Electronic Supplementary Information

β-$(C_3H_7N_6)_2Cl_2·H_2O$ and $(C_3H_7N_6)F·H_2O$: two UV birefringent crystals induced by the uniformly aligned structural groups

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Contents

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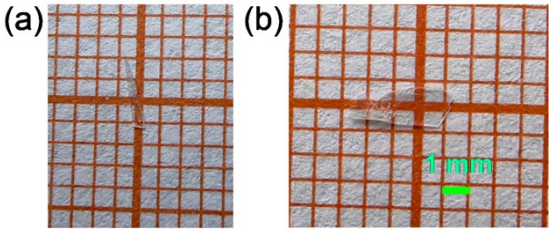

Fig. S1 The as-grown crystals for (a) **MELCl** and (b) **MELF**.

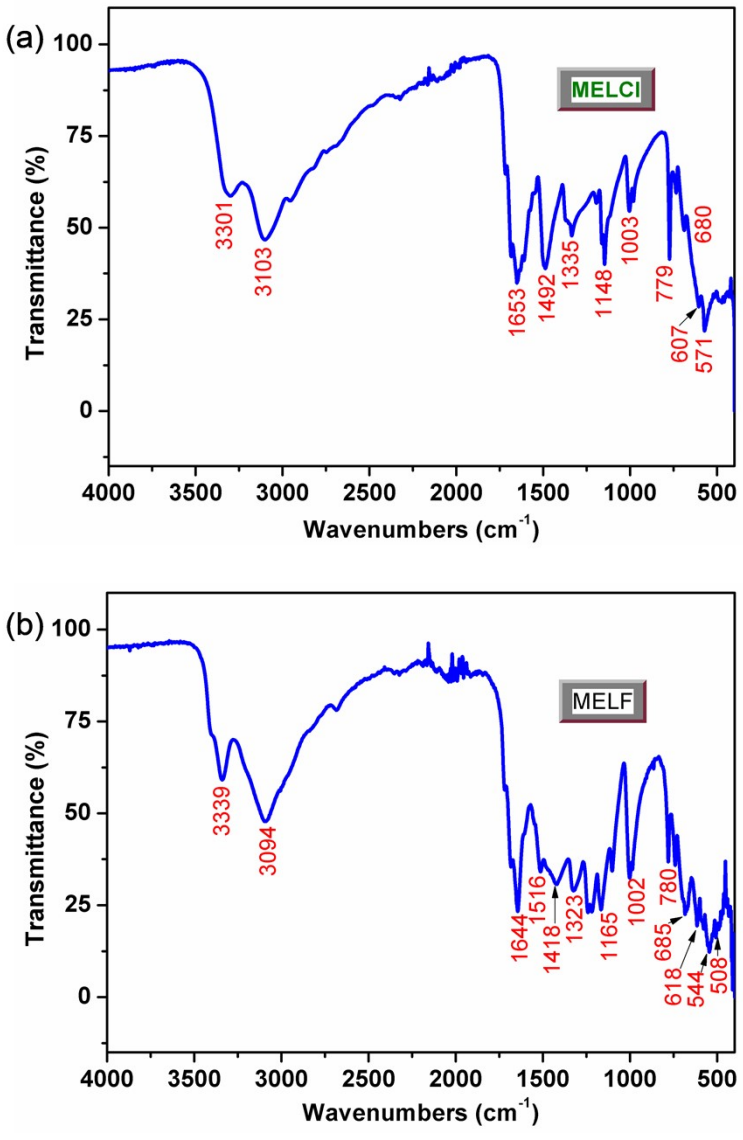

Fig. S2 Infrared spectra for (a) **MELCl** and (b) **MELF**.

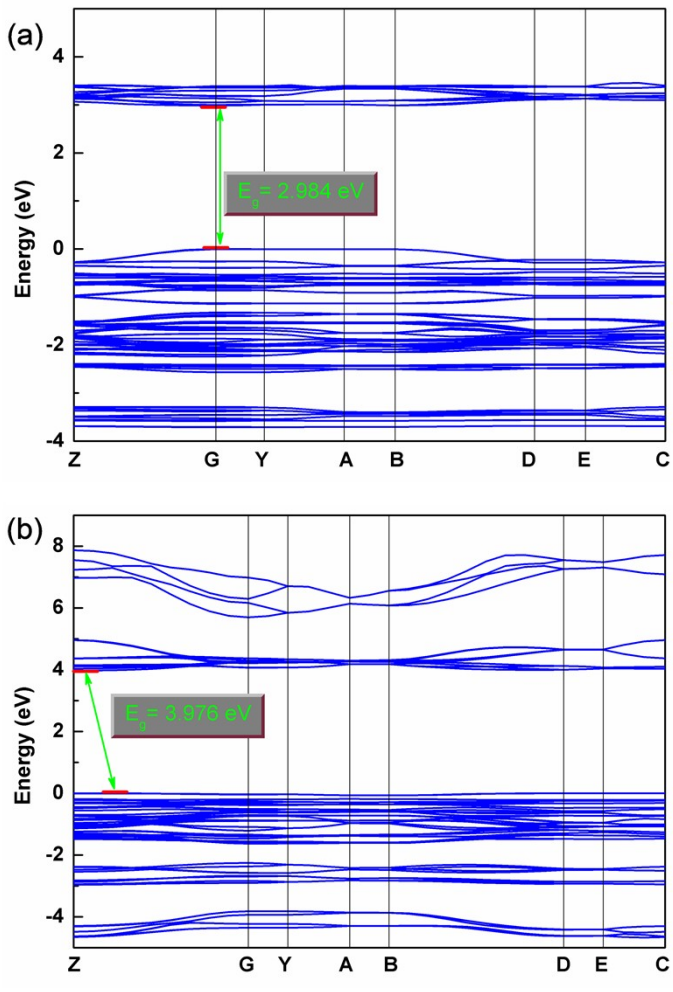

Fig. S3 Electronic band structures for (a) **MELCl** and (b) **MELF**.

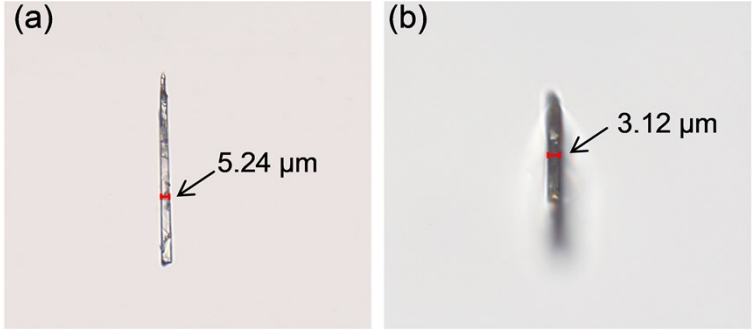

Fig. S4 The crystal thickness for the birefringence measurements (a) **MELCl** and (b) **MELF**.

Table S1. The Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for β-$(C_3H_7N_6)_2Cl_2 \cdot H_2O$. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl	7067.5(9)	5000	772(2)	56.6(4)
Cl2	9431.1(9)	5000	7140.8(14)	44.5(3)
O1	6601(3)	5000	4871(6)	70.8(10)
N1	5000	1566.0(14)	5000	32.3(6)
N2	3108.4(17)	1556.4(10)	4795(3)	37.5(5)
N3	4013.0(15)	2702.5(9)	4938(3)	24.7(4)
N4	5000	3798.2(14)	5000	41.3(8)
C1	4028.7(18)	1954.7(11)	4909(3)	24.7(5)
C2	5000	3052.5(16)	5000	24.0(6)
N5	10000	6522.8(13)	0	30.8(6)
N6	8123.8(17)	6518.0(10)	-116(3)	37.4(5)
N7	9011.2(15)	7659.4(9)	-68(3)	24.3(4)
N8	10000	8755.3(14)	0	38.7(7)
C3	9035.7(18)	6910.6(11)	-62(3)	24.1(5)
C4	10000	8009.2(15)	0	23.4(6)
H1A	6628.99	5000	3567.86	85
H1B	7372.59	5000	5987.16	85
H1	5000	1079.38	5000	39
H2A	2483.03	1782.66	4735.54	45
H2B	3132.33	1070.26	4777.64	45
H4A	5607.2	4041.56	5038	50
H4B	4392.8	4041.56	4962	50
H5	10000	6036.18	0	37
H6A	7505.3	6748.06	-157.77	45
H6B	8146.5	6031.66	-111.07	45
H8A	9391.9	8998.61	-42	46
H8B	10608.1	8998.61	42	46

Table S2. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for β-$(C_3H_7N_6)_2Cl_2 \cdot H_2O$. 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}
Cl	48.8(6)	20.2(4)	122.1(10)	0	56.9(6)	0
Cl2	56.4(6)	20.2(4)	47.2(6)	0	12.5(4)	0
O1	49.0(18)	41.2(15)	134(3)	0	51(2)	0
N1	24.6(13)	17.2(12)	57.9(18)	0	20.3(13)	0
N2	26.6(10)	20.0(9)	72.1(15)	4.0(9)	27.0(10)	-1.3(7)
N3	22.9(9)	20.5(9)	35.5(11)	1.0(7)	17.2(8)	0.1(7)
N4	36.6(16)	20.3(13)	81(2)	0	38.9(16)	0
C1	22.2(11)	22.6(10)	30.4(11)	2.2(8)	12.4(9)	0.6(8)
C2	24.0(15)	21.7(13)	29.5(16)	0	14.3(13)	0
N5	28.6(14)	14.4(11)	53.8(18)	0	21.8(13)	0
N6	30.5(10)	21.7(9)	67.4(15)	0.9(9)	27.8(10)	-4.6(7)
N7	22.4(9)	19.0(8)	36.1(11)	0.8(7)	17.0(8)	-0.1(7)
N8	31.3(15)	17.7(12)	79(2)	0	34.9(15)	0
C3	23.0(11)	22.0(10)	28.9(11)	0.3(8)	12.6(9)	-1.4(8)
C4	23.4(15)	19.6(13)	31.3(16)	0	15.5(13)	0

Table S3. Bond Lengths for β-$(C_3H_7N_6)_2Cl_2 \cdot H_2O$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C1[1]	1.368(2)	N5	C3[2]	1.367(2)
N1	C1	1.368(2)	N5	C3	1.367(2)
N2	C1	1.317(3)	N6	C3	1.317(3)
N3	C1	1.322(3)	N7	C3	1.324(3)
N3	C2	1.359(2)	N7	C4	1.360(2)
N4	C2	1.318(4)	N8	C4	1.319(4)

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

Table S4. Bond Angles for *β*-$(C_3H_7N_6)_2Cl_2 \cdot H_2O$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C1[1]	119.7(2)	C3	N5	C3[2]	119.8(2)
C1	N3	C2	115.87(18)	C3	N7	C4	115.80(18)
N2	C1	N1	117.55(19)	N6	C3	N5	118.10(19)
N2	C1	N3	121.13(19)	N6	C3	N7	120.55(19)
N3	C1	N1	121.32(19)	N7	C3	N5	121.35(18)
N3	C2	N3[1]	125.9(2)	N7[2]	C4	N7	125.9(2)
N4	C2	N3[1]	117.07(12)	N8	C4	N7	117.05(12)
N4	C2	N3	117.07(12)	N8	C4	N7[2]	117.05(12)

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

Table S5. The Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for $(C_3H_7N_6)F\cdot H_2O$. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
sF1	6330(3)	5000	4930(7)	55.2(8)
O1	3098(2)	10000	2131(7)	33.6(7)
N1	5000	6480.9(18)	5000	31.9(8)
N2	5999.4(18)	7691.1(12)	6870(6)	30.7(6)
N3	5000	8859.0(19)	5000	43.3(9)
N4	6905(2)	6473.9(14)	8532(6)	38.2(7)
C1	5984(2)	6892.1(15)	6802(6)	27.4(6)
C2	5000	8063(2)	5000	29.8(8)
H1A	2633.89	10128.6	3704.2	50
H1B	2852.29	10071.5	-68.7	50
H1	4999.99	5962.34	4999.98	38
H3A	4382.5	9118.3	3844.79	52
H3B	5617.5	9118.3	6155.21	52
H4B	7530.13	6717.77	9729.9	46
H4A	6884.8	5955.61	8468.93	46

Table S6. Anisotropic Displacement Parameters (Å^2×10^3) for $(C_3H_7N_6)F\cdot H_2O$. 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}
F1	57.1(16)	29.4(13)	77.2(18)	0	1.7(14)	0
O1	30.2(13)	24.0(13)	43.2(15)	0	-7.8(11)	0
N1	31.6(16)	20.6(15)	41.2(17)	0	-4.5(13)	0
N2	26.6(12)	25.1(12)	38.1(13)	0.4(9)	-5.3(10)	0.6(8)
N3	34.0(17)	23.5(17)	67(2)	0	-15.3(16)	0
N4	36.7(13)	26.0(12)	47.8(14)	3.3(10)	-10.2(11)	2.4(10)
C1	25.4(13)	26.1(14)	30.5(13)	1.3(10)	2.5(11)	0.8(10)
C2	26.1(17)	24.8(18)	37.0(19)	0	-2.0(15)	0

Table S7. Bond Lengths for $(C_3H_7N_6)F\cdot H_2O$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C1[1]	1.363(3)	N2	C2	1.354(3)
N1	C1	1.363(3)	N3	C2	1.320(5)
N2	C1	1.325(3)	N4	C1	1.311(3)
N2	C1	1.325(3)	N4	C1	1.311(3)

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

Table S8. Bond Angles for $(C_3H_7N_6)F{\cdot}H_2O$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1[1]	N1	C1	119.9(3)	N4	C1	N2	120.8(2)
C1	N2	C2	116.0(2)	N2[1]	C2	N2	125.8(3)
N2	C1	N1	121.1(2)	N3	C2	N2[1]	117.09(16)
N4	C1	N1	118.0(2)	N3	C2	N2	117.09(16)

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

Table S9. Hydrogen Bonds for $(C_3H_7N_6)F{\cdot}H_2O$.

D	H	A	d(D−H)/Å	d(H−A)/Å	d(D−A)/Å	D−H−A/°
O1	H1A	F1[1]	0.85	1.54	2.281(4)	144.0
N1	H1	F1	0.86	2.14	2.840(3)	138.2
N1	H1	F1[2]	0.86	2.14	2.840(3)	138.2
N3	H3A	O1	0.86	2.05	2.888(3)	163.0
N3	H3B	O1[2]	0.86	2.05	2.888(3)	163.0
N4	H4A	F1	0.86	2.11	2.829(3)	140.5

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