

Electronic supplementary information

Topological isomers in lanthanide-chloranilate coordination polymers: synthesis, structure and CO₂ adsorption properties

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Table S1Lanthanide geometry analysis by SHAPE software for **1Ln** and **2Ln**

Geometry	Enneagon (D_{9h})	Octagonal pyramid (C_{8v})	Heptagonal bipyramid (D_{7h})	Johnson triangular cupola (C_{3v})	Capped cube (C_{4v})
	EP-9	OPY-9	HBPY-9	JTC-9	JCCU-9
1Pr	43.903	33.050	34.108	30.735	27.656
1Nd	43.937	33.115	34.200	30.863	27.694
2Sm	34.190	32.735	31.742	23.884	31.158
2Eu	34.383	32.914	31.865	24.064	31.167
2Gd	34.635	33.139	32.057	24.273	31.183
2Tb	34.860	33.354	32.187	24.468	31.238
2Dy	35.095	33.546	32.332	24.626	31.259
2Er	35.499	33.989	32.583	24.995	31.315
2Tm	35.633	34.127	32.676	25.158	31.382
2Yb	35.760	34.277	32.752	25.291	31.455

Lanthanide geometry analysis by SHAPE software for **3Ln**

Geometry	Octagon (D_{8h})	Heptagonal pyramid (C_{7v})	Hexagonal bipyramid (D_{6h})	Cube (O_h)	Square antiprism (D_{4d})
	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8
3Tm	42.881	37.264	40.062	43.604	41.535
3Yb	42.943	37.389	40.157	43.685	41.590

Table S2 Selected bond lengths (Å) and bond angles (°) for **1Ln** and **2Ln**.

	1Pr	1Nd	2Sm	2Eu	2Gd
Ln1–O1	2.466(2)	2.451(3)	2.447(1)	2.435(2)	2.427(3)
Ln1–O2 ⁱ	2.500(2)	2.483(3)	2.456(1)	2.445(2)	2.439(3)
Ln1–O3	2.501(2)	2.484(3)	2.422(2)	2.411(2)	2.407(3)
Ln1–O4 ⁱⁱ	2.507(2)	2.492(3)	2.471(2)	2.458(2)	2.455(3)
Ln1–O5	2.506(2)	2.489(3)	2.466(1)	2.451(2)	2.439(3)
Ln1–O6 ⁱⁱⁱ	2.529(2)	2.518(3)	2.545(2)	2.541(2)	2.537(3)
Ln1–O7	2.574(2)	2.557(3)	2.421(2)	2.406(2)	2.390(3)
Ln1–O8	2.480(3)	2.458(3)	2.502(2)	2.489(2)	2.477(4)
Ln1–O9	2.541(3)	2.520(3)	2.442(2)	2.424(2)	2.393(4)
O1–Ln1–O2 ⁱ	63.88(7)	64.20(10)	64.78(5)	65.04(6)	65.26(10)
O1–Ln1–O3	141.67(8)	141.66(10)	126.37(5)	126.77(7)	127.09(11)
O1–Ln1–O4 ⁱⁱ	129.92(8)	129.91(11)	72.25(5)	72.16(7)	72.13(10)
O1–Ln1–O5	92.45(7)	92.27(10)	138.05(5)	137.97(7)	138.06(11)
O1–Ln1–O6 ⁱⁱⁱ	67.86(7)	67.90(10)	122.06(5)	121.94(7)	121.83(11)
O1–Ln1–O7	72.60(8)	72.45(10)	71.57(5)	91.59(7)	71.56(11)
O1–Ln1–O8	78.39(9)	78.21(12)	125.82(5)	125.71(7)	125.61(11)
O2 ⁱ –Ln1–O3	94.62(7)	94.59(10)	74.84(5)	74.93(7)	74.90(11)
O2 ⁱ –Ln1–O4 ⁱⁱ	73.44(7)	73.27(10)	76.31(5)	76.37(7)	76.39(11)
O2 ⁱ –Ln1–O5	137.82(7)	137.78(10)	144.93(5)	144.65(7)	144.46(11)
O2 ⁱ –Ln1–O6 ⁱⁱⁱ	126.89(7)	127.08(10)	136.13(5)	136.13(7)	136.13(11)
O2 ⁱ –Ln1–O7	69.89(7)	69.75(10)	82.67(6)	83.07(8)	83.29(12)
O3–Ln1–O4 ⁱⁱ	63.07(7)	63.50(9)	64.83(5)	65.23(7)	65.57(11)
O3–Ln1–O5	83.13(7)	82.91(9)	95.00(5)	94.70(7)	94.31(11)
O3–Ln1–O6 ⁱⁱⁱ	138.05(7)	137.94(10)	68.08(5)	68.07(7)	68.18(11)
O3–Ln1–O7	70.15(7)	70.19(9)	137.14(6)	137.32(8)	137.30(12)
O4 ⁱⁱ –Ln1–O6 ⁱⁱⁱ	128.68(7)	128.18(10)	67.32(5)	67.37(6)	67.40(10)
O4 ⁱⁱ –Ln1–O7	116.36(7)	116.55(10)	143.24(5)	143.24(7)	143.20(11)
O5–Ln1–O4 ⁱⁱ	137.60(7)	137.80(10)	130.18(5)	130.38(6)	130.36(10)
O5–Ln1–O6 ⁱⁱⁱ	62.81(7)	63.10(9)	130.18(5)	63.01(6)	62.98(10)
O5–Ln1–O7	69.82(7)	69.85(10)	82.89(5)	82.53(7)	82.53(12)
O6 ⁱⁱⁱ –Ln1–O7	114.95(7)	115.27(10)	141.05(6)	140.66(8)	140.44(12)
O8–Ln1–O2 ⁱ	78.88(10)	78.64(13)	73.76(5)	73.57(7)	73.44(11)
O8–Ln1–O3	130.86(8)	131.14(10)	68.96(5)	68.97(7)	68.90(11)
O8–Ln1–O4 ⁱⁱ	68.49(8)	68.30(11)	129.81(5)	130.07(7)	130.26(11)
O8–Ln1–O5	132.72(9)	132.97(12)	71.29(5)	71.19(7)	71.10(11)
O8–Ln1–O6 ⁱⁱⁱ	70.92(8)	70.78(11)	111.89(5)	114.64(7)	112.37(11)
O8–Ln1–O7	144.26(10)	143.76(13)	69.92(6)	69.92(8)	69.87(12)
O9–Ln1–O1	141.78(8)	141.75(12)	69.49(5)	69.40(7)	69.33(11)
O9–Ln1–O2 ⁱ	147.38(9)	146.83(12)	134.15(5)	134.34(7)	134.51(11)
O9–Ln1–O3	72.44(9)	72.51(11)	140.41(6)	140.14(8)	139.96(12)
O9–Ln1–O4 ⁱⁱ	74.02(9)	73.65(12)	93.20(6)	92.83(8)	92.49(13)
O9–Ln1–O5	71.72(9)	72.28(12)	73.84(6)	74.02(8)	74.28(12)
O9–Ln1–O6 ⁱⁱⁱ	74.00(9)	73.94(12)	73.17(6)	72.87(8)	72.56(12)
O9–Ln1–O7	128.49(9)	129.07(11)	80.18(6)	80.12(9)	80.23(13)
O9–Ln1–O8	87.25(11)	87.17(14)	136.12(6)	136.26(8)	136.42(13)

Table S2 (Continued).

	2Tb	2Dy	2Er	2Tm	2Yb
Ln1-O1	2.419(2)	2.412(2)	2.394(2)	2.389(2)	2.417(2)
Ln1-O2 ⁱ	2.417(2)	2.410(3)	2.390(2)	2.376(2)	2.356(1)
Ln1-O3	2.385(2)	2.373(3)	2.350(2)	2.340(2)	2.336(2)
Ln1-O4 ⁱⁱ	2.431(2)	2.424(3)	2.396(2)	2.385(2)	2.413(2)
Ln1-O5	2.423(2)	2.417(3)	2.385(2)	2.374(2)	2.374(2)
Ln1-O6 ⁱⁱⁱ	2.528(2)	2.530(3)	2.519(2)	2.523(2)	2.584(2)
Ln1-O7	2.377(2)	2.367(3)	2.337(2)	2.327(2)	2.373(2)
Ln1-O8	2.468(2)	2.461(3)	2.439(2)	2.436(2)	2.439(2)
Ln1-O9	2.372(2)	2.356(3)	2.316(3)	2.304(2)	2.261(2)
O1-Ln1-O2 ⁱ	65.53(6)	65.70(8)	66.29(7)	66.43(6)	65.32(5)
O1-Ln1-O3	127.58(7)	127.88(9)	128.90(8)	129.21(7)	130.08(5)
O1-Ln1-O4 ⁱⁱ	72.00(7)	71.77(9)	71.87(7)	71.75(7)	72.55(5)
O1-Ln1-O8	137.90(7)	125.40(9)	125.08(8)	125.03(7)	124.17(5)
O2 ⁱ -Ln1-O4 ⁱⁱ	121.51(7)	76.36(9)	76.38(8)	76.36(7)	77.38(5)
O2 ⁱ -Ln1-O8	71.46(7)	73.15(9)	72.63(8)	72.60(7)	73.30(5)
O3-Ln1-O2 ⁱ	125.47(7)	75.38(9)	75.48(8)	75.69(7)	77.97(5)
O3-Ln1-O4 ⁱⁱ	75.15(7)	66.24(9)	67.02(7)	67.27(7)	67.14(5)
O3-Ln1-O8	76.30(7)	69.24(9)	68.92(8)	69.05(7)	70.59(5)
O4 ⁱⁱ -Ln1-O8	144.24(7)	130.80(9)	130.91(8)	131.13(7)	132.39(5)
O5-Ln1-O1	135.99(7)	137.89(9)	137.60(8)	137.76(7)	138.45(5)
O5-Ln1-O2 ⁱ	83.46(8)	144.04(9)	143.61(8)	143.45(7)	143.23(5)
O5-Ln1-O3	65.90(7)	93.67(9)	93.00(8)	92.51(7)	90.95(6)
O5-Ln1-O4 ⁱⁱ	93.98(7)	130.87(9)	131.13(7)	131.15(7)	130.38(5)
O5-Ln1-O6 ⁱⁱⁱ	67.99(7)	63.58(8)	63.76(7)	63.96(6)	64.33(5)
O5-Ln1-O7	137.49(8)	82.24(10)	81.69(8)	81.68(7)	82.29(6)
O5-Ln1-O8	67.35(6)	70.95(9)	71.02(8)	70.87(7)	69.95(5)
O6 ⁱⁱⁱ -Ln1-O1	142.99(7)	121.20(9)	121.09(8)	120.70(7)	121.47(5)
O6 ⁱⁱⁱ -Ln1-O2 ⁱ	130.68(6)	136.00(9)	135.94(8)	135.84(7)	135.87(5)
O6 ⁱⁱⁱ -Ln1-O3	63.35(6)	67.91(9)	67.94(8)	67.89(7)	65.80(5)
O6 ⁱⁱⁱ -Ln1-O4 ⁱⁱ	82.36(7)	67.30(8)	67.39(7)	67.22(6)	66.09(5)
O6 ⁱⁱⁱ -Ln1-O8	140.44(8)	113.25(9)	113.71(8)	114.15(7)	114.26(5)
O7-Ln1-O1	73.29(7)	71.60(9)	71.45(8)	71.49(7)	70.91(6)
O7-Ln1-O2 ⁱ	69.09(7)	83.45(10)	84.21(9)	84.45(8)	83.33(6)
O7-Ln1-O3	130.51(7)	137.46(10)	137.58(9)	137.75(8)	138.41(6)
O7-Ln1-O4 ⁱⁱ	71.02(7)	142.89(9)	142.92(8)	142.88(7)	143.15(6)
O7-Ln1-O6 ⁱⁱⁱ	112.85(7)	140.45(10)	139.76(9)	139.64(8)	140.74(6)
O7-Ln1-O8	69.73(7)	69.46(10)	69.59(8)	69.53(8)	68.54(6)
O9-Ln1-O1	69.03(7)	69.02(9)	68.62(8)	68.51(7)	68.64(6)
O9-Ln1-O2 ⁱ	134.50(7)	134.67(9)	134.89(8)	134.93(7)	133.95(6)
O9-Ln1-O3	139.66(8)	139.29(10)	138.76(9)	138.44(8)	136.86(6)
O9-Ln1-O4 ⁱⁱ	92.21(8)	91.92(10)	91.05(9)	90.77(8)	89.80(7)
O9-Ln1-O5	74.55(7)	74.64(10)	75.21(9)	75.52(8)	76.57(6)
O9-Ln1-O6 ⁱⁱⁱ	72.40(8)	72.06(10)	71.47(8)	71.16(8)	71.64(6)
O9-Ln1-O7	80.22(9)	80.49(11)	80.61(10)	80.62(9)	81.36(7)
O9-Ln1-O8	136.54(8)	136.57(11)	137.39(9)	137.48(8)	137.15(7)

Symmetry codes: **(1Ln)** (i) $-x+1, -y+1, -z$; (ii) $-x+1, -y+2, -z+1$; (iii) $-x, -y+1, -z+1$; (iv) $x, y+1, z$.
(2Ln) (i) $-x+1, -y+1, -z+2$; (ii) $-x+2, -y, -z+2$; (iii) $-x+2, -y, -z+1$.

Table S3 Selected bond lengths (Å) and bond angles (°) for **3Ln**.

	3Tm	3Yb
Ln1–O1	2.357(2)	2.349(2)
Ln1–O2 ⁱ	2.356(2)	2.352(2)
Ln1–O3	2.324(2)	2.309(2)
Ln1–O4 ⁱⁱ	2.363(2)	2.353(2)
Ln1–O5	2.333(2)	2.317(2)
Ln1–O6 ⁱⁱⁱ	2.385(2)	2.375(2)
Ln1–O7	2.275(3)	2.260(3)
Ln1–O8	2.257(3)	2.247(3)
O1–Ln1–O2 ⁱ	66.74(8)	66.99(8)
O1–Ln1–O3	74.40(8)	74.44(8)
O1–Ln1–O4 ⁱⁱ	126.86(8)	127.18(8)
O1–Ln1–O8	141.18(9)	141.22(9)
O2 ⁱ –Ln1–O4 ⁱⁱ	129.83(8)	130.01(8)
O2 ⁱ –Ln1–O8	74.45(9)	74.24(9)
O3–Ln1–O2 ⁱ	74.21(8)	74.07(8)
O3–Ln1–O4 ⁱⁱ	66.92(8)	67.46(7)
O3–Ln1–O8	94.55(10)	94.54(10)
O4 ⁱⁱ –Ln1–O8	78.22(9)	78.18(9)
O5–Ln1–O1	79.39(8)	79.15(8)
O5–Ln1–O2 ⁱ	78.50(8)	78.37(8)
O5–Ln1–O3	147.82(8)	147.48(8)
O5–Ln1–O4 ⁱⁱ	145.26(8)	145.06(8)
O5–Ln1–O6 ⁱⁱⁱ	67.08(7)	67.42(7)
O5–Ln1–O7	91.37(10)	91.45(10)
O5–Ln1–O8	94.28(10)	94.29(10)
O6 ⁱⁱⁱ –Ln1–O1	131.94(8)	131.81(8)
O6 ⁱⁱⁱ –Ln1–O2 ⁱ	132.78(8)	132.90(8)
O6 ⁱⁱⁱ –Ln1–O3	145.10(8)	145.10(7)
O6 ⁱⁱⁱ –Ln1–O4 ⁱⁱ	78.19(7)	77.65(7)
O6 ⁱⁱⁱ –Ln1–O8	76.89(9)	77.01(10)
O7–Ln1–O1	73.50(9)	73.28(9)
O7–Ln1–O2 ⁱ	140.10(9)	140.15(9)
O7–Ln1–O3	98.66(10)	98.69(10)
O7–Ln1–O4 ⁱⁱ	77.77(10)	77.74(9)
O7–Ln1–O6 ⁱⁱⁱ	73.94(9)	73.92(10)
O7–Ln1–O8	145.29(10)	145.46(10)

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x+2, -y+1, -z+2$; (iii) $-x+1, -y+1, -z+1$.

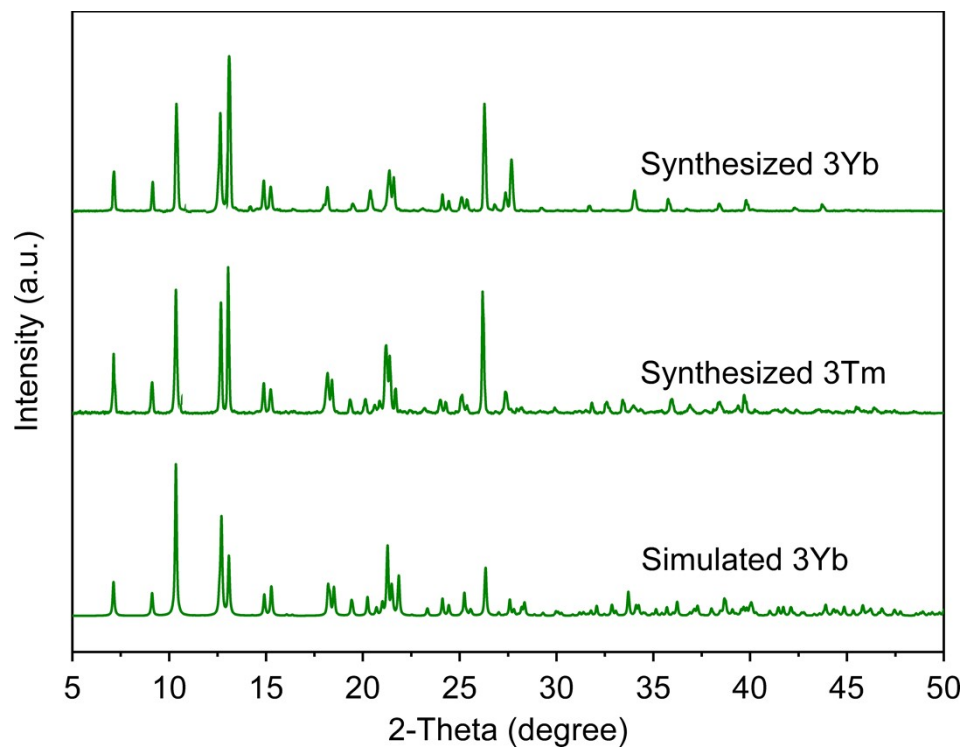
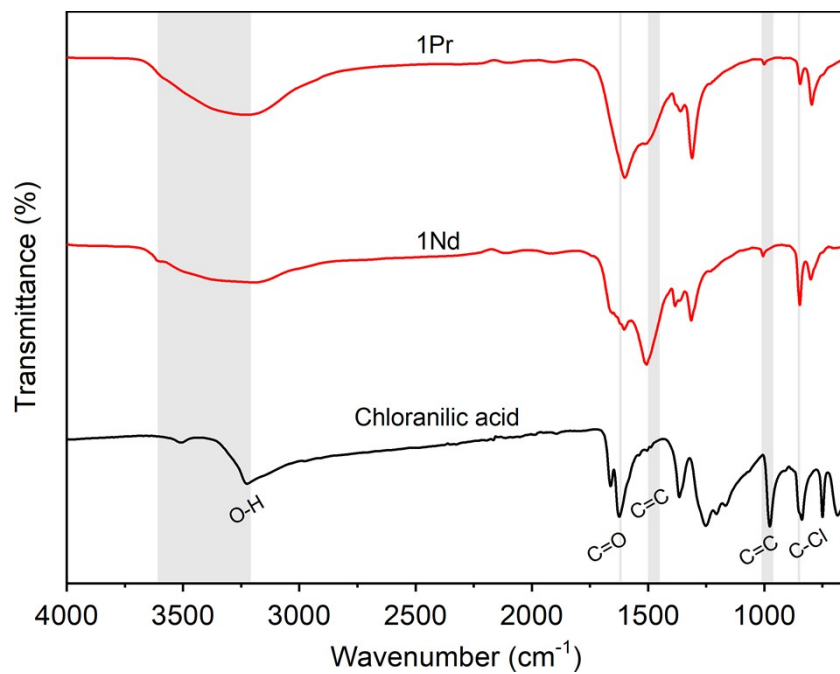
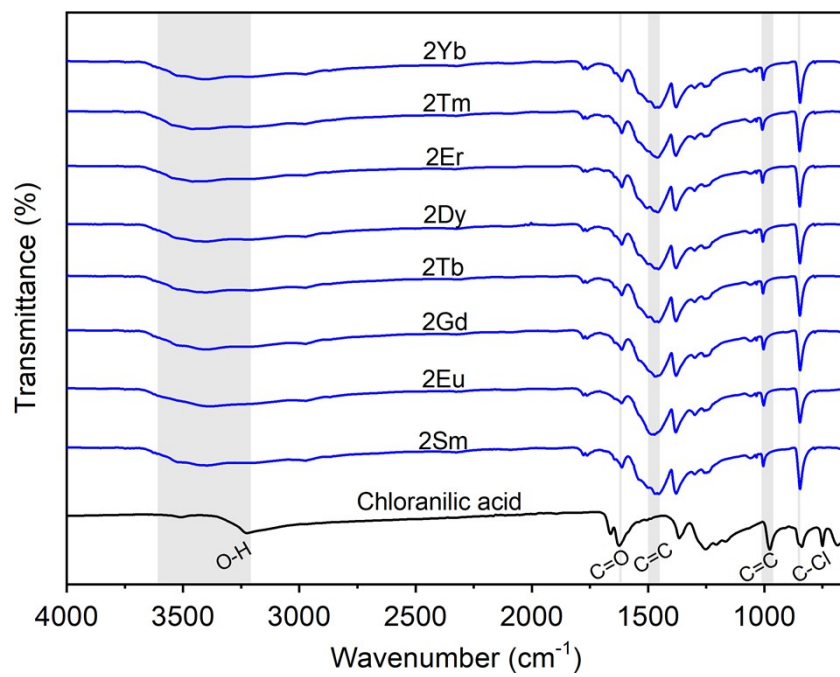


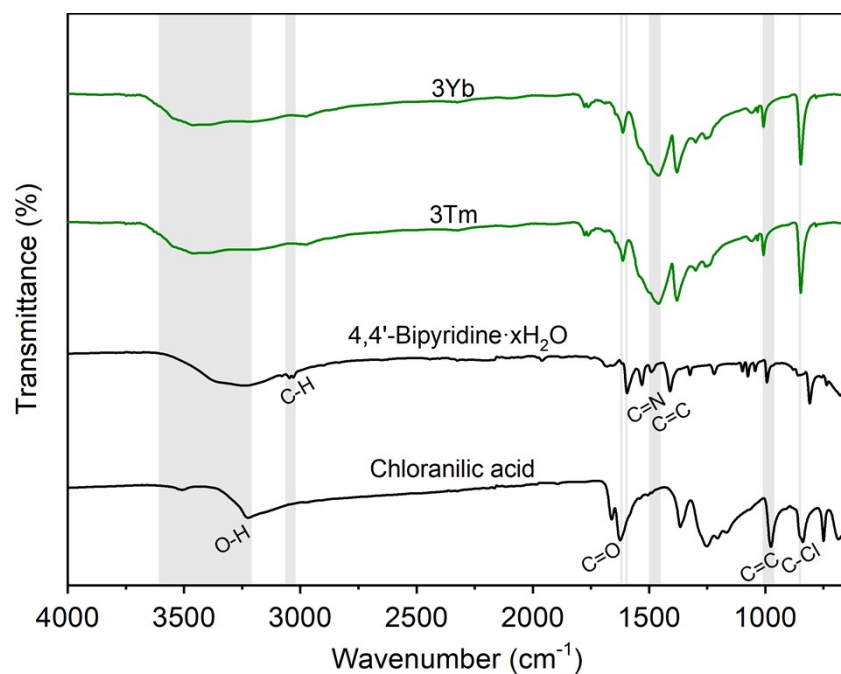
Fig. S1 Comparison of the simulated and synthesized PXRD patterns of all compounds in the series **3Ln**.



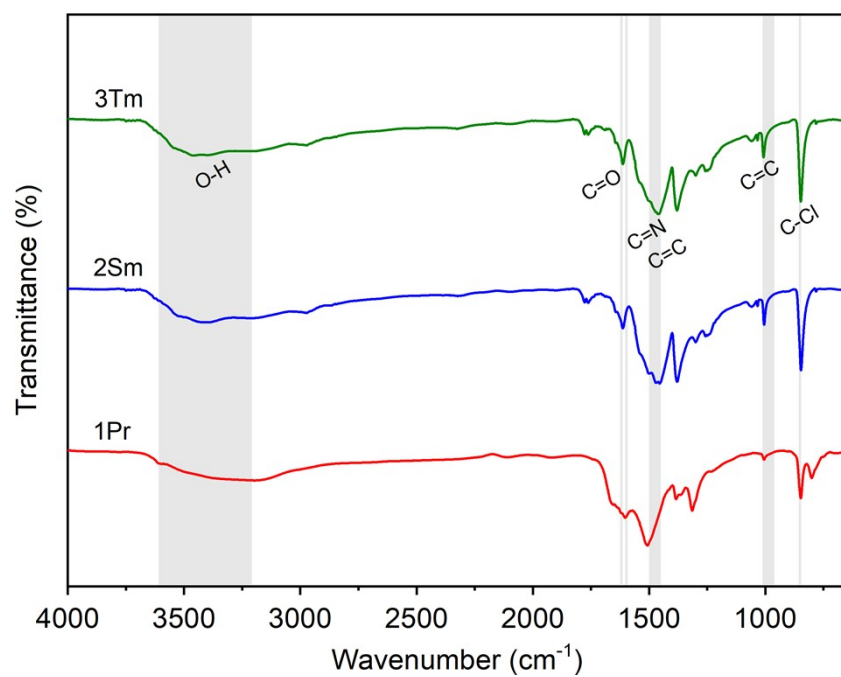
(a)



(b)



(c)



(d)

Fig. S2 FT-IR spectra recorded at room temperature for (a) chloranilic acid and **1Ln** compounds, (b) chloranilic acid and **2Ln** compounds, (c) chloranilic acid, 4,4'-bipyridine·xH₂O, and **3Ln** compounds, and (d) a comparative analysis of **1Pr**, **2Sm**, and **3Tm**.

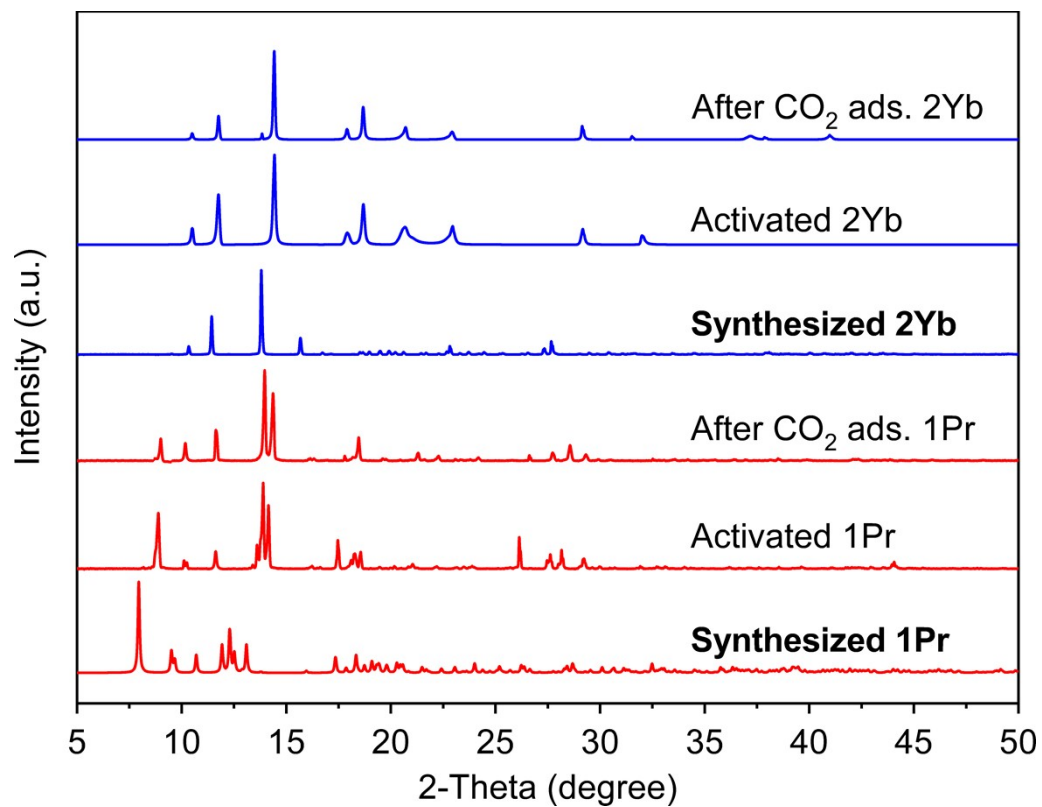


Fig. S3 Comparison of as-synthesized, thermally activated, and after CO₂ sorption PXR D patterns at an ambient temperature of **1Pr** and **2Yb**.