Structural Diversity of Lead Halide Chain Compounds, $APbX_3$, Templated by Isomeric Molecular Cations

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Supplementary Information

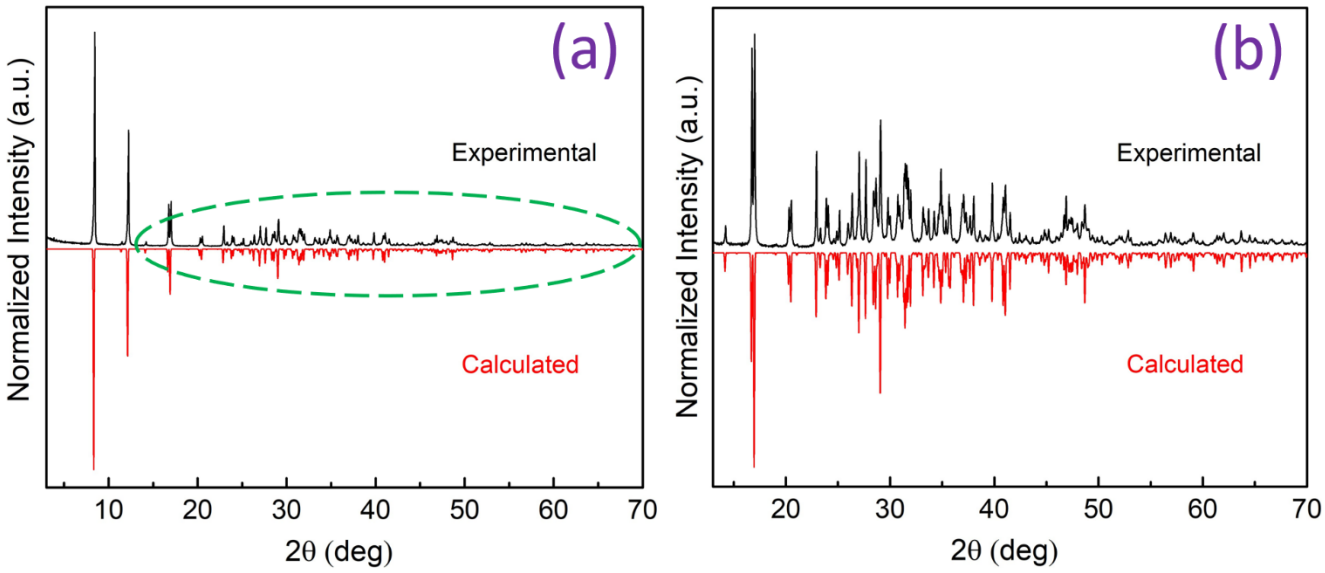

Figure S1. The full-range (a) and expanded (b) P-XRD data for $IQPbBr_3$ at room temperature, the corresponding colours represent the experimental (black) and the calculated (red) pattens.

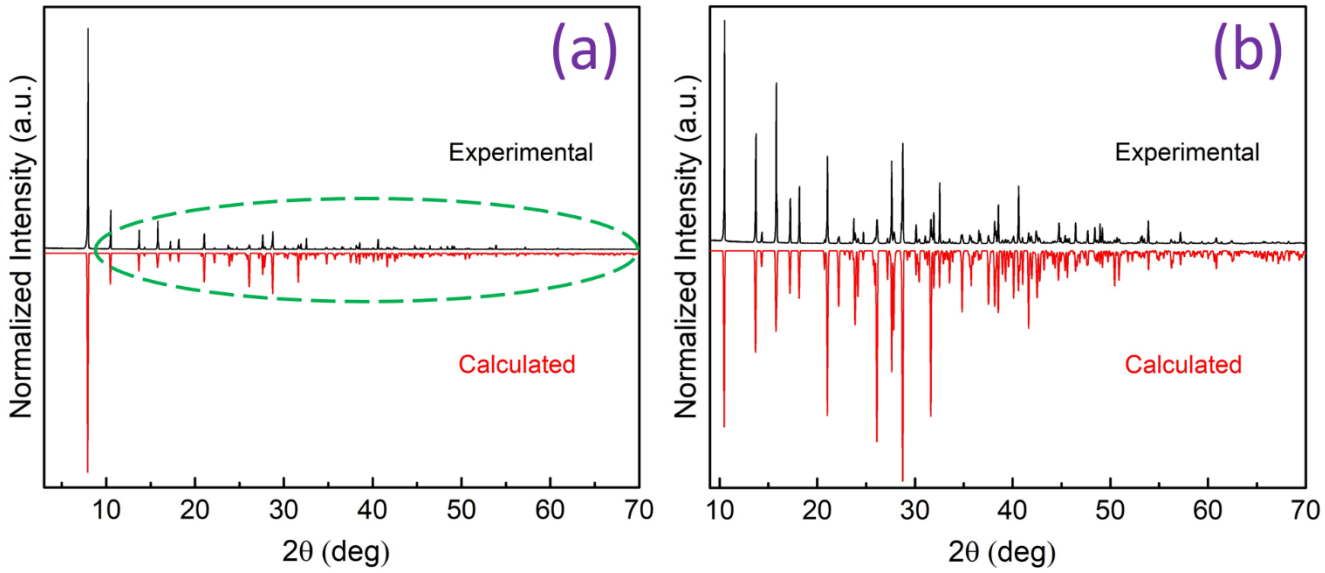

Figure S2. The full-range (a) and expanded (b) P-XRD data for $QPbBr_3$ at room temperature, the corresponding colours represent the experimental (black) and the calculated (red) pattens.

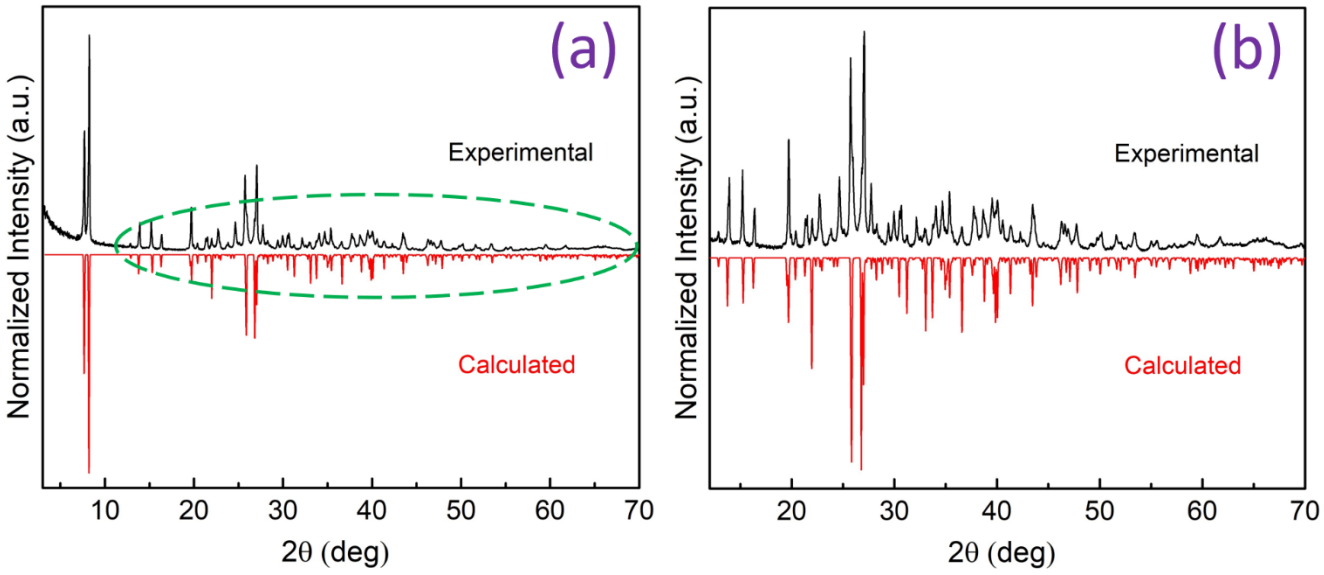

Figure S3. The full-range (a) and expanded (b) P-XRD data for $QPbI_3$ at room temperature, the corresponding colours represent the experimental (black) and the calculated (red) pattens.

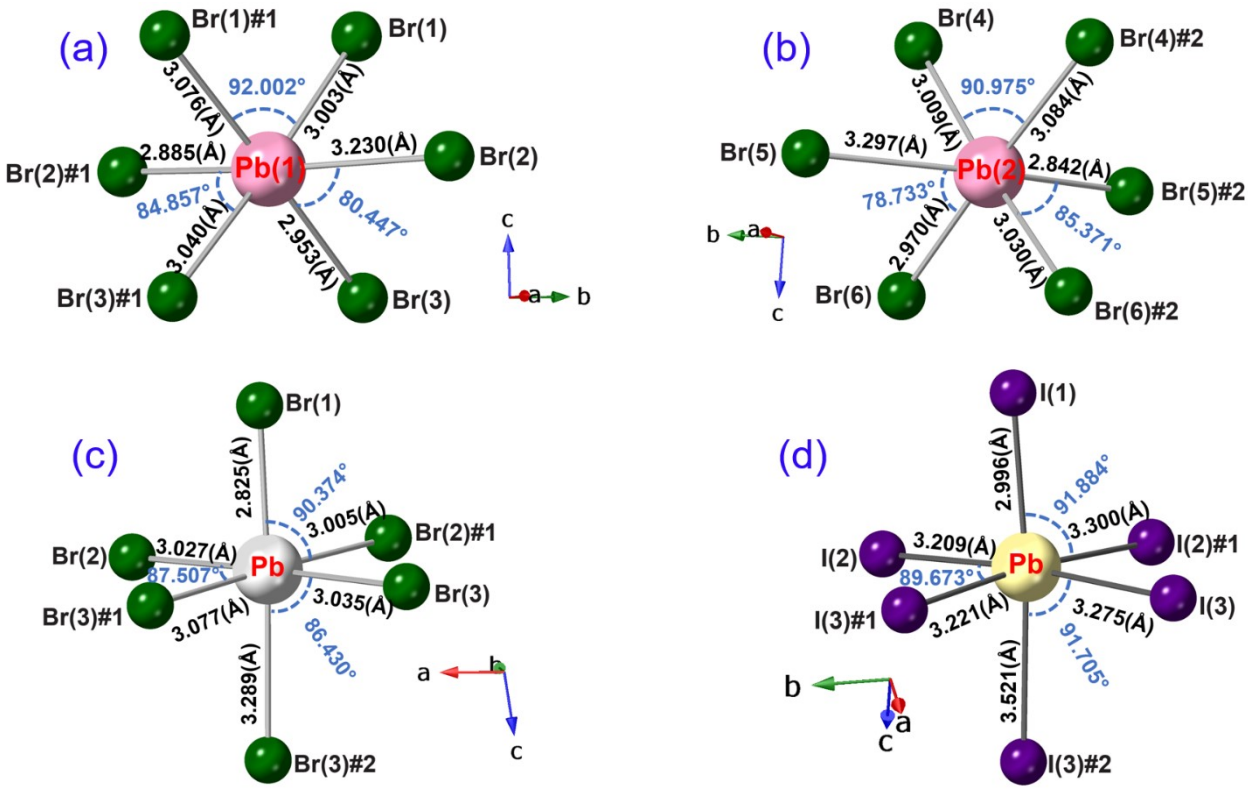

Figure S4. The nature of the distortions within the inorganic PbX_6 octahedra of the three compounds at 298 K. (a) $Pb(1)Br_6$ octahedra for $IQPbBr_3$, (b) $Pb(2)Br_6$ octahedra for $IQPbBr_3$, (c) $PbBr_6$ octahedra for $QPbBr_3$, (d) PbI_6 octahedra for $QPbI_3$.

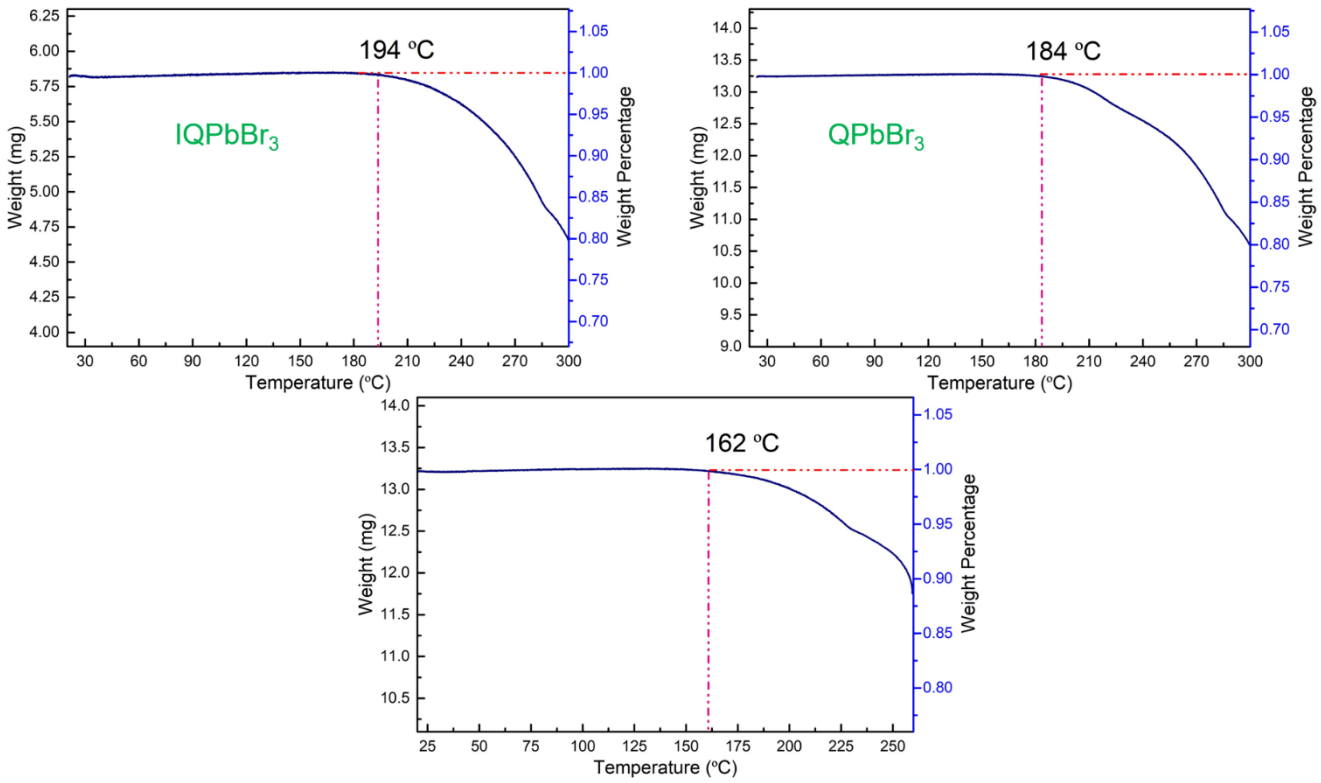

Figure S5. Thermal Gravimetric Analysis (TGA) of $IQPbBr_3$, $QPbBr_3$ and $QPbI_3$.

Table S1. Single crystal and structure refinement data for $IQPbBr_3$, $QPbBr_3$ and $QPbI_3$ at 173 K.

	$IQPbBr_3$	**$QPbBr_3$**	**$QPbI_3$**
Formula	$C_9H_8NPbBr_3$	$C_9H_8NPbBr_3$	$C_9H_8NPbI_3$
Formula weight	577.08	577.08	718.05
Colour/Habit	Colorless/Chip	Colorless/Prism	Yellow/Prism
Crystal size (mm^3)	0.32 × 0.24 × 0.09	0.25 × 0.06 × 0.04	0.32 × 0.09 × 0.05
Crystal system	Orthorhombic	Monoclinic	Monoclinic
Space group	*Pbca*	$P2_1/n$	$C2/c$
***a* (Å)**	21.1904(15)	4.3397(2)	25.767(2)
***b* (Å)**	7.7771(5)	22.5309(17)	4.6411(4)
***c* (Å)**	30.828(2)	13.0048(10)	25.931(2)
α (°)	90	90	90
β (°)	90	98.941(6)	115.396(7)
γ (°)	90	90	90
***V* ($Å^3$)**	5080.5(6)	1256.12(15)	2801.3(4)
Z	16	4	8
ρ_{calc} (g/cm^3)	3.018	3.052	3.405
μ (mm^{-1})	22.684	22.937	18.625
F(000)	4096	1024	2480
Reflns collected	47986	9972	12590
Independent reflns	5808	2192	3132
	0.099	0.1118	0.086
Goodness of Fit	1.072	0.944	0.909
Final *R* indices ($I > 2\sigma(I)$)	R_1 = 0.0397	R_1 = 0.0349	R_1 = 0.0400
	wR_2 = 0.0966	wR_2 = 0.0768	wR_2 = 0.0954
Largest diff. peak/hole (e $Å^{-3}$)	2.408/-2.586	1.955/-1.922	2.360/-1.679

Table S2. Selected bond lengths (Å) and bond angles (°) for $IQPbBr_3$ at 173 K and 298 K.

Temperature	173 K	298 K
Pb(1)-Br(1)	2.9955(7)	3.0034(11)
Pb(1)-Br(1)#1	3.0752(8)	3.0763(11)
Pb(1)-Br(2)	3.2403(8)	3.2299(12)
Pb(1)-Br(2)#1	2.8753(8)	2.8846(12)
Pb(1)-Br(3)	2.9449(8)	2.9535(11)
Pb(1)-Br(3)#1	3.0364(8)	3.0398(11)
Pb(2)-Br(4)	3.0923(8)	3.0837(11)
Pb(2)-Br(4)#2	2.9921(8)	3.0088(11)
Pb(2)-Br(5)	2.8328(8)	2.8425(11)
Pb(2)-Br(5)#2	3.3111(8)	3.2973(12)
Pb(2)-Br(6)	3.0377(8)	3.0295(11)
Pb(2)-Br(6)#2	2.9515(8)	2.9704(11)
Br(2)#1-Pb(1)-Br(3)	95.50(2)	95.80(3)
Br(2)#1-Pb(1)-Br(1)	93.95(2)	94.23(3)
Br(3)-Pb(1)-Br(1)	88.38(2)	88.14(3)
Br(2)#1-Pb(1)-Br(3)#1	84.87(2)	84.86(3)
Br(3)-Pb(1)-Br(3)#1	94.52(3)	94.55(4)
Br(2)#1-Pb(1)-Br(1)#1	82.36(2)	82.49(3)
Br(1)-Pb(1)-Br(1)#1	91.78(2)	92.00(3)
Br(3)#1-Pb(1)-Br(1)#1	85.30(2)	85.29(3)
Br(3)-Pb(1)-Br(2)	80.21(2)	80.45(3)
Br(1)-Pb(1)-Br(2)	77.81(2)	78.14(3)
Br(3)#1-Pb(1)-Br(2)	103.56(2)	102.93(3)
Br(1)#1-Pb(1)-Br(2)	101.91(2)	101.24(3)
Br(5)-Pb(2)-Br(6)#2	92.21(2)	93.52(3)
Br(5)-Pb(2)-Br(4)#2	94.04(2)	95.05(3)
Br(6)#2-Pb(2)-Br(4)#2	88.90(2)	88.23(3)
Br(5)-Pb(2)-Br(6)	85.20(2)	85.37(3)
Br(6)#2-Pb(2)-Br(6)	94.89(3)	95.01(4)
Br(5)-Pb(2)-Br(4)	84.15(2)	84.34(3)
Br(4)#2-Pb(2)-Br(4)	90.64(2)	90.97(3)
Br(6)-Pb(2)-Br(4)	85.53(2)	85.81(3)
Br(6)#2-Pb(2)-Br(5)#2	78.60(2)	78.73(3)
Br(4)#2-Pb(2)-Br(5)#2	78.02(2)	78.18(3)
Br(6)-Pb(2)-Br(5)#2	103.33(2)	101.83(3)
Br(4)-Pb(2)-Br(5)#2	103.90(2)	103.28(3)
Pb(1)-Br(1)-Pb(1)#2	79.66(2)	79.53(3)
Pb(2)-Br(4)-Pb(2)#1	79.43(2)	79.33(3)
Pb(1)#2-Br(2)-Pb(1)	78.72(2)	78.77(3)
Pb(2)-Br(5)-Pb(2)#1	78.11(2)	78.22(3)
Pb(2)#1-Br(6)-Pb(2)	80.96(2)	80.81(3)
Pb(1)-Br(3)-Pb(1)#2	81.09(2)	80.91(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,y+1/2,z #2 -x+1/2,y-1/2,z

Table S3. Selected bond lengths (Å) and bond angles (°) for $QPbBr_3$ at 173 K and 298 K.

Temperature	173 K	298 K
Pb(1)-Br(1)	2.8241(9)	2.8247(6)
Pb(1)-Br(2)#1	2.9985(9)	3.0046(6)
Pb(1)-Br(2)	3.0201(9)	3.0267(6)
Pb(1)-Br(3)	3.0317(9)	3.0352(6)
Pb(1)-Br(3)#1	3.2822(9)	3.2890(6)
Pb(1)-Br(3)#2	3.0713(9)	3.0766(6)
Br(1)-Pb(1)-Br(2)#1	90.42(3)	90.37(2)
Br(1)-Pb(1)-Br(2)	88.91(3)	89.17(2)
Br(2)-Pb(1)-Br(3)	87.04(2)	86.43(2)
Br(2)#1-Pb(1)-Br(2)	92.28(2)	92.68(2)
Br(1)-Pb(1)-Br(3)	91.97(3)	92.27(2)
Br(2)#1-Pb(1)-Br(3)	89.10(2)	88.67(2)
Br(1)-Pb(1)-Br(3)#2	90.47(3)	91.05(2)
Br(2)#2-Pb(1)-Br(3)#1	92.06(3)	92.20(2)
Br(2)-Pb(1)-Br(3)#2	87.97(2)	87.51(2)
Br(3)-Pb(1)-Br(3)#1	92.07(2)	91.38(2)
Br(3)#1-Pb(1)-Br(3)#2	87.12(2)	87.19(2)
Br(3)-Pb(1)-Br(3)#2	90.64(2)	91.11(2)
Pb(1)#2-Br(2)-Pb(1)	92.28(2)	92.68(2)
Pb(1)#2-Br(3)-Pb(1)#1	92.88(2)	93.57(2)
Pb(1)#2-Br(3)-Pb(1)	87.93(2)	88.62(2)
Pb(1)-Br(3)-Pb(1)#1	90.64(2)	91.11(2)

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z #2 x+1,y,z

Table S4. Selected bond lengths (Å) and bond angles (°) for $QPbI_3$ at 173 K and 298 K.

Temperature	173 K	298 K
Pb(1)-I(1)	3.0001(7)	2.9956(6)
Pb(1)-I(2)	3.2051(6)	3.2092(5)
Pb(1)-I(2)#1	3.2945(6)	3.2996(5)
Pb(1)-I(3)	3.2174(6)	3.2207(5)
Pb(1)-I(3)#1	3.2732(6)	3.2749(5)
Pb(1)-I(3)#2	3.5061(6)	3.5212(5)
I(1)-Pb(1)-I(2)	90.87(2)	91.19(1)
I(1)-Pb(1)-I(3)	91.76(2)	92.40(1)
I(2)-Pb(1)-I(3)	89.92(2)	89.67(1)
I(1)-Pb(1)-I(3)#1	92.89(2)	93.08(1)
I(3)-Pb(1)-I(3)#1	91.29(2)	91.53(1)
I(1)-Pb(1)-I(2)#1	92.00(2)	91.88(1)
I(2)-Pb(1)-I(2)#1	91.12(2)	91.28(1)
I(3)#1-Pb(1)-I(2)#1	87.42(2)	87.20(1)
I(2)-Pb(1)-I(3)#2	89.16(2)	89.13(1)
I(3)-Pb(1)-I(3)#2	92.04(2)	91.71(1)
I(3)#1-Pb(1)-I(3)#2	87.19(2)	86.69(1)
I(2)#1-Pb(1)-I(3)#2	84.21(2)	84.04(1)
Pb(1)-I(2)-Pb(1)#2	91.12(2)	91.28(1)
Pb(1)-I(3)-Pb(1)#2	91.29(2)	91.53(1)
Pb(1)-I(3)-Pb(1)#3	92.81(2)	93.31(1)
Pb(1)#2-I(3)-Pb(1)#3	87.96(2)	88.29(1)

Symmetry transformations used to generate equivalent atoms:

#1 x,y+1,z #2 x,y-1,z #3 x-1/2,-y+1/2,-z+1

Table S5. Hydrogen bond lengths (Å) and angles (°) for $IQPbBr_3$, $QPbBr_3$ and $QPbI_3$ at 173 K.

$APbX_3$	**D-H...A**	**d(D-H)**	**d(H...A)**	**d(D...A)**	**<(DHA)**
	N(1)-H(2)...Br(1)	0.86	3.13	3.537(8)	111.8
	N(1)-H(2)...Br(1)#1	0.86	3.08	3.694(9)	129.9
$IQPbBr_3$	N(1)-H(2)...Br(6)#3	0.86	2.98	3.613(8)	132.3
	N(2)-H(10)...Br(3)	0.86	3.10	3.413(8)	104.4
	N(2)-H(10)...Br(4)	0.86	2.72	3.462(9)	145.5
$QPbBr_3$	N(1)-H(1)...Br(1)	0.86	2.50	3.324(8)	161.9
$QPbI_3$	N(1)-H(1)...I(1)	0.86	2.93	3.604(8)	136.5
	N(1)-H(1)...I(1)#3	0.86	3.24	3.829(8)	128.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,y+1/2,z #3 x,-y+1/2,z+1/2 (**$IQPbBr_3$**); #3 -x+1,y,-z+3/2 (**$QPbI_3$**)