

Supporting Information: Pressure-Induced Tuning of Physical Properties in High-throughput Metal Halide MSn_2Br_5 ($M = K, Cs$) perovskites for Optoelectronic Applications

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Structural properties

Table S1: Computed structural parameters of MSn_2Br_5 ($M = K, Cs$) perovskites.

Pressure P (GPa)	$CsSn_2Br_5$														
	Lattice constants					Volume Formation energy					Br-Sn distance				
	$a=b$ (Å)	c (Å)	V (Å ³)	ΔE_f (eV)/atom	ΔE_f (eV)/atom	$a=b$ (Å)	c (Å)	V (Å ³)	ΔE_f (eV)/atom	ΔE_f (eV)/atom	Br-Sn distance (Å)	Br-Sn distance (Å)	Br-Sn distance (Å)		
0	8.39	14.99	527.40	-2.735	-2.735	2.80	8.54	16.15	589.06	-1.385	-1.385	2.79	2.79		
5	7.97	13.42	426.55	-2.736	-2.736	2.85	8.11	14.00	460.03	-1.393	-1.393	2.87	2.87		
10	7.75	12.90	387.38	-2.738	-2.738	2.83	7.90	13.31	415.32	-1.394	-1.394	2.86	2.86		
15	7.58	12.60	362.43	-2.740	-2.740	2.81	7.75	12.96	387.81	-1.394	-1.394	2.83	2.83		
20	7.44	12.40	343.76	-2.742	-2.742	2.79	7.62	12.64	367.27	-1.399	-1.399	2.81	2.81		
25	7.33	12.24	329.08	-2.744	-2.744	2.77	7.52	12.43	351.29	-1.402	-1.402	2.79	2.79		

Elastic constants

Table S2: The calculated values of elastic constants C_{ij} (in GPa) for KSn_2Br_5 and $CsSn_2Br_5$ perovskites at various applied pressures.

Pressure P (GPa)	KSn_2Br_5						$CsSn_2Br_5$					
	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}
0	24.87	10.49	5.24	15.65	7.59	13.01	12.84	4.80	6.58	8.84	5.29	11.10
5	63.19	29.40	29.42	52.67	19.75	23.95	66.86	37.94	29.42	45.66	22.58	24.23
10	93.60	42.44	50.69	87.13	35.47	31.99	96.09	55.46	47.49	77.09	30.89	31.44
15	128.51	63.50	71.99	113.18	45.07	41.29	125.03	68.84	63.05	111.58	39.27	39.52
20	153.59	72.84	88.04	140.25	57.58	48.63	153.49	85.59	80.67	139.85	51.18	44.73
25	182.07	86.45	104.83	166.58	72.55	56.50	176.38	98.22	91.36	167.69	58.40	51.28

Mechanical Properties

Table S3: The calculated bulk modulus B (GPa), shear modulus G (GPa), Young's modulus E (GPa), Pugh's ratio B/G and Poisson's ratio ν of KSn_2Br_5 perovskite.

Pressure P (GPa)	Bulk modulus			Shear modulus			Young's modulus E	Pugh's ratio B/G	Poisson's ratio ν
	B_V	B_R	B	G_V	G_R	G			
0	11.93	10.91	11.42	8.60	8.03	8.32	20.07	1.37	0.21
5	39.51	39.19	39.35	18.75	18.02	18.38	47.71	2.14	0.29
10	62.45	62.44	62.44	29.29	27.39	28.34	73.85	2.20	0.30
15	87.24	87.16	87.20	37.14	34.39	35.76	94.38	2.44	0.32
20	105.03	105.03	105.03	45.99	42.08	44.04	115.91	2.38	0.32
25	124.77	124.76	124.77	55.96	50.46	53.21	139.76	2.34	0.31

Table S4: The calculated bulk modulus B (GPa), shear modulus G (GPa), Young's modulus E (GPa), Pugh's ratio B/G and Poisson's ratio ν of $CsSn_2Br_5$ perovskite.

Pressure P (GPa)	Bulk modulus			Shear modulus			Young's modulus E	Pugh's ratio B/G	Poisson's ratio ν
	B_V	B_R	B	G_V	G_R	G			
0	7.83	7.70	7.77	5.44	3.59	4.52	11.35	1.72	0.26
5	41.44	38.94	40.19	19.38	17.83	18.61	48.36	2.16	0.29
10	63.35	61.96	62.65	26.57	25.16	25.86	68.20	2.42	0.32
15	83.50	83.00	83.25	34.73	33.69	34.21	90.26	2.43	0.32
20	104.52	104.13	104.32	42.75	41.12	41.93	110.93	2.49	0.32
25	120.26	120.04	120.15	49.58	48.12	48.85	129.06	2.46	0.32

Table S5: Influence of pressure on the hardness of $M\text{Sn}_2\text{Br}_5$ ($M = K, Cs$) perovskites.

P (GPa)	Perovskites	H ₁	H ₂	H ₃	H ₄	H ₅	H ₆	H ₇	H ₈
0	$K\text{Sn}_2\text{Br}_5$	1.10	1.22	1.23	1.27	-1.43	0.91	1.60	7.01
	$Cs\text{Sn}_2\text{Br}_5$	0.75	0.69	0.67	0.72	-2.10	0.49	0.72	6.11
5	$K\text{Sn}_2\text{Br}_5$	3.79	2.90	2.71	3.03	0.35	2.14	2.59	23.76
	$Cs\text{Sn}_2\text{Br}_5$	3.87	2.94	2.74	3.07	0.39	2.18	2.62	24.23
10	$K\text{Sn}_2\text{Br}_5$	6.01	4.48	4.18	4.69	2.11	3.20	3.79	32.65
	$Cs\text{Sn}_2\text{Br}_5$	6.03	4.14	3.81	4.33	1.68	2.85	3.10	34.76
15	$K\text{Sn}_2\text{Br}_5$	8.40	5.73	5.27	5.99	3.43	3.96	4.29	42.99
	$Cs\text{Sn}_2\text{Br}_5$	8.02	5.48	5.05	5.73	3.15	3.78	4.10	41.71
20	$K\text{Sn}_2\text{Br}_5$	10.11	7.04	6.50	7.36	4.89	4.77	5.27	47.62
	$Cs\text{Sn}_2\text{Br}_5$	10.05	6.73	6.18	7.04	4.52	4.74	5.04	48.68
25	$K\text{Sn}_2\text{Br}_5$	12.02	8.48	7.85	8.87	6.51	6.03	6.76	52.43
	$Cs\text{Sn}_2\text{Br}_5$	11.57	7.83	7.21	8.20	5.74	5.46	5.87	52.76