Electronic supplementary information

Growth, Structure, Optical and Electronic Transport Properties of Tetragonal CH$_3$NH$_3$SnBr$_3$ Perovskite Single Crystal

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Table S1.   Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for MASnBr$_3$.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Sn(1)	5000	5000	5000	25(1)
Sn(2)	5000	5000	0	37(1)
Br(1)	5000	5000	2493(1)	101(1)
Br(3)	5000	0	0	101(1)
Br(2)	5000	0	5000	99(1)
C(1)	0	0	2790(1)	151(1)
N(1)	0	770(5)	1599(1)	314(1)

Table S2.   Bond lengths [A] and angles [deg] for MASnBr$_3$.

Bond	Bond lengths [A] and angles [deg]
Sn(1)-Br(2)#1	2.9347(4)
Sn(1)-Br(2)#2	2.9346(4)

Sn(1)-Br(2)	2.9346(4)
Sn(1)-Br(2)#3	2.9346(4)
Sn(1)-Br(1)	2.9389(5)
Sn(1)-Br(1)#4	2.9389(5)
Sn(2)-Br(1)#5	2.9225(5)
Sn(2)-Br(1)	2.9225(5)
Sn(2)-Br(3)#1	2.9346(4)
Sn(2)-Br(3)	2.9346(4)
Sn(2)-Br(3)#3	2.9346(4)
Sn(2)-Br(3)#2	2.9346(4)
Br(3)-Sn(2)#6	2.9346(4)
Br(2)-Sn(1)#6	2.9346(4)
C(1)-N(1)	1.4679(17)
C(1)-H(1A)	0.9602
C(1)-H(1B)	0.9602
C(1)-H(1C)	0.9602
N(1)-H(1D)	0.8900
N(1)-H(1E)	0.8900
N(1)-H(1F)	0.8900
Br(2)#1-Sn(1)-Br(2)#2	180.0
Br(2)#1-Sn(1)-Br(2)	90.0
Br(2)#2-Sn(1)-Br(2)	90.0
Br(2)#1-Sn(1)-Br(2)#3	90.0
Br(2)#2-Sn(1)-Br(2)#3	90.0
Br(2)-Sn(1)-Br(2)#3	180.0
Br(2)#1-Sn(1)-Br(1)	90.0
Br(2)#2-Sn(1)-Br(1)	90.0
Br(2)-Sn(1)-Br(1)	90.0
Br(2)#3-Sn(1)-Br(1)	90.0
Br(2)#1-Sn(1)-Br(1)#4	90.0
Br(2)#2-Sn(1)-Br(1)#4	90.0
Br(2)-Sn(1)-Br(1)#4	90.0
Br(2)#3-Sn(1)-Br(1)#4	90.0
Br(1)-Sn(1)-Br(1)#4	180.0
Br(1)#5-Sn(2)-Br(1)	180.0
Br(1)#5-Sn(2)-Br(3)#1	90.0
Br(1)-Sn(2)-Br(3)#1	90.0
Br(1)#5-Sn(2)-Br(3)	90.0
Br(1)-Sn(2)-Br(3)	90.0
Br(3)#1-Sn(2)-Br(3)	90.0
Br(1)#5-Sn(2)-Br(3)#3	90.0
Br(1)-Sn(2)-Br(3)#3	90.0
Br(3)#1-Sn(2)-Br(3)#3	90.0

Br(3)-Sn(2)-Br(3)#3	180.0
Br(1)#5-Sn(2)-Br(3)#2	90.0
Br(1)-Sn(2)-Br(3)#2	90.0
Br(3)#1-Sn(2)-Br(3)#2	180.0
Br(3)-Sn(2)-Br(3)#2	90.0
Br(3)#3-Sn(2)-Br(3)#2	90.0
Sn(2)-Br(1)-Sn(1)	180.0
Sn(2)#6-Br(3)-Sn(2)	180.0
Sn(1)#6-Br(2)-Sn(1)	180.0
N(1)-C(1)-H(1A)	109.5
N(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
N(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(1)-N(1)-H(1D)	109.5
C(1)-N(1)-H(1E)	109.5
H(1D)-N(1)-H(1E)	109.5
C(1)-N(1)-H(1F)	109.5
H(1D)-N(1)-H(1F)	109.5
H(1E)-N(1)-H(1F)	109.5

Symmetry transformations used to generate equivalent atoms:

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

#4 -x+1,-y+1,-z+1   #5 -x+1,-y+1,-z

#6 x,y-1,z

Table S3.   Anisotropic displacement parameters (A^2 x 10^3) for MASnBr$_3$.
The anisotropic displacement factor exponent takes the form:
$$-2 \pi^2 [\, h^2 a^{*2} U11 + ... + 2\, h\, k\, a^*\, b^*\, U12 \,]$$

	U11	U22	U33	U23	U13	U12
Sn(1)	22(1)	22(1)	31(1)	0	0	0
Sn(2)	40(1)	40(1)	32(1)	0	0	0
Br(1)	123(1)	123(1)	57(1)	0	0	0
Br(3)	127(1)	53(1)	123(1)	0	0	0
Br(2)	118(1)	49(1)	128(1)	0	0	0
C(1)	151(1)	151(1)	149(1)	0	0	0
N(1)	313(1)	314(1)	315(1)	-1(1)	0	0

Table S4.   Hydrogen coordinates (x 10^4) and isotropic
displacement parameters (A^2 x 10^3) for MASnBr$_3$.

	x	y	z	U(eq)
H(1A)	432	1240	3278	226
H(1B)	1066	-1228	2878	226
H(1C)	-1498	-516	2994	226
H(1D)	380	-385	1146	471
H(1E)	1004	1894	1515	471
H(1F)	-1383	1269	1414	471

Table S5.   Torsion angles [deg] for MASnBr$_3$.

Bond	Bond lengths [A] and angles [deg]
Br(1)#5-Sn(2)-Br(1)-Sn(1)	0(19)
Br(3)#1-Sn(2)-Br(1)-Sn(1)	136(5)
Br(3)-Sn(2)-Br(1)-Sn(1)	-134(5)
Br(3)#3-Sn(2)-Br(1)-Sn(1)	46(5)
Br(3)#2-Sn(2)-Br(1)-Sn(1)	-44(5)
Br(2)#1-Sn(1)-Br(1)-Sn(2)	-136(36)
Br(2)#2-Sn(1)-Br(1)-Sn(2)	44(10)
Br(2)-Sn(1)-Br(1)-Sn(2)	134(10)
Br(2)#3-Sn(1)-Br(1)-Sn(2)	-46(10)
Br(1)#4-Sn(1)-Br(1)-Sn(2)	0(22)
Br(1)#5-Sn(2)-Br(3)-Sn(2)#6	0.0
Br(1)-Sn(2)-Br(3)-Sn(2)#6	0.0
Br(3)#1-Sn(2)-Br(3)-Sn(2)#6	0.0
Br(3)#3-Sn(2)-Br(3)-Sn(2)#6	0.0
Br(3)#2-Sn(2)-Br(3)-Sn(2)#6	0.0
Br(2)#1-Sn(1)-Br(2)-Sn(1)#6	180.0
Br(2)#2-Sn(1)-Br(2)-Sn(1)#6	0.0
Br(2)#3-Sn(1)-Br(2)-Sn(1)#6	0.0
Br(1)-Sn(1)-Br(2)-Sn(1)#6	-90.0
Br(1)#4-Sn(1)-Br(2)-Sn(1)#6	90.0

Symmetry transformations used to generate equivalent atoms:

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

#4 -x+1,-y+1,-z+1   #5 -x+1,-y+1,-z   #6 x,y-1,z