Supporting Information

Lead-Free and Stable Antimony-Silver-Halide Double Perovskite MA_2AgSbI_6

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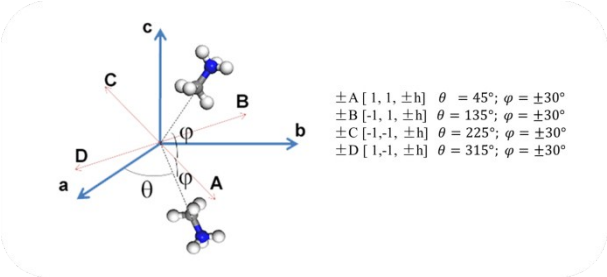
Scheme S1. Preferred Orientations of MA Cation in the Perovskite Cavity



a, b and c are the crystallographics axes of the perovskite with tetragonal phase. A, B, C, and D represent the projection of the MA cation orientations within the ab plane, as measured by the angle θ. The tilting of the molecule with respect to the c-axis is measured by the φ angle.

Table S1. Orientation of MA Cations in Ten Structural Models

Structure	MA Cation Orientation			
	A	**B**	**C**	**D**
1	1-	1-	1-	1-
2	1-	1-;1-	1-	
3	2-	2-		
4	1+	1-	1-	1+
5	2+		2-	
6	1+;1-		1+;1-	
7	1+;1-		1+;1-	
8	1+;1-		1+;1-	
9	2-		2-	
10	Oriented along c axis			

There are four MA cations in the unit cell of MA_2AgSbI_6 (see Figure 1).

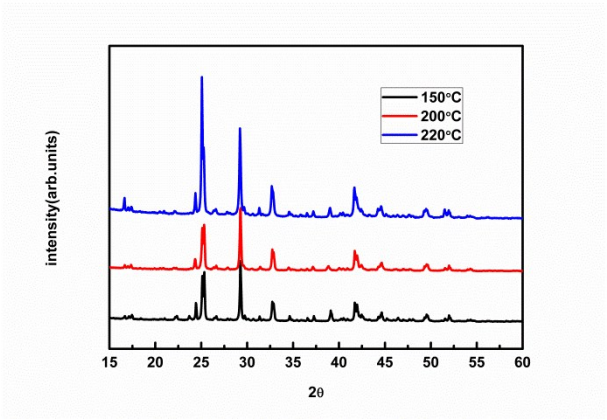


Figure S1. The XRD spectra of powder reacted at different temperature 150℃, 200℃and 220℃, respectively.

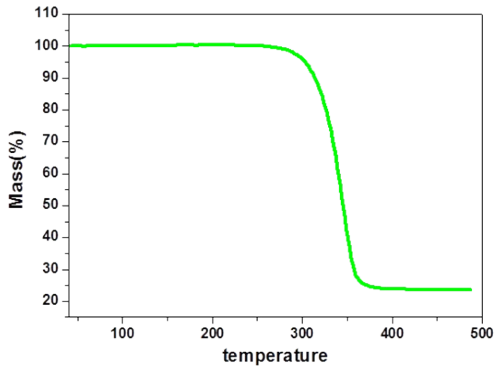


Figure S2. The thermogravimetric spectrum of MA_2AgSbI_6 under N_2

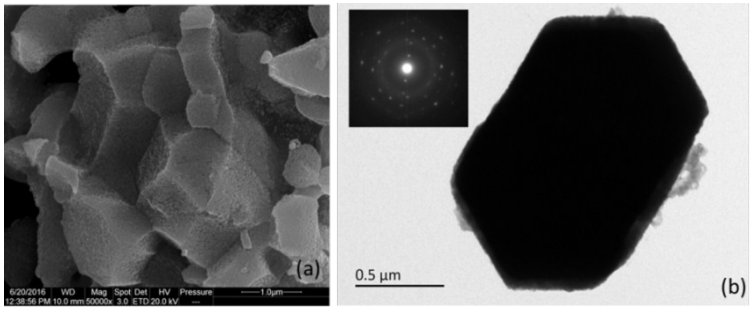


Figure S3. (a) SEM image of powder MA_2AgSbI_6. (b) TEM image and SAED patterns of powder MA_2AgSbI_6. The powder was suspended in n-hexane.