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Pressure Dependent Polymorphism and Bandgap Tuning of Methylammonium Lead Iodide Perovskite

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Dedication ((optional))

Abstract: We report the pressure-induced crystallographic transitions and optical behavior of $MAPbI_3$ (MA = $CH_3NH_3^+$) using in-situ synchrotron X-ray diffraction and laser-excited photoluminescence spectroscopy, supported by Density Functional Theory (DFT) calculations using the hybrid functional B3PW91 with spin-orbit coupling. The tetragonal polymorph determined at ambient pressure transforms to a ReO_3-type cubic phase at 0.3 GPa. Upon continuous compression to 2.7 GPa this cubic polymorph converts to a putative orthorhombic structure. Beyond 4.7 GPa it separates into crystalline and amorphous fractions. During decompression, this phase-mixed material undergoes distinct restoration pathways depending on the peak pressure. In-situ pressure-photoluminescence investigation suggests a reduction in bandgap with increasing pressure up to ~0.3 GPa and then an increase in bandgap up to a pressure of 2.7 GPa, in excellent agreement with our DFT calculation prediction. This work lays the foundation for understanding the pressure-dependent phase transition of $MAPbI_3$ and potentially enriches the toolkit for engineering perovskite polymorphs with exceptional optical properties.

Organic-inorganic metal halide perovskite-based photovoltaic (PV) cells show potential for the direct conversion of sunlight into electricity, due to their high charge-carrier mobilities and electron/hole diffusion lengths of hundreds of nanometers![1-3] The power conversion efficiency (PCE) of perovskite PV cells has rapidly increased from ~6% in 2011 towards ~20% presently, although device reproducibility is questionable.[3-8] PCE can be enhanced by modifying charge-carrier mobility and direct bandgap through tuning crystal chemistry.[9-10] Nonetheless, to date, extensive synthesis campaigns have revealed a limited range of materials. Alternatively, pressurization is a straightforward and robust way to transform crystal structures, where changes in bond strength and geometry are induced without the complication of chemical adjustments. By monitoring changes in PV, strategies for selecting ions of appropriate size and charge can be devised.[11-12] To this end, pressure-dependent structural behaviors of stable and metastable polymorphs can guide design strategies.[13]

The perovskite prototype has the general formula of ABX_3, where corner-sharing BX_6 octahedra create a 3D framework with an A component providing charge compensation if necessary (Figure 1a). The aristotype is cubic $Pm\bar{3}m$ (space group, No. 221), where all the BX_6 octahedra show B-X-B angles of 90°. This arrangement of untilted octahedra can be described in Glazer notation[14-15] as $a^0a^0a^0$. Among the Pb-based methylammonium (MA) halide perovskites (ionic A = $CH_3NH_3^+$ or MA; X = Cl^-, Br^-, I^-; B = Pb^{2+}), the bandgaps of $MAPbCl_3$, $MAPbBr_3$ and $MAPbI_3$ are reported as around 3.1, 2.3 and 1.5 eV, respectively.[10, 16] For single junction PV cells a bandgap in the range between 1.1 and 1.4 eV is desired.[17] Therefore, $MAPbI_3$ is the preferred material. Previous studies of pressure-induced transformations in hybrid perovskites illustrate the crystallographic richness and bandgap changes. Although pressure-induced synchrotron powder X-ray diffraction (XRD) of $MAPbI_3$ was reported recently,[18] extraction of high-pressure lattice parameters, the unambiguous determination of crystal symmetry and the refinement of atomic fractional coordinate are challenging.

In this work, $MAPbI_3$ was synthesized as reported previously.[19] In brief, polycrystalline $MAPbI_3$ was precipitated by 6-hour cooling from 100 to 46 °C after mixing PbI_2 and MA-I solutions in a Pyrex test tube. The PbI_2 solution was prepared by dissolving 2.5 g of lead(II) acetate (Chemical Reagents, Sigma-Aldrich) in 10 ml of aqueous HI solution (57 wt%), whereas the MA-I solution was formed by dissolving 0.597 g of aqueous CH_3NH_2 solution (40%, Merck) in 2 mL of HI solution. The Diamond Anvil cells (DAC) with a size of 500 μm were aligned, assembled and pressurized before conducting XRD (Figure 1b). A stainless steel gasket was indented before drilling a ~200 μm diameter hole that served as the compaction chamber. Ruby fluorescence was used to calibrate pressure[20] and ruby chips were distributed on the sample surface before closing the DAC. At each pressure, an XRD pattern (λ = 0.485946 Å) was collected at the B1 station of the Cornell High Energy Synchrotron Source (CHESS),[21] with a data accumulation time of 10 mins at each pressure, subsequent to maintaining the pressure for approximate 20 min.

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Supporting information for this article is given via a link at the end of the document.

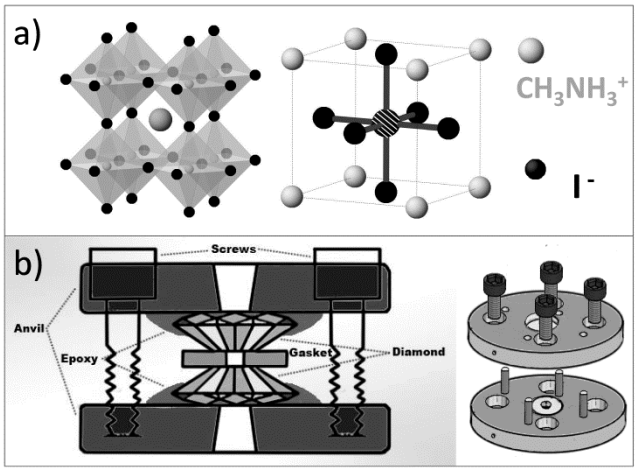


Figure 1. (a) $MAPbI_3$ perovskite $Pm\bar{3}m$ polymorph (left, polyhedral model; right, Pb-I bonds emphasized); (b) DAC holder system with balanced compression screws (left, side view; right, top-down view).

Synchrotron XRD patterns of $MAPbI_3$ collected at room temperature (Figure 2a) and ambient pressure confirms a tetragonal polymorph (*I*4/*mcm,* No. 140) with lattice constants of a_t = 8.8648(6) Å and c_t = 12.6746(8) Å. For this phase, octahedral tilting is about the unique *c* axis only and the Glazer notation is $a^0a^0c^-$. For the tetragonal (*t*) heterotype derived from the cubic (*c*) aristotype, $a_t = a_c\sqrt{2}$ and $c_t = 2a_c$. At ~0.3 GPa, additional reflections appear at 2θ = ~ 7.1° and 8.4 °, which Pawley fitting (Figure S1) shows to be consistent with a cubic bilayer supercell (*s*) ($Im\bar{3}$, No. 204), where $a_s = 2a_c$ as previously observed for the $MAPbBr_3$ analogue,[22] and a high pressure polymorph of ReO_3, where A site in ABX_3 is vacant.[23-24] No evidence was found for the $Pm\bar{3}m$ aristotype identified in a previous variable temperature study.[19] Although the $Pm\bar{3}m$ reflections may substantially overlap with those of the $Im\bar{3}$ supercell, the conventional primitive unit cell was not observed as a separate phase (Figure S1). For comparison, temperature-dependent XRD measurements were collected to 60°C (Figure S2) to demonstrate the conventional $Pm\bar{3}m$ polymorph is stable at elevated temperature (Figure 2a and Figure S1).

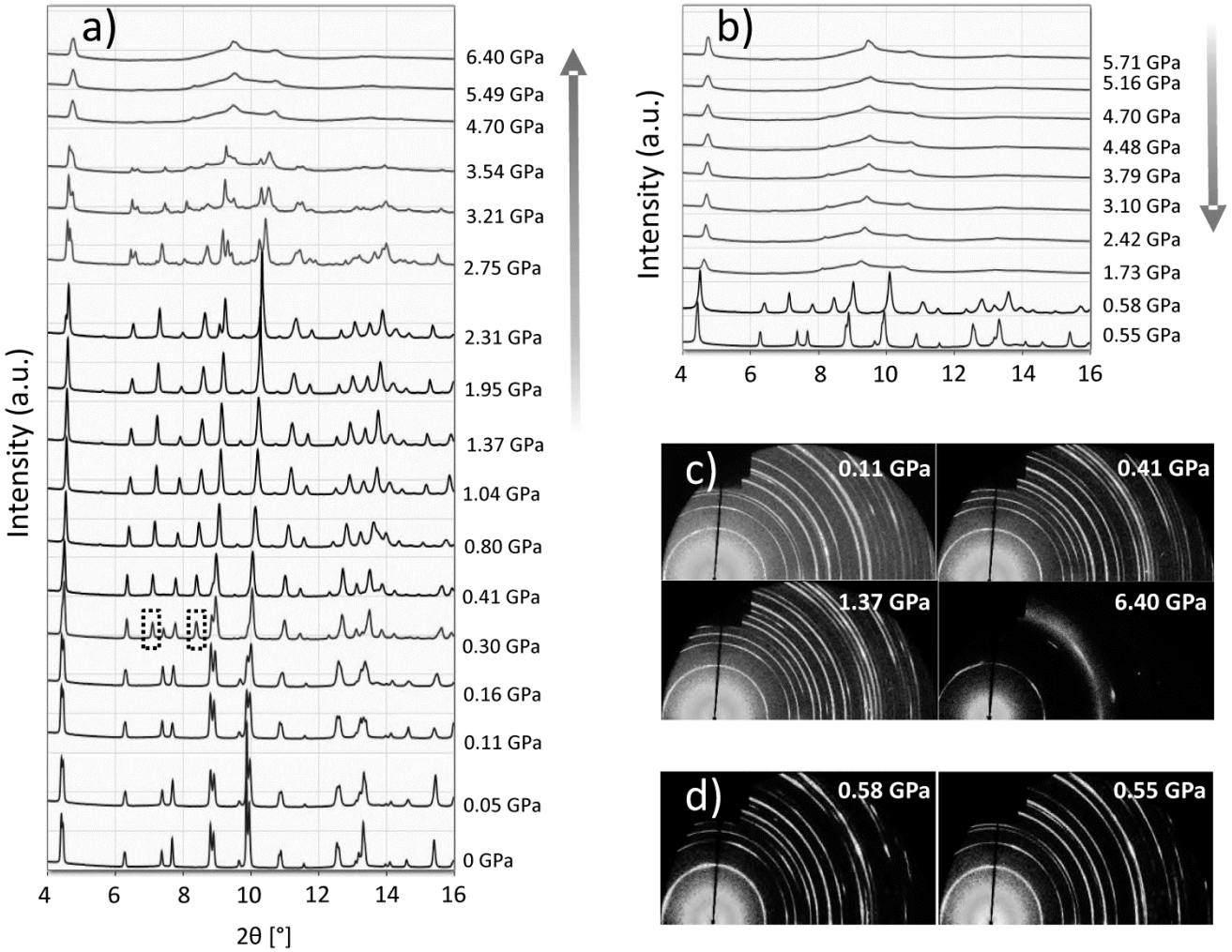


Figure 2. Conventional XRD patterns of $MAPbI_3$ during (a) compression and (b) decompression. (a), The ReO_3-type cubic supercell (a_s) appears at 0.3 GPa and becomes more abundant to 2.3 GPa, before conversion to the putative orthorhombic polymorph at 2.7 GPa, and finally approaches X-ray amorphicity above 3.5 GPa. (b), decompression from the amorphous mass restores the tetragonal phase at 0.5_8 GPa. (c) and (d), Representative 2D XRD patterns at specific pressures.

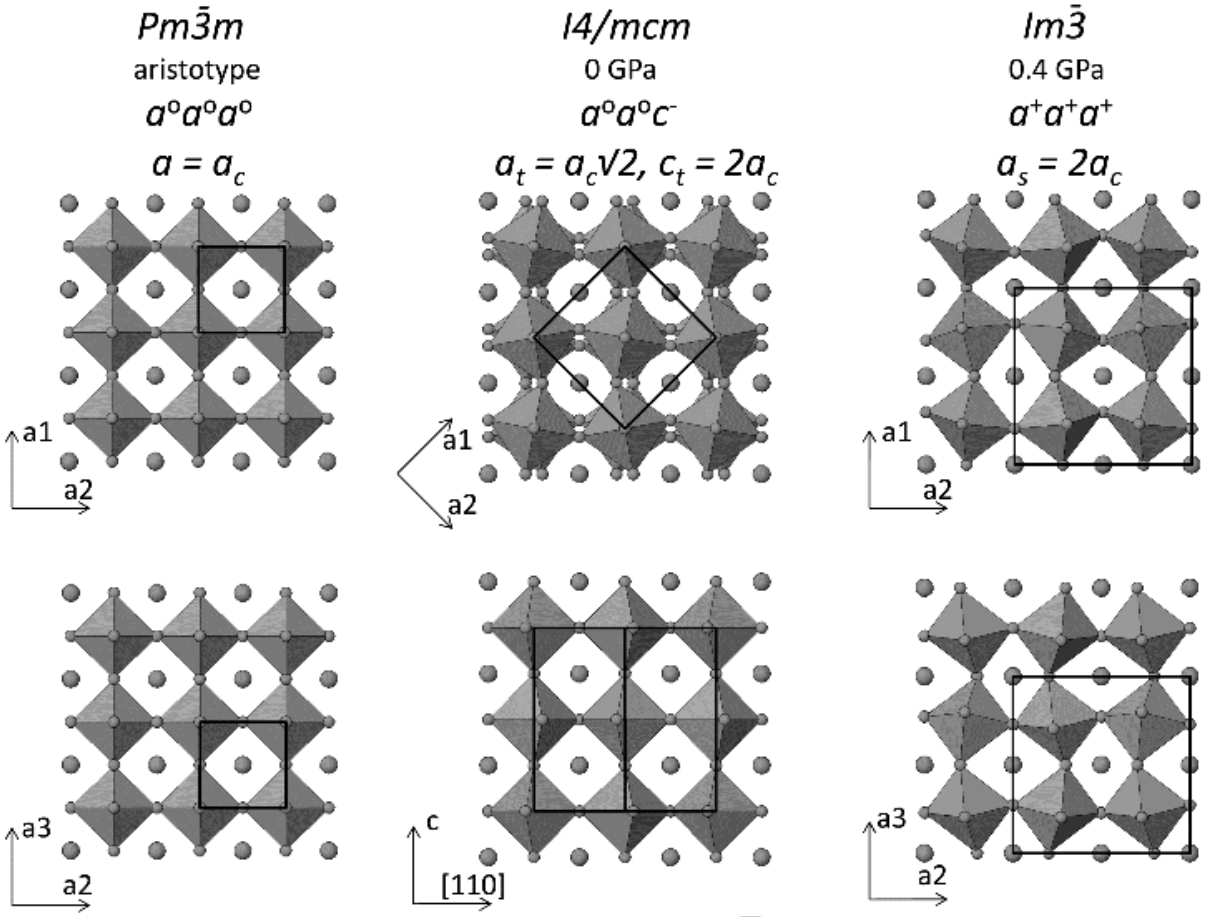


Figure 3. Characteristic PbI_6 octahedral and Glazer symbols of some typical pressure-related polymorphs. The figure for *Immm* polymorph should be similar to that of $Im\bar{3}$ with slightly different lattice parameters along each axis and an octahedral tilt change (Glazer symbol: $a^+b^+c^+$).

Beyond 0.4 GPa, $MAPbI_3$ completely transforms to the $Im\bar{3}$ phase with a_s = 12.4076(0) Å and tilt character $a^+a^+a^+$, with octahedral tilt of equal magnitude about all three axes (Figure S1). For this polymorph, the cell volume contracts and the Bragg reflections broaden as a function of the applied pressure until 2.3 GPa. Prior to amorphization at 4.7 GPa, an additional phase appearing at 2.7 GPa was identified, with 00*l* reflections becoming triply degenerate (Figure S3). Such splitting would be consistent with orthorhombic symmetry, and by analogy with $MASnI_3$[25] may be an *Immm* (No. 77) polymorph with $a^+b^+c^+$ PbI_6 tilting. Reports of an orthorhombic high-pressure form of $MAPbBr_3$ remain ambiguous.[22, 26] Beyond 2.7 GPa $MAPbI_3$ continues to amorphize to near completion at 4.7 GPa, with no further change in X-ray scattering character up to 6.4 GPa (also refer to 2D diffraction patterns in Figure 2c). Upon a gradual release of pressure, the sample remains partially amorphous until 0.5_8 GPa without the appearance of the putative *Immm* polymorph (Figure 2b). However, the $Im\bar{3}$ phase appeared at 0.5_8 GPa, and the *I*4/*mcm* was restored at 0.5_5 GPa (Figure 2b,d).

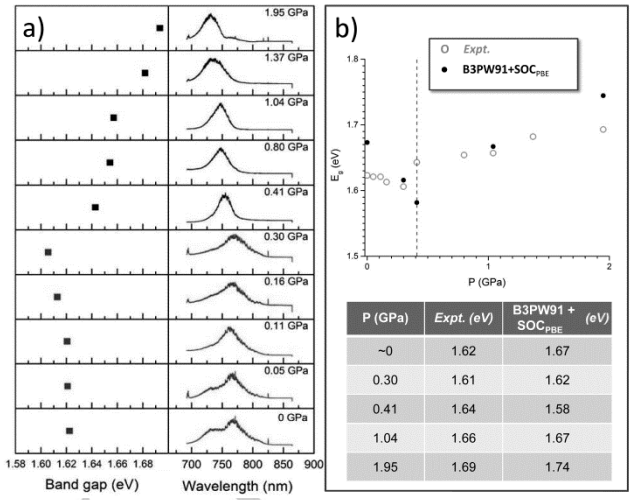
In order to determine the influence of the maximum applied pressure and microstructural evolution during decompression, a series of experiments with different peak-pressures were conducted. For example, using 3.5 GPa as the peak pressure (Figure S4) the *Immm* structure was favored at 2.8 GPa, and the $Im\bar{3}$ polymorph was recovered when the pressure was reduced to 0.9 GPa. This confirms the recovered structure during decompression is controlled by the peak pressure. The decompression pattern collected at 1.3_7 GPa was modelled using both *Immm and* $Im\bar{3}$ polymorphs (Figure S5). However, the poor Pawley fit of the 004 reflection (at 2θ = ~9°) for the cubic polymorph indicates this phase(s) resides on the borderline of the orthorhombic → cubic transition. This evidence supports the existence of the *Immm* polymorph, but suggests it is metastable with respect to the $Im\bar{3}$ and *I*4/*mcm* polymorphs. The tetragonal structure forms reversibly when the applied pressure does not exceed 8.0 GPa. Taken alone, Pawley fitted cell metrics do not show a clear discontinuity as the symmetry varies (Figure S6), but optical microscopy does show some distinct changes (Figure S7).

Using the refined atomic fractional coordinates for Pb and I in the ReO_3-type $Im\bar{3}$ cubic supercell as a basis, the octahedral topologies in the cubic (*c*), tetragonal (*t*) and ReO_3-type cubic supercell (*s*) of the $MAPbI_3$ can be derived (Figure 3).[24] It should be noted that only the MA groups are dynamic[27] and not included. The octahedral tilt angle in the cubic supercells approaches ~15° in advance of the appearance of the orthorhombic polymorph (refer to Table S1).[24] The cif files generated from the Density Functional Theory (DFT) calculations (*vide infra*) also present all the relevant coordinates (Table S2).

The $MAPbI_3$ polymorphs show discrete bandgaps that can be calculated from *in-situ* pressure-photoluminescence (PL) spectra during a compression (Figure 4a and Table S3) but are typically slightly larger than those determined by absorption,[28] as the Tauc plot[29] was calculated. At ambient conditions, the PL spectrum shows a broad band at 764 nm, equivalent to the bandgap of 1.62 eV and in agreement with previous reports.[29-32] The PL band of tetragonal perovskite is believed to originate from a near-band-edge transition.[30-31, 33] Up to 0.3 GPa, PL of the *I*4/*mcm* structure shows a progressive red shift (1.62 to 1.61 eV). In this pressure regime, the DFT calculations find the bandgap to decrease from 1.67 to 1.62 eV, in accord with the PL (Figure 4b).

With increasing PbI_6 octahedral tilt angles, the transition of the $Im\bar{3}$ polymorph to the suggested orthorhombic *Immm* structure at 0.4 GPa leads to a blue-shifted PL spectra accompanying an increase of the bandgap from 1.64 to 1.69 eV. The pressure-dependent PL variations are similar to those in the $MAPbBr_3$ system reported recently.[26] The PL band weakens substantially beyond 2.0 GPa, and vanishes at 2.7 GPa with the destabilization of the $Im\bar{3}$ supercell. The PL spectra during decompression are also instructive. For example, when a peak-pressure of 6.4 GPa was applied, the PL was annihilated upon release of pressure. In contrast, from a peak-pressure of 3.5 GPa, weak PL band appears at 1.7 GPa, near the incipient recovery of the cubic supercell (Figures S4, S5).

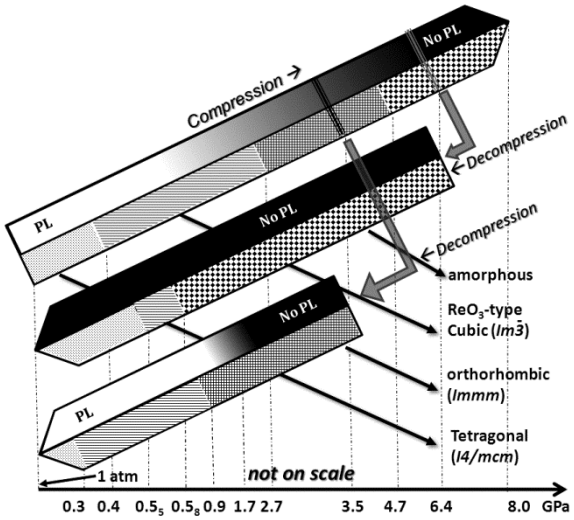
As PL correlates directly with polymorphism, conversion from the low-pressure *I*4/*mcm* phase to the cubic $Im\bar{3}$ supercell (< 0.4 GPa) offers a chemically-independent means of reducing $MAPbI_3$ bandgaps, or directing the design of novel organic-inorganic hybrid chemistries. When these two strategies are applied in tandem, the judicious selection of ionic ratios near polymorphic boundaries and the application of relatively low pressures could be deployed to extend the absorption range over the long wavelength region for the future photovoltaic device design.



P (GPa)	Expt. (eV)	B3PW91 + SOC$_{PBE}$ (eV)
~0	1.62	1.67
0.30	1.61	1.62
0.41	1.64	1.58
1.04	1.66	1.67
1.95	1.69	1.74

Figure 4. (a) Measured photoluminescence spectra (right panel) and calculated bandgaps (left panel) of $MAPbI_3$ as a function of compression pressure at room temperature; (b) comparison of bandgaps between the measurement and B3PW91+SOC$_{PBE}$ calculations (also refer to Table S2 in supporting information).

To better understand the atomistic origin of PL in $MAPbI_3$, DFT calculations using the Perdew-Burke-Ernzerhof (PBE)[34] approach were undertaken to optimize atomic positions, including London dispersion (van der Waals attraction) using the empirical D3 correction of Grimme et al.[35] to account for the strong hydrogen bonding between MA cations and the tilted octahedra in $MAPbI_3$.[36] The bandgaps were then calculated using the B3PW91 flavour of DFT, which has been validated to yield bandgaps accurate to ~0.09 eV.[37] Spin-orbit coupling (SOC) makes a significant contribution in the $MAPbI_3$ system and was also included.[38] Due to the rotational disorder of MA, the high symmetry tetragonal and cubic phases were modelled using a 2x2x2 supercell, with two sets of MA cation configurations that are energetically close (Figure S8), and the bandgap results were averaged according to Boltzmann distribution at room temperature (Table S4). The predicted pressure-dependent bandgaps (Figure 4b), decreasing from 1.67 to 1.62 eV up to 0.3 GPa, while increasing from 1.58 to 1.74 eV between 0.4 to 2.0 GPa, are in excellent agreement with the experimental values (1.62 to 1.61 eV, 1.64 to 1.69 eV, respectively). The success of our prediction from averaging over configurations is consistent with the fact that both tetragonal and cubic phases are of thermally averaged structures.



Scheme 1. A schematic illustration of structure transition of $MAPbI_3$ as a function of pressure (not on scale). "PL" represents photoluminescence observation.

In summary, the pressure-induced polymorphism and bandgap tuning of $MAPbI_3$ were investigated using synchrotron XRD, and the trends in bandgap extracted from laser-excited PL spectra compared with the DFT calculations. As illustrated in Scheme 1, $MAPbI_3$ undergoes two high-pressure phase transformations from a tetragonal polymorph (*I*4/*mcm*) at ambient pressure, to a suggested orthorhombic (*Immm*) form (2.7 GPa), through to an ReO_3-type ($Im\bar{3}$) cubic supercell (0.4 - 2.7 GPa), and finally amorphization above 2.7 GPa. Te transition from *I*4/*mcm* to $Im\bar{3}$ leads to a smaller bandgap energy, whereas conversion from the $Im\bar{3}$ polymorph to the suggested *Immm* polymorph reverses this trend. During decompression,

crystallographic restoration was dependent on the peak-pressure achieved. Recovery from 6.4 GPa restored the $Im\bar{3}$ polymorph from the partially amorphized state at ~0.5 GPa. However, from a peak pressure of 3.5 GPa the same structure was recovered at 0.9 GPa due to better preservation of long range order at the 3.5 GPa compared to 6.4 MPa. These studies provide insights into the correlations between structure and bandgap, uncompromised by changes in chemistry. Changes in PCE through the application of external pressure can be mimicked through chemical tailoring, where the introduction of ions in different sizes can effectively modify internal pressure and stabilize new polymorphs. By chemically adjusting hybrid perovskite compositions near to polymorphic boundaries, the application of modest pressure can be sufficient to initiate phase changes and bandgap adjustments. This combined chemical-pressure strategy may prove valuable in design of new perovskites for photovoltaic applications.

Experimental Section

Experimental details and computation results are described in Supporting Information.

Acknowledgements

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Keywords: high pressure • halide perovskite • bandgap • photoluminescence • phase transition

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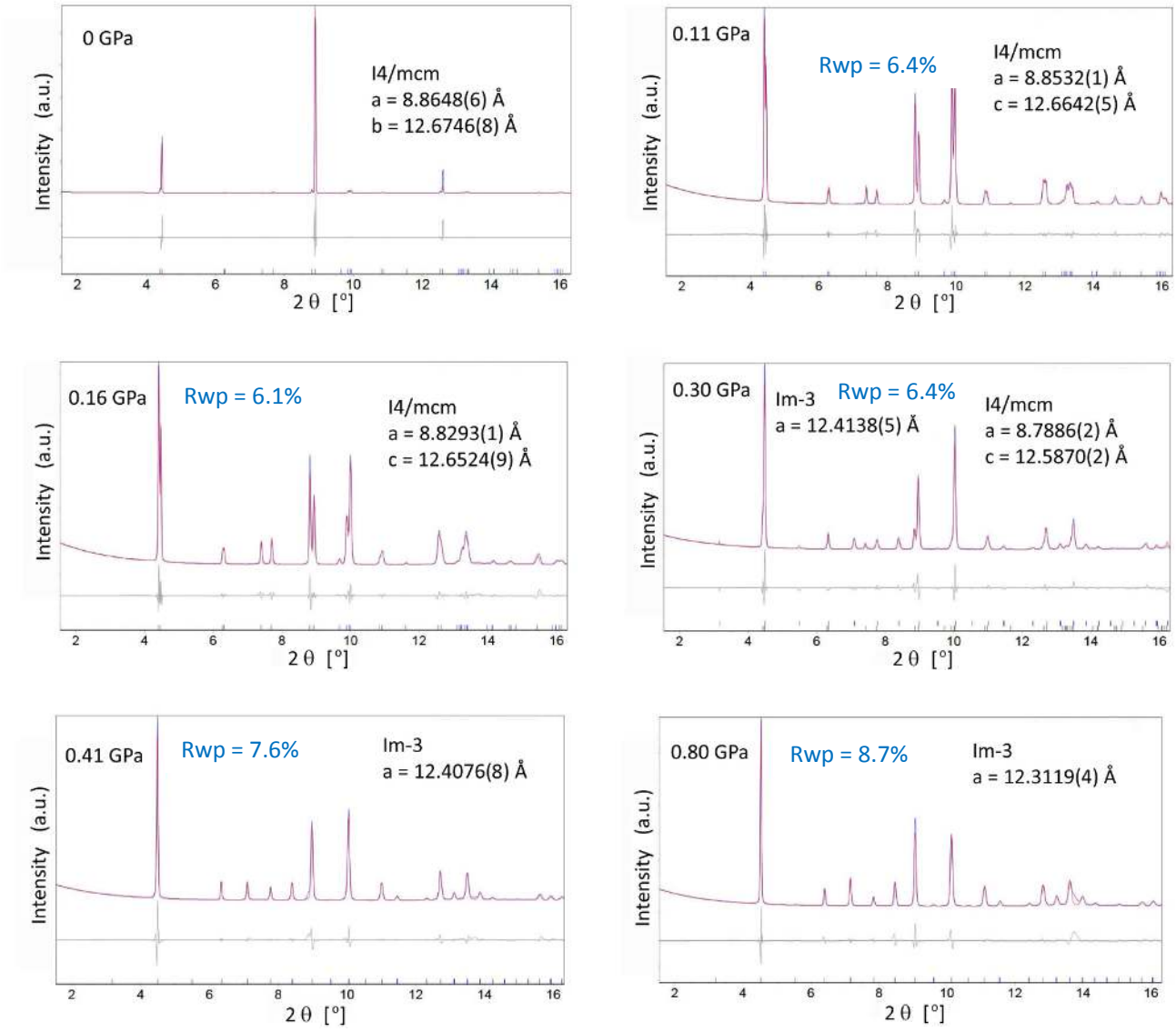
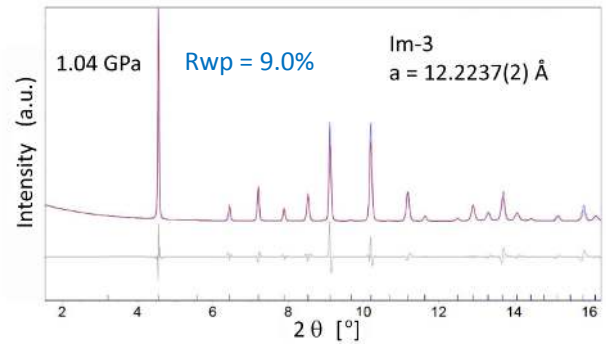
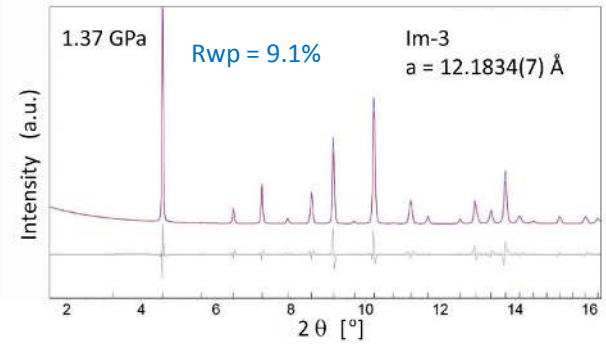
I. Results:

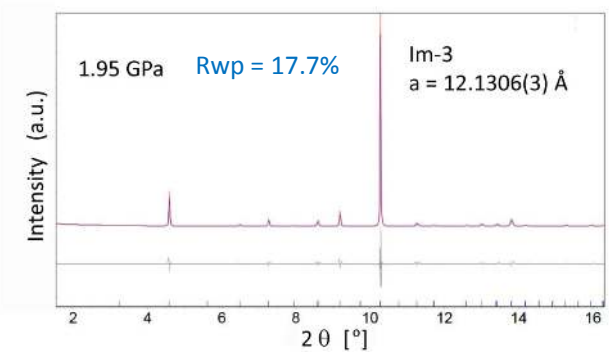
Fig. S1. Lattice parameters of $MAPbI_3$, received from Pawley fitting, during the compression and decompression runs. "Rwp" means R-weighted pattern.[S1] (Peak pressure: 6.4 GPa).

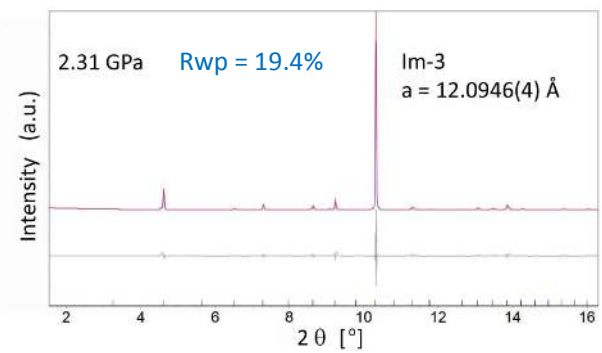
Compression:

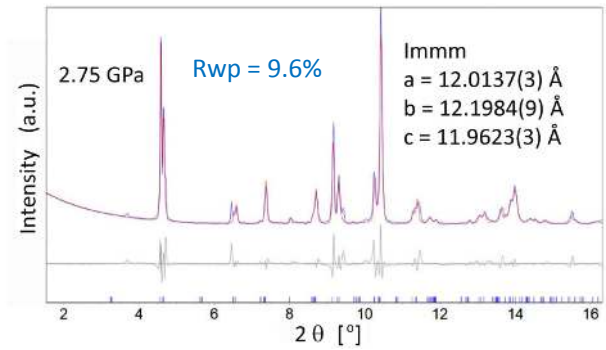


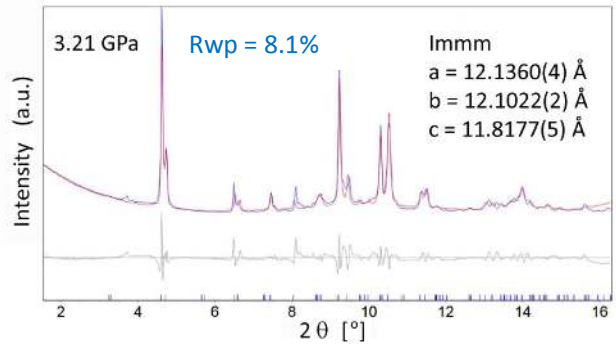




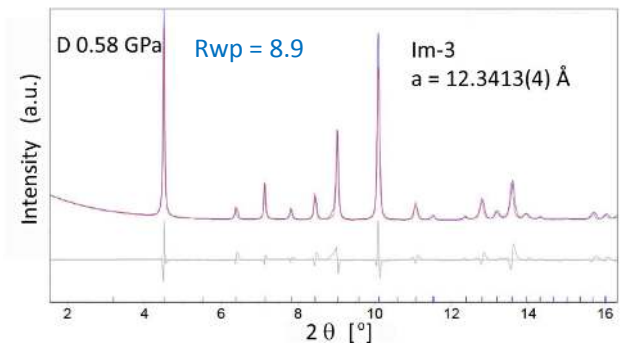








Decompression:



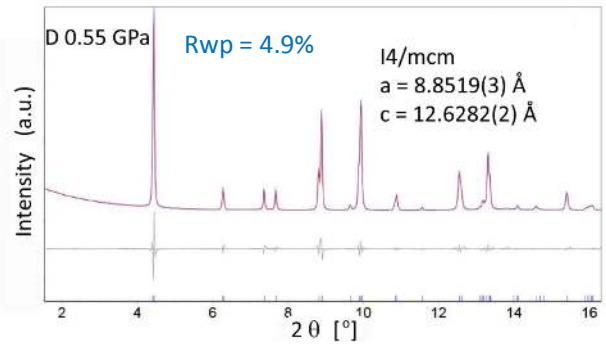
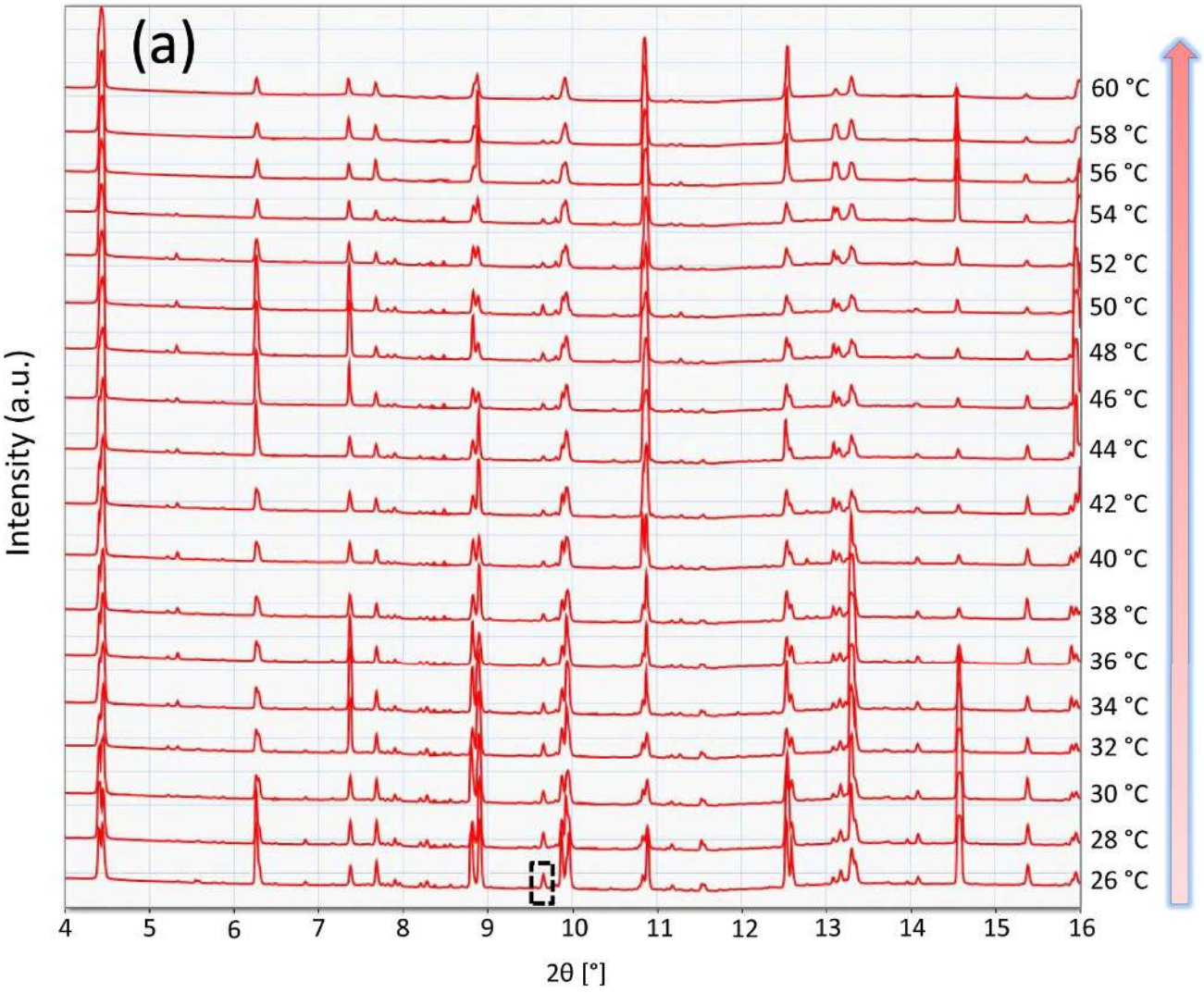


Fig. S2. Integrated synchrotron XRD pattern of $MAPbI_3$ as a function of temperature. (a) Series of patterns recorded at increasing temperatures; (b) series of patterns recorded at decreasing temperatures. The marked peaks in (a) and (b) are attributed to (123) of $MAPbI_3$ tetragonal structure.



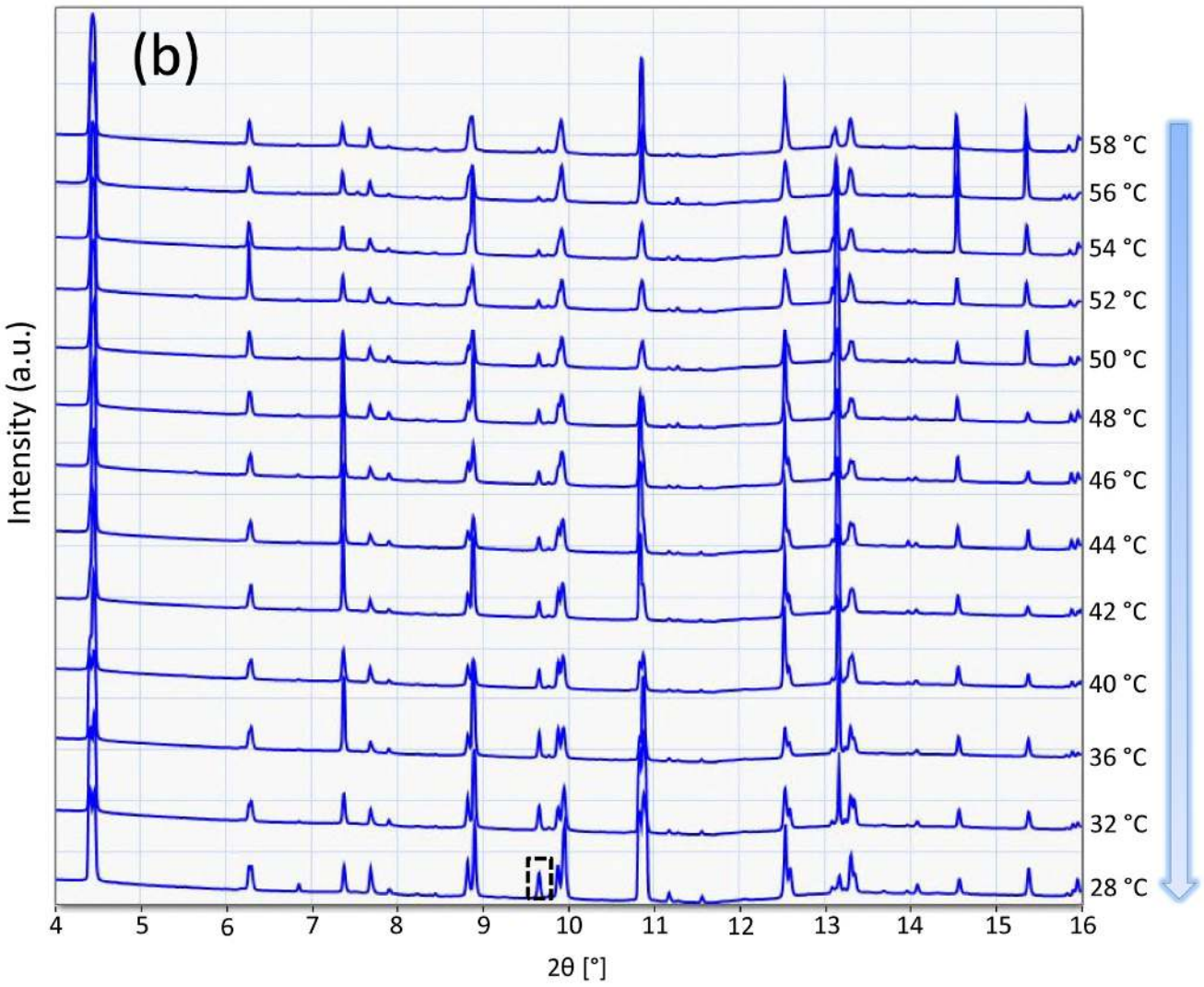
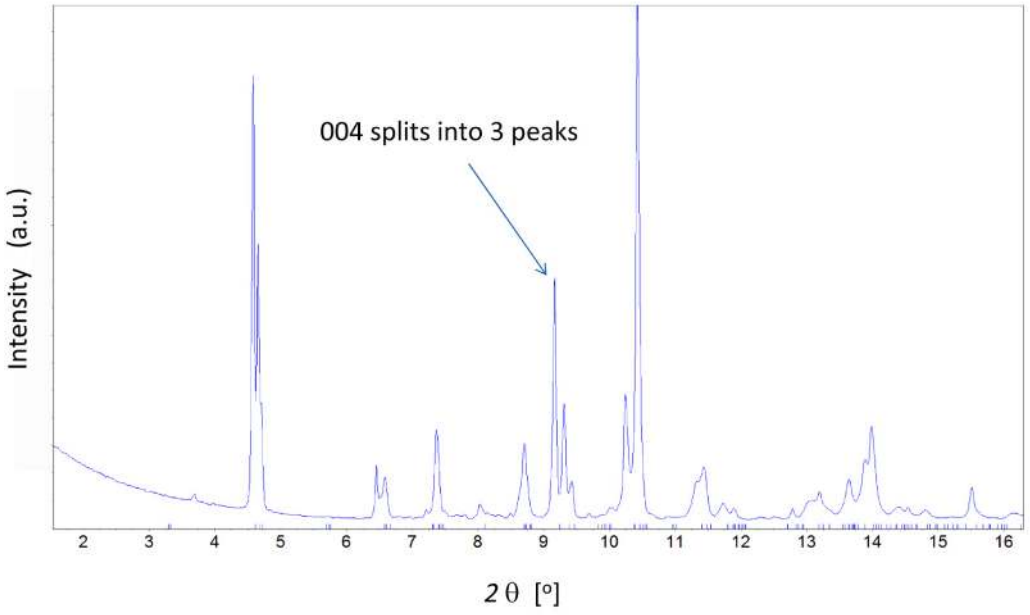

(b)
Intensity (a.u.)
58 °C
56 °C
54 °C
52 °C
50 °C
48 °C
46 °C
44 °C
42 °C
40 °C
36 °C
32 °C
28 °C
4
5
6
7
8
9
10
11
12
13
14
15
16
2θ [°]

Fig. S3. Integrated synchrotron XRD pattern of $MAPbI_3$ at pressure of 2.7_5 GPa (top) and zoon-in patterns under different pressures around $2\theta = 9^o$ (bottom).



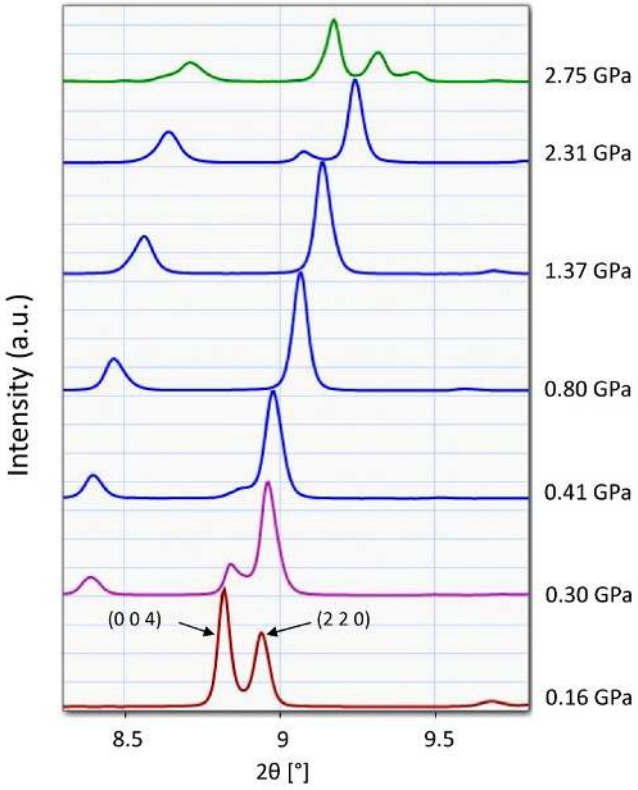


Fig. S4. Additional integrated synchrotron XRD patterns of $MAPbI_3$ (peak pressure: 3.5 GPa) during (a) compression and (b) decompression runs; and its 2D patterns during (c) compression and (d) decompression runs.

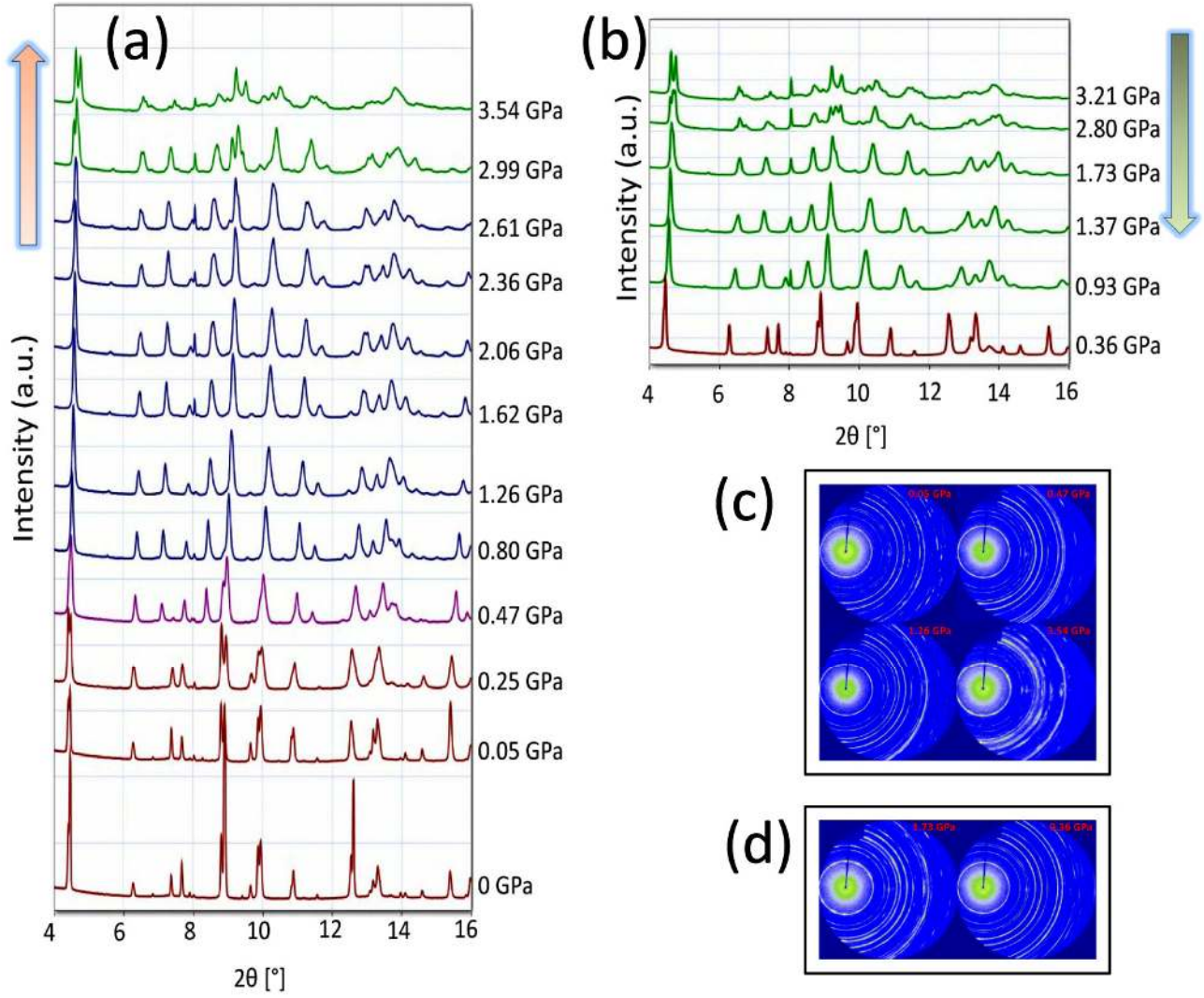
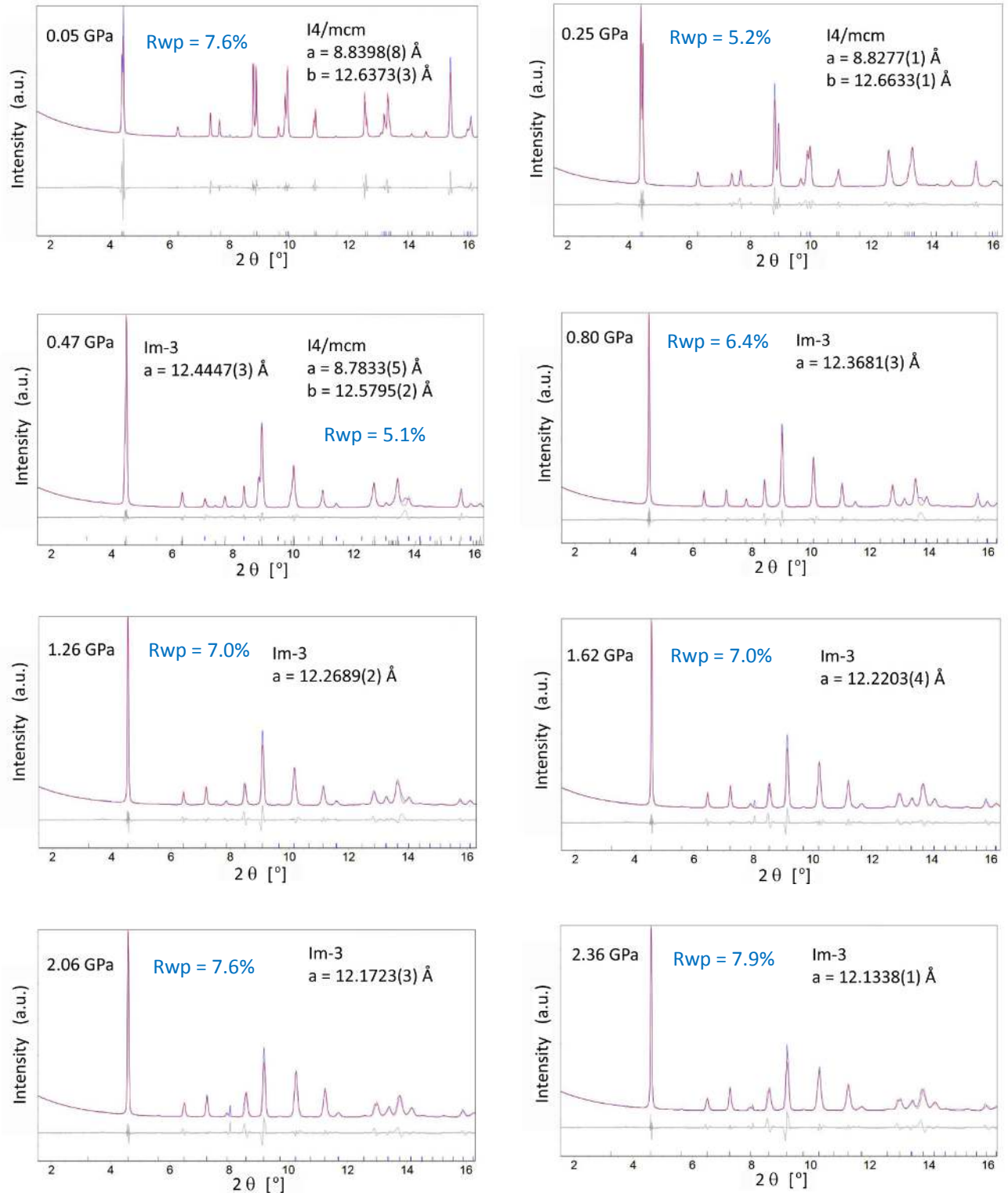
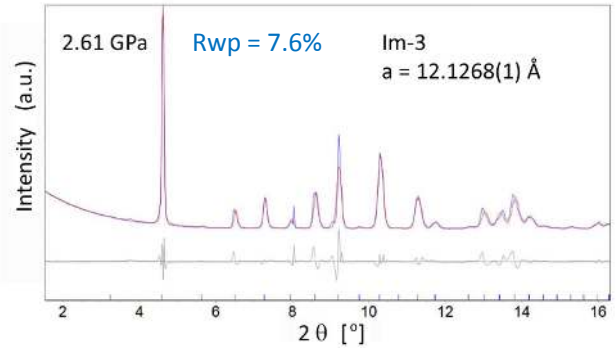
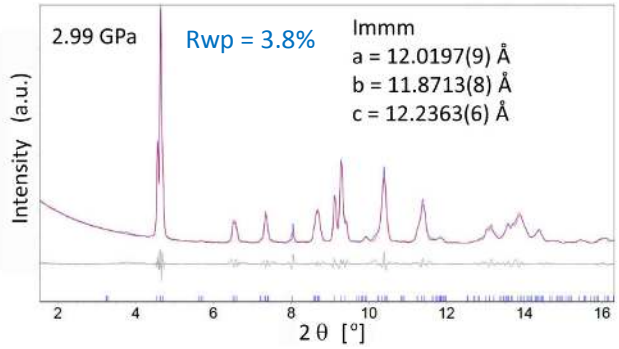


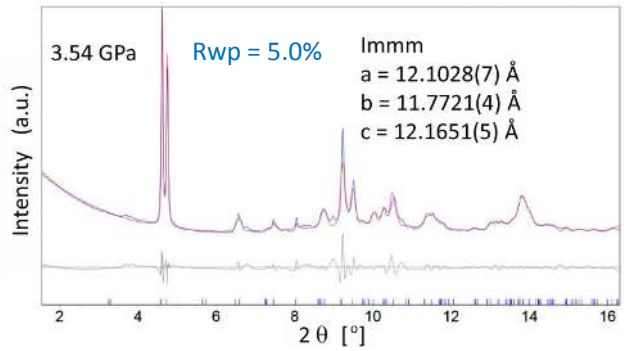
Fig. S5. Lattice parameters of $MAPbI_3$, received from Pawley fitting using data presented in Fig. S4, during the compression and decompression runs. "Rwp" means R-weighted pattern.[S1] (Peak pressure: 3.5 GPa).

Compression:

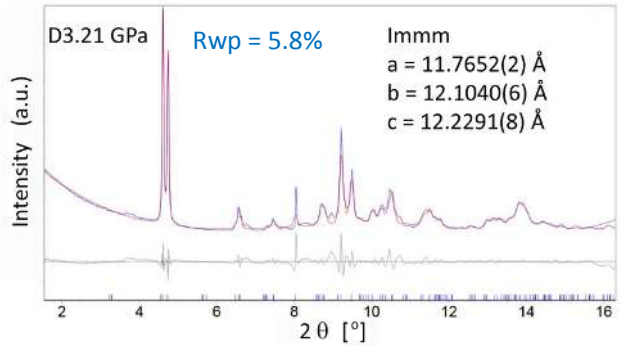


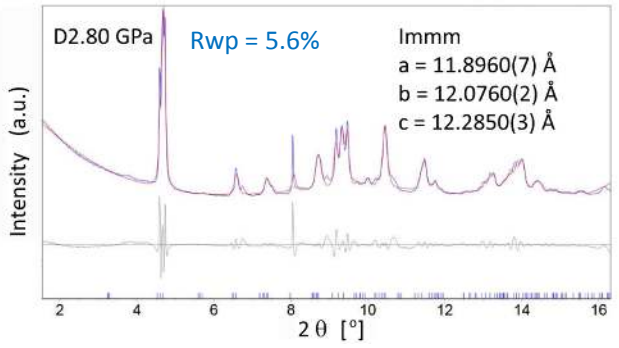

2.61 GPa
Rwp = 7.6%
Im-3
a = 12.1268(1) Å
Intensity (a.u.)
2 θ [°]

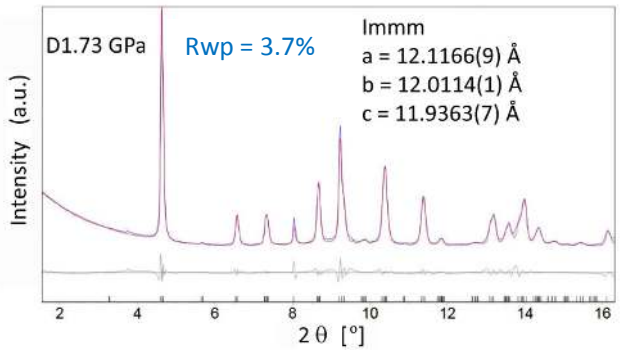

2.99 GPa
Rwp = 3.8%
Immm
a = 12.0197(9) Å
b = 11.8713(8) Å
c = 12.2363(6) Å
Intensity (a.u.)
2 θ [°]

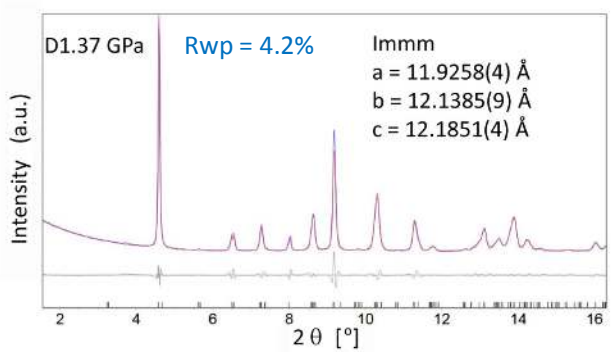

3.54 GPa
Rwp = 5.0%
Immm
a = 12.1028(7) Å
b = 11.7721(4) Å
c = 12.1651(5) Å
Intensity (a.u.)
2 θ [°]

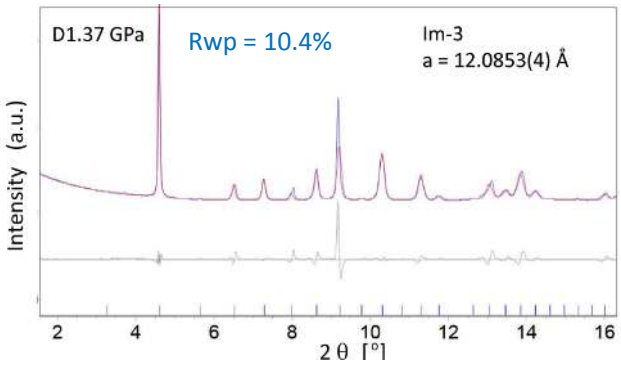
Decompression:

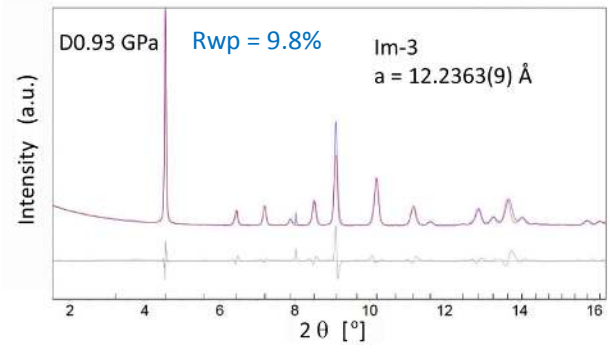












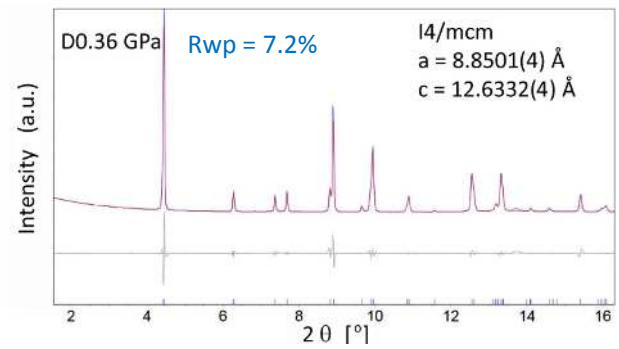


Fig. S6. Plot of unit cell volume calculated from the Pawley fittings as function of the applied pressure in two sets of compressions with different peak pressures.

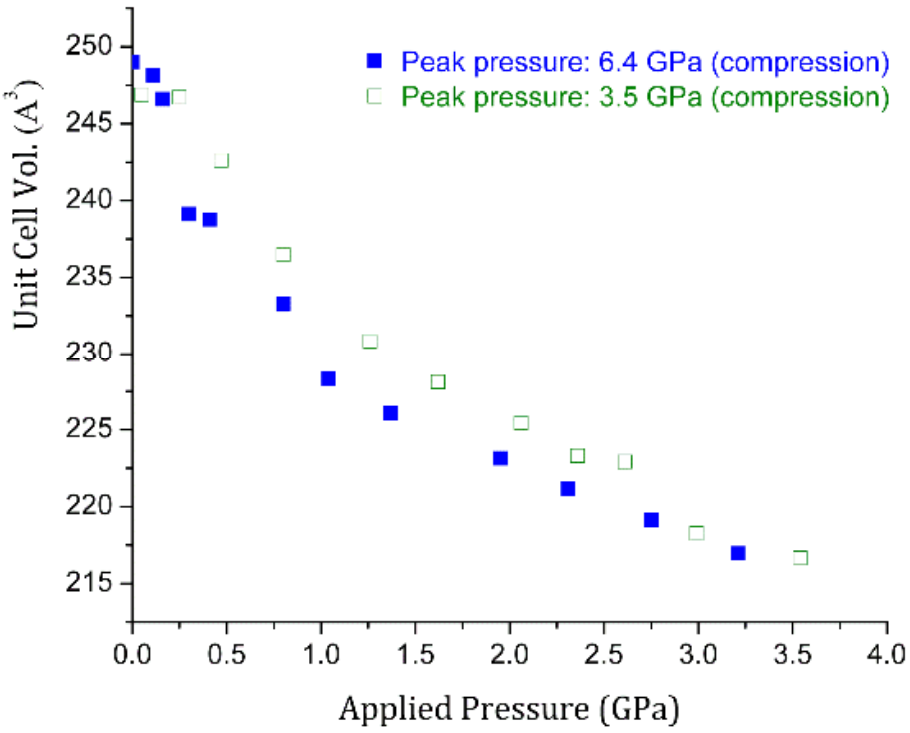


Fig. S7. Optical images of a pressed $MAPbI_3$ sample in DACs under white light. (a), compressed at 0.1_6 GPa; (b), decompressed at 3.7_1 GPa; (c), decompressed at 2.5_5 GPa; (d), decompressed at 1.9_8 GPa; and (e), decompressed to ambient pressure.

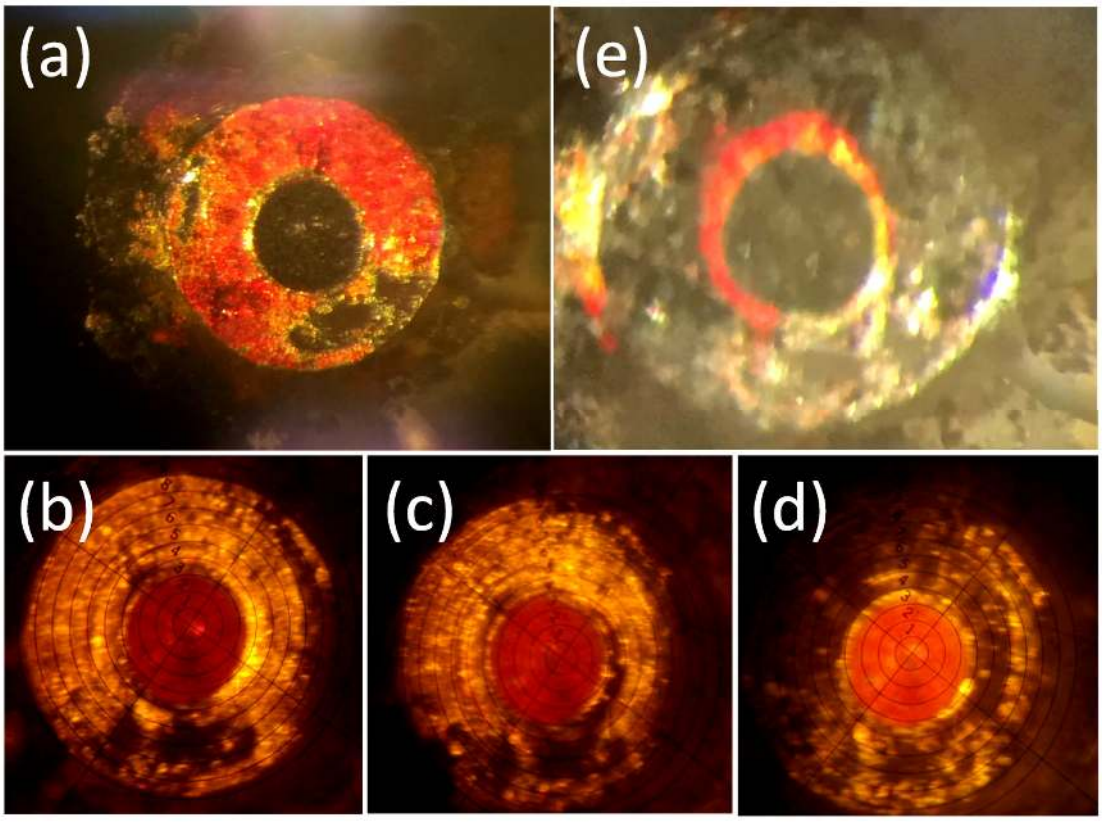


Table S1. Approximate values for the octahedral tilt angles in the cubic $Im\bar{3}$ phase using Rietveld refinements of selected data. The octahedral tilt angle was calculated using the same procedure described by Jorgensen *et al.* [ref.24]

Refined atomic positions for 0.80 GPa data

Site	Np	*x*	*y*	*z*	Atom	Occ.	Beq.
Pb1	8	0.25	0.25	0.25	Pb^{+2}	1	1
I1	24	0	0.2026(9)	0.2717(1)	I^{-1}	1	1
C/N1	2	0	0	0	Al	0.5	20
C/N2	6	0	0.5	0	Al	0.5	20

Refined atomic coordinates for I used to calculate the tilt angle (ϕ), Pb-I bond lengths and octahedral tilt angle for selected pressures.

Pressure	***y***	***z***	**Pb-I**	**ϕ**
0.8	0.2026(9)	0.2717(1)	3.145(2)	14.16
1.04	0.1961(8)	0.2705(1)	3.137(2)	15.44
1.37	0.1958(7)	0.2664(8)	3.121(2)	14.82

Table S2. Optimized CIFs of tetragonal and cubic phases of $MAPbI_3$ under selected pressures.

C H I N Pb

P1_0.00GPa_tetragonal.cif

```
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_cell_length_b                         12.52993
_cell_length_c                         12.69000
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_cell_angle_beta                       90
_cell_angle_gamma                      90
_symmetry_space_group_name_H-M         'P 1'
_symmetry_Int_Tables_number            1

loop_
_symmetry_equiv_pos_as_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   H1          1.0     0.166330      0.293205      0.687173     Biso  1.000000 H
   H2          1.0     0.670187      0.802096      0.665659     Biso  1.000000 H
   H3          1.0     0.327476      0.188924      0.660773     Biso  1.000000 H
   H4          1.0     0.823517      0.690374      0.705330     Biso  1.000000 H
   H5          1.0     0.218981      0.336110      0.812069     Biso  1.000000 H
   H6          1.0     0.617516      0.777672      0.786272     Biso  1.000000 H
   H7          1.0     0.376969      0.230944      0.778388     Biso  1.000000 H
   H8          1.0     0.768351      0.667424      0.834178     Biso  1.000000 H
   H9          1.0     0.186213      0.198282      0.791592     Biso  1.000000 H
   H10         1.0     0.629493      0.678382      0.699345     Biso  1.000000 H
   H11         1.0     0.359017      0.317565      0.679490     Biso  1.000000 H
   H12         1.0     0.810600      0.799069      0.796890     Biso  1.000000 H
   H13         1.0     0.687274      0.302214      0.810723     Biso  1.000000 H
   H14         1.0     0.181878      0.878554      0.733732     Biso  1.000000 H
   H15         1.0     0.753859      0.124531      0.774759     Biso  1.000000 H
   H16         1.0     0.270176      0.751252      0.852404     Biso  1.000000 H
   H17         1.0     0.754952      0.348495      0.694368     Biso  1.000000 H
   H18         1.0     0.232856      0.816125      0.628817     Biso  1.000000 H
   H19         1.0     0.818622      0.168800      0.665280     Biso  1.000000 H
   H20         1.0     0.319769      0.682887      0.737488     Biso  1.000000 H
   H21         1.0     0.830235      0.300248      0.805113     Biso  1.000000 H
   H22         1.0     0.315007      0.877618      0.714341     Biso  1.000000 H
   H23         1.0     0.685539      0.171099      0.668475     Biso  1.000000 H
   H24         1.0     0.178870      0.687057      0.763486     Biso  1.000000 H
   H25         1.0     0.336059      0.219099      0.312480     Biso  1.000000 H
   H26         1.0     0.777860      0.617507      0.286519     Biso  1.000000 H
   H27         1.0     0.230966      0.377040      0.278390     Biso  1.000000 H
   H28         1.0     0.667310      0.768129      0.334311     Biso  1.000000 H
   H29         1.0     0.293381      0.166266      0.187581     Biso  1.000000 H
   H30         1.0     0.801988      0.669991      0.165759     Biso  1.000000 H
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```

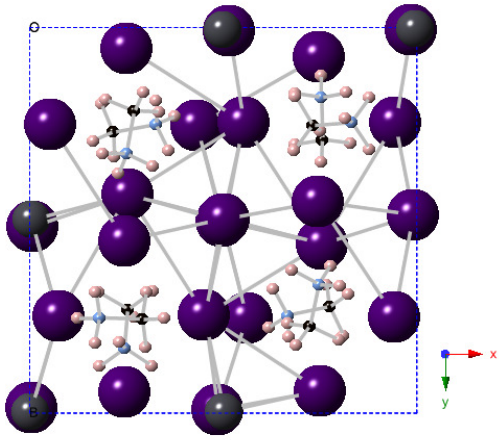

H32	1.0	0.689825	0.823076	0.205288	Biso	1.000000	H
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H34	1.0	0.678422	0.629020	0.199688	Biso	1.000000	H
H35	1.0	0.317809	0.358971	0.179732	Biso	1.000000	H
H36	1.0	0.798752	0.810690	0.296660	Biso	1.000000	H
H37	1.0	0.816770	0.234122	0.128893	Biso	1.000000	H
H38	1.0	0.348666	0.754786	0.194538	Biso	1.000000	H
H39	1.0	0.683533	0.319762	0.238767	Biso	1.000000	H
H40	1.0	0.169083	0.818517	0.164999	Biso	1.000000	H
H41	1.0	0.878983	0.181605	0.233235	Biso	1.000000	H
H42	1.0	0.302145	0.687388	0.310965	Biso	1.000000	H
H43	1.0	0.751451	0.267715	0.352912	Biso	1.000000	H
H44	1.0	0.124555	0.753958	0.274500	Biso	1.000000	H
H45	1.0	0.878117	0.315014	0.215599	Biso	1.000000	H
H46	1.0	0.300269	0.830333	0.305036	Biso	1.000000	H
H47	1.0	0.687180	0.178372	0.262086	Biso	1.000000	H
H48	1.0	0.171310	0.685438	0.168430	Biso	1.000000	H
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C2	1.0	0.756654	0.290994	0.759443	Biso	1.000000	C
C3	1.0	0.271182	0.216592	0.254680	Biso	1.000000	C
C4	1.0	0.291054	0.756656	0.259511	Biso	1.000000	C
C5	1.0	0.775137	0.724298	0.768923	Biso	1.000000	C
C6	1.0	0.254355	0.730912	0.769900	Biso	1.000000	C
C7	1.0	0.724025	0.774942	0.268919	Biso	1.000000	C
C8	1.0	0.731261	0.253595	0.270063	Biso	1.000000	C
N1	1.0	0.666376	0.747029	0.727256	Biso	1.000000	N
N2	1.0	0.245812	0.831650	0.708139	Biso	1.000000	N
N3	1.0	0.747007	0.666154	0.227435	Biso	1.000000	N
N4	1.0	0.832148	0.245880	0.208416	Biso	1.000000	N
N5	1.0	0.326915	0.250766	0.715764	Biso	1.000000	N
N6	1.0	0.753470	0.181249	0.714766	Biso	1.000000	N
N7	1.0	0.250915	0.326903	0.215874	Biso	1.000000	N
N8	1.0	0.181390	0.753441	0.214632	Biso	1.000000	N
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Pb2	1.0	0.005405	0.498359	0.503735	Biso	1.000000	Pb
Pb3	1.0	-0.003163	0.001839	0.004716	Biso	1.000000	Pb
Pb4	1.0	0.499082	0.504473	-0.010048	Biso	1.000000	Pb
Pb5	1.0	0.498527	0.005060	0.003424	Biso	1.000000	Pb
Pb6	1.0	-0.003143	0.503500	-0.006025	Biso	1.000000	Pb
Pb7	1.0	0.001979	-0.003173	0.504717	Biso	1.000000	Pb
Pb8	1.0	0.504994	0.498873	0.489959	Biso	1.000000	Pb
I1	1.0	0.486281	-0.008682	0.751706	Biso	1.000000	I
I2	1.0	0.009363	0.515047	0.750450	Biso	1.000000	I
I3	1.0	-0.014464	0.006180	0.257600	Biso	1.000000	I
I4	1.0	0.501938	0.496439	0.241846	Biso	1.000000	I
I5	1.0	0.514798	0.009530	0.250133	Biso	1.000000	I
I6	1.0	-0.008182	0.486268	0.252066	Biso	1.000000	I
I7	1.0	0.006295	-0.014680	0.757602	Biso	1.000000	I
I8	1.0	0.497183	0.501804	0.741824	Biso	1.000000	I
I9	1.0	0.944951	0.246072	0.513741	Biso	1.000000	I
I10	1.0	0.452590	0.746575	0.513799	Biso	1.000000	I
I11	1.0	0.553213	0.245962	0.522635	Biso	1.000000	I
I12	1.0	0.074824	0.747859	0.480987	Biso	1.000000	I
I13	1.0	0.255124	0.433212	0.483011	Biso	1.000000	I
I14	1.0	0.750750	0.942234	0.534373	Biso	1.000000	I
I15	1.0	0.252294	0.054109	0.515703	Biso	1.000000	I
I16	1.0	0.755054	0.561152	0.496304	Biso	1.000000	I
I17	1.0	0.747612	0.074863	0.981093	Biso	1.000000	I
I18	1.0	0.246136	0.553153	0.022676	Biso	1.000000	I
I19	1.0	0.746750	0.452222	0.014160	Biso	1.000000	I
I20	1.0	0.245782	0.944779	0.013606	Biso	1.000000	I
I21	1.0	0.054265	0.252211	0.015697	Biso	1.000000	I
I22	1.0	0.561127	0.754506	0.996055	Biso	1.000000	I
I23	1.0	0.433115	0.254525	0.982836	Biso	1.000000	I
I24	1.0	0.942195	0.750621	0.034573	Biso	1.000000	I

P4n_0.00GPa_tetragonal.cif

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#======================================================================

# CRYSTAL DATA

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   H3          1.0     0.806429     0.681610     0.338357     Biso  1.000000 H
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   H6          1.0     0.681610     0.193571     0.661643     Biso  1.000000 H
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   H10         1.0     0.877665     0.271498     0.222601     Biso  1.000000 H
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   H14         1.0     0.622335     0.228502     0.777399     Biso  1.000000 H
   H15         1.0     0.728502     0.877665     0.777399     Biso  1.000000 H
   H16         1.0     0.271498     0.122335     0.777399     Biso  1.000000 H
   H17         1.0     0.160825     0.822237     0.308807     Biso  1.000000 H
   H18         1.0     0.839175     0.177763     0.308807     Biso  1.000000 H
   H19         1.0     0.677763     0.660825     0.308807     Biso  1.000000 H
   H20         1.0     0.322237     0.339175     0.308807     Biso  1.000000 H
   H21         1.0     0.339175     0.677763     0.691193     Biso  1.000000 H
   H22         1.0     0.660825     0.322237     0.691193     Biso  1.000000 H
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   H26         1.0     0.717008     0.191565     0.157760     Biso  1.000000 H
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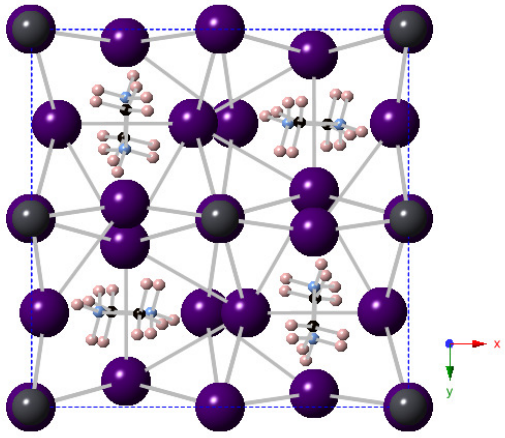

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H42	1.0	0.652731	0.219540	0.281380	Biso	1.000000	H
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H45	1.0	0.152731	0.719540	0.718620	Biso	1.000000	H
H46	1.0	0.847269	0.280460	0.718620	Biso	1.000000	H
H47	1.0	0.780460	0.652731	0.718620	Biso	1.000000	H
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N3	1.0	0.751091	0.681354	0.277070	Biso	1.000000	N
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N7	1.0	0.748909	0.818646	0.722930	Biso	1.000000	N
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Pb5	1.0	0.500000	0.000000	0.482956	Biso	1.000000	Pb
Pb6	1.0	0.000000	0.500000	0.517044	Biso	1.000000	Pb
Pb7	1.0	0.000000	0.000000	-0.000000	Biso	1.000000	Pb
Pb8	1.0	0.500000	0.500000	-0.000000	Biso	1.000000	Pb
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I3	1.0	0.250510	0.931330	0.502664	Biso	1.000000	I
I4	1.0	0.749490	0.068670	0.502664	Biso	1.000000	I
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I6	1.0	0.931330	0.749490	0.497336	Biso	1.000000	I
I7	1.0	0.249490	0.568670	0.497336	Biso	1.000000	I
I8	1.0	0.750510	0.431330	0.497336	Biso	1.000000	I
I9	1.0	0.249898	0.036436	0.965710	Biso	1.000000	I
I10	1.0	0.750102	0.963564	0.965710	Biso	1.000000	I
I11	1.0	0.463564	0.749898	0.965710	Biso	1.000000	I
I12	1.0	0.536436	0.250102	0.965710	Biso	1.000000	I
I13	1.0	0.250102	0.463564	0.034290	Biso	1.000000	I
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I15	1.0	0.036436	0.750102	0.034290	Biso	1.000000	I
I16	1.0	0.963564	0.249898	0.034290	Biso	1.000000	I
I17	1.0	0.500000	0.000000	0.237231	Biso	1.000000	I
I18	1.0	0.000000	0.500000	0.762769	Biso	1.000000	I
I19	1.0	0.000000	0.000000	0.747113	Biso	1.000000	I
I20	1.0	0.500000	0.500000	0.747113	Biso	1.000000	I
I21	1.0	0.500000	0.500000	0.252887	Biso	1.000000	I
I22	1.0	0.000000	0.000000	0.252887	Biso	1.000000	I
I23	1.0	0.000000	0.500000	0.266156	Biso	1.000000	I
I24	1.0	0.500000	0.000000	0.733844	Biso	1.000000	I

P1_0.30GPa_tetragonal.cif

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# CRYSTAL DATA

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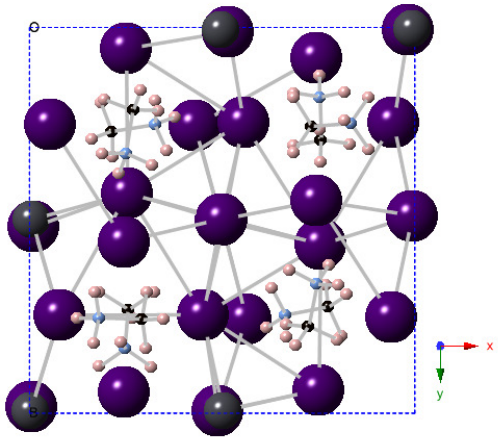

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H40	1.0	0.166898	0.819062	0.167273	Biso	1.000000	H
H41	1.0	0.879550	0.181913	0.233928	Biso	1.000000	H
H42	1.0	0.304364	0.687273	0.311250	Biso	1.000000	H
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H44	1.0	0.124727	0.753494	0.278430	Biso	1.000000	H
H45	1.0	0.880842	0.316925	0.220739	Biso	1.000000	H
H46	1.0	0.302086	0.831251	0.305562	Biso	1.000000	H
H47	1.0	0.685798	0.181516	0.262189	Biso	1.000000	H
H48	1.0	0.169792	0.684962	0.170583	Biso	1.000000	H
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C3	1.0	0.269036	0.214521	0.254140	Biso	1.000000	C
C4	1.0	0.291995	0.757077	0.259767	Biso	1.000000	C
C5	1.0	0.775364	0.724936	0.772303	Biso	1.000000	C
C6	1.0	0.256655	0.731989	0.773519	Biso	1.000000	C
C7	1.0	0.724591	0.775327	0.272177	Biso	1.000000	C
C8	1.0	0.732018	0.255686	0.273374	Biso	1.000000	C
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N3	1.0	0.746298	0.665283	0.231054	Biso	1.000000	N
N4	1.0	0.833422	0.248272	0.211143	Biso	1.000000	N
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N7	1.0	0.251192	0.325978	0.215154	Biso	1.000000	N
N8	1.0	0.180662	0.753502	0.216882	Biso	1.000000	N
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Pb2	1.0	0.006540	0.497332	0.505904	Biso	1.000000	Pb
Pb3	1.0	-0.005090	0.002117	0.006568	Biso	1.000000	Pb
Pb4	1.0	0.498088	0.505395	-0.008205	Biso	1.000000	Pb
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Pb7	1.0	0.002249	-0.004962	0.506590	Biso	1.000000	Pb
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I2	1.0	0.010718	0.516262	0.751559	Biso	1.000000	I
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I8	1.0	0.497104	0.500535	0.743447	Biso	1.000000	I
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I12	1.0	0.078214	0.746622	0.484095	Biso	1.000000	I
I13	1.0	0.255363	0.429361	0.484411	Biso	1.000000	I
I14	1.0	0.750818	0.939420	0.535922	Biso	1.000000	I
I15	1.0	0.252222	0.054375	0.514869	Biso	1.000000	I
I16	1.0	0.755518	0.562472	0.499965	Biso	1.000000	I
I17	1.0	0.746601	0.077681	0.984221	Biso	1.000000	I
I18	1.0	0.245936	0.555334	0.022960	Biso	1.000000	I
I19	1.0	0.746052	0.449532	0.016228	Biso	1.000000	I
I20	1.0	0.245206	0.945024	0.014993	Biso	1.000000	I
I21	1.0	0.054554	0.252155	0.014746	Biso	1.000000	I
I22	1.0	0.562391	0.755009	0.999847	Biso	1.000000	I
I23	1.0	0.429514	0.254929	0.984328	Biso	1.000000	I
I24	1.0	0.939465	0.750700	0.035991	Biso	1.000000	I

P4n_0.30GPa_tetragonal.cif

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   H5          1.0     0.319112     0.808196     0.664110     Biso  1.000000 H
   H6          1.0     0.680888     0.191804     0.664110     Biso  1.000000 H
   H7          1.0     0.691804     0.819112     0.664110     Biso  1.000000 H
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   H18         1.0     0.846469     0.178522     0.312066     Biso  1.000000 H
   H19         1.0     0.678522     0.653531     0.312066     Biso  1.000000 H
   H20         1.0     0.321478     0.346469     0.312066     Biso  1.000000 H
   H21         1.0     0.346469     0.678522     0.687934     Biso  1.000000 H
   H22         1.0     0.653531     0.321478     0.687934     Biso  1.000000 H
   H23         1.0     0.821478     0.846469     0.687934     Biso  1.000000 H
   H24         1.0     0.178522     0.153531     0.687934     Biso  1.000000 H
   H25         1.0     0.273631     0.822640     0.159167     Biso  1.000000 H
   H26         1.0     0.726369     0.177360     0.159167     Biso  1.000000 H
   H27         1.0     0.677360     0.773631     0.159167     Biso  1.000000 H
   H28         1.0     0.322640     0.226369     0.159167     Biso  1.000000 H
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   H31         1.0     0.822640     0.726369     0.840833     Biso  1.000000 H
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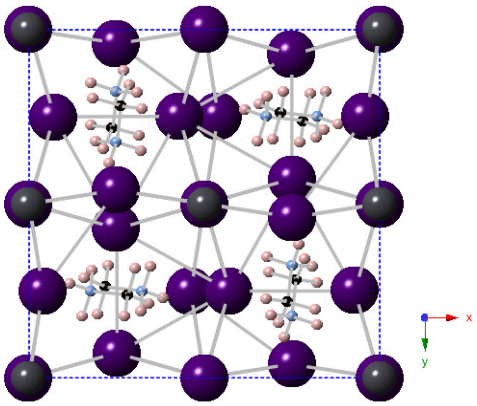

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H42	1.0	0.657051	0.213817	0.279005	Biso	1.000000	H
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H45	1.0	0.157051	0.713817	0.720995	Biso	1.000000	H
H46	1.0	0.842949	0.286183	0.720995	Biso	1.000000	H
H47	1.0	0.786183	0.657051	0.720995	Biso	1.000000	H
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C3	1.0	0.738409	0.781841	0.221292	Biso	1.000000	C
C4	1.0	0.261591	0.218160	0.221292	Biso	1.000000	C
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C6	1.0	0.781841	0.261591	0.778708	Biso	1.000000	C
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C8	1.0	0.238409	0.281841	0.778708	Biso	1.000000	C
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Pb5	1.0	0.500000	0.000000	0.485367	Biso	1.000000	Pb
Pb6	1.0	-0.000000	0.500000	0.514633	Biso	1.000000	Pb
Pb7	1.0	-0.000000	0.000000	-0.000000	Biso	1.000000	Pb
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I2	1.0	0.571300	0.750305	0.502562	Biso	1.000000	I
I3	1.0	0.250305	0.928700	0.502562	Biso	1.000000	I
I4	1.0	0.749695	0.071300	0.502562	Biso	1.000000	I
I5	1.0	0.071300	0.250305	0.497438	Biso	1.000000	I
I6	1.0	0.928700	0.749695	0.497438	Biso	1.000000	I
I7	1.0	0.249695	0.571300	0.497438	Biso	1.000000	I
I8	1.0	0.750305	0.428700	0.497438	Biso	1.000000	I
I9	1.0	0.249978	0.039058	0.972936	Biso	1.000000	I
I10	1.0	0.750022	0.960942	0.972936	Biso	1.000000	I
I11	1.0	0.460942	0.749978	0.972936	Biso	1.000000	I
I12	1.0	0.539058	0.250022	0.972936	Biso	1.000000	I
I13	1.0	0.250022	0.460942	0.027064	Biso	1.000000	I
I14	1.0	0.749978	0.539058	0.027064	Biso	1.000000	I
I15	1.0	0.039058	0.750022	0.027064	Biso	1.000000	I
I16	1.0	0.960942	0.249978	0.027064	Biso	1.000000	I
I17	1.0	0.500000	0.000000	0.240346	Biso	1.000000	I
I18	1.0	-0.000000	0.500000	0.759654	Biso	1.000000	I
I19	1.0	-0.000000	0.000000	0.747784	Biso	1.000000	I
I20	1.0	0.500000	0.500000	0.747784	Biso	1.000000	I
I21	1.0	0.500000	0.500000	0.252216	Biso	1.000000	I
I22	1.0	-0.000000	0.000000	0.252216	Biso	1.000000	I
I23	1.0	-0.000000	0.500000	0.262606	Biso	1.000000	I
I24	1.0	0.500000	0.000000	0.737394	Biso	1.000000	I

P1_0.41GPa_tetragonal.cif

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# CRYSTAL DATA

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_symmetry_Int_Tables_number            1

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   H7          1.0     0.378726      0.233000      0.782873     Biso  1.000000 H
   H8          1.0     0.774079      0.668284      0.831001     Biso  1.000000 H
   H9          1.0     0.187975      0.195706      0.797038     Biso  1.000000 H
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   H25         1.0     0.335635      0.217335      0.317636     Biso  1.000000 H
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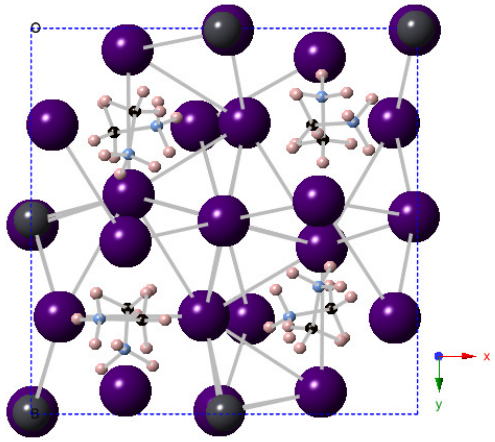

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H41	1.0	0.882832	0.183561	0.243058	Biso	1.000000	H
H42	1.0	0.300584	0.686138	0.311548	Biso	1.000000	H
H43	1.0	0.743169	0.272266	0.351351	Biso	1.000000	H
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H45	1.0	0.876309	0.316398	0.216906	Biso	1.000000	H
H46	1.0	0.298837	0.830454	0.307312	Biso	1.000000	H
H47	1.0	0.688950	0.171508	0.263887	Biso	1.000000	H
H48	1.0	0.168928	0.685531	0.168101	Biso	1.000000	H
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C4	1.0	0.289604	0.756693	0.260472	Biso	1.000000	C
C5	1.0	0.778949	0.727558	0.766682	Biso	1.000000	C
C6	1.0	0.250895	0.727675	0.768069	Biso	1.000000	C
C7	1.0	0.727319	0.778819	0.266652	Biso	1.000000	C
C8	1.0	0.728483	0.250353	0.268253	Biso	1.000000	C
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Pb3	1.0	-0.003677	0.002342	0.004832	Biso	1.000000	Pb
Pb4	1.0	0.499562	0.504387	-0.010446	Biso	1.000000	Pb
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I2	1.0	0.006291	0.510162	0.750889	Biso	1.000000	I
I3	1.0	-0.006841	0.004709	0.257439	Biso	1.000000	I
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I11	1.0	0.554606	0.246576	0.522265	Biso	1.000000	I
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I14	1.0	0.750872	0.942218	0.531598	Biso	1.000000	I
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I16	1.0	0.754193	0.566120	0.494885	Biso	1.000000	I
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I18	1.0	0.246644	0.554507	0.022442	Biso	1.000000	I
I19	1.0	0.746936	0.447827	0.015101	Biso	1.000000	I
I20	1.0	0.246179	0.939244	0.007532	Biso	1.000000	I
I21	1.0	0.058028	0.251693	0.018416	Biso	1.000000	I
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I23	1.0	0.430647	0.253582	0.987046	Biso	1.000000	I
I24	1.0	0.942145	0.750726	0.031814	Biso	1.000000	I

P4n_0.41GPa_tetragonal.cif

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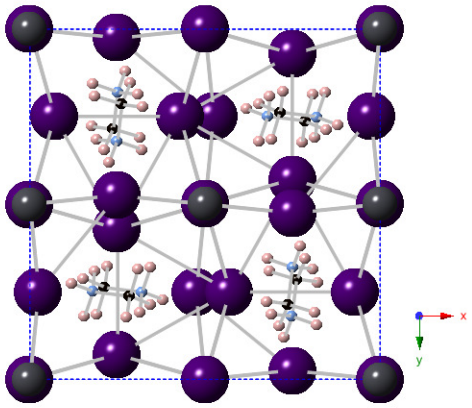

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H38	1.0	0.808344	0.185288	0.817100	Biso	1.000000	H
H39	1.0	0.685288	0.691656	0.817100	Biso	1.000000	H
H40	1.0	0.314712	0.308344	0.817100	Biso	1.000000	H
H41	1.0	0.346038	0.787772	0.276840	Biso	1.000000	H
H42	1.0	0.653962	0.212228	0.276840	Biso	1.000000	H
H43	1.0	0.712228	0.846038	0.276840	Biso	1.000000	H
H44	1.0	0.287772	0.153962	0.276840	Biso	1.000000	H
H45	1.0	0.153962	0.712228	0.723160	Biso	1.000000	H
H46	1.0	0.846038	0.287772	0.723160	Biso	1.000000	H
H47	1.0	0.787772	0.653962	0.723160	Biso	1.000000	H
H48	1.0	0.212228	0.346038	0.723160	Biso	1.000000	H
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C2	1.0	0.714377	0.237538	0.218550	Biso	1.000000	C
C3	1.0	0.737538	0.785623	0.218550	Biso	1.000000	C
C4	1.0	0.262462	0.214377	0.218550	Biso	1.000000	C
C5	1.0	0.214377	0.737538	0.781450	Biso	1.000000	C
C6	1.0	0.785623	0.262462	0.781450	Biso	1.000000	C
C7	1.0	0.762462	0.714377	0.781450	Biso	1.000000	C
C8	1.0	0.237538	0.285623	0.781450	Biso	1.000000	C
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N6	1.0	0.680050	0.249418	0.726672	Biso	1.000000	N
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Pb2	1.0	0.500000	0.500000	0.500000	Biso	1.000000	Pb
Pb3	1.0	0.500000	0.000000	-0.005177	Biso	1.000000	Pb
Pb4	1.0	-0.000000	0.500000	0.005177	Biso	1.000000	Pb
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Pb6	1.0	-0.000000	0.500000	0.512894	Biso	1.000000	Pb
Pb7	1.0	-0.000000	0.000000	0.000000	Biso	1.000000	Pb
Pb8	1.0	0.500000	0.500000	0.000000	Biso	1.000000	Pb
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I2	1.0	0.570846	0.749986	0.504921	Biso	1.000000	I
I3	1.0	0.249986	0.929154	0.504921	Biso	1.000000	I
I4	1.0	0.750014	0.070846	0.504921	Biso	1.000000	I
I5	1.0	0.070846	0.249986	0.495079	Biso	1.000000	I
I6	1.0	0.929154	0.750014	0.495079	Biso	1.000000	I
I7	1.0	0.250014	0.570846	0.495079	Biso	1.000000	I
I8	1.0	0.749986	0.429154	0.495079	Biso	1.000000	I
I9	1.0	0.249996	0.025098	0.966354	Biso	1.000000	I
I10	1.0	0.750004	0.974902	0.966354	Biso	1.000000	I
I11	1.0	0.474902	0.749996	0.966354	Biso	1.000000	I
I12	1.0	0.525098	0.250004	0.966354	Biso	1.000000	I
I13	1.0	0.250004	0.474902	0.033646	Biso	1.000000	I
I14	1.0	0.749996	0.525098	0.033646	Biso	1.000000	I
I15	1.0	0.025098	0.750004	0.033646	Biso	1.000000	I
I16	1.0	0.974902	0.249996	0.033646	Biso	1.000000	I
I17	1.0	0.500000	0.000000	0.240442	Biso	1.000000	I
I18	1.0	-0.000000	0.500000	0.759558	Biso	1.000000	I
I19	1.0	-0.000000	0.000000	0.747636	Biso	1.000000	I
I20	1.0	0.500000	0.500000	0.747636	Biso	1.000000	I
I21	1.0	0.500000	0.500000	0.252364	Biso	1.000000	I
I22	1.0	-0.000000	0.000000	0.252364	Biso	1.000000	I
I23	1.0	-0.000000	0.500000	0.262106	Biso	1.000000	I
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P1_0.41GPa_cubic.cif

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# CRYSTAL DATA

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   H3          1.0     0.329637      0.190465      0.663034     Biso  1.000000 H
   H4          1.0     0.830452      0.697737      0.701550     Biso  1.000000 H
   H5          1.0     0.216903      0.335564      0.818359     Biso  1.000000 H
   H6          1.0     0.618221      0.774174      0.784518     Biso  1.000000 H
   H7          1.0     0.378915      0.234094      0.783284     Biso  1.000000 H
   H8          1.0     0.774682      0.668215      0.831793     Biso  1.000000 H
   H9          1.0     0.188237      0.195376      0.798284     Biso  1.000000 H
   H10         1.0     0.635492      0.677053      0.692764     Biso  1.000000 H
   H11         1.0     0.357753      0.321187      0.682283     Biso  1.000000 H
   H12         1.0     0.811366      0.804019      0.798010     Biso  1.000000 H
   H13         1.0     0.685853      0.300701      0.811928     Biso  1.000000 H
   H14         1.0     0.186256      0.882898      0.746835     Biso  1.000000 H
   H15         1.0     0.754400      0.121816      0.775635     Biso  1.000000 H
   H16         1.0     0.277231      0.740734      0.851329     Biso  1.000000 H
   H17         1.0     0.755814      0.348043      0.694269     Biso  1.000000 H
   H18         1.0     0.222465      0.822882      0.632138     Biso  1.000000 H
   H19         1.0     0.820035      0.166879      0.664088     Biso  1.000000 H
   H20         1.0     0.308740      0.676012      0.725413     Biso  1.000000 H
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   H25         1.0     0.335534      0.217045      0.318749     Biso  1.000000 H
   H26         1.0     0.774265      0.618188      0.284568     Biso  1.000000 H
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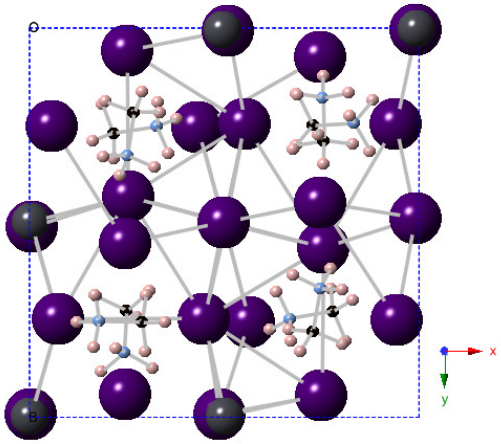

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H40	1.0	0.167069	0.819857	0.163824	Biso	1.000000	H
H41	1.0	0.883006	0.184695	0.244878	Biso	1.000000	H
H42	1.0	0.300665	0.686045	0.312220	Biso	1.000000	H
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H46	1.0	0.298910	0.830440	0.308108	Biso	1.000000	H
H47	1.0	0.688918	0.171032	0.264635	Biso	1.000000	H
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C2	1.0	0.756648	0.289667	0.760498	Biso	1.000000	C
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C4	1.0	0.289721	0.756699	0.260576	Biso	1.000000	C
C5	1.0	0.779448	0.727824	0.766917	Biso	1.000000	C
C6	1.0	0.250804	0.727060	0.768309	Biso	1.000000	C
C7	1.0	0.727588	0.779311	0.266909	Biso	1.000000	C
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N2	1.0	0.244297	0.832879	0.712353	Biso	1.000000	N
N3	1.0	0.746794	0.669155	0.223886	Biso	1.000000	N
N4	1.0	0.833549	0.244326	0.212258	Biso	1.000000	N
N5	1.0	0.327608	0.252685	0.719403	Biso	1.000000	N
N6	1.0	0.754059	0.179165	0.714409	Biso	1.000000	N
N7	1.0	0.252775	0.327594	0.219529	Biso	1.000000	N
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Pb2	1.0	0.004693	0.497348	0.504126	Biso	1.000000	Pb
Pb3	1.0	-0.003682	0.002775	0.005035	Biso	1.000000	Pb
Pb4	1.0	0.499876	0.504736	-0.009954	Biso	1.000000	Pb
Pb5	1.0	0.497219	0.004486	0.003734	Biso	1.000000	Pb
Pb6	1.0	-0.003254	0.502360	-0.004167	Biso	1.000000	Pb
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Pb8	1.0	0.505057	0.499903	0.490069	Biso	1.000000	Pb
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I2	1.0	0.006309	0.510732	0.750915	Biso	1.000000	I
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I4	1.0	0.500082	0.498765	0.241939	Biso	1.000000	I
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I9	1.0	0.941234	0.246441	0.507582	Biso	1.000000	I
I10	1.0	0.449097	0.747108	0.514953	Biso	1.000000	I
I11	1.0	0.553539	0.246602	0.521662	Biso	1.000000	I
I12	1.0	0.074696	0.747715	0.484621	Biso	1.000000	I
I13	1.0	0.254285	0.432750	0.488415	Biso	1.000000	I
I14	1.0	0.751032	0.942896	0.530864	Biso	1.000000	I
I15	1.0	0.251932	0.056943	0.517419	Biso	1.000000	I
I16	1.0	0.754543	0.564366	0.495560	Biso	1.000000	I
I17	1.0	0.747575	0.074643	0.984579	Biso	1.000000	I
I18	1.0	0.246630	0.553335	0.021884	Biso	1.000000	I
I19	1.0	0.747109	0.448749	0.015052	Biso	1.000000	I
I20	1.0	0.246258	0.940673	0.006895	Biso	1.000000	I
I21	1.0	0.057198	0.251762	0.017333	Biso	1.000000	I
I22	1.0	0.564233	0.754274	0.995365	Biso	1.000000	I
I23	1.0	0.432490	0.254023	0.988328	Biso	1.000000	I
I24	1.0	0.942879	0.750802	0.031061	Biso	1.000000	I

P4n_0.41GPa_cubic.cif

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# CRYSTAL DATA

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   H5          1.0     0.319790      0.809408      0.664375     Biso  1.000000 H
   H6          1.0     0.680210      0.190592      0.664375     Biso  1.000000 H
   H7          1.0     0.690592      0.819790      0.664375     Biso  1.000000 H
   H8          1.0     0.309408      0.180210      0.664375     Biso  1.000000 H
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   H29         1.0     0.227090      0.675267      0.841776     Biso  1.000000 H
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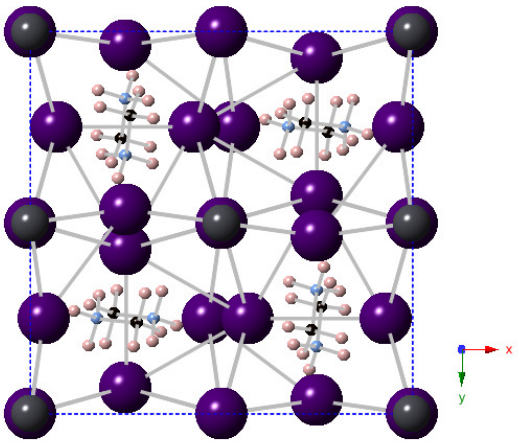

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H37	1.0	0.198854	0.814987	0.818340	Biso	1.000000	H
H38	1.0	0.801145	0.185013	0.818340	Biso	1.000000	H
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H44	1.0	0.284740	0.157010	0.278417	Biso	1.000000	H
H45	1.0	0.157010	0.715260	0.721583	Biso	1.000000	H
H46	1.0	0.842990	0.284740	0.721583	Biso	1.000000	H
H47	1.0	0.784740	0.657010	0.721583	Biso	1.000000	H
H48	1.0	0.215260	0.342990	0.721583	Biso	1.000000	H
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C3	1.0	0.737959	0.781021	0.219819	Biso	1.000000	C
C4	1.0	0.262041	0.218979	0.219819	Biso	1.000000	C
C5	1.0	0.218979	0.737959	0.780181	Biso	1.000000	C
C6	1.0	0.781021	0.262041	0.780181	Biso	1.000000	C
C7	1.0	0.762041	0.718979	0.780181	Biso	1.000000	C
C8	1.0	0.237959	0.281021	0.780181	Biso	1.000000	C
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N2	1.0	0.824056	0.249675	0.276698	Biso	1.000000	N
N3	1.0	0.749675	0.675944	0.276698	Biso	1.000000	N
N4	1.0	0.250325	0.324056	0.276698	Biso	1.000000	N
N5	1.0	0.324056	0.749675	0.723302	Biso	1.000000	N
N6	1.0	0.675944	0.250325	0.723302	Biso	1.000000	N
N7	1.0	0.750325	0.824056	0.723302	Biso	1.000000	N
N8	1.0	0.249675	0.175944	0.723302	Biso	1.000000	N
Pb1	1.0	0.000000	0.000000	0.500000	Biso	1.000000	Pb
Pb2	1.0	0.500000	0.500000	0.500000	Biso	1.000000	Pb
Pb3	1.0	0.500000	0.000000	-0.005096	Biso	1.000000	Pb
Pb4	1.0	0.000000	0.500000	0.005096	Biso	1.000000	Pb
Pb5	1.0	0.500000	0.000000	0.487102	Biso	1.000000	Pb
Pb6	1.0	0.000000	0.500000	0.512898	Biso	1.000000	Pb
Pb7	1.0	0.000000	0.000000	0.000000	Biso	1.000000	Pb
Pb8	1.0	0.500000	0.500000	0.000000	Biso	1.000000	Pb
I1	1.0	0.430089	0.249771	0.502394	Biso	1.000000	I
I2	1.0	0.569911	0.750229	0.502394	Biso	1.000000	I
I3	1.0	0.250229	0.930089	0.502394	Biso	1.000000	I
I4	1.0	0.749771	0.069911	0.502394	Biso	1.000000	I
I5	1.0	0.069911	0.250229	0.497606	Biso	1.000000	I
I6	1.0	0.930089	0.749771	0.497606	Biso	1.000000	I
I7	1.0	0.249771	0.569911	0.497606	Biso	1.000000	I
I8	1.0	0.750229	0.430089	0.497606	Biso	1.000000	I
I9	1.0	0.249923	0.035319	0.974264	Biso	1.000000	I
I10	1.0	0.750077	0.964681	0.974264	Biso	1.000000	I
I11	1.0	0.464681	0.749923	0.974264	Biso	1.000000	I
I12	1.0	0.535319	0.250077	0.974264	Biso	1.000000	I
I13	1.0	0.250077	0.464681	0.025736	Biso	1.000000	I
I14	1.0	0.749923	0.535319	0.025736	Biso	1.000000	I
I15	1.0	0.035319	0.750077	0.025736	Biso	1.000000	I
I16	1.0	0.964681	0.249923	0.025736	Biso	1.000000	I
I17	1.0	0.500000	0.000000	0.241480	Biso	1.000000	I
I18	1.0	0.000000	0.500000	0.758520	Biso	1.000000	I
I19	1.0	0.000000	0.000000	0.748102	Biso	1.000000	I
I20	1.0	0.500000	0.500000	0.748102	Biso	1.000000	I
I21	1.0	0.500000	0.500000	0.251898	Biso	1.000000	I
I22	1.0	0.000000	0.000000	0.251898	Biso	1.000000	I
I23	1.0	0.000000	0.500000	0.261436	Biso	1.000000	I
I24	1.0	0.500000	0.000000	0.738564	Biso	1.000000	I

P1_1.04GPa_cubic.cif

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# CRYSTAL DATA

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_cell_length_c                         12.22000
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_symmetry_Int_Tables_number            1

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   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
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   H3          1.0     0.328229      0.166508      0.666446     Biso  1.000000 H
   H4          1.0     0.821267      0.695528      0.715865     Biso  1.000000 H
   H5          1.0     0.189651      0.333277      0.778858     Biso  1.000000 H
   H6          1.0     0.603319      0.770216      0.795352     Biso  1.000000 H
   H7          1.0     0.372711      0.255426      0.762391     Biso  1.000000 H
   H8          1.0     0.766015      0.671033      0.850227     Biso  1.000000 H
   H9          1.0     0.193774      0.190756      0.813331     Biso  1.000000 H
   H10         1.0     0.622766      0.662979      0.712645     Biso  1.000000 H
   H11         1.0     0.325673      0.300238      0.639482     Biso  1.000000 H
   H12         1.0     0.796210      0.807978      0.806852     Biso  1.000000 H
   H13         1.0     0.708523      0.326458      0.794318     Biso  1.000000 H
   H14         1.0     0.183337      0.867830      0.746393     Biso  1.000000 H
   H15         1.0     0.754515      0.135019      0.783310     Biso  1.000000 H
   H16         1.0     0.305476      0.768262      0.869512     Biso  1.000000 H
   H17         1.0     0.785474      0.350178      0.671484     Biso  1.000000 H
   H18         1.0     0.238516      0.805529      0.637643     Biso  1.000000 H
   H19         1.0     0.830156      0.156732      0.668387     Biso  1.000000 H
   H20         1.0     0.364545      0.702474      0.751510     Biso  1.000000 H
   H21         1.0     0.853715      0.307348      0.794969     Biso  1.000000 H
   H22         1.0     0.315140      0.890465      0.714190     Biso  1.000000 H
   H23         1.0     0.694723      0.176222      0.664439     Biso  1.000000 H
   H24         1.0     0.225043      0.676019      0.788558     Biso  1.000000 H
   H25         1.0     0.333640      0.190071      0.279218     Biso  1.000000 H
   H26         1.0     0.770513      0.603766      0.295977     Biso  1.000000 H
   H27         1.0     0.255493      0.372906      0.262019     Biso  1.000000 H
   H28         1.0     0.670896      0.766445      0.349983     Biso  1.000000 H
   H29         1.0     0.233332      0.143367      0.182126     Biso  1.000000 H
   H30         1.0     0.790112      0.654685      0.168645     Biso  1.000000 H
   H31         1.0     0.166597      0.327935      0.166309     Biso  1.000000 H
   H32         1.0     0.694933      0.820976      0.215251     Biso  1.000000 H
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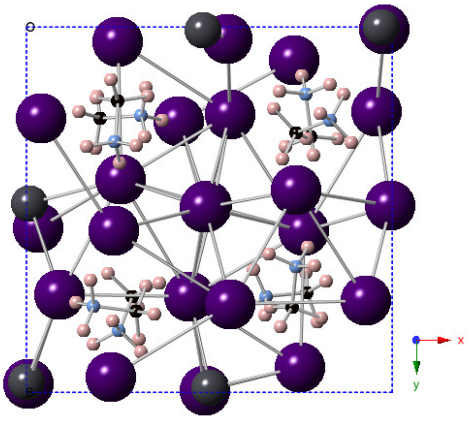

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H37	1.0	0.806076	0.238333	0.137661	Biso	1.000000	H
H38	1.0	0.350593	0.785068	0.171079	Biso	1.000000	H
H39	1.0	0.701538	0.363061	0.251404	Biso	1.000000	H
H40	1.0	0.157120	0.830105	0.167861	Biso	1.000000	H
H41	1.0	0.869141	0.183914	0.246378	Biso	1.000000	H
H42	1.0	0.326723	0.708940	0.294409	Biso	1.000000	H
H43	1.0	0.768563	0.305485	0.369458	Biso	1.000000	H
H44	1.0	0.135386	0.754773	0.282999	Biso	1.000000	H
H45	1.0	0.890369	0.315879	0.214018	Biso	1.000000	H
H46	1.0	0.307815	0.854156	0.294092	Biso	1.000000	H
H47	1.0	0.677219	0.223375	0.289177	Biso	1.000000	H
H48	1.0	0.176606	0.694660	0.164290	Biso	1.000000	H
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C2	1.0	0.779077	0.300345	0.745799	Biso	1.000000	C
C3	1.0	0.250706	0.202494	0.247400	Biso	1.000000	C
C4	1.0	0.300727	0.779210	0.245417	Biso	1.000000	C
C5	1.0	0.767836	0.727199	0.780406	Biso	1.000000	C
C6	1.0	0.290064	0.737600	0.786838	Biso	1.000000	C
C7	1.0	0.726939	0.768081	0.280062	Biso	1.000000	C
C8	1.0	0.737860	0.289268	0.286953	Biso	1.000000	C
N1	1.0	0.655262	0.738087	0.736045	Biso	1.000000	N
N2	1.0	0.254382	0.830486	0.717285	Biso	1.000000	N
N3	1.0	0.738240	0.655283	0.236363	Biso	1.000000	N
N4	1.0	0.831013	0.254517	0.217248	Biso	1.000000	N
N5	1.0	0.314622	0.242743	0.701560	Biso	1.000000	N
N6	1.0	0.763916	0.184200	0.713988	Biso	1.000000	N
N7	1.0	0.242858	0.314557	0.201447	Biso	1.000000	N
N8	1.0	0.184570	0.763988	0.213654	Biso	1.000000	N
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Pb2	1.0	0.008674	0.483144	0.506921	Biso	1.000000	Pb
Pb3	1.0	-0.027837	0.000352	0.001519	Biso	1.000000	Pb
Pb4	1.0	0.490879	0.509493	-0.007303	Biso	1.000000	Pb
Pb5	1.0	0.483209	0.008294	0.006967	Biso	1.000000	Pb
Pb6	1.0	-0.011506	0.503378	-0.010789	Biso	1.000000	Pb
Pb7	1.0	0.000175	-0.028053	0.501548	Biso	1.000000	Pb
Pb8	1.0	0.509814	0.490539	0.492698	Biso	1.000000	Pb
I1	1.0	0.489885	-0.004558	0.751319	Biso	1.000000	I
I2	1.0	0.033202	0.551489	0.748704	Biso	1.000000	I
I3	1.0	-0.020773	0.007031	0.254087	Biso	1.000000	I
I4	1.0	0.489072	0.494543	0.243803	Biso	1.000000	I
I5	1.0	0.550910	0.032904	0.248851	Biso	1.000000	I
I6	1.0	-0.004100	0.490095	0.251243	Biso	1.000000	I
I7	1.0	0.006401	-0.021987	0.754161	Biso	1.000000	I
I8	1.0	0.494140	0.489067	0.743757	Biso	1.000000	I
I9	1.0	0.957890	0.230749	0.507648	Biso	1.000000	I
I10	1.0	0.447287	0.738135	0.511464	Biso	1.000000	I
I11	1.0	0.557179	0.238591	0.525470	Biso	1.000000	I
I12	1.0	0.091987	0.732052	0.481231	Biso	1.000000	I
I13	1.0	0.258661	0.417694	0.477475	Biso	1.000000	I
I14	1.0	0.749391	0.930752	0.542977	Biso	1.000000	I
I15	1.0	0.250852	0.040418	0.501306	Biso	1.000000	I
I16	1.0	0.759494	0.559224	0.510499	Biso	1.000000	I
I17	1.0	0.732148	0.091742	0.981687	Biso	1.000000	I
I18	1.0	0.238858	0.557117	0.025449	Biso	1.000000	I
I19	1.0	0.738483	0.447336	0.011635	Biso	1.000000	I
I20	1.0	0.230874	0.957630	0.006931	Biso	1.000000	I
I21	1.0	0.040534	0.251057	0.000985	Biso	1.000000	I
I22	1.0	0.559397	0.759175	0.010110	Biso	1.000000	I
I23	1.0	0.417933	0.258397	0.977601	Biso	1.000000	I
I24	1.0	0.930763	0.749529	0.043191	Biso	1.000000	I

P4n_1.04GPa_cubic.cif

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# CRYSTAL DATA

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_symmetry_Int_Tables_number            1

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   H3         1.0     0.838476     0.663629     0.265805     Biso  1.000000 H
   H4         1.0     0.161524     0.336371     0.265805     Biso  1.000000 H
   H5         1.0     0.336371     0.838476     0.734195     Biso  1.000000 H
   H6         1.0     0.663629     0.161524     0.734195     Biso  1.000000 H
   H7         1.0     0.661524     0.836371     0.734195     Biso  1.000000 H
   H8         1.0     0.338476     0.163629     0.734195     Biso  1.000000 H
   H9         1.0     0.113522     0.753854     0.178281     Biso  1.000000 H
   H10        1.0     0.886478     0.246146     0.178281     Biso  1.000000 H
   H11        1.0     0.746146     0.613522     0.178281     Biso  1.000000 H
   H12        1.0     0.253854     0.386478     0.178281     Biso  1.000000 H
   H13        1.0     0.386478     0.746146     0.821719     Biso  1.000000 H
   H14        1.0     0.613522     0.253854     0.821719     Biso  1.000000 H
   H15        1.0     0.753854     0.886478     0.821719     Biso  1.000000 H
   H16        1.0     0.246146     0.113522     0.821719     Biso  1.000000 H
   H17        1.0     0.107719     0.776151     0.313027     Biso  1.000000 H
   H18        1.0     0.892281     0.223849     0.313027     Biso  1.000000 H
   H19        1.0     0.723849     0.607719     0.313027     Biso  1.000000 H
   H20        1.0     0.276151     0.392281     0.313027     Biso  1.000000 H
   H21        1.0     0.392281     0.723849     0.686973     Biso  1.000000 H
   H22        1.0     0.607719     0.276151     0.686973     Biso  1.000000 H
   H23        1.0     0.776151     0.892281     0.686973     Biso  1.000000 H
   H24        1.0     0.223849     0.107719     0.686973     Biso  1.000000 H
   H25        1.0     0.254737     0.886247     0.235929     Biso  1.000000 H
   H26        1.0     0.745263     0.113753     0.235929     Biso  1.000000 H
   H27        1.0     0.613753     0.754737     0.235929     Biso  1.000000 H
   H28        1.0     0.386247     0.245263     0.235929     Biso  1.000000 H
   H29        1.0     0.245263     0.613753     0.764071     Biso  1.000000 H
   H30        1.0     0.754737     0.386247     0.764071     Biso  1.000000 H
   H31        1.0     0.886247     0.745263     0.764071     Biso  1.000000 H
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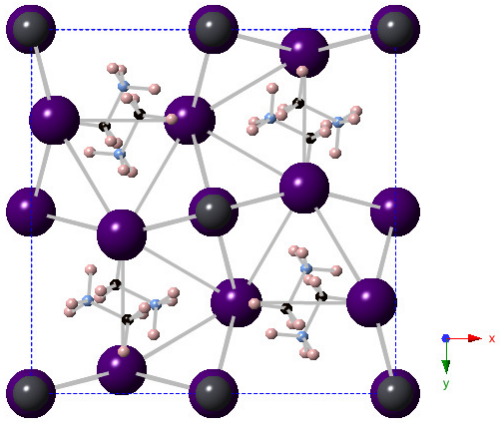

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H37	1.0	0.187832	0.736425	0.821103	Biso	1.000000	H
H38	1.0	0.812168	0.263575	0.821103	Biso	1.000000	H
H39	1.0	0.763575	0.687832	0.821103	Biso	1.000000	H
H40	1.0	0.236425	0.312168	0.821103	Biso	1.000000	H
H41	1.0	0.307928	0.782139	0.324907	Biso	1.000000	H
H42	1.0	0.692072	0.217861	0.324907	Biso	1.000000	H
H43	1.0	0.717861	0.807928	0.324907	Biso	1.000000	H
H44	1.0	0.282139	0.192072	0.324907	Biso	1.000000	H
H45	1.0	0.192072	0.717861	0.675093	Biso	1.000000	H
H46	1.0	0.807928	0.282139	0.675093	Biso	1.000000	H
H47	1.0	0.782139	0.692072	0.675093	Biso	1.000000	H
H48	1.0	0.217861	0.307928	0.675093	Biso	1.000000	H
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C2	1.0	0.733880	0.201722	0.247424	Biso	1.000000	C
C3	1.0	0.701722	0.766120	0.247424	Biso	1.000000	C
C4	1.0	0.298278	0.233880	0.247424	Biso	1.000000	C
C5	1.0	0.233880	0.701722	0.752576	Biso	1.000000	C
C6	1.0	0.766120	0.298278	0.752576	Biso	1.000000	C
C7	1.0	0.798278	0.733880	0.752576	Biso	1.000000	C
C8	1.0	0.201722	0.266120	0.752576	Biso	1.000000	C
N1	1.0	0.156847	0.744851	0.251089	Biso	1.000000	N
N2	1.0	0.843153	0.255149	0.251089	Biso	1.000000	N
N3	1.0	0.755149	0.656847	0.251089	Biso	1.000000	N
N4	1.0	0.244851	0.343153	0.251089	Biso	1.000000	N
N5	1.0	0.343153	0.755149	0.748911	Biso	1.000000	N
N6	1.0	0.656847	0.244851	0.748911	Biso	1.000000	N
N7	1.0	0.744851	0.843153	0.748911	Biso	1.000000	N
N8	1.0	0.255149	0.156847	0.748911	Biso	1.000000	N
Pb1	1.0	-0.000000	-0.000000	0.500000	Biso	1.000000	Pb
Pb2	1.0	0.500000	0.500000	0.500000	Biso	1.000000	Pb
Pb3	1.0	0.500000	-0.000000	0.004075	Biso	1.000000	Pb
Pb4	1.0	-0.000000	0.500000	-0.004075	Biso	1.000000	Pb
Pb5	1.0	0.500000	-0.000000	0.496244	Biso	1.000000	Pb
Pb6	1.0	-0.000000	0.500000	0.503756	Biso	1.000000	Pb
Pb7	1.0	-0.000000	-0.000000	-0.000000	Biso	1.000000	Pb
Pb8	1.0	0.500000	0.500000	-0.000000	Biso	1.000000	Pb
I1	1.0	0.434098	0.250190	0.528938	Biso	1.000000	I
I2	1.0	0.565902	0.749810	0.528938	Biso	1.000000	I
I3	1.0	0.249810	0.934098	0.528938	Biso	1.000000	I
I4	1.0	0.750190	0.065902	0.528938	Biso	1.000000	I
I5	1.0	0.065902	0.249810	0.471062	Biso	1.000000	I
I6	1.0	0.934098	0.750190	0.471062	Biso	1.000000	I
I7	1.0	0.250190	0.565902	0.471062	Biso	1.000000	I
I8	1.0	0.749810	0.434098	0.471062	Biso	1.000000	I
I9	1.0	0.250178	0.938067	0.969810	Biso	1.000000	I
I10	1.0	0.749822	0.061933	0.969810	Biso	1.000000	I
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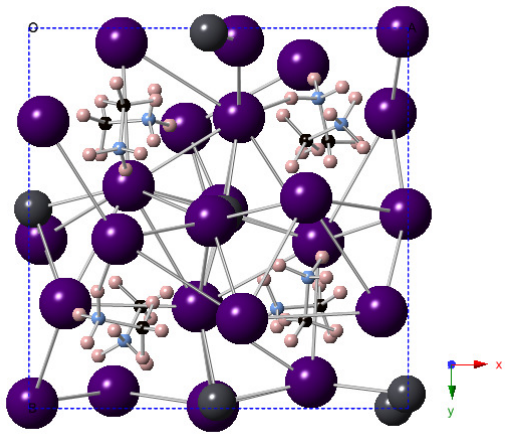

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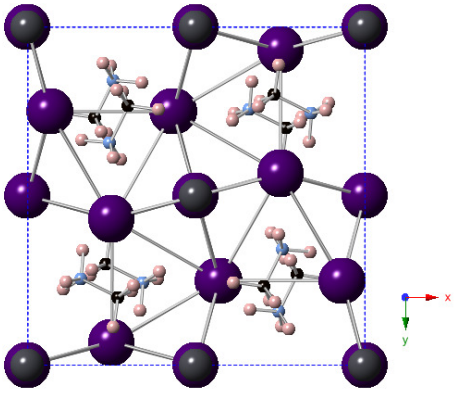

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H39	1.0	0.765191	0.685534	0.821474	Biso	1.000000	H
H40	1.0	0.234809	0.314466	0.821474	Biso	1.000000	H
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H46	1.0	0.809357	0.282356	0.674204	Biso	1.000000	H
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C4	1.0	0.299159	0.232410	0.247698	Biso	1.000000	C
C5	1.0	0.232410	0.700841	0.752302	Biso	1.000000	C
C6	1.0	0.767590	0.299159	0.752302	Biso	1.000000	C
C7	1.0	0.799159	0.732410	0.752302	Biso	1.000000	C
C8	1.0	0.200841	0.267590	0.752302	Biso	1.000000	C
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N3	1.0	0.755246	0.657919	0.250320	Biso	1.000000	N
N4	1.0	0.244754	0.342081	0.250320	Biso	1.000000	N
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N6	1.0	0.657919	0.244754	0.749680	Biso	1.000000	N
N7	1.0	0.744754	0.842081	0.749680	Biso	1.000000	N
N8	1.0	0.255246	0.157919	0.749680	Biso	1.000000	N
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Pb2	1.0	0.500000	0.500000	0.500000	Biso	1.000000	Pb
Pb3	1.0	0.500000	0.000000	0.004569	Biso	1.000000	Pb
Pb4	1.0	-0.000000	0.500000	0.995431	Biso	1.000000	Pb
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I3	1.0	0.249627	0.931213	0.529800	Biso	1.000000	I
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I5	1.0	0.068787	0.249627	0.470200	Biso	1.000000	I
I6	1.0	0.931213	0.750373	0.470200	Biso	1.000000	I
I7	1.0	0.250373	0.568787	0.470200	Biso	1.000000	I
I8	1.0	0.749627	0.431213	0.470200	Biso	1.000000	I
I9	1.0	0.250080	0.935159	0.969672	Biso	1.000000	I
I10	1.0	0.749920	0.064841	0.969672	Biso	1.000000	I
I11	1.0	0.564841	0.750080	0.969672	Biso	1.000000	I
I12	1.0	0.435159	0.249920	0.969672	Biso	1.000000	I
I13	1.0	0.249920	0.564841	0.030328	Biso	1.000000	I
I14	1.0	0.750080	0.435159	0.030328	Biso	1.000000	I
I15	1.0	0.935159	0.749920	0.030328	Biso	1.000000	I
I16	1.0	0.064841	0.250080	0.030328	Biso	1.000000	I
I17	1.0	0.500000	0.000000	0.250805	Biso	1.000000	I
I18	1.0	-0.000000	0.500000	0.749195	Biso	1.000000	I
I19	1.0	-0.000000	0.000000	0.749839	Biso	1.000000	I
I20	1.0	0.500000	0.500000	0.749839	Biso	1.000000	I
I21	1.0	0.500000	0.500000	0.250161	Biso	1.000000	I
I22	1.0	-0.000000	0.000000	0.250161	Biso	1.000000	I
I23	1.0	-0.000000	0.500000	0.249696	Biso	1.000000	I
I24	1.0	0.500000	0.000000	0.750304	Biso	1.000000	I

Table S3. Peak wavelength of $MAPbI_3$ photoluminescence spectra (Figure 4) collected under compression and their corresponding estimated band gaps.

Pressure(GPa)	Wavelength(nm)	Bandgap(eV)
1.95	732.1	1.693
1.37	737.3	1.682
1.04	748.2	1.657
0.80	749.5	1.654
0.41	754.7	1.643
0.30	772.1	1.606
0.16	768.7	1.613
0.11	765.1	1.621
0.05	764.8	1.621
~0	764.1	1.623

Fig. S8. Models for tetragonal and cubic phases of $MAPbI_3$. With explicit MA cations, symmetry is significantly lowered by orientations of C-N dipole and rotation of XH_3 groups. To model high symmetry I4/mcm and $Im\bar{3}$, we fixed the lattice parameters to experimental values, while all atomic positions were relaxed with P1 space group of no symmetry (a), or with a space group of P4/n (b) derived from the orthorhombic phase. The two models are energetically close, with (a) P1 of lower energy. The resulting band gaps were averaged over the two models according to Boltzmann distribution at room temperature.

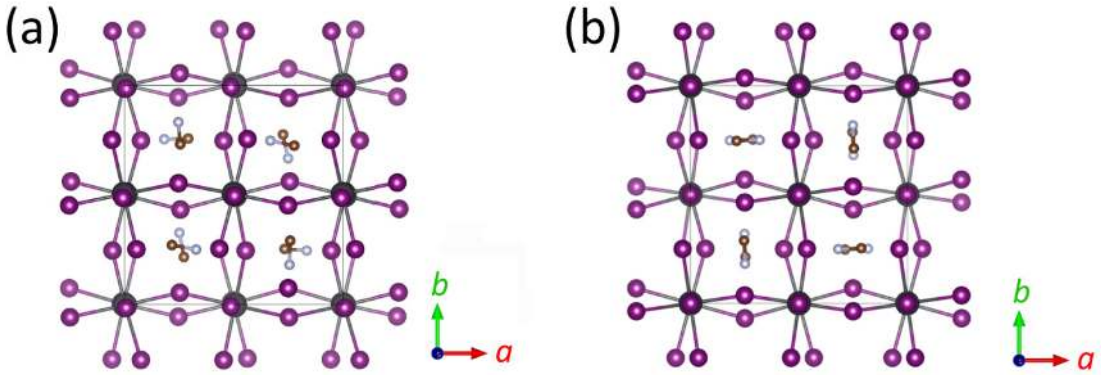

Table S4. The predicted band gaps E_g of $MAPbI_3$ with the two models P1 and P4/n for tetragonal and cubic phases, and the energy difference ΔE with the resulting ratios of structures, according to the Boltzmann distribution at room temperature.

P (GPa)	E_g (eV)				ΔE (eV/$MAPbI_3$)				Ratio				Averaged E_g (eV)
	Tetragonal		Cubic		Tetragonal		Cubic		Tetragonal		Cubic		
	P1	P4/n	P1	P4/n	P1	P4/n	P1	P4/n	P1	P4/n	P1	P4/n	
0	1.695	1.607			0.00000	0.02844			1	0.3306			1.67
0.30	1.659	1.497			0.00000	0.02594			1	0.3643			1.62
0.41	1.649	1.519	1.571	1.413	0.00000	0.02687	0.01914	0.03663	1	0.3514	0.4748	0.2403	1.58
1.04			1.703	1.542			0.00000	0.03177			1	0.2904	1.67
1.95			1.814	1.516			0.00000	0.03052			1	0.3049	1.74

II. Characterization and Fitting Software:

Synchrotron XRD and PL Characterization:

High Pressure Processing: The samples were loaded into a diamond anvil cell (DAC) for separate *in-situ* high pressure XRD runs. Stainless gaskets were pre-indented to reduce the thickness from 250 μm down to ~100 μm. A 200 μm diameter hole was drilled and served as the sample chamber. The samples were loaded into the gasket hole and then several small ruby chips were randomly distributed on the top of the samples for monitoring pressure. A laser-excited ruby fluorescence technique was used to measure the variation of the pressure, at which X-ray diffraction and photoluminescence were performed simultaneously. The optical images were taken from microscope directly at various pressures.

X-ray Diffraction Measurement: The X-ray diffraction was collected at B1 station, Cornell High Energy Synchrotron Source (CHESS), Cornell University. A monochromatic x-ray with the energy of 25.514 keV was collimated using a double pinhole-aligned circular tube into small x-ray beam with a diameter of 100 microns. X-ray scattering signals from the samples were collected using a large area Mar345 detector. The sample-to-detector distance and other detector sitting parameters were calibrated using the powder standard of CeO_2. The raw two-dimensional (2D) images were integrated and analyzed by the Fit2D[S2] package. Photoluminescence Characterization: The laser-excited photoluminescence spectra were recorded at Princeton Acton SP-300i system. The samples loaded in DAC were measured under compression or decompression as soon as each diffraction pattern was recorded. A 532 nm diode laser was used for excitation and the emitted light was collected through the spectrometer with 1200g/mm grating in the exposure time of 3s. In each snapshot, the collected PL spectrum covers only a very narrow wavelength range (40 nm), so the full spectrum presented in this work was technically synthesized by a feasible connection of several snapshots collected at nearby but different wavelength

range. This data processing technically involved slight adjustment of background intensities, but no modification was made on the peak position and intensity in each spectrum.

Fitting Software:

Pawley fitting of the lattice parameters and refinement of the atomic positions were carried out using a Topas (version 3) software package (1999-2000 Bruker AXS).

III. References:

(S1) Toby, B. H. *Powder Diffr.* **2007**, *21*, 67-70.

(S2) Hammersley, A. P. *ESRF97HA02T, "FIT2D: An Introduction and Overview"*, 1997.