Supporting information for

Influence of organic cation planarity on structural templating in hybrid metal-halides

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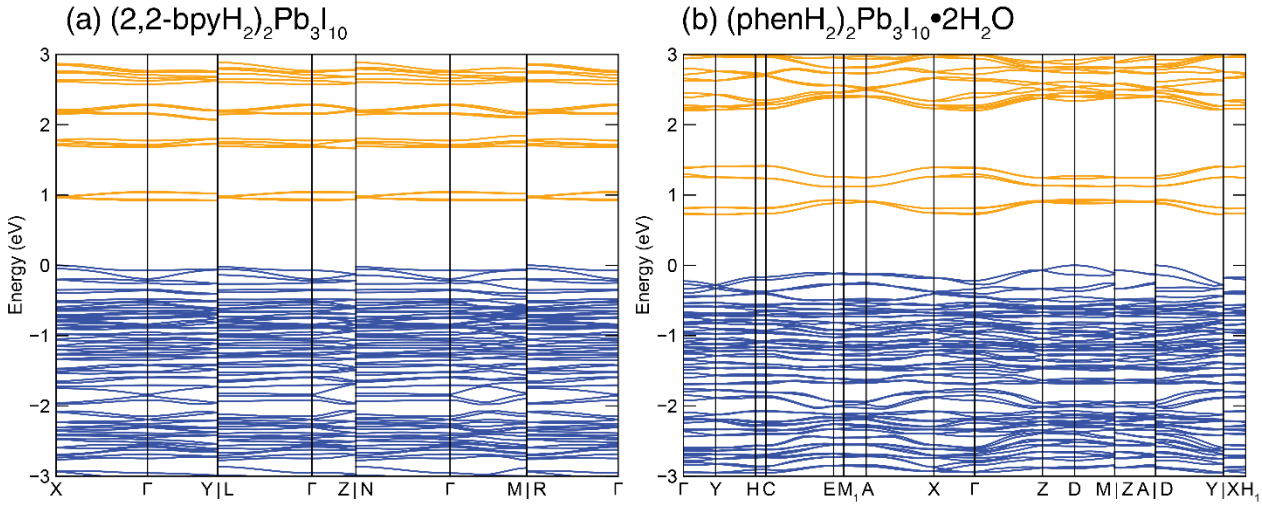

Figure S1. Band structures of (a) $(2,2\text{-bpyH}_2)_2Pb_3I_{10}$ and (b) $(phenH_2)_2Pb_3I_{10}\bullet 2H_2O$.

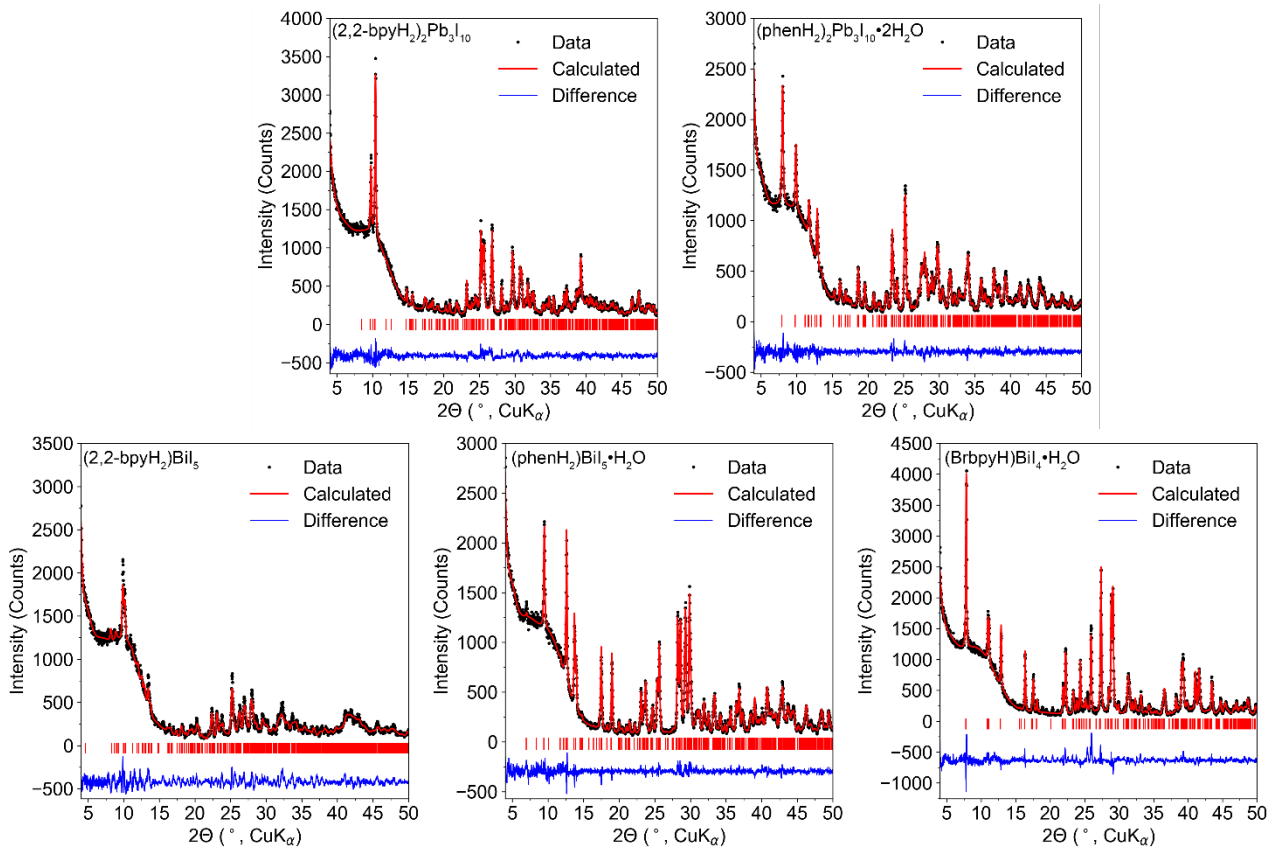

Figure S2. Powder diffraction patterns for all compounds.

Table S1. Atomic Positions and Thermal Parameters obtained from single crystal diffraction.

Compound/Atom	***x***	***y***	***z***	U_{iso}*/U_{eq}	**Occupancy (<1)**
$(2,2\text{-bpyH}_2)_2Pb_3I_{10}$					
Pb1	0.35414 (2)	0.73440 (3)	0.55324 (2)	0.03809 (9)	
Pb2	½	0.72704 (4)	¾	0.04067 (11)	
I1	0.24478 (2)	0.50023 (5)	0.49378 (2)	0.03932 (12)	
I2	0.46307 (2)	0.96512 (5)	0.62693 (3)	0.04497 (13)	
I3	0.34868 (3)	0.69645 (6)	0.71471 (3)	0.04736 (13)	
I4	0.46668 (2)	0.50470 (5)	0.62091 (3)	0.04738 (13)	
I5	0.35964 (3)	0.72084 (5)	0.40329 (3)	0.04879 (14)	
N1	0.1956 (3)	0.1828 (7)	0.3353 (4)	0.066 (2)	
H1A	0.211071	0.108885	0.360414	0.079*	
N2	0.3451 (3)	0.3628 (6)	0.4013 (3)	0.0429 (14)	
H2A	0.328379	0.444268	0.393051	0.051*	
C1	0.1325 (5)	0.1930 (10)	0.2985 (6)	0.078 (3)	
H1	0.106510	0.119972	0.299387	0.094*	
C2	0.1051 (4)	0.3085 (9)	0.2595 (5)	0.055 (2)	
H2	0.060768	0.316610	0.233651	0.066*	
C3	0.1446 (4)	0.4107 (8)	0.2597 (4)	0.055 (2)	
H3	0.127285	0.491669	0.233873	0.066*	
C4	0.2103 (4)	0.3977 (7)	0.2976 (4)	0.053 (2)	
H4	0.236717	0.469985	0.296962	0.063*	
C5	0.2370 (4)	0.2814 (7)	0.3356 (4)	0.0345 (15)	
C6	0.3055 (4)	0.2526 (7)	0.3761 (4)	0.0374 (16)	
C7	0.3329 (4)	0.1238 (7)	0.3899 (4)	0.0434 (17)	
H7	0.306999	0.045849	0.372904	0.052*	
C8	0.3981 (4)	0.1084 (8)	0.4284 (4)	0.0499 (19)	
H8	0.416151	0.020279	0.438099	0.060*	
C9	0.4368 (4)	0.2233 (9)	0.4526 (5)	0.055 (2)	
H9	0.481157	0.214692	0.478153	0.066*	
C10	0.4079 (4)	0.3518 (9)	0.4377 (4)	0.0498 (19)	
H10	0.432891	0.431175	0.453529	0.060*	
$(phenH_2)_2Pb_3I_{10}\bullet 2H_2O$					
Pb1	0.39548 (3)	0.65516 (2)	0.55077 (2)	0.03377 (9)	
Pb2	0	½	½	0.03677 (11)	
I1	0.41918 (6)	0.87036 (3)	0.54441 (3)	0.04281 (14)	

I2	0.32710 (6)	0.41678 (3)	0.56505 (3)	0.04477 (14)
I3	0.57536 (7)	0.64950 (4)	0.70231 (3)	0.04915 (15)
I4	0.18245 (6)	0.63098 (4)	0.38597 (3)	0.04802 (14)
I5	0.06379 (7)	0.67440 (4)	0.61182 (3)	0.05097 (15)
O1	0.1665 (9)	0.3217 (5)	0.7243 (5)	0.0522 (17)
H1B	0.116 (9)	0.285 (5)	0.749 (4)	0.03 (2)*
H2B	0.147 (14)	0.332 (7)	0.692 (6)	0.06 (4)*
N1	0.1298 (7)	0.5030 (4)	0.7812 (4)	0.0387 (14)
H1A	0.143512	0.454118	0.754046	0.046*
N2	0.4305 (7)	0.4119 (4)	0.7879 (3)	0.0360 (13)
H2A	0.357769	0.391089	0.757282	0.043*
C1	0.9919(10)	0.5460 (6)	0.7758 (5)	0.049 (2)
H1	0.08684	0.522767	0.743113	0.059*
C2	0.9644 (10)	0.6254 (5)	0.8183 (5)	0.0454 (18)
H2	0.867958	0.655600	0.814659	0.054*
C3	0.0820 (10)	0.6579 (5)	0.8656 (5)	0.0424 (18)
H3	0.065122	0.711156	0.894274	0.051*
C4	0.2296 (9)	0.6125 (4)	0.8720 (4)	0.0378 (16)
C5	0.3508 (10)	0.6437 (5)	0.9228 (5)	0.0447 (19)
H5	0.334695	0.696218	0.952431	0.054*
C6	0.4887 (10)	0.5986 (5)	0.9289 (5)	0.0484 (19)
H6	0.566775	0.619254	0.963070	0.058*
C7	0.5148 (9)	0.5189 (5)	0.8828 (4)	0.0400 (17)
C8	0.6631 (9)	0.4721 (5)	0.8868 (5)	0.0462 (19)
H8	0.742051	0.491538	0.920970	0.055*
C9	0.6872 (10)	0.3983 (6)	0.8396 (5)	0.051 (2)
H9	0.783197	0.367602	0.840928	0.062*
C10	0.5672 (10)	0.3701 (5)	0.7899 (5)	0.0470 (19)
H10	0.583688	0.320539	0.757397	0.056*
C11	0.3985 (8)	0.4863 (4)	0.8317 (4)	0.0306 (14)
C12	0.2502 (8)	0.5328 (4)	0.8279 (4)	0.0314 (14)
(2,2-bpy H_2)BiI_5				
Bi1	0.84182 (4)	0.89613 (3)	0.78618 (2)	0.04403 (10)
Bi2	0.81019 (4)	0.23816 (3)	0.63546 (2)	0.04626 (10)
I1	0.05312 (7)	0.12386 (6)	0.74055 (4)	0.05246 (17)
I2	0.58133 (8)	0.31398 (8)	0.54417 (4)	0.0668 (2)

I3	0.37961 (8)	0.40309 (8)	0.89835 (5)	0.0728 (2)
I4	0.62408 (9)	0.71195 (8)	0.81399 (5)	0.0759 (2)
I5	0.82469 (10)	0.48609 (8)	0.67677 (5)	0.0826 (3)
I6	0.87260 (10)	0.91509 (10)	0.93567 (4)	0.0821 (3)
I7	0.61998 (7)	0.12940 (7)	0.77021 (4)	0.05882 (18)
I8	0.81569 (7)	0.92277 (6)	0.62017 (3)	0.05373 (17)
I9	0.05784 (7)	0.69711 (6)	0.79158 (4)	0.06069 (19)
I10	0.00867 (7)	0.29120 (7)	0.51846 (3)	0.05360 (17)
N1	0.3920 (11)	0.0644 (11)	0.9306 (6)	0.0830 (15)
H1A	0.405955	0.143088	0.933310	0.100*
N2	0.0401 (12)	0.3958 (11)	0.9380 (6)	0.0889 (16)
H2A	0.125271	0.393495	0.944094	0.107*
N3	0.4209 (9)	0.5823 (9)	0.6894 (6)	0.0690 (9)
H3A	0.483428	0.627962	0.701164	0.083*
N4	0.2055 (9)	0.8444 (9)	0.6074 (5)	0.0690 (9)
H4A	0.132620	0.802876	0.608312	0.083*
C1	0.3103 (14)	0.0439 (14)	0.8837 (7)	0.0830 (15)
H1	0.270291	0.111643	0.853699	0.100*
C2	0.2853 (14)	0.9253 (14)	0.8796 (7)	0.0830 (15)
H2	0.221107	0.911205	0.848114	0.100*
C3	0.3441 (13)	0.8241 (14)	0.9169 (7)	0.0830 (15)
H3	0.327053	0.741621	0.909595	0.100*
C4	0.4452 (13)	0.8488 (14)	0.9746 (7)	0.0830 (15)
H4	0.490427	0.78385	0.995808	0.100*
C5	0.4580 (14)	0.9743 (15)	0.9758 (7)	0.0830 (15)
C6	0.9970 (14)	0.3293 (14)	0.8926 (8)	0.0889 (16)
H6	0.056796	0.283152	0.868065	0.107*
C7	0.8662 (14)	0.3290 (14)	0.8823 (8)	0.0889 (16)
H7	0. 832262	0.274951	0.854293	0.107*
C8	0.7835 (15)	0.4062 (14)	0.9122 (8)	0.0889 (16)
H8	0. 692356	0.410877	0.902861	0.107*
C9	0. 8367 (14)	0.4822 (14)	0.9590 (8)	0.0889 (16)
H9	0.781584	0.541598	0.977467	0.107*
C10	0.9653 (15)	0.4669 (14)	0.9759 (8)	0.0889 (16)
C11	0.4274 (12)	0.4545 (10)	0.7101 (7)	0.0690 (9)
H11	0.500141	0.417801	0.735931	0.083*

C12	0.3332 (11)	0.3798 (11)	0.6947 (7)	0.0690 (9)
H12	0.338096	0.291594	0.709598	0.083*
C13	0.2281 (12)	0.4366 (11)	0.6560 (7)	0.0690 (9)
H13	0.159761	0.386565	0.644578	0.083*
C14	0.2228 (12)	0.5676 (10)	0.6337 (7)	0.0690 (9)
H14	0.151702	0.604734	0.606612	0.083*
C15	0.3180 (12)	0.6416 (11)	0.6504 (7)	0.0690 (9)
C16	0.3182 (12)	0.7791 (11)	0.6298 (7)	0.0690 (9)
C17	0.4298 (12)	0.8500 (11)	0.6273 (7)	0.0690 (9)
H17	0.510791	0.809221	0.641579	0.083*
C18	0.4267 (12)	0.9800 (10)	0.6043 (7)	0.0690 (9)
H18	0.504436	0.026332	0.603674	0.083*
C19	0.3077 (11)	0.0414 (11)	0.5822 (7)	0.0690 (9)
H19	0.302471	0.129516	0.566816	0.083*
C20	0.2008 (12)	0.9693 (11)	0.5838 (7)	0.0690 (9)
H20	0.119788	0.007969	0.567923	0.083*
$(phenH_2)BiI_5 \cdot H_2O$				
Bi1	½	0.71572 (4)	¾	0.02875 (13)
Bi2	0	0.33968 (4)	¾	0.02972 (13)
I1	0.92366 (8)	0.34299 (6)	0.58652 (3)	0.04739 (19)
I2	0.37890 (9)	0.71449 (6)	0.58970 (3)	0.04663 (19)
I3	0.77106 (8)	0.18062 (6)	0.76121 (4)	0.0534 (2)
I4	0.25724 (8)	0.52978 (6)	0.76379 (5)	0.0589 (2)
I5	0.71907 (11)	0.87722 (8)	0.72499 (5)	0.0729 (3)
N2	0.9093 (9)	0.8490 (6)	0.5733 (4)	0.0399 (19)
H2A	0.940779	0.787550	0.587366	0.048*
N1	0.7570 (9)	0.6640 (6)	0.5085 (5)	0.0396 (19)
H1A	0.829618	0.655946	0.543550	0.047*
C5	0.5487 (12)	0.8794 (8)	0.4085 (6)	0.049 (3)
H5	0.468861	0.887723	0.371126	0.058*
C4	0.5959 (10)	0.7761 (8)	0.4308 (5)	0.037 (2)
C11	0.7907 (10)	0.8563 (8)	0.5204 (5)	0.038 (2)
C12	0.7152 (10)	0.7625 (7)	0.4870 (5)	0.0330 (19)
C7	0.7376 (10)	0.9537 (7)	0.4970 (5)	0.037 (2)
C9	0.9277 (14)	0.0316 (10)	0.5866 (6)	0.054 (3)
H9	0.972520	0.089887	0.610898	0.065*

C3	0.5261 (13)	0.6874 (9)	0.3988 (6)	0.051 (3)	
H3	0.445472	0.695152	0.361766	0.061*	
C2	0.5734 (13)	0.5876 (9)	0.4205 (7)	0.056 (3)	
H2	0.528719	0.528187	0.397658	0.067*	
C6	0.6169 (12)	0.9652 (8)	0.4401 (5)	0.043 (2)	
H6	0.584503	0.96808	0.424578	0.052*	
C10	0.9790 (12)	0.9311 (10)	0.6042 (6)	0.053 (3)	
H10	0.993571	0.921724	0.638606	0.063*	
C1	0.6896 (12)	0.5794 (9)	0.4773 (6)	0.050 (3)	
H1	0.721293	0.513098	0.494080	0.060*	
C8	0.8100 (12)	0.0424 (9)	0.5328 (6)	0.047 (2)	
H8	0.775721	0.109437	0.519016	0.056*	
O1	0.9928 (11)	0.6522 (8)	0.6221 (6)	0.076 (3)	
H1B	0.092 (4)	0.652 (12)	0.618 (8)	0.091*	
H2B	0.962 (15)	0.621 (11)	0.660 (5)	0.091*	
(BrbpyH)BiI$_4$•H$_2$O					
Bi1	½	0.91986 (2)	¾	0.03140 (10)	
I1	0.60717 (2)	0.93344 (2)	0.49435 (5)	0.03774 (11)	
I2	0.38325 (3)	0.79661 (2)	0.52703 (6)	0.04507 (12)	
Br1	0.31099 (5)	0.56428 (4)	0.43143 (10)	0.05210 (18)	
N1	0.4272 (3)	0.4506 (3)	0.6211 (7)	0.0357 (10)	
H1	0.453176	0.494432	0.670659	0.043*	0.5
C1	0.3547 (4)	0.4571 (4)	0.4895 (8)	0.0386 (13)	
C2	0.3102 (4)	0.3894 (5)	0.4018 (9)	0.0498 (16)	
H2	0.259475	0.395277	0.310000	0.060*	
C3	0.3444 (5)	0.3127 (5)	0.4567 (10)	0.0591 (19)	
H3	0.317121	0.265692	0.399241	0.071*	
C4	0.4188 (5)	0.3056 (4)	0.5962 (10)	0.0517 (17)	
H4	0.440964	0.253969	0.635590	0.062*	
C5	0.4603 (4)	0.3768 (3)	0.6774 (8)	0.0360 (12)	
O1	0.500000	0.6065 (4)	0.750000	0.080 (3)	
H5	0.537 (4)	0.653 (3)	0.770 (13)	0.097*	

[a] U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.