Inorganic-organic hybrid compounds based on face-sharing octahedral $[PbI_3]_\infty$ chains: self-assemblies, crystal structures, and ferroelectric, photoluminescence properties

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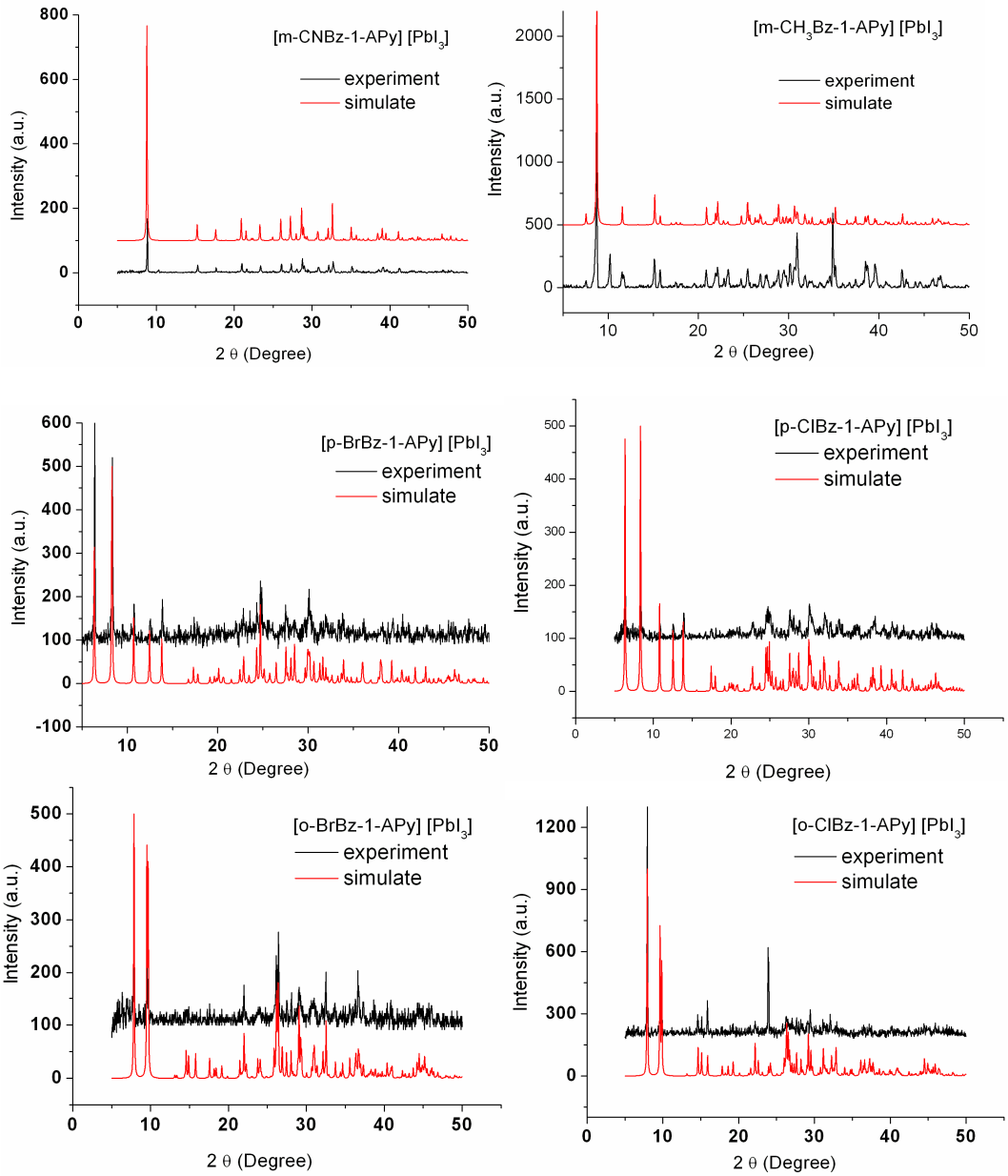

[m-CNBz-1-APy] [PbI3]
experiment
simulate
Intensity (a.u.)
2 θ (Degree)
[m-CH3Bz-1-APy] [PbI3]
experiment
simulate
Intensity (a.u.)
2 θ (Degree)
[p-BrBz-1-APy] [PbI3]
experiment
simulate
Intensity (a.u.)
2 θ (Degree)
[p-ClBz-1-APy] [PbI3]
experiment
simulate
Intensity (a.u.)
2 θ (Degree)
[o-BrBz-1-APy] [PbI3]
experiment
simulate
Intensity (a.u.)
2 θ (Degree)
[o-ClBz-1-APy] [PbI3]
experiment
simulate
Intensity (a.u.)
2 θ (Degree)

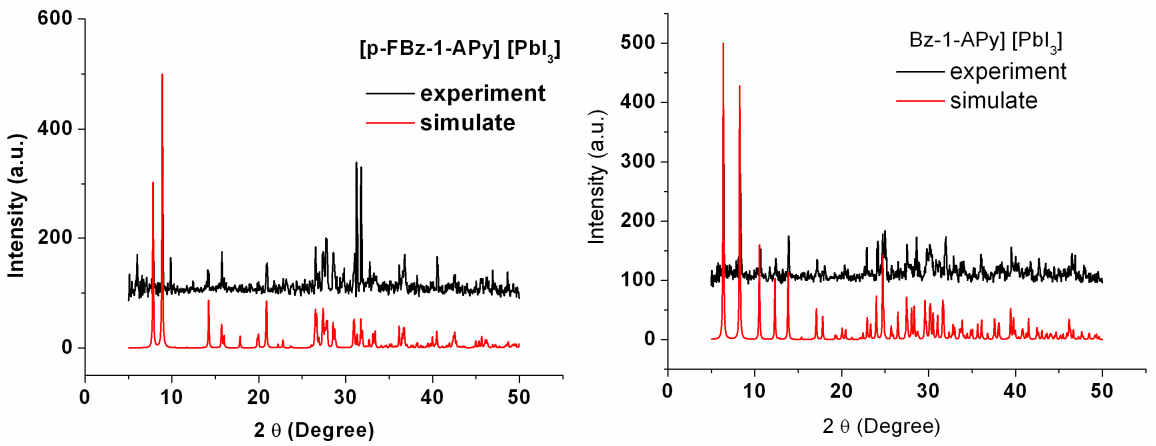


Figure S1 Both experimental and simulated Powder X-ray diffraction profiles for **1-8**.

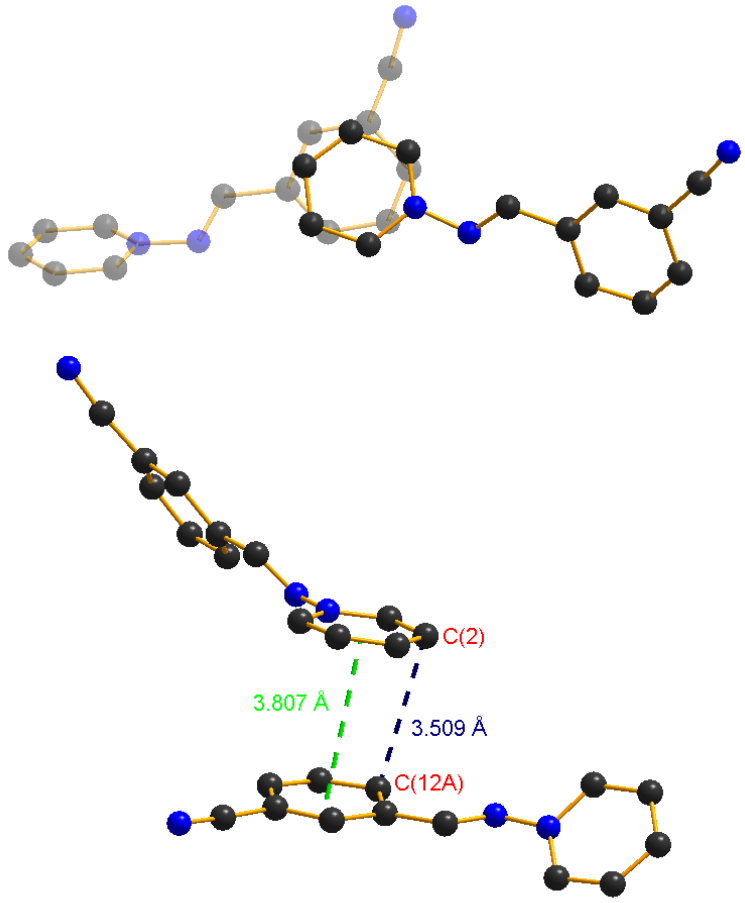


Figure S2 π…π interaction between the phenyl and pyridyl ring of the neighboring Schiff base cations in **1**.

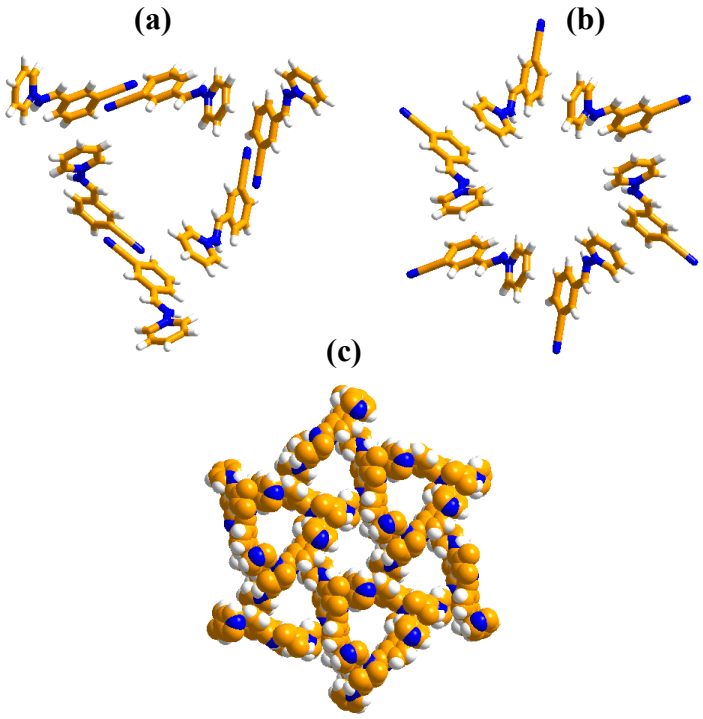


Figure S3 Perspective views of (a) trigonal cross-section (b) hexagonal cross-section (c) space-filling representation for Kagomé lattice of cations in the crystal of **1**.

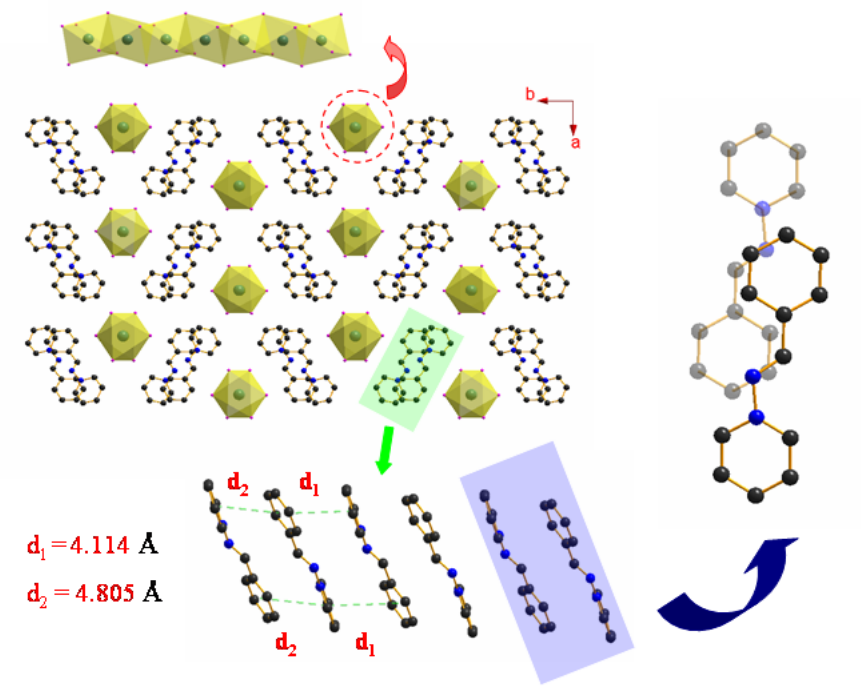


Figure S4 the alignment of inorganic and organic components in the crystals of **3**.

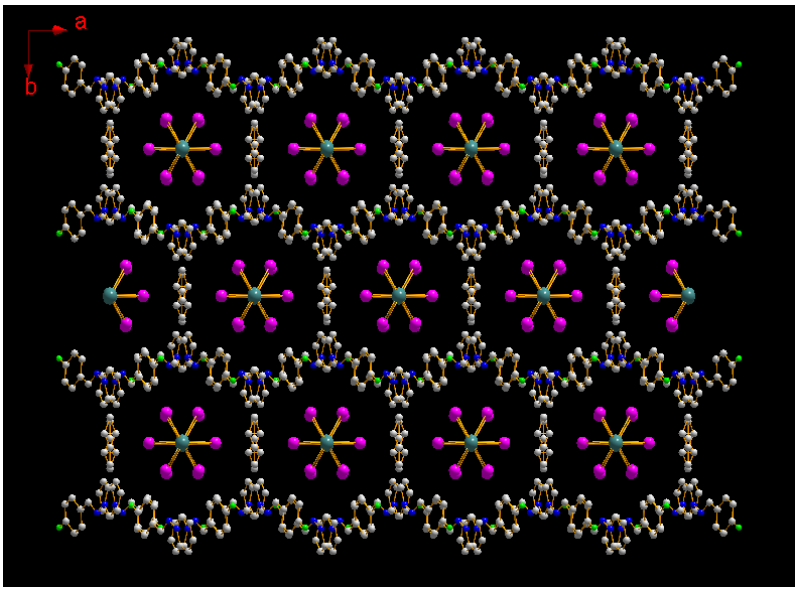


Figure S5 the alignment of inorganic and organic components in the crystal of **4**.

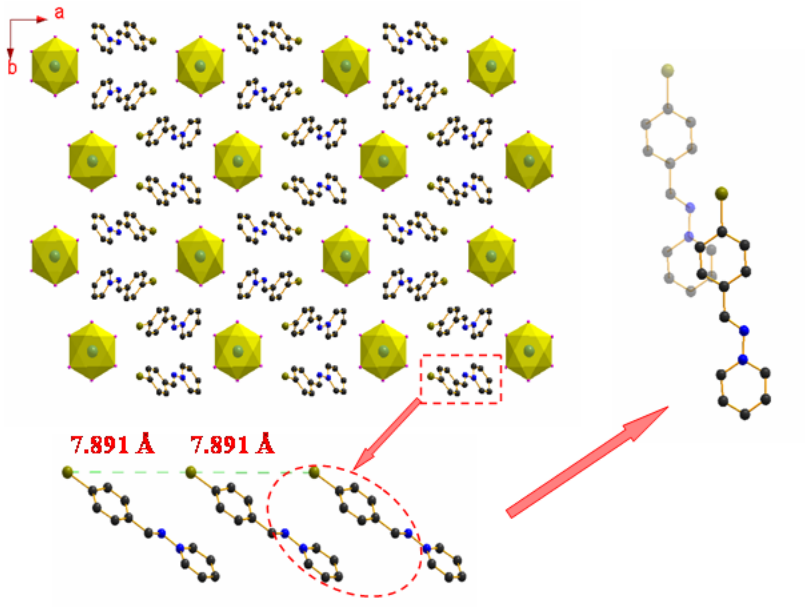


Figure S6 the alignment of inorganic and organic components in the crystal of **6**.

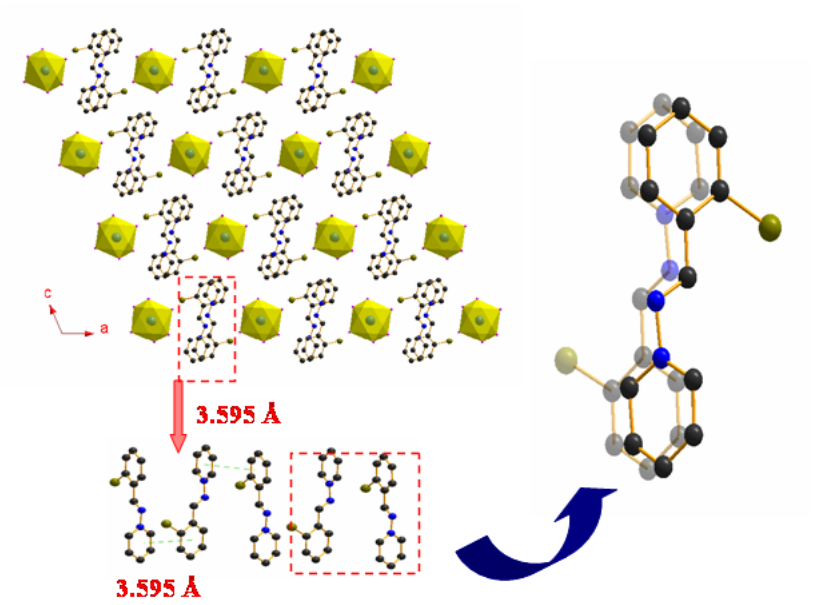
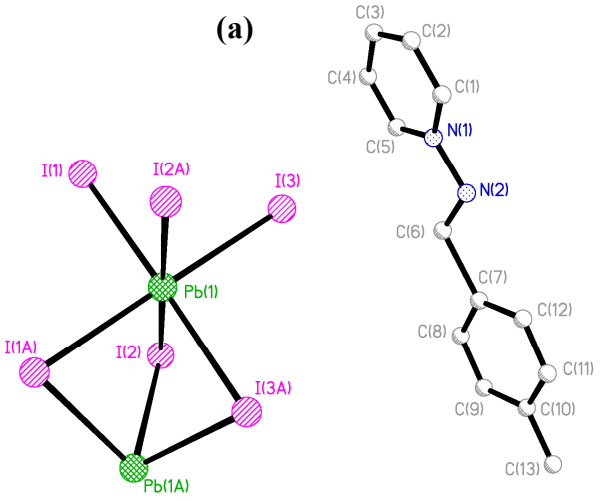


Figure S7 the alignment of inorganic and organic components in the crystal of **8**.



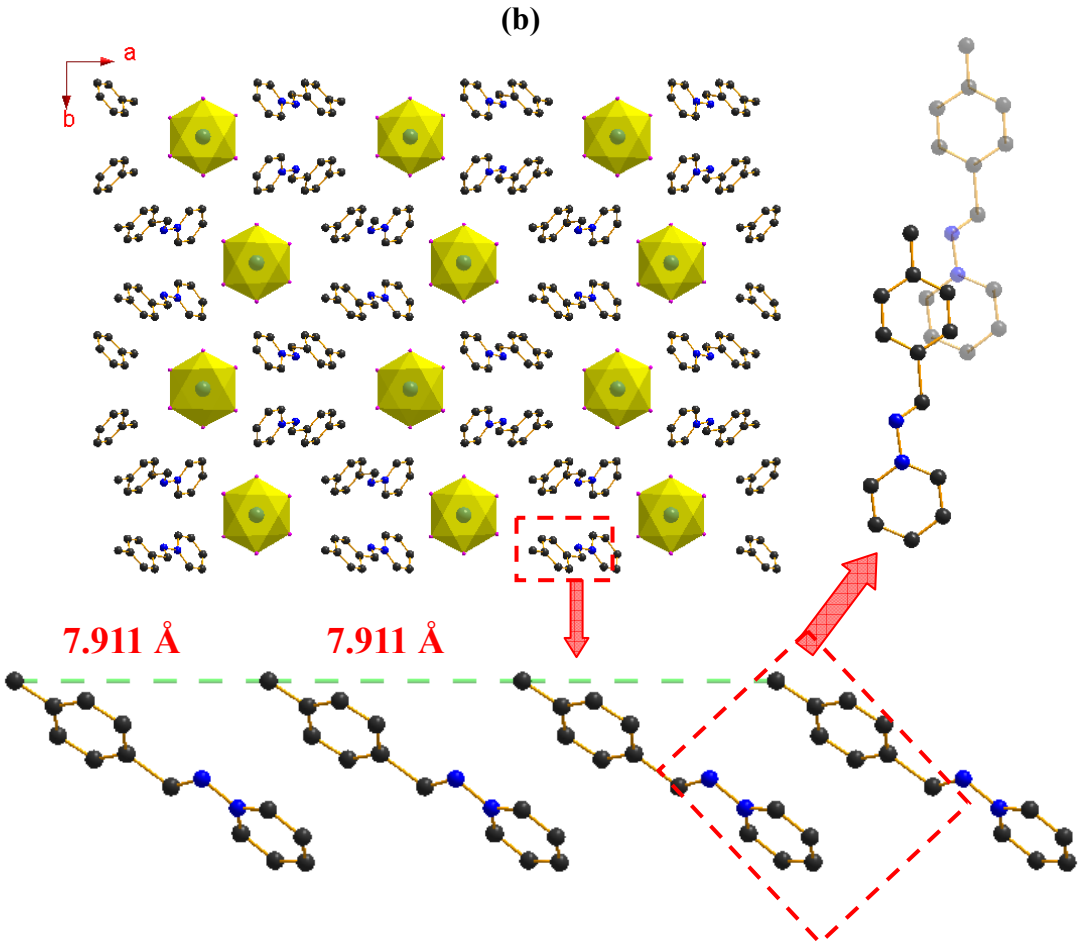
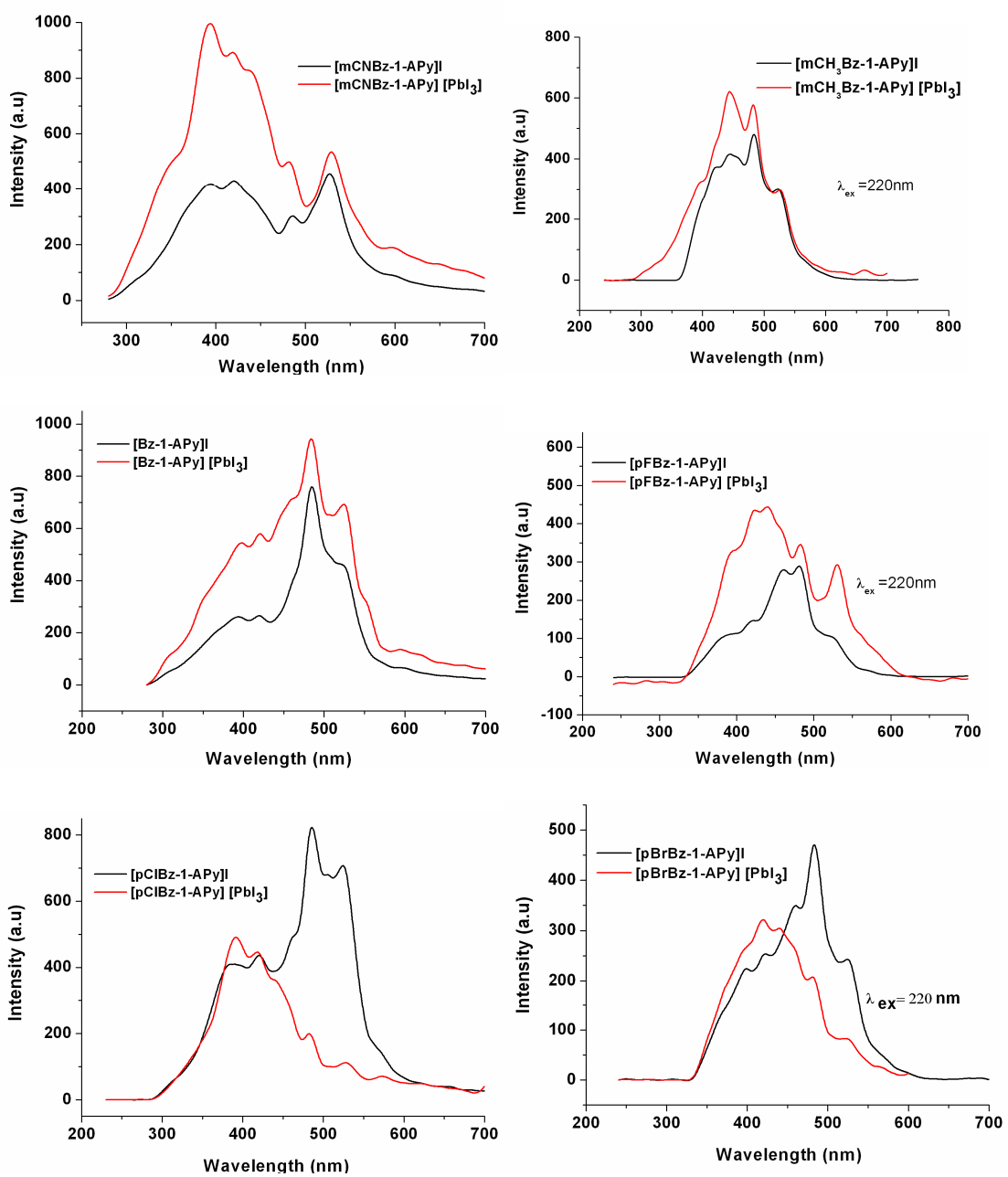


Figure S8 (a) the views of asymmetric unit with non-H atomic labeling and the thermal ellipsoids at the 20% probability (H atoms in the cation omitted for clarity) and (b) the arrangement of inorganic $[PbI_3]_\infty$ chains and Schiff base cation stacks for **[p-CH_3Bz-1-APy][PbI_3]**.


[mCNBz-1-APy]I
[mCNBz-1-APy] [PbI3]
Intensity (a.u)
Wavelength (nm)
[mCH3Bz-1-APy]I
[mCH3Bz-1-APy] [PbI3]
λex=220nm
[Bz-1-APy]I
[Bz-1-APy] [PbI3]
[pFBz-1-APy]I
[pFBz-1-APy] [PbI3]
[pClBz-1-APy]I
[pClBz-1-APy] [PbI3]
[pBrBz-1-APy]I
[pBrBz-1-APy] [PbI3]
λ ex= 220 nm

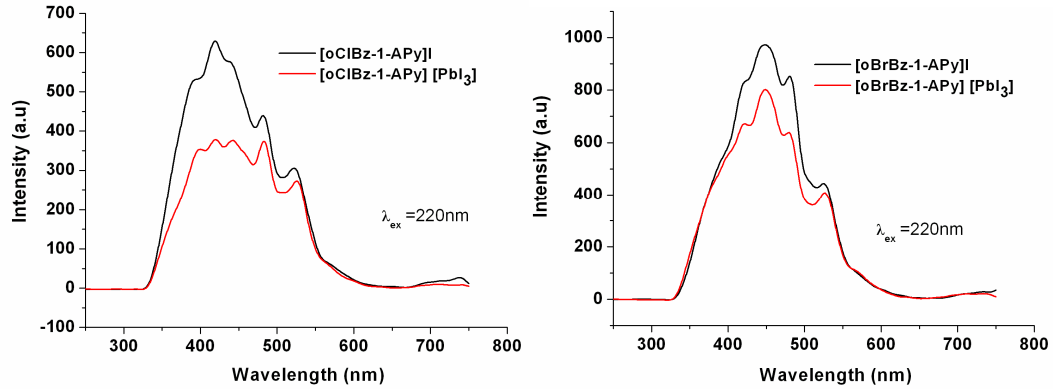
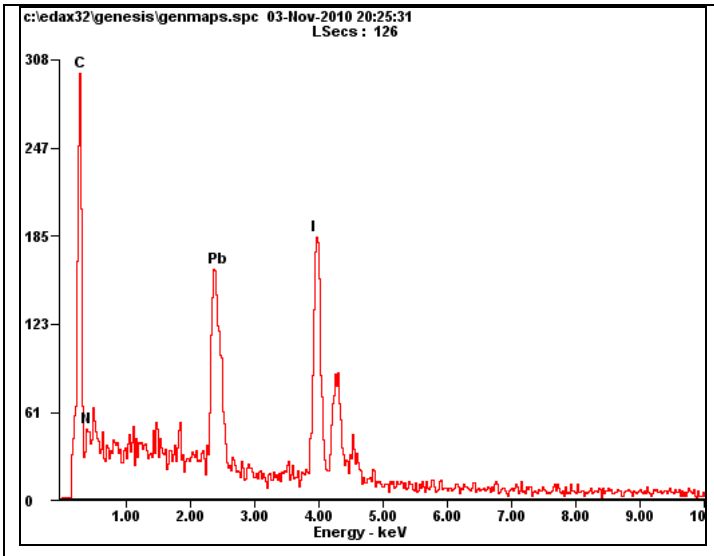
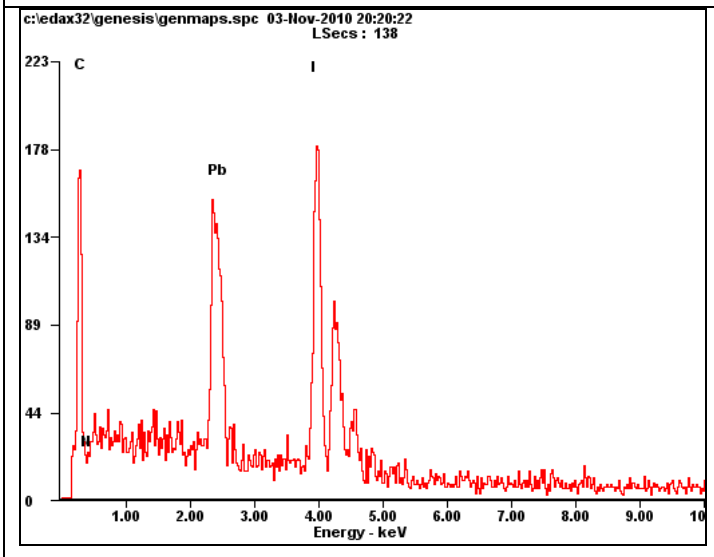


Figure S9 Emission spectra of Hybrid compounds and the corresponding Schiff base iodides in solid state at room temperature.



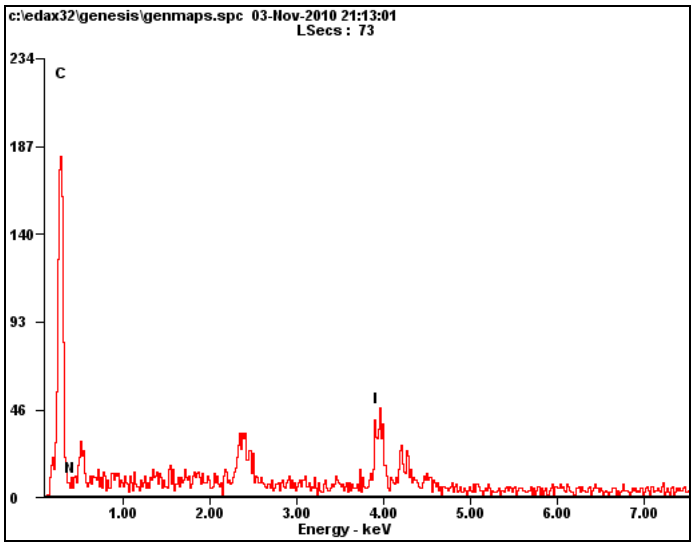
Element	*Wt%*	*At%*
CK	39.11	76.00
NK	09.76	16.27
IL	27.76	05.11
PbL	23.37	02.63
Matrix	Correction	ZAF

Compound **1**



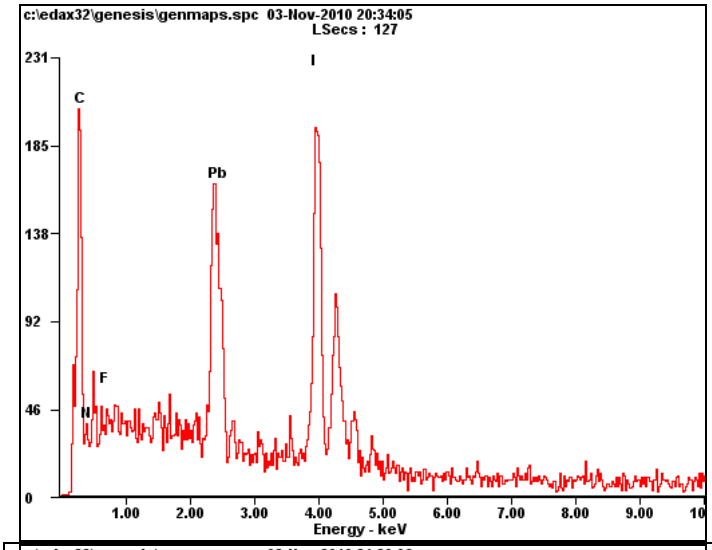
Element	*Wt%*	*At%*
CK	34.76	85.44
NK	00.85	01.78
IL	39.89	09.28
PbL	24.51	03.49
Matrix	Correction	ZAF

Compound **2**



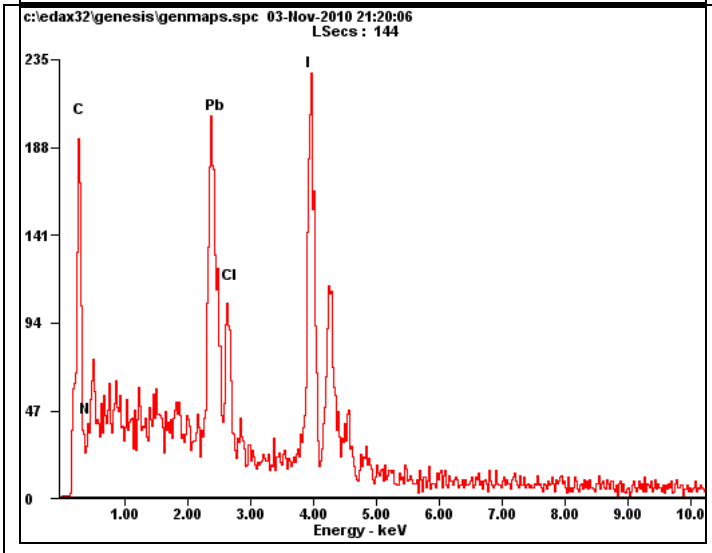
Element	Wt%	At%
CK	61.15	90.95
NK	03.95	05.03
IL	18.45	02.60
PbL	16.46	01.42
Matrix	Correction	ZAF

Compound **3**



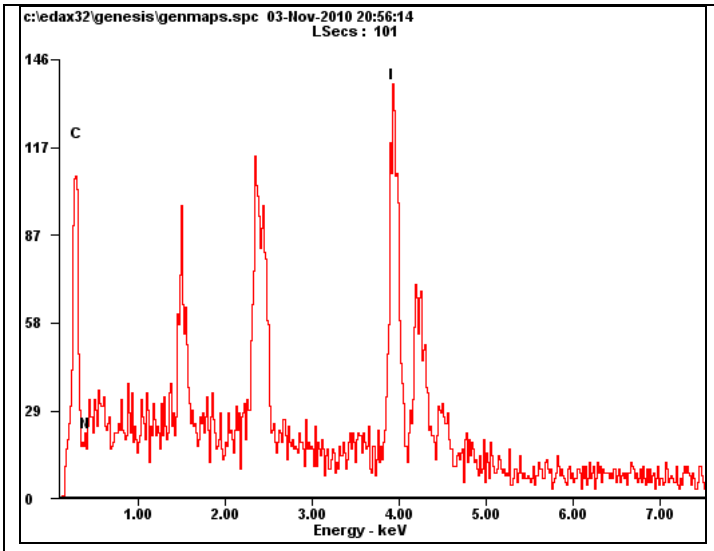
Element	Wt%	At%
CK	31.46	71.41
NK	06.86	13.34
FK	03.32	04.76
IL	33.69	07.24
PbL	24.67	03.25
Matrix	Correction	ZAF

Compound **4**



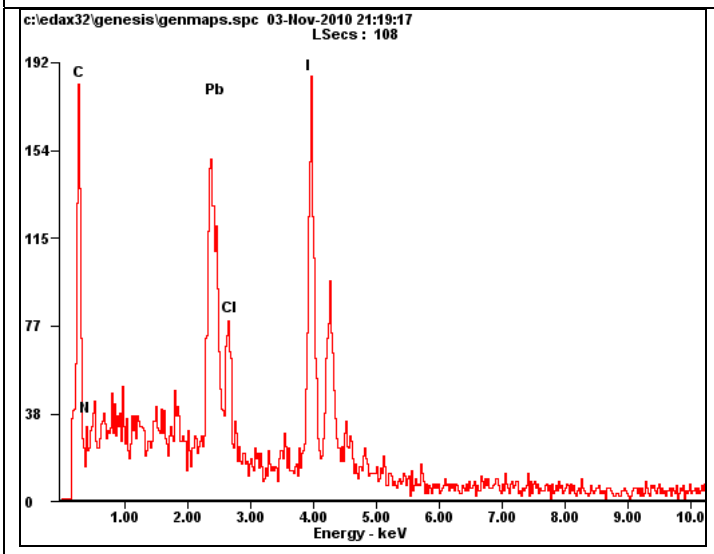
Element	Wt%	At%
CK	34.00	74.47
NK	07.08	13.29
ClK	03.56	02.64
IL	32.00	06.63
PbL	23.35	02.97
Matrix	Correction	ZAF

Compound **5**



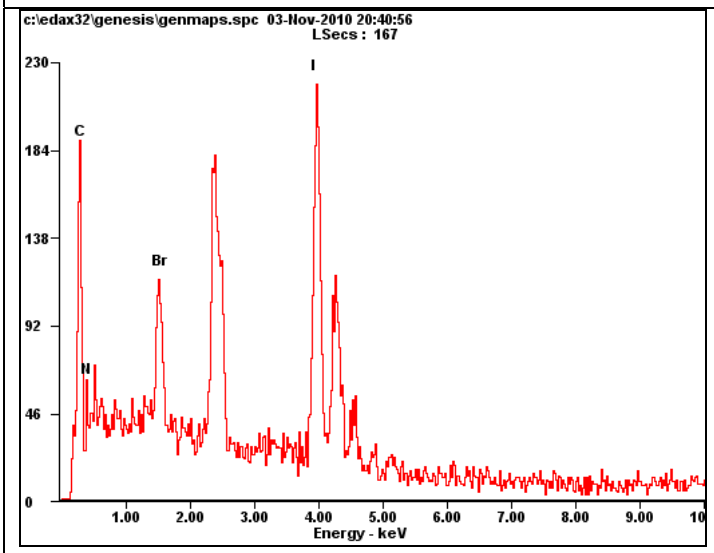
Element	Wt%	At%
CK	29.82	74.49
NK	05.24	11.23
IL	27.67	06.54
PbL	27.14	03.93
BrK	10.13	03.80
Matrix	Correction	ZAF

Compound **6**



Element	Wt%	At%
CK	36.63	75.12
NK	07.96	14.00
ClK	03.29	02.29
IL	31.87	06.19
PbL	20.26	02.41
Matrix	Correction	ZAF

Compound **7**



Element	Wt%	At%
CK	31.43	70.42
NK	09.30	17.86
BrL	06.50	02.19
IL	32.58	06.91
PbL	20.19	02.62
Matrix	Correction	ZAF

Compound **8**

Figure S10 EDS results for **1-8** which show the relative components of Pb and I.

Table S1 Selected bond lengths (Å) and bond angles (°) in **1**

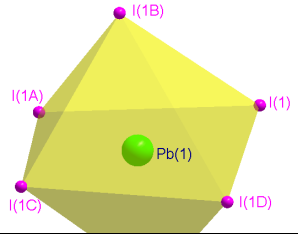
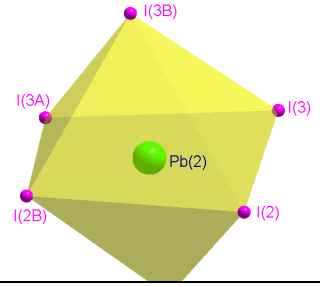
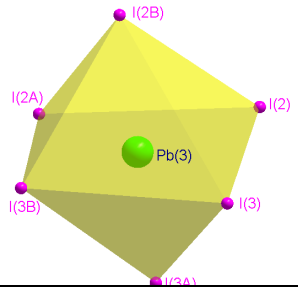
		1
	Pb(1)-I(1)	3.1894(17)
	Pb(1)-I(1A)	3.2581(17)
	I(1)-Pb(1)-I(1A)	87.32(5)
	I(1)-Pb(1)-I(1D)	93.81(2)
	I(1B)-Pb(1)-I(2B)	178.43(6)
	Pb(2)-I(2)	3.2214(18)
	Pb(2)-I(3)	3.2458(18)
	I(2)-Pb(2)-I(2A)	85.72(5)
	I(1)-Pb(2)-I(3)	89.85(4)
	I(2)-Pb(2)-I(3)	98.38(4)
	I(2)-Pb(2)-I(3A)	173.74(4)
	Pb(3)-I(2)	3.2151(18)
	Pb(3)-I(3)	3.2290(18)
	I(3)-Pb(3)-I(3A)	86.42(5)
	I(3A)-Pb(3)-I(3B)	86.98(5)
	I(2A)-Pb(3)-I(3A)	89.44(4)
	I(3A)-Pb(3)-I(2B)	173.69(4)

Table S2 Selected bond lengths (Å) and bond angles (°) in the PbI_6 octahedron of **2-8**

[m-CH_3Bz-1-APy] [PbI_3] (2)			
Pb(1)-I(2A)	3.1300(19)	Pb(1)-I(3A)	3.133(2)
Pb(1)-I(1A)	3.196(2)	Pb(1)-I(2)	3.354(2)
Pb(1)-I(1)	3.3422(19)	Pb(1)-I(3)	3.246(2)
I(2A)-Pb(1)-I(3A)	90.88(5)	I(2A)-Pb(1)-I(1A)	95.09(5)
I(3A)-Pb(1)-I(1A)	89.02(5)	I(2A)-Pb(1)-I(3)	88.07(5)
I(3A)-Pb(1)-I(3)	98.03(6)	I(1A)-Pb(1)-I(3)	172.24(6)
I(2A)-Pb(1)-I(1)	85.63(5)	I(3A)-Pb(1)-I(1)	175.52(6)
I(1A)-Pb(1)-I(1)	88.50(6)	I(3)-Pb(1)-I(1)	84.67(5)
I(3A)-Pb(1)-I(3)	176.97(6)	I(2B)-Pb(1)-I(3)	86.14(5)
I(1A)-Pb(1)-I(3)	84.39(5)	I(2)-Pb(1)-I(3)	92.83(5)
I(1)-Pb(1)-I(2)	97.33(5)		
Symmetry codes: 2A = x, -y+1/2, z+1/2; 1A = 3A = x, -y+1/2, z-1/2			
[p-FBz-1-APy][PbI_3] (4)			
Pb(1)-I(1)	3.2400(9)	Pb(1)-I(2)	3.1931(8)
Pb(1)-I(3)	3.2670(15)	Pb(2)-I(3)	3.1945(11)
Pb(2)-I(2)	3.2174(10)	Pb(2)-I(1)	3.2631(10)
I(2A)-Pb(1)-I(2)	180.0	I(2)-Pb(1)-I(1)	86.80(3)
I(2A)-Pb(1)-I(1)	93.20(3)	I(1)-Pb(1)-I(1A)	180.0
I(2)-Pb(1)-I(3)	84.95(3)	I(2)-Pb(1)-I(3A)	95.05(3)
I(1)-Pb(1)-I(3A)	95.12(3)	I(1)-Pb(1)-I(3)	84.88(3)
I(1)-Pb(2)-I(2)	86.01(4)	I(1)-Pb(2)-I(3)	85.68(4)
I(2)-Pb(2)-I(3)	85.75(3)	I(2B)-Pb(2)-I(3)	91.68(3)
I(1B)-Pb(2)-I(3)	96.82(3)	I(1B)-Pb(2)-I(2)	176.94(2)
Symmetry codes: B:-x+1,y,-z+1/2; A:-x+1, -y+1, -z			
[p-ClBz-1-APy][PbI_3] (5)			
Pb(1)-I(1)	3.2627(6)	Pb(1)-I(3)	3.2152(6)
Pb(1)-I(3A)	3.2284(6)	Pb(1)-I(1A)	3.2434(6)
Pb(1)-I(2)	3.2350(6)	Pb(1)-I(2A)	3.2047(6)
I(1)-Pb(1)-I(3)	87.036(15)	I(1)-Pb(1)-I(3A)	92.760(15)
I(3)-Pb(1)-I(3A)	177.436(17)	I(1)-Pb(1)-I(1A)	95.155(18)
I(3A)-Pb(1)-I(1A)	87.141(14)	I(1)-Pb(1)-I(2)	85.156(16)
I(3)-Pb(1)-I(2)	86.992(15)	I(3A)-Pb(1)-I(2)	95.540(15)
I(1A)-Pb(1)-I(2)	177.286(14)		
Symmetry codes: A = x, -y+1/2, z+1/2			
[p-BrBz-1-APy][PbI_3] (6)			

Pb(1)-I(2)	3.202(3)	Pb(1)-I(3)	3.203(3)
Pb(1)-I(2A)	3.229(3)	Pb(1)-I(3A)	3.231(3)
Pb(1)-I(1)	3.249(3)	Pb(1)-I(1A)	3.260(3)
I(2)-Pb(1)-I(3)	92.50(7)	I(2)-Pb(1)-I(2A)	93.92(8)
I(3)-Pb(1)-I(2A)	87.05(7)	I(3)-Pb(1)-I(3A)	177.01(9)
I(2A)-Pb(1)-I(3A)	95.92(7)	I(2)-Pb(1)-I(1)	85.60(7)
I(3)-Pb(1)-I(1)	89.85(7)	I(2A)-Pb(1)-I(1)	176.84(8)
I(3A)-Pb(1)-I(1)	87.17(7)	I(2)-Pb(1)-I(1A)	178.91(8)
I(3)-Pb(1)-I(1A)	87.46(7)	I(2A)-Pb(1)-I(1A)	84.99(6)
I(3A)-Pb(1)-I(1A)	93.08(7)	I(1)-Pb(1)-I(1A)	95.48(8)

Symmetry codes: 1A = 2A = x,-y+3/2,z-1/2; 3A = x, -y+3/2, z+1/2

[Bz-1-APy][PbI_3] (3)

Pb(1)-I(1)	3.1005(6)	Pb(1)-I(3)	3.1447(6)
Pb(1)-I(2)	3.1871(6)	Pb(1)-I(3A)	3.2486(6)
Pb(1)-I(2A)	3.2846(6)		
I(1)-Pb(1)-I(3)	93.428(17)	I(1)-Pb(1)-I(2)	97.332(15)
I(3)-Pb(1)-I(2)	91.010(19)	I(1)-Pb(1)-I(3A)	85.779(16)
I(3)-Pb(1)-I(3A)	93.510(20)	I(2)-Pb(1)-I(3A)	174.356(14)
I(1)-Pb(1)-I(2A)	84.871(16)	I(3)-Pb(1)-I(2A)	177.973(14)
I(2)-Pb(1)-I(2A)	88.118(19)	I(3A)-Pb(1)-I(2A)	87.470(19)

Symmetry codes: 2A = 3A = x,-y+1/2,z+1/2

[o-ClBz-1-APy][PbI_3] (7)

Pb(1)-I(2)	3.1767(5)	Pb(1)-I(3)	3.1778(5)
Pb(1)-I(3A)	3.2226(5)	Pb(1)-I(2A)	3.2440(5)
Pb(1)-I(1)	3.2736(6)		
I(2)-Pb(1)-I(3A)	91.272(14)	I(3)-Pb(1)-I(3A)	177.580(15)
I(2)-Pb(1)-I(2A)	178.155(10)	I(3)-Pb(1)-I(2A)	90.865(14)
I(3A)-Pb(1)-I(2A)	87.294(13)	I(2)-Pb(1)-I(1)	82.840(14)
I(3)-Pb(1)-I(1)	101.084(15)	I(3A)-Pb(1)-I(1)	80.742(14)
I(2A)-Pb(1)-I(1)	98.065(14)		

Symmetry codes: 1A = 3A = -x+1,y+1/2, -z+3/2; 2A= -x+1,y-1/2, -z+3/2

[o-BrBz-1-APy][PbI_3] (8)

Pb(1)-I(2)	3.1711(11)	Pb(1)-I(3A)	3.2044(10)
Pb(1)-I(3)	3.2109(10)	Pb(1)-I(2A)	3.2156(11)
Pb(1)-I(1)	3.2708(12)	Pb(1)-I(1A)	3.4252(12)
I(2)-Pb(1)-I(3A)	91.35(3)	I(2)-Pb(1)-I(3)	91.32(3)
I(3A)-Pb(1)-I(3)	176.93(3)	I(2)-Pb(1)-I(2A)	177.99(3)
I(3A)-Pb(1)-I(2A)	90.63(3)	I(3)-Pb(1)-I(2A)	86.69(3)

I(2)-Pb(1)-I(1)	81.35(3)	I(3A)-Pb(1)-I(1)	99.66(3)
I(3)-Pb(1)-I(1)	82.24(3)	I(2A)-Pb(1)-I(1)	98.64(3)
I(2)-Pb(1)-I(1A)	101.65(3)	I(3A)-Pb(1)-I(1A)	79.96(3)
I(3)-Pb(1)-I(1A)	98.02(3)	I(2A)-Pb(1)-I(1A)	78.38(3)
I(1)-Pb(1)-I(1A)	176.98(3)		

Symmetry codes: A = -x+2, y+1/2, -z+3/2

References

1. Kurtz, S. K.; Perry, T. T. *J. Appl. Phys.* **1968**, *39*, 3798-3813.
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