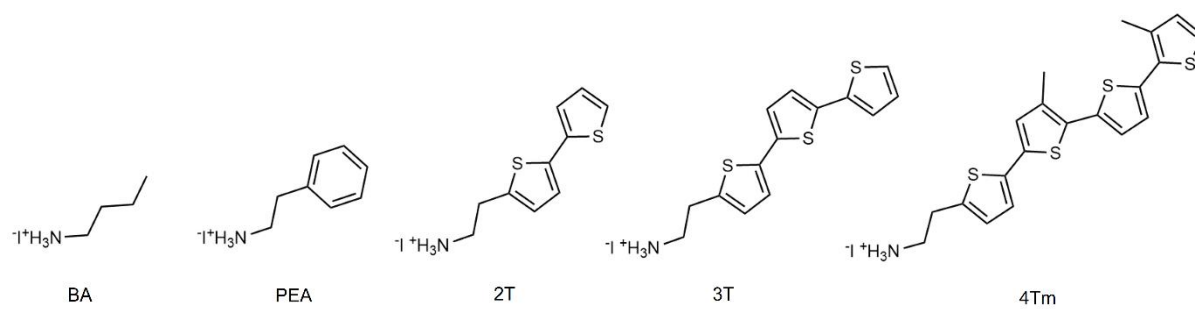

Thickness control of organic semiconductor-incorporated perovskites

In the format provided by the
authors and unedited

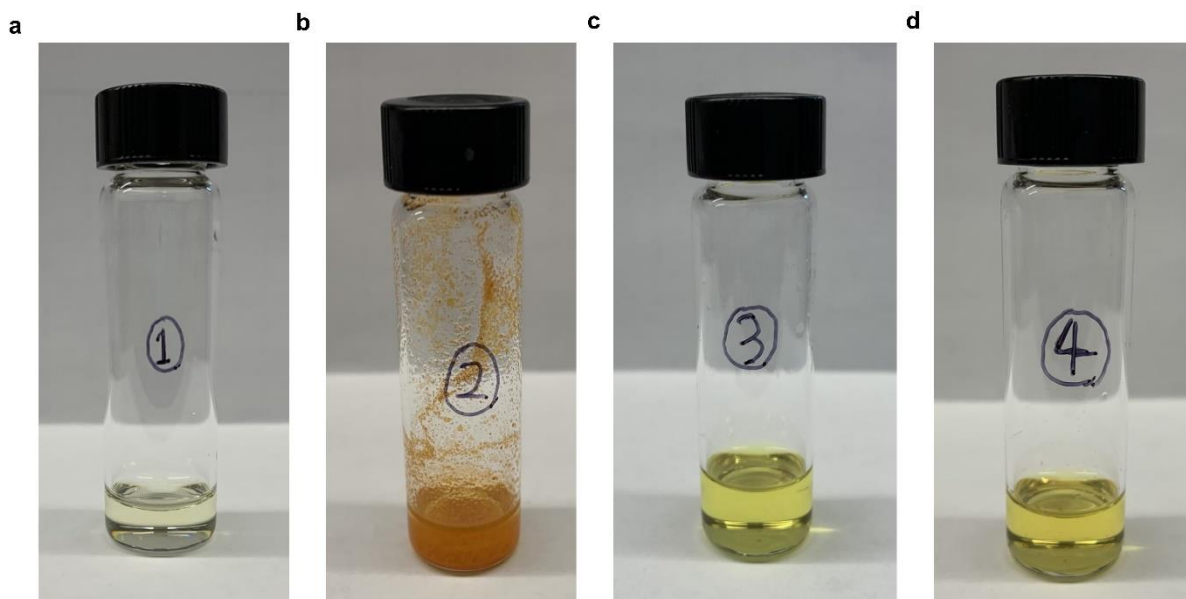
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1. Supplementary figures



Supplementary Fig. 1. The chemical structures of conjugated organic monoammonium ligands (BA, PEA, 2T, 3T, and 4Tm) investigated in this study.



Supplementary Fig. 2.

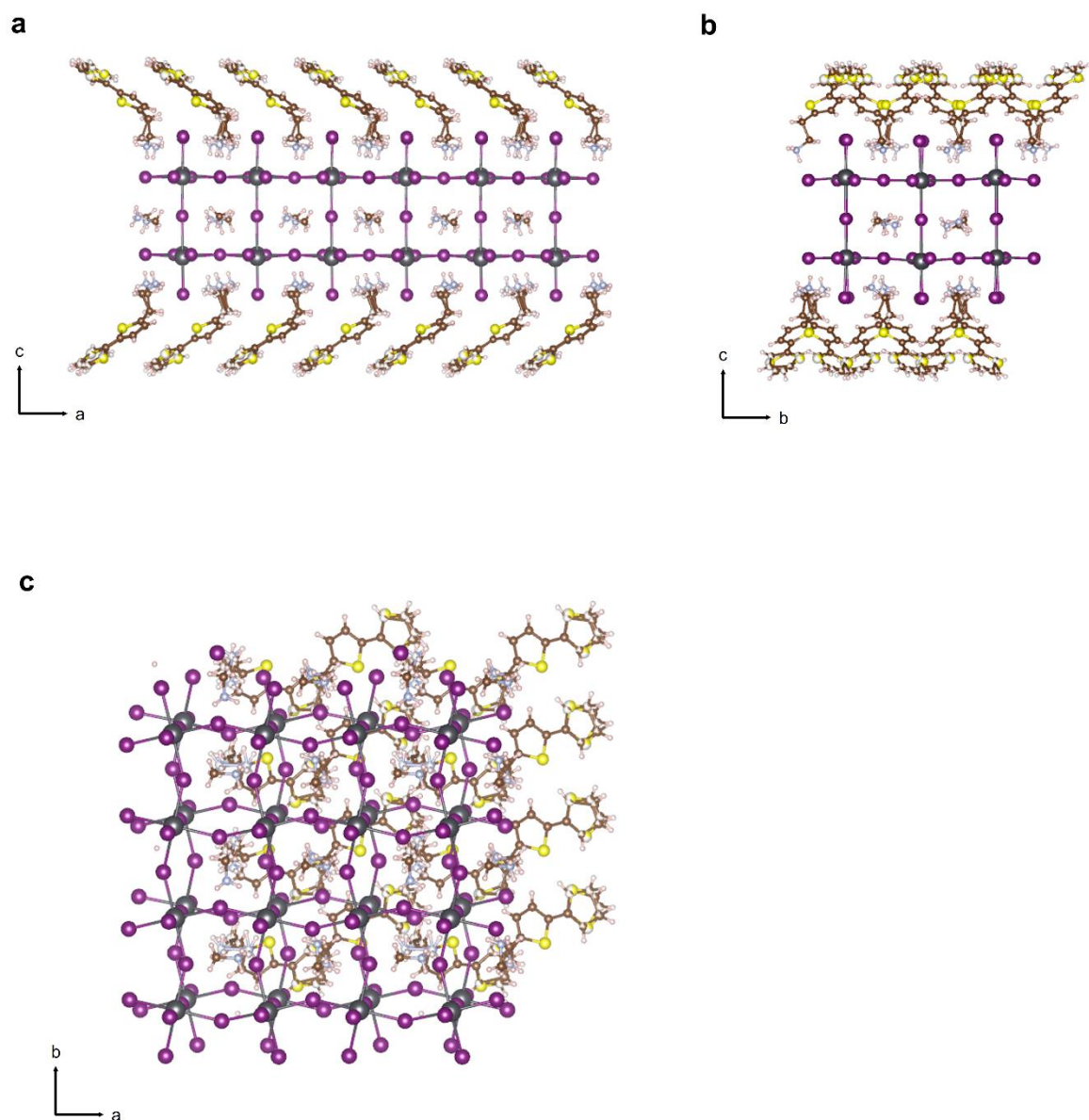
(a) 400 μ l HI + 200 μ l H_3PO_2 + 40 mg PbI_2 + 50 mg MAI

(b) 400 μ l HI + 200 μ l H_3PO_2 + 40 mg PbI_2 + 50 mg MAI + 5mg 2T·HI

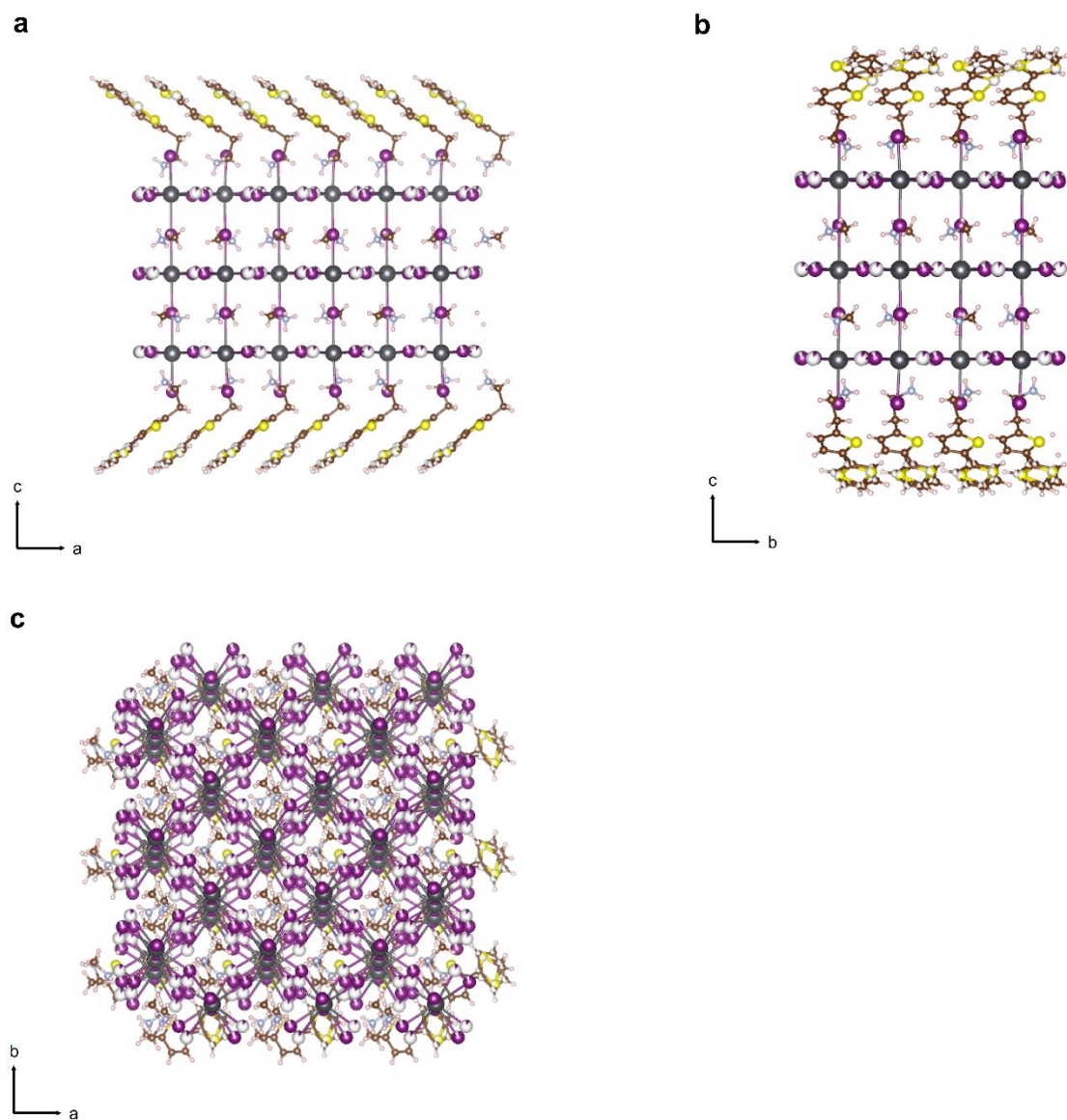
(c) 400 μ l HI + 200 μ l H_3PO_2 + 500 μ l IPA + 40 mg PbI_2 + 50mg MAI + 5mg 2T·HI

(d) 400 μ l HI + 200 μ l H_3PO_2 + 300 μ l EtOH + 40 mg + PbI_2 50 mg MAI + 5mg 2T·HI

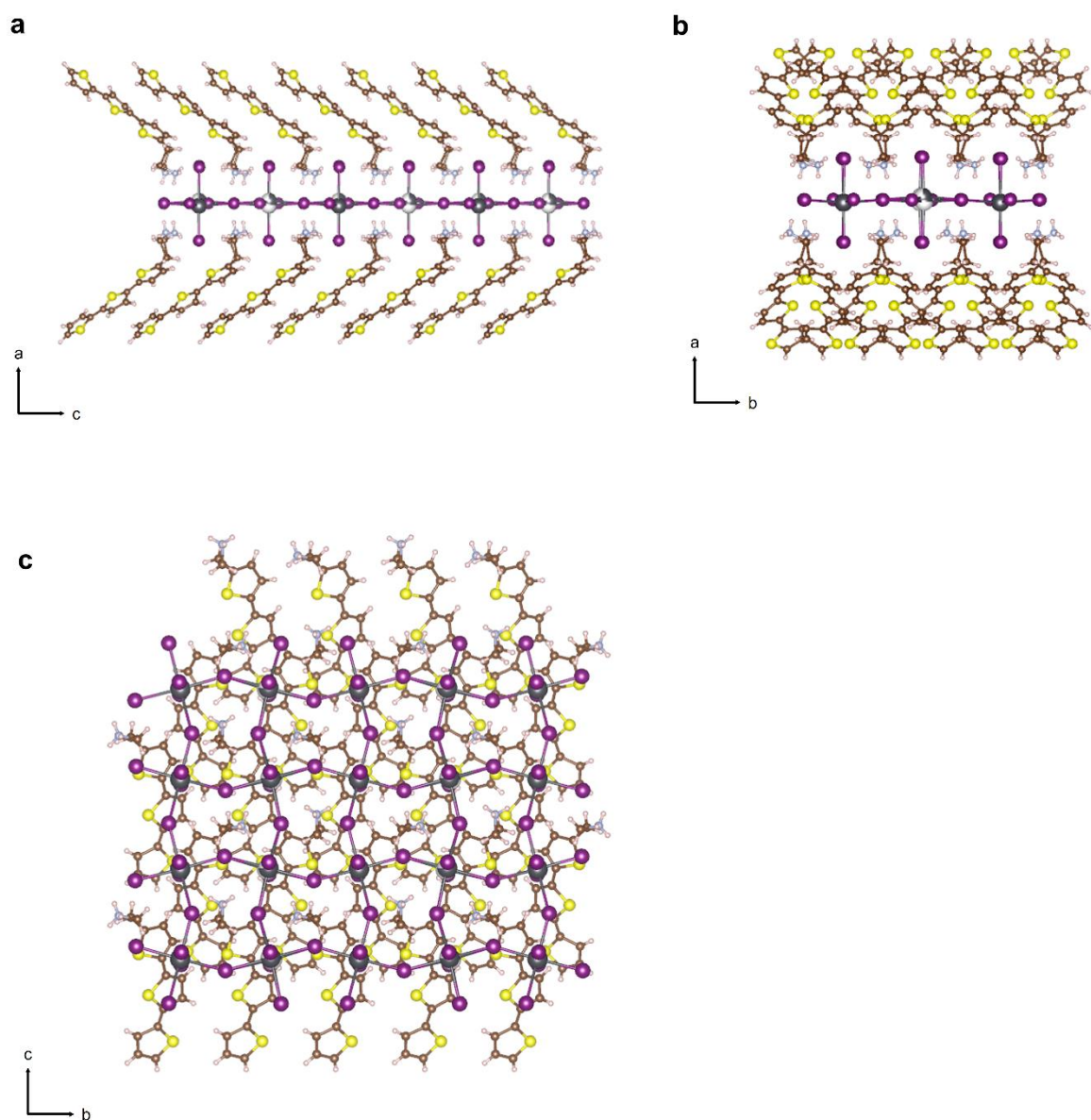
While a mixture of hydroiodic acid (HI) and hypo phosphorous acid (H_3PO_2) is capable of dissolving inorganic lead iodide (PbI_2) and methyl ammonium iodide (MAI) precursors, it is incapable of dissolving conjugated ligand precursors even when heating to 100 $^\circ\text{C}$. Thus, alcoholic solvents (isopropyl alcohol, ethanol) were added to assist the crystallization process. Above shows the mixture each vial is composed of. The vials were heated in a water bath until all precursors were dissolved typically within 5 mins. In case of (b) precursors were not dissolved even with 60 mins of heating (100 $^\circ\text{C}$).



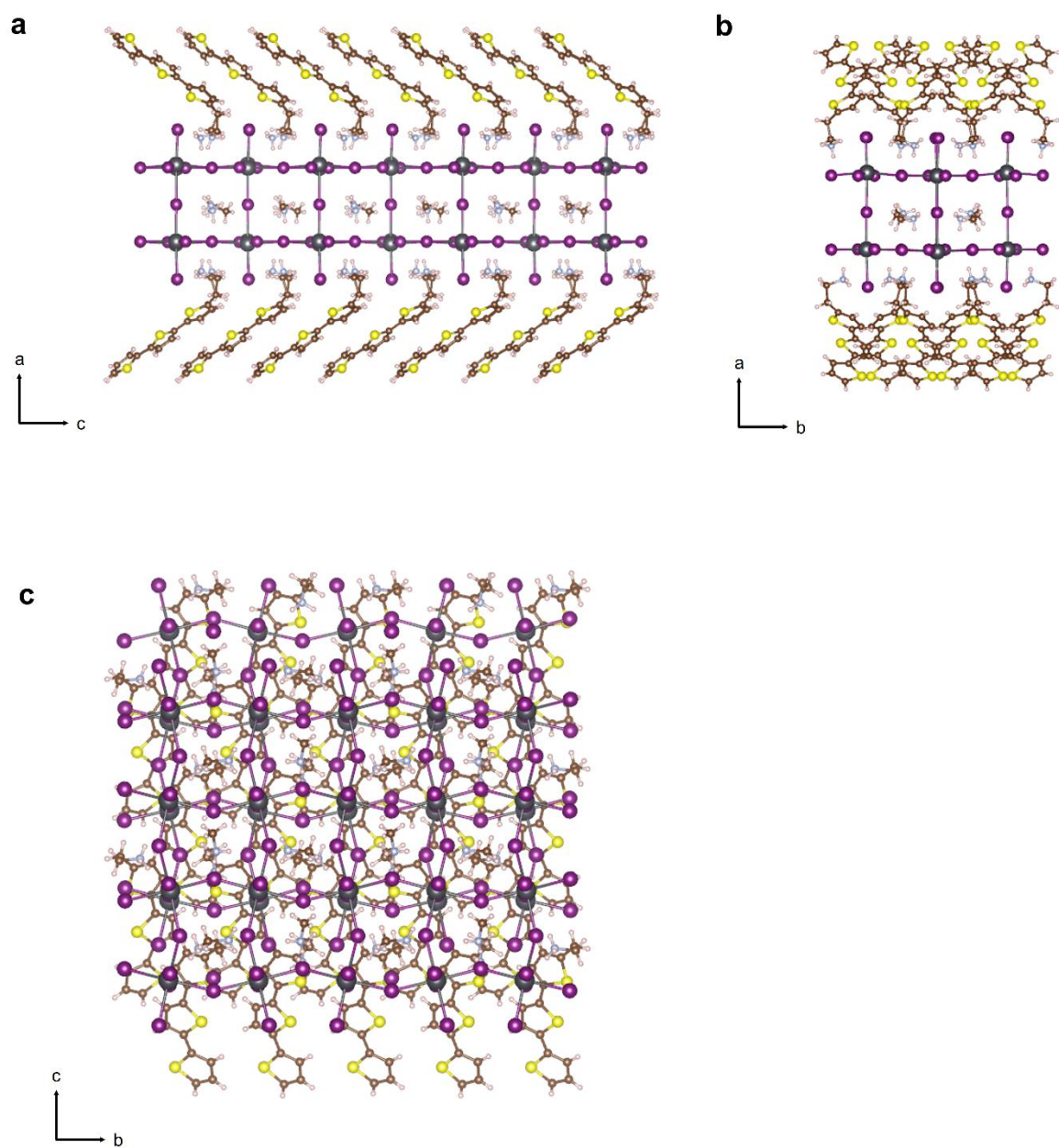
Supplementary Fig. 3. Single crystal structure of $(2T)_2(MA)Pb_2I_7$ solved from single crystal X-ray diffraction. View along (a) *b* axis (b) *a* axis (c) *c* axis.



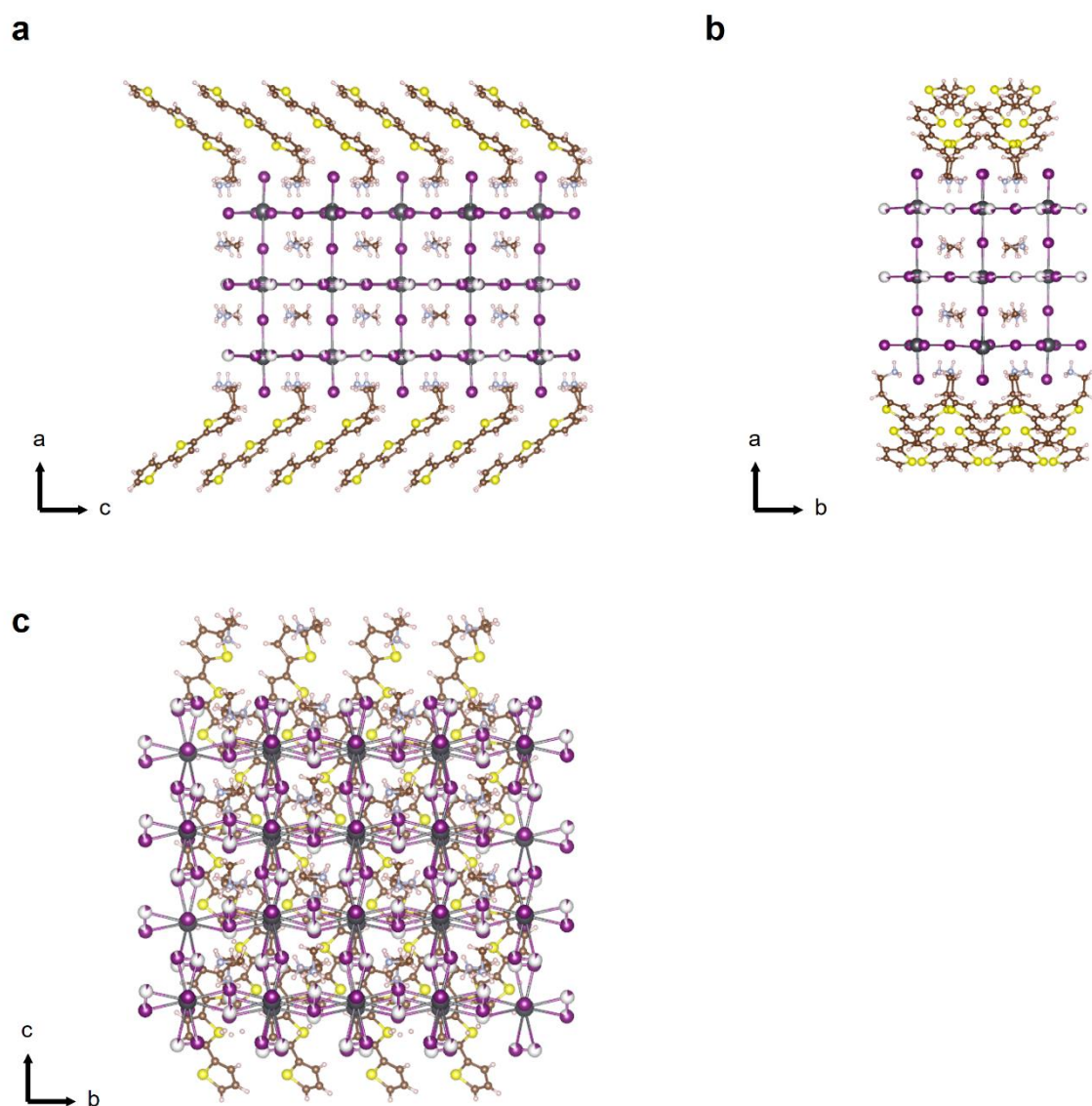
Supplementary Fig. 4. Single crystal structure of $(2T)_2(MA)_2Pb_3I_{10}$ solved from single crystal X-ray diffraction. View along (a) *b* axis (b) *a* axis (c) *c* axis.



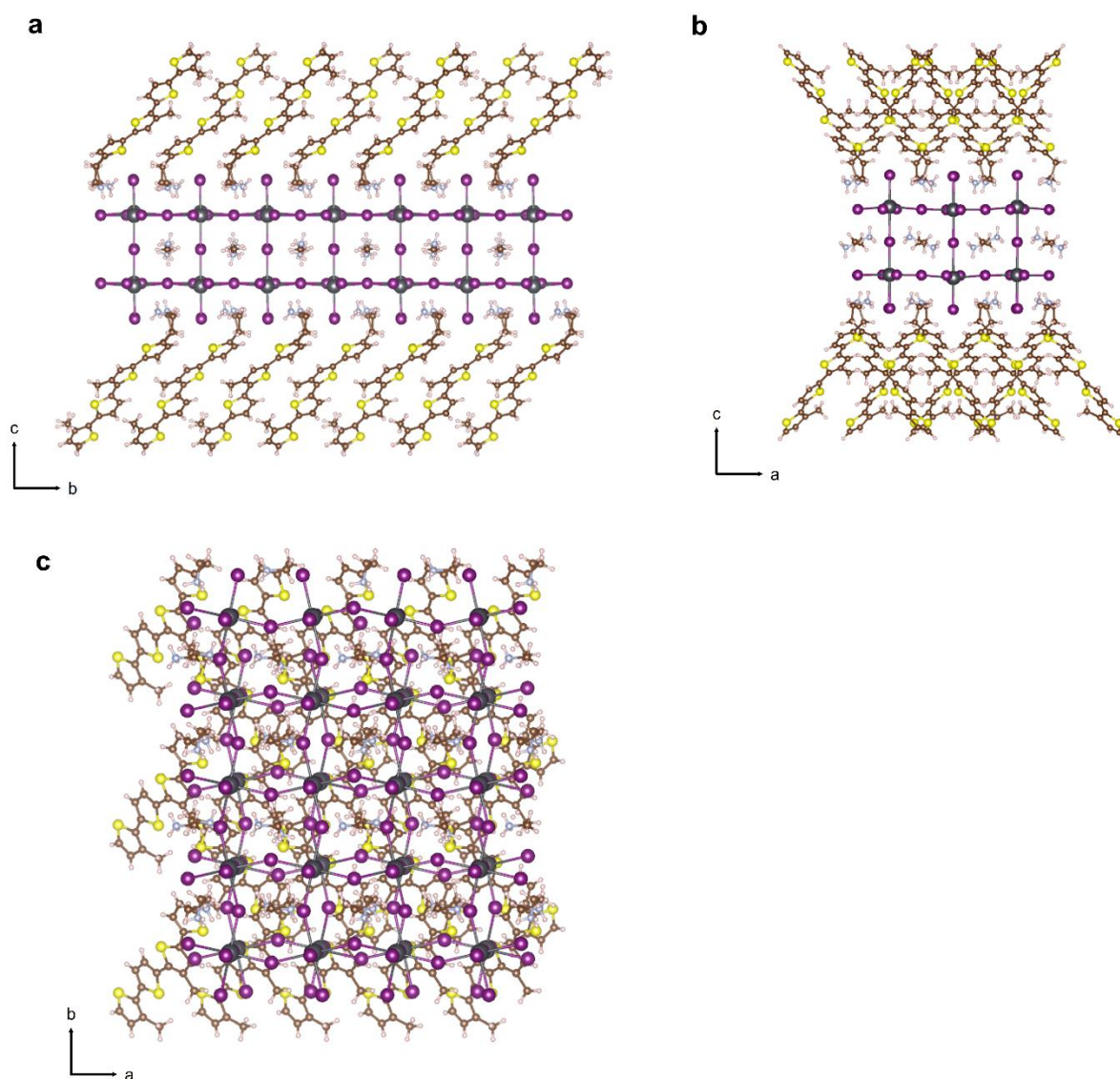
Supplementary Fig. 5. Single crystal structure of $(3T)_2PbI_4$ solved from single crystal X-ray diffraction. View along (a) b axis (b) c axis (c) a axis.



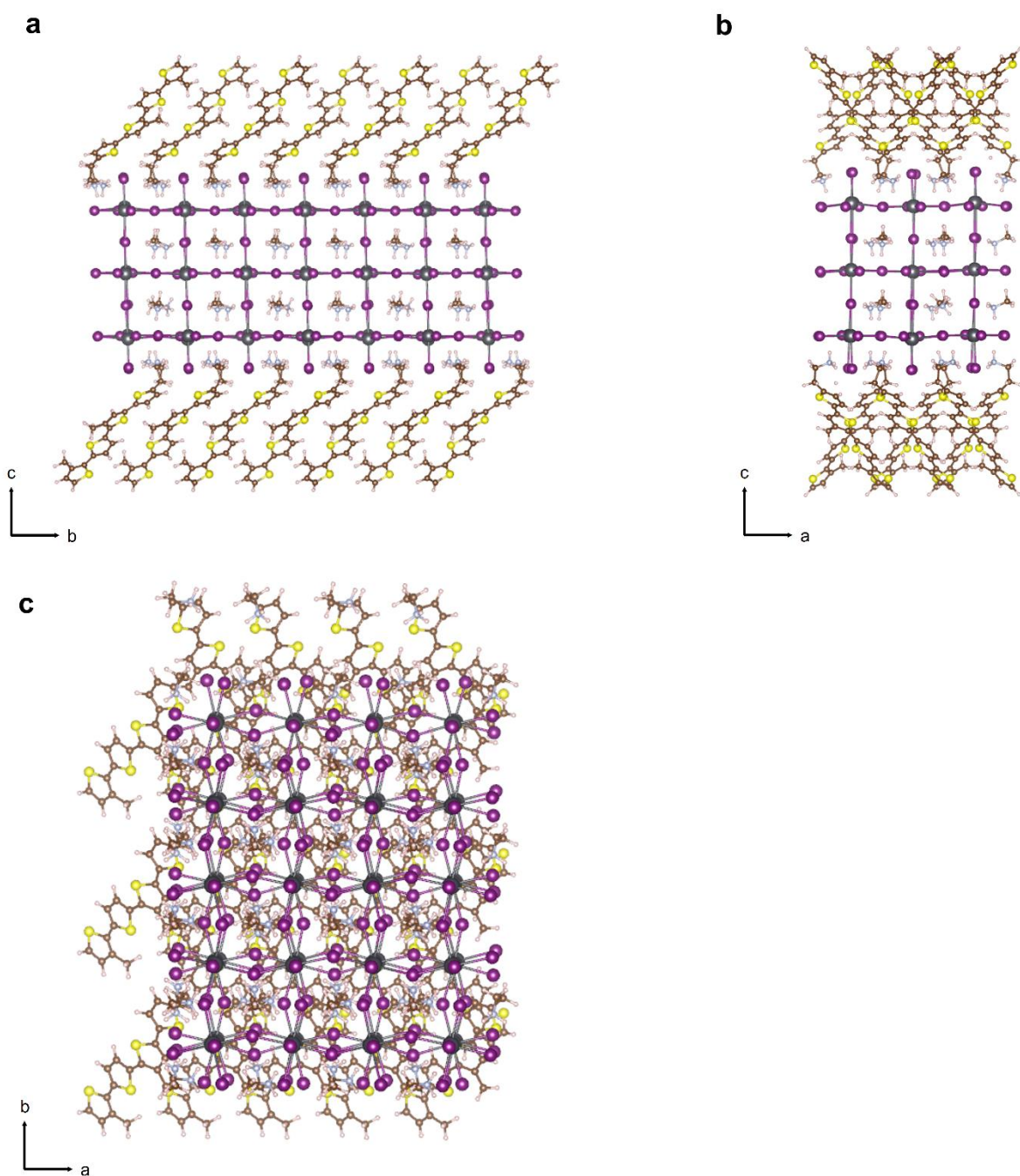
Supplementary Fig. 6. Single crystal structure of $(3T)_2(MA)Pb_2I_7$ solved from single crystal X-ray diffraction. View along (a) *b* axis (b) *c* axis (c) *a* axis.



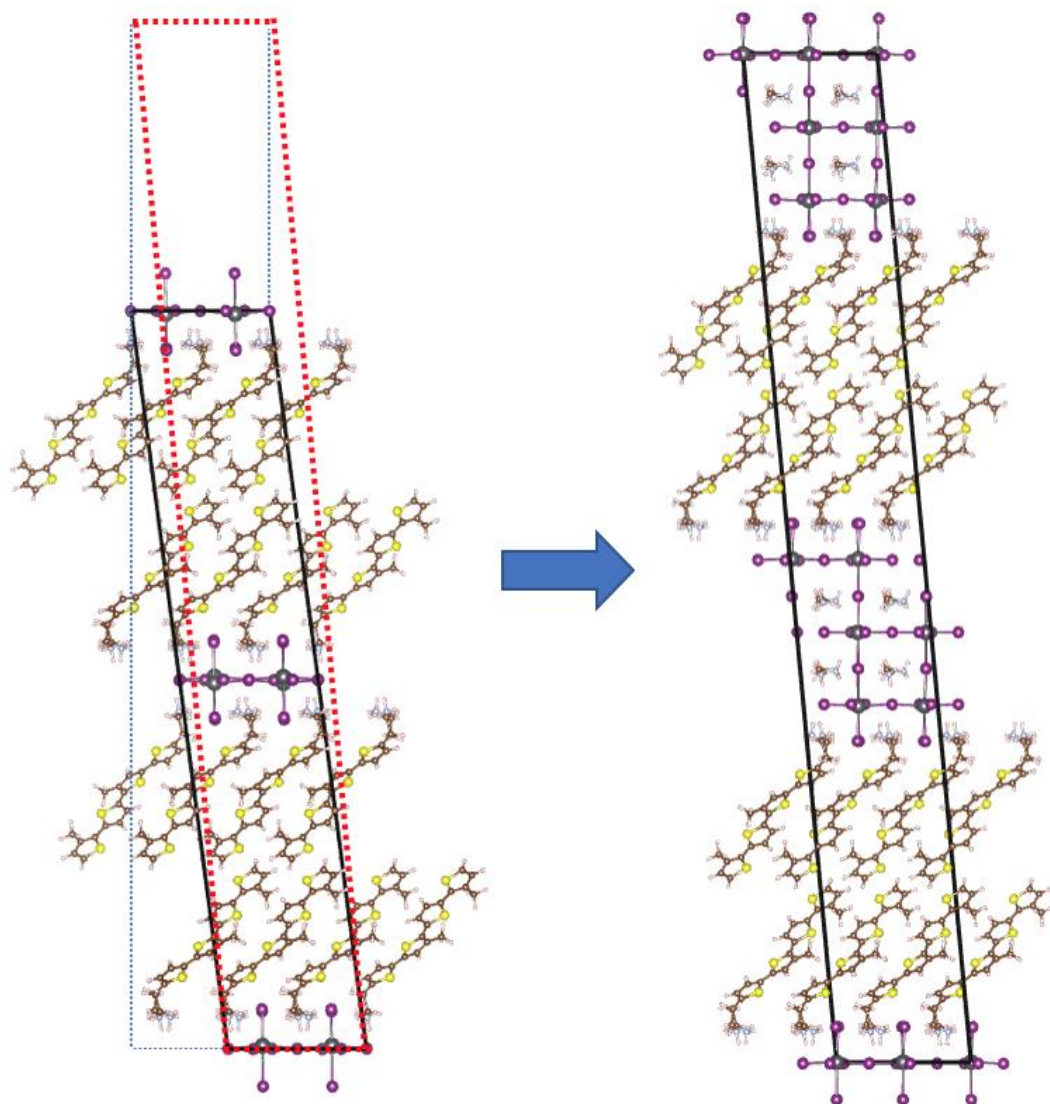
Supplementary Fig. 7. Single crystal structure of $(3T)_2(MA)_2Pb_3I_{10}$ solved from single crystal X-ray diffraction. View along (a) b axis (b) c axis (c) a axis.



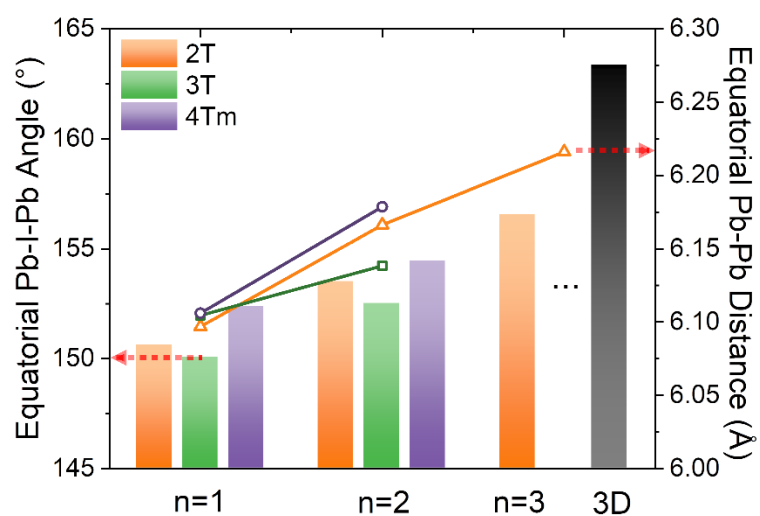
Supplementary Fig. 8. Single crystal structure of $(4Tm)_2(MA)Pb_2I_7$ solved from single crystal X-ray diffraction. View along (a) *a* axis (b) *b* axis (c) *c* axis.



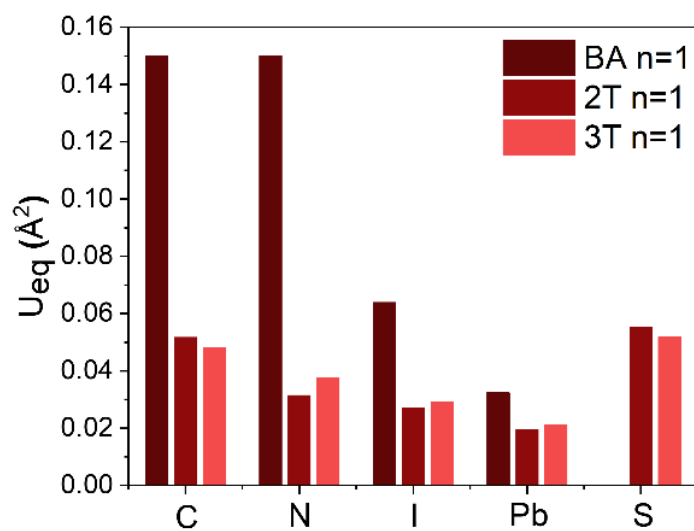
Supplementary Fig. 9. Single crystal structure of $(4Tm)_2(MA)_2Pb_3I_{10}$ simulated with computation. View along (a) *a* axis (b) *b* axis (c) *c* axis.



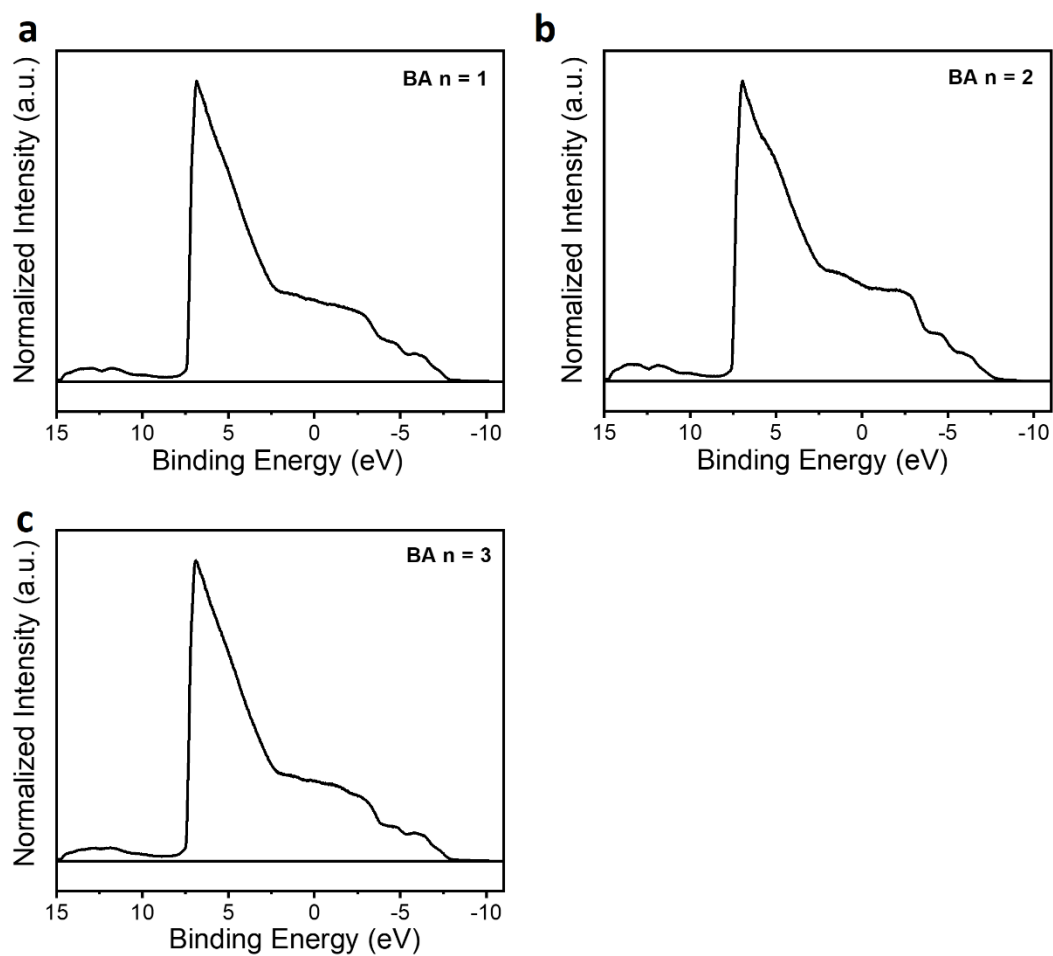
Supplementary Fig. 10. Construction of experimentally unknown structures for computational analysis. Taking the 4Tm based systems as an example, the organic cations of the 4Tm $n=1$ system were shifted upwards along the stacking direction and the 3-layer Pb-I inorganic framework together with the CH_3NH_3^+ cations were extracted from the 2T $n=3$ system and inserted to build the 4Tm $n=3$ structure.



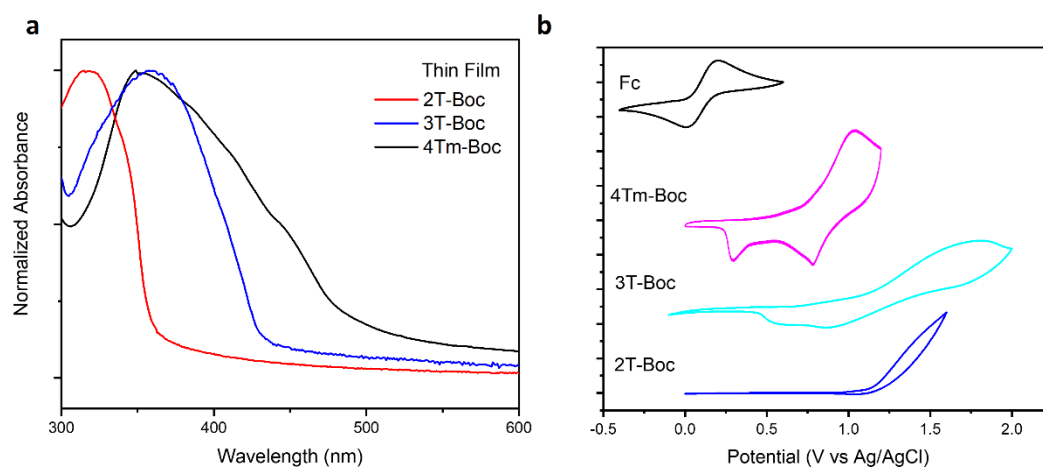
Supplementary Fig. 11. Change in the average equatorial Pb-I-Pb angle and Pb-Pb distance depending on the dimensionality (n) analyzed from experimentally resolved structures from single crystal XRD. The black bar on the far right represents MAPbI₃ (3D perovskite).



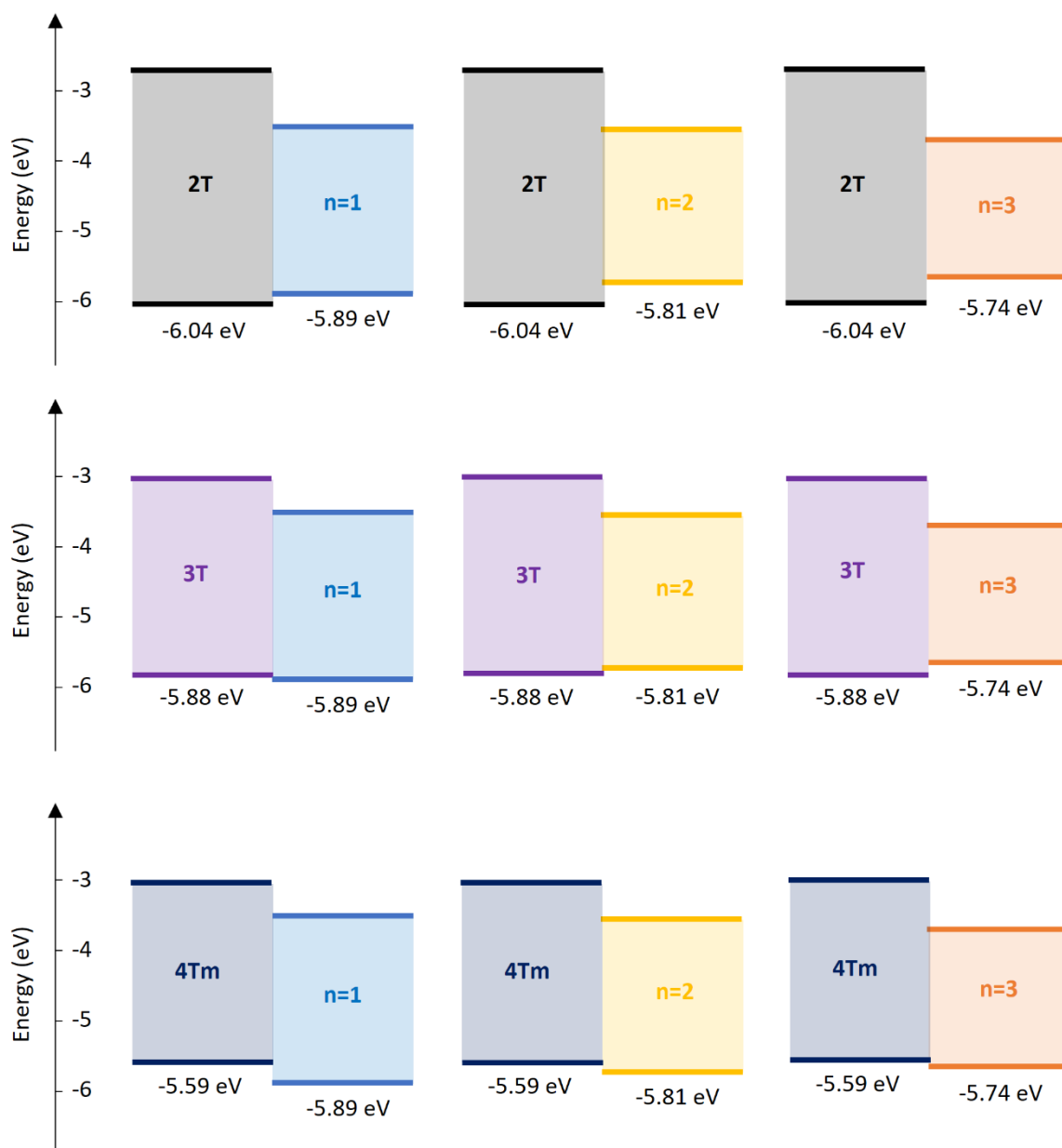
Supplementary Fig. 12. Equivalent isotropic displacement parameters extracted from single crystal XRD measurements of **BA n=1**, **2T n=1**, and **3T n=1** bulk crystals.



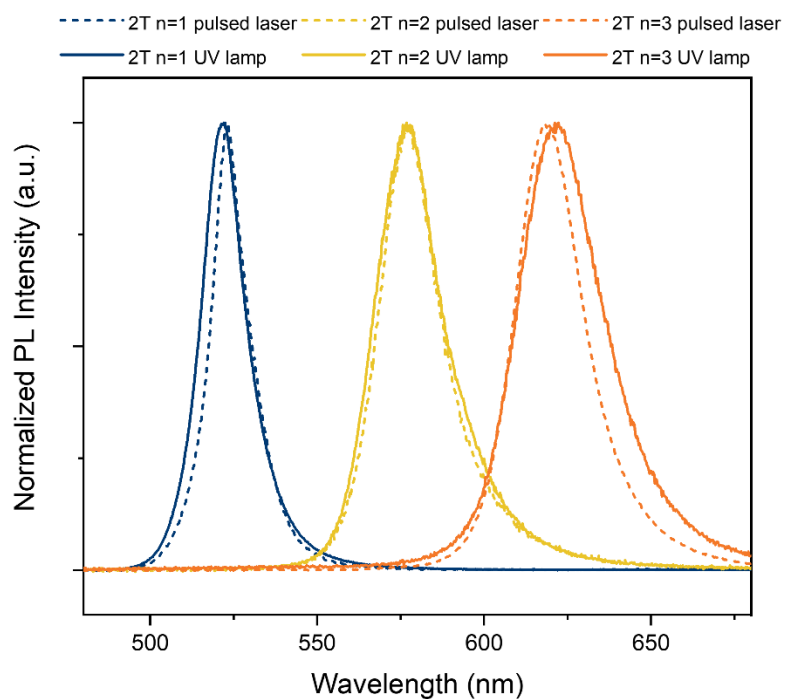
Supplementary Fig. 13. Ultraviolet photoelectron spectroscopy (UPS) measurement data of (BA)₂PbI₄, b) (BA)₂(MA)Pb₂I₇, and c) (BA)₂(MA)Pb₃I₁₀ thin films.



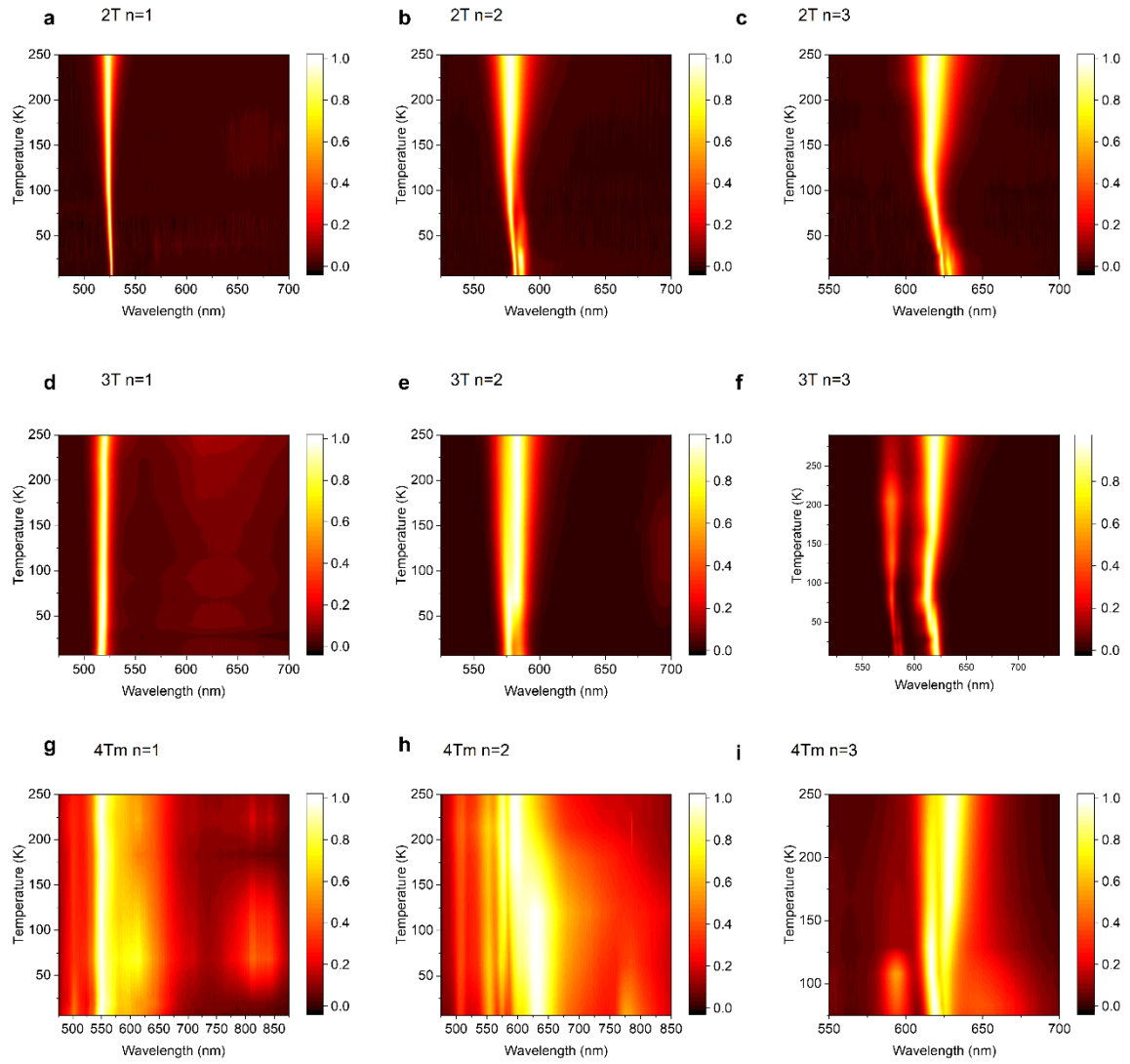
Supplementary Fig. 14. Thin film absorption and Cyclic voltammograms (CV). a) Thin film absorption data of 2T-Boc, 3T-Boc, and 4Tm-Boc thin films. b) Cyclic voltammograms of 2T-Boc, 3T-Boc, and 4Tm-Boc.



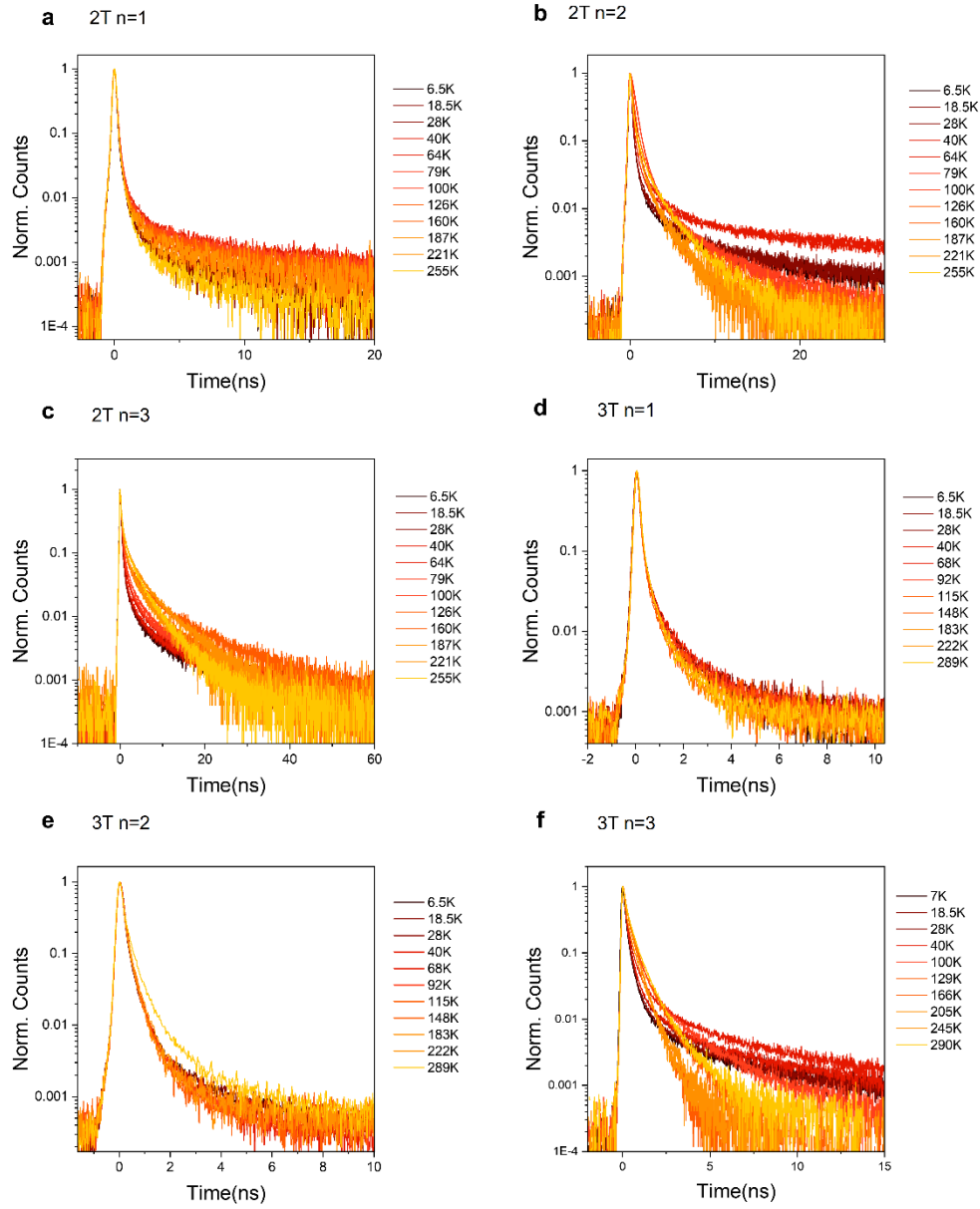
Supplementary Fig. 15. Estimated energy band alignments of 2T $n=1\sim3$, 3T $n=1\sim3$, and 4Tm $n=1\sim3$ based on UPS and CV measurements. First, UPS measurement were performed on BA $n=1\sim3$ films to determine the work function and valence band of these films. Then, CV was measured for 2T, 3T, and 4Tm. Ferrocene HOMO level was used as reference to acquire the HOMO level for the organic moieties. Lastly, valence band and HOMO energy levels, the onset of the absorption spectra was used to estimate the LUMO energy level of 2T, 3T, and 4Tm.



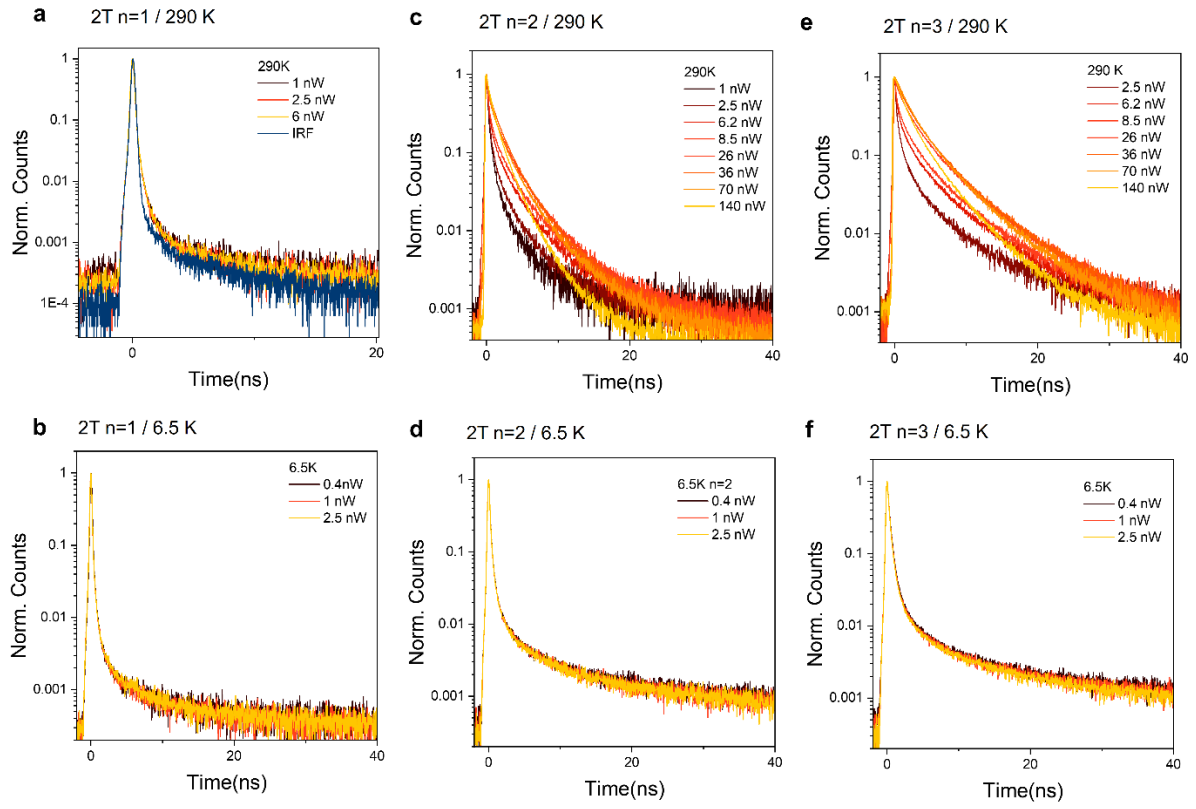
Supplementary Fig. 16. Comparison of 2T n=1~3 PL spectra taken with picosecond pulsed laser and UV lamp. It should be noted that the peak positions of the spectra from the same samples show negligible difference. The PL linewidth and intensity show slight differences due to the difference in the spectrometer specs and resolution.



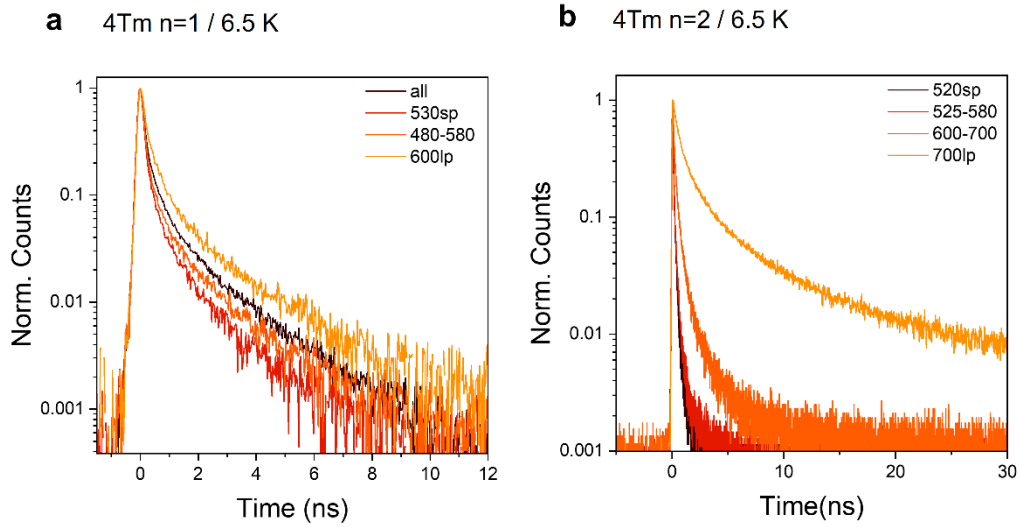
Supplementary Fig. 17. 2D plots of temperature dependent PL measurements of (a) 2T $n=1$, (b) 2T $n=2$, (c) 2T $n=3$, (d) 3T $n=1$, (e) 3T $n=2$, (f) 3T $n=3$, (g) 4Tm $n=1$, (h) 4Tm $n=2$, and (i) 4Tm $n=3$.



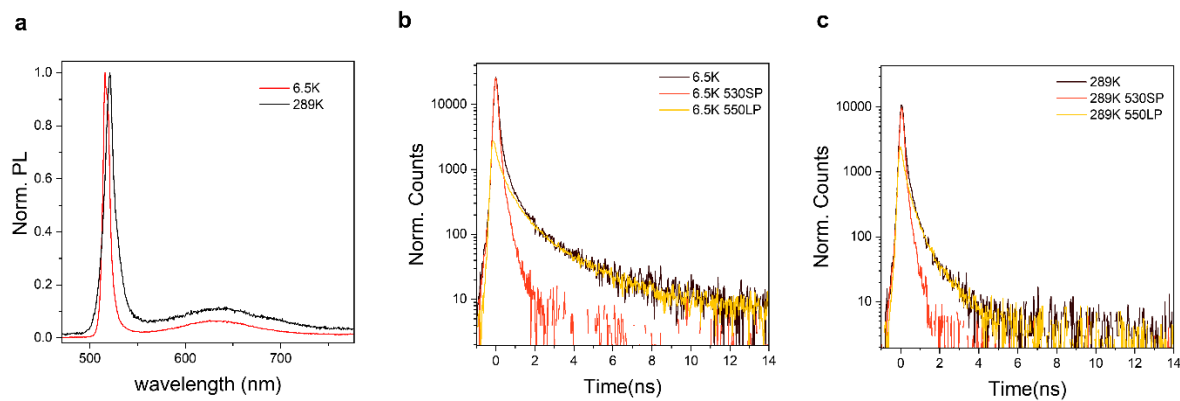
Supplementary Fig. 18. Temperature dependent TRPL measurements of (a) 2T n=1, (b) 2T n=2, (c) 2T n=3, (d) 3T n=1, (e) 3T n=2, and (f) 3T n=3.



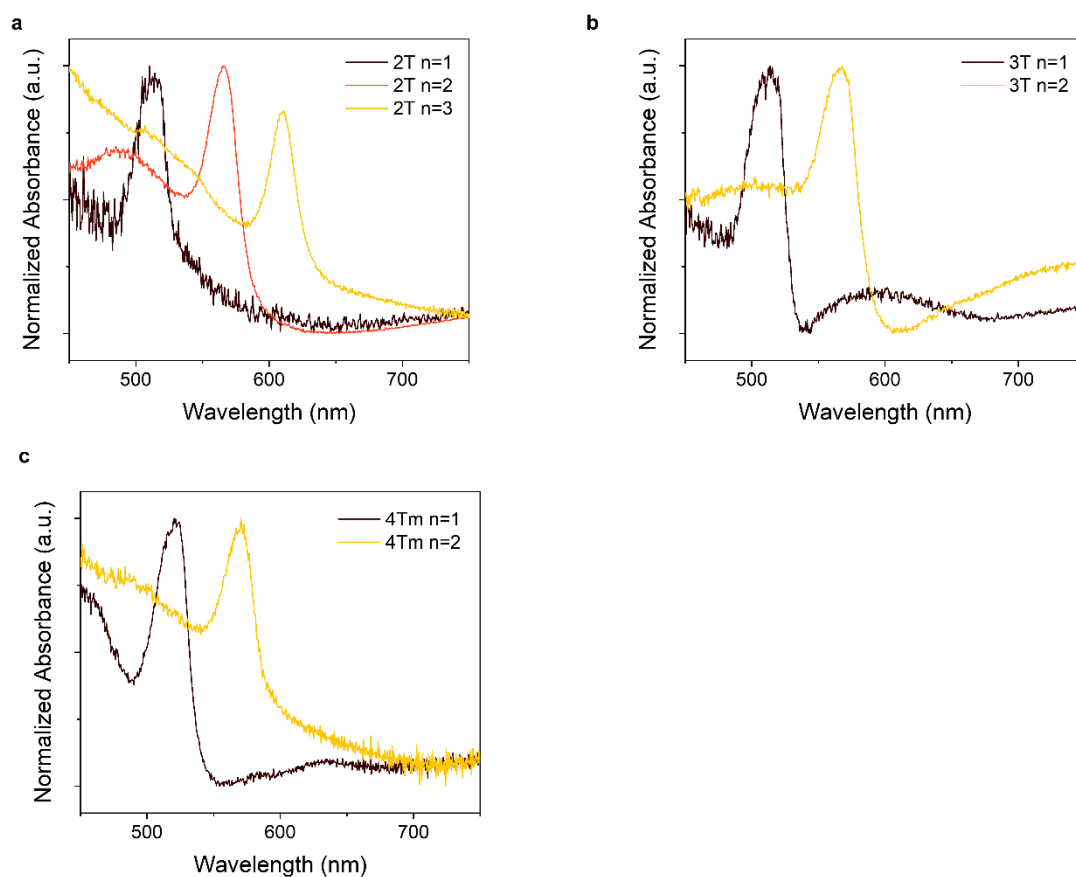
Supplementary Fig. 19. Power dependent TRPL measurements at 290 K and 6.5 K for (a, b) $2T\ n=1$, (c, d) $2T\ n=2$, and (e, f) $2T\ n=3$. The black line in (a) shows the instrument response function (IRF) limit range.



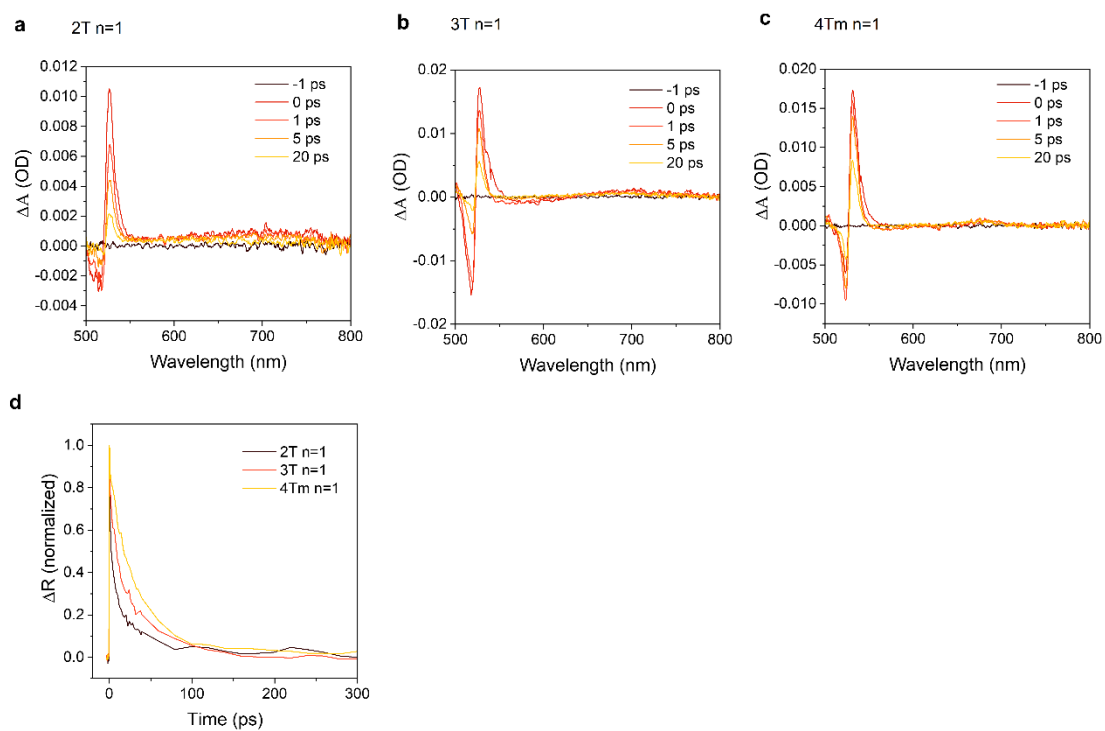
Supplementary Fig. 20. TRPL measurements of (a) **4Tm n=1** and (b) **4Tm n=2** at 6.5 K using band pass filters. For **4Tm n=1**, 3 ranges using 530 nm short pass, 480 nm long pass – 580 nm short pass, and 600nm long pass filters were measured. For 4Tmn2, 4 ranges using 520 nm short pass, 525 nm long pass – 580 nm short pass, 600 nm long pass – 700 nm short pass, and 700 nm long pass were measured.



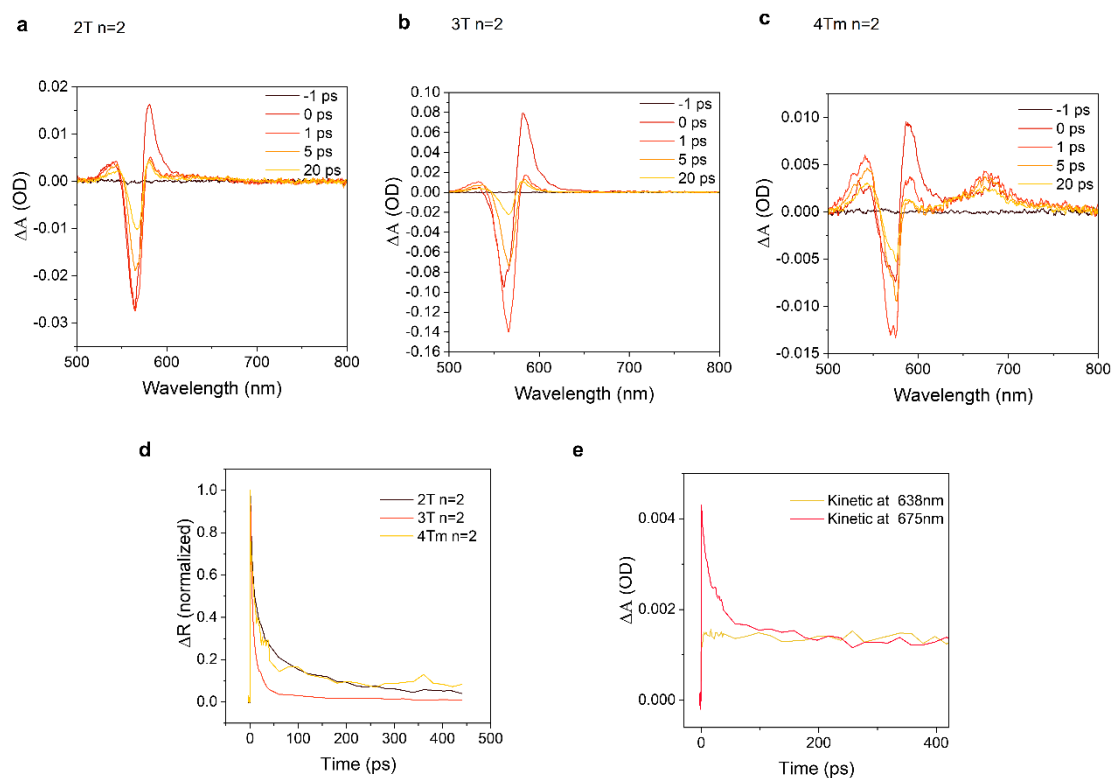
Supplementary Fig. 21. 3T n=1 (a) PL spectra, TRPL measurements at (b) 6.5 K and (c) 289 K. 530 nm short pass and 550 nm long pass filters were used to separately measure the lifetime of the broad peak and the narrow peak. These peaks with broad nature have been reported to be originating from self-trapped excitons or extrinsic defects.¹



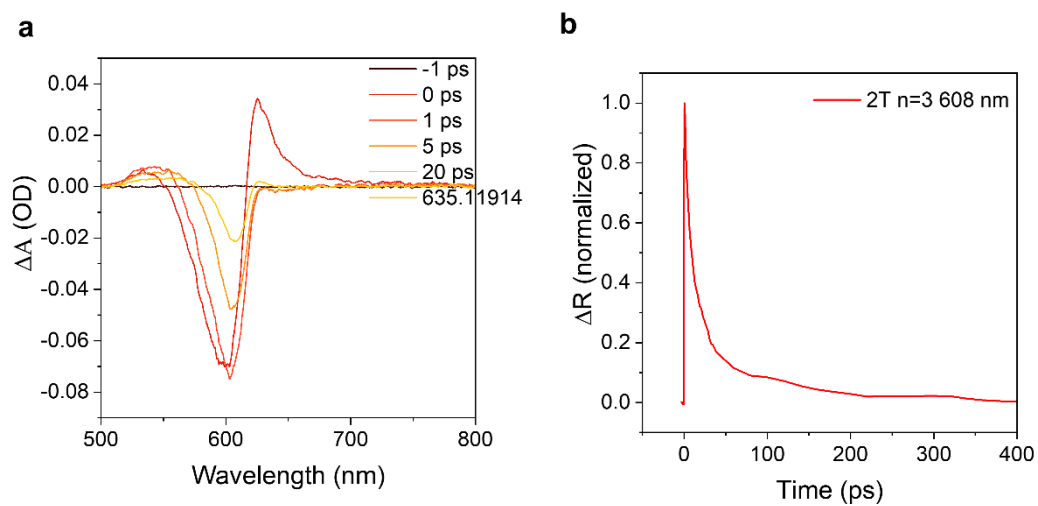
Supplementary Fig. 22. Normalized absorbance calculated from micro transmittance of mechanically exfoliated crystals of (a) **2T n=1**, **2T n=2**, **2T n=3**, (b) **3T n=1**, **3T n=2**, (c) **4Tm n=1** and **4Tm n=2**.



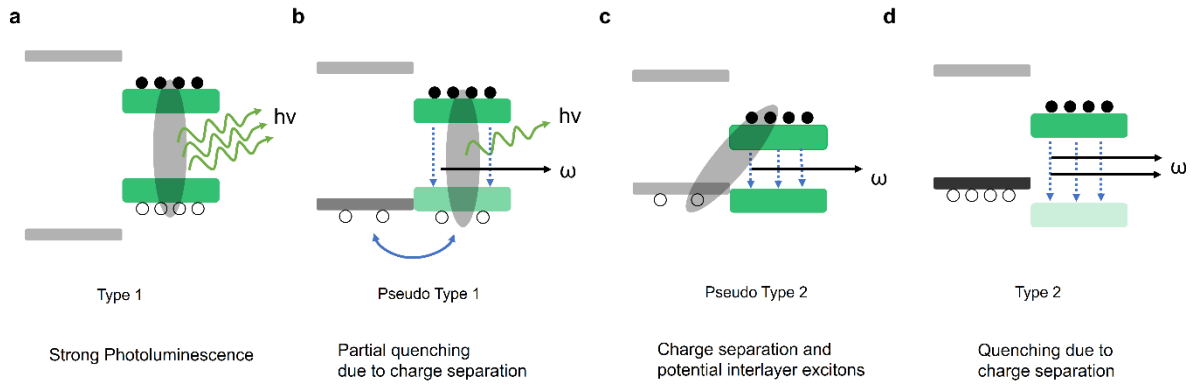
Supplementary Fig. 23. Transient absorption spectra acquired for (a) **2T $n=1$** (b) **3T $n=1$** , and (c) **4Tm $n=1$** at different delays from pump excitation of 450 nm with a fluence of 20 μW . (d) Decay dynamics of **2T $n=1$** , **3T $n=1$** , and **4Tm $n=1$** at 530 nm.



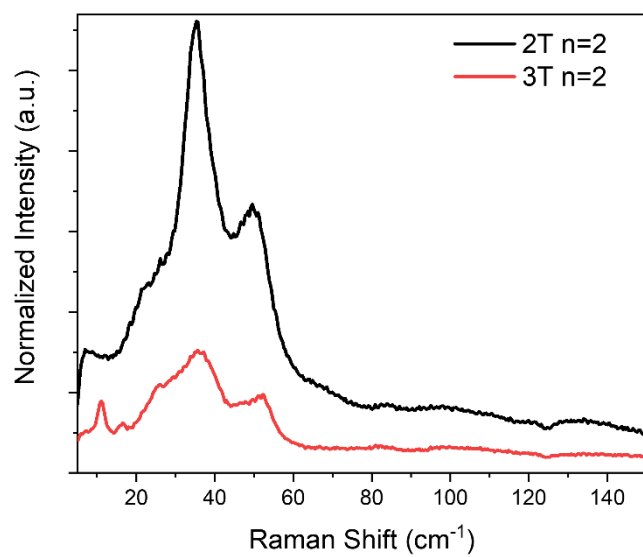
Supplementary Fig. 24. Transient absorption spectra acquired for (a) 2T n=2 (b) 3T n=2 (c) 4Tm n=2 at different delays from pump excitation of 450 nm with a fluence of 20 μW . (d) Decay dynamics of 2T n=2, 3T n=2, and 4Tm n=2 at 570 nm. (e) Decay dynamics of 4Tm n=2 at 638 nm and 675 nm showing long-lived components. This is likely due to the formation of interlayer excitons at the organic-inorganic interface.



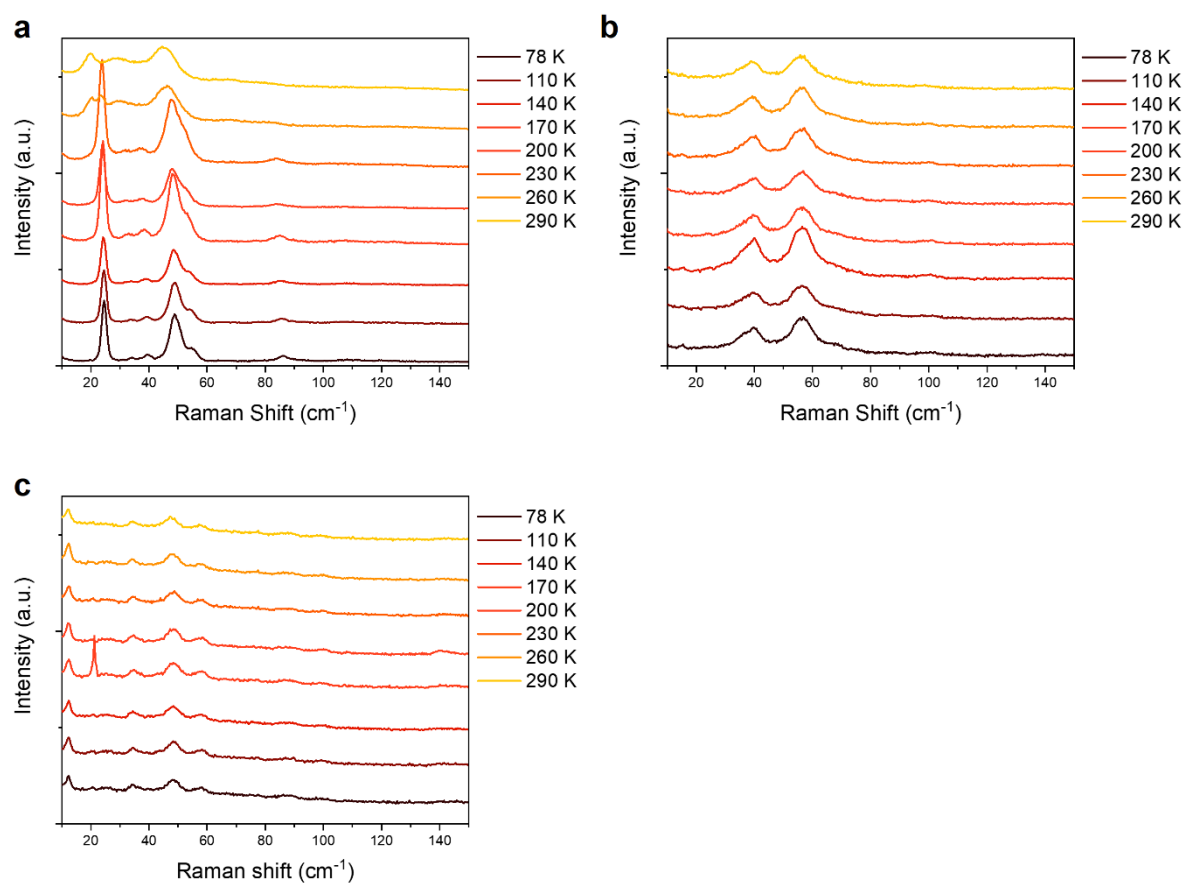
Supplementary Fig. 25. Transient absorption spectra acquired for a) **2T n=3** at different delays from pump excitation of 450 nm with a fluence of 20 μ W. (b) Decay dynamics of **2T n=3** at 608 nm.



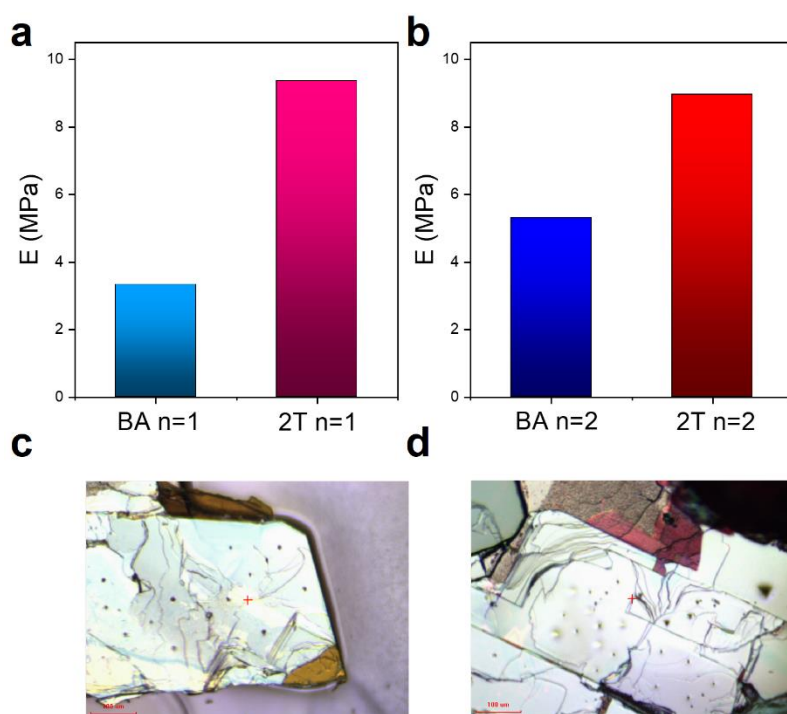
Supplementary Fig. 26. An illustration of different band alignment types in OSiP quantum wells. (a) Type I alignment leads to concentration of charge carriers in the inorganic layers resulting in a robust radiative recombination showing narrow and strong emissive properties. (b) Pseudo type I alignment shows partial quenching of photons due to charge separation between the hybrid interfaces. (c) Pseudo type II alignment also exhibits quenched PL properties due to charge transfer while potential weakly bound interlayer excitons can exist. (d) Type II alignments show quenched PL with very weak emissive properties due to rapid charge separation along the interface. $h\nu$ represent photons emitted through photoluminescence; ω represents energy dissipated through phonons.



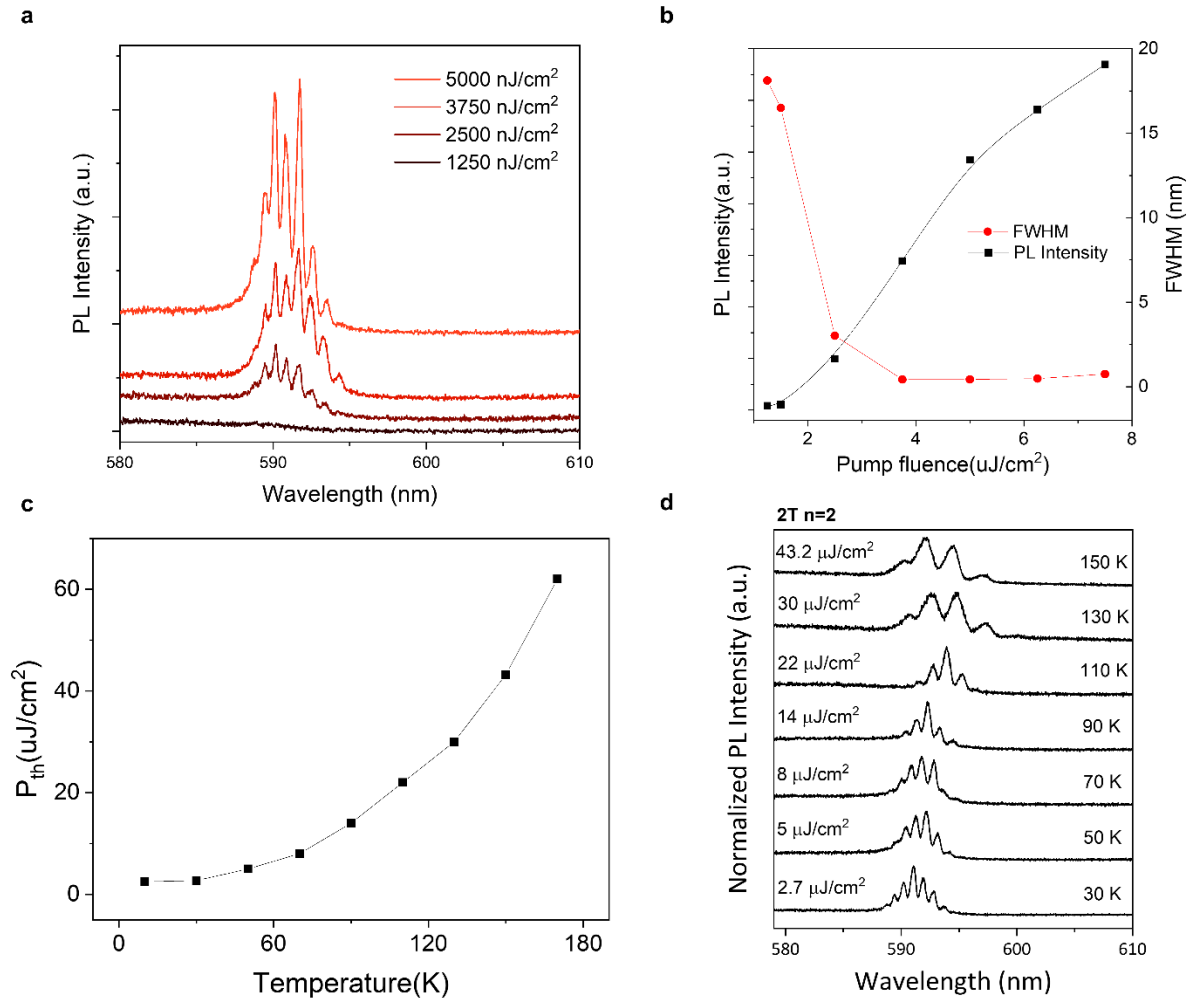
Supplementary Fig. 27. Low-frequency Raman spectrum of **2T n=2** and **3T n=2** at room temperature.



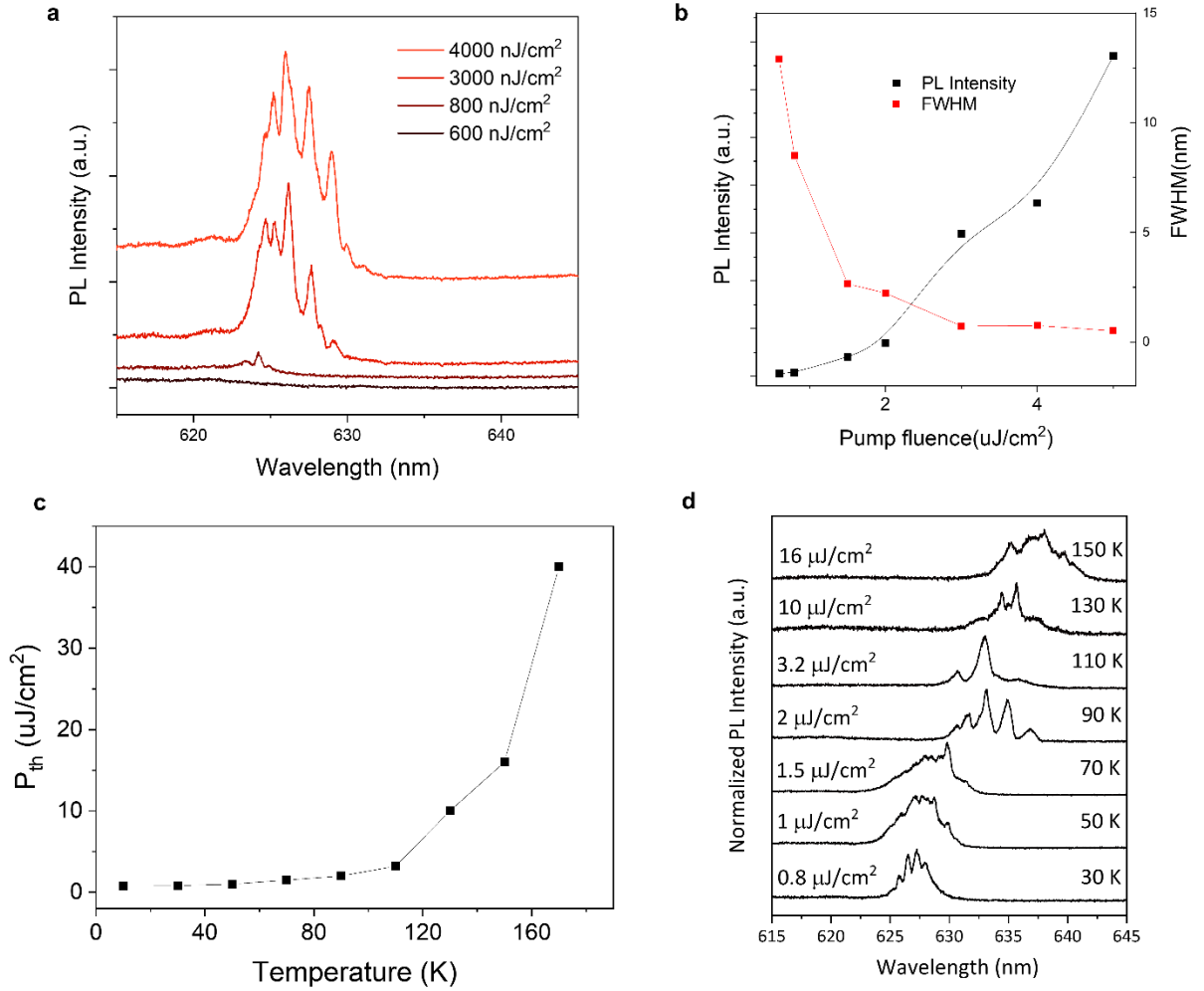
Supplementary Fig. 28. Temperature dependent low-frequency Raman spectra of (a) BA $n=1$, (b) 2T $n=1$, and (c) 3T $n=1$.



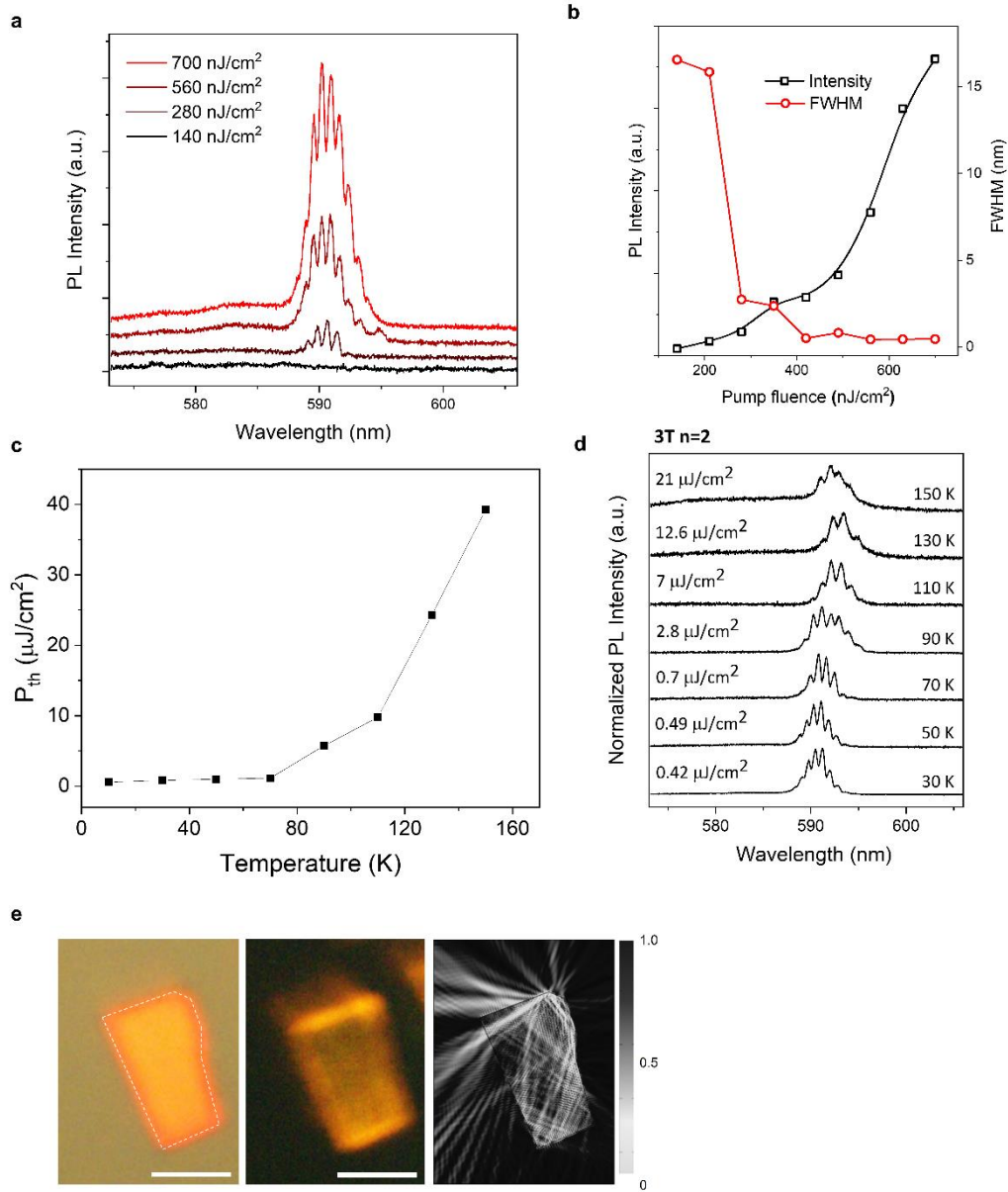
Supplementary Fig. 29. Comparison of out of plane Young's modulus and nanoindentation trial images. Comparison of (a) BA n=1 and 2T n=1, (b) BA n=2 and 2T n=2. The images of the crystal surface after nanoindentation trials: (c) 2T n=1 and (d) 2T n=2.



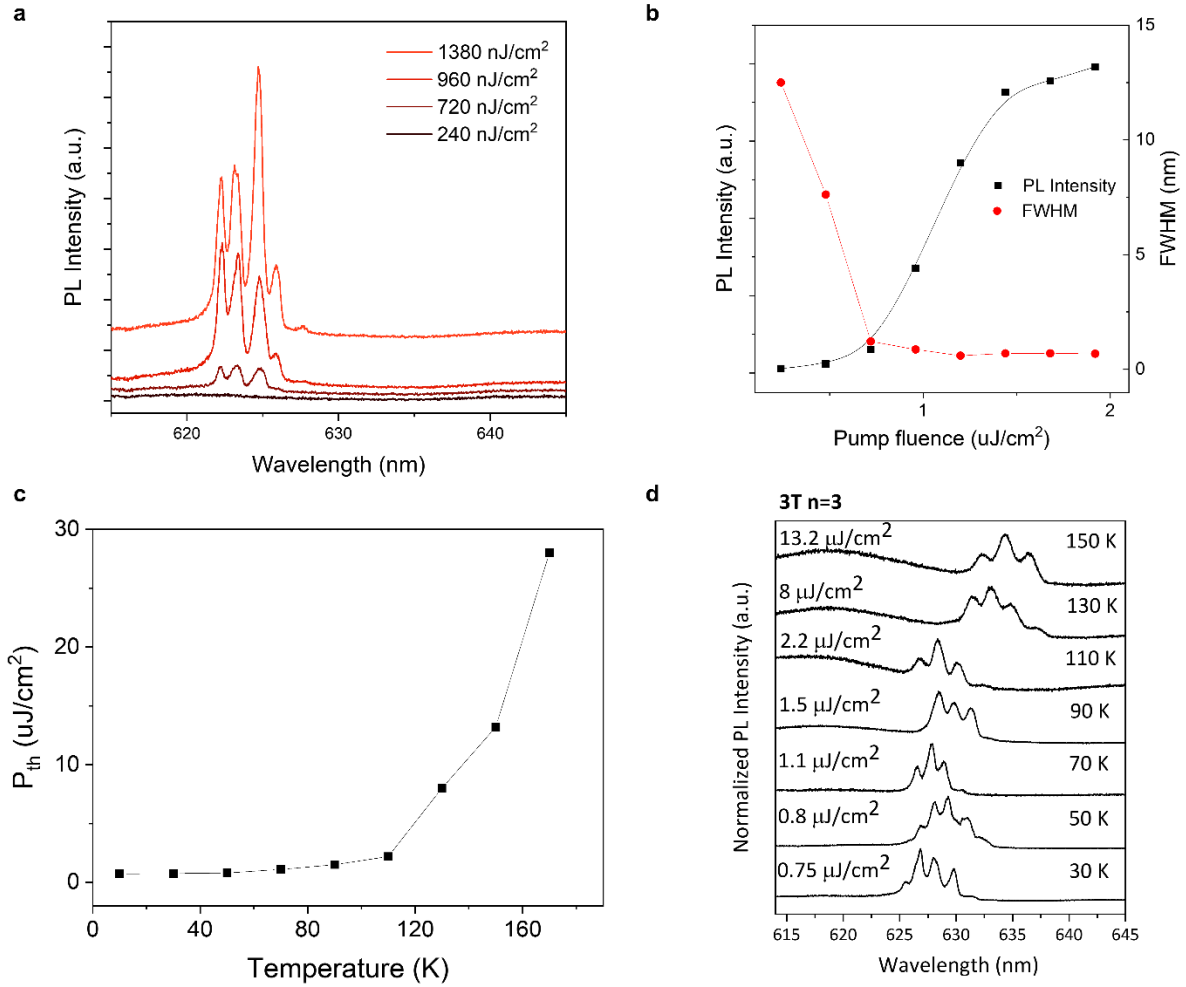
Supplementary Fig. 30. Lasing characteristics of **2T n=2** showing (a) lasing PL spectra at 10 K with pump fluence of 1250, 2500, 3750, and 5000 nJ/cm², (b) pump fluence dependent PL intensity, FWHM at 10K, (c) temperature dependent lasing pump thresholds, and (d) temperature dependent lasing PL spectra up to 150 K. Selective and strong amplification of several mode peaks were observed when the pump fluence reached around 2500 nJ/cm² at 10 K. Above the onset power for each temperature, FWHM dramatically narrowed down to less than 1 nm and the peak intensity showed nonlinear increase with the pump fluence, exhibiting a clear knee behavior and threshold characteristic indicative of lasing.



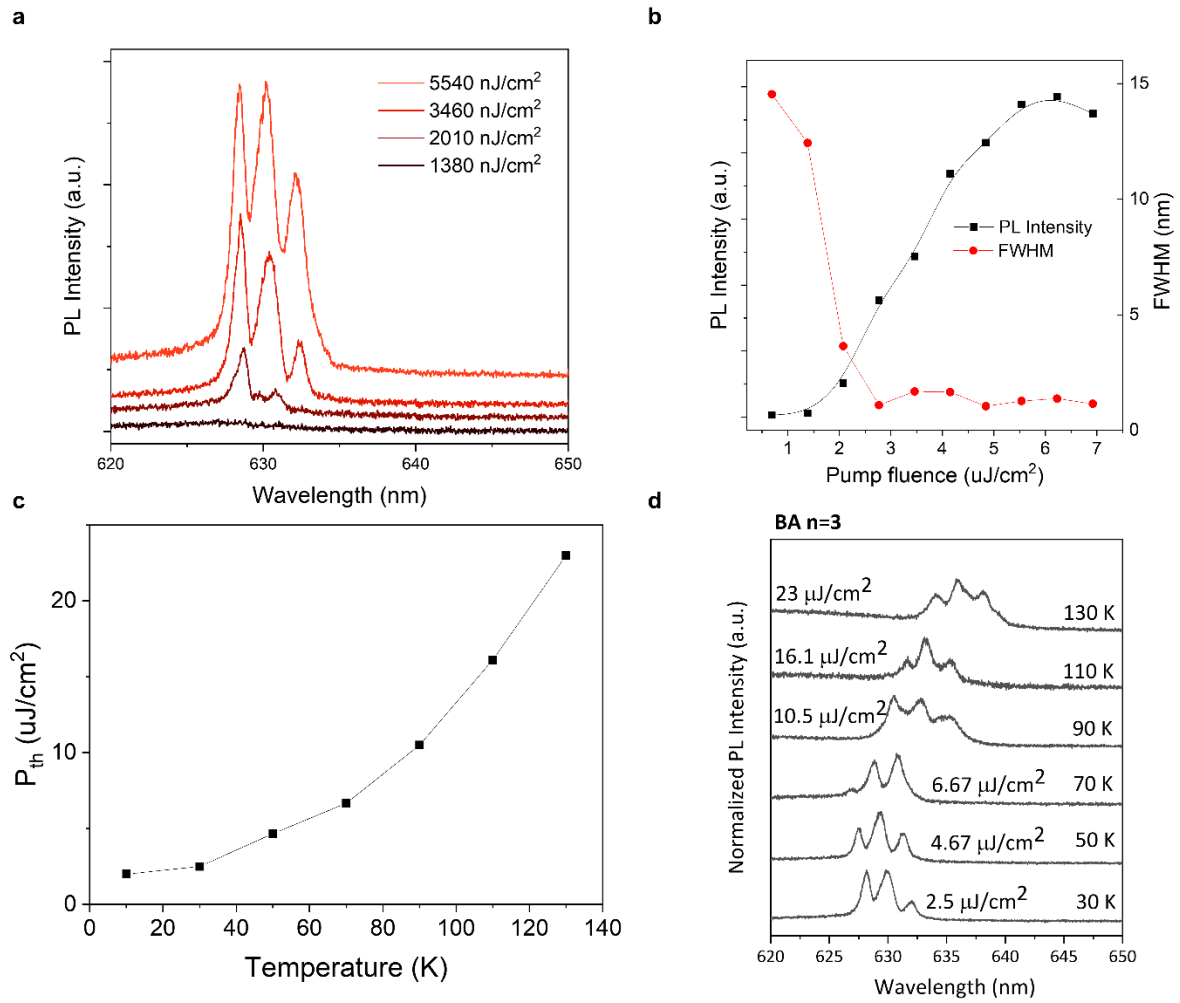
Supplementary Fig. 31. Lasing characteristics of **2T n=3** showing (a) lasing PL spectra at 10 K with pump fluence of 600, 800, 3000, and 4000 nJ/cm², (b) pump fluence dependent PL intensity, FWHM at 10K, (c) temperature dependent lasing pump thresholds, and (d) temperature dependent lasing PL spectra up to 150 K. Selective and strong amplification of several mode peaks were observed when the pump fluence reached around 800 nJ/cm² at 10 K. Above the onset power for each temperature, FWHM dramatically narrowed down to less than 1 nm and the peak intensity showed nonlinear increase with the pump fluence, exhibiting a clear knee behavior and threshold characteristic indicative of lasing.



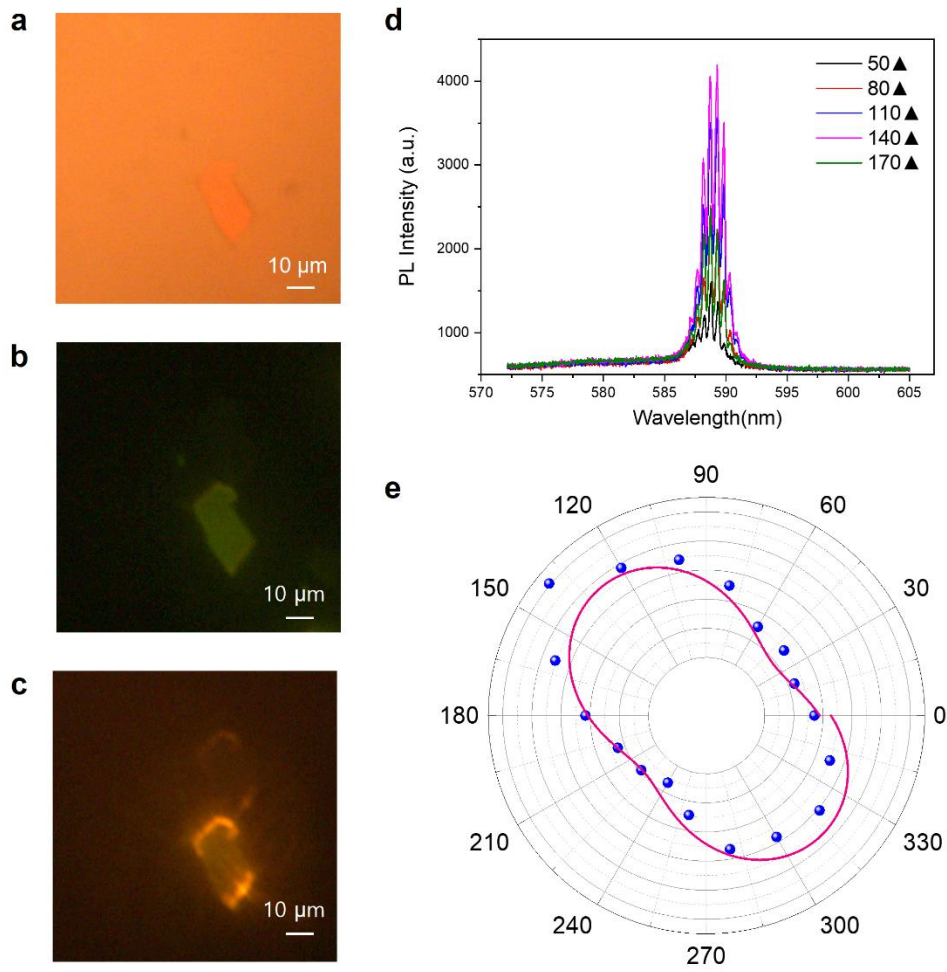
Supplementary Fig. 32. Lasing characteristics of **3T n=2** showing (a) lasing PL spectra at 10 K with pump fluence of 140, 280, 560, and 700 nJ/cm², (b) pump fluence dependent PL intensity, FWHM at 10K, (c) temperature dependent lasing pump thresholds, and (d) temperature dependent lasing PL spectra up to 150 K. Selective and strong amplification of several mode peaks were observed when the pump fluence reached around 280 nJ/cm² at 10 K. Above the onset power for each temperature, FWHM dramatically narrowed down to less than 1 nm and the peak intensity showed nonlinear increase with the pump fluence, exhibiting a clear knee behavior and threshold characteristic indicative of lasing. (e) Bright field image, lasing image, and simulated electric field intensity distribution in the 3T n=2 single crystal, scale bar: 10 μm.



Supplementary Fig. 33. Lasing characteristics of **3T n=3** showing (a) lasing PL spectra at 10 K with pump fluence of 240, 720, 960, and 1380 nJ/cm², (b) pump fluence dependent PL intensity, FWHM at 10K, (c) temperature dependent lasing pump thresholds, and (d) temperature dependent lasing PL spectra up to 150 K. Selective and strong amplification of several mode peaks were observed when the pump fluence reached around 720 nJ/cm² at 10 K. Above the onset power for each temperature, FWHM dramatically narrowed down to less than 1 nm and the peak intensity showed nonlinear increase with the pump fluence, exhibiting a clear knee behavior and threshold characteristic indicative of lasing.



Supplementary Fig. 34. Lasing characteristics of **BA n=3** showing (a) lasing PL spectra at 10 K with pump fluence of 1380, 2010, 3460, and 5540 nJ/cm², (b) pump fluence dependent PL intensity, FWHM at 10K, (c) temperature dependent lasing pump thresholds, and (d) temperature dependent lasing PL spectra up to 130 K. Selective and strong amplification of several mode peaks were observed when the pump fluence reached around 2010 nJ/cm² at 10 K. Above the onset power for each temperature, FWHM dramatically narrowed down to less than 1 nm and the peak intensity showed nonlinear increase with the pump fluence, exhibiting a clear knee behavior and threshold characteristic indicative of lasing.



Supplementary Fig. 35. Polarization characterization of lasing from 3T n=2. a, Bright field image. b, PL image below pump threshold. c, PL image above pump threshold. d, Polarization dependent PL spectra with the emission polarization oriented by each corresponding angle relative to the vertical direction. e, polar plot of the emission intensity.

2. Supplementary tables

Supplementary Table 1.

OSiP	(L)·HI	PbI ₂	MAI	HI	H ₃ PO ₂	IPA	EtOH
2T n=1	0.005 mmol	0.02 mmol	-	200 µl	100 µl	300 µl	-
2T n=2	0.005 mmol	0.05 mmol	0.1mmol	200 µl	100 µl	300 µl	-
2T n=3	0.005 mmol	0.07 mmol	0.18mmol	200 µl	100 µl	300 µl	-
3T n=1	0.005 mmol	0.02 mmol	-	200 µl	100 µl	-	1.5 ml
3T n=2	0.005 mmol	0.03 mmol	0.1mmol	200 µl	100 µl	-	1.5 ml
3T n=3	0.005 mmol	0.05 mmol	0.15mmol	200 µl	100 µl	-	1.5 ml
4Tm n=1	0.005 mmol	0.02 mmol	-	200 µl	100 µl	-	1.2 ml
4Tm n=2	0.015 mmol	0.08 mmol	0.3mmol	-	-	-	5 ml
4Tm n=3	0.015 mmol	0.1 mmol	0.4mmol	-	-	-	5 ml

Detailed crystal growth parameters using the slow cooling method. Alcoholic solvents were added to assist the reactivity between organic components and inorganic components. To obtain X-ray diffraction quality grade single crystals for **4Tm n=2** and **4Tm n=3**, non-acidic conditions were used. The alcoholic solvent crystallization conditions partially yield MAPbI₃. Pure mm scale OSiP single crystals were filtered and separated from the impurities before

characterization. All the solutions were contained in a vial, heated with a water bath, and then slow cooled in a Dewar flask for 72 hours until the solution temperature reaches room temperature.

Supplementary Table 2.

System		a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	V (Å ³)
2T n=1	Input (experimental)	12.09	12.27	20.81	98.42	98.77	89.97	3017
	Relaxed	12.07	12.24	20.95	98.32	98.98	89.99	3026
	Deviation (%)	-0.12	-0.23	0.69	-0.10	0.21	0.02	0.30
2T n=2	Input	12.32	12.34	26.82	83.53	96.46	90.06	4024
	Relaxed	12.30	12.31	27.13	85.85	95.99	91.04	4072
	Deviation (%)	-0.15	-0.25	1.14	2.77	-0.49	1.09	1.18
2T n=3	Input	12.42	12.44	33.14	95.32	95.50	90.01	5076
	Relaxed	12.34	12.39	33.32	91.86	94.88	91.25	5072
	Deviation (%)	-0.65	-0.40	0.53	-3.63	-0.65	1.37	-0.07
3T n=1	Input	12.28	12.10	24.92	90.00	97.08	90.00	3675
	Relaxed	12.25	12.05	25.32	90.00	96.88	90.00	3711
	Deviation (%)	-0.22	-0.46	1.63	0.00	-0.20	0.00	0.98
3T n=2	Input	12.20	12.35	30.94	90.00	95.71	90.00	4637
	Relaxed	12.33	12.17	31.28	89.99	95.72	90.01	4670
	Deviation (%)	1.09	-1.44	1.09	-0.01	0.01	0.01	0.72
3T n=3	Input	12.28	12.10	37.85	90.00	94.65	90.00	5607
	Relaxed	12.35	12.22	37.88	89.47	94.22	90.07	5703
	Deviation (%)	0.58	0.98	0.08	-0.59	-0.46	0.08	1.71
4Tm n=1	Input	12.21	12.19	64.19	90.00	97.77	90.00	9465
	Relaxed	12.27	12.15	63.71	90.00	97.68	90.00	9416
	Deviation (%)	0.52	-0.31	-0.75	-0.02	-0.08	0.02	-0.52
4Tm n=2	Input	12.38	12.32	37.71	94.60	87.82	90.03	5729
	Relaxed	12.33	12.25	37.87	94.64	87.46	89.99	5700
	Deviation (%)	-0.40	-0.53	0.45	0.04	-0.41	-0.04	-0.51
4Tm n=3	Input	12.15	12.27	93.35	97.45	95.28	89.98	13744
	Relaxed	12.31	12.38	89.66	100.06	94.15	90.28	13419
	Deviation (%)	1.32	0.88	-3.95	2.68	-1.18	0.34	-2.36

The lattice parameters of each system before and after DFT-PBE+TS based geometry relaxation. All numbers show small deviations after relaxation.

Supplementary Table 3.

Materials	τ_1 (ns) (weight)	τ_2 (ns) (weight)	τ_{avg} (ns)
2T n = 1	0.10 (77.27%)	0.32 (22.73%)	0.15
2T n = 2	0.19 (88.24%)	1.45 (11.76%)	0.34
2T n = 3	0.25 (88.19%)	2.24 (11.81%)	0.48
3T n=1	0.16 (96.41%)	0.78 (3.59%)	0.18
3T n=2	0.33 (77.01%)	0.99 (22.93%)	0.48
3T n=3	1.02 (72.28%)	2.99 (27.72%)	1.57
4Tm n=1	0.10 (90.48%)	0.69 (9.52%)	0.16
4Tm n=2	0.07 (90.72%)	0.35 (9.28%)	0.10
4Tm n=3	0.11 (81.54%)	0.876 (18.46%)	0.25

Calculated PL lifetimes from biexponential fitting of TRPL data shown in Fig. 3g, h and i.

Supplementary Table 4.**(a)**

2T	Γ_0 (eV)	Γ_{AC} (eV/K)	Γ_{LO} (eV)	E_{LO}(eV)
n = 1	0.0064	1.40E-4	0	-
n = 2	0.0110	0	0.066	0.015
n = 3	0.0098	0	0.028	0.008

(b)

3T	Γ_0 (eV)	Γ_{AC} (eV/K)	Γ_{LO} (eV)	E_{LO}(eV)
n = 1	0.0405	5.06E-5	0	-
n = 2	0.0311	0	0.029	0.015
n = 3	0.0208	0	0.016	0.008

Comparison of **(a)** the 2T series and **(b)** the 3T series showing the effect of different n numbers on the fitting parameters of FWHM values dependent on temperature. The parameters are defined as follows: Γ_0 is the inhomogeneous broadening factor, Γ_{AC} is the exciton-longitudinal acoustic phonon coupling strength, Γ_{LO} is the exciton-longitudinal optical (LO) phonon coupling strength, and E_{LO} is the longitudinal optical phonon energy.^{2,3}

Supplementary Table 5.

	2T n=2, (2T)₂(MA)Pb₂I₇
Crystal data	
Chemical formula	4(P ₂ I ₇)·8(C ₁₀ H ₁₂ NS ₂)·4(CH ₆ N)
<i>M_r</i>	7021.59
Crystal system, space group	Triclinic, <i>P</i> 1
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	12.3170 (8), 12.3373 (8), 26.8215 (18)
α , β , γ (°)	83.533 (2), 83.543 (2), 89.9379 (19)
<i>V</i> (Å ³)	4023.9 (5)
<i>Z</i>	1
<i>F</i> (000)	3104
<i>D_x</i> (Mg m ⁻³)	2.898
Radiation type	Mo <i>K</i> α
No. of reflections for cell measurement	9876
θ range (°) for cell measurement	3.1–33.2
μ (mm ⁻¹)	13.95
Crystal shape	Fragment
Colour	Red
Crystal size (mm)	0.09 × 0.08 × 0.04
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Radiation source	fine focus sealed tube X-ray source
Monochromator	Triumph curved graphite crystal
Detector resolution (pixels mm ⁻¹)	10.4167
Scan method	ω and ϕ scans
Absorption correction	Multi-scan SADABS 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D. (2015). <i>J. Appl. Cryst.</i> 48, 3-10.
<i>T_{min}</i> , <i>T_{max}</i>	0.158, 0.551
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	150143, 150143, 93257
<i>R_{int}</i>	0.052
θ values (°)	$\theta_{\max}$ = 33.3, $\theta_{\min}$ = 2.1

$(\sin \theta/\lambda)_{\max}$ ($\text{\AA}^{-1}$)	0.772
Range of h, k, l	$h = -18 - 18, k = -19 - 19, l = -41 - 41$
Refinement	
Refinement on	F^2
$R[F^2 > 2\sigma(F^2)],$ $wR(F^2), S$	0.070, 0.235, 1.04
No. of reflections	150143
No. of parameters	1454
No. of restraints	3442
H-atom treatment	H-atom parameters constrained
	$w = 1/[\sigma^2(F_o^2) + (0.0872P)^2 + 65.6296P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$	0.006
$\Delta\rho_{\max}, \Delta\rho_{\min}$ ($\text{e \AA}^{-3}$)	3.73, -4.88
Absolute structure	Flack x determined using 13593 quotients $[(I+)-(I-)]/[(I+)+(I-)]$ (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	0.200 (5)

Computer programs: Apex3 v2018.7-2 (Bruker, 2018), SAINT V8.38A (Bruker, 2018), SHELXM (Sheldrick, 2008), SHELXL2018/3 (Sheldrick, 2015, 2018), SHELXLE Rev1030 (Hübschle *et al.*, 2011).

The crystal under investigation was found to be non-merohedrally twinned. The orientation matrices for the two components were identified using the program Cell_Now, with the two components being related by a 180° rotation around the real a -axis or the $[4\ 0\ 1]$ reciprocal axis, with a transformation matrix of $1\ 0\ 0, 0\ -1\ 0, 0.5\ 0\ -1$. Diffraction spots are thus arranged in alternating rows of exactly overlapping reflections, and reflections spaced by half of the longest unit cell axis.

Integration proved problematic due to excessive multiple overlap of reflections for reflections that are not exactly overlapped, resulting in large numbers of rejected reflections. Attempts were made to adjust integration parameters to avoid excessive rejections (through adjustments to integration queue size, integration box slicing and twin overlap parameters, and omission of box size optimization), as well as crystal to detector distance, which led to less but still substantial numbers of rejected reflections.

With no complete data set obtainable through simultaneous integration of both twin domains, the data were instead handled as if not twinned, with only the major domain integrated, and

converted into an hklf 5 type format hkl file after integration using the "Make HKLF5 File" routine as implemented in the program WinGX.⁴ The twin law matrix used was $\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0.5 & 0 & -1 \end{pmatrix}$. The Overlap R1 and R2 values used were 0.25, i.e. reflections with a discriminator function less or equal to overlap radius of 0.25 were counted overlapped, all others as single. The discriminator function used was the "delta function on index non-integrality". No reflections were omitted and data are not merged.

The structure was solved using direct methods with the hklf 4 type file and was refined using the hklf 5 type file, resulting in a BASF value of 0.274(3) (this is known to be an underestimate. Simultaneous integration of both twin domains indicates a close to 1:1 intensity ratio of twin domains).

No R_{int} value is obtainable for the hklf 5 type file using the WinGX routine. The value from before use on WinGX is given instead.

The structure is pseudo C-centered emulating a monoclinic lattice with dimensions $a = 17.443$, $b = 17.424$, $c = 26.822 \text{ \AA}$ and $\beta = 99.15^\circ$. The structure also exhibits pseudo-translations within the Pb-I double layers along the in plane Pb-I-Pb-I directions. These directions coincide with the a and b -axis directions of the primitive cell (note the 90° gamma angle, creating on average square Pb nets). The pseudo-translations are obeyed by most atoms, but broken by a modulation of the Pb and I atoms, which extends to the methyl ammonium cations and the ammonium fragments of the organic ligands. Modulation is induced by a zig-zag distortion of iodine atoms of the the square Pb-I layers. Along the b -axis direction modulated iodine atoms are placed alternately to the right and left of the Pb ions (along the a -axis direction). This induces an alternating 90° rotation of both the methyl ammonium ions and the ammonium fragments of the organic ligands along this axis. The thiophene portions of the ligands obey exact translation. The lead ions are slightly displaced from average positions by distortion of octahedral coordination in a direction perpendicular to the double Pb-I layers, with half the Pb ions from the top and bottom Pb layer being bonded to the central iodine layer (with a PbI_6 coordination), and half being displaced away from the central iodine layer (with a PbI_5 coordination with a sixth iodine just out of bonding range). Along the a -axis direction modulation is absent for the lead ions, but more pronounced for all other fragments. Iodine atoms show the same modulation as along the b -axis, being placed alternately to the right and left of the Pb ions. Alternating 90° rotations of both the methyl ammonium ions and ammonium fragments of the organic ligands are again observed along

this axis. The thiophene fragments are not related by pseudotranslation but are arranged in a herringbone pattern when looking along a.

If pseudotranslations and satellite reflections are ignored the unit cell can be transformed into a smaller monoclinic C-centered cell with dimensions $a = 8.70$, $b = 8.715$, $c = 26.772$ Å, $\beta = 99.42^\circ$.

The outer thiophene ligands are disordered by rotation, which was included in the refinement model. Some of the ammonium fragments of the organic ligand were refined as disordered by approximate 90° rotations. Twinning, correlation due to pseudosymmetry and the overall low data quality required application of a series of restraints and constraints to ensure a stable and meaningful refinement. All organic ligands and disordered segments were restrained to have similar geometries. C atoms related by pseudotranslation were constrained to have identical ADPs. C and S atoms of the disordered outer thiophene rings were restrained to be coplanar. The distances of the nitrogen atoms to the second next carbon atom were restrained to be at least $2.60(2)$ Å (aka, the N-C-C angles were restrained to be meaningful). U^{ij} components of the ADPs of their C, N and S atoms closer to each other than 2.0 Å were restrained to be similar. ADPs of nitrogen atoms with similar orientations were constrained to be identical (N1A, N1C and N1K; N1B, N1D and N1L; N1E, N1G and N1O; and N1F, N1H and N1P). Torsion angles other than for the disordered outer thiophene ligands, and thus all modulation along pseudo-translation directions, were not restrained but always freely refined.

Subject to these conditions the disorder ratios for the outer thiophene ligands refined to $0.86(3)$ to $0.14(3)$, $0.77(3)$ to $0.23(3)$, $0.86(3)$ to $0.14(3)$, $0.81(3)$ to $0.19(3)$, $0.71(3)$ to $0.29(3)$, $0.70(3)$ to $0.70(3)$, $0.68(3)$ to $0.32(3)$ and $0.66(3)$ to $0.34(3)$ for ligands A through H, respectively.

C-N distances of methyl ammonium cations were restrained to be similar. U^{ij} components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar, and ADPs were restrained to be close to isotropic. No attempts were made to verify the placement of N versus C atoms for the methyl ammonium cations, but the C-N direction was allowed to freely refine.

Subject to these conditions the disorder ratios for the ammonium rotation of fragments C, D, G and H refined to $0.38(3)$ to $0.62(3)$, $0.51(4)$ to $0.49(4)$, $0.55(4)$ to $0.45(4)$, $0.58(3)$ to $0.42(3)$, respectively.

Supplementary Table 6.

	2T n=3, (2T)₂(MA)₂Pb₃I₁₀
Crystal data	
Chemical formula	I ₂₀ Pb ₆ ·4(C ₁₀ H ₁₂ NS ₂)·4(CH ₆ N)
<i>M_r</i>	4750.78
Crystal system, space group	Triclinic, <i>P</i> 1
Temperature (K)	273
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.7915 (18), 8.7897 (17), 33.141 (7)
α , β , γ (°)	97.664 (5), 90.116 (5), 90.095 (6)
<i>V</i> (Å ³)	2538.1 (9)
<i>Z</i>	1
<i>F</i> (000)	2072
<i>D_x</i> (Mg m ⁻³)	3.108
Radiation type	Mo <i>K</i> α
No. of reflections for cell measurement	9952
θ range (°) for cell measurement	2.5–33.8
μ (mm ⁻¹)	16.19
Crystal shape	Plate
Colour	Black
Crystal size (mm)	0.12 × 0.05 × 0.01
Data collection	
Diffractometer	Bruker AXS D8 Quest diffractometer with PhotonII charge-integrating pixel array detector (CPAD)
Radiation source	fine focus sealed tube X-ray source
Monochromator	Triumph curved graphite crystal
Detector resolution (pixels mm ⁻¹)	7.4074
Scan method	ω and ϕ scans
Absorption correction	Multi-scan SADABS 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
<i>T_{min}</i> , <i>T_{max}</i>	0.044, 0.105
No. of measured, independent and observed [<i>I</i> > 2s(<i>I</i>)] reflections	59201, 36853, 22936
<i>R_{int}</i>	0.057
θ values (°)	$\theta_{\max}$ = 33.8, $\theta_{\min}$ = 2.3

$(\sin \theta/\lambda)_{\max}$ ($\text{\AA}^{-1}$)	0.782
Range of h, k, l	$h = -13 - 13, k = -13 - 13, l = -51 - 51$
Refinement	
Refinement on	F^2
$R[F^2 > 2\sigma(F^2)],$ $wR(F^2), S$	0.059, 0.194, 1.04
No. of reflections	36853
No. of parameters	1076
No. of restraints	1777
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0726P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$	0.001
$\Delta\rho_{\max}, \Delta\rho_{\min}$ ($\text{e \AA}^{-3}$)	3.06, -2.26
Extinction method	<i>SHELXL2018/3</i> (Sheldrick 2018), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient	0.00055 (8)
Absolute structure	Twinning involves inversion, so Flack parameter cannot be determined

Computer programs: Apex3 v2019.1-0 (Bruker, 2019), *SAINT* V8.40A (Bruker, 2019), *SHELXS97* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2015, 2018), *SHELXLE* Rev1146 (Hübschle *et al.*, 2011).

Crystals are twinned by multiple twin operations. At room temperature twinning is close to pseudo-merohedral. Upon cooling to under 0 °C twinning transforms into non-merohedral with multiple ill-defined twin domains with excessive overlap that preempts data analysis and processing. Data were thus collected at 0 °C.

The main twin operation is a 180 ° rotation around $[0\ 1\ 2]$, twin transformation matrix $-1\ 0\ 0, 0\ 1\ 0, 0\ -1\ -1$. Additional minor twinning by positive and negative 90 ° rotations around the same axis is observed, twin transformation matrix $0\ 1\ 0, -1\ 0\ 0, 0.5\ 0.5\ 1$ as well as inversion twinning. Twinning was thus implemented by inclusion of four domains with successive application of three 90 ° rotations around $[0\ 1\ 2]$ combined with inversion twinning (8-component inversion twinning), using the Shelxl command "TWIN 0 1 0 -1 0 0 0.5 0.5 1 -8".

Twin components refined to the following fractions:

0.124(8) (original lattice)

0.038(8) (90 ° rotation, no inversion)

0.069(9) (180 ° rotation, no inversion)

0.000(8) (270 ° rotation, no inversion)

0.472(9) (original lattice, inversion)

0.030(8) (90 ° rotation, inversion)

0.190(9) (180 ° rotation, inversion)

0.077(8) (270 ° rotation, inversion)

The structure exhibits pseudo-translation by approximate C-centering. Exact translation is broken by modulation of the iodine atoms in layers (see below, 1:1 disorder would be required for a C-centered lattice), by modulation of the methyl ammonium cations, and by modulation of the H₃N-CH₂-CH₂ moieties. Lead atoms and terminal iodine atoms, and the thiophene rings obey exact lattice translation.

Disorder is observed for the iodine atoms in the infinite Pb-I layers (but not for the struts between layers or for terminal iodine atoms). A common occupancy ratio was applied for all disordered iodine atoms. U^{ij} components of ADPs for lead and iodine atoms closer to each other than 3.3 Å were restrained to be similar. Subject to these conditions the occupancy ratio refined to 0.9015(16) to 0.0985(16).

Methyl ammonium ions of the thiophene ammonium cations are ill defined and a rigid body approach was used for refinement of both. C-N bond distances were restrained to 1.53(2) Å. Methyl ammonium cations were restrained to have close to isotropic atoms, and U^{ij} components of ADPs closer to each other than 2.0 Å were restrained to be similar. Disorder induced by iodine disorder was not resolved and was ignored.

All thiophene ammonium cations were restrained to have similar geometries. The outer thiophene rings were refined as rotationally disordered. Most C-C and C-S bond distances were restrained to target values (1.36(2) Å for C=C, 1.43(2) Å for thiophene C-C, 1.71(2) Å for C-S), as were several bond angles by restraining 1,3 C...C distances to target values or minimum distances. Thiophene rings and directly adjacent atoms as well as their rotationally disordered counterparts were restrained to lie in a common plane. U^{ij} components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar. Subject to these conditions the occupancy ratios for the outer thiophene rings refined to 0.96(3) to 0.04(3) (cation A), 0.85(4) to 0.15(3) (cation B), 0.68(4) to 0.32(4) (cation C), 0.63(3) to 0.37(3) (cation D).

Supplementary Table 7.

	3T n=1, (3T)₂PbI₄
Crystal data	
Chemical formula	I ₄ Pb·2(C ₁₄ H ₁₄ NS ₃)
<i>M_r</i>	1299.67
Crystal system, space group	Monoclinic, <i>Pc</i>
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	24.9155 (19), 12.1019 (10), 12.2806 (9)
β (°)	97.080 (2)
<i>V</i> (Å ³)	3674.7 (5)
<i>Z</i>	4
<i>F</i> (000)	2400
<i>D_x</i> (Mg m ⁻³)	2.349
Radiation type	Mo <i>K</i> α
No. of reflections for cell measurement	9896
θ range (°) for cell measurement	2.5–30.6
μ (mm ⁻¹)	8.32
Crystal shape	Yellow
Colour	Plate
Crystal size (mm)	0.22 × 0.12 × 0.04
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Radiation source	fine focus sealed tube X-ray source
Monochromator	Triumph curved graphite crystal
Detector resolution (pixels mm ⁻¹)	10.4167
Scan method	ω and phi scans
Absorption correction	Multi-scan SADABS 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D. (2015). <i>J. Appl. Cryst.</i> 48 3-10.
<i>T_{min}</i> , <i>T_{max}</i>	0.047, 0.100
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	59215, 59215, 46013
<i>R_{int}</i>	0.052
θ values (°)	θ _{max} = 30.6, θ _{min} = 2.4

$(\sin \theta/\lambda)_{\max}$ ($\text{\AA}^{-1}$)	0.717
Range of h, k, l	$h = -34 - 35, k = -17 - 17, l = -17 - 17$
Refinement	
Refinement on	F^2
$R[F^2 > 2\sigma(F^2)],$ $wR(F^2), S$	0.085, 0.246, 1.04
No. of reflections	59215
No. of parameters	559
No. of restraints	796
H-atom treatment	H-atom parameters constrained
	$w = 1/[\sigma^2(F_o^2) + (0.087P)^2 + 160.9832P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$	0.001
$\Delta\rho_{\max}, \Delta\rho_{\min}$ ($\text{e \AA}^{-3}$)	4.92, -8.08
Extinction method	<i>SHELXL2018/3</i> (Sheldrick 2018), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient	0.00188 (14)
Absolute structure	Flack x determined using 5861 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons, Flack and Wagner, <i>Acta Cryst. B</i> 69 (2013) 249-259).
Absolute structure parameter	0.336 (5)

Computer programs: Apex3 v2018.7-2 (Bruker, 2018), *SAINT* V8.38A (Bruker, 2018), *SHELXS97* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2015, 2018), *SHELXLE* Rev1030 (Hübschle *et al.*, 2011).

The crystal under investigation was found to be non-merohedrally twinned. The orientation matrices for the two components were identified using the program *Cell_Now*, with the two components being related by a 180 ° rotation around the reciprocal a -axis or the real c -axis, with a transformation matrix of -1 0 -0.5, 0 -1 0, 0 0 1. Diffraction spots are thus arranged in alternating rows of exactly overlapping reflections, and rows of reflections spaced by half of the longest unit cell axis.

Integration proved problematic due to excessive multiple overlap of reflections for reflections that are not exactly overlapped, resulting in large numbers of rejected reflections. Attempts were made to adjust integration parameters to avoid excessive rejections (through adjustments to integration queue size, integration box slicing and twin overlap parameters, and omission of box size optimization), as well as crystal to detector distance, which led to less but still substantial numbers of rejected reflections.

With no complete data set obtainable through simultaneous integration of both twin domains, the data were instead handled as if not twinned, with only the major domain integrated, and converted into an hklf 5 type format hkl file after integration using the "Make HKLF5 File" routine as implemented in the program WinGX.⁴ The twin law matrix used was $\begin{pmatrix} -1 & 0 & -0.5 \\ 0 & 0 & 1 \end{pmatrix}$. The Overlap R1 and R2 values used were 0.15, i.e. reflections with a discriminator function less or equal to overlap radius of 0.15 were counted overlapped, all others as single. The discriminator function used was the "delta function on index non-integrality". No reflections were omitted and data are not merged.

The structure was solved using direct methods with the hklf 4 type file and was refined using the hklf 5 type file, resulting in a BASF value of 0.301(5) (this is known to be an underestimate. Simultaneous integration of both twin domains indicates a close to 1:1 intensity ratio of twin domains).

No R_{int} value is obtainable for the hklf 5 type file using the WinGX routine. The value from before use on WinGX is given instead.

The structure is pseudo A-centered emulating a monoclinic C-centered lattice with dimensions $a = 12.281$, $b = 12.102$, $c = 24.916$ Å and $\beta = 97.08^\circ$. The structure also exhibits pseudo-translations within the Pb-I double layers along the in plane Pb-I-Pb-I directions. These directions coincide with the a and b-axis directions of the unit cell. The pseudo-translations are obeyed by most atoms, but broken by a modulation of the Pb and I atoms, which extends to the methyl ammonium cations and the ammonium fragments of the organic ligands. Modulation is induced by a zig-zag distortion of iodine atoms of the square Pb-I layers. Along the b-axis direction modulated iodine atoms are placed alternatingly to the right and left of the Pb ions (along the a-axis direction). This induces an alternating 90° rotation of the ammonium fragments of the organic ligands along this axis. The thiophene portions of the ligands obey exact translation. The lead ions are slightly displaced from average positions by distortion of octahedral coordination in a direction perpendicular to the double Pb-I layers, with half the terminal iodine ions being bonded to the central layer lead atoms (with a PbI_5 coordination with a sixth iodine just out of bonding range). Pb ion Pb2 was refined as disordered over the two alternative positions, with Pb2 bonded to I4 and Pb2B to I3 instead. ADPs of the two Pb ions were constrained to be identical, leading to a disorder ratio of 0.74(2) to 0.26(2) in favor of Pb2. Along the a-axis direction modulation is absent for the lead ions, but more pronounced for all other fragments. Iodine atoms show the same

modulation as along the b-axis, being placed alternatingly to the right and left of the Pb ions. Alternating 90 ° rotations of ammonium fragments of the organic ligands are again observed along this axis. The thiophene fragments are not related by pseudotranslation but are arranged in a herringbone pattern when looking along a.

Twinning, correlation due to pseudosymmetry and the overall low data quality required application of a series of restraints and constraints to ensure a stable and meaningful refinement. All organic ligands were restrained to have similar geometries. C atoms related by pseudotranslation were constrained to have identical ADPs. The distances of the nitrogen atoms to the second next carbon atom were restrained to be at least 2.50(2) Å (aka, the N-C-C angles were restrained to be meaningful). All C1-C2 bond distances were restrained to a target value of 1.50(2) Å. U^{ij} components of the ADPs of their C, N and S atoms closer to each other than 2.0 Å were restrained to be similar. ADPs of all nitrogen atoms were constrained to be identical. Torsion angles, and thus all modulation along pseudo-translation directions, were not restrained but always freely refined.

Supplementary Table 8.

	3T n=2, (3T)₂(MA)Pb₂I₇
Crystal data	
Chemical formula	I ₁₄ Pb ₄ ·4(C ₁₄ H ₁₄ NS ₃)·2(CH ₆ N)
<i>M_r</i>	3839.26
Crystal system, space group	Monoclinic, <i>Pc</i>
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	30.944 (7), 12.196 (3), 12.347 (3)
β (°)	95.714 (5)
<i>V</i> (Å ³)	4636.4 (19)
<i>Z</i>	2
<i>F</i> (000)	3440
<i>D_x</i> (Mg m ⁻³)	2.750
Radiation type	Mo <i>K</i> α
No. of reflections for cell measurement	9882
θ range (°) for cell measurement	2.7–31.5
μ (mm ⁻¹)	12.21
Crystal shape	Wedge
Colour	Orange
Crystal size (mm)	0.09 × 0.03 × 0.003
Data collection	
Diffractometer	Bruker AXS D8 Quest diffractometer with PhotonII charge-integrating pixel array detector (CPAD)
Radiation source	fine focus sealed tube X-ray source
Monochromator	Triumph curved graphite crystal
Detector resolution (pixels mm ⁻¹)	7.4074
Scan method	ω and phi scans
Absorption correction	Multi-scan SADABS 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D. (2015). <i>J. Appl. Cryst.</i> 48, 3-10.
<i>T_{min}</i> , <i>T_{max}</i>	0.022, 0.055
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	196559, 196559, 80281
<i>R_{int}</i>	0.093
θ values (°)	θ _{max} = 30.5, θ _{min} = 2.1

$(\sin \theta/\lambda)_{\max}$ ($\text{\AA}^{-1}$)	0.714
Range of h, k, l	$h = -44 - 44, k = -17 - 17, l = -17 - 17$
Refinement	
Refinement on	F^2
$R[F^2 > 2\sigma(F^2)],$ $wR(F^2), S$	0.083, 0.293, 1.03
No. of reflections	196559
No. of parameters	824
No. of restraints	826
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$	0.001
$\Delta\rho_{\max}, \Delta\rho_{\min}$ ($\text{e \AA}^{-3}$)	5.86, -7.58
Absolute structure	Flack x determined using 4172 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	0.013 (5)

Computer programs: Apex3 v2019.1-0 (Bruker, 2019), SAINT V8.40A (Bruker, 2019), SHELXM (Sheldrick, 2008), SHELXL2018/3 (Sheldrick, 2015, 2018), SHELXLE Rev1146 (Hübschle *et al.*, 2011).

The crystal under investigation was found to be non-merohedrally twinned. The orientation matrices for the two components were identified using the program Cell_Now, with the two components being related by a 180 ° rotation around the reciprocal a-axis.

Integration proved problematic due to excessive multiple overlap of reflections along the long reciprocal axis, resulting in large numbers of rejected reflections. Attempts were made to adjust integration parameters to avoid excessive rejections (through adjustments to integration queue size, integration box slicing and twin overlap parameters, and omission of box size optimization), which led to less but still substantial numbers of rejected reflections. With no complete data set obtainable through simultaneous integration of both twin domains, the data were instead handled as if not twinned, with only the major domain integrated, and converted into an hklf 5 type format hkl file after integration using the "Make HKLF5 File" routine as implemented in the program WinGX.⁴ The twin law matrix was used as obtained from SAINT, see above. The Overlap R1 and R2 values used were 0.35, i.e. reflections with a

discriminator function less or equal to overlap radius of 0.35 were counted overlapped, all others as single. The discriminator function used was the "delta function on index non-integrality". No reflections were omitted.

The structure was solved using direct methods with the uncorrected hklf 4 type file and was refined using the hklf 5 type file, resulting in a BASF value of 0.199(4).

No R_{int} value is obtainable for the hklf 5 type file using the WinGX routine. The value from TWINABS is given instead, which is for all reflections available and is based on agreement between observed single and composite intensities and those calculated from refined unique intensities and twin fractions (TWINABS (Sheldrick, 2009)).

Omission of twinning resulted in slightly higher R values (R_1 being about 1% higher), and presence of large residual electron densities nearby Pb, I and S atoms in positions created by pseudo-translation (see below). The eight largest difference density peaks had been between 12.8 and 14.2 electrons per $\text{\AA}^3$.

The structure exhibits pseudo-translation along the b-axis direction with an 85% fit. Exact lattice translation is broken by modulation of the iodine atoms within each of the Pb-I layers, and by modulation of the ammonium and adjacent methylene fragments (following the iodine modulation that they are H-bonded to). The remaining organic fragments, the lead ions, the terminal iodines and the iodines bridging between the Pb-I layers obey translational symmetry.

Methyl ammonium cations are located within the voids of the double Pb-I layer. The cations are ill defined due to large thermal libration and correlation from pseudosymmetry. U^{ij} components of ADPs of all methyl ammonium C and N atoms were restrained to be similar and ADPs were restrained to be close to isotropic. The C-N distances were restrained to a target value of 1.50(2) $\text{\AA}$. H-atoms were initially allowed to rotate and were in the final refinement cycles set to ride on their respective carrier atom.

The four organic cations were restrained to have similar geometries. U^{ij} components of their atoms' ADPs closer to each other than 2.0 $\text{\AA}$ were restrained to be similar.

Supplementary Table 9.

	4Tm n=2, (4Tm)₂(MA)Pb₂I₇
Crystal data	
Chemical formula	I ₁₄ Pb ₄ ·4(C ₂₀ H ₂₀ NS ₄)·2(CH ₆ N)
<i>M_r</i>	4279.93
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	12.319 (3), 12.382 (3), 37.706 (12)
α , β , γ (°)	87.821 (15), 85.396 (10), 89.973 (11)
<i>V</i> (Å ³)	5729 (3)
<i>Z</i>	2
<i>F</i> (000)	3904
<i>D_x</i> (Mg m ⁻³)	2.481
Radiation type	Mo <i>K</i> α
No. of reflections for cell measurement	9880
θ range (°) for cell measurement	2.7–32.9
μ (mm ⁻¹)	9.97
Crystal shape	Plate
Colour	Red
Crystal size (mm)	0.06 × 0.05 × 0.003
Data collection	
Diffractometer	Bruker AXS D8 Quest diffractometer with PhotonII charge-integrating pixel array detector (CPAD)
Radiation source	fine focus sealed tube X-ray source
Monochromator	Triumph curved graphite crystal
Detector resolution (pixels mm ⁻¹)	7.4074
Scan method	ω and ϕ scans
Absorption correction	Multi-scan SADABS 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D. (2015). <i>J. Appl. Cryst.</i> 48, 3-10.
<i>T_{min}</i> , <i>T_{max}</i>	0.097, 0.359
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	113768, 113768, 46566
<i>R_{int}</i>	0.108
θ values (°)	$\theta_{\max}$ = 30.5, $\theta_{\min}$ = 2.2

$(\sin \theta/\lambda)_{\max}$ ($\text{\AA}^{-1}$)	0.714
Range of h, k, l	$h = -17 - 17, k = -17 - 17, l = -53 - 53$
Refinement	
Refinement on	F^2
$R[F^2 > 2\sigma(F^2)],$ $wR(F^2), S$	0.116, 0.346, 1.03
No. of reflections	113768
No. of parameters	1113
No. of restraints	1118
H-atom treatment	H-atom parameters constrained
	$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 257.6246P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$	0.001
$\Delta\rho_{\max}, \Delta\rho_{\min}$ ($\text{e \AA}^{-3}$)	5.17, -5.25

Computer programs: Apex3 v2019.11-0 (Bruker, 2019), SAINT V8.40B (Bruker, 2019), SHELXS97 (Sheldrick, 2008), SHELXL2018/3 (Sheldrick, 2015, 2018), SHELXLE Rev1183 (Hübschle *et al.*, 2011).

The crystal under investigation was found to be non-merohedrally twinned. The orientation matrices for the two components were identified using the program Cell_Now, with the two components being related by a 180° rotation around the real b-axis. Attempts were made to integrate the data using Saint, but integration proved problematic due to excessive multiple overlap of reflections, resulting in large numbers of rejected reflections. Attempts were made to adjust integration parameters to avoid excessive rejections (through adjustments to integration queue size, integration box slicing and twin overlap parameters, and omission of box size optimization), which led to less but still substantial numbers of rejected reflections.

With no complete data set obtainable through simultaneous integration of both twin domains, the data were instead handled as if not twinned, with only the major domain integrated, and converted into an hklf 5 type format hkl file after integration using the "Make HKLF5 File" routine as implemented in WinGX.⁴ The twin law matrix was used as obtained from Rotax⁵ within WinGX and was as follows:

-1.000 0.001 0.000

0.000 1.000 0.000

0.000 0.232 -1.000

The Overlap R1 and R2 values used were 0.16, i.e. reflections with a discriminator function less or equal to overlap radius of 0.16 were counted as overlapped, all others as single. The discriminator function used was the "delta function on index non-integrality". No reflections were omitted.

The structure was solved using direct methods with the hklf 4 type file and was refined using the hklf 5 type file, resulting in a BASF value of 0.234(3).

No R_{int} value is obtainable for the hklf 5 type file using the WinGX routine. The value from before correction in WinGX is given instead.

The structure exhibits pseudo-translation along the a-axis (88% fit). Exact translational symmetry is broken by modulation of the iodine atoms I1 through I8 (within each Pb-I layer) that also induces modulation of the ammonium end of the major organic cations, and by modulation of the intralayer methyl ammonium cations. Exact translation is obeyed by the main sections of the major organic cations, by the lead ions, and by the remainder of the iodine atoms (I9 through I14).

Due to the pseudo-translation, positions and ADPs of the organic cations are ill-defined. The four moieties were thus restrained to have similar geometries. U^{ij} components of ADPs for N, C and S atoms closer to each other than 2.0 Å were restrained to be similar. The C and N atoms of the methyl ammonium cations were further restrained to be close to isotropic, and their C-N bond distances were restrained to a target value of 1.50(2) Angstroms.

Supplementary Table 10.

	3T n=3, (3T)₂(MA)₂Pb₃I₁₀
Crystal data	
Chemical formula	I ₂₀ Pb ₆ ·4(C ₁₄ H ₁₄ NS ₃)·4(CH ₆ N)
<i>M_r</i>	5079.18
Crystal system, space group	Monoclinic, <i>Pc</i>
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	37.131 (6), 12.2609 (17), 12.375 (2)
β (°)	94.693 (7)
<i>V</i> (Å ³)	5614.7 (15)
<i>Z</i>	2
Radiation type	Synchrotron, λ = 0.7288 Å
μ (mm ⁻¹)	15.57
Crystal shape	Plate
Colour	Dark Red
Crystal size (mm)	0.04 × 0.04 × 0.01
Data collection	
Diffractometer	Bruker D8 with PHOTONII detector
Absorption correction	Multi-scan SADABS 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
<i>T_{min}</i> , <i>T_{max}</i>	0.055, 0.104
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	148428, 38586, 24810
<i>R_{int}</i>	0.054
(sin θ/λ) _{max} (Å ⁻¹)	0.748
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.069, 0.236, 1.06
No. of reflections	38586
No. of parameters	833
No. of restraints	840
H-atom treatment	H-atom parameters constrained
	<i>w</i> = 1/[σ ² (<i>F_o</i> ²) + (0.056 <i>P</i>) ² + 257.6246 <i>P</i>] where <i>P</i> = (<i>F_o</i> ² + 2 <i>F_c</i> ²)/3
Δρ _{max} , Δρ _{min} (e Å ⁻³)	3.49, -3.48

Computer programs: Apex3 v2019.11-0 (Bruker, 2019), *SAINT* V8.40B (Bruker, 2019), *SHELXS97* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2015, 2018), *SHELXLE* Rev1183 (Hübschle *et al.*, 2011).

Data were collected at the Advanced Light Source beamline 12.2.1 using a wavelength of 0.72880 Angstrom. Frequency dependent components of the elemental X-ray scattering factors were based on the used wavelength (L. Kissel and R. H. Pratt (1990) *Acta Cryst A* 46, 170).

The crystal under investigation was found to be pseudo-merohedrally twinned. The orientation matrices for the two components were identified using the program *Cell_Now*, with the two components being related by a 180 degree rotation around the reciprocal c-axis. Attempts were made to integrate the two components using *Saint*. However, integration proved problematic due to excessive multiple overlap of reflections, resulting in large numbers of rejected reflections. Attempts were made to adjust integration parameters to avoid excessive rejections (through adjustments to integration queue size, integration box slicing and twin overlap parameters, and omission of box size optimization), which led to less but still substantial numbers of rejected reflections. The data quality that could be obtained was less than satisfactory. Twinning was thus considered post-processing by application of a *Shelxl* TWIN transformation matrix. The matrix as obtained from *Cell Now* was used.

Systematic absences indicated space group *P2(1)/c* to be the most likely. Attempts to solve and refine the structure in this space group resulted in a good fit for the lead and iodine fraction of the structure, but incompatible positions for the outermost thiophene rings, large thermal ellipsoids for the thiophene rings, large residuals in this area as well as elevated R values (> 10% for *R*₁). Refinement in *Pc* resulted in substantially lower R values and no incompatible atom positions for the thiophene rings. A *Platon* *Addsym* check (after removal of all minor disordered atoms as well as the methyl ammonium ions) revealed no missed symmetry. The solution in *Pc* was thus used.

Application of pseudo-merohedral twinning under inclusion of inversion (TWIN 1 0 0.458 0 -1 0 0 0 -1 -4) resulted in BASF values of 0.077(8), 0.467(9) and 0.070(8) (the latter two involving inversion), indicating close to 1:1 inversion twinning. The structure was refined in space group *Pc* under inclusion of minor disorder for the in-plane iodine atoms. ADPs of major and minor disordered iodine atoms were constrained to be identical. Initially disorder was refined for each of the three layers with different occupancy values for each layer.

Values were highly correlated due to pseudo-symmetry. Minor disorder values for the lowest layer (I15 to I18) refined to less than 3% and minor iodine atom positions drifted to unreasonable positions. Disorder for these atoms was thus omitted from the refinement model. Subject to these conditions the occupancy ratio refined to 0.841(3) to 0.159(3) for the top layer (I1 through I4) and to 0.922(2) to 0.078(2) for the medium layer (I9 through I12).

Pseudo-translation by pseudo-A centering is observed. Exact translational symmetry is broken by ordering of the major moiety of the in-plane iodine atoms (which refined to be 84, 92 and 100% occupied). Exact translational symmetry is also broken by ordering of the ammonium nitrogen atoms of the outer cations. The four outer cations were restrained to have similar geometries. Their C and S atoms related by pseudo-translation were constrained to have identical ADPs (residues 1 and 2, and residues 3 and 4). Uij components of ADPs closer to each other than 2.0 Angstrom were also restrained to be similar.

Methyl ammonium cations within the Pb-I layers are ill-defined due to large libration and tumbling as well as correlation due to pseudo-symmetry, and thus no attempts were made to refine disorder. Their C-N distances were restrained to a target value (1.45(2)

Angstrom), Uij components of ADPs closer to each other than 2.0 Angstrom were restrained to be similar and atoms were restrained to be close to isotropic. H-atoms were initially refined as rotating while a damping factor was applied. In the final refinement cycles the damping factor was removed and the H atoms were constrained to ride on their C and N carrier atoms.

General method used for resolving crystal structures from single crystal XRD:

Single crystal data were collected using a Bruker Quest diffractometer with a fixed chi angle, a sealed tube fine focus X-ray tube, single crystal curved graphite incident beam monochromator, and either a Photon100 (2T n=2, 3T n=1) or a Photon II area detector area detector (2T n=3, 3T n=2, 4Tm n=2). Instruments were equipped with an Oxford Cryosystems low temperature device and examination and data collection were performed with Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$) at either 150 or 273 K.

Data were collected, reflections were indexed and processed, and the files scaled and corrected for absorption using APEX3⁶ and SADABS.⁷ The space groups were assigned using XPREP within the SHELXTL suite of programs^{8,9} and solved by direct methods using ShelXS or dual methods using ShelXT¹⁰ and refined by full matrix least squares against F^2 with all reflections using Shelxl2018¹¹ using the graphical interface Shelxle.¹² If not specified otherwise H atoms

attached to carbon and nitrogen atoms were positioned geometrically and constrained to ride on their parent atoms. C-H bond distances were constrained to 0.95 Å for aromatic and alkene C-H C-H moieties, and to 1.00, 0.99 and 0.98 Å for aliphatic C-H, CH₂ and CH₃ moieties, respectively. N-H bond distances were constrained to 0.91 Å for pyramidal (sp³ hybridized) ammonium NH₃⁺ groups. Methyl CH₃ and ammonium NH₃⁺ H atoms were allowed to rotate but not to tip to best fit the experimental electron density. U_{iso}(H) values were set to a multiple of U_{eq}(C) with 1.5 for CH₃ and NH₃⁺, and 1.2 for C-H and CH₂ units, respectively.

3. References

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Appendix

Input geometry.in file of (2T)₂PbI₄

lattice_vector	12.0719299316	0.0000000000	0.0000000000
lattice_vector	0.0166684428	12.2423277868	0.0000000000
lattice_vector	-6.5422005594	-6.0510283723	40.9431343323
atom	4.453380585	6.474589825	8.614877701 Pb
atom	1.182280183	3.449075699	29.086446762 Pb
atom	4.437623501	0.388776094	8.144691467 Pb
atom	1.166523099	-2.636738062	28.616258621 Pb
atom	10.463127136	0.342526108	8.175242424 Pb
atom	7.192026615	-2.682987928	28.646808624 Pb
atom	10.501770020	6.519457817	8.629413605 Pb
atom	7.230669498	3.493943691	29.100980759 Pb
atom	3.574370861	3.430657864	8.463286400 I
atom	0.303270698	0.405143648	28.934852600 I
atom	7.447041512	1.260124087	8.444230080 I
atom	4.175941467	-1.765389919	28.915796280 I
atom	5.239512920	9.555176735	8.381636620 I
atom	1.968412757	6.529662609	28.853202820 I
atom	1.414590716	-0.501458228	8.397115707 I
atom	-1.856509686	-3.526972532	28.868684769 I
atom	-0.809900880	3.428421259	8.441392899 I
atom	-4.081001282	0.402907044	28.912960052 I
atom	7.473784924	5.639883518	8.437805176 I
atom	4.202684879	2.614369392	28.909370422 I
atom	9.586524963	9.549621582	8.375460625 I
atom	6.315424919	6.524106979	28.847028732 I
atom	1.435809851	7.381331921	8.378184319 I
atom	-1.835290551	4.355817795	28.849752426 I
atom	4.415406227	6.532109261	11.723504066 I
atom	1.144305944	3.506594896	32.195072174 I
atom	4.388848305	6.624402046	5.145284653 I

atom	1.117747903	3.598887920	25.616851807 I
atom	4.392817497	0.304741561	5.023305416 I
atom	1.121717095	-2.720772743	25.494873047 I
atom	4.381012440	0.210395798	11.636236191 I
atom	1.109912038	-2.815118551	32.107803345 I
atom	-1.654321313	0.511828303	11.660289764 I
atom	-4.925421715	-2.513685942	32.131855011 I
atom	10.398535728	0.410513103	5.070146084 I
atom	7.127436161	-2.615000963	25.541711807 I
atom	-1.608497024	6.460362434	11.737597466 I
atom	-4.879597187	3.434848309	32.209163666 I
atom	10.462310791	6.330344200	5.148644924 I
atom	7.191210270	3.304829836	25.620212555 I
atom	7.520423412	8.444152832	5.646518230 N
atom	4.249323368	5.418639183	26.118083954 N
atom	2.424180984	9.618000984	5.648097515 N
atom	-0.846919358	6.592486382	26.119665146 N
atom	1.487778425	4.459718704	5.739481449 N
atom	-1.783321857	1.434204340	26.211048126 N
atom	8.472588539	3.384402275	5.732386112 N
atom	5.201488018	0.358888209	26.203952789 N
atom	2.442528725	9.478291512	11.138084412 N
atom	-0.828571320	6.452777386	31.609649658 N
atom	1.469707251	2.338959932	11.136837959 N
atom	-1.801393032	-0.686554253	31.608406067 N
atom	8.476172447	3.505045891	11.172633171 N
atom	5.205071926	0.479531676	31.644201279 N
atom	7.506304264	-1.615011573	11.093446732 N
atom	4.235203743	-4.640525818	31.565015793 N
atom	8.264611244	7.865037918	5.205462456 H
atom	4.993511200	4.839523315	25.677030563 H
atom	6.610393524	7.941743851	5.546836376 H
atom	3.339293003	4.916229725	26.018404007 H

atom	7.754624367	8.496466637	6.654923439 H
atom	4.483523846	5.470952034	27.126491547 H
atom	8.470228195	10.265224457	5.207951069 H
atom	5.199128151	7.239710331	25.679519653 H
atom	6.765106678	10.403543472	5.691062450 H
atom	3.494005919	7.378029346	26.162631989 H
atom	5.997832298	9.468063354	3.541636229 H
atom	2.726732254	6.442549229	24.013204575 H
atom	7.010942459	10.877375603	3.290402889 H
atom	3.739842415	7.851861477	23.761968613 H
atom	6.690002918	7.217987061	2.419343710 H
atom	3.418902874	4.192472935	22.890909195 H
atom	8.594545364	6.272045135	0.882979393 H
atom	5.323445797	3.246531248	21.354545593 H
atom	11.870826721	9.896306992	0.484047234 H
atom	8.599726677	6.870793343	20.955614090 H
atom	-1.541686416	5.885402203	19.477666855 H
atom	-4.812786579	2.859888315	39.949234009 H
atom	-1.962584615	3.335413218	18.906421661 H
atom	-5.233684540	0.309899271	39.377986908 H
atom	2.969141245	10.403157234	5.225146770 H
atom	-0.301959187	7.377643108	25.696714401 H
atom	2.988326073	8.741821289	5.555394173 H
atom	-0.282774329	5.716306686	26.026962280 H
atom	2.338053942	9.838196754	6.655964851 H
atom	-0.933046162	6.812683105	27.127531052 H
atom	0.576056242	10.460682869	5.118037701 H
atom	-2.695044041	7.435168743	25.589605331 H
atom	0.501811504	8.771908760	5.671384335 H
atom	-2.769288778	5.746394634	26.142951965 H
atom	1.543291330	7.964745045	3.588126659 H
atom	-1.727808833	4.939230919	24.059694290 H
atom	0.095741689	8.898582458	3.245895386 H

atom	-3.175358534	5.873068810	23.717460632 H
atom	0.714882672	11.678147316	2.547550678 H
atom	-2.556217670	8.652632713	23.019119263 H
atom	2.561440706	0.473659277	1.027830720 H
atom	-0.709659696	-2.551854849	21.499397278 H
atom	5.899764061	9.156062126	0.396213561 H
atom	2.628664017	6.130547523	20.867780685 H
atom	4.555766582	7.234264851	19.468675613 H
atom	1.284666538	4.208751202	39.940242767 H
atom	4.083786488	-2.433087349	19.053314209 H
atom	0.812686384	-5.458601475	39.524879456 H
atom	0.564231575	4.929859161	5.616217613 H
atom	-2.706868649	1.904345155	26.087783813 H
atom	2.214523554	5.046535015	5.280096054 H
atom	-1.056576610	2.021020889	25.751663208 H
atom	1.715999246	4.453143597	6.750375271 H
atom	-1.555101156	1.427629352	27.221942902 H
atom	0.815813780	2.472586870	5.861173630 H
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Input geometry.in file of (2T)₂(MA)₂Pb₃I₁₀

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Input geometry.in file of (3T)₂(MA)Pb₂I₇

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#Cartesian

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Input geometry.in file of (3T)₂(MA)₂Pb₃I₁₀

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Input geometry.in file of (4Tm)₂(MA)Pb₂I₇

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Input geometry.in file of (4Tm)₂(MA)₂Pb₃I₁₀

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