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A Melamine-Based Organic-Inorganic Hybrid Material Revealing Excellent Optical Performance and Moderate Thermal Stability

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Table S1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 1. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Zn1	9115.3(11)	4349(2)	7445.3(8)	28.6(3)
Cl1	9919(2)	2555(3)	9047.0(15)	33.5(4)
Cl2	10016(2)	7455(3)	7775.4(18)	38.3(5)
Cl3	9827(2)	2721(4)	6011.4(16)	37.9(5)
C1	4046(8)	5759(12)	6685(6)	26.4(15)
C2	6133(8)	5094(11)	7955(6)	23.8(15)
C3	6118(8)	5127(12)	6058(6)	25.2(16)
C4	5871(8)	5669(12)	1973(6)	26.8(16)
C5	3787(8)	5090(12)	2619(6)	23.8(15)
C6	3783(8)	5153(12)	668(6)	25.5(16)
N1	4719(7)	5605(11)	7763(5)	27.1(14)
N2	4708(7)	5520(11)	5805(5)	30.6(16)
N3	6898(6)	4838(10)	7117(5)	23.9(14)
N4	6831(7)	5094(13)	5219(5)	40(2)
N5	2650(7)	6211(14)	6459(6)	41.4(19)
N6	6815(7)	4901(11)	9011(5)	32.8(17)
N7	3054(7)	4859(11)	1524(5)	29.2(16)
N8	5201(7)	5502(12)	878(5)	29.7(15)
N9	5187(7)	5532(11)	2852(5)	28.8(14)
N10	3057(7)	4843(10)	3428(5)	31.2(16)
N11	3037(8)	5090(13)	-367(5)	42(2)
N12	7271(7)	6028(13)	2201(6)	39.1(18)

Table S2. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn1	21.9(5)	37.1(6)	25.6(5)	-0.4(5)	2.3(4)	0.4(6)
Cl1	25.5(8)	42.2(11)	31.3(9)	6.9(9)	2.1(7)	1.3(8)
Cl2	28.0(9)	35.7(11)	50.9(12)	-5.2(10)	7.5(8)	-3.5(9)
Cl3	29.1(10)	53.0(13)	30.2(9)	-5.9(10)	2.7(7)	7.3(10)
C1	21(3)	32(4)	26(4)	-1(3)	4(3)	1(3)
C2	22(3)	28(4)	22(3)	1(3)	4(3)	4(3)
C3	21(3)	34(4)	20(4)	0(3)	3(3)	0(3)
C4	24(4)	35(4)	20(3)	3(3)	0(3)	-3(3)
C5	21(3)	30(4)	19(3)	-2(3)	1(3)	1(3)
C6	23(4)	33(4)	19(3)	-2(3)	1(3)	0(3)
N1	23(3)	38(4)	19(3)	2(3)	3(2)	-1(3)
N2	22(3)	48(5)	20(3)	-1(3)	2(2)	4(3)
N3	17(3)	37(4)	16(3)	0(3)	2(2)	1(3)
N4	22(3)	81(6)	15(3)	5(3)	1(2)	14(3)
N5	23(3)	75(6)	25(3)	3(4)	2(3)	5(4)
N6	24(3)	56(5)	17(3)	1(3)	3(2)	6(3)
N7	17(3)	44(4)	25(3)	-2(3)	1(2)	-1(3)
N8	21(3)	47(4)	19(3)	0(3)	2(2)	-1(3)
N9	26(3)	38(4)	22(3)	-1(3)	5(2)	1(3)
N10	25(3)	44(5)	25(3)	2(3)	6(3)	-2(3)
N11	24(3)	77(6)	21(3)	-1(3)	-2(3)	-6(3)
N12	22(3)	64(5)	30(4)	6(4)	3(3)	-4(4)

Table S3. Bond Lengths for compound 1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn1	Cl1	2.282(2)	N9	C5	1.316(9)
Zn1	Cl2	2.260(3)	N8	C6	1.319(9)
Zn1	Cl3	2.269(2)	N9	C4	1.355(9)
Zn1	N3	2.057(6)	N8	C4	1.353(9)
N1	C1	1.336(10)	N6	C2	1.316(9)
N1	C2	1.340(9)	N11	C6	1.307(9)
N2	C1	1.349(9)	N12	C4	1.305(10)
N2	C3	1.319(9)	N4	C3	1.327(9)
N3	C2	1.369(9)	N7	C5	1.374(9)
N3	C3	1.356(9)	N7	C6	1.368(9)
N10	C5	1.316(9)	N5	C1	1.313(10)

Table S4. Bond Angles for compound 1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl3	Zn1	Cl1	107.53(10)	N6	C2	N1	117.4(7)
Cl2	Zn1	Cl1	107.01(9)	N2	C3	N3	124.7(7)
Cl2	Zn1	Cl3	115.20(10)	N2	C3	N4	117.3(7)
N3	Zn1	Cl1	113.18(18)	N4	C3	N3	117.9(7)
N3	Zn1	Cl3	111.75(18)	N10	C5	N9	120.8(7)
N3	Zn1	Cl2	102.2(2)	N10	C5	N7	118.4(7)
C2	N3	Zn1	122.4(5)	N9	C5	N7	120.7(7)
C3	N3	Zn1	122.2(5)	N8	C6	N7	121.0(6)
C3	N3	C2	115.2(6)	N11	C6	N8	120.6(7)
C1	N1	C2	116.2(6)	N11	C6	N7	118.3(7)
C3	N2	C1	116.0(6)	N8	C4	N9	124.7(7)
C5	N9	C4	117.1(6)	N12	C4	N9	117.4(7)
C6	N8	C4	116.8(6)	N12	C4	N8	117.9(7)
C6	N7	C5	119.4(6)	N1	C1	N2	124.5(7)
N1	C2	N3	123.3(6)	N5	C1	N1	118.1(7)
N6	C2	N3	119.2(6)	N5	C1	N2	117.4(7)

Table S5. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for compound 1.

Atom	*x*	*y*	*z*	U(eq)
H4A	6371.87	5322.84	4542.08	48
H4B	7751.81	4842.53	5351.99	48
H5A	2195.93	6398.66	6999.14	50
H5B	2191.16	6319.94	5772.26	50
H6A	6352.49	5100.81	9544.39	39
H6B	7722.84	4574.24	9166.33	39
H7	2146.35	4532.24	1378.58	35
H10A	3495.69	4969.75	4119.71	37
H10B	2142.69	4554.08	3265.69	37
H11A	3470.72	5276.17	-918.28	50
H11B	2113.21	4861.61	-495.66	50
H12A	7738.44	6151.01	1664.19	47
H12B	7726.77	6142.34	2889.22	47

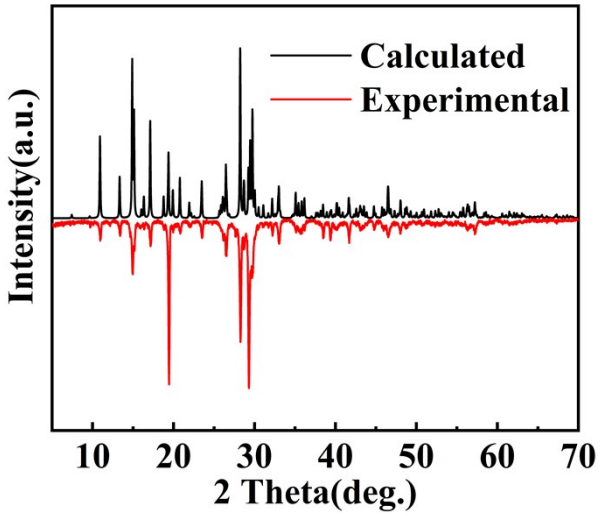

Figure S1. The Powder X-ray diffraction of compound **1**.

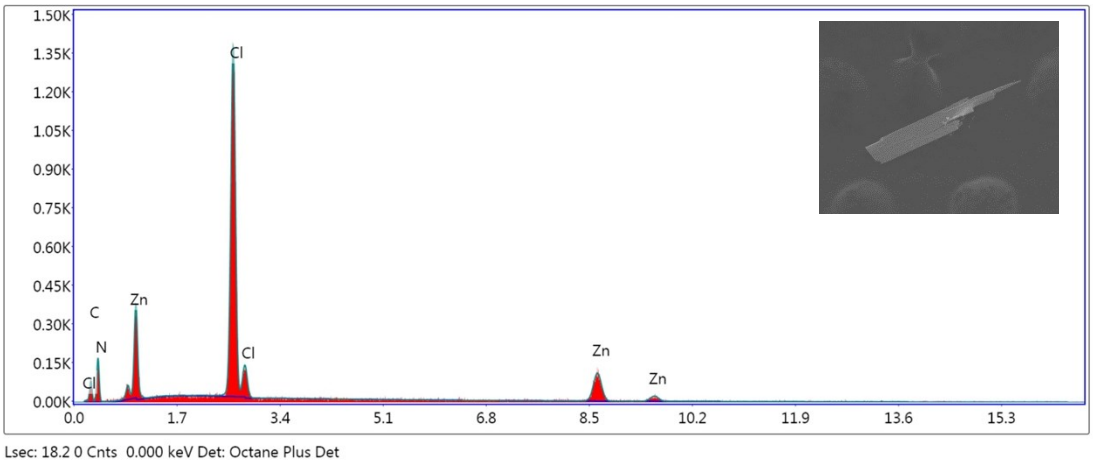

Figure S2. The Energy-dispersive X-ray Spectroscopy of compound **1**.

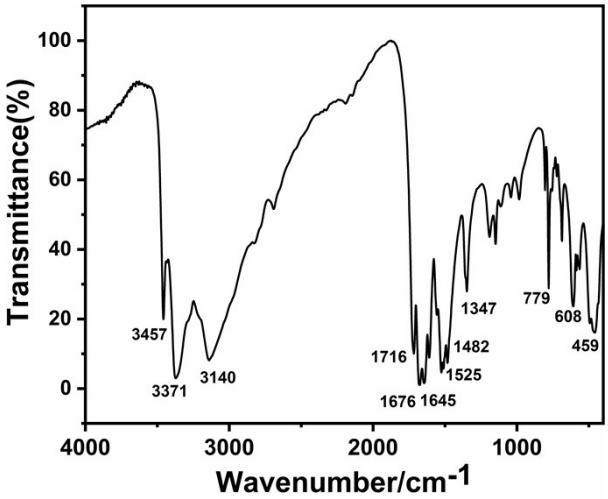

Figure S3. Room temperature powder IR spectrum of compound **1**.

Table S6 Wavenumbers of the bands observed in the powder infrared spectra of compound **1**.

Wavenumbers (cm^{-1})	Tentative assignment
3457	NH_2 asym stretch
3371	NH_2 asym stretch and N-H…Cl stretch
3140	N-H…N stretch
1716, 1676, 1645	NH_2 bend
1525, 1482	Side-chain asym C-N stretch
1347	Ring: semi-circle stretch
779	Side-chain out-of-plane C-N bend
608	NH_2 bend
459	Combination tone: NH_2 bend-NH_2 rock

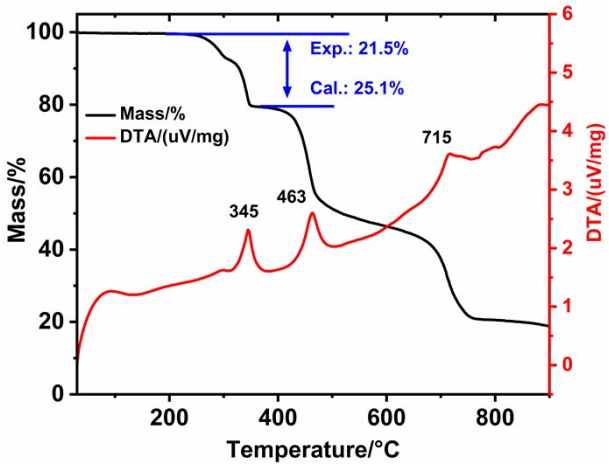

Figure S4. The thermal gravimetric analysis (TGA) and differential thermal analysis (DTA) curves of compound **1**.

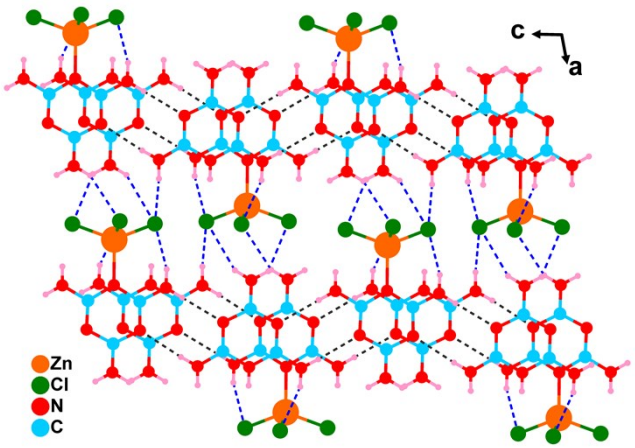

Figure S5. The H-Bonds of compound **1**.

Table S7. Hydrogen-bonding geometry (A, °) of compound 1.

Donor --- H...Acceptor	[ARU]	D - H	H...A	D...A	D - H...A
N4---H4A···N9	[1555.02]	0.86	2.13	2.984(9)	173
N4---H4B···Cl3	[-]	0.86	2.41	3.198(8)	152
N5---H5A···Cl2	[1455.01]	0.86	2.52	3.306(7)	153
N5---H5B···Cl3	[2656.01]	0.86	2.73	3.544(8)	158
N6---H6A···N8	[1556.02]	0.86	2.14	2.996(9)	178
N6---H6B···Cl1	[-]	0.86	2.49	3.297(7)	156
N7---H7···Cl1	[2656.01]	0.86	2.78	3.274(7)	118
N7---H7···Cl2	[2646.01]	0.86	2.82	3.547(7)	143
N10---H10A···N2	[1555.01]	0.86	2.16	3.017(9)	175
N10---H10B···Cl2	[2646.01]	0.86	2.57	3.356(7)	152
N11---H11A···N1	[1554.01]	0.86	2.18	3.034(9)	175
N11---H11B···Cl1	[1454.01]	0.86	2.54	3.328(8)	152
N12---H12A···Cl1	[2756.01]	0.86	2.69	3.447(7)	148
N12---H12B···Cl3	[2756.01]	0.86	2.63	3.312(7)	137

Translation of ARU-Code to CIF and Equivalent Position Code：

[2646.] = [2_646] = 1-x, -1/2 +y, 1-z; [1556.] = [1_556] = x, y, 1 +z; [1455.] = [1_455] = -1 +x, y, z'; [2656.] = [2_656] = 1-x, 1/2 +y, 1-z; [1554.] = [1_554] = x, y, -1 +z; [1454.] = [1_454] = -1 +x, y, -1 +z; [2756.] = [2_756] = 2-x, 1/2 +y, 1-z.

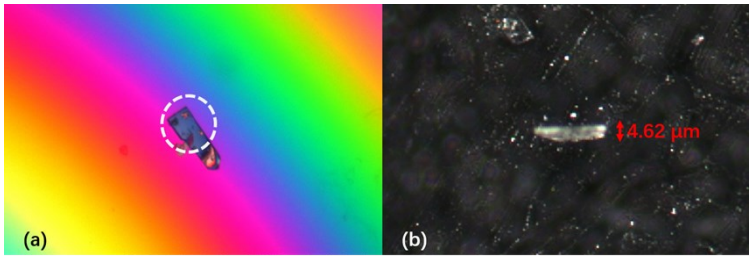

Figure S6. (a)Compound **1** achieving extinction. (b)The thickness of the crystal.

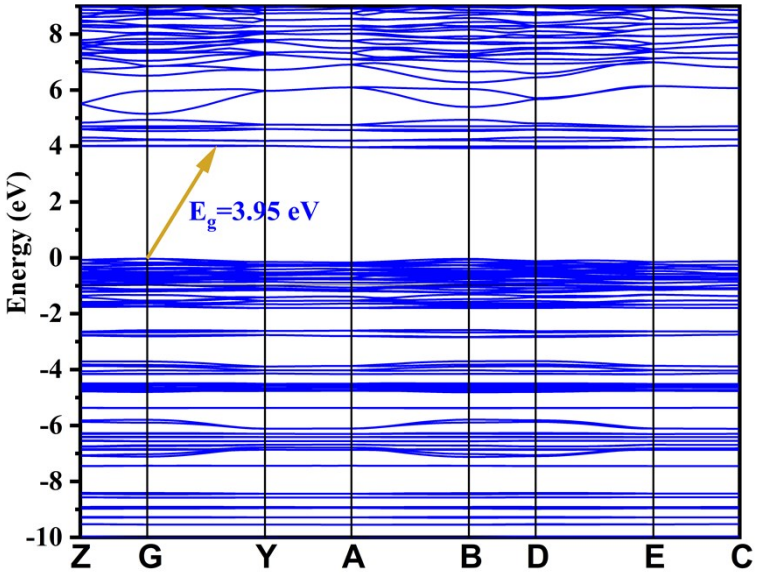

Figure. S7 Electronic band structures of compound **1**.

Table S8. Calculation of dipole moment for [$ZnNCl_3$] polyhedral for unit cells.

Species	x-component	y-component	z-component	Total magnitude
[Zn(1)NCl_3]	-3.3878598	0.2800433	-1.42552	3.686207
[Zn(2)NCl_3]	3.3878924	0.2800701	1.425489	3.686228