Supporting Information

Violet Light Excitable Organic Halides with Short ~ns Emissions for Multiple Optoelectronic Applications

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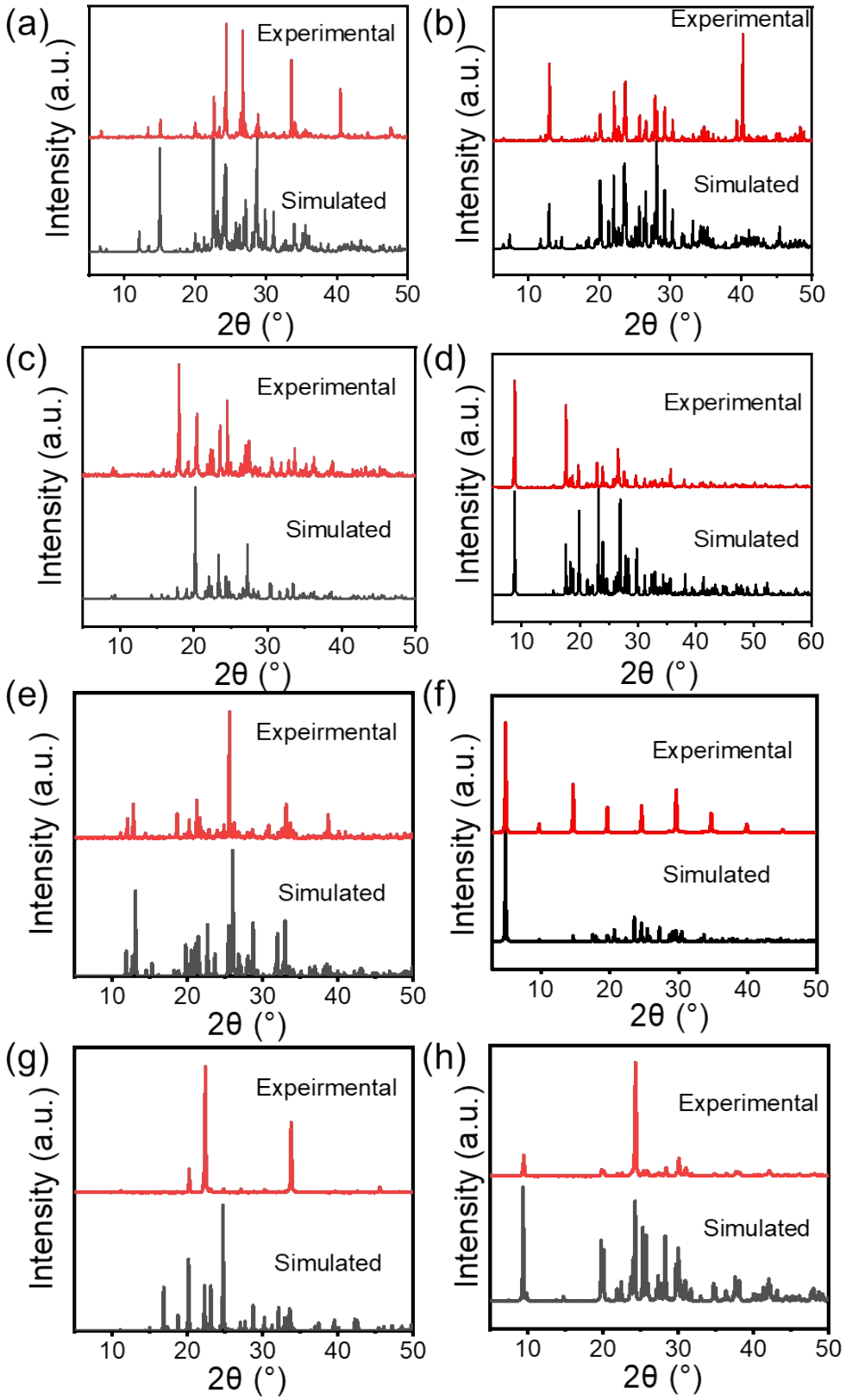

Fig. S1. Powder X-ray diffraction patterns of (a) MXDA-Cl, (b) MXDA-Br, (c) OHPEA-Cl, (d) OHPEA-Br, (e) 4AMP-Cl, (f) MPEA-Br, (g) 2ABT-Cl, (h) APEA-Br, and corresponding simulated patterns.

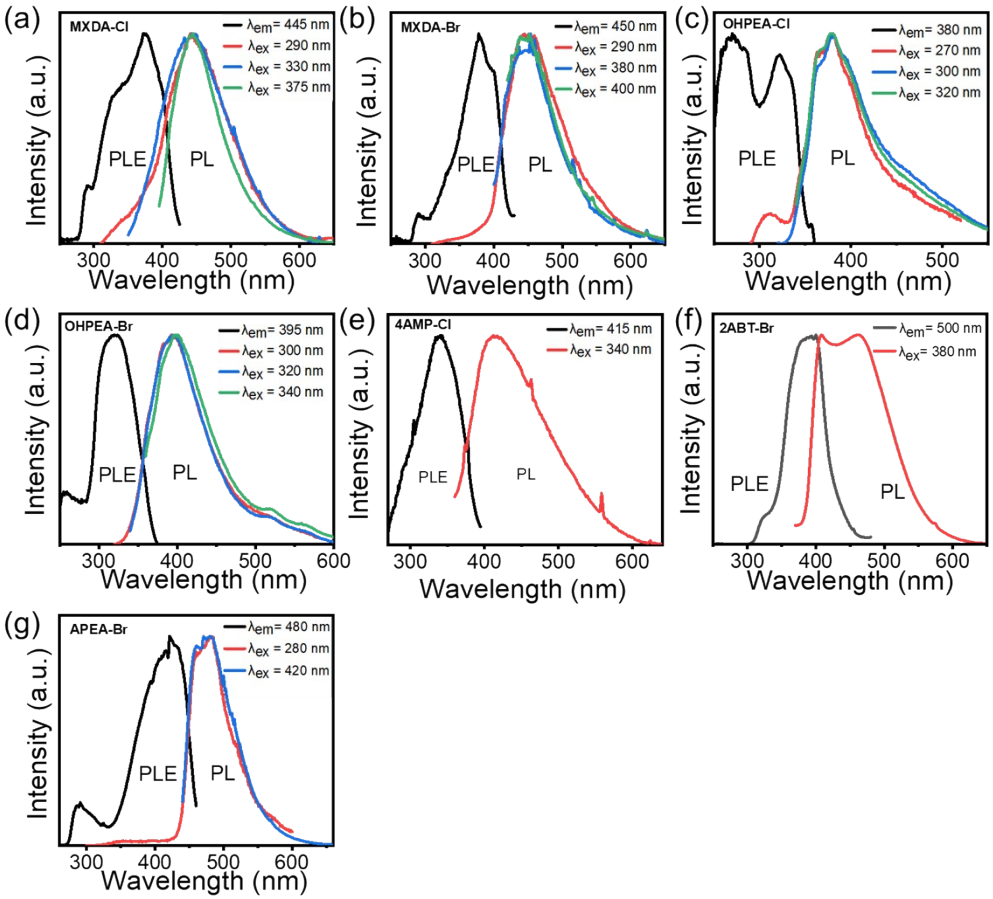

Fig. S2. Excitation and emission spectra of powder X-ray diffraction patterns of (a) MXDA-Cl, (b) MXDA-Br, (c) OHPEA-Cl, (d) OHPEA-Br, (e) 4AMP-Br, (f) 2ABT-Cl, (g) APEA-Br.

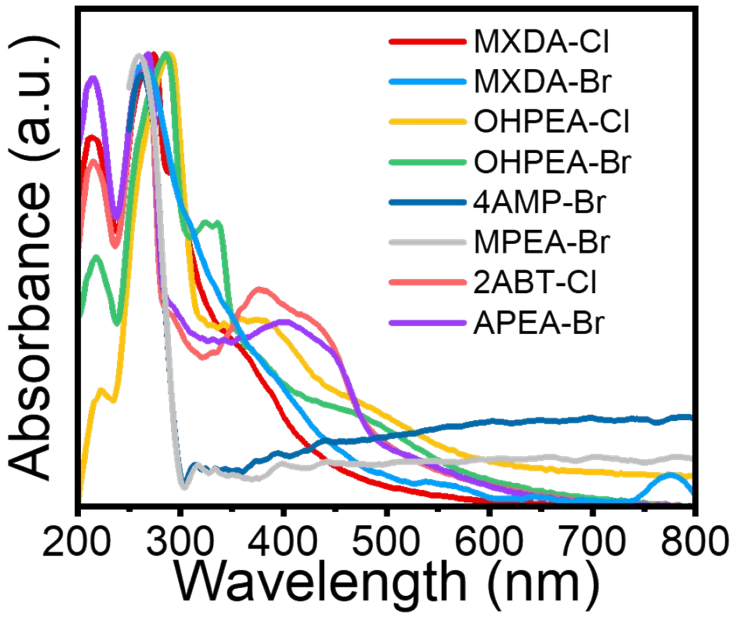

Fig. S3. Absorbance spectra of MXDA-Cl, MXDA-Br, OHPEA-Cl, OHPEA-Br, 4AMP-Cl, MPEA-Br, 2ABT-Cl, and APEA-Br.

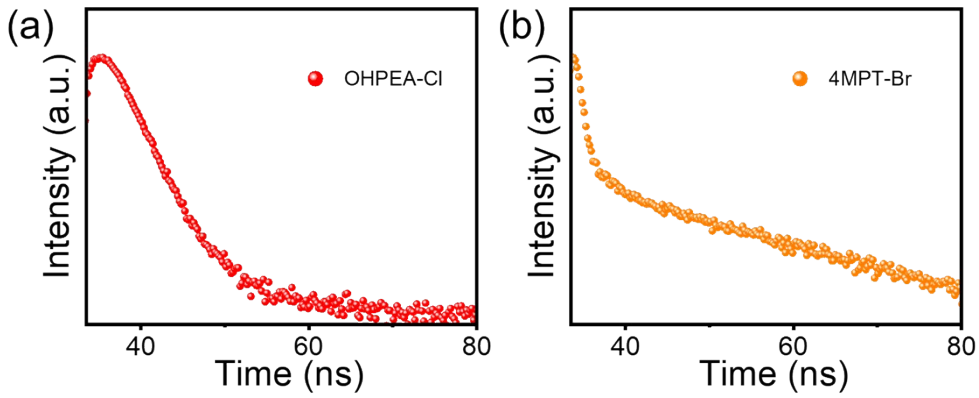

Fig. S4. Photoluminescence lifetime decay curves of OHPEA-Cl and 4MPT-Br.

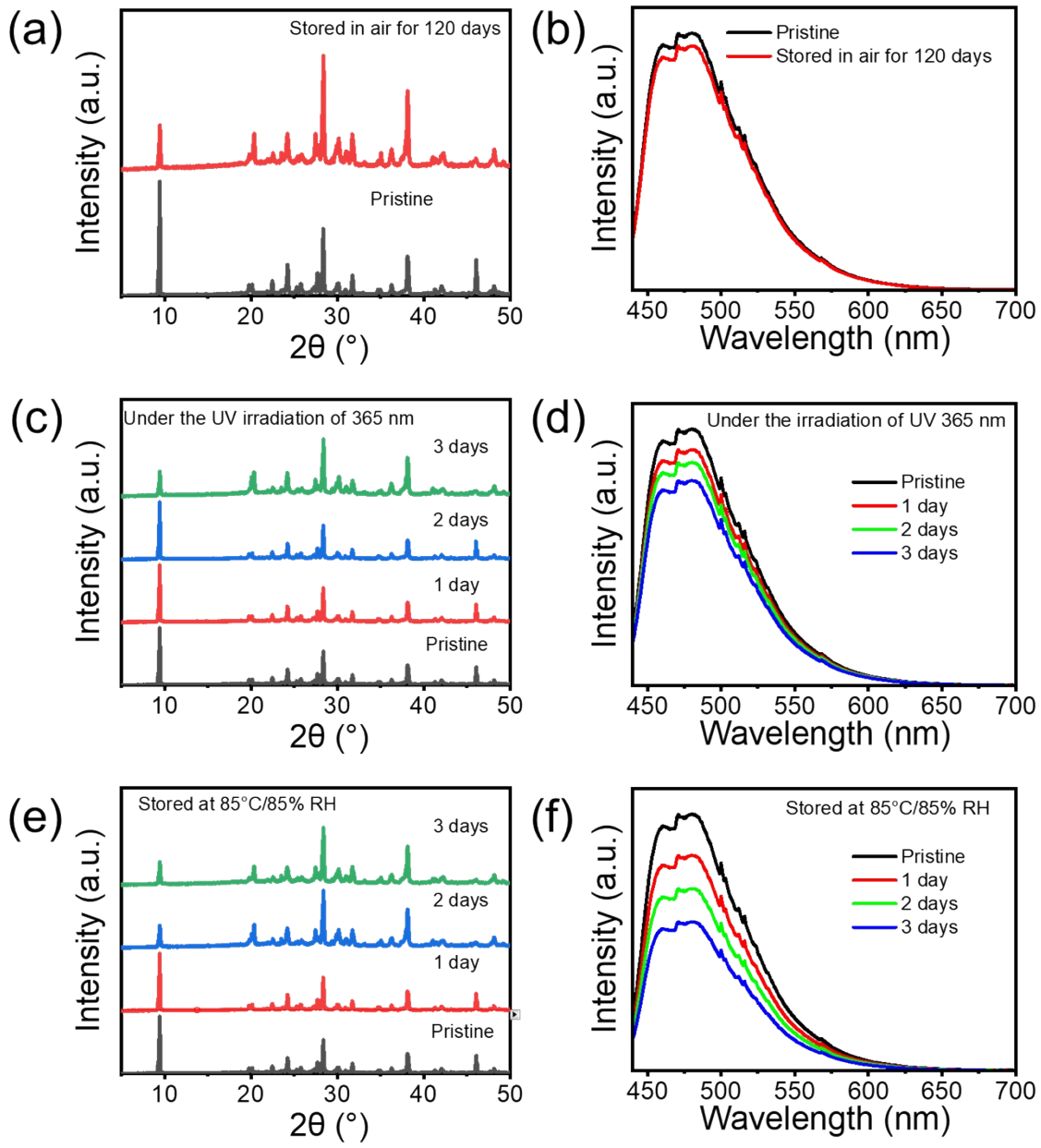

Fig. S5 Powder X-ray diffraction patterns and Photoluminescence spectra of APEA-Br preserved under different conditions ((a, b) Stored in air for 120 days; (c, d) Under the irradiation of UV 365 nm; (e, f) Stored at 85℃/85% RH).).

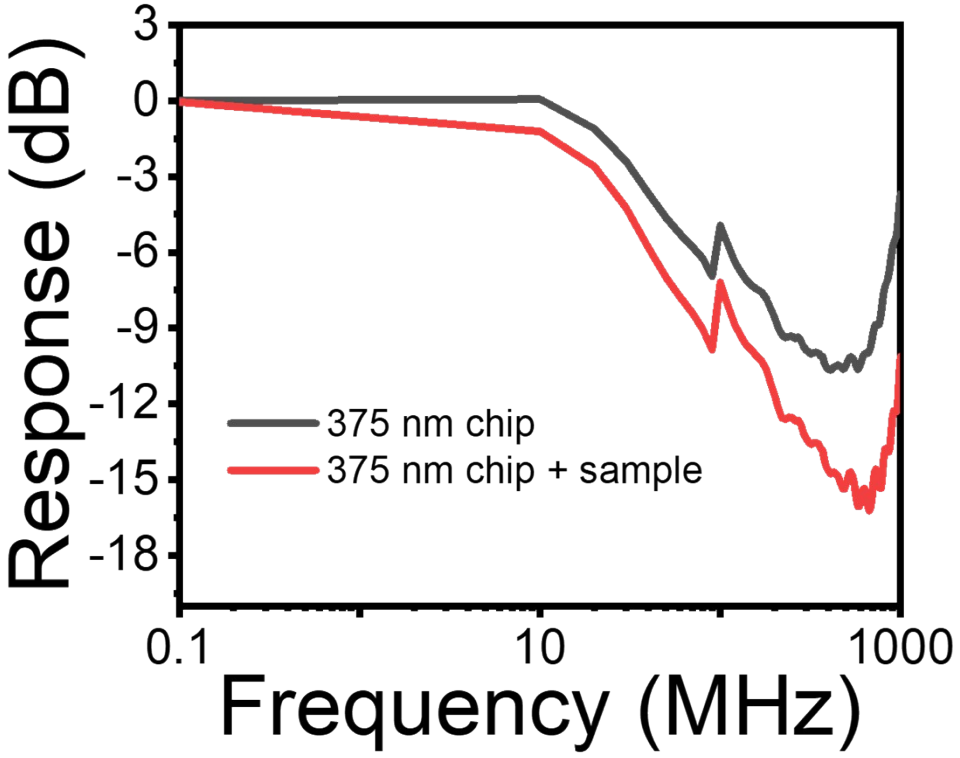

Fig. S6 Electrical-optical-electrical (EOE) frequency response of the VLC system under high-frequency.

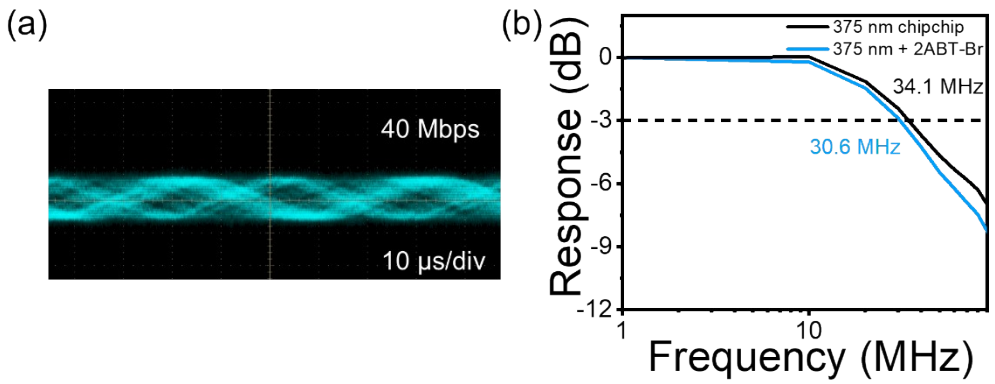

Fig. S7 (a) Opened-eye diagrams of the VLC experiment constructed by 2ABT-Br operating at transmission rates of 40 Mbps. (b) Electrical-optical-electrical (EOE) frequency response of the system.

Table S1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for 4AMP-Cl at 298.00 K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}*
Cl(2)	18(2)	4032(1)	6097(1)	1	52(1)
Cl(1)	5112(2)	6012(1)	6626(1)	1	53(1)
N(1)	4321(3)	4129(2)	6208(2)	1	49(1)
H(1A)	4637	4667	6246	1	59
H(1B)	3085	4099	6217	1	59
N(2)	5518(3)	905(2)	6565(2)	1	53(1)
H(2A)	5260	372	6460	1	64
H(2B)	5033	1039	7014	1	64
H(2C)	6745	976	6580	1	64
C(6)	4518(4)	2877(2)	5407(2)	1	46(1)
H(6A)	5027	2659	4936	1	55
H(6B)	3177	2816	5386	1	55
C(2)	5270(4)	2367(2)	6068(2)	1	41(1)
H(2)	6631	2401	6060	1	49
C(1)	4715(4)	1451(2)	5972(2)	1	47(1)
H(1C)	3370	1407	5988	1	57
H(1D)	5125	1256	5478	1	57
C(3)	4585(4)	2747(2)	6812(2)	1	50(1)
H(3A)	3246	2683	6845	1	59
H(3B)	5138	2448	7235	1	59
C(5)	5001(4)	3797(2)	5474(2)	1	48(1)
H(5A)	6339	3868	5442	1	58
H(5B)	4435	4106	5060	1	58
C(4)	5078(4)	3666(2)	6867(2)	1	52(1)
H(4A)	4572	3898	7333	1	62
H(4B)	6419	3729	6882	1	62

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Anisotropic displacement parameters ($Å^2x10^3$) for 4AMP-Cl at 298.00 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl(2)	50(1)	57(1)	50(1)	0(1)	0(1)	-10(1)
Cl(1)	61(1)	52(1)	47(1)	0(1)	-2(1)	-5(1)
N(1)	48(2)	46(2)	53(2)	-8(2)	-2(2)	-2(2)
N(2)	61(2)	47(2)	51(2)	-4(2)	7(2)	-4(2)
C(6)	46(2)	59(2)	33(2)	3(2)	-1(2)	-3(2)
C(2)	32(2)	52(2)	39(2)	-3(2)	-2(2)	-3(2)
C(1)	48(2)	53(2)	42(2)	-1(2)	-3(2)	-4(2)
C(3)	59(2)	55(2)	35(2)	-5(2)	3(2)	1(2)
C(5)	51(2)	59(2)	35(2)	-1(2)	-1(2)	6(2)
C(4)	61(2)	58(2)	36(2)	-7(2)	-2(2)	-3(2)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S3. Bond lengths [Å] for 4AMP-Cl at 298.00 K with estimated standard deviations in parentheses.

Label	Distances
N(1)-H(1A)	0.8900
N(1)-H(1B)	0.8900
N(1)-C(5)	1.479(4)
N(1)-C(4)	1.479(4)
N(2)-H(2A)	0.8900
N(2)-H(2B)	0.8900
N(2)-H(2C)	0.8900
N(2)-C(1)	1.477(4)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(6)-C(2)	1.520(4)
C(6)-C(5)	1.512(4)
C(2)-H(2)	0.9800
C(2)-C(1)	1.523(4)
C(2)-C(3)	1.525(4)
C(1)-H(1C)	0.9700
C(1)-H(1D)	0.9700
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(3)-C(4)	1.510(4)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700

Symmetry transformations used to generate equivalent atoms:

Table S4. Bond angles [°] for 4AMP-Cl at 298.00 K with estimated standard deviations in parentheses.

Label	Angles
H(1A)-N(1)-H(1B)	107.8
C(5)-N(1)-H(1A)	109.1
C(5)-N(1)-H(1B)	109.1
C(4)-N(1)-H(1A)	109.1
C(4)-N(1)-H(1B)	109.1
C(4)-N(1)-C(5)	112.7(2)
H(2A)-N(2)-H(2B)	109.5
H(2A)-N(2)-H(2C)	109.5
H(2B)-N(2)-H(2C)	109.5
C(1)-N(2)-H(2A)	109.5
C(1)-N(2)-H(2B)	109.5
C(1)-N(2)-H(2C)	109.5
H(6A)-C(6)-H(6B)	107.9
C(2)-C(6)-H(6A)	109.2
C(2)-C(6)-H(6B)	109.2
C(5)-C(6)-H(6A)	109.2
C(5)-C(6)-H(6B)	109.2
C(5)-C(6)-C(2)	112.2(2)
C(6)-C(2)-H(2)	108.3
C(6)-C(2)-C(1)	109.5(2)
C(6)-C(2)-C(3)	109.3(2)
C(1)-C(2)-H(2)	108.3
C(1)-C(2)-C(3)	113.1(2)
C(3)-C(2)-H(2)	108.3
N(2)-C(1)-C(2)	112.6(2)
N(2)-C(1)-H(1C)	109.1
N(2)-C(1)-H(1D)	109.1
C(2)-C(1)-H(1C)	109.1
C(2)-C(1)-H(1D)	109.1
H(1C)-C(1)-H(1D)	107.8
C(2)-C(3)-H(3A)	109.3
C(2)-C(3)-H(3B)	109.3
H(3A)-C(3)-H(3B)	108.0
C(4)-C(3)-C(2)	111.4(2)
C(4)-C(3)-H(3A)	109.3

C(4)-C(3)-H(3B)	109.3
N(1)-C(5)-C(6)	109.9(2)
N(1)-C(5)-H(5A)	109.7
N(1)-C(5)-H(5B)	109.7
C(6)-C(5)-H(5A)	109.7
C(6)-C(5)-H(5B)	109.7
H(5A)-C(5)-H(5B)	108.2
N(1)-C(4)-C(3)	110.3(2)
N(1)-C(4)-H(4A)	109.6
N(1)-C(4)-H(4B)	109.6
C(3)-C(4)-H(4A)	109.6
C(3)-C(4)-H(4B)	109.6
H(4A)-C(4)-H(4B)	108.1

Symmetry transformations used to generate equivalent atoms:

Table S5. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for MPEA-Br at 298.00 K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}*
Br(1)	713(1)	2330(1)	686(1)	1	49(1)
N(1)	712(2)	7264(3)	2203(2)	1	48(1)
H(1A)	785	6029	1716	1	58
H(1B)	654	8363	1556	1	58
H(1C)	307	7137	2683	1	58
C(4)	2656(2)	9025(4)	3651(3)	1	47(1)
C(9)	1356(2)	7698(4)	3286(3)	1	48(1)
H(9A)	1432	6459	3954	1	58
H(9B)	1254	8964	3880	1	58
C(8)	2059(2)	8104(5)	2540(3)	1	52(1)
H(8A)	2228	6744	2136	1	62
H(8B)	1958	9123	1722	1	62
C(3)	3281(2)	7850(5)	4133(3)	1	59(1)
H(3)	3347	6461	3750	1	71
C(5)	2580(2)	11088(5)	4240(3)	1	57(1)
H(5)	2168	11929	3922	1	68
C(6)	3109(2)	11916(5)	5296(4)	1	63(1)
H(6)	3041	13297	5691	1	76
C(2)	3811(2)	8705(6)	5179(4)	1	69(1)
H(2)	4229	7881	5483	1	83
C(1)	3733(2)	10747(5)	5776(3)	1	63(1)
C(7)	4313(2)	11709(7)	6915(4)	1	96(2)
H(7A)	4314	13271	6821	1	144
H(7B)	4791	11147	6745	1	144
H(7C)	4200	11317	7900	1	144

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S6. Anisotropic displacement parameters ($Å^2x10^3$) for MPEA-Br at 298.00 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br(1)	58(1)	38(1)	52(1)	-1(1)	12(1)	0(1)
N(1)	54(2)	41(2)	51(2)	-2(1)	12(1)	-5(1)
C(4)	48(2)	49(2)	44(2)	3(2)	14(2)	3(2)
C(9)	58(2)	47(2)	42(2)	-5(2)	10(2)	-2(2)
C(8)	54(2)	57(2)	46(2)	2(2)	12(2)	-1(2)
C(3)	65(2)	56(2)	57(2)	12(2)	11(2)	-4(2)
C(5)	53(2)	49(2)	68(2)	4(2)	10(2)	-1(2)
C(6)	68(2)	52(2)	72(2)	-6(2)	20(2)	-10(2)
C(2)	55(2)	84(2)	67(2)	15(2)	0(2)	6(2)
C(1)	54(2)	76(2)	60(2)	-10(2)	12(2)	-1(2)
C(7)	76(3)	130(4)	82(3)	-25(2)	3(2)	-19(2)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S7. Bond lengths [Å] for MPEA-Br at 298.00 K with estimated standard deviations in parentheses.

Label	Distances
N(1)-H(1A)	0.8900
N(1)-H(1B)	0.8900
N(1)-H(1C)	0.8900
N(1)-C(9)	1.476(3)
C(4)-C(8)	1.513(4)
C(4)-C(3)	1.378(4)
C(4)-C(5)	1.382(4)
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(9)-C(8)	1.517(4)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(3)-H(3)	0.9300
C(3)-C(2)	1.385(4)
C(5)-H(5)	0.9300
C(5)-C(6)	1.384(4)
C(6)-H(6)	0.9300
C(6)-C(1)	1.375(4)
C(2)-H(2)	0.9300
C(2)-C(1)	1.373(4)
C(1)-C(7)	1.519(4)
C(7)-H(7A)	0.9600
C(7)-H(7B)	0.9600
C(7)-H(7C)	0.9600

Symmetry transformations used to generate equivalent atoms:

Table S8. Bond angles [°] for MPEA-Br at 298.00 K with estimated standard deviations in parentheses.

Label	Angles
H(1A)-N(1)-H(1B)	109.5
H(1A)-N(1)-H(1C)	109.5
H(1B)-N(1)-H(1C)	109.5
C(9)-N(1)-H(1A)	109.5
C(9)-N(1)-H(1B)	109.5
C(9)-N(1)-H(1C)	109.5
C(3)-C(4)-C(8)	122.1(2)
C(3)-C(4)-C(5)	117.7(3)
C(5)-C(4)-C(8)	120.2(3)
N(1)-C(9)-H(9A)	109.1
N(1)-C(9)-H(9B)	109.1
N(1)-C(9)-C(8)	112.6(2)
H(9A)-C(9)-H(9B)	107.8
C(8)-C(9)-H(9A)	109.1
C(8)-C(9)-H(9B)	109.1
C(4)-C(8)-C(9)	110.4(2)
C(4)-C(8)-H(8A)	109.6
C(4)-C(8)-H(8B)	109.6
C(9)-C(8)-H(8A)	109.6
C(9)-C(8)-H(8B)	109.6
H(8A)-C(8)-H(8B)	108.1
C(4)-C(3)-H(3)	119.5
C(4)-C(3)-C(2)	121.1(3)
C(2)-C(3)-H(3)	119.5
C(4)-C(5)-H(5)	119.7
C(4)-C(5)-C(6)	120.7(3)
C(6)-C(5)-H(5)	119.7
C(5)-C(6)-H(6)	119.2
C(1)-C(6)-C(5)	121.6(3)
C(1)-C(6)-H(6)	119.2
C(3)-C(2)-H(2)	119.4
C(1)-C(2)-C(3)	121.3(3)
C(1)-C(2)-H(2)	119.4
C(6)-C(1)-C(7)	120.6(3)
C(2)-C(1)-C(6)	117.6(3)

C(2)-C(1)-C(7)	121.8(3)
C(1)-C(7)-H(7A)	109.5
C(1)-C(7)-H(7B)	109.5
C(1)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S9. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for 2ABT-Br at 304.00 K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}*
Br(1)	5124(2)	3669(1)	899(1)	1	74(1)
S(1)	7164(2)	6362(1)	5785(2)	1	47(1)
N(1)	5610(9)	6573(5)	2793(6)	1	52(2)
H(1A)	6164.07	6500.76	2052.5	1	63
H(1B)	5750.44	7176.95	3113.54	1	63
H(1C)	4330.77	6430.27	2447.44	1	63
N(2)	6855(7)	5086(4)	3755(5)	1	42(2)
H(2)	6567.39	4805.84	2888.37	1	51
C(1)	6466(8)	6007(4)	3909(6)	1	39(2)
C(2)	7761(8)	4613(4)	5102(6)	1	42(2)
C(3)	8306(10)	3664(4)	5264(9)	1	54(2)
H(3)	8075.06	3263.1	4425.84	1	65
C(4)	9215(12)	3321(6)	6721(10)	1	69(2)
H(4)	9598.92	2682.92	6861.49	1	82
C(5)	9556(13)	3930(7)	7976(10)	1	75(2)
H(5)	10192.53	3697.26	8940.39	1	90
C(6)	8950(12)	4875(7)	7789(8)	1	67(2)
H(6)	9138.05	5274.77	8624.12	1	80
C(7)	8062(8)	5218(5)	6343(6)	1	46(2)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S10. Anisotropic displacement parameters ($Å^2x10^3$) for 2ABT-Br at 304.00 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br(1)	148(2)	40(1)	29(1)	-8(1)	18(1)	-6(1)
S(1)	65(1)	48(1)	28(1)	-3(1)	12(1)	-11(1)
N(1)	70(3)	53(3)	32(3)	7(2)	11(2)	-5(2)
N(2)	49(2)	49(3)	29(2)	-7(2)	12(2)	-13(2)
C(1)	45(3)	41(3)	33(3)	-9(2)	13(2)	-7(2)
C(2)	42(3)	49(3)	35(3)	-4(2)	12(2)	-5(2)
C(3)	50(3)	48(4)	64(5)	-1(2)	18(3)	-4(3)
C(4)	64(4)	63(4)	76(5)	13(3)	16(4)	17(4)
C(5)	72(5)	91(6)	51(5)	4(4)	1(4)	18(4)
C(6)	77(5)	84(6)	33(3)	5(4)	6(3)	-2(3)
C(7)	51(3)	56(3)	31(3)	-4(2)	13(2)	-4(3)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S11. Bond lengths [Å] for 2ABT-Br at 304.00 K with estimated standard deviations in parentheses.

Label	Distances
S(1)-C(1)	1.729(5)
S(1)-C(7)	1.742(7)
N(1)-H(1A)	0.8900
N(1)-H(1B)	0.8900
N(1)-H(1C)	0.8900
N(1)-C(1)	1.299(8)
N(2)-H(2)	0.8600
N(2)-C(1)	1.333(8)
N(2)-C(2)	1.387(8)
C(2)-C(3)	1.378(9)
C(2)-C(7)	1.389(8)
C(3)-H(3)	0.9300
C(3)-C(4)	1.395(11)
C(4)-H(4)	0.9300
C(4)-C(5)	1.400(14)
C(5)-H(5)	0.9300
C(5)-C(6)	1.385(14)
C(6)-H(6)	0.9300
C(6)-C(7)	1.383(9)

Symmetry transformations used to generate equivalent atoms:

Table S12. Bond angles [°] for 2ABT-Br at 304.00 K with estimated standard deviations in parentheses.

Label	Angles
C(1)-S(1)-C(7)	90.2(3)
H(1A)-N(1)-H(1B)	109.5
H(1A)-N(1)-H(1C)	109.5
H(1B)-N(1)-H(1C)	109.5
C(1)-N(1)-H(1A)	109.5
C(1)-N(1)-H(1B)	109.5
C(1)-N(1)-H(1C)	109.5
C(1)-N(2)-H(2)	122.6
C(1)-N(2)-C(2)	114.8(5)
C(2)-N(2)-H(2)	122.6
N(1)-C(1)-S(1)	123.3(5)
N(1)-C(1)-N(2)	124.5(5)
N(2)-C(1)-S(1)	112.2(4)
N(2)-C(2)-C(7)	111.6(5)
C(3)-C(2)-N(2)	126.6(6)
C(3)-C(2)-C(7)	121.8(6)
C(2)-C(3)-H(3)	121.0
C(2)-C(3)-C(4)	118.0(7)
C(4)-C(3)-H(3)	121.0
C(3)-C(4)-H(4)	119.7
C(3)-C(4)-C(5)	120.6(7)
C(5)-C(4)-H(4)	119.7
C(4)-C(5)-H(5)	119.8
C(6)-C(5)-C(4)	120.4(8)
C(6)-C(5)-H(5)	119.8
C(5)-C(6)-H(6)	120.4
C(7)-C(6)-C(5)	119.1(8)
C(7)-C(6)-H(6)	120.4
C(2)-C(7)-S(1)	111.1(5)
C(6)-C(7)-S(1)	128.7(6)
C(6)-C(7)-C(2)	120.1(7)

Symmetry transformations used to generate equivalent atoms:

Table S13. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for APEA-Br at 297.00 K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}*
Br(1B)	6865(2)	11594(1)	4267(1)	1	43(1)
Br(2B)	13077(2)	9056(1)	1064(1)	1	45(1)
N(2N)	10585(10)	9025(5)	3477(3)	1	39(2)
H(2NA)	11729	9024	2914	1	47
H(2NB)	11650	8986	4054	1	47
H(2NC)	9877	9814	3685	1	47
N(1N)	-613(10)	1640(5)	1673(4)	1	43(2)
H(1NA)	-1679	1567	1056	1	51
H(1NB)	-1758	1743	2244	1	51
H(1NC)	104	860	1561	1	51
C(3C)	6647(11)	5146(6)	2424(4)	1	36(2)
C(1C)	8085(12)	7778(6)	3104(5)	1	40(2)
H(1CA)	6869	7845	2499	1	48
H(1CB)	6857	7771	3721	1	48
C(6C)	1865(12)	2881(5)	1935(4)	1	36(2)
C(7C)	2911(13)	3608(6)	3031(5)	1	48(2)
H(7C)	2026	3340	3609	1	57
C(4C)	5543(13)	4397(6)	1333(4)	1	48(2)
H(4C)	6424	4664	755	1	58
C(2C)	9191(12)	6428(6)	2711(5)	1	45(2)
H(2CA)	10545	6400	3294	1	54
H(2CB)	10275	6399	2053	1	54
C(5C)	3177(13)	3267(6)	1076(5)	1	48(2)
H(5C)	2472	2770	333	1	57
C(8C)	5276(14)	4734(7)	3266(5)	1	53(2)
H(8C)	5972	5233	4010	1	64

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S14. Anisotropic displacement parameters ($Å^2x10^3$) for APEA-Br at 297.00 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br(1B)	46(1)	47(1)	37(1)	7(1)	5(1)	18(1)
Br(2B)	47(1)	52(1)	31(1)	3(1)	4(1)	13(1)
N(2N)	43(3)	40(3)	32(2)	4(2)	8(2)	11(2)
N(1N)	40(3)	43(3)	39(3)	0(2)	2(2)	11(2)
C(3C)	27(3)	39(3)	43(3)	7(2)	4(2)	14(3)
C(1C)	37(3)	36(3)	47(3)	0(2)	-1(3)	16(3)
C(6C)	34(3)	30(3)	42(3)	7(2)	2(2)	7(2)
C(7C)	56(4)	50(4)	36(3)	0(3)	2(3)	20(3)
C(4C)	50(4)	55(4)	31(3)	-3(3)	7(3)	11(3)
C(2C)	37(3)	41(3)	50(4)	-3(3)	-3(3)	11(3)
C(5C)	49(4)	48(4)	36(3)	0(3)	5(3)	5(3)
C(8C)	61(4)	51(4)	36(3)	-10(3)	-12(3)	13(3)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S15. Bond lengths [Å] for APEA-Br at 297.00 K with estimated standard deviations in parentheses.

Label	Distances
N(2N)-H(2NA)	0.8900
N(2N)-H(2NB)	0.8900
N(2N)-H(2NC)	0.8900
N(2N)-C(1C)	1.482(6)
N(1N)-H(1NA)	0.8900
N(1N)-H(1NB)	0.8900
N(1N)-H(1NC)	0.8900
N(1N)-C(6C)	1.474(6)
C(3C)-C(4C)	1.377(7)
C(3C)-C(2C)	1.517(7)
C(3C)-C(8C)	1.381(7)
C(1C)-H(1CA)	0.9700
C(1C)-H(1CB)	0.9700
C(1C)-C(2C)	1.497(8)
C(6C)-C(7C)	1.372(7)
C(6C)-C(5C)	1.378(7)
C(7C)-H(7C)	0.9300
C(7C)-C(8C)	1.371(7)
C(4C)-H(4C)	0.9300
C(4C)-C(5C)	1.372(7)
C(2C)-H(2CA)	0.9700
C(2C)-H(2CB)	0.9700
C(5C)-H(5C)	0.9300
C(8C)-H(8C)	0.9300

Symmetry transformations used to generate equivalent atoms:

Table S16. Bond angles [°] for APEA-Br at 297.00 K with estimated standard deviations in parentheses.

Label	Angles
H(2NA)-N(2N)-H(2NB)	109.5
H(2NA)-N(2N)-H(2NC)	109.5
H(2NB)-N(2N)-H(2NC)	109.5
C(1C)-N(2N)-H(2NA)	109.5
C(1C)-N(2N)-H(2NB)	109.5
C(1C)-N(2N)-H(2NC)	109.5
H(1NA)-N(1N)-H(1NB)	109.5
H(1NA)-N(1N)-H(1NC)	109.5
H(1NB)-N(1N)-H(1NC)	109.5
C(6C)-N(1N)-H(1NA)	109.5
C(6C)-N(1N)-H(1NB)	109.5
C(6C)-N(1N)-H(1NC)	109.5
C(4C)-C(3C)-C(2C)	121.7(5)
C(4C)-C(3C)-C(8C)	117.8(5)
C(8C)-C(3C)-C(2C)	120.4(5)
N(2N)-C(1C)-H(1CA)	109.4
N(2N)-C(1C)-H(1CB)	109.4
N(2N)-C(1C)-C(2C)	111.1(5)
H(1CA)-C(1C)-H(1CB)	108.0
C(2C)-C(1C)-H(1CA)	109.4
C(2C)-C(1C)-H(1CB)	109.4
C(7C)-C(6C)-N(1N)	119.6(5)
C(7C)-C(6C)-C(5C)	120.7(5)
C(5C)-C(6C)-N(1N)	119.7(5)
C(6C)-C(7C)-H(7C)	120.4
C(8C)-C(7C)-C(6C)	119.3(5)
C(8C)-C(7C)-H(7C)	120.4
C(3C)-C(4C)-H(4C)	119.1
C(5C)-C(4C)-C(3C)	121.8(5)
C(5C)-C(4C)-H(4C)	119.1
C(3C)-C(2C)-H(2CA)	109.4
C(3C)-C(2C)-H(2CB)	109.4
C(1C)-C(2C)-C(3C)	111.2(5)
C(1C)-C(2C)-H(2CA)	109.4
C(1C)-C(2C)-H(2CB)	109.4

H(2CA)-C(2C)-H(2CB)	108.0
C(6C)-C(5C)-H(5C)	120.5
C(4C)-C(5C)-C(6C)	118.9(5)
C(4C)-C(5C)-H(5C)	120.5
C(3C)-C(8C)-H(8C)	119.2
C(7C)-C(8C)-C(3C)	121.5(5)
C(7C)-C(8C)-H(8C)	119.2

Symmetry transformations used to generate equivalent atoms: