Supporting Information for

$Ba_2M(C_3N_3O_3)_2$ (M = Mg, Ca): Potential UV Birefringent Materials with Strengthened Optical Anisotropy Originated from $(C_3N_3O_3)^{3-}$ Group

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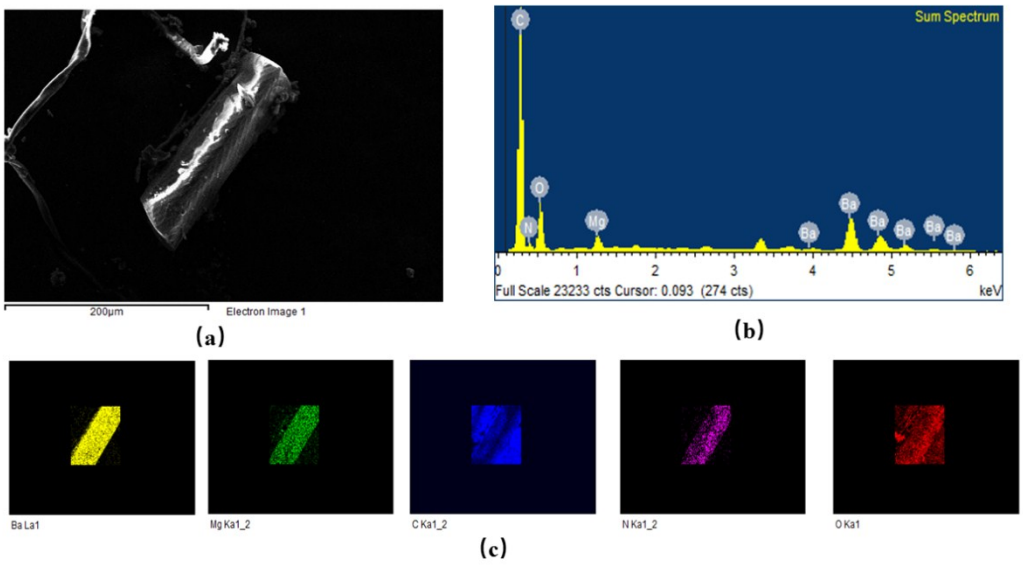

Figure S1. (a) Scanning electron microscopy (SEM) image of BMCY. (b) Elemental analysis of BMCY by EDX spectroscopy. (c) Elemental distribution of the as-grown crystal (from left to right: Ba Mg C N O).

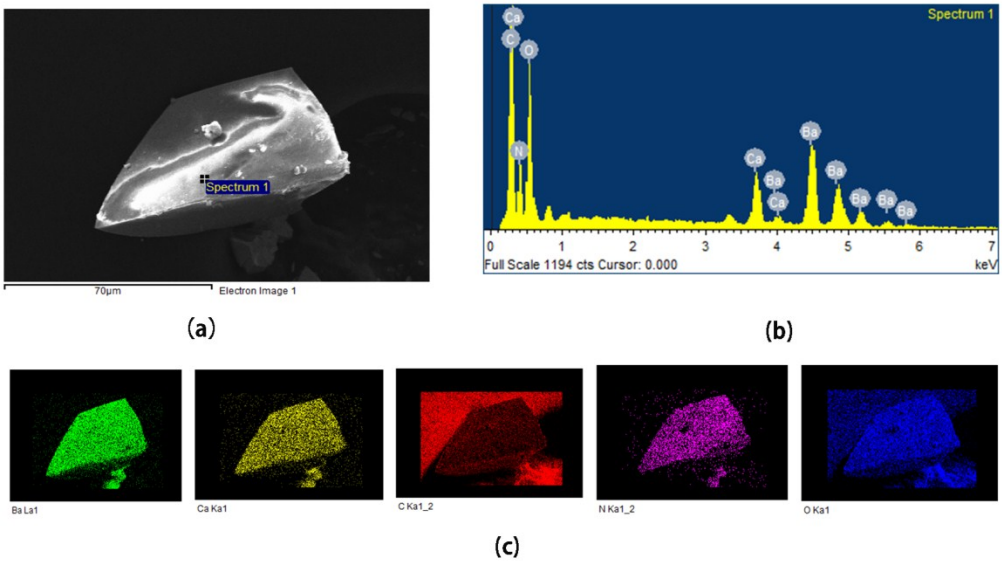

Figure S2. (a) Scanning electron microscopy (SEM) image of BCCY. (b) Elemental analysis of BCCY by EDX spectroscopy. (c) Elemental distribution of the as-grown crystal (from left to right: Ba Ca C N O).

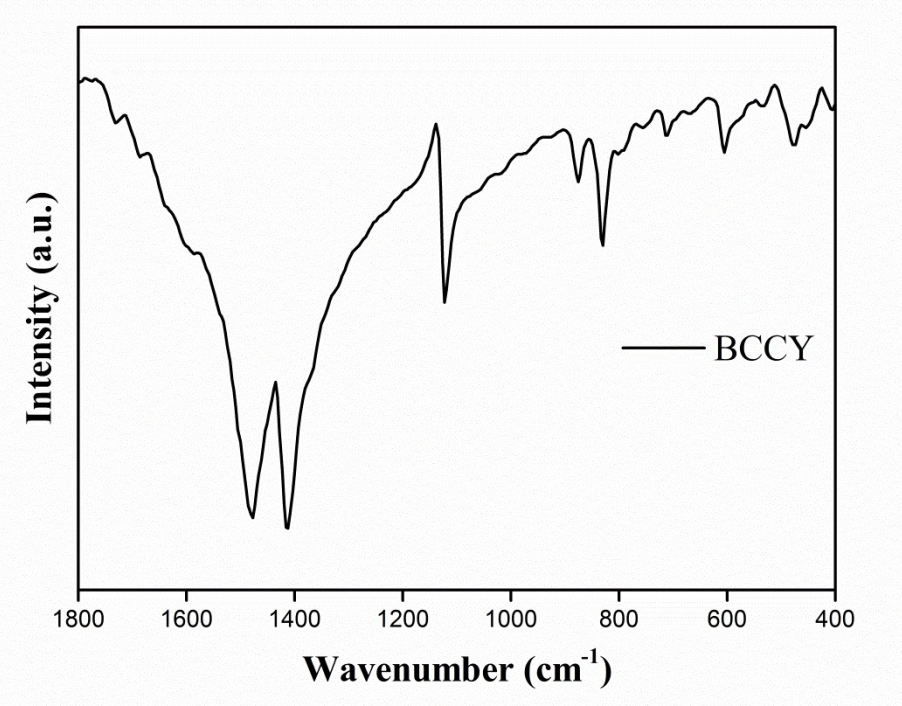

Figure S3 The infrared spectrum of BCCY.

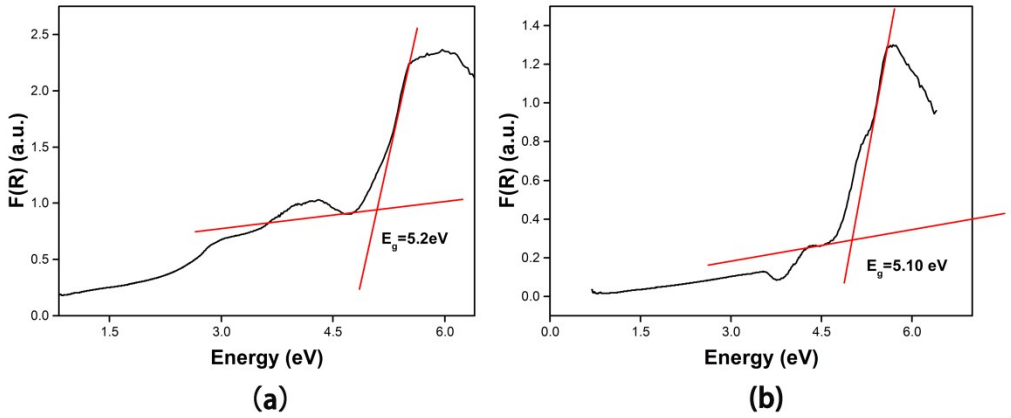

Figure S3 Band gap of BMCY (a) and BCCY (b), deduced from UV−vis/NIR diffuse reflectance spectrum.

Table S1. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Ba_2Mg(C_3N_3O_3)_2$. U_{eq} is defined as 1/3 of of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	Wyckoff site	U(eq)
Ba	0	0	7834.4(2)	6c	13.3(2)
Mg	3333	6667	6667	3a	10.5(6)

O	3583(4)	4420(4)	7452.9(14)	18f	14.2(6)
N	4465(5)	1735(5)	7436.8(18)	18f	14.6(7)
C	5111(6)	3904(6)	7436.7(18)	18f	9.6(7)

Table S2. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Ba_2Ca(C_3N_3O_3)_2$. U_{eq} is defined as 1/3 of of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	Wyckoff site	U(eq)
Ba	3333.3	6666.7	4535.9	6c	14.6
Ca	6666.7	3333.3	3333.3	3a	12.1
O	6836(3)	5939(3)	4189.7	18f	16.1
N	10488(4)	8336(4)	4140.1(15)	18f	14.3(5)
C	8408(5)	7942(5)	4153.0(16)	18f	12.3(6)

Table S3. Selected bond lengths (Å) and angles (°) for $Ba_2Mg(C_3N_3O_3)_2$.

Mg−O×1	2.131(3)	Ba−O×3	2.871(2)
Mg−O×5	2.132(3)	Ba−O×3	2.911(3)
C−O×1	1.285(4)	C−N−C	116.7(4)
C−N×1	1.346(5)	O−C−N	117.2(3)
C−N×2	1.361(5)	O−C−N	119.5(3)
Ba−N×3	2.803(3)	N−C−N	123.3(3)

Table S4. Selected bond lengths (Å) and angles (°) for $Ba_2Ca(C_3N_3O_3)_2$.

Ca−O×6	2.356(2)	Ba−O×3	2.835(2)
C−O×1	1.291(4)	Ba−O×3	2.903(2)
C−N×2	1.351(4)	N−C−O	118.5(3)
Ba−N×3	2.881(2)	N−C−O	117.1(3)

Table S5. Atom-cutting analysis and calculated refractive index of BMCY and BMBO.

		n_o	n_e	Δn
BMBO	cal	1.7273	1.6272	0.1011
	exp	1.6966	1.5886	0.1080
atom-cutting results		Ba^{2+}	Mg^{2+}	$(B_3O_6)^{3-}$
		0.010	0.013	0.103
		n_o	n_e	Δn
BMCY	cal	1.9903	1.6452	0.3451
	exp	-	-	-
atom-cutting results		Ba^{2+}	Mg^{2+}	$(C_3N_3O_3)^{3-}$
		0.08	0.078	0.347

Table S6. The selected bond length and band population of BMBO and BMCY.

BMBO			BMCY		
bond	length	population	bond	length	population
Ba−O	2.766	0.06	Ba−O	2.875	0.04
Ba−O	2.880	0.04	Ba−O	2.912	0.02
Ba−O	2.895	0.05	Ba−N	2.803	0.13