Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

$RE(H_2C_3N_3O_3)_2 \cdot (OH) \cdot xH_2O$ (RE = La, Y and Gd): potential UV birefringent materials with strong optical anisotropy originating from the $(H_2C_3N_3O_3)^-$ group

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Table S1. Atomic coordinates (×10⁴) and equivalent isotropic displacement parameters (Å²×10³) for **I**, **II** and **III**.

I

Atom	x	y	z	U(eq)
La1	3531.3(4)	4506.0(2)	2913.2(4)	13.73(10)
O1	6235(5)	4728(2)	1817(5)	29.6(10)
O2	551(5)	4826(2)	1686(5)	29.6(10)
O3	1857(5)	5141(2)	4929(5)	28.2(9)
O4	1697(5)	3511(2)	3740(5)	25.5(9)
O5	4899(4)	4250.3(19)	5745(4)	18.1(8)
O6	-1175(5)	1629(2)	831(5)	25.2(9)
O7	2849(5)	984(2)	4995(5)	27.4(9)
O8	5009(5)	1775(2)	7686(5)	24.4(9)
O9	8156(5)	3655(2)	10390(5)	23.2(9)
N1	6450(5)	4004(2)	8084(5)	14.6(9)
N2	4793(5)	2994(2)	6628(5)	16.9(9)
N3	6698(5)	2709(2)	8933(5)	18.2(10)
N4	210(5)	2567(2)	2319(6)	19.9(10)
N5	2298(5)	2259(2)	4400(5)	18.4(9)
N6	855(5)	1245(2)	2851(6)	20.6(10)
C1	5377(6)	3734(3)	6804(7)	16.0(11
C2	7141(6)	3479(3)	9172(6)	15.8(10)
C3	5466(6)	2473(3)	7740(6)	16.9(11)
C4	1423(6)	2812(3)	3497(7)	16.4(11)
C5	2006(6)	1464(3)	4093(6)	18.6(11)
C6	-67(6)	1786(3)	1959(7)	18.6(11)

II

Atom	x	y	z	U(eq)
Y1	6336.3(4)	1045.8(3)	-6.8(3)	13.43(11)
O1	2612(4)	584(4)	5539(3)	38.4(7)
O2	4365(4)	4240(3)	6482(3)	29.7(6)
O3	4805(4)	2638(3)	1990(2)	28.4(6)
O5	8145(4)	62(4)	1778(3)	35.9(7)
O6	5482(3)	-656(3)	1150(2)	24.7(5)
O7	8402(4)	-1358(3)	-952(3)	40.5(7)
O8	4638(3)	3734(3)	-672(3)	29.0(6)
O9	8067(4)	2402(4)	46(3)	39.2(7)
O10	7318(3)	1275(3)	-2411(3)	29.6(6)
O11	9226(4)	1950(4)	-6816(3)	36.4(7)
O12	9227(4)	4981(3)	-3251(3)	32.2(6)
N1	3473(4)	2373(4)	6132(3)	25.7(6)
N2	3706(4)	1582(4)	3754(3)	25.5(7)
N3	4542(4)	3474(3)	4239(3)	23.3(6)
N4	8272(4)	3150(4)	-2693(3)	25.6(6)
N5	8249(4)	1623(4)	-4594(3)	26.0(6)
N6	9209(4)	3500(4)	-5036(3)	25.8(6)
C1	3233(5)	1507(4)	5186(4)	24.4(7)
C2	4114(5)	3369(4)	5675(4)	22.9(7)
C3	4376(4)	2564(4)	3253(4)	21.4(7)
C4	7920(4)	2025(4)	-3176(4)	23.0(7)
C5	8920(4)	2334(4)	-5559(4)	24.0(7)
C6	8908(4)	3902(4)	-3616(4)	23.8(7)

O4	1460(4)	4195(4)	507(3)	40.1(7)

III

Atom	x	y	z	U(eq)
Gd1	6347.7(3)	1066.5(3)	-1.7(2)	14.04(10)
O1	2617(6)	590(5)	5528(4)	32.3(10)
O2	4369(5)	4238(5)	6480(4)	26.4(9)
O3	4784(5)	2667(5)	2023(4)	24.3(8)
O4	5490(5)	-657(4)	1166(4)	20.0(8)
O5	8179(5)	68(5)	1819(4)	29.8(9)
O7	8452(5)	-1385(5)	-950(4)	32.0(10)
O8	4617(5)	3788(4)	-678(4)	23.1(8)
O9	8139(6)	2424(5)	20(4)	32.4(10)
O10	7332(5)	1270(5)	-2425(4)	24.4(9)
O11	9256(6)	1946(5)	-6797(4)	30.7(10)
O12	9222(5)	4984(5)	-3261(4)	26.3(9)
N1	3477(6)	2379(5)	6124(5)	22.5(10)
N2	3696(6)	1591(5)	3760(5)	20.7(9)
N3	4530(6)	3491(5)	4253(5)	20.0(9)
N4	8256(6)	1629(6)	-4602(5)	22.3(10)
N5	8261(6)	3168(5)	-2712(4)	21.3(10)
N6	9224(6)	3489(6)	-5038(4)	21.1(9)
C1	3239(7)	1504(6)	5187(6)	20.4(11)
C2	4118(6)	3381(6)	5677(5)	17.7(10)
C3	4364(6)	2587(6)	3268(5)	18.0(10)
C4	7920(6)	2035(6)	-3192(5)	19.3(11)
C5	8908(7)	3906(6)	-3623(5)	17.7(10)
C6	8938(7)	2327(6)	-5555(5)	20.0(11)
O6	1447(5)	4214(5)	525(4)	31.3(10)

Table S2. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **I**, **II** and **III.** The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

I

Atom	U11	U22	U33	U23	U13	U12
La1	16.99(16)	8.88(14)	13.94(17)	0.04(12)	-1.48(11)	-0.04(11)
O1	34(2)	19.0(18)	39(3)	-3.1(18)	17(2)	-1.1(17)
O2	23(2)	22.3(19)	38(3)	-3.1(19)	-11.9(19)	3.8(16)
O3	33(2)	24(2)	27(2)	-1.6(18)	2.9(19)	2.4(17)
O4	25(2)	13.2(17)	36(3)	-2.0(17)	-1.2(18)	-2.6(15)
O5	24.6(19)	13.4(16)	14.1(19)	3.8(15)	-3.2(16)	0.0(14)
O6	25(2)	22.2(19)	24(2)	2.4(17)	-9.6(18)	-2.1(16)
O7	34(2)	17.2(18)	26(2)	5.3(17)	-10.0(19)	0.5(16)
O8	35(2)	12.3(16)	25(2)	2.1(16)	0.0(18)	-6.6(16)
O9	32(2)	15.3(18)	18(2)	0.8(15)	-9.6(17)	0.9(15)
N1	19(2)	11.9(19)	11(2)	0.7(17)	-3.8(18)	-0.6(16)
N2	19(2)	12.4(19)	17(2)	2.2(18)	-2.6(19)	-0.2(16)
N3	24(2)	11.1(19)	17(2)	-0.2(18)	-4.2(19)	-3.9(17)
N4	22(2)	12.5(19)	24(3)	0.4(19)	0(2)	-4.5(17)
N5	20(2)	16(2)	19(2)	2.9(18)	-0.1(19)	-0.4(17)
N6	22(2)	17(2)	20(3)	4.5(19)	-4(2)	-2.1(18)
C1	15(2)	13(2)	20(3)	0(2)	2(2)	0.5(18)
C2	18(2)	13(2)	16(3)	-2(2)	3(2)	1(2)

C3	20(3)	12(2)	18(3)	-1(2)	2(2)	-2.8(19)
C4	17(2)	12(2)	20(3)	3(2)	3(2)	-1.4(19)
C5	20(3)	18(2)	18(3)	0(2)	2(2)	-3(2)
C6	19(3)	15(2)	21(3)	2(2)	5(2)	0(2)

II

Atom	U11	U22	U33	U23	U13	U12
Y1	19.43(17)	14.41(16)	10.10(16)	0.15(10)	0.71(10)	-11.34(12)
O1	64(2)	42.5(17)	28.1(14)	4.3(12)	-3.4(14)	-42.2(16)
O2	51.6(17)	29.4(13)	19.5(12)	1.5(10)	-6.2(11)	-27.7(13)
O3	42.1(16)	27.4(13)	14.7(12)	-1.2(10)	1.7(11)	-15.1(12)
O5	43.1(17)	43.2(17)	32.1(15)	12.2(12)	-13.0(13)	-26.7(14)
O6	35.8(14)	28.2(13)	20.4(12)	7.2(10)	-5.9(10)	-23.2(12)
O7	50.8(19)	27.3(14)	32.9(15)	0.0(12)	14.8(13)	-11.4(14)
O8	39.8(15)	24.4(13)	21.9(13)	1.4(10)	-0.6(11)	-13.4(12)
O9	53.7(19)	52.0(18)	33.8(15)	14.9(13)	-15.2(14)	-41.6(16)
O10	39.2(15)	28.7(14)	25.6(13)	2.3(11)	7.0(11)	-21.8(12)
O11	52.4(18)	45.2(17)	22.5(13)	-8.4(12)	11.5(12)	-34.7(15)
O12	50.2(17)	33.1(14)	24.6(13)	-3.9(11)	4.3(12)	-30.5(14)
N1	39.0(18)	25.9(15)	18.3(14)	0.9(12)	-1.7(12)	-20.0(14)
N2	38.8(18)	26.6(16)	18.1(14)	-0.7(12)	-2.3(12)	-20.9(14)
N3	33.9(16)	24.7(15)	16.0(14)	0.1(11)	-1.0(12)	-17.4(13)
N4	34.4(17)	26.4(15)	20.0(14)	1.9(12)	2.9(12)	-18.4(14)
N5	34.6(17)	27.4(16)	21.4(15)	-0.1(12)	5.0(12)	-20.4(14)
N6	35.0(17)	27.6(15)	21.1(15)	0.4(12)	3.7(12)	-21.4(14)
C1	32.7(19)	24.2(17)	21.7(17)	3.2(13)	-4.6(14)	-17.0(16)
C2	30.2(18)	21.1(16)	18.8(16)	0.7(13)	-2.0(13)	-12.5(15)
C3	25.4(17)	19.3(16)	18.8(16)	0.3(12)	-1.4(13)	-9.0(14)
C4	23.0(17)	22.4(17)	23.8(17)	2.8(13)	2.8(13)	-11.5(14)
C5	26.5(18)	26.0(17)	21.9(17)	-2.0(14)	3.9(14)	-15.2(15)
C6	27.2(18)	23.2(17)	24.1(17)	0.3(14)	1.4(14)	-14.8(15)
O4	44.7(18)	37.8(16)	36.3(16)	-1.1(13)	-3.8(13)	-16.0(14)

III

Atom	U11	U22	U33	U23	U13	U12
Gd1	18.81(15)	15.25(14)	11.41(14)	0.43(9)	0.12(9)	-10.93(10)
O1	58(3)	35(2)	23(2)	4.9(18)	-6(2)	-37(2)
O2	47(3)	29(2)	16.0(18)	1.5(16)	-6.3(17)	-27(2)
O3	37(2)	22(2)	13.7(18)	-0.9(15)	1.8(16)	-13.8(18)
O4	26(2)	26(2)	17.9(18)	8.3(15)	-7.7(15)	-20.1(17)
O5	35(2)	38(3)	27(2)	8.5(18)	-11.8(18)	-24(2)
O7	36(2)	24(2)	26(2)	-2.8(17)	11.5(18)	-6.4(19)
O8	29(2)	20.0(19)	18.8(18)	2.6(15)	-2.1(15)	-8.7(17)
O9	41(3)	46(3)	29(2)	13(2)	-13.3(19)	-34(2)
O10	32(2)	27(2)	18.5(19)	1.3(16)	7.2(16)	-19.3(19)
O11	44(3)	41(3)	18.5(19)	-7.8(18)	7.7(18)	-31(2)
O12	43(3)	25(2)	19.9(19)	-1.6(16)	1.8(17)	-25(2)
N1	34(3)	23(2)	17(2)	2.8(18)	-3.5(19)	-19(2)
N2	32(3)	21(2)	16(2)	1.5(17)	-2.5(18)	-18(2)
N3	27(2)	20(2)	15(2)	0.1(17)	-2.3(17)	-13(2)
N4	30(3)	24(2)	17(2)	0.0(18)	4.0(18)	-17(2)

N5	31(3)	23(2)	15(2)	1.3(18)	3.2(18)	-18(2)
N6	29(2)	24(2)	17(2)	-1.8(18)	3.8(18)	-18(2)
C1	28(3)	18(3)	18(2)	2(2)	-4(2)	-11(2)
C2	23(3)	19(3)	14(2)	2.4(19)	-4.9(19)	-10(2)
C3	20(3)	17(2)	15(2)	0.8(19)	-1.8(19)	-6(2)
C4	19(3)	20(3)	18(2)	1(2)	4(2)	-9(2)
C5	24(3)	17(2)	14(2)	-1.3(19)	0.3(19)	-11(2)
C6	22(3)	22(3)	19(2)	-1(2)	2(2)	-13(2)
O6	33(2)	32(2)	28(2)	-4.4(18)	-2.2(18)	-14(2)

Table S3. Select bond lengths (Å) and angles (degree) for **I**, **II** and **III**.

I

La1-O1	2.555(4)	O9-C2	1.254(6)
La1-O2	2.538(4)	N1-C1	1.362(7)
La1-O3	2.603(4)	N1-C2	1.349(6)
La1-O4	2.449(4)	N2-C1	1.358(6)
La1-O5	2.527(4)	N2-C3	1.353(7)
La1-O5[1]	2.651(3)	N3-C2	1.378(6)
La1-O7[2]	2.600(4)	N3-C3	1.367(7)
La1-O8[2]	2.532(3)	N4-C4	1.354(7)
La1-N1[1]	2.701(4)	N4-C6	1.388(6)
O4-C4	1.233(6)	N5-C4	1.352(6)
O5-C1	1.280(6)	N5-C5	1.405(6)
O6-C6	1.234(6)	N6-C5	1.347(7)
O7-C5	1.253(6)	N6-C6	1.349(7)
O8-C3	1.254(6)		
O1-La1-O3	138.95(13)	O82-La1-O7[2]	70.99(12)
O1-La1-O5[1]	69.85(12)	O82-La1-N1[1]	140.72(13)
O1-La1-O7[2]	76.03(14)	C4-O4-La1	137.2(4)
O1-La1-N1[1]	72.12(12)	La1-O5-La1[1]	112.18(12)
O2-La1-O1	129.58(15)	C1-O5-La1	146.1(3)
O2-La1-O3	67.30(14)	C1-O5-La1[1]	100.7(3)
O2-La1-O5[1]	111.26(11)	C5-O7-La1[3]	144.1(4)
O2-La1-O7[2]	68.66(13)	C3-O8-La1[3]	166.1(4)
O2-La1-N1[1]	73.66(12)	C1-N1-La1[1]	96.1(3)
O3-La1-O5[1]	69.10(12)	C2-N1-La1[1]	145.9(3)
O3-La1-N1[1]	80.84(13)	C2-N1-C1	117.6(4)
O4-La1-O1	144.24(12)	C3-N2-C1	116.7(4)
O4-La1-O2	71.62(13)	C3-N3-C2	122.5(4)
O4-La1-O3	72.13(13)	C4-N4-C6	122.5(4)
O4-La1-O5[1]	135.38(13)	C4-N5-C5	121.5(4)
O4-La1-O5	78.24(12)	C5-N6-C6	120.1(4)
O4-La1-O7[2]	90.33(13)	O5-C1-N1	114.2(4)
O4-La1-O82	74.53(13)	O5-C1-N2	120.8(5)
O4-La1-N1[1]	142.08(13)	N2-C1-N1	125.0(5)
O5-La1-O1	96.10(14)	O9-C2-N1	123.5(4)
O5-La1-O2	132.28(14)	O9-C2-N3	118.4(5)
O5-La1-O3	68.70(12)	N1-C2-N3	118.1(5)
O5-La1-O5[1]	67.82(12)	O8-C3-N2	121.6(5)
O5-La1-O7[2]	148.26(11)	O8-C3-N3	119.2(5)
O5-La1-O8[2]	77.41(12)	N2-C3-N3	119.2(4)
O5[1]-La1-N1[1]	48.98(11)	O4-C4-N4	121.2(5)
O5-La1-N1[1]	116.23(12)	O4-C4-N5	121.8(5)
O7[2]-La1-O3	135.75(13)	N5-C4-N4	117.1(4)

O7[2]-La1-O5[1]	133.32(12)	O7-C5-N5	117.9(5)
O7[2]-La1-N1[1]	90.96(12)	O7-C5-N6	122.6(5)
O8[2]-La1-O1	69.79(13)	N6-C5-N5	119.5(5)
O8[2]-La1-O2	126.16(12)	O6-C6-N4	117.0(5)
O8[2]-La1-O3	136.21(13)	O6-C6-N6	123.8(5)
O8[2]-La1-O5[1]	122.27(12)	N6-C6-N4	119.2(5)

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

II

Y1-Y1[1]	3.7083(6)	O12-C6	1.242(4)
Y1-O3	2.366(2)	N1-C1	1.334(4)
Y1-O5	2.407(3)	N1-C2	1.339(4)
Y1-O6	2.273(2)	N2-C1	1.395(4)
Y1-O6[1]	2.237(2)	N2-C3	1.357(4)
Y1-O7	2.370(3)	N3-C2	1.395(4)
Y1-O8	2.477(3)	N3-C3	1.358(4)
Y1-O9	2.409(3)	N4-C4	1.341(4)
Y1-O10	2.402(2)	N4-C6	1.344(4)
O1-C1	1.242(4)	N5-C4	1.383(4)
O2-C2	1.251(4)	N5-C5	1.360(4)
O3-C3	1.234(4)	N6-C5	1.358(4)
O10-C4	1.240(4)	N6-C6	1.386(4)
O11-C5	1.232(4)		
O3-Y1-Y1[1]	94.44(7)	O10-Y1-Y1[1]	107.96(6)
O3-Y1-O5	76.82(10)	O10-Y1-O5	122.51(10)
O3-Y1-O7	148.91(10)	O10-Y1-O8	73.55(9)
O3-Y1-O8	68.54(9)	O10-Y1-O9	73.42(9)
O3-Y1-O9	84.50(10)	C3-O3-Y1	141.6(2)
O3-Y1-O10	139.91(9)	Y1[1]-O6-Y1	110.62(10)
O5-Y1-Y1[1]	110.16(7)	C4-O10-Y1	142.3(2)
O5-Y1-O8	131.54(9)	C1-N1-C2	118.6(3)
O5-Y1-O9	68.73(10)	C3-N2-C1	122.1(3)
O6[1]-Y1-Y1[1]	35.01(6)	C3-N3-C2	122.5(3)
O6-Y1-Y1[1]	34.37(6)	C4-N4-C6	118.8(3)
O6-Y1-O3	81.53(9)	C5-N5-C4	122.8(3)
O6[1]-Y1-O3	106.15(10)	C5-N6-C6	122.8(3)
O6-Y1-O5	76.23(9)	O1-C1-N1	121.7(3)
O6[1]-Y1-O5	144.42(9)	O1-C1-N2	117.3(3)
O6[1]-Y1-O6	69.38(10)	N1-C1-N2	120.9(3)
O6-Y1-O7	79.03(10)	O2-C2-N1	123.1(3)
O6[1]-Y1-O7	89.38(11)	O2-C2-N3	116.5(3)
O6[1]-Y1-O8	79.29(9)	N1-C2-N3	120.3(3)
O6-Y1-O8	128.10(9)	O3-C3-N2	122.8(3)

O6-Y1-O9	144.39(9)	O3-C3-N3	121.8(3)
O6[1]-Y1-O9	146.21(9)	N2-C3-N3	115.4(3)
O6[1]-Y1-O10	78.54(9)	O10-C4-N4	123.6(3)
O6-Y1-O10	134.31(9)	O10-C4-N5	116.1(3)
O7-Y1-Y1[1]	82.93(8)	N4-C4-N5	120.3(3)
O7-Y1-O5	75.13(11)	O11-C5-N5	122.0(3)
O7-Y1-O8	142.05(9)	O11-C5-N6	122.9(3)
O7-Y1-O9	97.51(12)	N6-C5-N5	115.1(3)
O7-Y1-O10	68.71(9)	O12-C6-N4	122.4(3)
O8-Y1-Y1[1]	105.44(7)	O12-C6-N6	117.4(3)
O9-Y1-Y1[1]	178.61(7)	N4-C6-N6	120.2(3)
O9-Y1-O8	75.03(10)		

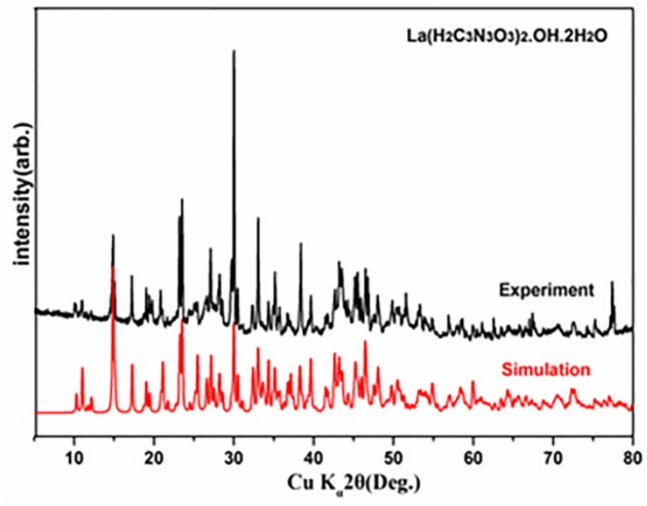
[1]1-X,-Y,-Z

III

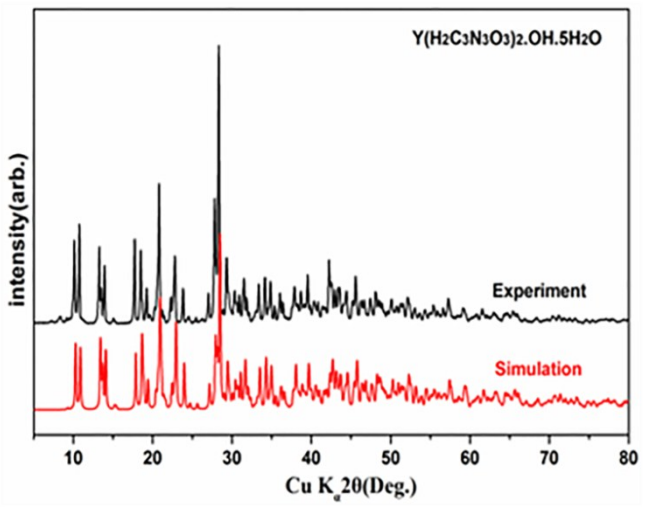
Gd1-Gd1[1]	3.7713(5)	O12-C5	1.241(6)
Gd1-O3	2.411(4)	N1-C1	1.340(7)
Gd1-O4	2.309(3)	N1-C2	1.348(7)
Gd1-O4[1]	2.282(4)	N2-C1	1.402(7)
Gd1-O5	2.462(4)	N2-C3	1.371(7)
Gd1-O7	2.421(4)	N3-C2	1.395(6)
Gd1-O8	2.521(4)	N3-C3	1.361(7)
Gd1-O9	2.463(4)	N4-C4	1.387(7)
Gd1-O10	2.435(4)	N4-C6	1.359(7)
O1-C1	1.238(7)	N5-C4	1.346(7)
O2-C2	1.244(6)	N5-C5	1.342(7)
O3-C3	1.227(6)	N6-C5	1.395(6)
O10-C4	1.251(6)	N6-C6	1.355(7)
O11-C6	1.226(6)		
O3-Gd1-Gd1[1]	94.16(10)	O10-Gd1-Gd1[1]	107.24(9)
O3-Gd1-O5	76.50(14)	O10-Gd1-O5	123.06(14)
O3-Gd1-O7	148.39(14)	O10-Gd1-O8	73.86(13)
O3-Gd1-O8	68.98(12)	O10-Gd1-O9	73.25(14)
O3-Gd1-O9	85.89(15)	C3-O3-Gd1	141.7(4)
O3-Gd1-O10	140.89(13)	Gd1[1]-O4-Gd1	110.46(14)
O4[1]-Gd1-Gd1[1]	35.00(9)	C4-O10-Gd1	141.7(4)
O4-Gd1-Gd11	34.53(9)	C1-N1-C2	119.2(4)
O4-Gd1-O3	80.98(13)	C3-N2-C1	121.8(4)
O4[1]-Gd1-O3	106.18(14)	C3-N3-C2	122.9(5)
O4[1]-Gd1-O4	69.54(14)	C6-N4-C4	122.8(5)
O4-Gd1-O5	75.79(13)	C5-N5-C4	118.8(4)
O4[1]-Gd1-O5	144.12(14)	C6-N6-C5	122.8(4)
O4-Gd1-O7	78.79(14)	O1-C1-N1	122.4(5)
O4[1]-Gd1-O7	89.13(15)	O1-C1-N2	117.1(5)

O4[1]-Gd1-O8	79.33(13)	N1-C1-N2	120.6(5)
O4-Gd1-O8	128.14(13)	O2-C2-N1	123.1(5)
O4-Gd1-O9	144.57(13)	O2-C2-N3	117.0(5)
O4[1]-Gd1-O9	145.88(13)	N1-C2-N3	119.9(5)
O4[1]-Gd1-O10	77.89(13)	O3-C3-N2	122.6(5)
O4-Gd1-O10	133.74(13)	O3-C3-N3	121.9(5)
O5-Gd1-Gd1[1]	109.87(10)	N3-C3-N2	115.5(4)
O5-Gd1-O8	131.70(14)	O10-C4-N4	116.2(5)
O5-Gd1-O9	69.18(14)	O10-C4-N5	123.5(5)
O7-Gd1-Gd1[1]	82.64(11)	N5-C4-N4	120.3(5)
O7-Gd1-O5	75.16(15)	O12-C5-N5	122.4(5)
O7-Gd1-O8	142.22(13)	O12-C5-N6	117.6(5)
O7-Gd1-O9	96.80(16)	N5-C5-N6	120.0(5)
O7-Gd1-O10	68.55(14)	O11-C6-N4	122.5(5)
O8-Gd1-Gd1[1]	105.43(9)	O11-C6-N6	122.3(5)
O9-Gd1-Gd1[1]	179.01(10)	N6-C6-N4	115.2(5)
O9-Gd1-O8	75.51(14)		

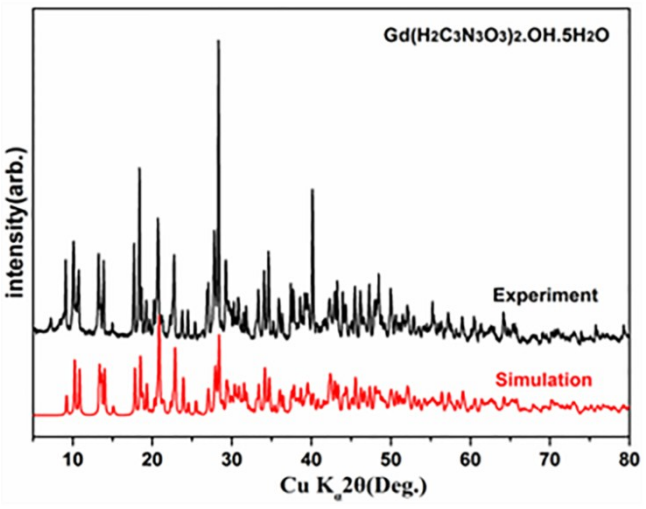
[1]1-X,-Y,-Z



(a)



(b)



(c)

Figure S1. Calculated and experimental powder X-ray diffraction patterns of **I** (a), **II** (b) and **III** (c). The black curves are the patterns of samples, the red are the calculated ones.

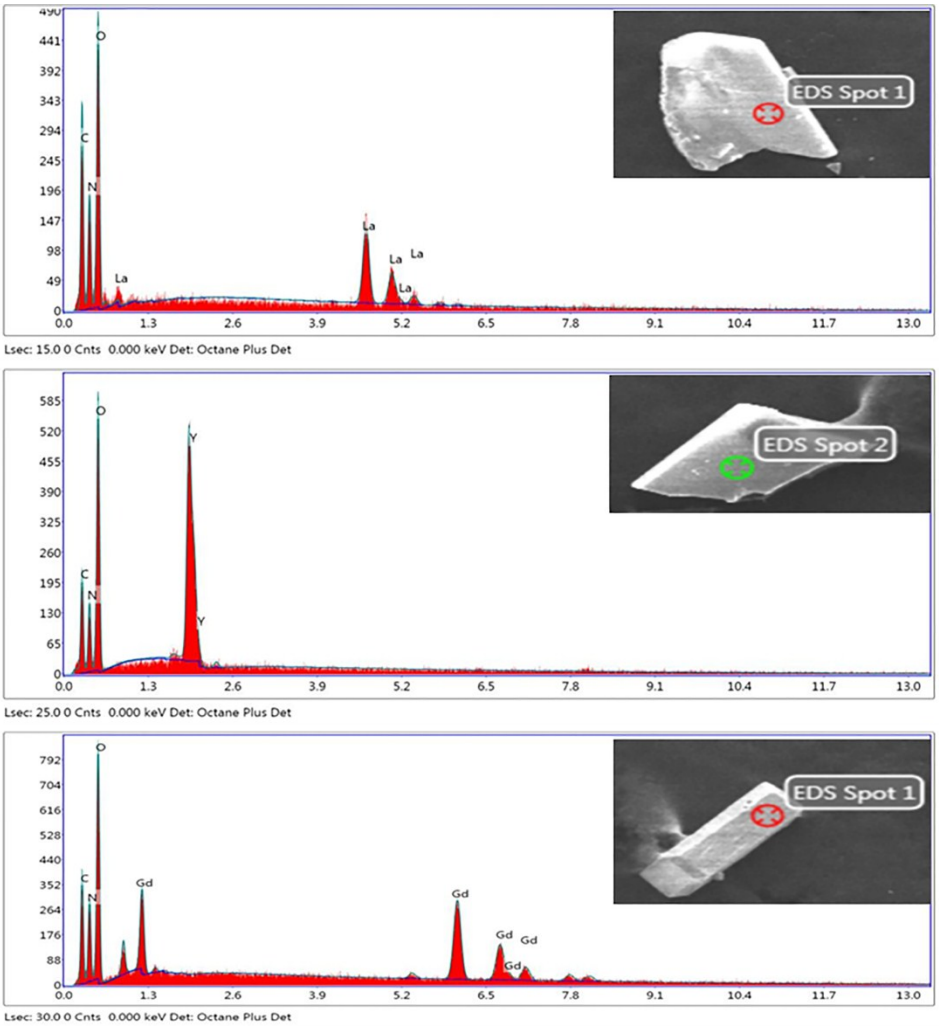
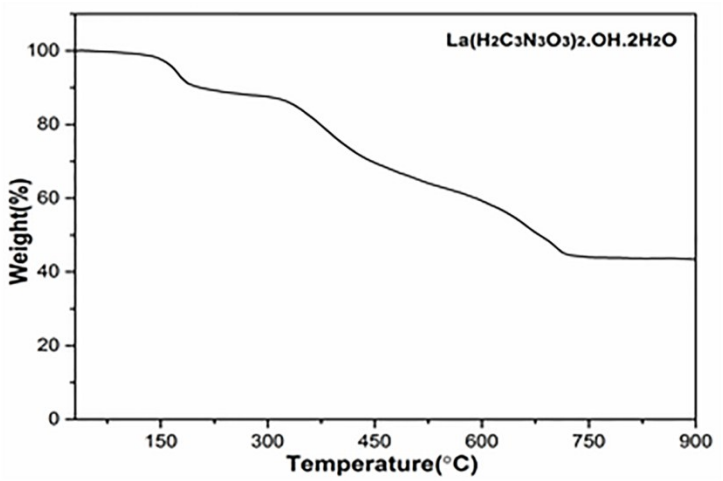
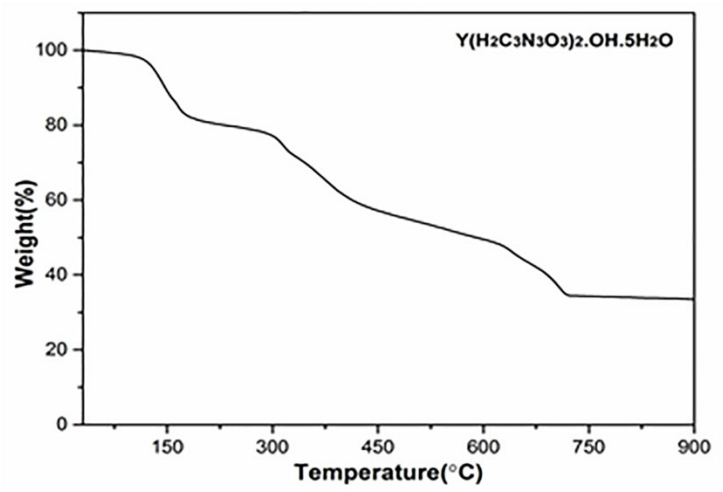


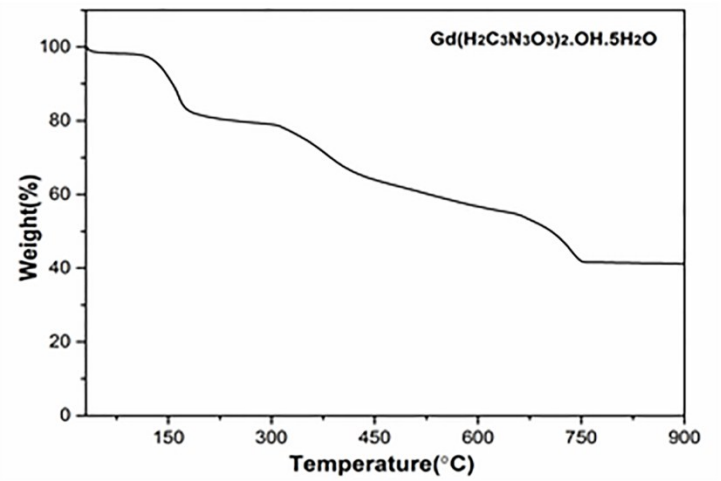
Figure S2. Energy dispersive X-ray spectroscopy analysis of **I**, **II** and **III.**



(a)



(b)



(c)

Figure S3. The TG diagrams for **I** (a), **II** (b) and **III** (c).

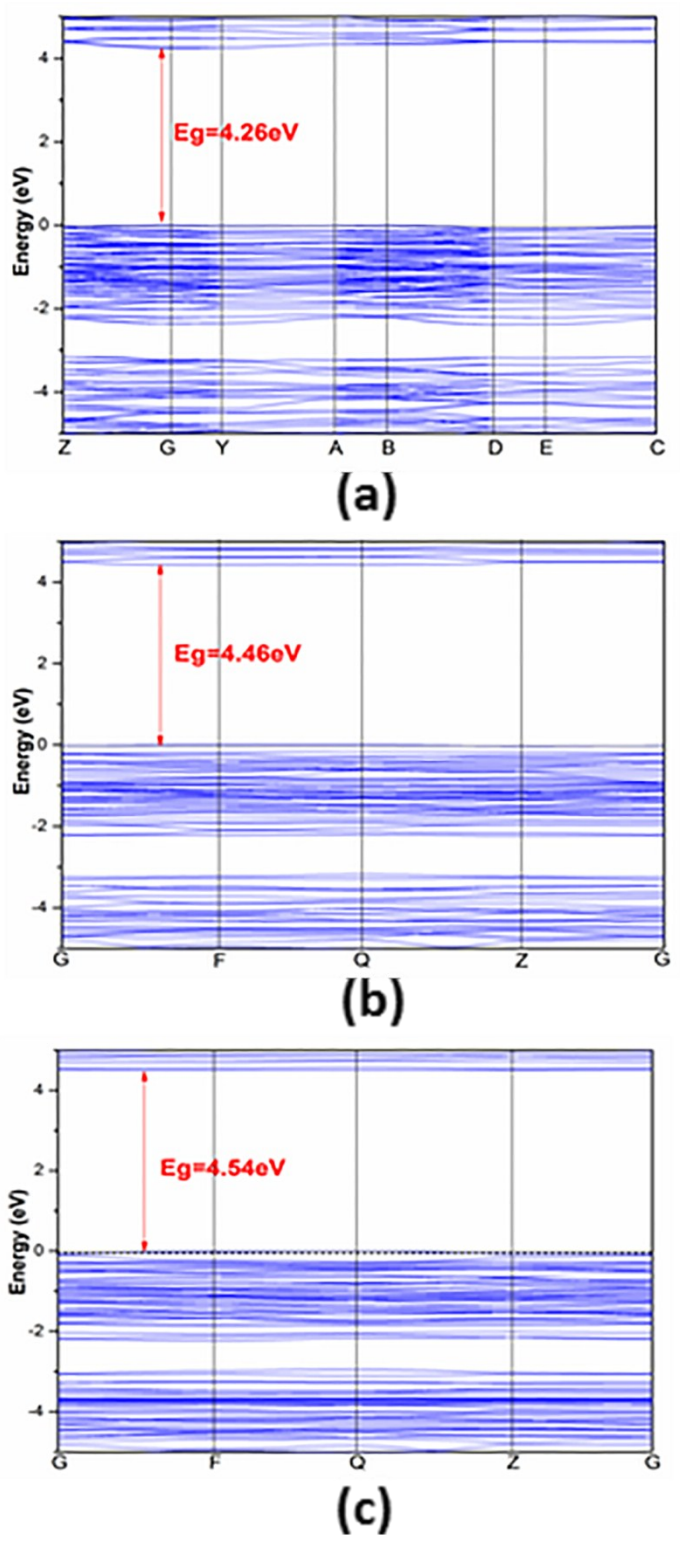


Figure S4. The band structure of **I** (a), **II** (b) and **III** (c).

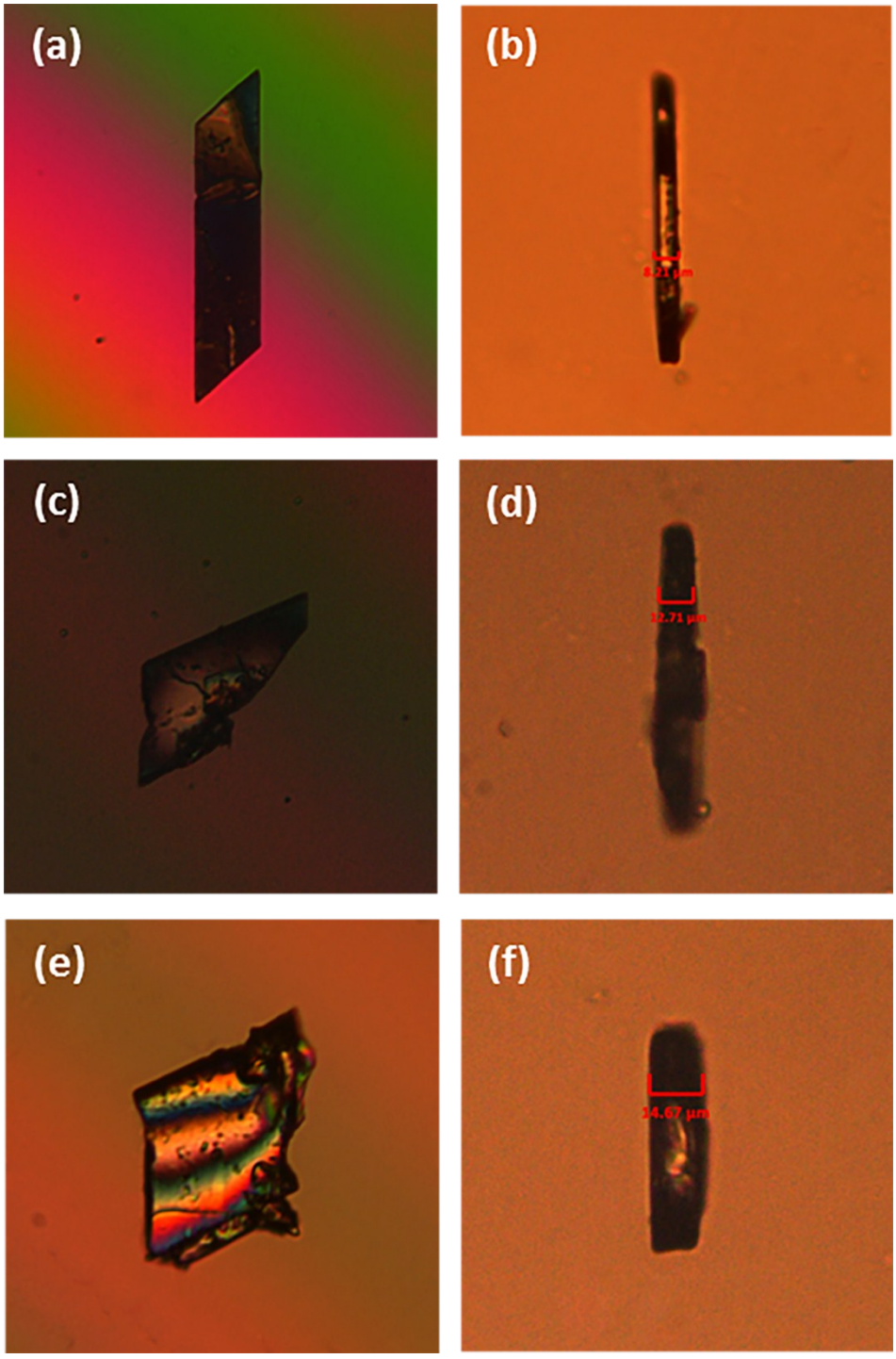


Figure S5. Photograph of crystals **I** (a, b), **II** (c, d) and **III** (e, f) for the measurement of birefringence.

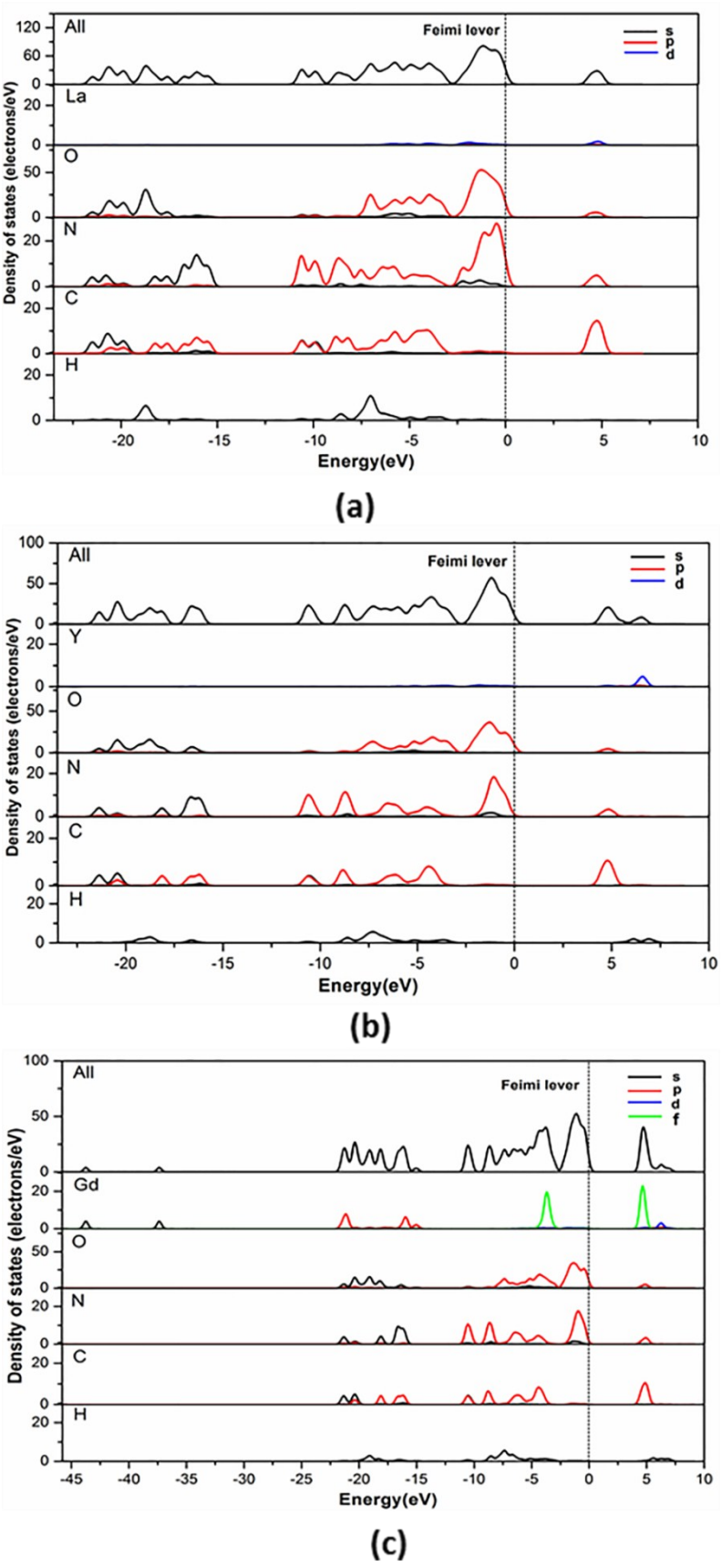


Figure S6. Densities of states for **I** (a), **II** (b) and **III** (c).

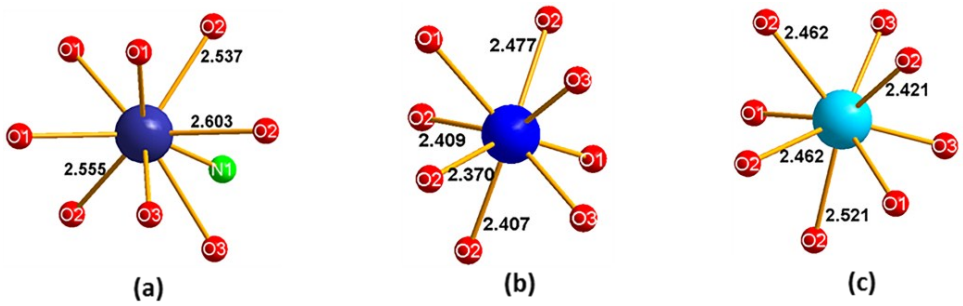


Figure S7. The bond length of La-O2 (a), Y-O2 (b) and Gd-O2 (c), O2 participates in the formation of water molecules.

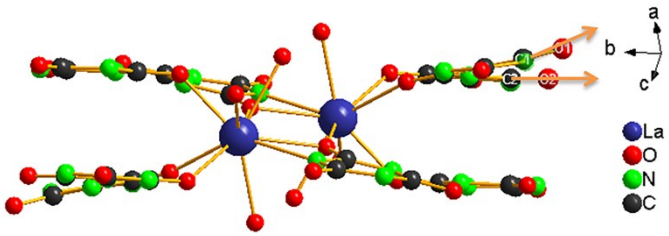


Figure S8. The 3D framework of **I** with the calculational inclination angle (θ) of anion groups $(H_2C_3N_3O_3)^-$, θ = 15.87°.