

Electronic Supplementary Information for: Bulk Crystal Growth of Hybrid Perovskite Material $\text{CH}_3\text{NH}_3\text{PbI}_3$

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Fig. S1 The photograph of white MAI.

Fig. S2 The photograph of white with yellow MAI.

Fig. S3 Calculated and experimental powder X-ray diffraction patterns for MAI.

Fig. S4 ¹H-NMR spectrum of MAI.

Fig. S5 ¹³C-NMR spectrum of MAI.

Fig.S6 The photograph of residue light yellow PbI_2 .

Table S1 Selected bond length(Å) and bond angles(deg) for β -MAPbI₃¹

Table S2 Atomic coordinates and equivalent isotropic displacement parameters for MAPbI₃

Table S3 Anisotropic displacement parameters for MAPbI₃



Fig. S1 The photograph of white MAI.

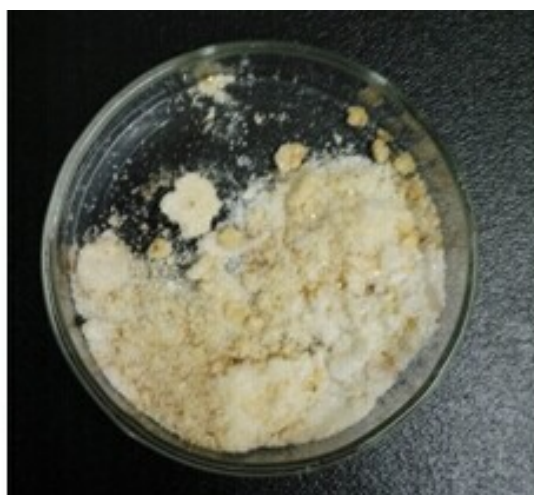


Fig. S2 The photograph of white with yellow MAI.

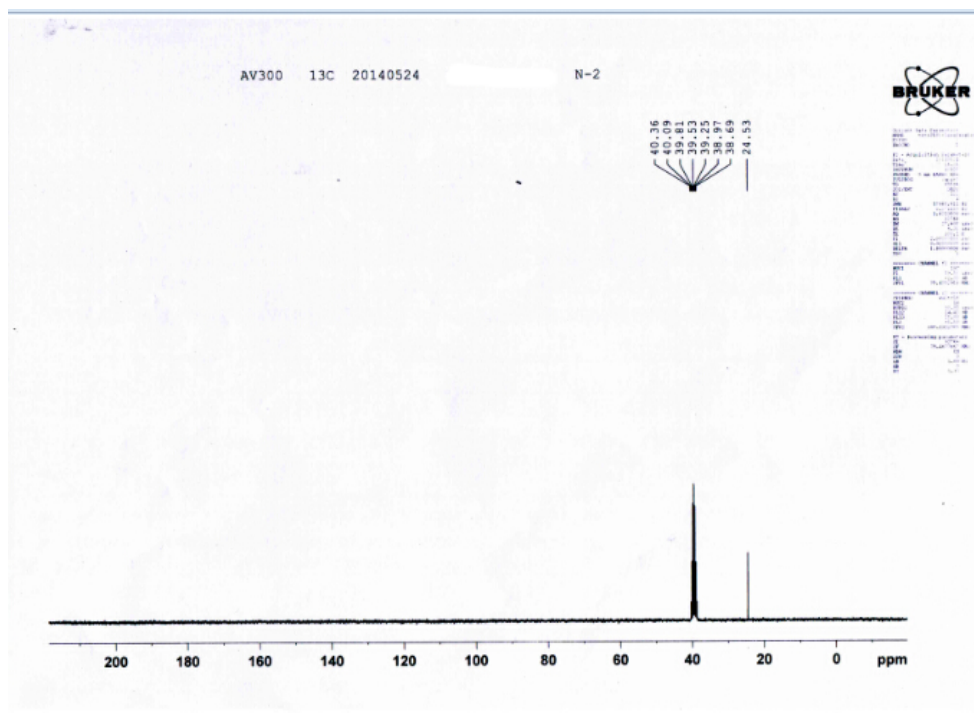


Fig. S5 ¹³C-NMR spectrum of MAI.

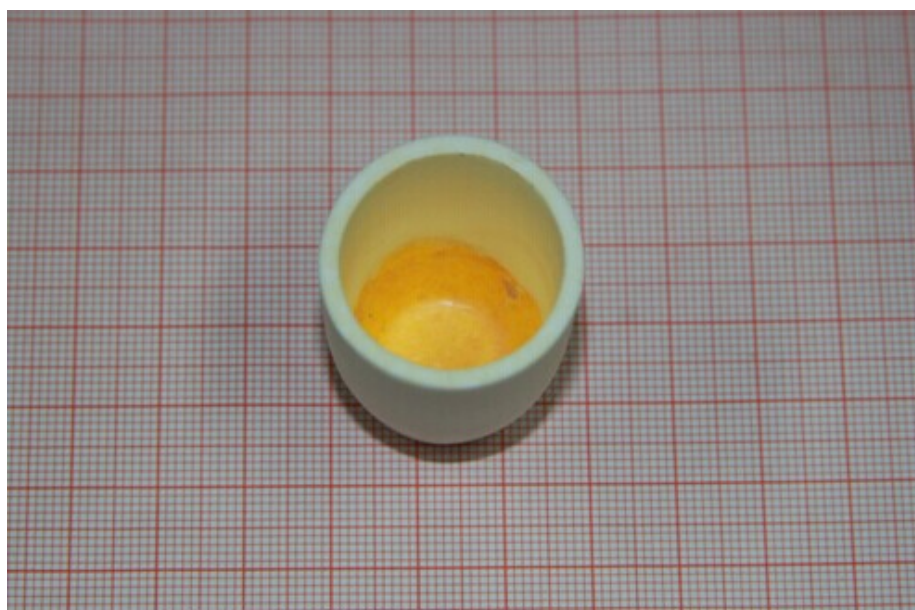


Fig.S6 The photograph of residue PbI₂.

Table S1 Selected bond length(Å) and bond angles(deg) for β -MAPbI₃¹

Pb-I(1)	3.125(8)
Pb-I(2)#1	3.1613(8)
Pb-I(2)#2	3.1613(8)
Pb-I(2)#3	3.1613(8)
Pb-I(2)#4	3.1613(8)
Pb-I(1)#5	3.196(8)
I(1)-Pb#6	3.196(8)
I(2)-Pb#7	3.1613(8)
I(2)-Pb#8	3.1613(8)
C-N	1.39(2)
I(1)-Pb-I(2)#1	88.94(13)
I(1)-Pb-I(2)#2	88.94(13)
I(2)#1-Pb-I(2)#2	177.9(3)
I(1)-Pb-I(2)#3	88.94(13)
I(2)#1-Pb-I(2)#3	89.980(5)
I(1)-Pb-I(2)#4	88.94(13)
I(2)#1-Pb-I(2)#4	89.980(5)
I(2)#3-Pb-I(2)#4	177.9(3)
I(1)-Pb-I(1)#5	180.0
I(2)#4-Pb-I(1)#5	91.06(13)

Pb-I(1)-Pb#6

180.0

Pb#7-I(2)-Pb#8

163.55(6)

Symmetry transformations used to generate equivalent atoms:

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

#4 $-x, -y+1, z$ #5 $x, -y, z-1/2$ #6 $x, -y, z+1/2$

#7 $x+1/2, -y+1/2, z+0$ #8 $x, y+1, z$

Table S2 Atomic coordinates and equivalent isotropic displacement parameters for MAPbI₃

Atom	x	y	z	U(eq)(Å ²)
Pb(01)	0	0	0.1274	0.033(1)
I(002)	0	0	-0.1226(8)	0.122(2)
I(003)	0.2769(4)	0.2231(4)	0.1311(8)	0.104(2)
N(1)	0.4480(4)	0.9480(4)	0.8480(30)	0.063(15)
C(1)	0.4480(4)	0.9480(4)	0.8480(30)	0.063(15)

^aU_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S3. Anisotropic displacement parameters for MAPbI₃

Atom	U11	U22	U33	U23	U13	U12
Pb(01)	0.032(1)	0.032(1)	0.035(10)	0	0	0
I(002)	0.156(3)	0.156(3)	0.025(2)	0	0	0
I(003)	0.081(2)	0.081(2)	0.150(4)	0.055(3)	-0.055(3)	-0.053(2)
N(1)	0.070(2)	0.070(2)	0.05(2)	0.016(15)	0.016(15)	0.050(2)
C(1)	0.070(2)	0.070(2)	0.05(2)	0.016(15)	0.016(15)	0.050(2)

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

Reference

1. C. C. Stoumpos, C. D. Malliakas, and M. G. Kanatzidis, *Inorg. Chem.*, 2013, **52**, 9019.