	Ho1	O11	84.18(9)	C47	C48	C43	121.2(3)
O40	Ho1	O31	131.51(7)	C18	C17	C16	121.0(3)
O40	Ho1	O51	74.32(7)	C17	C16	C15	118.2(3)
O40	Ho1	O30	78.37(8)	C17	C16	N22	119.3(3)
O60	Ho1	O11	174.37(9)	C15	C16	N22	122.5(3)
O60	Ho1	O31	81.22(7)	C38	C33	C39	120.7(2)
O60	Ho1	O51	86.65(8)	C38	C33	C34	117.6(3)
O60	Ho1	O30	81.00(8)	C34	C33	C39	121.6(3)
O60	Ho1	O40	91.44(8)	C45	C44	C43	121.1(3)
O31	Ho2	O51[1]	154.26(7)	C25	C24	C23	120.6(3)
O31	Ho2	O50	147.03(7)	C54	C55	C56	120.5(3)
O41	Ho2	O31	78.22(7)	C37	C38	C33	121.9(3)
O41	Ho2	O51[1]	77.69(7)	C14	C15	C16	120.6(3)
O41	Ho2	O50	130.18(7)	O41	C39	C33	118.8(2)
O41	Ho2	O20	153.12(7)	O40[1]	C39	O41	123.3(3)
O50	Ho2	O51[1]	53.27(7)	O40[1]	C39	C33	117.9(2)
O61	Ho2	O31	99.63(7)	C38	C37	C36	120.9(3)
O61	Ho2	O41	92.67(8)	C8	C7	C6	120.7(3)
O61	Ho2	O51[1]	90.43(7)	C4	C3	C8	118.1(3)
O61	Ho2	O50	95.66(9)	C4	C3	C9	122.2(3)

O61	Ho2	O20	89.74(8)	C8	C3	C9	119.7(3)
O10	Ho2	O31	81.63(10)	C5	C4	C3	121.0(3)
O10	Ho2	O41	86.18(10)	C4	C5	C6	120.9(3)
O10	Ho2	O51[1]	87.84(9)	C28	C23	C24	118.1(3)
O10	Ho2	O50	83.95(11)	C28	C23	C29	121.1(3)
O10	Ho2	O61	178.10(9)	C24	C23	C29	120.8(3)
O10	Ho2	O20	91.96(10)	C59[2]	O60	Ho1	146.2(2)
O20	Ho2	O31	74.98(7)	C7	C8	C3	120.8(3)
O20	Ho2	O51[1]	129.08(7)	C48	C43	C49	121.7(3)
O20	Ho2	O50	76.06(7)	C48	C43	C44	117.7(3)
C9	O11	Ho1	118.8(2)	C44	C43	C49	120.5(3)
C19	O21	Ho1	142.8(2)	O31	C29	Ho1	63.27(14)
Ho2	O31	Ho1	114.86(8)	O31	C29	C23	119.7(3)
C29	O31	Ho1	89.34(16)	O30	C29	Ho1	57.16(14)
C29	O31	Ho2	134.27(16)	O30	C29	O31	118.1(3)
C39	O41	Ho2	138.68(18)	O30	C29	C23	122.1(2)
Ho1	O51	Ho2[2]	117.05(8)	C23	C29	Ho1	161.57(17)
C49[2]	O51	Ho1	139.08(17)	C34	C35	C36	121.0(3)
C49[2]	O51	Ho2[2]	90.13(15)	C55	C54	C53	121.9(3)
C49	O50	Ho2	96.98(17)	N12	C6	C7	119.5(3)
C59	O61	Ho2	130.6(2)	N12	C6	C5	122.1(4)
C29	O30	Ho1	96.39(16)	C7	C6	C5	118.3(3)
C9	O10	Ho2	159.4(3)	N32	C26	C27	120.2(3)
C19	O20	Ho2	134.88(19)	N32	C26	C25	121.6(3)
O51[1]	C49	Ho2	62.57(13)	C25	C26	C27	118.1(3)
O51[1]	C49	C43	121.5(3)	N62	C56	C57	120.0(3)
O50	C49	Ho2	56.49(14)	N62	C56	C55	121.9(3)
O50	C49	O51[1]	117.3(2)	C55	C56	C57	118.2(3)
O50	C49	C43	121.1(3)	C35	C34	C33	120.8(3)
C43	C49	Ho2	163.1(2)	O21	C19	C13	118.0(3)
C28	C27	C26	120.4(3)	O20	C19	O21	123.7(3)
C39[2]	O40	Ho1	133.50(19)	O20	C19	C13	118.3(3)
C58	C53	C59	121.0(3)	O61	C59	C53	120.0(3)
C54	C53	C58	117.4(3)	O61	C59	O60[1]	121.7(3)
C54	C53	C59	121.6(3)	O60[1]	C59	C53	118.3(3)
C24	C25	C26	121.3(3)	O11	C9	O10	121.4(3)
N52	C46	C47	120.6(3)	O11	C9	C3	120.1(3)
N52	C46	C45	121.2(3)	O10	C9	C3	118.5(3)
C45	C46	C47	118.1(3)	C44	C45	C46	121.2(3)

[1]-1+X,+Y,+Z; [2]1+X,+Y,+Z

Table S16. Hydrogen Bonds for Ho-CP.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N62	H62A	O11[1]	0.87	2.35	3.172(4)	157.5
N12	H12A	O20[2]	0.82	2.47	3.169(5)	144.2
N22	H22A	O50[3]	0.87	2.27	3.090(4)	157.1

[1]-1+X,1+Y,+Z; [2]+X,-1+Y,+Z; [3]1-X,1-Y,-Z

Table S17. Torsion Angles for Ho-CP.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ho1	O11	C9	O10	2.9(4)	C28	C23	C29	Ho1	90.5(6)
Ho1	O11	C9	C3	-178.4(2)	C28	C23	C29	O31	-3.6(4)
Ho1	O21	C19	O20	-34.0(5)	C28	C23	C29	O30	172.4(2)
Ho1	O21	C19	C13	148.2(3)	C17	C16	C15	C14	1.6(6)
Ho1	O31	C29	O30	-16.9(2)	C33	C38	C37	C36	4.7(6)
Ho1	O31	C29	C23	159.3(2)	C24	C25	C26	N32	-175.2(3)
Ho1	O30	C29	O31	18.0(2)	C24	C25	C26	C27	1.3(4)
Ho1	O30	C29	C23	-158.1(2)	C24	C23	C29	Ho1	-87.0(7)
Ho2	O31	C29	Ho1	125.2(2)	C24	C23	C29	O31	178.9(2)
Ho2	O31	C29	O30	108.3(3)	C24	C23	C29	O30	-5.1(4)
Ho2	O31	C29	C23	-75.5(3)	C38	C33	C39	O41	-160.3(3)
Ho2	O41	C39	O40[1]	-48.7(5)	C38	C33	C39	O40[1]	20.8(4)
Ho2	O41	C39	C33	132.5(3)	C38	C33	C34	C35	-1.1(5)
Ho2	O50	C49	O51[1]	15.7(3)	C15	C14	C13	C18	0.7(6)
Ho2	O50	C49	C43	-160.2(2)	C15	C14	C13	C19	177.1(3)
Ho2	O61	C59	C53	167.24(19)	C39	C33	C38	C37	179.5(3)
Ho2	O61	C59	O60[1]	-11.0(4)	C39	C33	C34	C35	176.4(3)
Ho2	O10	C9	O11	-72.3(8)	C37	C36	C35	C34	-2.0(5)
Ho2	O10	C9	C3	108.9(7)	C3	C4	C5	C6	-2.2(5)
Ho2	O20	C19	O21	-7.1(5)	C4	C3	C8	C7	0.4(5)
Ho2	O20	C19	C13	170.68(19)	C4	C3	C9	O11	-19.3(5)
Ho2	C49	C43	C48	93.5(7)	C4	C3	C9	O10	159.5(3)
Ho2	C49	C43	C44	-83.2(8)	C4	C5	C6	N12	179.9(4)
O51[1]	C49	C43	C48	-5.6(5)	C4	C5	C6	C7	2.6(5)
O51[1]	C49	C43	C44	177.6(3)	N52	C46	C47	C48	-177.7(4)
O50	C49	C43	C48	170.1(3)	N52	C46	C45	C44	178.0(4)
O50	C49	C43	C44	-6.6(5)	N22	C16	C15	C14	-179.4(4)
C27	C28	C23	C24	1.0(4)	C8	C7	C6	N12	-179.0(4)
C27	C28	C23	C29	-176.5(3)	C8	C7	C6	C5	-1.6(5)
C53	C58	C57	C56	2.9(5)	C8	C3	C4	C5	0.6(5)

C25	C24	C23	C28	-1.3(4)	C8	C3	C9	O11	160.2(3)
C25	C24	C23	C29	176.2(3)	C8	C3	C9	O10	-21.0(5)
C46	C47	C48	C43	0.3(6)	C43	C44	C45	C46	-0.9(5)
C36	C35	C34	C33	3.6(5)	C35	C36	C37	C38	-2.1(5)
C14	C13	C18	C17	0.4(5)	C54	C53	C58	C57	-1.8(5)
C14	C13	C19	O21	-18.2(5)	C54	C53	C59	O61	174.6(3)
C14	C13	C19	O20	163.8(3)	C54	C53	C59	O60[1]	-7.1(4)
C58	C53	C54	C55	-0.4(5)	C54	C55	C56	N62	-179.5(3)
C58	C53	C59	O61	-6.1(4)	C54	C55	C56	C57	-0.5(5)
C58	C53	C59	O60[1]	172.2(3)	C6	C7	C8	C3	0.1(5)
C58	C57	C56	N62	177.3(3)	C26	C27	C28	C23	0.4(4)
C58	C57	C56	C55	-1.7(5)	C26	C25	C24	C23	0.1(4)
N42	C36	C37	C38	-179.3(4)	C56	C55	C54	C53	1.6(6)
N42	C36	C35	C34	175.2(3)	C34	C33	C38	C37	-3.1(5)
C47	C46	C45	C44	-0.5(5)	C34	C33	C39	O41	22.3(4)
C47	C48	C43	C49	-178.6(3)	C34	C33	C39	O40[1]	-156.5(3)
C47	C48	C43	C44	-1.8(5)	C19	C13	C18	C17	-176.2(3)
C13	C14	C15	C16	-1.7(6)	C59	C53	C58	C57	178.8(3)
C13	C18	C17	C16	-0.4(6)	C59	C53	C54	C55	178.9(3)
C18	C13	C19	O21	158.1(3)	C9	C3	C4	C5	-179.8(3)
C18	C13	C19	O20	-19.8(4)	C9	C3	C8	C7	-179.2(3)
C18	C17	C16	C15	-0.5(6)	C45	C46	C47	C48	0.9(6)
C18	C17	C16	N22	-179.6(3)	C45	C44	C43	C49	178.9(3)
C28	C27	C26	N32	175.0(3)	C45	C44	C43	C48	2.1(5)
C28	C27	C26	C25	-1.5(4)					

[1]-1+X,+Y,+Z

Table S18. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Ho-CP.

Atom	***x***	***y***	***z***	**U(eq)**
H32A	-15.41	6613.91	5349.5	70
H32B	1150.86	6090.67	5789.53	70
H27	555.99	6462.56	4219.75	52
H62A	-4247.98	9838.54	3328.58	76
H62B	-5684.25	9422.63	3597.7	76
H25	3105.17	4584.37	5559.46	55
H14	7705.44	4999.68	1249.24	57
H58	-502.84	7027.61	2780.6	49
H57	-1712.64	8765.54	3040.99	57
H42A	3396.99	-1014.45	5563.1	76

H42B	2423.74	-1817.76	5327.98	76
H47	-3342.14	-241.68	782.74	62
H18	2807.83	5639.29	737.99	49
H28	1820.94	5309.07	3467.31	44
H48	-2422.75	870.72	1545.54	52
H17	3575.42	6756.88	-66.87	54
H44	-135.61	2576.88	221.08	53
H24	4349.62	3425.29	4804.75	46
H55	-5858.88	7481.16	3697.95	62
H38	-554.98	-253.77	3730.32	55
H15	8467.85	6163.13	460.28	65
H37	770.5	-1544.54	4411.81	59
H12A	2083.92	-3524.92	1872.06	105
H7	-122.34	-1079.69	1929.6	60
H4	5706.24	-983.4	2024.25	50
H5	4637.58	-2605.56	1792.54	59
H52A	-2284.52	-89.89	-751.14	77
H52B	-2824.28	-809.73	-285.63	77
H22A	7485.84	7001.7	-561.52	71
H22B	5739.24	7314.4	-682.82	71
H8	947.11	558.65	2133.04	52
H35	3648.95	719.75	5033.1	50
H54	-4709.5	5765.8	3375.03	54
H34	2534.1	1942.94	4261.61	42
H45	-1070.41	1481.27	-539.37	58
H12B	290(70)	-2990(50)	1730(20)	88(16)

Section 3: Photocatalytic studies

^{1}H-NMR analysis of the photocatalytic reactions over Ln-CPs photocatalyst.

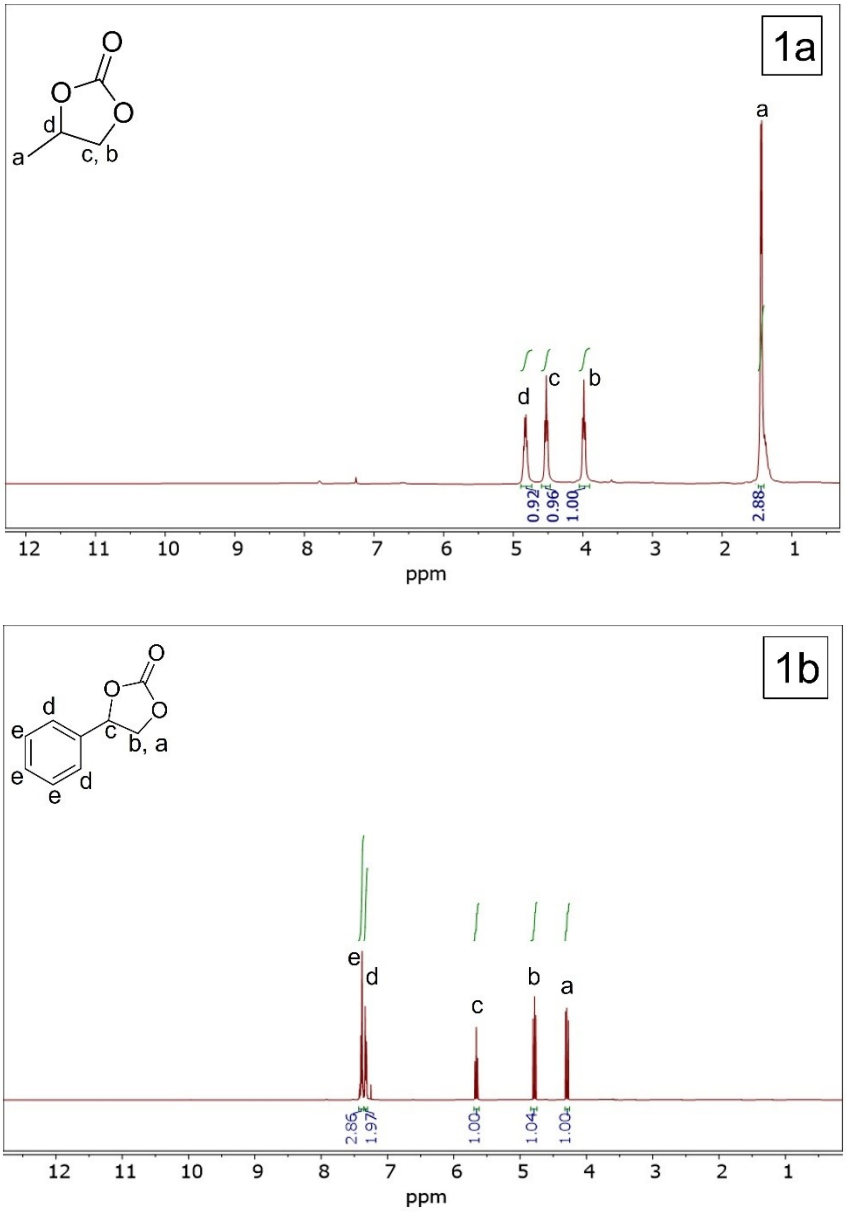

Figure S10. ^{1}H-NMR spectrum with assigned peaks of cyclic carbonates produced using Ln-CPs . Both Ho-CP and Er-CP show full product conversions (continued).

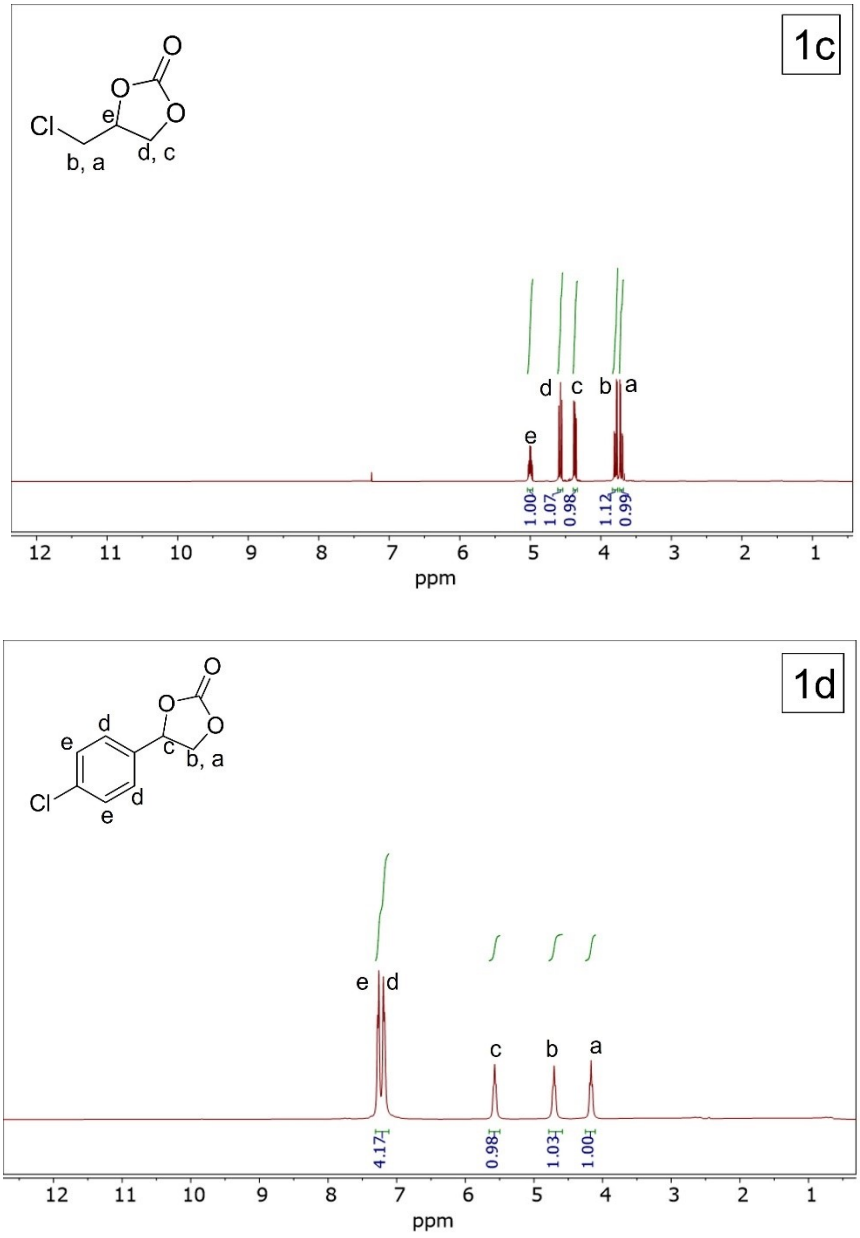

Figure S10. ^{1}H-NMR spectrum with assigned peaks of cyclic carbonates produced using Ln-CPs. Both Ho-CP and Er-CP show full product conversions (continued).

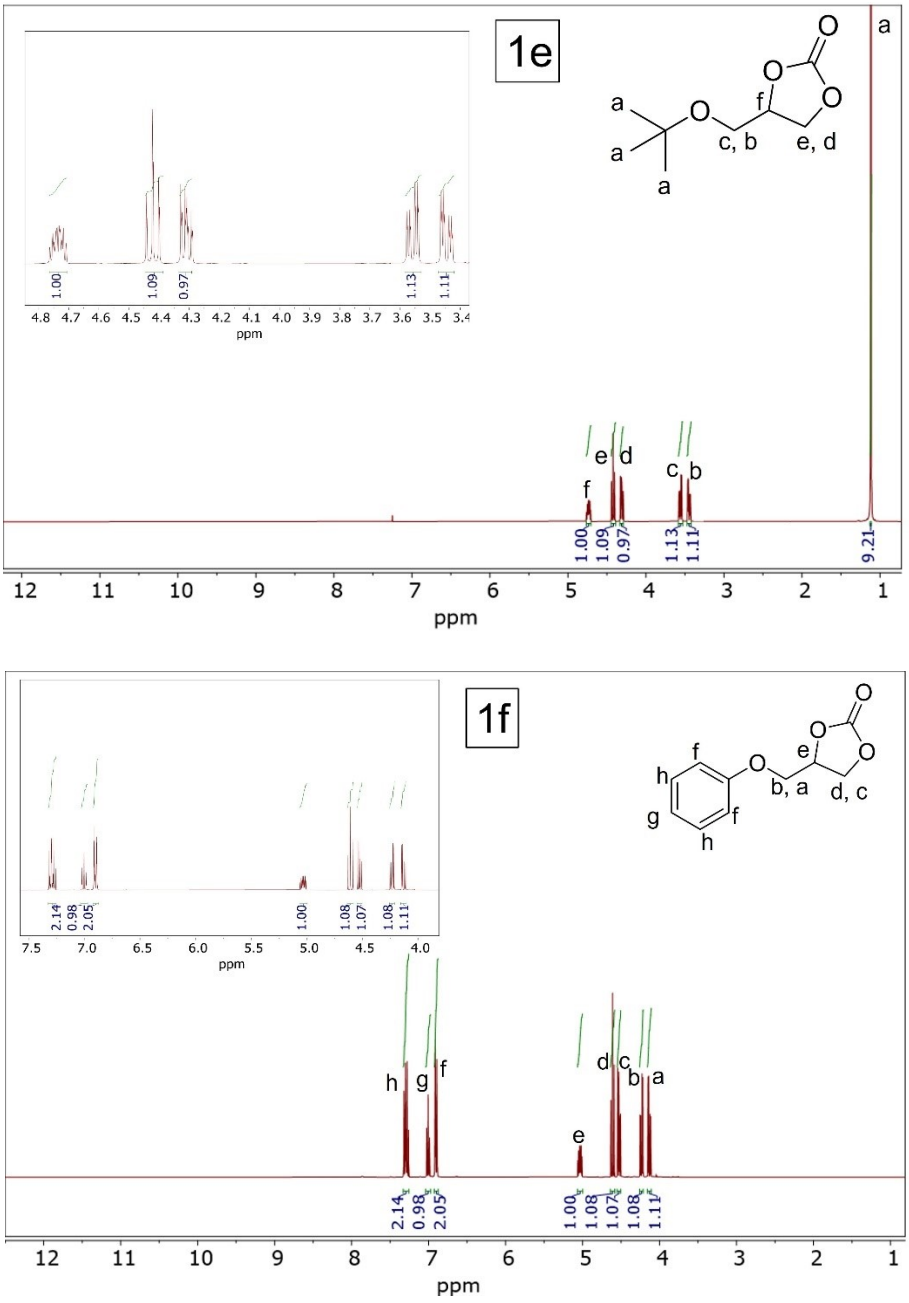

Figure S10. [1]H-NMR spectrum with assigned peaks of cyclic carbonates produced using Ln-CPs. Both Ho-CP and Er-CP show full product conversions (continued).

^{13}C-NMR analysis of the photocatalytic reactions over Ln-CPs photocatalyst.

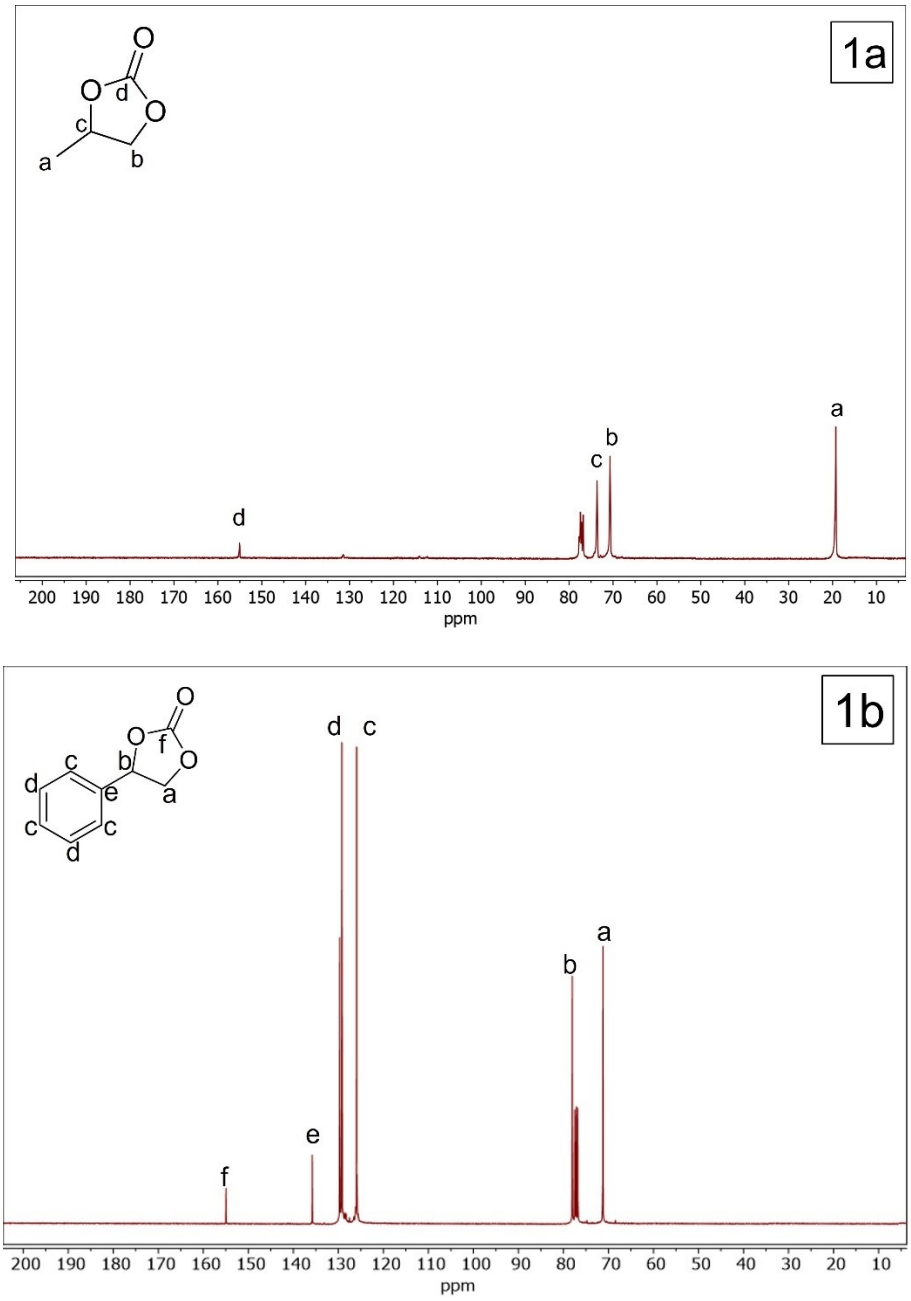

Figure S11. ^{13}C-NMR spectrum with assigned peaks of cyclic carbonates produced using Ln-CPs. Both Ho-CP and Er-CP show full product conversions (continued).

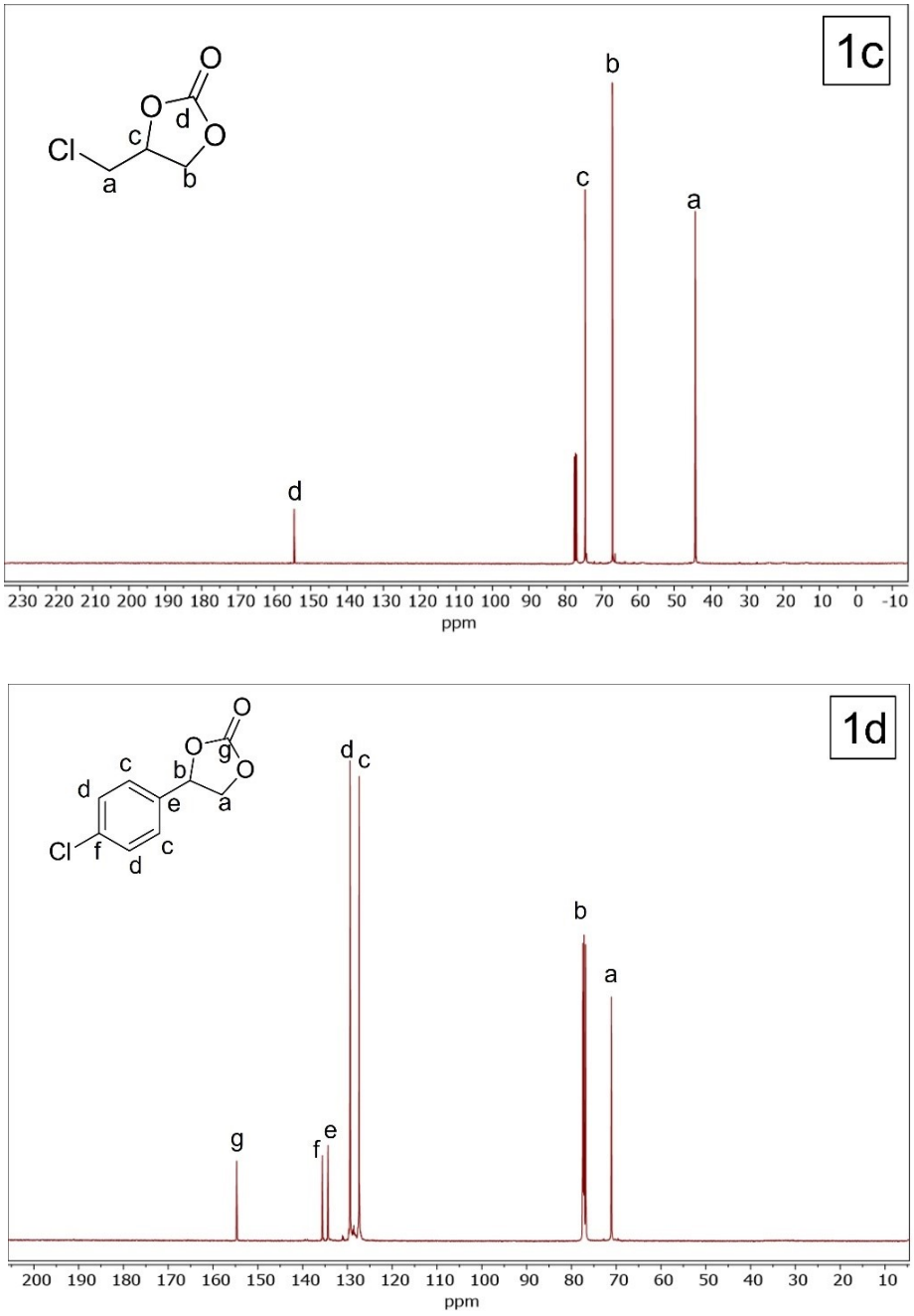

Figure S11. ^{13}C-NMR spectrum with assigned peaks of cyclic carbonates produced using Ln-CPs. Both Ho-CP and Er-CP show full product conversions (continued).

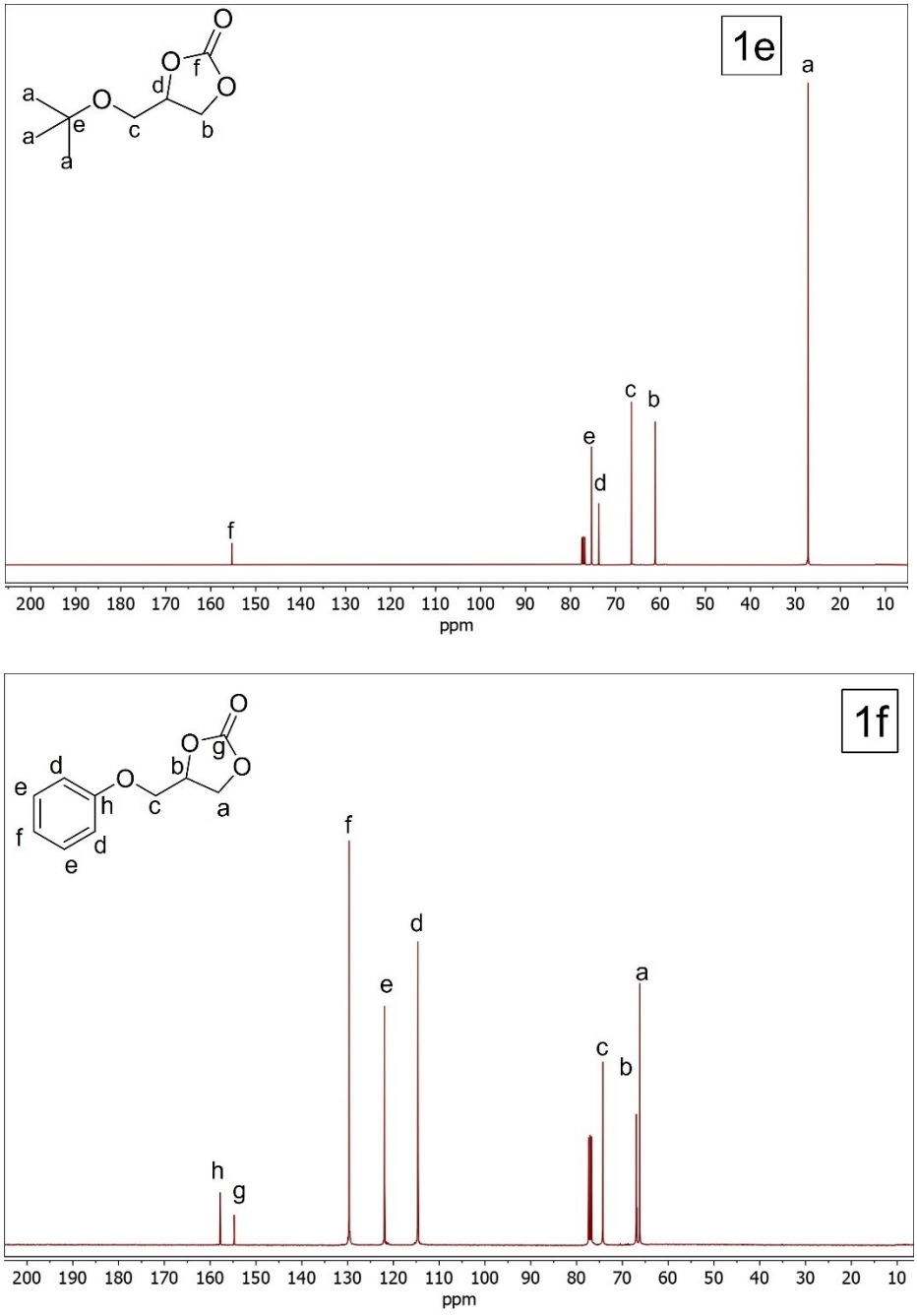

Figure S11. ^{13}C-NMR spectrum with assigned peaks of cyclic carbonates produced using Ln-CPs. Both Ho-CP and Er-CP show full product conversions.

PXRD patterns of recycled Ln-CPs photocatalysts.

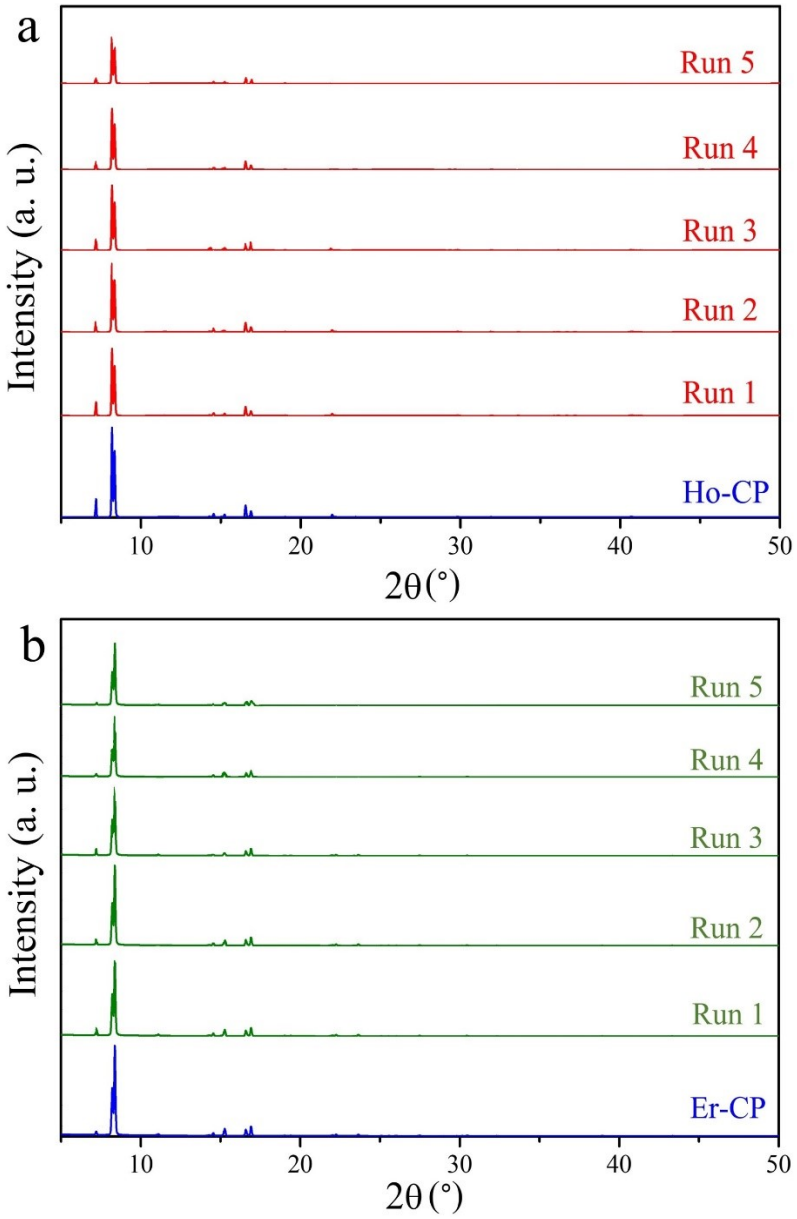

Figure S12. PXRD patterns of the regenerated Ho-CP (a) and Er-CP (b) after each recycling run.

SEM images of recycled Ln-CPs photocatalysts.

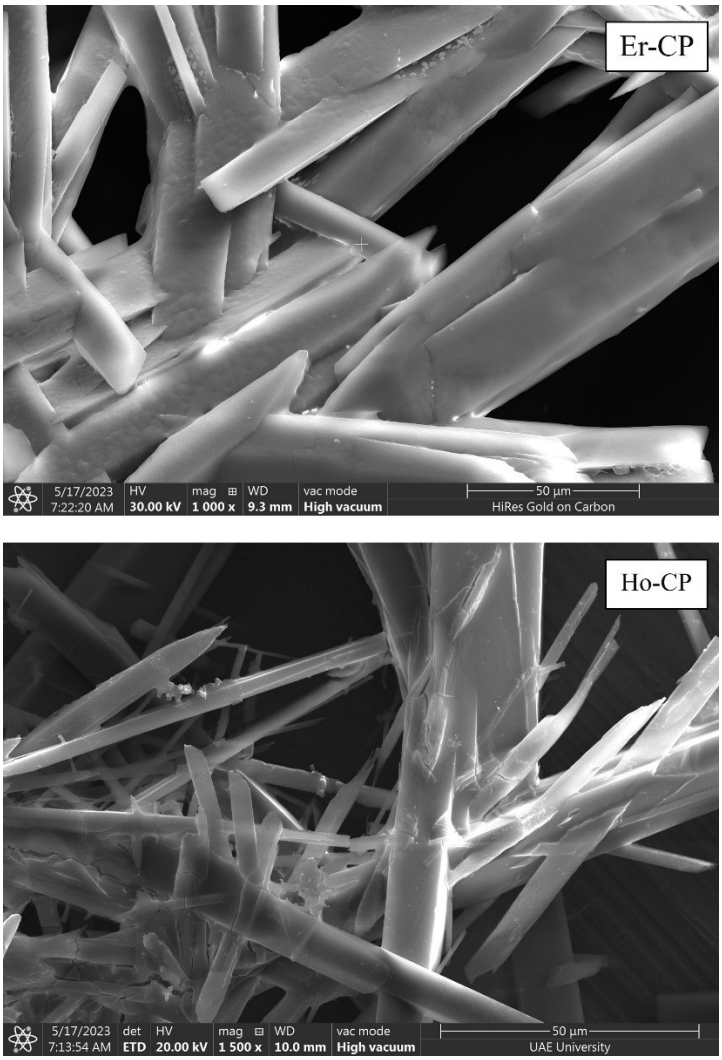

Figure S13. SEM images of recycled Ho and Er-CPs samples at 50 µm resolution.

Summary of previously published photocatalysts used in CO_2 cycloaddition reaction.

Table S19. Previous reports on cycloaddition of CO_2 photocatalytic reaction

Photocatalyst	Substrate (epoxide)	Conversion yield (the highest obtained)	Reference
ZISe mixed metal sulfides	Multiple epoxides	99.9%	[1]
FeTPyP MOF	Styrene oxide	106.13 mmol/(g h).	[2]
B−N coordinated phenanthroimidazole-based zinc salen	Multiple epoxides	90.0%	[3]
Mg-centered porphyrin-based MOF	Multiple epoxides	99.9%	[4]
$Ti_{18}Bi_4O_{29}Bz_{26}$ cluster	Multiple epoxides	99.9%	[5]
Mn-MOF (UAEU-50)	Multiple epoxides	90.0%	[6]
TiO_2 derived from NH_2-MIL-125 MOF	Propylene oxide	99.9%	[7]
Bi-gallate MOF	Multiple epoxides	99.9%	[8]
Bi-PCN-224 MOF	Propylene oxide	99.9%	[9]
$BiNbO_4/NH_2$-MIL-125(Ti)	Propylene oxide	74.0%	[10]
$FeNbO_4$/reduced graphene oxide composites	Propylene oxide	57.0%	[11]
CoPc/TiO_2 hybrid materials	Multiple epoxides	94.0%	[12]

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