Blue Emission from Charge Transfer Excitons in Hybrid Organic-Inorganic Quantum Wires: (ABT) [$PbCl_3$]

Supplementary information

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Table S1. Crystallographic data for $ABTPbCl_3$

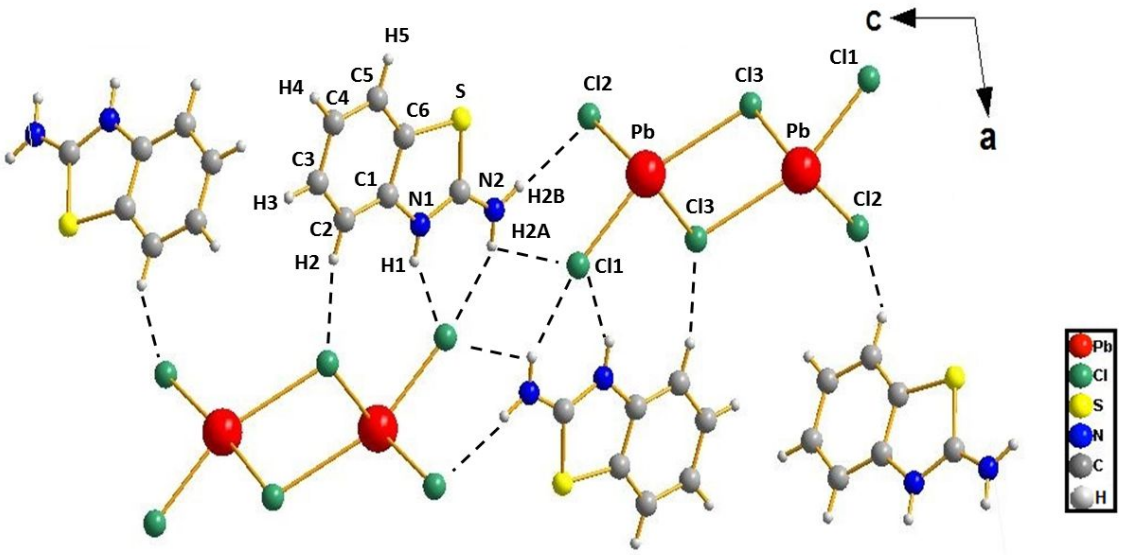
	Temperature (K)		
	100	**180**	**220**
Chemical formula	**$C_7H_7Cl_3N_2SPb$**	**$C_7H_7Cl_3N_2SPb$**	**$C_7H_7Cl_3N_2SPb$**
M(g.mol^{-1})	464.75	464.75	464.75
Space group	P21/n	P21/n	P21/n
a (Å)	11.4398(9)	11.4693(2)	11.4949(2)
b (Å)	4.3445(3)	4.35001(9)	4.35479(8)
c (Å)	24.0300(18)	24.0723(5)	24.1198(4)
α (°)	90	90	90
β (°)	99.311(2)	99.515(2)	99.5773(17)
γ (°)	90	90	90
V (Å^3)	1178.56(15)	1184.48(4)	1190.56(4)
Z	4	4	4
Ref. measured	33973	11121	27019
Θ_{max}	36.493	30.506	32.960
R_{int}	0.0395	0.0298	0.0479
μ/mm^{-1}	15.134	15.058	14.981
Ref. independent [F^2>2s(F^2)]	5744 [5272]	3628 [3354]	4283 [3897]
wR2 [F^2>2s(F^2)]	0.0689 [0.0676]	0.0805 [0.0696]	0.0712 [0.0590]
R1[F^2>2s(F^2)]	0.0429 [0.0375]	0.0252 [0.0214]	0.0260 [0.0219]
G.o.F	1.338	1.267	1.206
$\Delta_{\rho\ min}/\Delta_{\rho\ max}$	2.836/ -4.794	0.973/ -2.174	0.664 / -1.662

Table S2: Bond distances (Å) and angles (°) in $PbCl_6$and centroid-centroid distance between two adjacent organic rings in the 100-220 K temperature range.

	Temperature (K)		
	100	**180**	**220**
Bond length(Å)			
Pb-Cl1	2.667(9)	2.6625(10)	2.6653(8)
Pb-Cl2	2.934(1)	2.9369(10)	2.9407(8)
Pb-Cl2	2.897(1)	2.8979(10)	2.8991(9)
Pb-Cl3	2.861(1)	2.8657(10)	2.8688(9)
Pb-Cl3	2.965(1)	2.9669(11)	2.9698(9)
Pb-Cl3	3.136(1)	3.1358(12)	3.1392(10)
d Pb …Pb	4.345	4.350	4.355
d’ Pb …Pb	4.615	4.615	4.617
Bond angles (°)			
Pb-Cl2-Pb	84.67(3)	96.41(3)	96.44(3)
Pb-Cl3-Pb	85.99(3)	96.44(3)	96.45(3)
Pb-Cl3-Pb	96.43(3)	100.42(3)	100.34(3)
Pb-Cl3-Pb	81.34(3)	98.21(4)	98.15(3)
dCentroid-centroid (Å)	3.448	3.460	3.469

Table S3: Hydrogen bond geometry for $ABTPbCl_3$at180 K.

D-H	A	d (D-H)	d (H…A)	< DHA	(D…A)
N_2-H_{2A}	Cl_1	0.860	2.425	153.91	3.220
N_2-H_{2B}	Cl_2	0.859	4.422	156.70	3.228
N_1-H_1	Cl_1	0.861	2.709	139.49	3.410
C_2-H_2	Cl_3	0.930	2.725	121.94	3.590
C_5-H_5	Cl_2	0.930	2.881	111.94	3.597



FigureS1: Packing diagram of the title compound $ABTPbCl_3$viewed down the b-axis. The hydrogen bondsN-H … Cl and C-H … Clare shown as dashed lines.

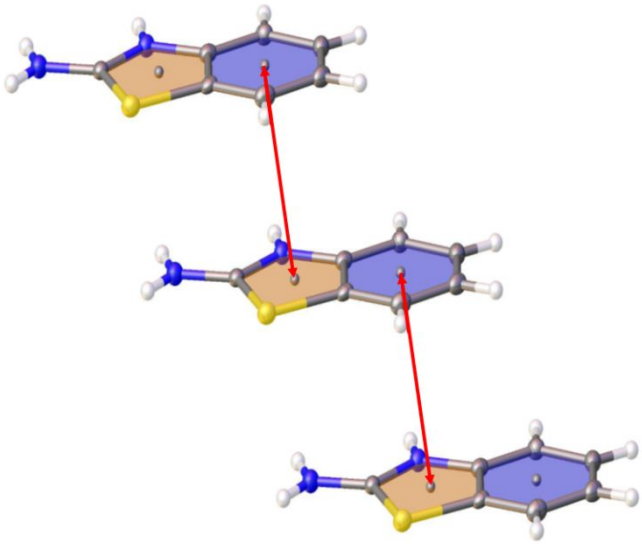


Figure S2: The alternating rows of π-π interaction of organic cation in $ABTPbCl_3$.

Table S4: Time-resolved PL lifetime data fitted to exponential decay function $I(t) = A_1 \times \exp(-t/\tau_1) + A_2 \times \exp(-t/\tau_2)$.

Excitation wavelength=375 nm		
$ABTPbCl_3$	Emission wavelength Rise time	483 nm 5.64 ns
Fitting parameters of exponential curve	A_1	21.16 (±3.3007)
	τ_1	6.072 (±6.1866 e^{-1})
	A_2	181.70 (±3.4072)
	τ_2	1.5510 (±4.3078e^{-2})
	Chi^2	1.325
ABT(HCl)	Emission wavelength Rise time	423 nm 3.81 ns
Fitting parameters of exponential curve	A_1	5027 (±9.1283e^{+2})
	τ_1	1.3570 (5.0187e^{-2})
	A_2	28.46 (2.2673)
	τ_2	9.928 (5.5090e^{-1})
	Chi^2	1.492