

Electronic Supplementary Information (ESI) for Dalton Transactions

Facile synthesis of $\text{Sb}^{3+}:(\text{Bmim})_2\text{InCl}_5(\text{H}_2\text{O})$ through a grinding method for light-emitting diodes

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Supporting Tables

Table S1. The single crystal X-ray diffraction data of (Bmim)₂InCl₅(H₂O)

Empirical formula	C ₁₆ H ₃₂ Cl ₅ InN ₄ O
Formula weight	588.52
Temperature/K	173
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	8.7805(3)
b/Å	13.8362(5)
c/Å	21.0836(8)
α /°	90
β /°	96.1830(10)
γ /°	90
Volume/Å ³	2546.52(16)
Z	4
ρ_{calc} / cm ³	1.535
μ / mm ⁻¹	1.466
Radiation	Mo K α (λ = 0.71073)
Reflections collected	74745
Goodness of fit on F ²	1.078
Final R indexes [$I \geq 2\sigma(I)$]	R ₁ = 0.0304, wR ₂ = 0.0640
Final R indexes [all data]	R ₁ = 0.0387, wR ₂ = 0.0679

Table S2. Bond lengths of (Bmim)₂InCl₅(H₂O)

bond	lengths (Å)	bond	lengths (Å)
In1-Cl1	2.4753(6)	N3-C11	1.382(3)
In1-Cl2	2.5441(5)	N3-C13	1.472(3)
In1-Cl4	2.5368(5)	N4-C9	1.462(3)
In1-Cl5	2.4825(5)	N4-C10	1.326(3)
In1-Cl6	2.4518(6)	N4-C12	1.382(3)
In1-O1	2.2984(15)	C9-H9A	0.9800
O1-H1D	0.8695	C9-H9B	0.9800
O1-H1E	0.8701	C9-H9C	0.9800
N1-C3	1.374(3)	C10-H10	0.9500
N1-C4	1.329(3)	C11-H11	0.9500
N1-C5	1.473(3)	C11-C12	1.346(4)
N2-C1	1.466(3)	C12-H12	0.9500
N2-C2	1.370(3)	C13-H13A	0.9900
N2-C4	1.322(3)	C13-H13B	0.9900
C1-H1A	0.9800	C13-C14	1.516(5)
C1-H1B	0.9800	C14-H14C	0.9900
C1-H1C	0.9800	C14-H14D	0.9900
C2-H2	0.9500	C14-H14A	0.9900
C2-C3	1.345(4)	C14-H14B	0.9900
C3-H3	0.9500	C14-C17	1.360(9)
C4-H4	0.9500	C14-C15	1.296(7)
C5-H5A	0.9900	C17-H17A	0.9900
C5-H5B	0.9900	C17-H17B	0.9900
C5-C6	1.514(4)	C17-C18	1.850(15)
C6-H6A	0.9900	C18-H18A	0.9800
C6-H6B	0.9900	C18-H18B	0.9800
C6-C7	1.528(4)	C18-H18C	0.9800

C7-H7A	0.9900	C15-H15A	0.9900
C7-H7B	0.9900	C15-H15B	0.9900
C7-C8	1.507(5)	C15-C16	1.956(13)
C8-H8A	0.9800	C16-H16A	0.9800
C8-H8B	0.9800	C16-H16B	0.9800
C8-H8C	0.9800	C16-H16C	0.9800
N3-C10	1.331(3)		

Table S3. Bond angles of (Bmim)₂InCl₅(H₂O)

Atom	Angle / °	Atom	Angle / °
C11-In1-Cl2	87.325(19)	C10-N3-C11	108.5(2)
C11-In1-Cl4	171.70(2)	C10-N3-C13	126.2(2)
C11-In1-Cl5	92.21(2)	C11-N3-C13	125.3(2)
C14-In1-Cl2	89.860(17)	C10-N4-C9	125.9(2)
C15-In1-Cl2	165.768(19)	C10-N4-C12	108.6(2)
C15-In1-Cl4	88.606(18)	C12-N4-C9	125.5(2)
C16-In1-Cl1	94.47(2)	N4-C9-H9A	109.50
C16-In1-Cl2	96.03(2)	N4-C9-H9B	109.50
C16-In1-Cl4	93.59(2)	N4-C9-H9C	109.50
C16-In1-Cl5	98.19(2)	H9A-C9-H9B	109.50
O1-In1-Cl1	86.33(4)	H9A-C9-H9C	109.50
O1-In1-Cl2	82.02(4)	H9B-C9-H9C	109.50
O1-In1-Cl4	85.54(4)	N3-C10-H10	125.60
O1-In1-Cl5	83.76(4)	N4-C10-N3	108.8(2)
O1-In1-Cl6	177.86(4)	N4-C10-H10	125.60
In1-O1-H1D	109.30	N3-C11-H11	126.50
In1-O1-H1E	109.40	C12-C11-N3	107.1(2)
H1D-O1-H1E	104.50	C12-C11-H11	126.50
C3-N1-C5	125.8(2)	N4-C12-H12	126.40
C4-N1-C3	108.40(19)	C11-C12-N4	107.2(2)
C4-N1-C5	125.76(19)	C11-C12-H12	126.40
C2-N2-C1	125.1(2)	N3-C13-H13A	109.40
C4-N2-C1	126.6(2)	N3-C13-H13B	109.40
C4-N2-C2	108.3(2)	N3-C13-C14	111.0(3)
N2-C1-H1A	109.50	H13A-C13-H13B	108.00
N2-C1-H1B	109.50	C14-C13-H13A	109.40
N2-C1-H1C	109.50	C14-C13-H13B	109.40

H1A-C1-H1B	109.50	C13-C14-H14C	103.60
H1A-C1-H1C	109.50	C13-C14-H14D	103.60
H1B-C1-H1C	109.50	C13-C14-H14A	107.90
N2-C2-H2	126.20	C13-C14-H14B	107.90
C3-C2-N2	107.6(2)	H14C-C14-H14D	105.30
C3-C2-H2	126.20	H14A-C14-H14B	107.20
N1-C3-H3	126.60	C17-C14-C13	134.3(6)
C2-C3-N1	106.8(2)	C17-C14-H14C	103.60
C2-C3-H3	126.60	C17-C14-H14D	103.60
N1-C4-H4	125.60	C15-C14-C13	117.8(4)
N2-C4-N1	108.88(19)	C15-C14-H14A	107.90
N2-C4-H4	125.60	C15-C14-H14B	107.90
N1-C5-H5A	109.10	C14-C17-H17A	113.10
N1-C5-H5B	109.10	C14-C17-H17B	113.10
N1-C5-C6	112.4(2)	C14-C17-C18	92.9(6)
H5A-C5-H5B	107.90	H17A-C17-H17B	110.50
C6-C5-H5A	109.10	C18-C17-H17A	113.10
C6-C5-H5B	109.10	C18-C17-H17B	113.10
C5-C6-H6A	109.00	C17-C18-H18A	109.50
C5-C6-H6B	109.00	C17-C18-H18B	109.50
C5-C6-C7	113.1(2)	C17-C18-H18C	109.50
H6A-C6-H6B	107.80	H18A-C18-H18B	109.50
C7-C6-H6A	109.00	H18A-C18-H18C	109.50
C7-C6-H6B	109.00	H18B-C18-H18C	109.50
C6-C7-H7A	109.10	C14-C15-H15A	112.10
C6-C7-H7B	109.10	C14-C15-H15B	112.10
H7A-C7-H7B	107.80	C14-C15-C16	98.4(5)
C8-C7-C6	112.7(3)	H15A-C15-H15B	109.70
C8-C7-H7A	109.10	C16-C15-H15A	112.10

C8-C7-H7B	109.10	C16-C15-H15B	112.10
C7-C8-H8A	109.50	C15-C16-H16A	109.50
C7-C8-H8B	109.50	C15-C16-H16B	109.50
C7-C8-H8C	109.50	C15-C16-H16C	109.50
H8A-C8-H8B	109.50	H16A-C16-H16B	109.50
H8A-C8-H8C	109.50	H16A-C16-H16C	109.50
H8B-C8-H8C	109.50		

Table S4. ICP-OES data of Sb:(Bmim)₂InCl₅(H₂O)

Feeding ratio (%)		Actual ratio (%)	
In	Sb	In	Sb
80	20	94.26	5.74
85	15	97.38	2.62
90	10	99.14	0.86
95	5	99.28	0.72
99	1	99.82	0.18

Supporting Figure

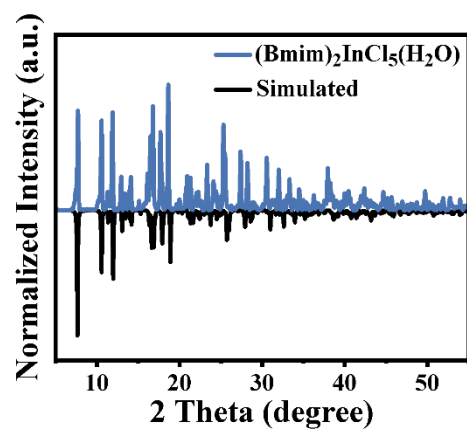


Fig. S1 The simulated and the experimentally obtained PXRD patterns of $(\text{Bmim})_2\text{InCl}_5(\text{H}_2\text{O})$.

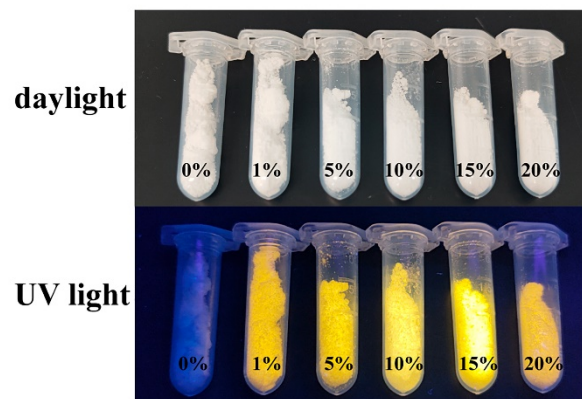


Fig. S2 Photographs of $x\% \text{Sb}^{3+}:(\text{Bmim})_2\text{InCl}_5(\text{H}_2\text{O})$ ($x = 0, 1, 5, 10, 15, 20$) powder under daylight (top) and UV light (bottom).