

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 MAPbI₃ (MA = CH₃NH₃⁺) 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 ReO₃-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 MAPbI₃ 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 ABX₃, where corner-sharing BX₆ 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 BX₆ octahedra show B-X-B angles of 90°. This arrangement of untilted octahedra can be described in Glazer notation^[14-15] as *a*⁰*a*⁰*a*⁰. Among the Pb-based methylammonium (MA) halide perovskites (ionic A = CH₃NH₃⁺ or MA; X = Cl⁻, Br⁻, I⁻; B = Pb²⁺), the bandgaps of MAPbCl₃, MAPbBr₃ and MAPbI₃ 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, MAPbI₃ 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 MAPbI₃ 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, MAPbI₃ was synthesized as reported previously.^[19] In brief, polycrystalline MAPbI₃ was precipitated by 6-hour cooling from 100 to 46 °C after mixing PbI₂ and MA-I solutions in a Pyrex test tube. The PbI₂ 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 CH₃NH₂ 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 ($\lambda = 0.485946$ 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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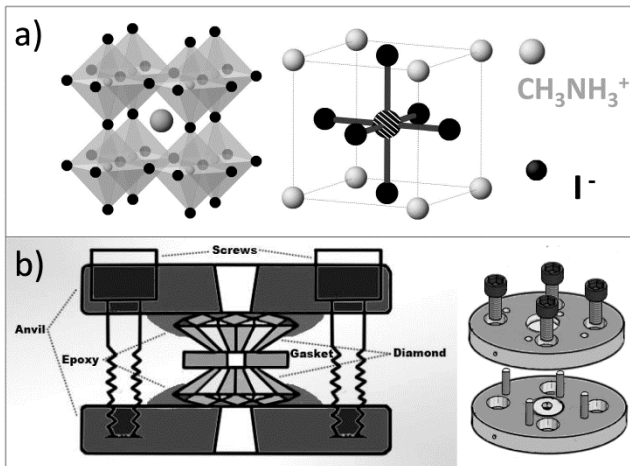


Figure 1. (a) MAPbI₃ perovskite $Pm\bar{3}m$ polymorph (left, polyhedral model; right, Pb-I bonds emphasized); (b) DAC holder system with balanced compression screws (left, side view; right, top-down view).

Synchrotron XRD patterns of MAPbI₃ collected at room temperature (Figure 2a) and ambient pressure confirms a tetragonal polymorph ($I4/mcm$, 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 $2\theta = \sim 7.1^\circ$ 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 MAPbBr₃ analogue,^[22] and a high pressure polymorph of ReO₃, where A site in ABX₃ 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).

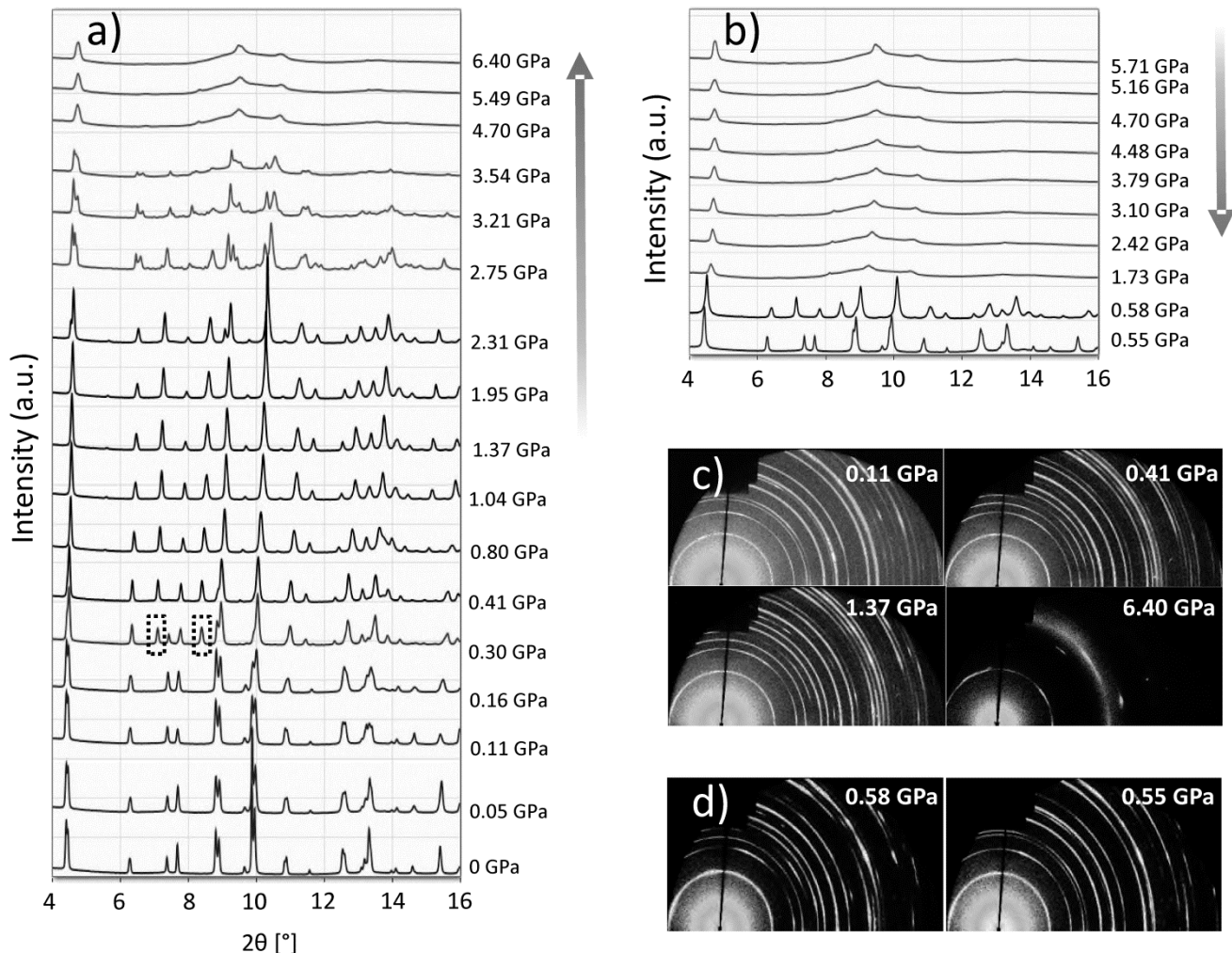


Figure 2. Conventional XRD patterns of MAPbI₃ during (a) compression and (b) decompression. (a), The ReO₃-type cubic supercell (a_s) appears at 0.3 GPa and becomes more abundant to 2.3 GPa, before conversion to the putative orthorhombic polymorph at 2.7 GPa, and finally approaches X-ray amorphicity above 3.5 GPa. (b), decompression from the amorphous mass restores the tetragonal phase at 0.5₈ GPa. (c) and (d), Representative 2D XRD patterns at specific pressures.

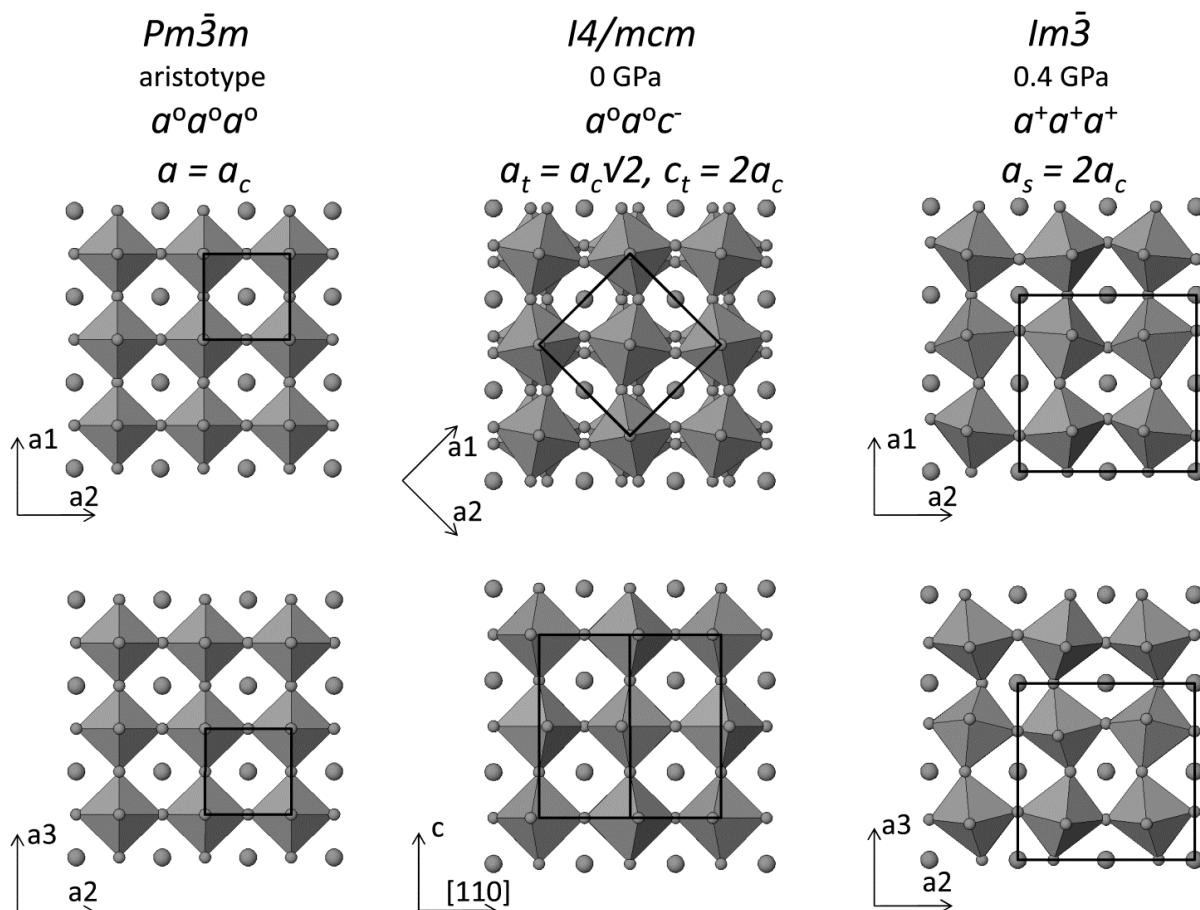


Figure 3. Characteristic PbI₆ octahedral and Glazer symbols of some typical pressure-related polymorphs. The figure for $Immm$ polymorph should be similar to that of $Im\bar{3}$ with slightly different lattice parameters along each axis and an octahedral tilt change (Glazer symbol: $a^+b^+c^+$).

Beyond 0.4 GPa, MAPbI₃ 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 MASnI₃^[25] may be an $Immm$ (No. 77) polymorph with $a^+b^+c^+$ PbI₆ tilting. Reports of an orthorhombic high-pressure form of MAPbBr₃ remain ambiguous.^[22, 26] Beyond 2.7 GPa MAPbI₃ 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 0.5₈ GPa without the appearance of the putative $Immm$ polymorph (Figure 2b). However, the $Im\bar{3}$ phase appeared at 0.5₈ GPa, and the $I4/mcm$ was restored at 0.5₅ 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 1.3₇ GPa was modelled using both $Immm$ and $Im\bar{3}$ polymorphs (Figure S5). However, the poor Pawley fit of the 004 reflection (at $2\theta = -9^\circ$) for the cubic polymorph indicates this phase(s) resides on the borderline of the orthorhombic \rightarrow cubic transition. This evidence supports the existence of the $Immm$ polymorph, but suggests it is metastable with respect to the $Im\bar{3}$ and $I4/mcm$ 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 ReO₃-type $Im\bar{3}$ cubic supercell as a basis, the octahedral topologies in the cubic (c), tetragonal (t) and ReO₃-type cubic supercell (s) of the MAPbI₃ 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 $\sim 15^\circ$ 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 MAPbI₃ 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 *I4/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 PbI₆ 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 MAPbBr₃ 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 *I4/mcm* phase to the cubic *Im* $\bar{3}$ supercell (< 0.4 GPa) offers a chemically-independent means of reducing MAPbI₃ 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.

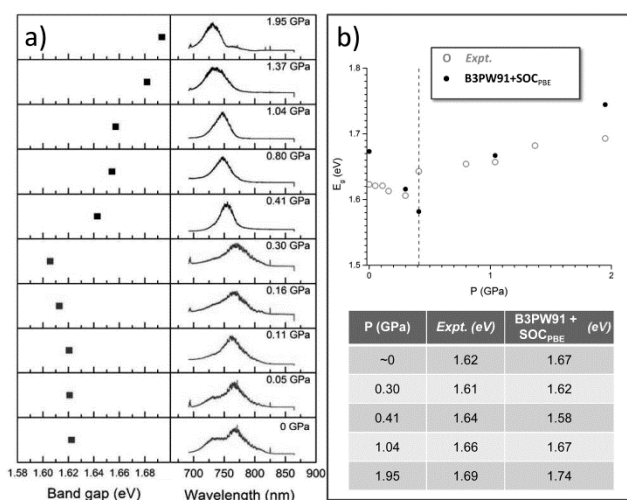
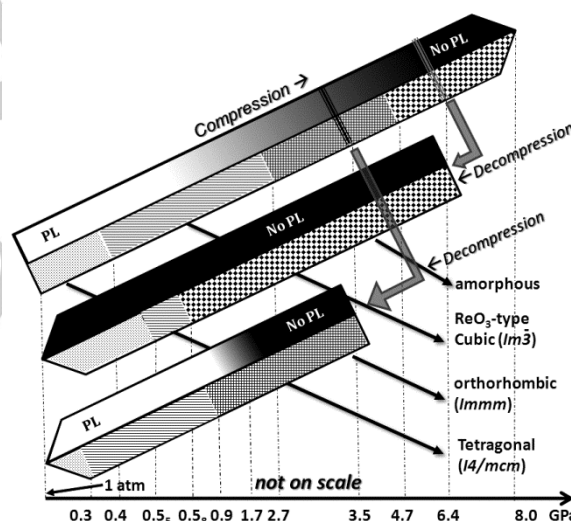


Figure 4. (a) Measured photoluminescence spectra (right panel) and calculated bandgaps (left panel) of MAPbI₃ as a function of compression pressure at room temperature; (b) comparison of bandgaps between the measurement and B3PW91+SOC_{PBE} calculations (also refer to Table S2 in supporting information).

To better understand the atomistic origin of PL in MAPbI₃, 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 MAPbI₃.^[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 MAPbI₃ 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 MAPbI₃ as a function of pressure (not on scale). “PL” represents photoluminescence observation.

In summary, the pressure-induced polymorphism and bandgap tuning of MAPbI₃ 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, MAPbI₃ undergoes two high-pressure phase transformations from a tetragonal polymorph (*I4/mcm*) at ambient pressure, to a suggested orthorhombic (*Immm*) form (2.7 GPa), through to an ReO₃-type (*Im* $\bar{3}$) cubic supercell (0.4 - 2.7 GPa), and finally amorphization above 2.7 GPa. The transition from *I4/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

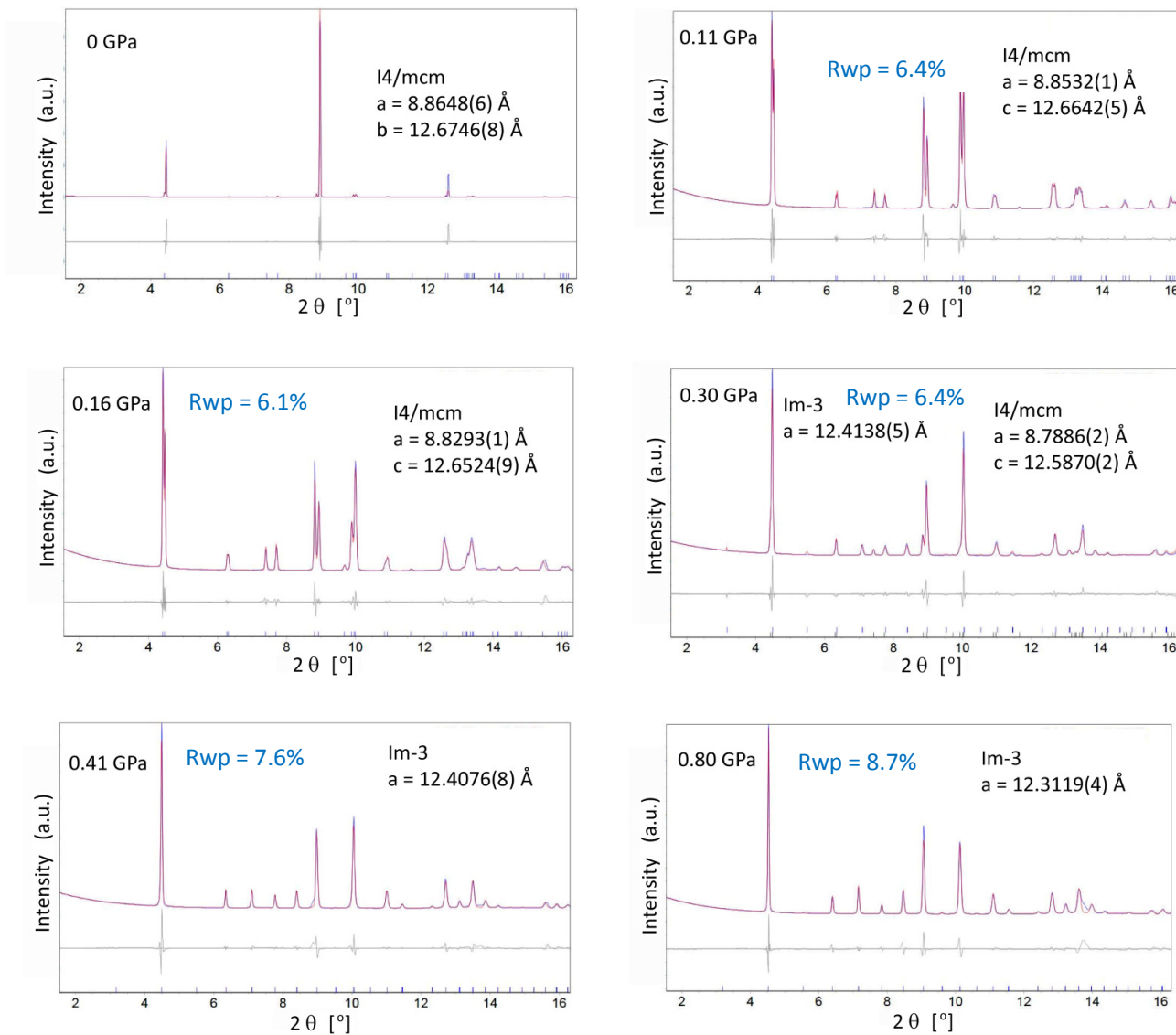
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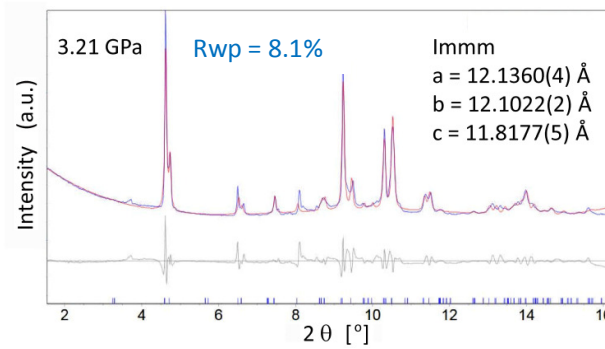
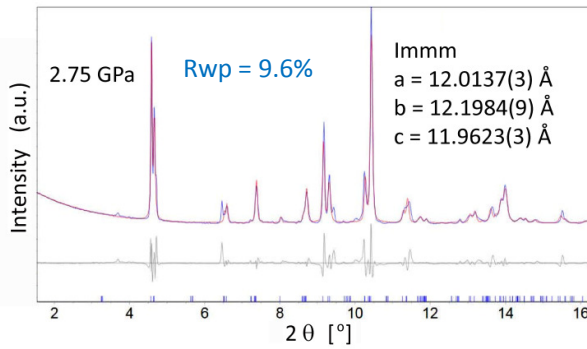
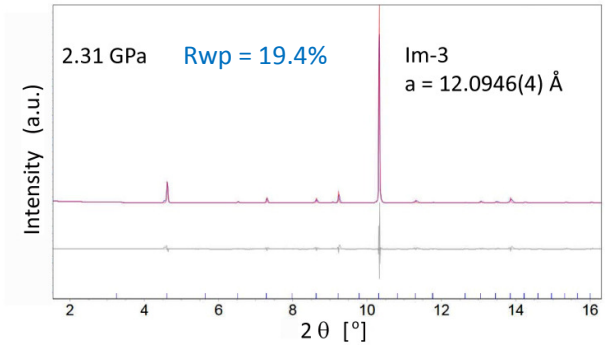
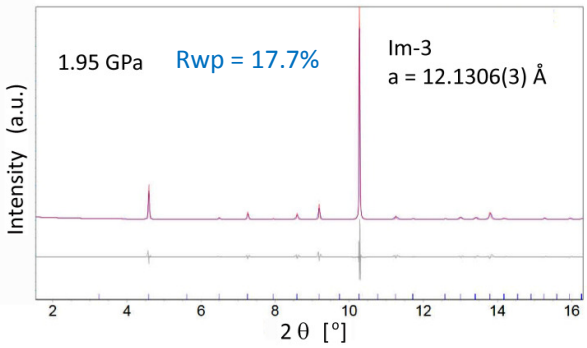
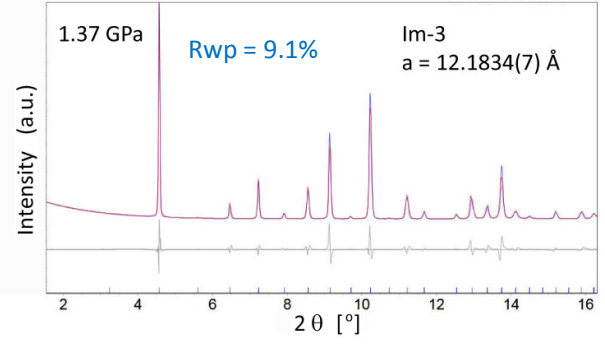
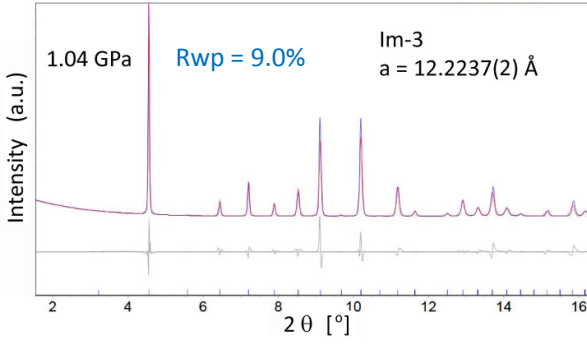
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I. Results:

Fig. S1. Lattice parameters of MAPbI₃, received from Pawley fitting, during the compression and decompression runs. “Rwp” means R-weighted pattern.^[S1] (Peak pressure: 6.4 GPa).

Compression:





Decompression:

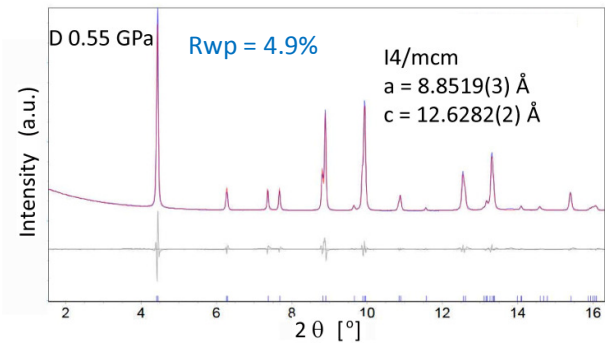
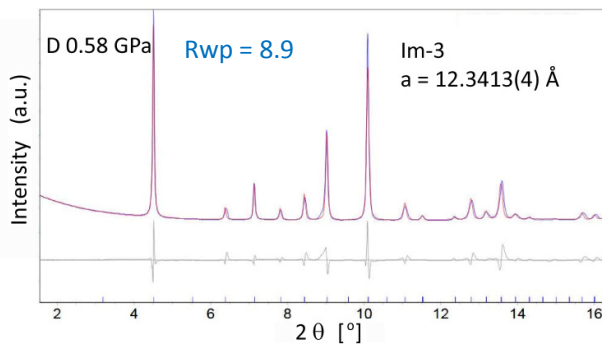
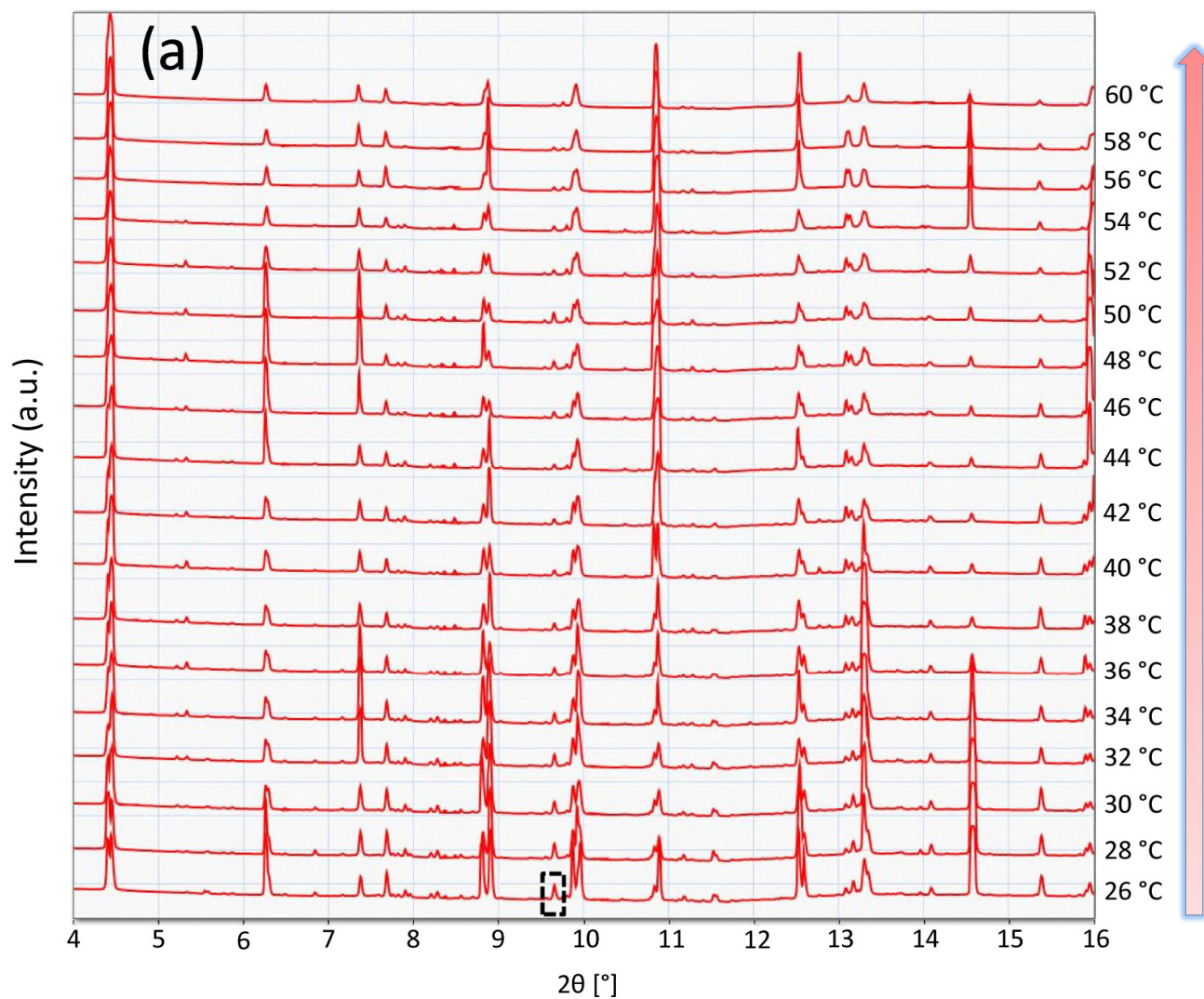


Fig. S2. Integrated synchrotron XRD pattern of MAPbI₃ as a function of temperature. (a) Series of patterns recorded at increasing temperatures; (b) series of patterns recorded at decreasing temperatures. The marked peaks in (a) and (b) are attributed to (123) of MAPbI₃ tetragonal structure.



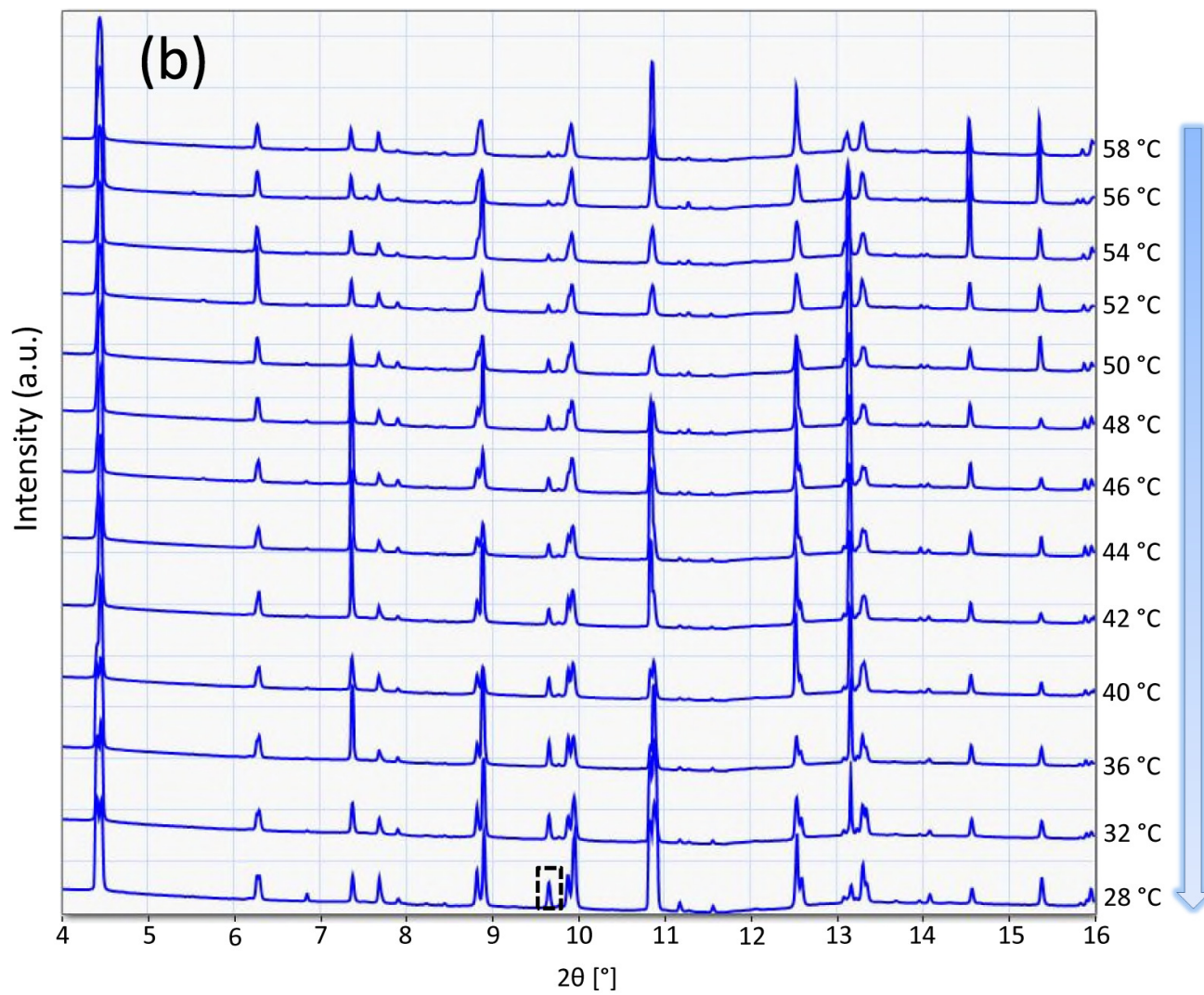


Fig. S3. Integrated synchrotron XRD pattern of MAPbI₃ at pressure of 2.7₅ GPa (top) and zoom-in patterns under different pressures around 2 θ = 9° (bottom).

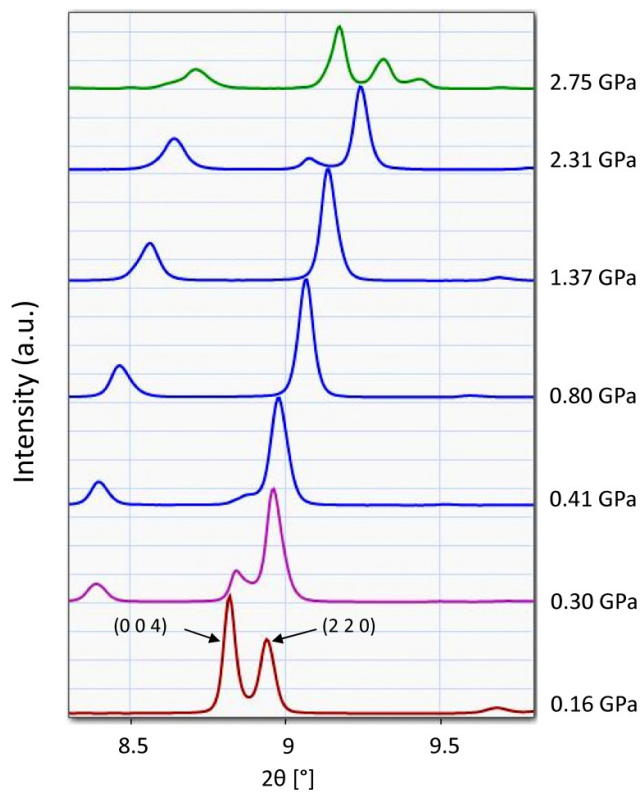
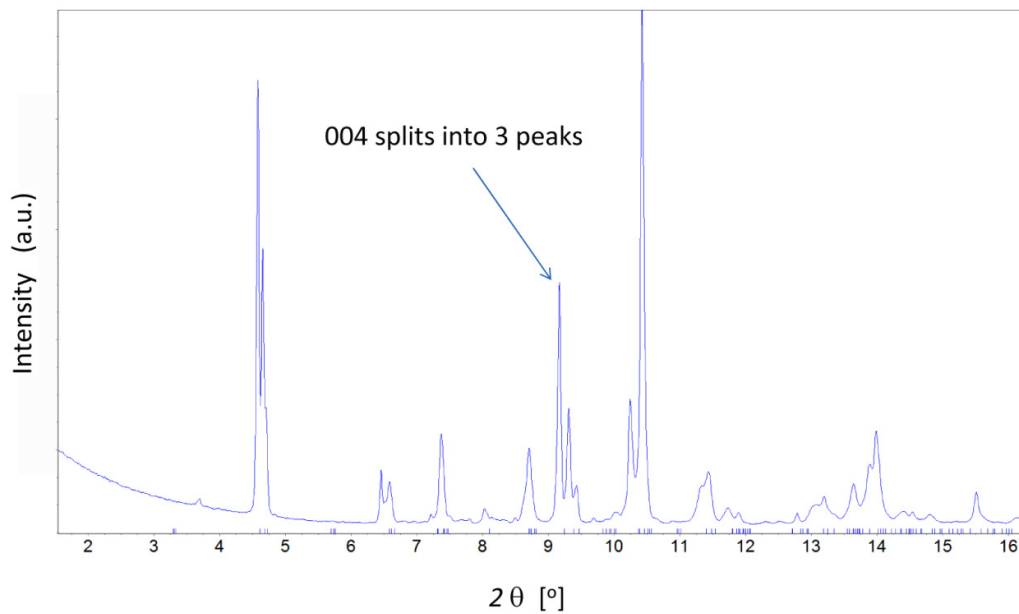


Fig. S4. Additional integrated synchrotron XRD patterns of MAPbI₃ (peak pressure: 3.5 GPa) during (a) compression and (b) decompression runs; and its 2D patterns during (c) compression and (d) decompression runs.

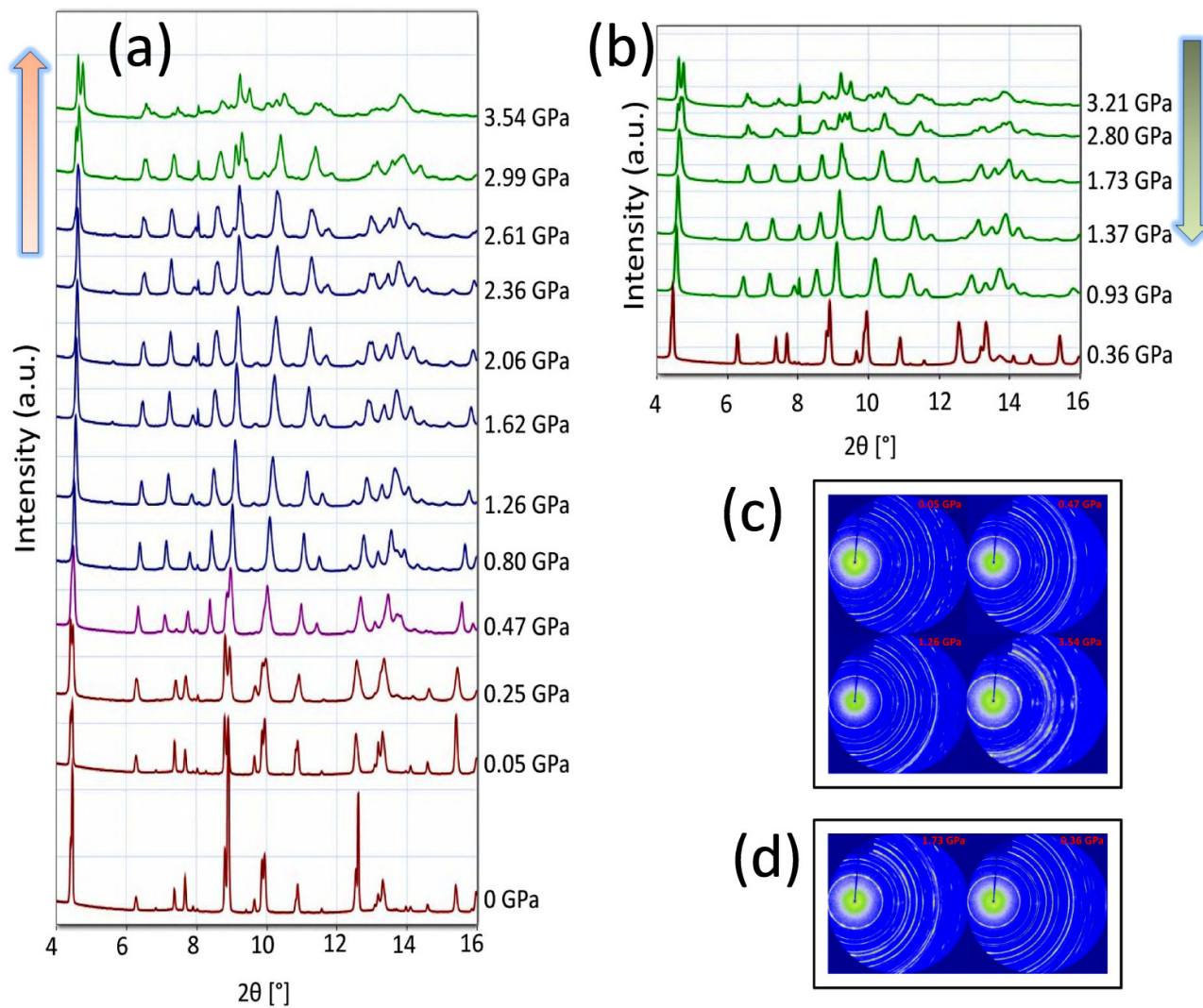
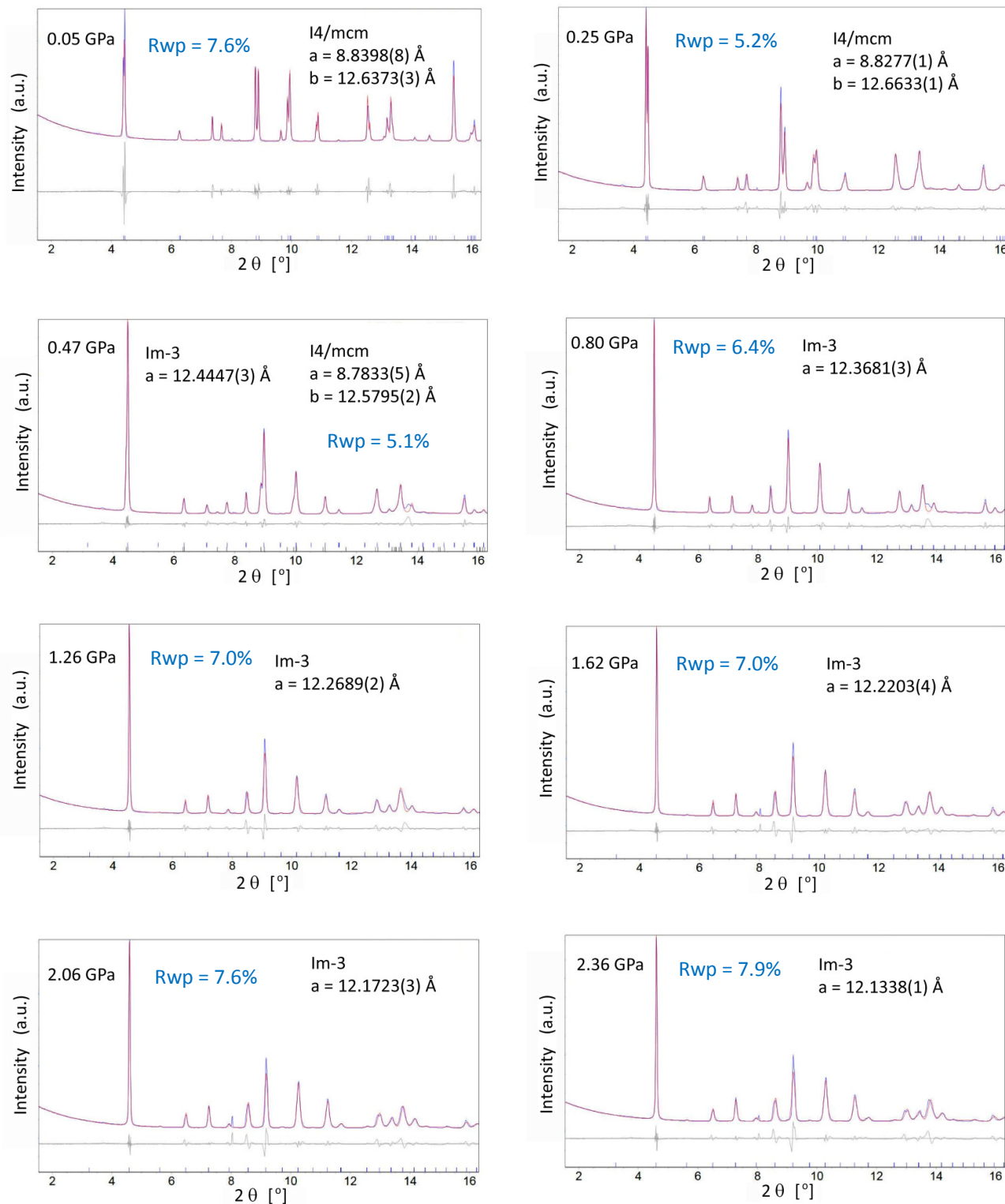
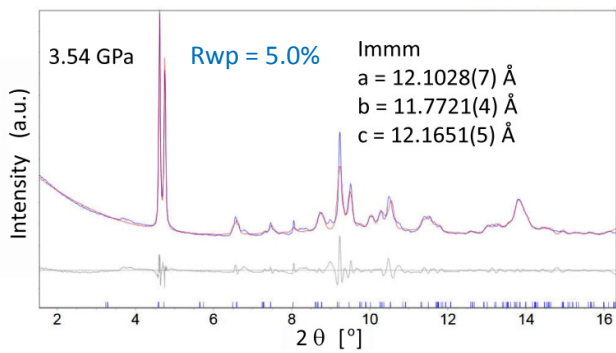
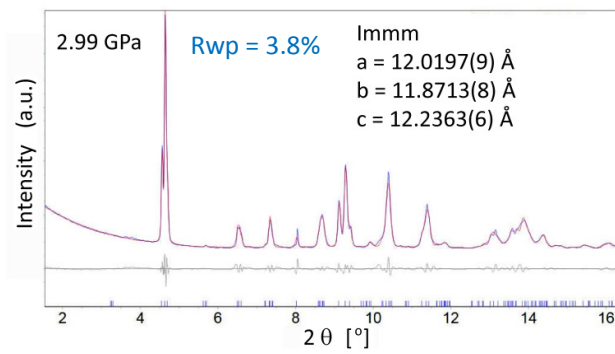
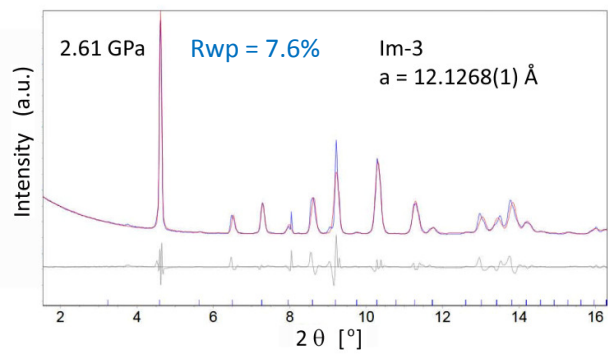


Fig. S5. Lattice parameters of MAPbI₃, received from Pawley fitting using data presented in Fig. S4, during the compression and decompression runs. “Rwp” means R-weighted pattern.^[S1] (Peak pressure: 3.5 GPa).

Compression:





Decompression:

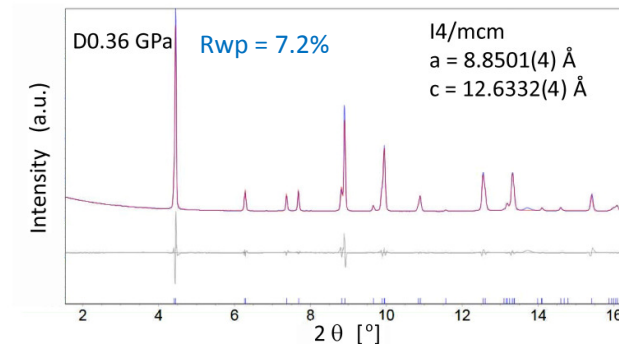
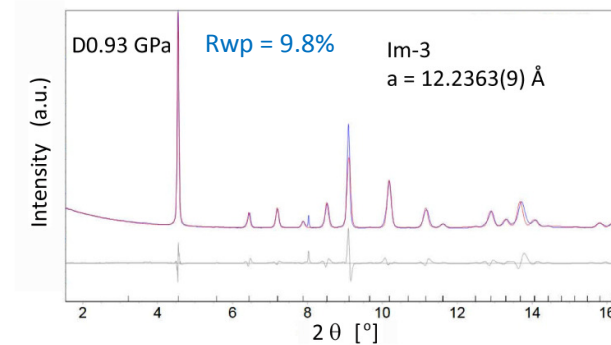
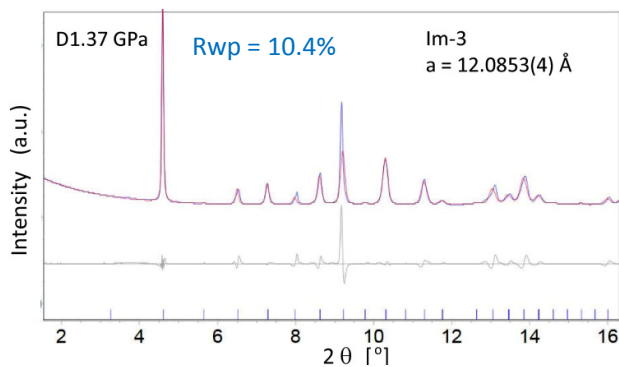
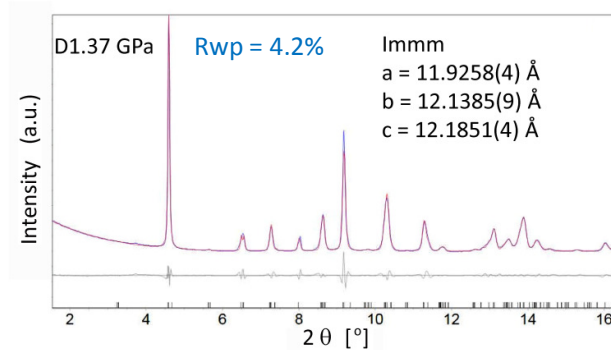
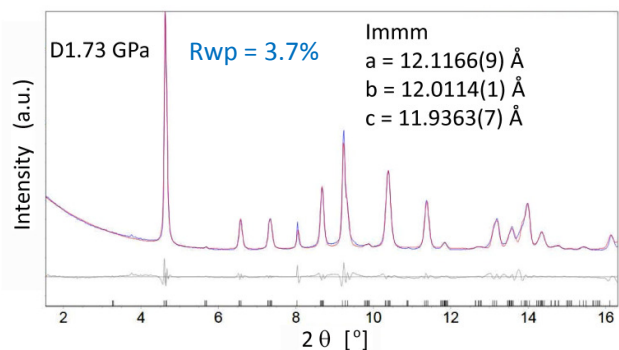
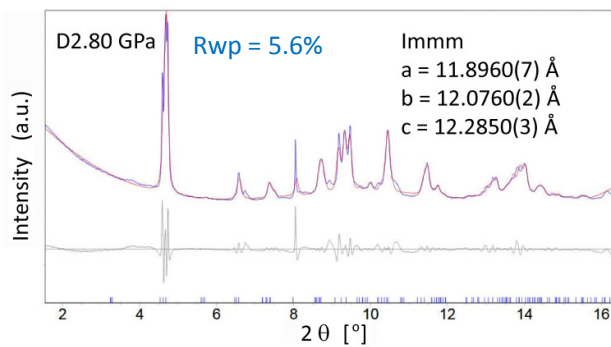
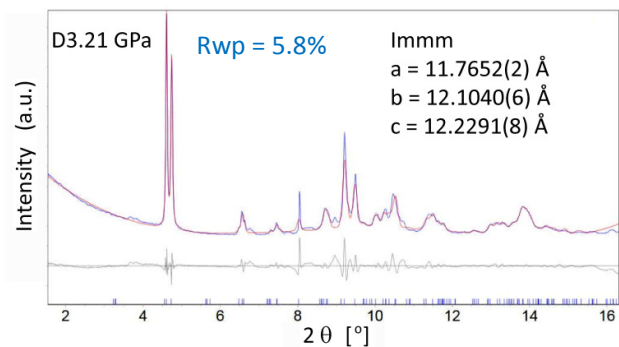


Fig. S6. Plot of unit cell volume calculated from the Pawley fittings as function of the applied pressure in two sets of compressions with different peak pressures.

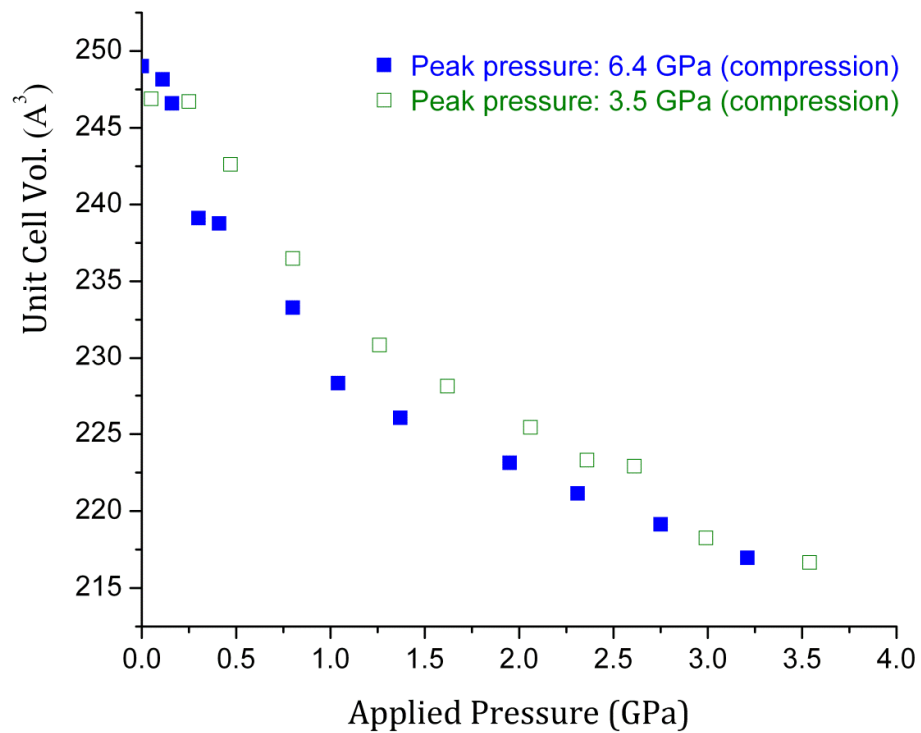


Fig. S7. Optical images of a pressed MAPbI₃ sample in DACs under white light. (a), compressed at 0.1₆ GPa; (b), decompressed at 3.7₁ GPa; (c), decompressed at 2.5₅ GPa; (d), decompressed at 1.9₈ GPa; and (e), decompressed to ambient pressure.

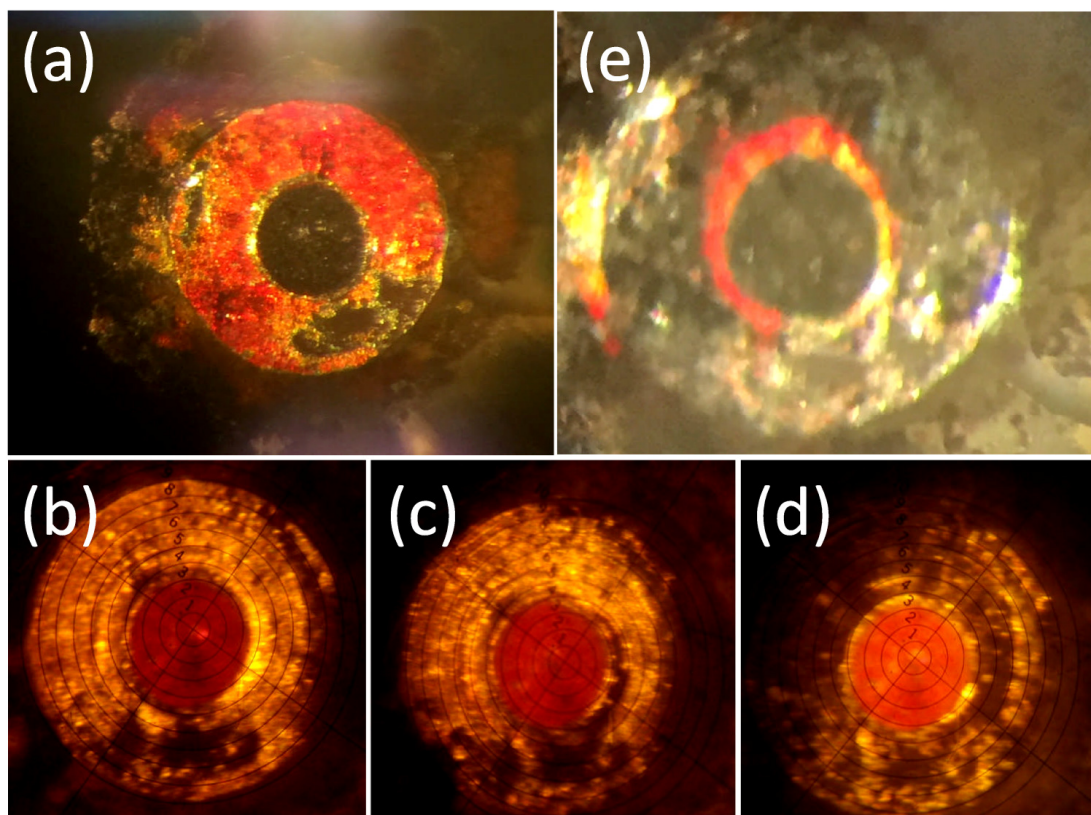


Table S1. Approximate values for the octahedral tilt angles in the cubic $Im\bar{3}$ phase using Rietveld refinements of selected data. The octahedral tilt angle was calculated using the same procedure described by Jorgensen *et al.* [ref.24]

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

H32	1.0	0.689825	0.823076	0.205288	Biso	1.000000	H
H33	1.0	0.198269	0.186316	0.291810	Biso	1.000000	H
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
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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
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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
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I23	1.0	0.433115	0.254525	0.982836	Biso	1.000000	I
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P4n_0.00GPa_tetragonal.cif

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CRYSTAL DATA

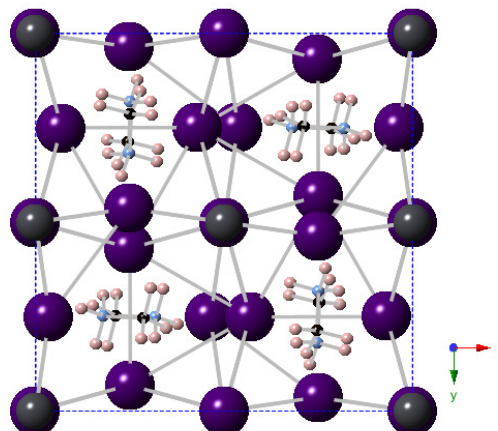
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N7	1.0	0.748909	0.818646	0.722930	Biso	1.000000	N
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Pb8	1.0	0.500000	0.500000	-0.000000	Biso	1.000000	Pb
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I2	1.0	0.568670	0.750510	0.502664	Biso	1.000000	I
I3	1.0	0.250510	0.931330	0.502664	Biso	1.000000	I
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P1_0.30GPa_tetragonal.cif

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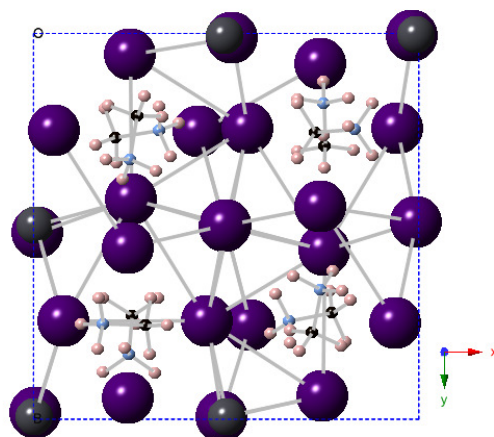
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loop_
_symmetry_equiv_pos_as_xyz
  'x, y, z'
  
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loop_
_atom_site_label
_atom_site_occupancy
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_adp_type
_atom_site_B_iso_or_equiv
_atom_site_type_symbol
H1      1.0      0.162960      0.288360      0.685969      Biso  1.000000  H
H2      1.0      0.668093      0.801632      0.668823      Biso  1.000000  H
H3      1.0      0.328108      0.188147      0.660431      Biso  1.000000  H
H4      1.0      0.824607      0.692484      0.707812      Biso  1.000000  H
H5      1.0      0.215106      0.335622      0.810735      Biso  1.000000  H
H6      1.0      0.616239      0.776808      0.790727      Biso  1.000000  H
H7      1.0      0.377059      0.233133      0.778076      Biso  1.000000  H
H8      1.0      0.769836      0.666929      0.837487      Biso  1.000000  H
H9      1.0      0.186225      0.195564      0.792750      Biso  1.000000  H
H10     1.0      0.628669      0.676559      0.703447      Biso  1.000000  H
H11     1.0      0.356210      0.318816      0.677338      Biso  1.000000  H
H12     1.0      0.809698      0.800587      0.801160      Biso  1.000000  H
H13     1.0      0.687321      0.304393      0.811170      Biso  1.000000  H
H14     1.0      0.181901      0.879059      0.734064      Biso  1.000000  H
H15     1.0      0.753380      0.124639      0.778760      Biso  1.000000  H
H16     1.0      0.267870      0.752960      0.857175      Biso  1.000000  H
H17     1.0      0.755519      0.348558      0.693264      Biso  1.000000  H
H18     1.0      0.238771      0.816807      0.630660      Biso  1.000000  H
H19     1.0      0.819174      0.166516      0.667651      Biso  1.000000  H
H20     1.0      0.325425      0.685500      0.744192      Biso  1.000000  H
H21     1.0      0.831295      0.301958      0.805722      Biso  1.000000  H
H22     1.0      0.316714      0.880765      0.719673      Biso  1.000000  H
H23     1.0      0.685083      0.169581      0.670724      Biso  1.000000  H
H24     1.0      0.182384      0.685552      0.763610      Biso  1.000000  H
H25     1.0      0.335478      0.215227      0.311170      Biso  1.000000  H
H26     1.0      0.777038      0.616425      0.290870      Biso  1.000000  H
H27     1.0      0.233059      0.377133      0.278165      Biso  1.000000  H
H28     1.0      0.666737      0.769688      0.337483      Biso  1.000000  H
H29     1.0      0.288431      0.162944      0.186364      Biso  1.000000  H
H30     1.0      0.801634      0.668140      0.168859      Biso  1.000000  H
H31     1.0      0.188321      0.328101      0.160466      Biso  1.000000  H
H32     1.0      0.691811      0.824297      0.207643      Biso  1.000000  H
H33     1.0      0.195458      0.186350      0.292966      Biso  1.000000  H
  
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H34	1.0	0.676710	0.628324	0.203614	Biso	1.000000	H
H35	1.0	0.318979	0.356219	0.177648	Biso	1.000000	H
H36	1.0	0.800152	0.810041	0.300814	Biso	1.000000	H
H37	1.0	0.817626	0.239614	0.130739	Biso	1.000000	H
H38	1.0	0.348787	0.755251	0.193285	Biso	1.000000	H
H39	1.0	0.685558	0.324794	0.244717	Biso	1.000000	H
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
H43	1.0	0.752563	0.265814	0.357252	Biso	1.000000	H
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
C1	1.0	0.214451	0.269069	0.753837	Biso	1.000000	C
C2	1.0	0.757191	0.291885	0.759827	Biso	1.000000	C
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
N1	1.0	0.665320	0.746268	0.730994	Biso	1.000000	N
N2	1.0	0.248209	0.833054	0.710876	Biso	1.000000	N
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
N5	1.0	0.325955	0.251132	0.714994	Biso	1.000000	N
N6	1.0	0.753565	0.180449	0.717107	Biso	1.000000	N
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
Pb1	1.0	0.503526	-0.004917	0.495550	Biso	1.000000	Pb
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
Pb5	1.0	0.497233	0.005883	0.005704	Biso	1.000000	Pb
Pb6	1.0	-0.004493	0.503379	-0.004221	Biso	1.000000	Pb
Pb7	1.0	0.002249	-0.004962	0.506590	Biso	1.000000	Pb
Pb8	1.0	0.506020	0.497771	0.491853	Biso	1.000000	Pb
I1	1.0	0.488171	-0.005406	0.753441	Biso	1.000000	I
I2	1.0	0.010718	0.516262	0.751559	Biso	1.000000	I
I3	1.0	-0.016417	0.004729	0.258110	Biso	1.000000	I
I4	1.0	0.500933	0.496599	0.243430	Biso	1.000000	I
I5	1.0	0.515588	0.010807	0.251383	Biso	1.000000	I
I6	1.0	-0.005246	0.488227	0.253539	Biso	1.000000	I
I7	1.0	0.004845	-0.016203	0.758162	Biso	1.000000	I
I8	1.0	0.497104	0.500535	0.743447	Biso	1.000000	I
I9	1.0	0.945045	0.245310	0.514945	Biso	1.000000	I
I10	1.0	0.449963	0.745621	0.516129	Biso	1.000000	I
I11	1.0	0.555253	0.245512	0.523078	Biso	1.000000	I
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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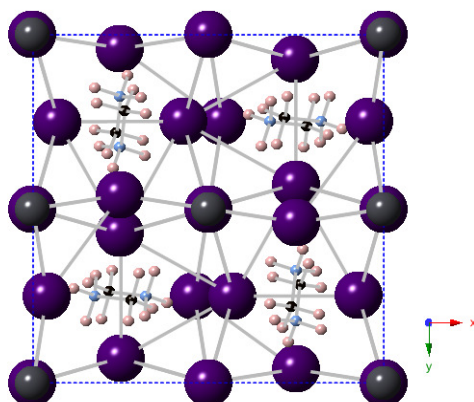
CRYSTAL DATA

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data_VESTA_phase_1

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_cell_length_b           12.43094
_cell_length_c           12.60000
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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
  
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loop_
_symmetry_equiv_pos_as_xyz
  'x, y, z'
  
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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
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H2      1.0      0.819112      0.308196      0.335890      Biso  1.000000  H
H3      1.0      0.808196      0.680888      0.335890      Biso  1.000000  H
H4      1.0      0.191804      0.319112      0.335890      Biso  1.000000  H
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
H8      1.0      0.308196      0.180888      0.664110      Biso  1.000000  H
H9      1.0      0.116854      0.728975      0.222234      Biso  1.000000  H
H10     1.0      0.883146      0.271025      0.222234      Biso  1.000000  H
H11     1.0      0.771025      0.616854      0.222234      Biso  1.000000  H
H12     1.0      0.228975      0.383146      0.222234      Biso  1.000000  H
H13     1.0      0.383146      0.771025      0.777766      Biso  1.000000  H
H14     1.0      0.616854      0.228975      0.777766      Biso  1.000000  H
H15     1.0      0.728975      0.883146      0.777766      Biso  1.000000  H
H16     1.0      0.271025      0.116854      0.777766      Biso  1.000000  H
H17     1.0      0.153531      0.821478      0.312066      Biso  1.000000  H
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
H29     1.0      0.226369      0.677360      0.840833      Biso  1.000000  H
H30     1.0      0.773631      0.322640      0.840833      Biso  1.000000  H
H31     1.0      0.822640      0.726369      0.840833      Biso  1.000000  H
H32     1.0      0.177360      0.273631      0.840833      Biso  1.000000  H
H33     1.0      0.303137      0.684205      0.185508      Biso  1.000000  H
  
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H34	1.0	0.696863	0.315795	0.185508	Biso	1.000000	H
H35	1.0	0.815795	0.803137	0.185508	Biso	1.000000	H
H36	1.0	0.184205	0.196863	0.185508	Biso	1.000000	H
H37	1.0	0.196863	0.815795	0.814492	Biso	1.000000	H
H38	1.0	0.803137	0.184205	0.814492	Biso	1.000000	H
H39	1.0	0.684205	0.696863	0.814492	Biso	1.000000	H
H40	1.0	0.315795	0.303137	0.814492	Biso	1.000000	H
H41	1.0	0.342949	0.786183	0.279005	Biso	1.000000	H
H42	1.0	0.657051	0.213817	0.279005	Biso	1.000000	H
H43	1.0	0.713817	0.842949	0.279005	Biso	1.000000	H
H44	1.0	0.286183	0.157051	0.279005	Biso	1.000000	H
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
H48	1.0	0.213817	0.342949	0.720995	Biso	1.000000	H
C1	1.0	0.281841	0.761591	0.221292	Biso	1.000000	C
C2	1.0	0.718159	0.238409	0.221292	Biso	1.000000	C
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
C5	1.0	0.218160	0.738409	0.778708	Biso	1.000000	C
C6	1.0	0.781841	0.261591	0.778708	Biso	1.000000	C
C7	1.0	0.761591	0.718159	0.778708	Biso	1.000000	C
C8	1.0	0.238409	0.281841	0.778708	Biso	1.000000	C
N1	1.0	0.176614	0.749974	0.276542	Biso	1.000000	N
N2	1.0	0.823386	0.250026	0.276542	Biso	1.000000	N
N3	1.0	0.750026	0.676614	0.276542	Biso	1.000000	N
N4	1.0	0.249974	0.323386	0.276542	Biso	1.000000	N
N5	1.0	0.323386	0.750026	0.723458	Biso	1.000000	N
N6	1.0	0.676614	0.249974	0.723458	Biso	1.000000	N
N7	1.0	0.749974	0.823386	0.723458	Biso	1.000000	N
N8	1.0	0.250026	0.176614	0.723458	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	-0.005810	Biso	1.000000	Pb
Pb4	1.0	-0.000000	0.500000	0.005810	Biso	1.000000	Pb
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
Pb8	1.0	0.500000	0.500000	-0.000000	Biso	1.000000	Pb
I1	1.0	0.428700	0.249695	0.502562	Biso	1.000000	I
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

#=====

CRYSTAL DATA

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data_VESTA_phase_1

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_cell_length_b           12.41679
_cell_length_c           12.57000
_cell_angle_alpha        90
_cell_angle_beta         90
_cell_angle_gamma        90
_symmetry_space_group_name_H-M 'P 1'
_symmetry_Int_Tables_number 1
    
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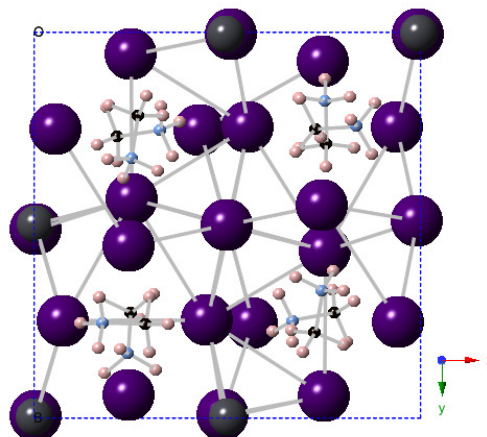
loop_
_symmetry_equiv_pos_as_xyz
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loop_

```

_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
    
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H1	1.0	0.164655	0.290809	0.691687	Biso	1.000000	H
H2	1.0	0.671348	0.803620	0.662988	Biso	1.000000	H
H3	1.0	0.329761	0.190942	0.663715	Biso	1.000000	H
H4	1.0	0.829492	0.696870	0.702080	Biso	1.000000	H
H5	1.0	0.217187	0.335672	0.817256	Biso	1.000000	H
H6	1.0	0.618276	0.775647	0.784061	Biso	1.000000	H
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
H10	1.0	0.634195	0.677123	0.694840	Biso	1.000000	H
H11	1.0	0.358823	0.321286	0.684034	Biso	1.000000	H
H12	1.0	0.811519	0.803616	0.796945	Biso	1.000000	H
H13	1.0	0.685961	0.300622	0.811232	Biso	1.000000	H
H14	1.0	0.184868	0.882618	0.744830	Biso	1.000000	H
H15	1.0	0.754349	0.121602	0.775468	Biso	1.000000	H
H16	1.0	0.276253	0.741963	0.850266	Biso	1.000000	H
H17	1.0	0.755753	0.347809	0.694851	Biso	1.000000	H
H18	1.0	0.223717	0.822216	0.632606	Biso	1.000000	H
H19	1.0	0.819951	0.166708	0.665363	Biso	1.000000	H
H20	1.0	0.309663	0.676867	0.726658	Biso	1.000000	H
H21	1.0	0.830279	0.298834	0.807415	Biso	1.000000	H
H22	1.0	0.316777	0.874972	0.715079	Biso	1.000000	H
H23	1.0	0.685758	0.168772	0.667965	Biso	1.000000	H
H24	1.0	0.171375	0.689306	0.766699	Biso	1.000000	H
H25	1.0	0.335635	0.217335	0.317636	Biso	1.000000	H
H26	1.0	0.775787	0.618257	0.284097	Biso	1.000000	H
H27	1.0	0.233049	0.378861	0.282899	Biso	1.000000	H
H28	1.0	0.668169	0.773881	0.331082	Biso	1.000000	H
H29	1.0	0.290851	0.164609	0.192123	Biso	1.000000	H
H30	1.0	0.803406	0.671282	0.162916	Biso	1.000000	H
H31	1.0	0.191088	0.329711	0.163789	Biso	1.000000	H
H32	1.0	0.696420	0.829246	0.202055	Biso	1.000000	H
H33	1.0	0.195676	0.188150	0.297369	Biso	1.000000	H



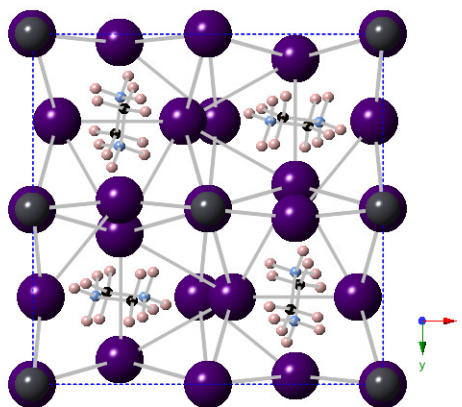
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H41	1.0	0.882832	0.183561	0.243058	Biso	1.000000	H
H42	1.0	0.300584	0.686138	0.311548	Biso	1.000000	H
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H44	1.0	0.121628	0.754435	0.275341	Biso	1.000000	H
H45	1.0	0.876309	0.316398	0.216906	Biso	1.000000	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
C1	1.0	0.216309	0.269946	0.759211	Biso	1.000000	C
C2	1.0	0.756659	0.289562	0.760373	Biso	1.000000	C
C3	1.0	0.269954	0.216385	0.259545	Biso	1.000000	C
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
N1	1.0	0.668810	0.747089	0.724388	Biso	1.000000	N
N2	1.0	0.244044	0.833089	0.712063	Biso	1.000000	N
N3	1.0	0.747001	0.668673	0.224429	Biso	1.000000	N
N4	1.0	0.833780	0.244122	0.211974	Biso	1.000000	N
N5	1.0	0.327927	0.252674	0.719806	Biso	1.000000	N
N6	1.0	0.754031	0.178964	0.715070	Biso	1.000000	N
N7	1.0	0.252762	0.327943	0.219943	Biso	1.000000	N
N8	1.0	0.179068	0.753944	0.215031	Biso	1.000000	N
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Pb2	1.0	0.004494	0.497692	0.504110	Biso	1.000000	Pb
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
Pb5	1.0	0.497547	0.004191	0.003638	Biso	1.000000	Pb
Pb6	1.0	-0.003225	0.502141	-0.005087	Biso	1.000000	Pb
Pb7	1.0	0.002486	-0.003495	0.504898	Biso	1.000000	Pb
Pb8	1.0	0.504830	0.499584	0.489571	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
I4	1.0	0.500502	0.498862	0.241596	Biso	1.000000	I
I5	1.0	0.509937	0.006351	0.250422	Biso	1.000000	I
I6	1.0	-0.007662	0.489368	0.252694	Biso	1.000000	I
I7	1.0	0.004894	-0.006921	0.757462	Biso	1.000000	I
I8	1.0	0.499037	0.500357	0.741605	Biso	1.000000	I
I9	1.0	0.939740	0.246373	0.508113	Biso	1.000000	I
I10	1.0	0.448227	0.746889	0.514932	Biso	1.000000	I
I11	1.0	0.554606	0.246576	0.522265	Biso	1.000000	I
I12	1.0	0.076564	0.747932	0.484166	Biso	1.000000	I
I13	1.0	0.253908	0.430984	0.487163	Biso	1.000000	I
I14	1.0	0.750872	0.942218	0.531598	Biso	1.000000	I
I15	1.0	0.251829	0.057825	0.518380	Biso	1.000000	I
I16	1.0	0.754193	0.566120	0.494885	Biso	1.000000	I
I17	1.0	0.747769	0.076389	0.984067	Biso	1.000000	I
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
I22	1.0	0.565995	0.753796	0.994772	Biso	1.000000	I
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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# CRYSTAL DATA
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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
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_atom_site_B_iso_or_equiv
_atom_site_type_symbol
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H2      1.0      0.815125      0.308769      0.332901      Biso  1.000000  H
H3      1.0      0.808769      0.684875      0.332901      Biso  1.000000  H
H4      1.0      0.191231      0.315125      0.332901      Biso  1.000000  H
H5      1.0      0.315125      0.808769      0.667099      Biso  1.000000  H
H6      1.0      0.684875      0.191231      0.667099      Biso  1.000000  H
H7      1.0      0.691231      0.815125      0.667099      Biso  1.000000  H
H8      1.0      0.308769      0.184875      0.667099      Biso  1.000000  H
H9      1.0      0.120753      0.727397      0.218640      Biso  1.000000  H
H10     1.0      0.879247      0.272603      0.218640      Biso  1.000000  H
H11     1.0      0.772603      0.620753      0.218640      Biso  1.000000  H
H12     1.0      0.227397      0.379247      0.218640      Biso  1.000000  H
H13     1.0      0.379247      0.772603      0.781360      Biso  1.000000  H
H14     1.0      0.620753      0.227397      0.781360      Biso  1.000000  H
H15     1.0      0.727397      0.879247      0.781360      Biso  1.000000  H
H16     1.0      0.272603      0.120753      0.781360      Biso  1.000000  H
H17     1.0      0.155566      0.820814      0.308519      Biso  1.000000  H
H18     1.0      0.844434      0.179186      0.308519      Biso  1.000000  H
H19     1.0      0.679186      0.655566      0.308519      Biso  1.000000  H
H20     1.0      0.320814      0.344434      0.308519      Biso  1.000000  H
H21     1.0      0.344434      0.679186      0.691481      Biso  1.000000  H
H22     1.0      0.655566      0.320814      0.691481      Biso  1.000000  H
H23     1.0      0.820814      0.844434      0.691481      Biso  1.000000  H
H24     1.0      0.179186      0.155566      0.691481      Biso  1.000000  H
H25     1.0      0.277271      0.823580      0.156273      Biso  1.000000  H
H26     1.0      0.722729      0.176420      0.156273      Biso  1.000000  H
H27     1.0      0.676420      0.777271      0.156273      Biso  1.000000  H
H28     1.0      0.323580      0.222729      0.156273      Biso  1.000000  H
H29     1.0      0.222729      0.676420      0.843727      Biso  1.000000  H
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H31     1.0      0.823580      0.722729      0.843727      Biso  1.000000  H
H32     1.0      0.176420      0.277271      0.843727      Biso  1.000000  H
H33     1.0      0.308344      0.685288      0.182900      Biso  1.000000  H
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H34	1.0	0.691656	0.314712	0.182900	Biso	1.000000	H
H35	1.0	0.814712	0.808344	0.182900	Biso	1.000000	H
H36	1.0	0.185288	0.191656	0.182900	Biso	1.000000	H
H37	1.0	0.191656	0.814712	0.817100	Biso	1.000000	H
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
C1	1.0	0.285623	0.762462	0.218550	Biso	1.000000	C
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
N1	1.0	0.180050	0.749418	0.273328	Biso	1.000000	N
N2	1.0	0.819950	0.250582	0.273328	Biso	1.000000	N
N3	1.0	0.750582	0.680050	0.273328	Biso	1.000000	N
N4	1.0	0.249418	0.319950	0.273328	Biso	1.000000	N
N5	1.0	0.319950	0.750582	0.726672	Biso	1.000000	N
N6	1.0	0.680050	0.249418	0.726672	Biso	1.000000	N
N7	1.0	0.749418	0.819950	0.726672	Biso	1.000000	N
N8	1.0	0.250582	0.180050	0.726672	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	-0.005177	Biso	1.000000	Pb
Pb4	1.0	-0.000000	0.500000	0.005177	Biso	1.000000	Pb
Pb5	1.0	0.500000	0.000000	0.487106	Biso	1.000000	Pb
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
I1	1.0	0.429154	0.250014	0.504921	Biso	1.000000	I
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
I24	1.0	0.500000	0.000000	0.737894	Biso	1.000000	I

P1_0.41GPa_cubic.cif

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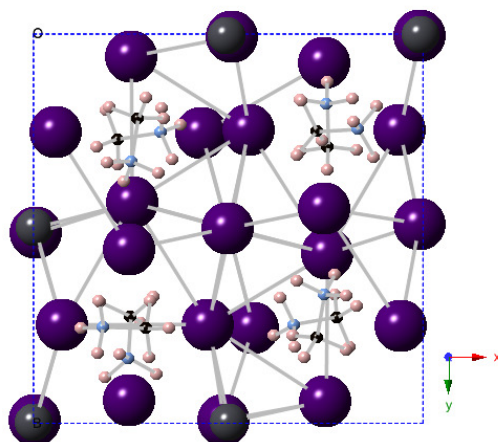
CRYSTAL DATA

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_atom_site_fract_x
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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
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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
H21     1.0      0.830259      0.298883      0.808226      Biso  1.000000  H
H22     1.0      0.317594      0.873965      0.714421      Biso  1.000000  H
H23     1.0      0.685721      0.168996      0.666700      Biso  1.000000  H
H24     1.0      0.170898      0.689376      0.767569      Biso  1.000000  H
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
H27     1.0      0.234152      0.379035      0.283288      Biso  1.000000  H
H28     1.0      0.668098      0.774486      0.331886      Biso  1.000000  H
H29     1.0      0.290145      0.163914      0.191916      Biso  1.000000  H
H30     1.0      0.803980      0.671513      0.162217      Biso  1.000000  H
H31     1.0      0.190611      0.329555      0.163100      Biso  1.000000  H
H32     1.0      0.697301      0.830208      0.201554      Biso  1.000000  H
H33     1.0      0.195350      0.188401      0.298641      Biso  1.000000  H
  
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H37	1.0	0.823279	0.225139	0.131440	Biso	1.000000	H
H38	1.0	0.348177	0.755653	0.194420	Biso	1.000000	H
H39	1.0	0.677697	0.310655	0.228081	Biso	1.000000	H
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
H43	1.0	0.742033	0.273091	0.352534	Biso	1.000000	H
H44	1.0	0.121847	0.754528	0.275491	Biso	1.000000	H
H45	1.0	0.875395	0.317127	0.216477	Biso	1.000000	H
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
H48	1.0	0.169154	0.685557	0.166806	Biso	1.000000	H
C1	1.0	0.216071	0.269693	0.759676	Biso	1.000000	C
C2	1.0	0.756648	0.289667	0.760498	Biso	1.000000	C
C3	1.0	0.269703	0.216127	0.260026	Biso	1.000000	C
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
C8	1.0	0.727868	0.250245	0.268537	Biso	1.000000	C
N1	1.0	0.669296	0.746903	0.723832	Biso	1.000000	N
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
N8	1.0	0.179275	0.754020	0.214353	Biso	1.000000	N
Pb1	1.0	0.502602	-0.003217	0.495494	Biso	1.000000	Pb
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
Pb7	1.0	0.002887	-0.003501	0.505126	Biso	1.000000	Pb
Pb8	1.0	0.505057	0.499903	0.490069	Biso	1.000000	Pb
I1	1.0	0.488171	-0.008637	0.752010	Biso	1.000000	I
I2	1.0	0.006309	0.510732	0.750915	Biso	1.000000	I
I3	1.0	-0.006955	0.005059	0.257132	Biso	1.000000	I
I4	1.0	0.500082	0.498765	0.241939	Biso	1.000000	I
I5	1.0	0.510438	0.006283	0.250551	Biso	1.000000	I
I6	1.0	-0.008343	0.488082	0.252367	Biso	1.000000	I
I7	1.0	0.005168	-0.007098	0.757148	Biso	1.000000	I
I8	1.0	0.498882	0.499919	0.741942	Biso	1.000000	I
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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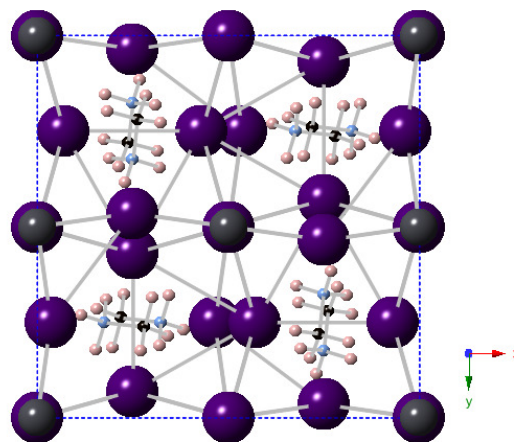
CRYSTAL DATA

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data_VESTA_phase_1

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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
_atom_site_B_iso_or_equiv
_atom_site_type_symbol
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H2      1.0      0.819790      0.309408      0.335625      Biso  1.000000  H
H3      1.0      0.809408      0.680210      0.335625      Biso  1.000000  H
H4      1.0      0.190592      0.319790      0.335625      Biso  1.000000  H
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
H9      1.0      0.115365      0.731339      0.221482      Biso  1.000000  H
H10     1.0      0.884635      0.268661      0.221482      Biso  1.000000  H
H11     1.0      0.768661      0.615365      0.221482      Biso  1.000000  H
H12     1.0      0.231339      0.384635      0.221482      Biso  1.000000  H
H13     1.0      0.384635      0.768661      0.778518      Biso  1.000000  H
H14     1.0      0.615365      0.231339      0.778518      Biso  1.000000  H
H15     1.0      0.731339      0.884635      0.778518      Biso  1.000000  H
H16     1.0      0.268661      0.115365      0.778518      Biso  1.000000  H
H17     1.0      0.154305      0.821432      0.314793      Biso  1.000000  H
H18     1.0      0.845695      0.178568      0.314793      Biso  1.000000  H
H19     1.0      0.678568      0.654305      0.314793      Biso  1.000000  H
H20     1.0      0.321432      0.345695      0.314793      Biso  1.000000  H
H21     1.0      0.345695      0.678568      0.685207      Biso  1.000000  H
H22     1.0      0.654305      0.321432      0.685207      Biso  1.000000  H
H23     1.0      0.821432      0.845695      0.685207      Biso  1.000000  H
H24     1.0      0.178568      0.154305      0.685207      Biso  1.000000  H
H25     1.0      0.272910      0.824733      0.158224      Biso  1.000000  H
H26     1.0      0.727090      0.175267      0.158224      Biso  1.000000  H
H27     1.0      0.675267      0.772910      0.158224      Biso  1.000000  H
H28     1.0      0.324733      0.227090      0.158224      Biso  1.000000  H
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H31     1.0      0.824733      0.727090      0.841776      Biso  1.000000  H
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H33     1.0      0.301146      0.685013      0.181660      Biso  1.000000  H
    
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H35	1.0	0.814987	0.801145	0.181660	Biso	1.000000	H
H36	1.0	0.185013	0.198854	0.181660	Biso	1.000000	H
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
H39	1.0	0.685013	0.698855	0.818340	Biso	1.000000	H
H40	1.0	0.314987	0.301146	0.818340	Biso	1.000000	H
H41	1.0	0.342990	0.784740	0.278417	Biso	1.000000	H
H42	1.0	0.657010	0.215260	0.278417	Biso	1.000000	H
H43	1.0	0.715260	0.842990	0.278417	Biso	1.000000	H
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
C1	1.0	0.281021	0.762041	0.219819	Biso	1.000000	C
C2	1.0	0.718979	0.237959	0.219819	Biso	1.000000	C
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
N1	1.0	0.175944	0.750325	0.276698	Biso	1.000000	N
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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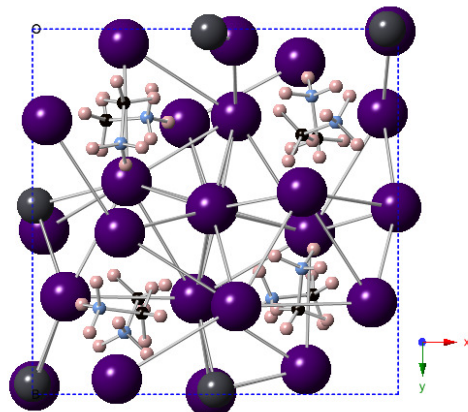
CRYSTAL DATA

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data_VESTA_phase_1

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_symmetry_Int_Tables_number 1
    
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loop_
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_atom_site_fract_x
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_atom_site_type_symbol
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H2      1.0      0.654875      0.789970      0.668336      Biso  1.000000  H
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
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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
H33     1.0      0.191145      0.194121      0.313772      Biso  1.000000  H
    
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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
Pb1	1.0	0.503105	-0.011851	0.489332	Biso	1.000000	Pb
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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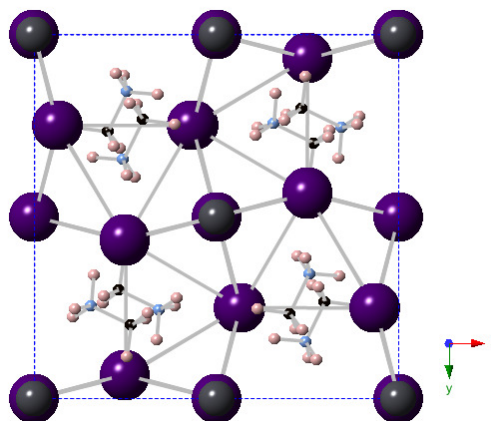
CRYSTAL DATA

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data_VESTA_phase_1

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_cell_length_b           12.22000
_cell_length_c           12.22000
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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
    
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loop_
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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      0.163629      0.661524      0.265805      Biso  1.000000  H
H2      1.0      0.836371      0.338476      0.265805      Biso  1.000000  H
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
H32     1.0      0.113753      0.254737      0.764071      Biso  1.000000  H
H33     1.0      0.312168      0.763575      0.178897      Biso  1.000000  H
    
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H35	1.0	0.736425	0.812168	0.178897	Biso	1.000000	H
H36	1.0	0.263575	0.187832	0.178897	Biso	1.000000	H
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
C1	1.0	0.266120	0.798278	0.247424	Biso	1.000000	C
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
I11	1.0	0.561933	0.750178	0.969810	Biso	1.000000	I
I12	1.0	0.438067	0.249822	0.969810	Biso	1.000000	I
I13	1.0	0.249822	0.561933	0.030190	Biso	1.000000	I
I14	1.0	0.750178	0.438067	0.030190	Biso	1.000000	I
I15	1.0	0.938067	0.749822	0.030190	Biso	1.000000	I
I16	1.0	0.061933	0.250178	0.030190	Biso	1.000000	I
I17	1.0	0.500000	-0.000000	0.250346	Biso	1.000000	I
I18	1.0	-0.000000	0.500000	0.749654	Biso	1.000000	I
I19	1.0	-0.000000	-0.000000	0.749688	Biso	1.000000	I
I20	1.0	0.500000	0.500000	0.749688	Biso	1.000000	I
I21	1.0	0.500000	0.500000	0.250312	Biso	1.000000	I
I22	1.0	-0.000000	-0.000000	0.250312	Biso	1.000000	I
I23	1.0	-0.000000	0.500000	0.250442	Biso	1.000000	I
I24	1.0	0.500000	-0.000000	0.749558	Biso	1.000000	I

P1_1.95GPa_cubic.cif

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CRYSTAL DATA

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data_VESTA_phase_1

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_symmetry_space_group_name_H-M 'P 1'
_symmetry_Int_Tables_number 1
    
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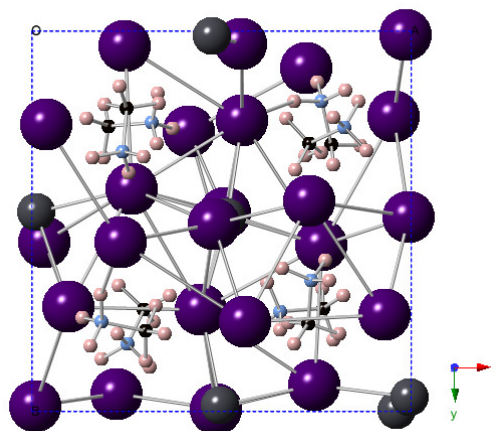
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loop_
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loop_
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H2	1.0	0.655935	0.785309	0.663193	Biso	1.000000	H
H3	1.0	0.332555	0.162503	0.676479	Biso	1.000000	H
H4	1.0	0.822790	0.694307	0.717864	Biso	1.000000	H
H5	1.0	0.189152	0.334002	0.778793	Biso	1.000000	H
H6	1.0	0.603066	0.774757	0.791418	Biso	1.000000	H
H7	1.0	0.373362	0.257194	0.769197	Biso	1.000000	H
H8	1.0	0.766246	0.676078	0.853476	Biso	1.000000	H
H9	1.0	0.191961	0.191399	0.816950	Biso	1.000000	H
H10	1.0	0.622638	0.660798	0.716316	Biso	1.000000	H
H11	1.0	0.329255	0.295579	0.641958	Biso	1.000000	H
H12	1.0	0.796805	0.811735	0.803630	Biso	1.000000	H
H13	1.0	0.722644	0.328645	0.798222	Biso	1.000000	H
H14	1.0	0.185119	0.861869	0.755746	Biso	1.000000	H
H15	1.0	0.754136	0.134444	0.777937	Biso	1.000000	H
H16	1.0	0.321687	0.764611	0.867164	Biso	1.000000	H
H17	1.0	0.796014	0.352191	0.672262	Biso	1.000000	H
H18	1.0	0.227331	0.796247	0.641967	Biso	1.000000	H
H19	1.0	0.828400	0.154738	0.660784	Biso	1.000000	H
H20	1.0	0.366033	0.694534	0.743943	Biso	1.000000	H
H21	1.0	0.867332	0.299912	0.791284	Biso	1.000000	H
H22	1.0	0.312753	0.883543	0.708353	Biso	1.000000	H
H23	1.0	0.693774	0.183761	0.661570	Biso	1.000000	H
H24	1.0	0.231024	0.670246	0.798492	Biso	1.000000	H
H25	1.0	0.334576	0.189651	0.278982	Biso	1.000000	H
H26	1.0	0.774081	0.603075	0.291648	Biso	1.000000	H
H27	1.0	0.256570	0.373377	0.269089	Biso	1.000000	H
H28	1.0	0.675994	0.766494	0.353476	Biso	1.000000	H
H29	1.0	0.231476	0.145013	0.182375	Biso	1.000000	H
H30	1.0	0.785076	0.655793	0.163347	Biso	1.000000	H
H31	1.0	0.162200	0.331818	0.176381	Biso	1.000000	H
H32	1.0	0.694159	0.822880	0.217784	Biso	1.000000	H
H33	1.0	0.191964	0.191651	0.317171	Biso	1.000000	H



H34	1.0	0.660402	0.622817	0.216193	Biso	1.000000	H
H35	1.0	0.295314	0.329329	0.141983	Biso	1.000000	H
H36	1.0	0.811645	0.796764	0.303445	Biso	1.000000	H
H37	1.0	0.797153	0.227443	0.141797	Biso	1.000000	H
H38	1.0	0.352400	0.795324	0.171542	Biso	1.000000	H
H39	1.0	0.694318	0.364770	0.244211	Biso	1.000000	H
H40	1.0	0.155099	0.828687	0.160810	Biso	1.000000	H
H41	1.0	0.863191	0.185268	0.255335	Biso	1.000000	H
H42	1.0	0.328965	0.721855	0.297470	Biso	1.000000	H
H43	1.0	0.765035	0.320976	0.367253	Biso	1.000000	H
H44	1.0	0.134799	0.754420	0.277959	Biso	1.000000	H
H45	1.0	0.883929	0.313238	0.208425	Biso	1.000000	H
H46	1.0	0.300940	0.866693	0.290879	Biso	1.000000	H
H47	1.0	0.671419	0.229493	0.298647	Biso	1.000000	H
H48	1.0	0.183452	0.693917	0.161382	Biso	1.000000	H
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C2	1.0	0.789605	0.299651	0.745330	Biso	1.000000	C
C3	1.0	0.250316	0.202556	0.249397	Biso	1.000000	C
C4	1.0	0.300102	0.789043	0.244810	Biso	1.000000	C
C5	1.0	0.768456	0.729253	0.780683	Biso	1.000000	C
C6	1.0	0.296112	0.731554	0.787271	Biso	1.000000	C
C7	1.0	0.729085	0.768547	0.280617	Biso	1.000000	C
C8	1.0	0.732094	0.295175	0.287400	Biso	1.000000	C
N1	1.0	0.655573	0.737857	0.734726	Biso	1.000000	N
N2	1.0	0.252546	0.823246	0.719334	Biso	1.000000	N
N3	1.0	0.737468	0.655607	0.234776	Biso	1.000000	N
N4	1.0	0.824075	0.252515	0.219249	Biso	1.000000	N
N5	1.0	0.316853	0.240797	0.706922	Biso	1.000000	N
N6	1.0	0.765259	0.185413	0.709751	Biso	1.000000	N
N7	1.0	0.240570	0.316664	0.206927	Biso	1.000000	N
N8	1.0	0.185613	0.765344	0.209614	Biso	1.000000	N
Pb1	1.0	0.497591	0.984912	0.488752	Biso	1.000000	Pb
Pb2	1.0	0.012028	0.476657	0.508959	Biso	1.000000	Pb
Pb3	1.0	0.962819	0.997638	0.996179	Biso	1.000000	Pb
Pb4	1.0	0.487796	0.517239	0.989387	Biso	1.000000	Pb
Pb5	1.0	0.476286	0.012198	0.008593	Biso	1.000000	Pb
Pb6	1.0	0.984400	0.497981	0.989047	Biso	1.000000	Pb
Pb7	1.0	0.997213	0.963045	0.496178	Biso	1.000000	Pb
Pb8	1.0	0.516888	0.488201	0.489500	Biso	1.000000	Pb
I1	1.0	0.487772	0.993508	0.752112	Biso	1.000000	I
I2	1.0	0.033945	0.553992	0.749675	Biso	1.000000	I
I3	1.0	0.987478	0.009404	0.248379	Biso	1.000000	I
I4	1.0	0.480051	0.507936	0.241666	Biso	1.000000	I
I5	1.0	0.553571	0.033817	0.249360	Biso	1.000000	I
I6	1.0	0.994130	0.487868	0.252280	Biso	1.000000	I
I7	1.0	0.008956	0.986114	0.748466	Biso	1.000000	I
I8	1.0	0.510153	0.479625	0.741864	Biso	1.000000	I
I9	1.0	0.954656	0.225092	0.498342	Biso	1.000000	I
I10	1.0	0.447166	0.733737	0.512769	Biso	1.000000	I
I11	1.0	0.554928	0.234906	0.524839	Biso	1.000000	I
I12	1.0	0.097898	0.725731	0.479037	Biso	1.000000	I
I13	1.0	0.263299	0.414936	0.483178	Biso	1.000000	I
I14	1.0	0.745907	0.931234	0.541433	Biso	1.000000	I
I15	1.0	0.246427	0.040167	0.503848	Biso	1.000000	I
I16	1.0	0.765070	0.562965	0.510352	Biso	1.000000	I
I17	1.0	0.725492	0.098166	0.979178	Biso	1.000000	I
I18	1.0	0.234644	0.554928	0.024795	Biso	1.000000	I
I19	1.0	0.733482	0.447153	0.013292	Biso	1.000000	I
I20	1.0	0.224950	0.954416	0.997862	Biso	1.000000	I
I21	1.0	0.040240	0.246769	0.003313	Biso	1.000000	I
I22	1.0	0.562781	0.765188	0.010592	Biso	1.000000	I
I23	1.0	0.414671	0.263461	0.982857	Biso	1.000000	I
I24	1.0	0.931025	0.746319	0.041997	Biso	1.000000	I

P4n_1.95GPa_cubic.cif

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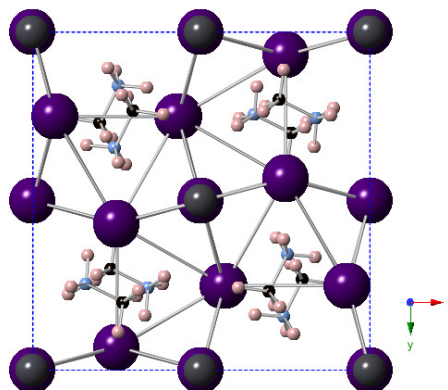
CRYSTAL DATA

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data_VESTA_phase_1

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_cell_length_b          12.14000
_cell_length_c          12.14000
_cell_angle_alpha       90
_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      0.164987      0.660946      0.265693      Biso  1.000000  H
H2      1.0      0.835013      0.339054      0.265693      Biso  1.000000  H
H3      1.0      0.839054      0.664987      0.265693      Biso  1.000000  H
H4      1.0      0.160946      0.335013      0.265693      Biso  1.000000  H
H5      1.0      0.335013      0.839054      0.734307      Biso  1.000000  H
H6      1.0      0.664987      0.160946      0.734307      Biso  1.000000  H
H7      1.0      0.660946      0.835013      0.734307      Biso  1.000000  H
H8      1.0      0.339054      0.164987      0.734307      Biso  1.000000  H
H9      1.0      0.115133      0.753278      0.176520      Biso  1.000000  H
H10     1.0      0.884867      0.246722      0.176520      Biso  1.000000  H
H11     1.0      0.746722      0.615133      0.176520      Biso  1.000000  H
H12     1.0      0.253278      0.384867      0.176520      Biso  1.000000  H
H13     1.0      0.384867      0.746722      0.823480      Biso  1.000000  H
H14     1.0      0.615133      0.253278      0.823480      Biso  1.000000  H
H15     1.0      0.753278      0.884867      0.823480      Biso  1.000000  H
H16     1.0      0.246722      0.115133      0.823480      Biso  1.000000  H
H17     1.0      0.107517      0.776451      0.311860      Biso  1.000000  H
H18     1.0      0.892483      0.223549      0.311860      Biso  1.000000  H
H19     1.0      0.723549      0.607517      0.311860      Biso  1.000000  H
H20     1.0      0.276451      0.392483      0.311860      Biso  1.000000  H
H21     1.0      0.392483      0.723549      0.688140      Biso  1.000000  H
H22     1.0      0.607517      0.276451      0.688140      Biso  1.000000  H
H23     1.0      0.776451      0.892483      0.688140      Biso  1.000000  H
H24     1.0      0.223549      0.107517      0.688140      Biso  1.000000  H
H25     1.0      0.255434      0.887748      0.236946      Biso  1.000000  H
H26     1.0      0.744566      0.112252      0.236946      Biso  1.000000  H
H27     1.0      0.612252      0.755434      0.236946      Biso  1.000000  H
H28     1.0      0.387748      0.244566      0.236946      Biso  1.000000  H
H29     1.0      0.244566      0.612252      0.763054      Biso  1.000000  H
H30     1.0      0.755434      0.387748      0.763054      Biso  1.000000  H
H31     1.0      0.887748      0.744566      0.763054      Biso  1.000000  H
H32     1.0      0.112252      0.255434      0.763054      Biso  1.000000  H
H33     1.0      0.314466      0.765191      0.178526      Biso  1.000000  H
  
```

H34	1.0	0.685534	0.234809	0.178526	Biso	1.000000	H
H35	1.0	0.734809	0.814466	0.178526	Biso	1.000000	H
H36	1.0	0.265191	0.185534	0.178526	Biso	1.000000	H
H37	1.0	0.185534	0.734809	0.821474	Biso	1.000000	H
H38	1.0	0.814466	0.265191	0.821474	Biso	1.000000	H
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
H41	1.0	0.309357	0.782356	0.325796	Biso	1.000000	H
H42	1.0	0.690643	0.217644	0.325796	Biso	1.000000	H
H43	1.0	0.717644	0.809357	0.325796	Biso	1.000000	H
H44	1.0	0.282356	0.190643	0.325796	Biso	1.000000	H
H45	1.0	0.190643	0.717644	0.674204	Biso	1.000000	H
H46	1.0	0.809357	0.282356	0.674204	Biso	1.000000	H
H47	1.0	0.782356	0.690643	0.674204	Biso	1.000000	H
H48	1.0	0.217644	0.309357	0.674204	Biso	1.000000	H
C1	1.0	0.267590	0.799159	0.247698	Biso	1.000000	C
C2	1.0	0.732410	0.200841	0.247698	Biso	1.000000	C
C3	1.0	0.700841	0.767590	0.247698	Biso	1.000000	C
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
N1	1.0	0.157919	0.744754	0.250320	Biso	1.000000	N
N2	1.0	0.842081	0.255246	0.250320	Biso	1.000000	N
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
N5	1.0	0.342081	0.755246	0.749680	Biso	1.000000	N
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
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	0.004569	Biso	1.000000	Pb
Pb4	1.0	-0.000000	0.500000	0.995431	Biso	1.000000	Pb
Pb5	1.0	0.500000	0.000000	0.497163	Biso	1.000000	Pb
Pb6	1.0	-0.000000	0.500000	0.502837	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	0.431213	0.250373	0.529800	Biso	1.000000	I
I2	1.0	0.568787	0.749627	0.529800	Biso	1.000000	I
I3	1.0	0.249627	0.931213	0.529800	Biso	1.000000	I
I4	1.0	0.750373	0.068787	0.529800	Biso	1.000000	I
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 MAPbI₃ 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 MAPbI₃. With explicit MA cations, symmetry is significantly lowered by orientations of C-N dipole and rotation of XH₃ 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.

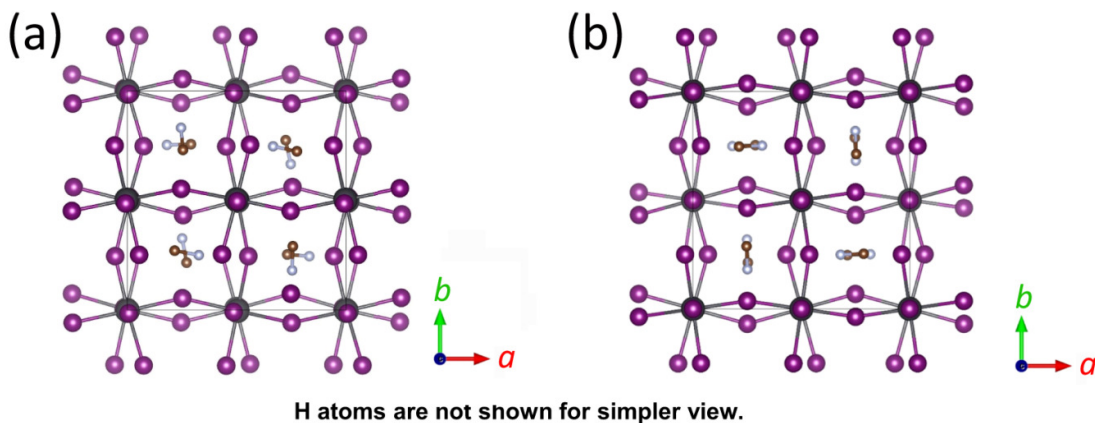


Table S4. The predicted band gaps E_g of MAPbI₃ with the two models P1 and P4/n for tetragonal and cubic phases, and the energy difference ΔE with the resulting ratios of structures, according to the Boltzmann distribution at room temperature.

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 CeO₂. 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.