Direct Single Crystal to Amorphous Transformation and Memory Effect in $AlPO_4$-17.

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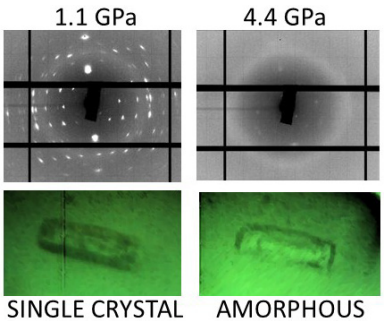
ABSTRACT: Pressure induced amorphization provides a distinct route to prepare novel amorphous materials. Single crystals of the porous aluminophosphate AlPO4-17 directly transform to an amorphous state beginning at 0.6 GPa, without fragmentation into polycrystalline material. Apart from a reduction in dimensions, the amorphous material retains the form of the initial single crystal. Remnant crystalline domains in the amorphous material also preserve the initial orientation of the single crystal. X-ray diffraction indicates the compression of the structure around the empty pores in the *xy* plane and such an amorphization mechanism is consistent with a direct structural relationship between the single crystal and amorphous forms. The collapse of the initial pore volume is almost complete at 2.5 GPa. A memory effect is observed in the amorphous form, which strongly expands on decompression. The present process opens the way for the synthesis of topologically-ordered amorphous materials approaching "perfect glasses" with improved mechanical properties.



The use of high pressure is a powerful tool to obtain new amorphous materials with distinct structural and physical properties with respect to standard glasses[1-3]. In particular, pressure was found to produce a novel amorphous form of ice[4]. There was also considerable interest placed in the amorphization of quartz SiO_2[5-7] and various minerals[1]. Pressure-induced elastic softening has been identified in materials with the unusual property of negative thermal expansion[8] followed in a large number of cases by amorphization such as in the case of zirconium tungstate ZrW_2O_8[9-10]. Both negative thermal expansion[11-13] and pressure-induced amorphization[14-21] occur in a large number of porous materials, such as zeolites. Additionally, in the case of zeolites, slow compression opens the way for the synthesis of "perfect" or ordered glasses[16]. Such "perfect glasses" exhibit a degree of structural order, low entropy and low fragility. The dense amorphous form obtained by the room temperature compression of the pure silica zeolite, silicalite-1, with the Mobil-five structure, was found to retain the framework topology of the starting zeolite, but is amorphous due to strong geometrical distortions[17]. This topologically ordered amorphous form exhibits permanent densification after compression at room temperature in contrast to silica glass[22].

The aluminophosphate, $AlPO_4$-17, with the porous hexagonal erionite (ERI) structure (space group $P6_3/m$), is the zeolite-type material with the highest coefficient of negative thermal expansion[23] and exhibits an elastic instability and pressure-induced amorphization beginning near 1 GPa[20]. In the present study, single crystals of this material are found to transform directly to the amorphous state retaining the form and orientation of the initial crystal. Single-crystal x-ray diffraction indicates a collapse of the pore network leading to amorphization.

Single crystals (110-160 μm maximum dimensions) of AlPO4-17 (Figure 1a) were studied under hydrostatic pressure in DAPHNE 7474 oil[24] by single-crystal x-ray diffraction (XRD) in a diamond anvil cell at the Xpress beamline at the Elettra Sincrotrone Trieste. The ERI structure of AlPO4-17[23] is built up of columns of alternating cancrinite (can) cages and double 6-membered ring (D6MR) secondary building units along the c direction with larger erionite (eri) cages between the columns (Figure 2a,b).

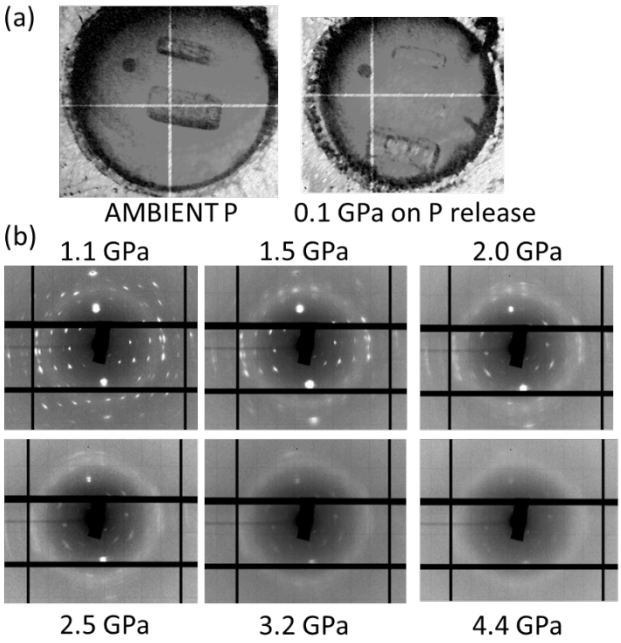


Figure 1. Optical images of investigated single crystal and amorphous $AlPO_4$-17 in the diamond anvil cell (a). X-ray rotation photographs (λ=0.4956 Å) of $AlPO_4$-17 at selected pressures (b).

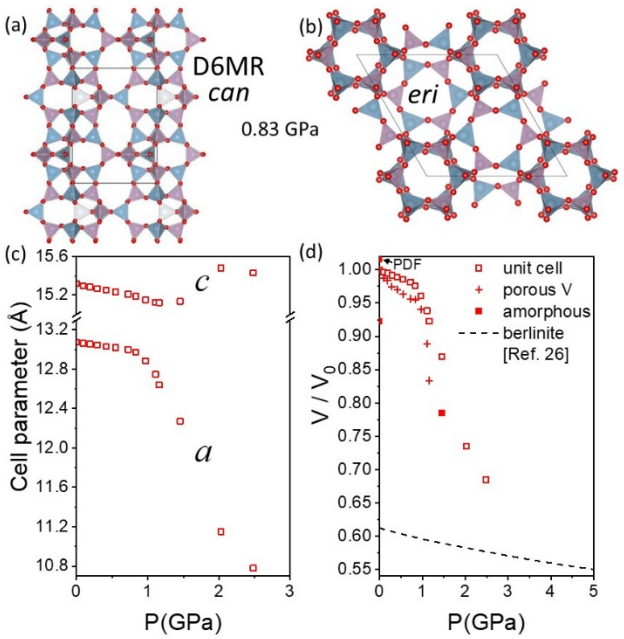


Figure 2. Projection of the polyhedral representation of the crystal structure of $AlPO_4$-17 along *x* (a) and *z* (b). Cell parameters of single-crystal $AlPO_4$-17 as a function of pressure (c). Relative unit cell volume and relative pore volume of $AlPO_4$-17 as a function of pressure (d). Data for the dense crystalline form of $AlPO_4$, berlinite, from the literature are given for comparison[26].

The XRD data were of high quality with very good agreement factors for the structure refinements up to 0.6 GPa (Tables S1-S55). Up to this pressure, compression proceeded in a conventional manner (Figure 2c, S1) with similar compressibilities along the **a** (0.0081(2) GPa^{-1}) and **c** (0.0111(5) GPa^{-1}) directions and no direct evidence of elastic softening. The pressure dependence of the unit cell volume (Figure 2d) can easily be fitted to a standard second-order Birch-Murnaghan[25] equation of state with a bulk modulus of 36(1) GPa and an implied first pressure derivative of 4 (Figure S2a). The Al-O-P angles most affected over this pressure range are the angles in the *xy* plane in the 4 membered rings (4MR) in the D6MR (Figure S3). The other angles remain quite stable. The main change is to the porous volume corresponding to the empty pores and cages (Figure 2d), which with a bulk modulus of 14(4) GPa (Figure 2b) decreases 2.6 times more rapidly than the unit cell volume and considering that the porous volume accounts for 38% of the unit cell volume, the compression mechanism correspond almost entirely to the collapse of the structure around the empty pores. At 0.55 GPa, for example, the reduction in pore volume of 32 $Å^3$ corresponds exactly to the total reduction in unit cell volume.

Beginning above 0.7 GPa, elastic softening begins in the *xy* plane (Figure 2c) with decreases in the in-plane Al-O-P angles in the large *eri* cages (Figure S3). Concomitantly, a close to 30% decrease in intensity (Figure 3a) and broadening of the reflections of the single crystal are observed without the formation of polycrystalline material. At the same time, values of the agreement R-factors for the single crystal double (see supporting information). Another major decrease in intensity by more than a factor of two follows above 1.1 GPa. At this pressure, the diffuse signal of the amorphous form (Figure 1b) is clearly visible in x-ray rotation images, and based on its intensity, the majority of the material is already amorphous at this pressure. Additionally, in the remaining crystalline phase above 0.9 GPa a large number of superlattice *hkl* reflections (Figure S4) with half integer indices in *h* and *k* (i.e. 1/2 0 8, 3/2 0 2, 3/2 5/2 4, etc.) with a maximum relative intensity of 4% appear indicating cell doubling along **a** and **b** as has also been found in oxygen filled $AlPO_4$-17 at much higher pressure[27]. No clear distortion from a hexagonal unit cell metric is observed and any eventual lowering in symmetry could not be reliably determined due to the reduction in data quality at this pressure. Due to this reduced data quality, structure refinements were performed using the undoubled hexagonal subcell over the 0.9-1.2 GPa pressure interval, above which only the unit cell parameters could be refined. Cell doubling enables increased flexibility and subsequent rapid collapse of the decreasing amount of remnant crystalline material, which is progressively becoming amorphous with each further increase in pressure. Even though there is a decrease in crystal quality, the diffraction data continue to correspond to a single crystal albeit with a degree of strain corresponding the stress gradients experienced by the single crystal domains embedded in the amorphous material (Figure 1b). In addition, the orientation of the remnant crystal domains and the form of the macroscopic amorphous material are the same as that of the initial single crystal. These results are evidence for a direct relationship between the structure of the single crystal $AlPO_4$-17 and the collapsed network of the amorphous form around the empty pores, similar to the process in which the silicalite-1 structure collapses upon amorphization while retaining the structural topology of the crystalline phase[17]. The first stages of this collapse in $AlPO_4$-17 around the empty pores are clearly demonstrated by refined structures of the crystal up to 1.2 GPa (Figure 2d and Tables S2-S55).

The diffuse halo corresponding to the first sharp diffraction peak (FSDP) increases in intensity and shifts to higher Q values with increasing pressure (Figure 3b). The increase in FSDP is an indication of a modification of the intermediate range structure of the amorphous form and for higher pressures, the values are similar to those of silica glass[28]. A large decrease in the FSDP occurs on pressure release with a value similar to that of recovered amorphous $AlPO_4$-17[20] (Figure S5). This decrease indicates that the changes in intermediate range structure are reversible. The relative volume and density of the amorphous form at ambient pressure, estimated by the reduction in single crystal dimensions upon transformation to the amorphous form (Figure 1a), are 0.92 and 1.7 g/cm^3, respectively. An independent determination of the density based on the initial slope of the reduced pair distribution function $G(r)$ from a previously-obtained, recovered, amorphous powder sample (Figures S6 and S7) yields a density of close to 1.6 g/cm^3. This is essentially the same as that of the initial crystal of $AlPO_4$-17 (1.607 g/cm^3). This low density is consistent with recovery of a significant degree of pore volume providing evidence for the retention of the initial structural topology in the amorphous form. The changes in intermediate range structure corresponding to the large decrease in the position of the FSDP in Q can be expected to arise from geometrical

changes (bond angles etc.) yielding voids in the structure. This recovered structure is not periodic and remains amorphous. This recovery of an amorphous material with a similar density to the initial crystalline phase is an indication of a memory effect at the level of the local and intermediate range order. It is distinct from the memory effect reported in crystalline, non-porous $AlPO_4$ berlinite, which was proposed to transform reversibly to an amorphous form under pressure[29]. Later studies by Raman spectroscopy[30] and x-ray powder diffraction[31] indicated that instead the high-pressure form was a poorly-crystallized phase with a $CrVO_4$ structure with Al in octahedral coordination, which retransformed to berlinite on decompression.

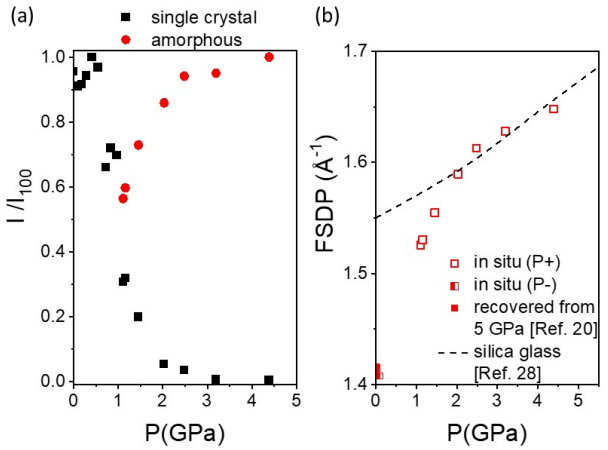


Figure 3. Normalized intensity of diffraction signals (with respect to maximum values for single crystal and amorphous) of $AlPO_4$-17 as a function of pressure (a). Position of the FSDP in Q of $AlPO_4$-17 as a function of pressure (b). Data for silica glass[28] are given for comparison.

Based on x-ray diffraction, the unit cell volume of the crystalline phase decreases by 32% between ambient pressure and 2.5 GPa. This can be compared with initial pore volume, which represents 38% of the total volume of the $AlPO_4$-17 structure. The dimensions of the sample at 1.45 GPa, which was then predominantly amorphous, give a relative volume of 0.78 for the amorphous form. This is 8% lower than the remnant crystalline domains at the same pressure. Based on these results, the amorphous form can be expected to exhibit almost no porosity at 2.5 GPa. It can be noted that starting from this pressure, the position of the FSDP is similar to that of non-porous silica glass.

The present results provide a coherent overall picture of a direct transformation of a single crystal to an amorphous material. The retained shape of the crystal and the orientation of remnant crystal domains upon transformation are consistent with a direct transformation pathway. Single-crystal x-ray diffraction indicates the collapse of the structure around the empty pores. The estimation of the density of the amorphous form provides evidence that the pressure-induced volume changes are reversible. This collapse of the structure and the observation that the reversible volume change essentially corresponds to the initial porous volume of the crystal can be indirectly used to infer that the transformation mechanism corresponds to pore collapse while keeping the network topology of the $AlPO_4$ framework. A memory effect is observed in the amorphous form, which strongly expands on decompression returning to the density of the initial crystalline form without recovering long-range order. The amorphous form thus exhibits a very high degree of flexibility. Such a new topologically ordered amorphous phase could approach a low-entropy "perfect" glass with improved mechanical properties as compared to standard glasses.

ASSOCIATED CONTENT

Supporting Information

Experimental details, additional figures and tables of crystallographic data are supplied as Supporting Information. This material is available free of charge via the Internet at http://pubs.acs.org.

Accession Codes

CSD 2323675-2323684 contain the supplementary crystallographic data for this paper. These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service.

Notes

The authors declare no competing financial interest.

Acknowledgment

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Experimental

Synthesis. Single crystals of hydrated $AlPO_4$-17 with maximum dimensions of 250 × 70 × 70 μm^3 were synthesized under hydrothermal conditions from aluminum triisopropoxide and phosphoric acid using N,N,N′,N′-tetramethyl-1,6-hexanediamine as a structure directing agent as described previously[1,2]. The crystals were calcined in air at 500 °C for 24 h.

High-pressure experiment. Two $AlPO_4$-17 single crystals (dimensions 154 × 76 × 76 μm^3 and 110 × 35 × 35 μm^3) were placed in 400 µm diameter and a 150 µm thick, stainless steel gasket along with a ruby pressure calibrant in a membrane diamond anvil cell (DAC) with 800 µm culets and an opening angle of 80°. The DAC was placed in a cryogenic gas loading system and the sample was dehydrated for 1h30 at 110 °C under vacuum (4 Pa). DAPHNE7474 oil[3] was then added. Crystal dimensions were obtained from analysis of optical images.

High-pressure x-ray diffraction. X-ray diffraction measurements (λ=0.4956 Å) under pressure were performed with an 80 µm beam on the Xpress beamline equipped with a PILATUS3 S 6M (DECTRIS) detector at the Elettra Sincrotrone Trieste (Trieste, Italy). The detector was placed at 255 mm from the sample. The pressure was measured based on the shift in the R_1 fluorescence line of ruby[4]. Diffraction data were collected from the $AlPO_4$-17 single crystals using phi scans from –38° to +37°. Data reduction was performed with CrysalisPro 1.171.43.92a (Rigaku OD, 2023). The crystal structure was refined using ShelxI-2017/129[5] with the OLEX[6] interface. Data are given for the larger crystal as they are of better quality due to higher measured intensities. The void volume was calculated with Platon Squeeze[7] using the OLEX interface. Crystal structures plotted using Vesta[8]. Equation of state parameters were calculated with EosFit7_GUI[9].

High energy X-ray total scattering. Data from the amorphous powder sample recovered from 5 GPa[1] in a belt-type apparatus were obtained using the two-axis, horizontal diffractometer built for liquid and glass samples on the bending magnet beamline BL04B2 with 61.6 keV X-rays at the SPring-8 synchrotron as described previously[1]. The pair distribution function was obtained in the form of the total radial distribution function G(r) by direct Fourier transformation of the total scattering data S(Q) obtained up to a maximum Q of 20 $Å^{-1}$. The details of experiment and standard data analysis are described elsewhere[10-11].

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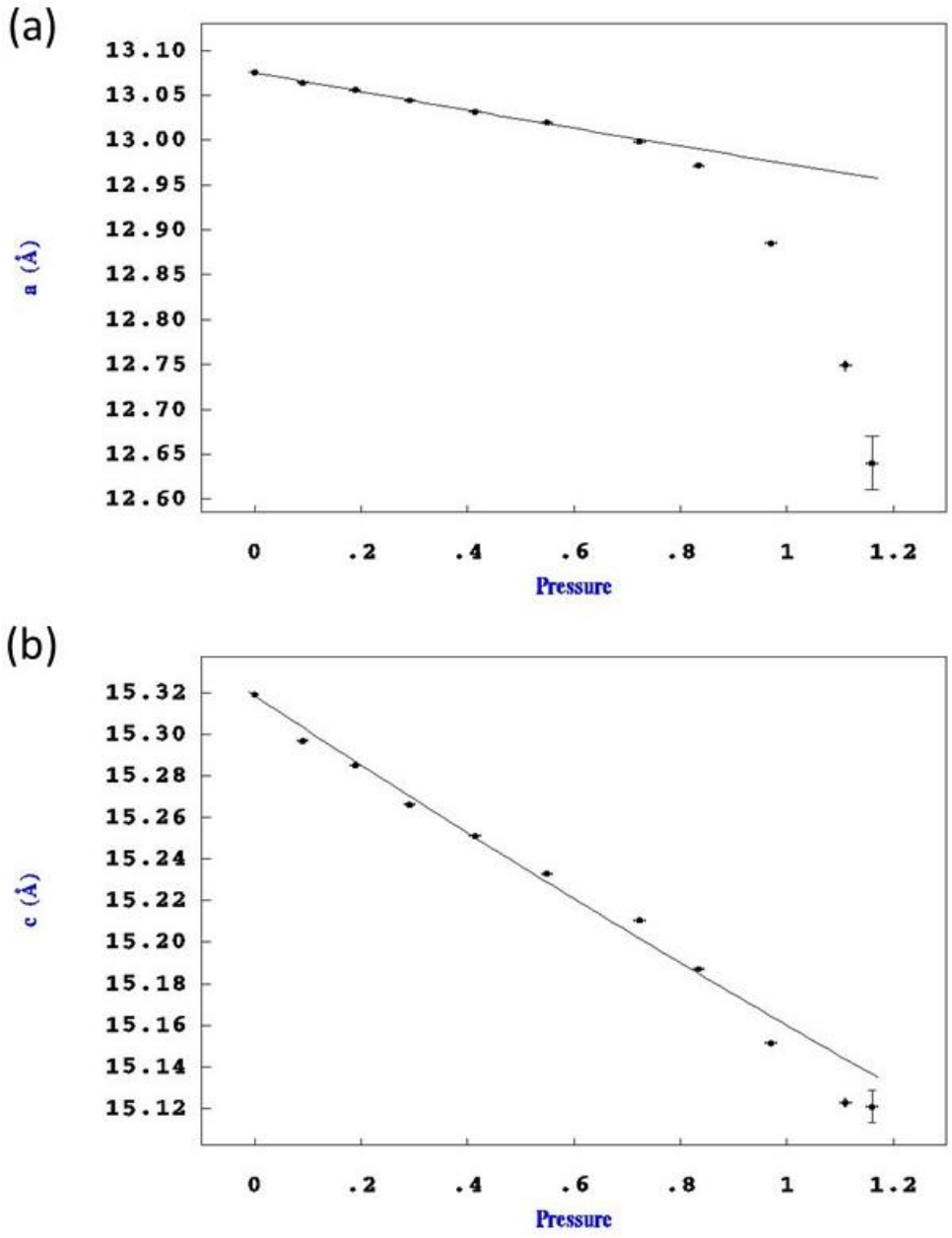

Figure S1. Cell parameters *a* of single-crystal $AlPO_4$-17 as a function of pressure (a). Cell parameters *c* of single-crystal $AlPO_4$-17 as a function of pressure (b). The solid lines represent 2nd order Birch-Murnaghan EOS fits to the data up to the onset of amorphization at 0.6 GPa giving the following compressibilities along **a** (0.0081(2) GPa^{-1}) and **c** (0.0111(5) GPa^{-1}).

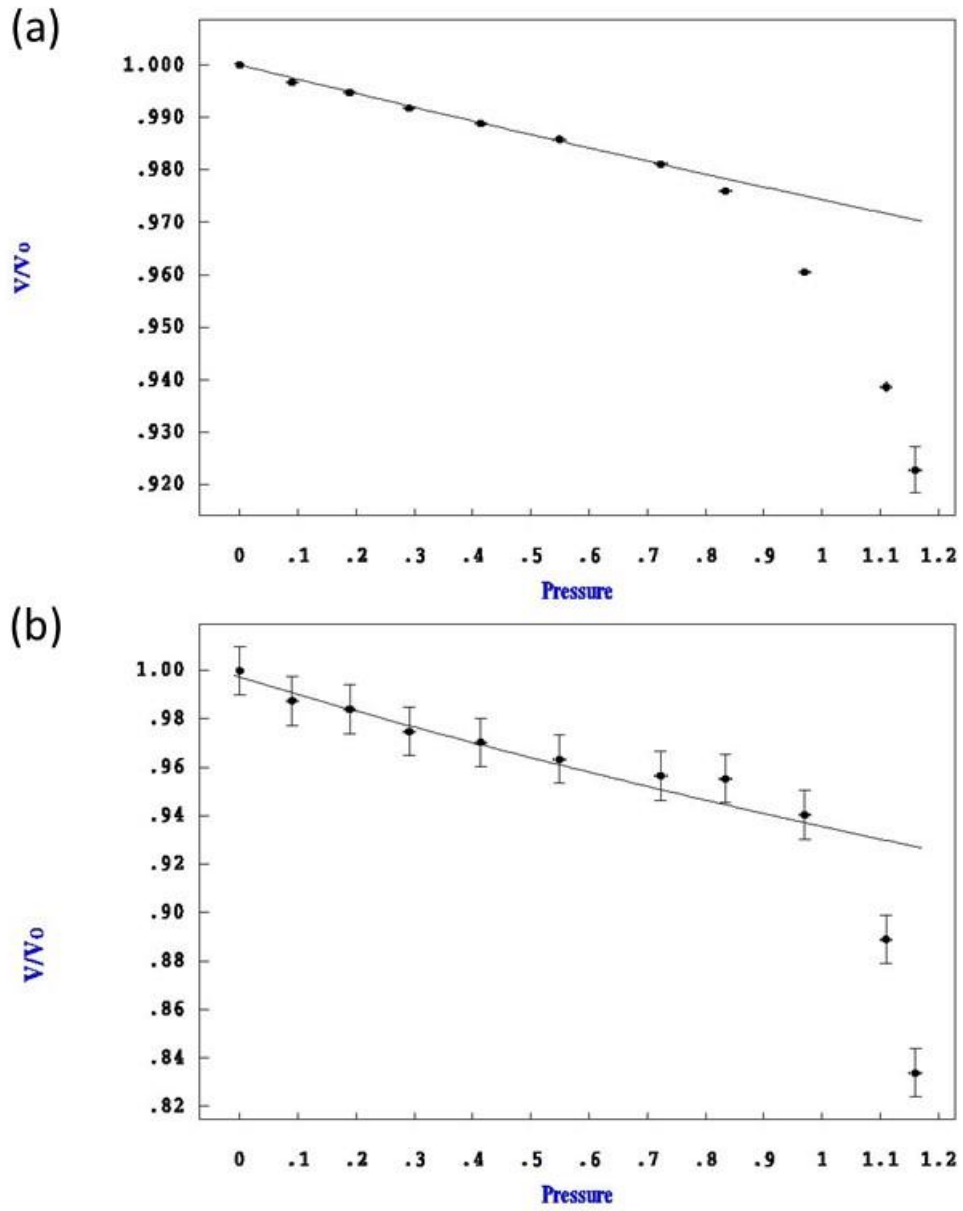

Figure S2. Relative unit cell volume of single-crystal $AlPO_4$-17 as a function of pressure (a). Relative porous volume of single-crystal $AlPO_4$-17 as a function of pressure (b). The solid lines represent 2nd order Birch-Murnaghan EOS fits to the data up to the onset of amorphization at 0.6 GPa giving the following bulk moduli for the unit cell, 36(1) GPa, and the pores, 14(4) GPa.

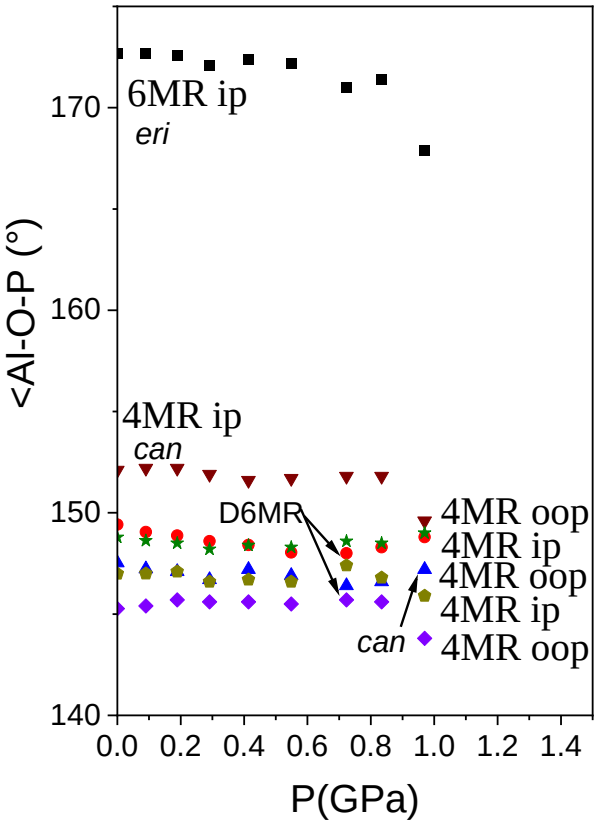

Figure S3. In-plane (ip-*xy*) and out-of-plane (oop) Al-O-P angles in the 4MR and 6MR of $AlPO_4$-17 as a function of pressure.

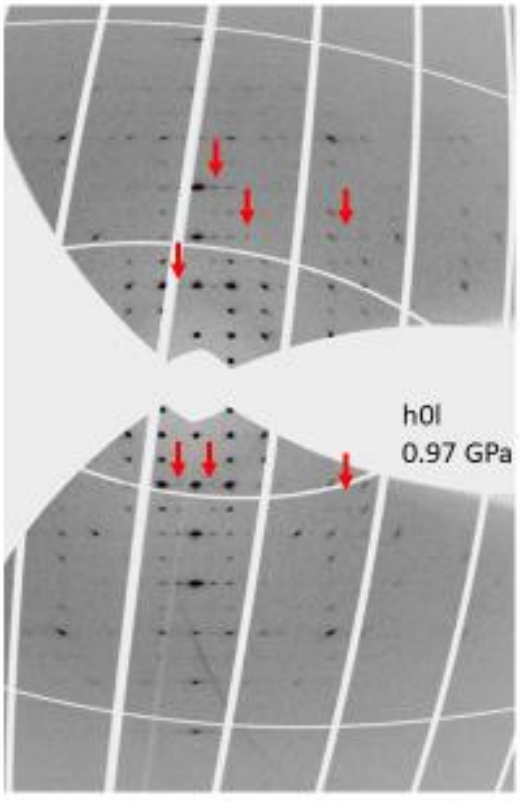

Figure S4. (h0*l*) Reciprocal space reconstruction for $AlPO_4$-17 at 0.97 GPa. Arrows indicate the principal rows of superlattice reflections.

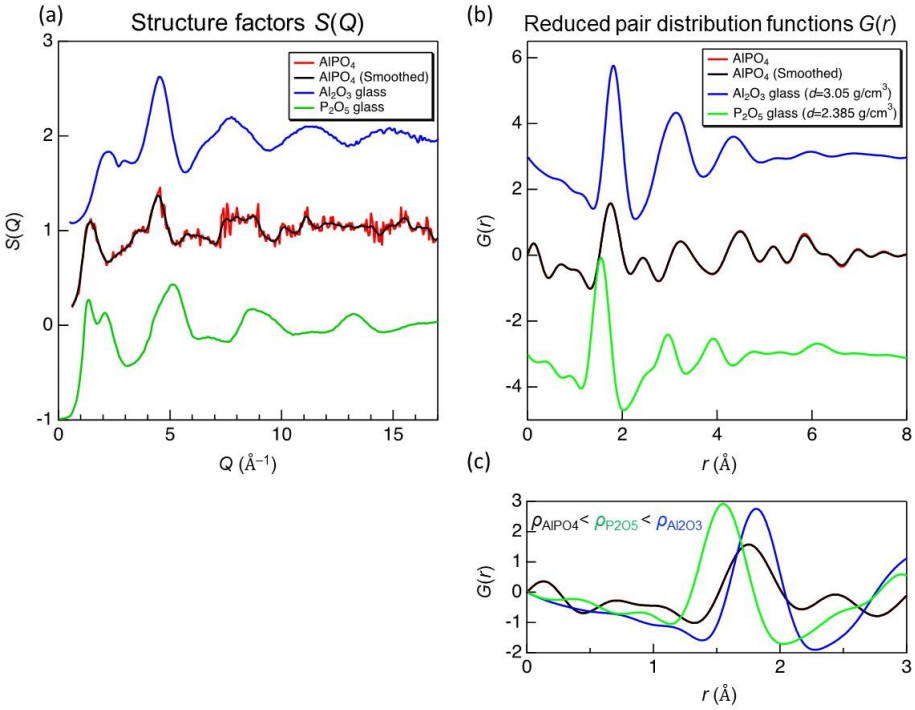

Figure S5. Structure factors $S(Q)$ (a), reduced pair distribution functions $G(r)$ (b) and detail of the low r region of $G(r)$ (c) for amorphous $AlPO_4$-17 recovered from 5 GPa[1], Al_2O_3[12] and P_2O_5[13] glasses.

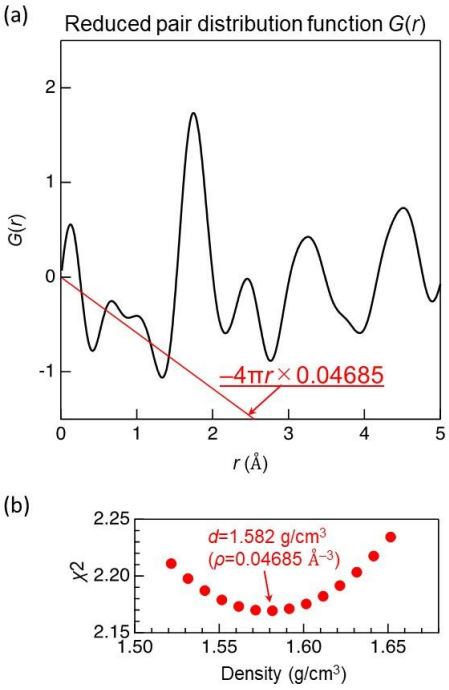

Figure S6. Reduced pair distribution function $G(r)$ for amorphous $AlPO_4$-17 recovered from 5 GPa[1] showing the determination of the initial slope used to estimate the sample density (a) and dependence of χ^2 on the fitted density (b).

Table S1. Hexagonal unit cell parameters of an $AlPO_4$-17 single crystal as a function of pressure.

P(GPa)	*a*(Å)	*c*(Å)	*V*(Å^3)
0.0001	13.0758(9)	15.3189(4)	2268.3(3)
0.09	13.0641(8)	15.2968(5)	2260.9(3)
0.189	13.0556(9)	15.285(5)	2256.3(3)
0.291	13.0443(10)	15.2662(5)	2249.6(3)
0.414	13.0318(11)	15.2511(6)	2243.1(4)
0.549	13.0191(11)	15.2329(6)	2236.0(4)
0.723	12.9981(13)	15.2105(7)	2225.5(5)
0.834	12.9715(14)	15.1870(7)	2213.5(5)
0.97	12.885(3)	15.1515(11)	2178.7(10)
1.11	12.749(5)	15.123(2)	2129(2)
1.16	12.64(3)	15.121(8)	2093(10)
1.454*	12.27(2)	15.136(15)	1973(6)
2.03*	11.15(9)	15.48(3)	1667(20)
2.481*	10.89	15.31	1573

*Cell parameters corresponding to the strongest diffracting remanent crystalline domain in the amorphous matrix. Other minor domains exhibited a distribution of cell parameters due to stress gradients as the external pressure in the surrounding fluid is transmitted by the rigid amorphous matrix surrounding the crystallites.

Table S2 Crystal data and structure refinement for $AlPO_4$-17 at 0.1 MPa

Identification code	17hyd_SC5
Empirical formula	O_4AlP
Formula weight	121.95
Temperature/K	293(2)
Crystal system	hexagonal
Space group	$P6_3/m$
a/Å	13.0758(9)
b/Å	13.0758(9)
c/Å	15.3189(4)
α/°	90
β/°	90
γ/°	120
Volume/$Å^3$	2268.3(3)
Z	18
$\rho_{calc}g/cm^3$	1.607
μ/mm^{-1}	0.223
F(000)	1080.0
Crystal size/mm^3	0.154 × 0.74 × 0.74
Radiation	synchrotron (λ = 0.49555)
2Θ range for data collection/°	3.708 to 38.566
Index ranges	$-8 \le h \le 13$, $-13 \le k \le 8$, $-20 \le l \le 20$
Reflections collected	5001
Independent reflections	1406 [R_{int} = 0.0278, R_{sigma} = 0.0305]
Data/restraints/parameters	1406/0/88
Goodness-of-fit on F^2	1.094
Final R indexes [I>=2σ (I)]	R_1 = 0.0384, wR_2 = 0.1029
Final R indexes [all data]	R_1 = 0.0492, wR_2 = 0.1076
Largest diff. peak/hole / e $Å^{-3}$	0.32/-0.33

Table S3 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for $AlPO_4$-17 at 0.1 MPa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	9973.9(6)	2373.1(6)	1013.3(4)	18.8(2)
P2	5747.3(8)	9080.5(9)	2500	17.4(2)
Al2	918.7(10)	4232.2(10)	2500	17.1(3)
Al1	7610.1(7)	9974.7(7)	1006.5(4)	18.3(2)
O1	229(2)	3416.5(19)	1586.2(11)	29.1(5)

Table S3 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for AlPO$_4$-17 at 0.1 MPa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1B	6464.0(19)	9694(2)	1689.0(11)	30.8(5)
O2	910(2)	2016(2)	1140.8(13)	35.0(5)
O3	1326.3(19)	2540(2)	6261.2(11)	29.7(5)
O4	2769(2)	37(2)	10066.6(10)	32.8(5)
O5	2374(3)	4586(3)	2500	32.5(7)
O6	4645(2)	9170(3)	2500	26.2(6)

Table S4 Anisotropic Displacement Parameters (Å^2×10^3) for AlPO$_4$-17 at 0.1 MPa. The Anisotropic displacement factor exponent takes the form: -2π^2[h^{2}a*^{2}U$_{11}$+2hka*b*U$_{12}$+…].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	17.3(4)	19.6(4)	17.2(3)	-2.7(2)	-0.5(2)	7.3(3)
P2	15.4(5)	19.0(5)	18.3(4)	0	0	8.8(4)
Al2	19.4(6)	15.2(6)	16.8(4)	0	0	8.7(5)
Al1	19.0(4)	17.8(4)	16.2(3)	0.6(2)	2.2(2)	7.7(3)
O1	36.1(13)	23.9(11)	23.7(8)	-6.4(7)	-2.4(7)	12.3(10)
O1B	26.1(12)	37.0(13)	27.7(9)	5.6(8)	8.6(7)	14.6(11)
O2	27.2(13)	36.6(14)	43.8(11)	2.7(9)	2.0(8)	17.9(11)
O3	24.4(12)	36.1(14)	34.5(9)	-7.4(8)	-4.6(7)	19.4(11)
O4	38.6(13)	44.6(14)	19.7(8)	2.2(7)	2.4(7)	24.1(12)
O5	23.5(17)	25.4(18)	49.2(16)	0	0	12.6(14)
O6	20.4(15)	33.4(18)	29.5(12)	0	0	16.8(14)

Table S5 Bond Lengths for AlPO$_4$-17 at 0.1 MPa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	O1^1	1.513(2)	Al2	O1^4	1.7172(19)
P1	O2^1	1.525(2)	Al2	O1	1.7172(19)
P1	O3^2	1.518(2)	Al2	O5	1.720(3)
P1	O4^3	1.5264(18)	Al2	O6^5	1.686(3)
P2	O1B	1.5211(19)	Al1	O1B	1.710(2)
P2	O1B^4	1.5212(19)	Al1	O2^5	1.723(2)
P2	O5^5	1.519(3)	Al1	O3^6	1.709(2)
P2	O6	1.503(3)	Al1	O4^7	1.7149(18)

^{1}1+X,+Y,+Z; ^{2}1-Y+X,+X,-1/2+Z; ^{3}1-Y,+X-Y,-1+Z; ^{4}+X,+Y,1/2-Z; ^{5}1-Y,1+X-Y,+Z; ^{6}1-Y+X,1+X,-1/2+Z; ^{7}1-X,1-Y,1-Z

Table S6 Bond Angles for $AlPO_4$-17 at 0.1 MPa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1[1]	P1	O2[1]	110.69(12)	O6[5]	Al2	O1	109.32(10)
O1[1]	P1	O3[2]	109.44(12)	O6[5]	Al2	O5	109.93(16)
O1[1]	P1	O4[3]	107.80(13)	O1B	Al1	O2[5]	109.21(11)
O2[1]	P1	O4[3]	110.38(12)	O1B	Al1	O3[6]	108.72(11)
O3[2]	P1	O2[1]	107.93(13)	O1B	Al1	O4[7]	111.45(12)
O3[2]	P1	O4[3]	110.61(12)	O3[6]	Al1	O2[5]	110.07(12)
O1B	P2	O1B[4]	109.53(18)	O3[6]	Al1	O4[7]	109.56(10)
O1B[4]	P2	O5[5]	110.20(11)	O4[7]	Al1	O2[5]	107.84(11)
O1B	P2	O5[5]	110.20(11)	P1[8]	O1	Al2	147.53(15)
O6	P2	O1B[4]	108.71(11)	P2	O1B	Al1	148.79(16)
O6	P2	O1B	108.71(11)	P1[8]	O2	Al1[9]	146.99(17)
O6	P2	O5[5]	109.47(17)	P1[10]	O3	Al1[11]	149.42(13)
O1[4]	Al2	O1	109.22(16)	P1[12]	O4	Al1[7]	145.27(17)
O1[4]	Al2	O5	109.52(10)	P2[9]	O5	Al2	152.1(2)
O1	Al2	O5	109.52(10)	P2	O6	Al2[9]	172.7(2)
O6[5]	Al2	O1[4]	109.32(10)				

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-Y+X,1+X,-1/2+Z; [7]1-X,1-Y,1-Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S7 Crystal data and structure refinement for $AlPO_4$-17 at 0.09 GPa.

Identification code	17_SC05_P1b
Empirical formula	O_4AlP
Formula weight	121.95
Temperature/K	293(2)
Crystal system	hexagonal
Space group	$P6_3/m$
a/Å	13.0641(8)
b/Å	13.0641(8)
c/Å	15.2968(5)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	2260.9(3)
Z	18
ρ_{calc}g/cm^3	1.612
μ/mm^{-1}	0.224
F(000)	1080.0
Crystal size/mm^3	? × ? × ?
Radiation	synchrotron (λ = 0.49555)

2Θ range for data collection/°	3.712 to 38.512
Index ranges	$-8 \le h \le 13$, $-12 \le k \le 7$, $-20 \le l \le 20$
Reflections collected	4770
Independent reflections	1390 [R_{int} = 0.0337, R_{sigma} = 0.0395]
Data/restraints/parameters	1390/0/88
Goodness-of-fit on F^2	1.140
Final R indexes [I>=2σ (I)]	R_1 = 0.0469, wR_2 = 0.1195
Final R indexes [all data]	R_1 = 0.0656, wR_2 = 0.1263
Largest diff. peak/hole / e $Å^{-3}$	0.48/-0.36

Table S8 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for $AlPO_4$-17 at 0.09 GPa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	9972.5(8)	2371.0(8)	1014.2(4)	14.2(3)
P2	5747.1(11)	9080.8(11)	2500	12.8(3)
Al2	919.4(12)	4233.3(12)	2500	12.1(3)
Al1	7611.1(9)	9974.3(9)	1007.4(5)	13.9(3)
O1	227(2)	3419(2)	1585.6(13)	25.5(6)
O1B	6460(2)	9692(3)	1688.7(13)	26.8(6)
O2	909(2)	2015(3)	1142.8(16)	31.2(7)
O3	1326(2)	2541(2)	6265.3(14)	24.8(6)
O4	2767(3)	38(2)	10066.8(13)	28.8(7)
O5	2377(3)	4586(3)	2500	29.1(9)
O6	4645(3)	9170(3)	2500	22.8(8)

Table S9 Anisotropic Displacement Parameters (Å^2×10^3) for $AlPO_4$-17 at 0.09 GPa. The Anisotropic displacement factor exponent takes the form: -2π^2[h^{2}a*^{2}U_{11}+2hka*b*U_{12}+…].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	11.7(5)	12.8(5)	16.0(4)	-2.8(3)	-0.6(3)	4.5(4)
P2	7.9(6)	12.7(7)	18.0(5)	0	0	5.3(5)
Al2	12.3(8)	8.3(8)	16.0(5)	0	0	5.4(6)
Al1	13.3(6)	12.5(6)	14.3(4)	0.6(3)	2.1(3)	5.2(5)
O1	32.5(17)	18.9(15)	21.8(10)	-5.1(8)	-2.0(9)	10.3(13)
O1B	18.7(15)	33.7(17)	26.5(11)	6.5(10)	10.2(9)	12.1(13)
O2	21.0(17)	28.1(18)	45.5(14)	4.2(11)	3.6(10)	13.1(14)
O3	15.9(14)	28.4(17)	34.8(11)	-7.9(10)	-4.5(9)	14.7(13)
O4	34.3(17)	38.1(18)	17.4(10)	0.8(9)	1.6(9)	20.7(15)
O5	19(2)	19(2)	50(2)	0	0	10.5(18)

Table S9 Anisotropic Displacement Parameters ($Å^2×10^3$) for $AlPO_4$-17 at 0.09 GPa. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O6	16(2)	29(2)	28.9(15)	0	0	15.1(18)

Table S10 Bond Lengths for $AlPO_4$-17 at 0.09 GPa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	O1[1]	1.514(2)	Al1	O2[5]	1.721(3)
P1	O2[1]	1.523(3)	Al1	O3[6]	1.708(3)
P1	O3[2]	1.517(3)	Al1	O4[7]	1.714(2)
P1	O4[3]	1.525(2)	O1	P1[8]	1.514(2)
P2	O1B	1.517(2)	O2	P1[8]	1.523(3)
P2	O1B[4]	1.517(2)	O2	Al1[9]	1.721(3)
P2	O5[5]	1.515(4)	O3	P1[10]	1.517(3)
P2	O6	1.501(3)	O3	Al1[11]	1.708(3)
Al2	O1[4]	1.716(2)	O4	P1[12]	1.525(2)
Al2	O1	1.716(2)	O4	Al1[7]	1.714(2)
Al2	O5	1.721(4)	O5	P2[9]	1.515(4)
Al2	O6[5]	1.684(4)	O6	Al2[9]	1.684(4)
Al1	O1B	1.711(2)			

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-Y+X,1+X,-1/2+Z; [7]1-X,1-Y,1-Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S11 Bond Angles for $AlPO_4$-17 at 0.09 GPa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1[1]	P1	O2[1]	110.73(15)	O6[5]	Al2	O1	109.20(12)
O1[1]	P1	O3[2]	109.34(14)	O6[5]	Al2	O5	110.02(19)
O1[1]	P1	O4[3]	107.63(16)	O1B	Al1	O2[5]	109.19(14)
O2[1]	P1	O4[3]	110.38(15)	O1B	Al1	O4[6]	111.33(14)
O3[2]	P1	O2[1]	108.00(15)	O3[7]	Al1	O1B	108.67(13)
O3[2]	P1	O4[3]	110.77(14)	O3[7]	Al1	O2[5]	110.12(14)
O1B[4]	P2	O1B	109.8(2)	O3[7]	Al1	O4[6]	109.69(13)
O5[5]	P2	O1B[4]	110.16(14)	O4[6]	Al1	O2[5]	107.84(13)
O5[5]	P2	O1B	110.16(14)	P1[8]	O1	Al2	147.23(19)
O6	P2	O1B	108.63(13)	P2	O1B	Al1	148.63(19)
O6	P2	O1B[4]	108.63(13)	P1[8]	O2	Al1[9]	147.0(2)
O6	P2	O5[5]	109.4(2)	P1[10]	O3	Al1[11]	149.05(15)
O1[4]	Al2	O1	109.20(19)	P1[12]	O4	Al1[6]	145.4(2)
O1[4]	Al2	O5	109.60(12)	P2[9]	O5	Al2	152.2(3)
O1	Al2	O5	109.60(12)	P2	O6	Al2[9]	172.7(3)
O6[5]	Al2	O1[4]	109.20(12)				

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-X,1-Y,1-Z; [7]1-Y+X,1+X,-1/2+Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S12 Crystal data and structure refinement for $AlPO_4$-17 at 0.189 GPa.

Identification code	17_SC05_P2
Empirical formula	O_4AlP
Formula weight	121.95
Temperature/K	293(2)
Crystal system	hexagonal
Space group	$P6_3/m$
a/Å	13.0556(9)
b/Å	13.0556(9)
c/Å	15.2850(5)
α/°	90
β/°	90
γ/°	120
Volume/$Å^3$	2256.3(3)
Z	18
$\rho_{calc}g/cm^3$	1.616
μ/mm^{-1}	0.224
F(000)	1080.0
Crystal size/mm^3	? × ? × ?
Radiation	synchrotron (λ = 0.49555)
2Θ range for data collection/°	3.716 to 38.54
Index ranges	$-8 \leq h \leq 13$, $-12 \leq k \leq 7$, $-20 \leq l \leq 20$
Reflections collected	4694
Independent reflections	1388 [R_{int} = 0.0337, R_{sigma} = 0.0393]
Data/restraints/parameters	1388/0/88
Goodness-of-fit on F^2	1.123
Final R indexes [I>=2σ (I)]	R_1 = 0.0494, wR_2 = 0.1195
Final R indexes [all data]	R_1 = 0.0687, wR_2 = 0.1269
Largest diff. peak/hole / e $Å^{-3}$	0.47/-0.34

Table S13 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for $AlPO_4$-17 at 0.189 GPa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	9973.1(8)	2371.1(8)	1014.3(5)	15.0(3)

Table S13 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for AlPO$_4$-17 at 0.189 GPa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P2	5746.2(11)	9080.4(11)	2500	13.8(3)
Al2	920.8(13)	4232.4(13)	2500	13.1(3)
Al1	7611.0(10)	9973.9(9)	1008.1(5)	14.9(3)
O1	226(3)	3418(2)	1585.2(14)	26.7(7)
O1B	6460(3)	9694(3)	1688.5(15)	28.4(7)
O2	908(3)	2017(3)	1143.6(17)	32.5(7)
O3	1326(2)	2544(3)	6266.5(15)	26.5(6)
O4	2764(3)	38(3)	10067.3(14)	30.5(7)
O5	2377(3)	4586(4)	2500	30.7(9)
O6	4644(3)	9171(4)	2500	23.6(8)

Table S14 Anisotropic Displacement Parameters (Å^2×10^3) for AlPO$_4$-17 at 0.189 GPa. The Anisotropic displacement factor exponent takes the form: -2π^2[h^{2}a*^{2}U$_{11}$+2hka*b*U$_{12}$+…].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	12.6(5)	14.0(5)	16.1(4)	-2.8(3)	-0.4(3)	4.9(4)
P2	9.7(7)	13.8(7)	18.2(5)	0	0	6.2(6)
Al2	13.9(8)	9.5(8)	16.7(6)	0	0	6.4(7)
Al1	14.2(6)	14.3(6)	14.6(4)	0.5(3)	2.4(3)	6.0(5)
O1	36.2(18)	17.4(15)	22.6(11)	-5.9(9)	-2.1(10)	10.5(14)
O1B	20.1(16)	35.1(18)	29.1(13)	6.1(11)	10.5(10)	13.2(14)
O2	22.9(18)	31.2(19)	45.8(15)	4.6(12)	3.9(11)	15.3(15)
O3	17.7(16)	33.4(18)	34.5(12)	-8.3(11)	-5.2(10)	17.4(14)
O4	36.6(18)	41.4(19)	18.1(11)	1.7(10)	2.9(10)	22.9(16)
O5	18(2)	20(2)	53(2)	0	0	8.5(19)
O6	14(2)	32(2)	31.3(16)	0	0	16.4(19)

Table S15 Bond Lengths for AlPO$_4$-17 at 0.189 GPa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	O1^1	1.513(3)	Al1	O2^5	1.721(3)
P1	O2^1	1.519(3)	Al1	O3^6	1.706(3)
P1	O3^2	1.519(3)	Al1	O4^7	1.713(2)
P1	O4^3	1.522(2)	O1	P1^8	1.513(3)
P2	O1B	1.517(2)	O2	P1^8	1.519(3)
P2	O1B^4	1.517(2)	O2	Al1^9	1.721(3)
P2	O5^5	1.514(4)	O3	P1^{10}	1.519(3)
P2	O6	1.502(4)	O3	Al1^{11}	1.706(3)
Al2	O1^4	1.715(2)	O4	P1^{12}	1.522(2)

Table S15 Bond Lengths for $AlPO_4$-17 at 0.189 GPa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Al2	O1	1.715(2)	O4	$Al1^{7}$	1.713(2)
Al2	O5	1.717(4)	O5	$P2^{9}$	1.514(4)
Al2	$O6^{5}$	1.683(4)	O6	$Al2^{9}$	1.683(4)
Al1	O1B	1.710(3)			

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-Y+X,1+X,-1/2+Z; [7]1-X,1-Y,1-Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S16 Bond Angles for $AlPO_4$-17 at 0.189 GPa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
$O1^{1}$	P1	$O2^{1}$	110.75(16)	$O6^{5}$	Al2	O1	109.06(13)
$O1^{1}$	P1	$O3^{2}$	109.18(15)	$O6^{5}$	Al2	O5	110.1(2)
$O1^{1}$	P1	$O4^{3}$	107.75(16)	O1B	Al1	$O2^{5}$	109.25(15)
$O2^{1}$	P1	$O4^{3}$	110.34(16)	O1B	Al1	$O4^{6}$	111.44(15)
$O3^{2}$	P1	$O2^{1}$	108.13(16)	$O3^{7}$	Al1	O1B	108.51(14)
$O3^{2}$	P1	$O4^{3}$	110.69(15)	$O3^{7}$	Al1	$O2^{5}$	110.30(15)
$O1B^{4}$	P2	O1B	109.7(2)	$O3^{7}$	Al1	$O4^{6}$	109.61(14)
$O5^{5}$	P2	$O1B^{4}$	110.22(15)	$O4^{6}$	Al1	$O2^{5}$	107.74(14)
$O5^{5}$	P2	O1B	110.22(15)	$P1^{8}$	O1	Al2	147.1(2)
O6	P2	O1B	108.59(14)	P2	O1B	Al1	148.5(2)
O6	P2	$O1B^{4}$	108.59(14)	$P1^{8}$	O2	$Al1^{9}$	147.1(2)
O6	P2	$O5^{5}$	109.5(2)	$P1^{10}$	O3	$Al1^{11}$	148.88(17)
$O1^{4}$	Al2	O1	109.2(2)	$P1^{12}$	O4	$Al1^{6}$	145.7(2)
$O1^{4}$	Al2	O5	109.73(13)	$P2^{9}$	O5	Al2	152.2(3)
O1	Al2	O5	109.73(13)	P2	O6	$Al2^{9}$	172.6(3)
$O6^{5}$	Al2	$O1^{4}$	109.06(13)				

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-X,1-Y,1-Z; [7]1-Y+X,1+X,-1/2+Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S17 Crystal data and structure refinement for $AlPO_4$-17 at 0.291 GPa.

Identification code	17_SC05_P3
Empirical formula	O_4AlP
Formula weight	121.95
Temperature/K	293(2)
Crystal system	hexagonal
Space group	$P6_3/m$
a/Å	13.0443(10)
b/Å	13.0443(10)

c/Å	15.2662(5)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	2249.6(3)
Z	18
ρ_{calc}g/cm^3	1.620
μ/mm^{-1}	0.225
F(000)	1080.0
Crystal size/mm^3	? × ? × ?
Radiation	synchrotron (λ = 0.49555)
2Θ range for data collection/°	3.72 to 38.58
Index ranges	-8 ≤ h ≤ 13, -12 ≤ k ≤ 7, -20 ≤ l ≤ 20
Reflections collected	4677
Independent reflections	1392 [R_{int} = 0.0358, R_{sigma} = 0.0459]
Data/restraints/parameters	1392/0/88
Goodness-of-fit on F^2	1.077
Final R indexes [I>=2σ (I)]	R_1 = 0.0584, wR_2 = 0.1444
Final R indexes [all data]	R_1 = 0.0824, wR_2 = 0.1539
Largest diff. peak/hole / e Å^{-3}	0.54/-0.46

Table S18 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for $AlPO_4$-17 at 0.291 GPa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	9972.3(10)	2371.1(10)	1015.4(6)	17.5(3)
P2	5745.1(13)	9079.2(14)	2500	15.9(4)
Al2	921.3(16)	4233.6(15)	2500	14.5(4)
Al1	7611.0(11)	9973.2(11)	1009.1(7)	17.1(4)
O1	228(3)	3424(3)	1583.5(18)	30.9(8)
O1B	6457(3)	9692(3)	1687.1(18)	30.7(8)
O2	904(3)	2011(3)	1146(2)	35.3(9)
O3	1329(3)	2548(3)	6269.4(18)	29.3(8)
O4	2765(3)	38(3)	10066.9(17)	33.7(9)
O5	2380(4)	4591(4)	2500	33.4(11)
O6	4644(4)	9176(4)	2500	26.1(10)

Table S19 Anisotropic Displacement Parameters ($Å^2×10^3$) for $AlPO_4$-17 at 0.291 GPa. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	16.5(7)	16.3(6)	17.9(5)	-2.9(4)	-0.3(3)	6.9(5)
P2	10.3(8)	17.7(9)	20.1(6)	0	0	7.5(7)
Al2	15.6(10)	9.9(9)	18.0(7)	0	0	6.3(8)
Al1	16.0(7)	16.4(8)	16.6(5)	0.9(4)	2.5(4)	6.4(6)
O1	39(2)	24(2)	25.6(14)	-6.4(11)	-1.2(12)	12.2(17)
O1B	23(2)	37(2)	31.2(16)	6.5(13)	10.8(12)	14.0(17)
O2	23(2)	35(2)	49.3(19)	5.3(15)	4.4(14)	15.2(18)
O3	21.6(19)	35(2)	37.8(15)	-10.5(13)	-6.7(12)	18.9(17)
O4	39(2)	47(2)	19.5(14)	1.8(12)	2.2(11)	24.8(19)
O5	18(3)	20(3)	60(3)	0	0	8(2)
O6	22(3)	35(3)	34(2)	0	0	24(2)

Table S20 Bond Lengths for $AlPO_4$-17 at 0.291 GPa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	$O1^1$	1.514(3)	Al1	$O2^5$	1.723(4)
P1	$O2^1$	1.519(4)	Al1	$O3^6$	1.707(3)
P1	$O3^2$	1.517(3)	Al1	$O4^7$	1.712(3)
P1	$O4^3$	1.523(3)	O1	$P1^8$	1.514(3)
P2	$O1B^4$	1.516(3)	O2	$P1^8$	1.519(4)
P2	O1B	1.516(3)	O2	$Al1^9$	1.723(4)
P2	$O5^5$	1.512(5)	O3	$P1^{10}$	1.517(3)
P2	O6	1.504(4)	O3	$Al1^{11}$	1.707(3)
Al2	O1	1.713(3)	O4	$P1^{12}$	1.523(3)
Al2	$O1^4$	1.713(3)	O4	$Al1^7$	1.712(3)
Al2	O5	1.718(5)	O5	$P2^9$	1.512(5)
Al2	$O6^5$	1.677(4)	O6	$Al2^9$	1.677(4)
Al1	O1B	1.709(3)			

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-Y+X,1+X,-1/2+Z; [7]1-X,1-Y,1-Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S21 Bond Angles for $AlPO_4$-17 at 0.291 GPa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
$O1^1$	P1	$O2^1$	111.0(2)	$O6^5$	Al2	$O1^4$	108.75(16)
$O1^1$	P1	$O3^2$	109.21(18)	$O6^5$	Al2	O5	110.2(2)
$O1^1$	P1	$O4^3$	107.4(2)	O1B	Al1	$O2^5$	109.44(18)
$O2^1$	P1	$O4^3$	110.47(19)	O1B	Al1	$O4^6$	111.18(18)
$O3^2$	P1	$O2^1$	108.0(2)	$O3^7$	Al1	O1B	108.45(17)
$O3^2$	P1	$O4^3$	110.78(19)	$O3^7$	Al1	$O2^5$	110.23(19)

Table S21 Bond Angles for $AlPO_4$-17 at 0.291 GPa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1B	P2	O1B[4]	109.9(3)	O3[7]	Al1	O4[6]	109.64(17)
O5[5]	P2	O1B	110.32(18)	O4[6]	Al1	O2[5]	107.90(17)
O5[5]	P2	O1B[4]	110.32(18)	P1[8]	O1	Al2	146.7(2)
O6	P2	O1B[4]	108.33(17)	P2	O1B	Al1	148.2(2)
O6	P2	O1B	108.33(17)	P1[8]	O2	Al1[9]	146.6(3)
O6	P2	O5[5]	109.6(3)	P1[10]	O3	Al1[11]	148.6(2)
O1	Al2	O1[4]	109.5(3)	P1[12]	O4	Al1[6]	145.6(3)
O1	Al2	O5	109.82(16)	P2[9]	O5	Al2	151.9(4)
O1[4]	Al2	O5	109.82(16)	P2	O6	Al2[9]	172.1(3)
O6[5]	Al2	O1	108.75(16)				

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-X,1-Y,1-Z; [7]1-Y+X,1+X,-1/2+Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S22 Crystal data and structure refinement for $AlPO_4$-17 at 0.414 GPa.

Identification code	17_SC05_P4
Empirical formula	O_4AlP
Formula weight	121.95
Temperature/K	293(2)
Crystal system	hexagonal
Space group	$P6_3/m$
a/Å	13.0318(11)
b/Å	13.0318(11)
c/Å	15.2511(6)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	2243.1(4)
Z	18
ρ_{calc}g/cm^3	1.625
μ/mm^{-1}	0.225
F(000)	1080.0
Crystal size/mm^3	? × ? × ?
Radiation	synchrotron (λ = 0.49555)
2Θ range for data collection/°	3.724 to 38.58
Index ranges	$-7 \le h \le 12$, $-16 \le k \le 16$, $-20 \le l \le 20$
Reflections collected	4729
Independent reflections	1400 [R_{int} = 0.0373, R_{sigma} = 0.0434]
Data/restraints/parameters	1400/0/88
Goodness-of-fit on F^2	1.105

Final R indexes [I>=2σ (I)]	R_1 = 0.0522, wR_2 = 0.1235
Final R indexes [all data]	R_1 = 0.0785, wR_2 = 0.1334
Largest diff. peak/hole / e Å^{-3}	0.45/-0.28

Table 23 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for AlPO$_4$-17 at 0.414 GPa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	9971.2(9)	2371.0(9)	1016.0(5)	19.6(3)
P2	5744.9(12)	9079.2(12)	2500	17.6(3)
Al2	922.0(14)	4234.9(14)	2500	16.8(4)
Al1	7612.4(10)	9973.9(10)	1009.6(6)	18.8(3)
O1	235(3)	3425(3)	1585.1(15)	32.0(7)
O1B	6456(3)	9690(3)	1687.7(15)	34.1(7)
O2	906(3)	2012(3)	1147.0(18)	39.0(8)
O3	1329(3)	2549(3)	6271.3(15)	31.6(7)
O4	2766(3)	40(3)	10066.5(14)	35.7(8)
O5	2381(4)	4596(4)	2500	36.7(10)
O6	4640(3)	9172(4)	2500	29.1(9)

Table S24 Anisotropic Displacement Parameters (Å^2×10^3) for AlPO$_4$-17 at 0.414 GPa. The Anisotropic displacement factor exponent takes the form: -2π^2[h^{2}a*^{2}U$_{11}$+2hka*b*U$_{12}$+…].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	17.4(6)	19.2(6)	19.9(4)	-3.3(3)	-0.3(3)	7.3(5)
P2	13.0(7)	17.9(8)	22.3(5)	0	0	8.0(6)
Al2	17.5(9)	14.0(9)	19.9(6)	0	0	8.6(7)
Al1	18.6(6)	17.6(7)	17.9(5)	0.5(4)	2.6(4)	7.5(5)
O1	40.5(19)	23.2(17)	27.7(12)	-6.3(10)	-1.6(11)	12.5(15)
O1B	28.1(18)	43(2)	31.5(14)	7.0(12)	11.4(11)	17.7(16)
O2	30.7(19)	39(2)	51.1(17)	5.7(13)	5.0(12)	20.0(16)
O3	23.4(17)	38.2(19)	39.9(13)	-9.3(11)	-4.8(11)	20.5(15)
O4	41(2)	47(2)	20.5(12)	2.3(11)	3.4(10)	22.7(17)
O5	23(3)	25(3)	63(3)	0	0	13(2)
O6	19(2)	38(3)	37.1(18)	0	0	20(2)

Table S25 Bond Lengths for $AlPO_4$-17 at 0.414 GPa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	O1[1]	1.512(3)	Al1	O2[5]	1.718(3)
P1	O2[1]	1.521(3)	Al1	O3[6]	1.705(3)
P1	O3[2]	1.516(3)	Al1	O4[7]	1.711(2)
P1	O4[3]	1.522(2)	O1	P1[8]	1.512(3)
P2	O1B	1.513(3)	O2	P1[8]	1.521(3)
P2	O1B[4]	1.513(3)	O2	Al1[9]	1.718(3)
P2	O5[5]	1.514(4)	O3	P1[10]	1.516(3)
P2	O6	1.503(4)	O3	Al1[11]	1.705(3)
Al2	O1	1.708(3)	O4	P1[12]	1.522(2)
Al2	O1[4]	1.708(3)	O4	Al1[7]	1.711(2)
Al2	O5	1.715(4)	O5	P2[9]	1.514(4)
Al2	O6[5]	1.672(4)	O6	Al2[9]	1.672(4)
Al1	O1B	1.708(3)			

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-Y+X,1+X,-1/2+Z; [7]1-X,1-Y,1-Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S26 Bond Angles for $AlPO_4$-17 at 0.414 GPa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1[1]	P1	O2[1]	110.57(17)	O6[5]	Al2	O1[4]	109.03(14)
O1[1]	P1	O3[2]	109.39(16)	O6[5]	Al2	O5	109.9(2)
O1[1]	P1	O4[3]	107.58(18)	O1B	Al1	O2[5]	109.28(16)
O2[1]	P1	O4[3]	110.46(17)	O1B	Al1	O4[6]	111.10(16)
O3[2]	P1	O2[1]	108.04(17)	O3[7]	Al1	O1B	108.45(15)
O3[2]	P1	O4[3]	110.81(16)	O3[7]	Al1	O2[5]	110.33(16)
O1B	P2	O1B[4]	109.9(3)	O3[7]	Al1	O4[6]	109.81(14)
O1B[4]	P2	O5[5]	110.30(16)	O4[6]	Al1	O2[5]	107.87(15)
O1B	P2	O5[5]	110.30(16)	P1[8]	O1	Al2	147.2(2)
O6	P2	O1B[4]	108.50(15)	P2	O1B	Al1	148.4(2)
O6	P2	O1B	108.50(15)	P1[8]	O2	Al1[9]	146.7(2)
O6	P2	O5[5]	109.3(2)	P1[10]	O3	Al1[11]	148.41(17)
O1	Al2	O1[4]	109.5(2)	P1[12]	O4	Al1[6]	145.6(2)
O1	Al2	O5	109.66(14)	P2[9]	O5	Al2	151.6(3)
O1[4]	Al2	O5	109.66(14)	P2	O6	Al2[9]	172.4(3)
O6[5]	Al2	O1	109.03(14)				

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-X,1-Y,1-Z; [7]1-Y+X,1+X,-1/2+Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S27 Crystal data and structure refinement for $AlPO_4$-17 at 0.549 GPa.

Identification code	17_SC05_P5
Empirical formula	O_4AlP
Formula weight	121.95
Temperature/K	293(2)
Crystal system	hexagonal
Space group	$P6_3/m$
a/Å	13.0191(11)
b/Å	13.0191(11)
c/Å	15.2329(6)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	2236.0(4)
Z	18
ρ_{calc}g/cm^3	1.630
μ/mm^{-1}	0.226
F(000)	1080.0
Crystal size/mm^3	? × ? × ?
Radiation	synchrotron (λ = 0.49555)
2Θ range for data collection/°	3.728 to 38.572
Index ranges	$-8 \le h \le 13$, $-12 \le k \le 7$, $-20 \le l \le 20$
Reflections collected	4785
Independent reflections	1402 [R_{int} = 0.0412, R_{sigma} = 0.0471]
Data/restraints/parameters	1402/0/88
Goodness-of-fit on F^2	1.109
Final R indexes [I>=2σ (I)]	R_1 = 0.0585, wR_2 = 0.1360
Final R indexes [all data]	R_1 = 0.0944, wR_2 = 0.1493
Largest diff. peak/hole / e Å^{-3}	0.36/-0.27

Table S28 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for $AlPO_4$-17 at 0.549 GPa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	9971.9(10)	2370.3(10)	1016.8(6)	26.8(3)
P2	5743.4(14)	9076.7(14)	2500	24.4(4)
Al2	925.4(16)	4236.1(16)	2500	23.7(4)
Al1	7613.5(12)	9975.2(12)	1010.4(7)	26.0(4)
O1	233(3)	3425(3)	1583.5(17)	41.1(9)
O1B	6454(3)	9688(3)	1686.2(17)	43.4(9)
O2	903(3)	2009(3)	1148(2)	46.1(9)
O3	1328(3)	2551(3)	6274.8(17)	38.5(8)

Table S28 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for AlPO$_4$-17 at 0.549 GPa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O4	2766(4)	40(3)	10065.4(16)	44.1(9)
O5	2384(4)	4594(4)	2500	45.3(12)
O6	4642(4)	9172(4)	2500	36.4(11)

Table S29 Anisotropic Displacement Parameters (Å^2×10^3) for AlPO$_4$-17 at 0.549 GPa. The Anisotropic displacement factor exponent takes the form: -2π^2[h^{2}a*^{2}U$_{11}$+2hka*b*U$_{12}$+…].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	25.4(7)	27.9(7)	24.5(5)	-3.8(4)	-0.6(4)	11.4(6)
P2	20.3(9)	25.9(9)	27.6(6)	0	0	12.0(7)
Al2	26.9(11)	20.9(10)	25.6(7)	0	0	13.6(9)
Al1	26.6(8)	25.8(8)	23.7(6)	1.0(4)	2.9(5)	11.6(6)
O1	49(2)	33(2)	35.1(15)	-7.1(12)	-0.5(13)	15.7(18)
O1B	36(2)	52(2)	37.6(16)	6.0(14)	11.8(13)	18.6(19)
O2	37(2)	49(2)	56.9(19)	6.5(15)	5.0(15)	25.7(19)
O3	29.7(19)	47(2)	45.5(15)	-11.1(13)	-8.2(13)	24.3(18)
O4	53(2)	58(2)	26.4(14)	1.4(13)	3.4(12)	31(2)
O5	32(3)	33(3)	71(3)	0	0	16(2)
O6	26(3)	44(3)	45(2)	0	0	22(2)

Table S30 Bond Lengths for AlPO$_4$-17 at 0.549 GPa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	O1[1]	1.510(3)	Al1	O2[5]	1.720(4)
P1	O2[1]	1.517(4)	Al1	O3[6]	1.700(3)
P1	O3[2]	1.519(3)	Al1	O4[7]	1.709(3)
P1	O4[3]	1.524(3)	O1	P1[8]	1.510(3)
P2	O1B[4]	1.513(3)	O2	P1[8]	1.517(4)
P2	O1B	1.513(3)	O2	Al1[9]	1.720(4)
P2	O5[5]	1.505(5)	O3	P1[10]	1.519(3)
P2	O6	1.500(4)	O3	Al1[11]	1.700(3)
Al2	O1	1.710(3)	O4	P1[12]	1.524(3)
Al2	O1[4]	1.710(3)	O4	Al1[7]	1.709(3)
Al2	O5	1.714(5)	O5	P2[9]	1.505(5)
Al2	O6[5]	1.673(5)	O6	Al2[9]	1.673(5)
Al1	O1B	1.707(3)			

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-Y+X,1+X,-1/2+Z; [7]1-X,1-Y,1-Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S31 Bond Angles for $AlPO_4$-17 at 0.549 GPa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
$O1^1$	P1	$O2^1$	110.8(2)	$O6^5$	Al2	$O1^4$	108.87(16)
$O1^1$	P1	$O3^2$	109.21(18)	$O6^5$	Al2	O5	110.1(2)
$O1^1$	P1	$O4^3$	107.4(2)	O1B	Al1	$O2^5$	109.33(18)
$O2^1$	P1	$O3^2$	108.0(2)	O1B	Al1	$O4^6$	110.92(19)
$O2^1$	P1	$O4^3$	110.50(19)	$O3^7$	Al1	O1B	108.41(17)
$O3^2$	P1	$O4^3$	110.85(18)	$O3^7$	Al1	$O2^5$	110.36(18)
O1B	P2	$O1B^4$	110.0(3)	$O3^7$	Al1	$O4^6$	110.00(17)
$O5^5$	P2	O1B	110.32(18)	$O4^6$	Al1	$O2^5$	107.83(17)
$O5^5$	P2	$O1B^4$	110.32(18)	$P1^8$	O1	Al2	146.9(2)
O6	P2	$O1B^4$	108.37(17)	P2	O1B	Al1	148.3(3)
O6	P2	O1B	108.37(17)	$P1^8$	O2	$Al1^9$	146.6(3)
O6	P2	$O5^5$	109.4(3)	$P1^{10}$	O3	$Al1^{11}$	148.04(19)
O1	Al2	$O1^4$	109.4(3)	$P1^{12}$	O4	$Al1^6$	145.5(3)
O1	Al2	O5	109.77(16)	$P2^9$	O5	Al2	151.7(4)
$O1^4$	Al2	O5	109.77(16)	P2	O6	$Al2^9$	172.2(3)
$O6^5$	Al2	O1	108.87(16)				

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-X,1-Y,1-Z; [7]1-Y+X,1+X,-1/2+Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S32 Crystal data and structure refinement for $AlPO_4$-17 at 0.723 GPa.

Identification code	17_SC05_P6b
Empirical formula	O_4AlP
Formula weight	121.95
Temperature/K	293(2)
Crystal system	hexagonal
Space group	$P6_3/m$
a/Å	12.9981(13)
b/Å	12.9981(13)
c/Å	15.2105(7)
α/°	90
β/°	90
γ/°	120
Volume/$Å^3$	2225.5(5)
Z	18
$\rho_{calc}g/cm^3$	1.638
μ/mm^{-1}	0.227
F(000)	1080.0

Crystal size/mm^3	? × ? × ?
Radiation	synchrotron (λ = 0.49555)
2Θ range for data collection/°	3.734 to 38.532
Index ranges	-8 ≤ h ≤ 13, -12 ≤ k ≤ 8, -20 ≤ l ≤ 20
Reflections collected	4741
Independent reflections	1375 [R_{int} = 0.0678, R_{sigma} = 0.0835]
Data/restraints/parameters	1375/0/88
Goodness-of-fit on F^2	1.130
Final R indexes [I>=2σ (I)]	R_1 = 0.1095, wR_2 = 0.2539
Final R indexes [all data]	R_1 = 0.1691, wR_2 = 0.2838
Largest diff. peak/hole / e Å^{-3}	1.00/-0.52

Table S33 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for AlPO$_4$-17 at 0.723 GPa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	9973(2)	2369(2)	1017.9(10)	41.5(7)
P2	5737(3)	9072(3)	2500	38.6(9)
Al2	930(3)	4241(3)	2500	39.0(10)
Al1	7617(2)	9977(2)	1010.7(12)	39.2(8)
O1	227(6)	3425(6)	1583(3)	62(2)
O1B	6455(6)	9688(7)	1689(3)	61(2)
O2	908(6)	2013(7)	1140(4)	65(2)
O3	1334(6)	2554(6)	6274(3)	56.6(17)
O4	2759(7)	34(6)	10059(3)	62(2)
O5	2384(8)	4599(8)	2500	58(2)
O6	4658(8)	9180(8)	2500	54(2)

Table S34 Anisotropic Displacement Parameters (Å^2×10^3) for AlPO$_4$-17 at 0.723 GPa. The Anisotropic displacement factor exponent takes the form: -2π^2[h^{2}a*^{2}U$_{11}$+2hka*b*U$_{12}$+…].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	47.7(15)	52.0(16)	24.2(9)	-3.6(8)	-0.7(8)	24.4(13)
P2	42(2)	48(2)	25.2(11)	0	0	22.7(16)
Al2	51(2)	44(2)	22.1(12)	0	0	23.5(19)
Al1	46.4(16)	47.4(17)	22.1(10)	1.4(8)	2.7(9)	22.2(13)
O1	83(5)	55(4)	32(2)	-6(2)	-3(3)	21(4)
O1B	64(5)	82(5)	30(2)	8(3)	13(2)	33(4)
O2	69(5)	78(5)	53(3)	10(3)	7(3)	40(4)
O3	60(4)	71(5)	42(3)	-9(3)	-6(3)	35(4)

Table S34 Anisotropic Displacement Parameters ($Å^2×10^3$) for $AlPO_4$-17 at 0.723 GPa. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O4	79(5)	72(5)	30(3)	2(2)	6(2)	34(4)
O5	62(7)	42(6)	69(5)	0	0	24(5)
O6	62(6)	61(6)	45(4)	0	0	35(5)

Table S35 Bond Lengths for $AlPO_4$-17 at 0.723 GPa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	O1[1]	1.510(6)	Al1	O2[5]	1.710(7)
P1	O2[1]	1.513(7)	Al1	O3[6]	1.699(7)
P1	O3[2]	1.511(6)	Al1	O4[7]	1.698(5)
P1	O4[3]	1.531(5)	O1	P1[8]	1.510(6)
P2	O1B[4]	1.512(5)	O2	P1[8]	1.513(7)
P2	O1B	1.513(5)	O2	Al1[9]	1.710(7)
P2	O5[5]	1.503(9)	O3	P1[10]	1.511(6)
P2	O6	1.478(9)	O3	Al1[11]	1.699(7)
Al2	O1	1.713(6)	O4	P1[12]	1.531(5)
Al2	O1[4]	1.713(6)	O4	Al1[7]	1.698(5)
Al2	O5	1.705(10)	O5	P2[9]	1.503(9)
Al2	O6[5]	1.684(9)	O6	Al2[9]	1.684(9)
Al1	O1B	1.708(6)			

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-Y+X,1+X,-1/2+Z; [7]1-X,1-Y,1-Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S36 Bond Angles for $AlPO_4$-17 at 0.723 GPa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1[1]	P1	O2[1]	111.4(4)	O6[5]	Al2	O1	108.5(3)
O1[1]	P1	O3[2]	108.9(3)	O6[5]	Al2	O5	110.6(4)
O1[1]	P1	O4[3]	107.4(4)	O1B	Al1	O2[5]	109.3(3)
O2[1]	P1	O4[3]	109.7(4)	O3[6]	Al1	O1B	108.4(3)
O3[2]	P1	O2[1]	108.6(4)	O3[6]	Al1	O2[5]	110.9(3)
O3[2]	P1	O4[3]	110.9(3)	O4[7]	Al1	O1B	111.0(4)
O1B[4]	P2	O1B	109.4(6)	O4[7]	Al1	O2[5]	107.5(3)
O5[5]	P2	O1B	110.3(3)	O4[7]	Al1	O3[6]	109.8(3)
O5[5]	P2	O1B[4]	110.3(3)	P1[8]	O1	Al2	146.4(5)
O6	P2	O1B	108.3(3)	P2	O1B	Al1	148.6(5)
O6	P2	O1B[4]	108.3(3)	P1[8]	O2	Al1[9]	147.4(5)
O6	P2	O5[5]	110.1(5)	P1[10]	O3	Al1[11]	148.0(3)
O1[4]	Al2	O1	109.0(5)	P1[12]	O4	Al1[7]	145.7(6)
O5	Al2	O1	110.2(3)	P2[9]	O5	Al2	151.8(6)

Table S36 Bond Angles for $AlPO_4$-17 at 0.723 GPa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O5	Al2	O1[4]	110.2(3)	P2	O6	Al2[9]	171.0(6)
O6[5]	Al2	O1[4]	108.5(3)				

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-Y+X,1+X,-1/2+Z; [7]1-X,1-Y,1-Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S37 Crystal data and structure refinement for $AlPO_4$-17 at 0.834 GPa.

Identification code	17_SC05_P7
Empirical formula	O_4AlP
Formula weight	121.95
Temperature/K	293(2)
Crystal system	hexagonal
Space group	$P6_3/m$
a/Å	12.9715(14)
b/Å	12.9715(14)
c/Å	15.1870(7)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	2213.0(5)
Z	18
ρ_{calc}g/cm^3	1.647
μ/mm^{-1}	0.228
F(000)	1080.0
Crystal size/mm^3	? × ? × ?
Radiation	synchrotron (λ = 0.49555)
2Θ range for data collection/°	3.74 to 38.572
Index ranges	-8 ≤ h ≤ 12, -16 ≤ k ≤ 16, -20 ≤ l ≤ 20
Reflections collected	4591
Independent reflections	1366 [R_{int} = 0.0779, R_{sigma} = 0.1022]
Data/restraints/parameters	1366/0/88
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.1148, wR_2 = 0.2657
Final R indexes [all data]	R_1 = 0.2009, wR_2 = 0.3112
Largest diff. peak/hole / e Å^{-3}	0.90/-0.54

Table S38 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for AlPO$_4$-17 at 0.834 GPa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	9970(3)	2369(2)	1019.3(12)	49.3(9)
P2	5731(3)	9065(4)	2500	45.0(10)
Al2	934(4)	4248(4)	2500	44.5(11)
Al1	7614(3)	9973(3)	1012.4(13)	46.8(9)
O1	229(8)	3429(7)	1586(3)	75(3)
O1B	6457(7)	9689(8)	1691(3)	72(3)
O2	898(7)	2004(8)	1140(4)	73(2)
O3	1328(7)	2554(7)	6272(3)	64(2)
O4	2768(8)	45(7)	10061(3)	70(2)
O5	2383(9)	4604(9)	2500	68(3)
O6	4652(10)	9170(9)	2500	67(3)

Table S39 Anisotropic Displacement Parameters (Å^2×10^3) for AlPO$_4$-17 at 0.834 GPa. The Anisotropic displacement factor exponent takes the form: -2π^2[h^{2}a*^{2}U$_{11}$+2hka*b*U$_{12}$+…].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	57.7(19)	60(2)	28.9(10)	-3.9(10)	-1.9(10)	28.3(16)
P2	52(3)	57(3)	30.6(13)	0	0	30(2)
Al2	57(3)	51(3)	27.4(15)	0	0	28(2)
Al1	57(2)	56(2)	26.3(12)	1.3(10)	2.8(11)	28.1(17)
O1	111(7)	74(6)	35(3)	-13(3)	-7(3)	42(5)
O1B	70(6)	92(6)	39(3)	4(3)	15(3)	29(5)
O2	72(6)	93(6)	58(4)	9(3)	6(3)	46(5)
O3	62(5)	78(6)	48(3)	-8(3)	-5(3)	33(4)
O4	92(6)	80(6)	32(3)	5(3)	3(3)	38(5)
O5	70(8)	54(7)	74(6)	0	0	26(6)
O6	85(8)	73(8)	50(5)	0	0	46(7)

Table S40 Bond Lengths for AlPO$_4$-17 at 0.834 GPa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	O1^1	1.511(7)	Al1	O2^5	1.714(8)
P1	O2^1	1.508(8)	Al1	O3^6	1.693(8)
P1	O3^2	1.510(7)	Al1	O4^7	1.701(6)
P1	O4^3	1.529(6)	O1	P1^8	1.511(7)
P2	O1B	1.513(6)	O2	P1^8	1.508(8)
P2	O1B^4	1.513(6)	O2	Al1^9	1.714(8)
P2	O5^5	1.500(11)	O3	P1^{10}	1.510(7)
P2	O6	1.473(11)	O3	Al1^{11}	1.693(8)

Table S40 Bond Lengths for $AlPO_4$-17 at 0.834 GPa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Al2	$O1^4$	1.709(7)	O4	$P1^{12}$	1.529(6)
Al2	O1	1.709(7)	O4	$Al1^7$	1.701(6)
Al2	O5	1.695(11)	O5	$P2^9$	1.500(11)
Al2	$O6^5$	1.673(11)	O6	$Al2^9$	1.673(11)
Al1	O1B	1.702(7)			

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-Y+X,1+X,-1/2+Z; [7]1-X,1-Y,1-Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S41 Bond Angles for $AlPO_4$-17 at 0.834 GPa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
$O1^1$	P1	$O4^2$	107.4(5)	$O6^5$	Al2	$O1^4$	108.7(4)
$O2^1$	P1	$O1^1$	111.5(4)	$O6^5$	Al2	O5	110.3(5)
$O2^1$	P1	$O3^3$	108.2(4)	O1B	Al1	$O2^5$	109.8(4)
$O2^1$	P1	$O4^2$	110.0(4)	$O3^6$	Al1	O1B	108.3(4)
$O3^3$	P1	$O1^1$	109.3(4)	$O3^6$	Al1	$O2^5$	110.6(4)
$O3^3$	P1	$O4^2$	110.4(4)	$O3^6$	Al1	$O4^7$	109.8(3)
$O1B^4$	P2	O1B	108.6(7)	$O4^7$	Al1	O1B	111.0(4)
$O5^5$	P2	$O1B^4$	110.6(4)	$O4^7$	Al1	$O2^5$	107.4(4)
$O5^5$	P2	O1B	110.6(4)	$P1^8$	O1	Al2	146.6(6)
O6	P2	O1B	108.5(4)	P2	O1B	Al1	148.5(6)
O6	P2	$O1B^4$	108.5(4)	$P1^8$	O2	$Al1^9$	146.8(6)
O6	P2	$O5^5$	110.0(6)	$P1^{10}$	O3	$Al1^{11}$	148.3(4)
$O1^4$	Al2	O1	108.7(6)	$P1^{12}$	O4	$Al1^7$	145.6(7)
O5	Al2	O1	110.2(4)	$P2^9$	O5	Al2	151.8(8)
O5	Al2	$O1^4$	110.2(4)	P2	O6	$Al2^9$	171.4(8)
$O6^5$	Al2	O1	108.7(4)				

[1]1+X,+Y,+Z; [2]1-Y,+X-Y,-1+Z; [3]1-Y+X,+X,-1/2+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-Y+X,1+X,-1/2+Z; [7]1-X,1-Y,1-Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S42 Crystal data and structure refinement for $AlPO_4$-17 at 0.97 GPa.

Identification code	17_SC05_P8
Empirical formula	O_4AlP
Formula weight	121.95
Temperature/K	293(2)
Crystal system	hexagonal
Space group	$P6_3/m$
a/Å	12.885(3)
b/Å	12.885(3)
c/Å	15.1515(11)

α/°	90
β/°	90
γ/°	120
Volume/Å^3	2178.7(10)
Z	18
ρ_{calc}g/cm^3	1.673
μ/mm^{-1}	0.232
F(000)	1080.0
Crystal size/mm^3	? × ? × ?
Radiation	synchrotron (λ = 0.49555)
2Θ range for data collection/°	3.748 to 28.58
Index ranges	-7 ≤ h ≤ 9, -9 ≤ k ≤ 6, -15 ≤ l ≤ 15
Reflections collected	2027
Independent reflections	590 [R_{int} = 0.0633, R_{sigma} = 0.0849]
Data/restraints/parameters	590/0/88
Goodness-of-fit on F^2	1.167
Final R indexes [I>=2σ (I)]	R_1 = 0.0907, wR_2 = 0.2016
Final R indexes [all data]	R_1 = 0.1438, wR_2 = 0.2265
Largest diff. peak/hole / e Å^{-3}	0.29/-0.34

Table S43 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for $AlPO_4$-17 at 0.834 GPa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	9964(5)	2375(5)	1012(2)	83.3(19)
P2	5728(6)	9053(6)	2500	71(2)
Al2	931(7)	4253(7)	2500	71(2)
Al1	7597(5)	9969(5)	1007(2)	79.4(19)
O1	246(12)	3450(12)	1584(6)	108(5)
O1B	6446(14)	9684(13)	1708(6)	123(6)
O2	910(11)	1997(12)	1128(6)	110(4)
O3	1325(10)	2558(10)	6264(5)	92(4)
O4	2802(13)	51(11)	10065(5)	104(4)
O5	2380(14)	4637(16)	2500	96(5)
O6	4669(16)	9208(16)	2500	115(6)

Table S44 Anisotropic Displacement Parameters ($Å^2×10^3$) for $AlPO_4$-17 at 0.834 GPa. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	95(4)	112(5)	48(2)	-10(3)	-12(2)	55(4)
P2	71(5)	88(6)	54(3)	0	0	40(4)
Al2	82(6)	78(6)	54(3)	0	0	40(5)
Al1	102(5)	90(4)	48(2)	9(2)	15(3)	49(4)
O1	111(11)	108(12)	94(7)	-37(7)	-13(6)	46(9)
O1B	148(14)	143(14)	77(6)	27(7)	51(7)	72(12)
O2	93(10)	170(13)	79(7)	8(6)	0(5)	74(10)
O3	92(10)	133(11)	62(5)	-20(5)	-3(5)	63(9)
O4	117(12)	102(9)	70(6)	6(5)	-6(6)	38(8)
O5	84(13)	112(15)	100(10)	0	0	56(12)
O6	80(14)	107(17)	169(15)	0	0	56(13)

Table S45 Bond Lengths for $AlPO_4$-17 at 0.834 GPa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	$O1^1$	1.517(13)	Al1	$O2^5$	1.695(12)
P1	$O2^1$	1.531(13)	Al1	$O3^6$	1.686(12)
P1	$O3^2$	1.506(11)	Al1	$O4^7$	1.699(9)
P1	$O4^3$	1.519(10)	O1	$P1^8$	1.517(13)
P2	O1B	1.485(10)	O2	$P1^8$	1.531(13)
P2	$O1B^4$	1.485(10)	O2	$Al1^9$	1.695(12)
P2	$O5^5$	1.508(17)	O3	$P1^{10}$	1.506(11)
P2	O6	1.475(18)	O3	$Al1^{11}$	1.686(12)
Al2	O1	1.692(12)	O4	$P1^{12}$	1.519(10)
Al2	$O1^4$	1.692(12)	O4	$Al1^7$	1.699(9)
Al2	O5	1.676(18)	O5	$P2^9$	1.508(17)
Al2	$O6^5$	1.653(19)	O6	$Al2^9$	1.653(19)
Al1	O1B	1.708(13)			

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-Y+X,1+X,-1/2+Z; [7]1-X,1-Y,1-Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S46 Bond Angles for $AlPO_4$-17 at 0.834 GPa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
$O1^1$	P1	$O2^1$	111.1(7)	$O6^5$	Al2	$O1^4$	107.9(6)
$O1^1$	P1	$O4^2$	106.4(8)	$O6^5$	Al2	O5	110.6(9)
$O3^3$	P1	$O1^1$	110.2(7)	$O2^5$	Al1	O1B	110.1(7)
$O3^3$	P1	$O2^1$	107.9(7)	$O2^5$	Al1	$O4^6$	107.7(6)
$O3^3$	P1	$O4^2$	110.8(6)	$O3^7$	Al1	O1B	108.0(6)
$O4^2$	P1	$O2^1$	110.4(7)	$O3^7$	Al1	$O2^5$	109.4(7)

Table S46 Bond Angles for $AlPO_4$-17 at 0.834 GPa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1B	P2	O1B[4]	107.8(12)	O3[7]	Al1	O4[6]	110.1(6)
O1B	P2	O5[5]	111.9(7)	O4[6]	Al1	O1B	111.6(7)
O1B[4]	P2	O5[5]	111.9(7)	P1[8]	O1	Al2	147.2(9)
O6	P2	O1B	106.9(8)	P2	O1B	Al1	149.0(11)
O6	P2	O1B[4]	106.9(8)	P1[8]	O2	Al1[9]	145.9(9)
O6	P2	O5[5]	111.1(10)	P1[10]	O3	Al1[11]	148.8(6)
O1[4]	Al2	O1	110.2(11)	P1[12]	O4	Al1[6]	143.8(11)
O5	Al2	O1	110.1(6)	P2[9]	O5	Al2	149.6(13)
O5	Al2	O1[4]	110.1(6)	P2	O6	Al2[9]	167.9(13)
O6[5]	Al2	O1	107.9(6)				

[1]1+X,+Y,+Z; [2]1-Y,+X-Y,-1+Z; [3]1-Y+X,+X,-1/2+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-X,1-Y,1-Z; [7]1-Y+X,1+X,-1/2+Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S47 Crystal data and structure refinement for $AlPO_4$-17 at 0.97 GPa.

Identification code	17_SC05_P9
Empirical formula	O_4AlP
Formula weight	121.95
Temperature/K	293(2)
Crystal system	hexagonal
Space group	$P6_3/m$
a/Å	12.749(5)
b/Å	12.749(5)
c/Å	15.1232(16)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	2128.7(18)
Z	18
ρ_{calc}g/cm^3	1.712
μ/mm^{-1}	0.238
F(000)	1080.0
Crystal size/mm^3	? × ? × ?
Radiation	synchrotron (λ = 0.49555)
2Θ range for data collection/°	3.756 to 24.884
Index ranges	$-6 \le h \le 8$, $-8 \le k \le 5$, $-13 \le l \le 13$
Reflections collected	1386
Independent reflections	382 [R_{int} = 0.0560, R_{sigma} = 0.0567]
Data/restraints/parameters	382/0/88
Goodness-of-fit on F^2	1.176

Final R indexes [I>=2σ (I)]	R_1 = 0.1371, wR_2 = 0.2148
Final R indexes [all data]	R_1 = 0.1782, wR_2 = 0.2317
Largest diff. peak/hole / e Å^{-3}	0.33/-0.28

Table S48 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for AlPO$_4$-17 at 0.97 GPa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	9961(18)	2470(20)	996(8)	174(7)
P2	5691(19)	9042(18)	2500	145(7)
Al2	910(20)	4263(19)	2500	145(7)
Al1	7570(20)	9942(18)	983(8)	177(8)
O1	200(40)	3450(40)	1645(18)	220(20)
O1B	6450(30)	9580(30)	1739(13)	230(20)
O2	910(30)	2070(30)	1117(13)	187(13)
O3	1330(40)	2510(20)	6243(10)	174(13)
O4	2950(30)	120(20)	10063(15)	165(12)
O5	2320(30)	4690(40)	2500	165(16)
O6	4680(50)	9200(50)	2500	260(30)

Table S49 Anisotropic Displacement Parameters (Å^2×10^3) for AlPO$_4$-17 at 0.97 GPa. The Anisotropic displacement factor exponent takes the form: -2π^2[h^{2}a*^{2}U$_{11}$+2hka*b*U$_{12}$+…].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	150(15)	220(20)	113(12)	10(10)	-30(9)	59(14)
P2	140(20)	150(19)	107(10)	0	0	45(17)
Al2	140(20)	124(17)	124(12)	0	0	32(13)
Al1	290(30)	141(14)	118(11)	41(9)	51(11)	119(17)
O1	230(50)	280(60)	190(20)	-110(30)	-90(30)	150(50)
O1B	190(40)	210(40)	119(16)	63(17)	85(19)	-40(30)
O2	160(30)	300(40)	140(20)	13(18)	-3(17)	140(30)
O3	220(40)	180(30)	58(13)	-16(12)	4(18)	50(30)
O4	200(30)	120(20)	122(13)	39(13)	15(18)	37(19)
O5	60(30)	240(50)	160(30)	0	0	60(30)
O6	80(50)	230(70)	460(90)	0	0	70(40)

Table S50 Bond Lengths for $AlPO_4$-17 at 0.97 GPa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	O1[1]	1.50(3)	Al1	O2[5]	1.69(3)
P1	O2[1]	1.55(3)	Al1	O3[6]	1.73(4)
P1	O3[2]	1.51(4)	Al1	O4[7]	1.70(3)
P1	O4[3]	1.50(3)	O1	P1[8]	1.50(3)
P2	O1B	1.44(2)	O2	P1[8]	1.55(3)
P2	O1B[4]	1.44(2)	O2	Al1[9]	1.69(3)
P2	O5[5]	1.61(4)	O3	P1[10]	1.51(4)
P2	O6	1.40(5)	O3	Al1[11]	1.73(4)
Al2	O1[4]	1.62(3)	O4	P1[12]	1.50(3)
Al2	O1	1.62(3)	O4	Al1[7]	1.70(3)
Al2	O5	1.60(4)	O5	P2[9]	1.61(4)
Al2	O6[5]	1.63(5)	O6	Al2[9]	1.63(5)
Al1	O1B	1.71(4)			

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-Y+X,1+X,-1/2+Z; [7]1-X,1-Y,1-Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

Table S51 Bond Angles for $AlPO_4$-17 at 0.97 GPa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1[1]	P1	O2[1]	109.6(19)	O5	Al2	O1	113(2)
O1[1]	P1	O3[2]	110(2)	O5	Al2	O6[5]	107(3)
O1[1]	P1	O4[3]	112(3)	O1B	Al1	O3[6]	109.9(16)
O3[2]	P1	O2[1]	101(2)	O2[5]	Al1	O1B	103(2)
O4[3]	P1	O2[1]	113.2(18)	O2[5]	Al1	O3[6]	110(2)
O4[3]	P1	O3[2]	110.3(15)	O2[5]	Al1	O4[7]	109.6(15)
O1B	P2	O1B[4]	106(3)	O4[7]	Al1	O1B	111(2)
O1B[4]	P2	O5[5]	107(2)	O4[7]	Al1	O3[6]	113.2(12)
O1B	P2	O5[5]	107(2)	P1[8]	O1	Al2	150(3)
O6	P2	O1B[4]	112(3)	P2	O1B	Al1	160(4)
O6	P2	O1B	112(3)	P1[8]	O2	Al1[9]	147(3)
O6	P2	O5[5]	112(3)	P1[10]	O3	Al1[11]	151.9(14)
O1[4]	Al2	O1	106(4)	P1[12]	O4	Al1[7]	138(2)
O1[4]	Al2	O6[5]	108(2)	Al2	O5	P2[9]	148(4)
O1	Al2	O6[5]	108(2)	P2	O6	Al2[9]	168(5)
O5	Al2	O1[4]	113(2)				

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-Y+X,1+X,-1/2+Z; [7]1-X,1-Y,1-Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

17_SC05_P10

Table S52 Crystal data and structure refinement for $AlPO_4$-17 at 1.11 GPa.

Identification code	17_SC05_P10
Empirical formula	AlO_4P
Formula weight	121.95
Temperature/K	293(2)
Crystal system	hexagonal
Space group	$P6_3/m$
a/Å	12.64(3)
b/Å	12.64(3)
c/Å	15.121(8)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	2093(10)
Z	18
ρ_{calc}g/cm^3	1.741
μ/mm^{-1}	0.242
F(000)	1080.0
Crystal size/mm^3	? × ? × ?
Radiation	synchrotron (λ = 0.49555)
2Θ range for data collection/°	3.756 to 20.378
Index ranges	$-5 \le h \le 6$, $-6 \le k \le 4$, $-10 \le l \le 10$
Reflections collected	719
Independent reflections	194 [R_{int} = 0.0736, R_{sigma} = 0.0645]
Data/restraints/parameters	194/0/41
Goodness-of-fit on F^2	1.226
Final R indexes [I>=2σ (I)]	R_1 = 0.1772, wR_2 = 0.4214
Final R indexes [all data]	R_1 = 0.2155, wR_2 = 0.4495
Largest diff. peak/hole / e Å^{-3}	0.30/-0.39

Table S53 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for $AlPO_4$-17 at 1.11 GPa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	9950(20)	2350(20)	1041(14)	142(10)
P2	5740(40)	9090(50)	2500	171(15)
Al2	1050(50)	4440(50)	2500	176(16)
Al1	7500(30)	9970(30)	971(15)	159(11)
O1	100(90)	3490(90)	1590(40)	250(30)
O1B	6340(90)	9810(90)	1720(40)	250(30)
O2	1030(50)	1910(60)	1030(30)	176(18)
O3	1300(40)	2530(30)	6228(19)	104(14)

Table S53 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for AlPO$_4$-17 at 1.11 GPa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O4	2840(60)	150(50)	10160(30)	190(30)
O5	2420(70)	4530(60)	2500	140(20)
O6	4750(190)	9300(130)	2500	330(60)

Table S54 Bond Lengths for AlPO$_4$-17 at 1.11 GPa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P1	O1^1	1.60(9)	Al1	O2^5	1.58(5)
P1	O2^1	1.71(5)	Al1	O3^6	1.68(5)
P1	O3^2	1.45(4)	Al1	O4^7	1.76(5)
P1	O4^3	1.42(5)	O1	P1^8	1.60(9)
P2	O1B	1.45(7)	O2	P1^8	1.71(5)
P2	O1B^4	1.45(7)	O2	Al1^9	1.58(5)
P2	O5^5	1.38(7)	O3	P1^{10}	1.45(4)
P2	O6	1.40(18)	O3	Al1^{11}	1.68(5)
Al2	O1	1.82(9)	O4	P1^{12}	1.42(5)
Al2	O1^4	1.82(9)	O4	Al1^7	1.76(5)
Al2	O5	1.68(7)	O5	P2^9	1.38(7)
Al2	O6^5	1.55(18)	O6	Al2^9	1.55(18)
Al1	O1B	1.78(9)			

^{1}1+X,+Y,+Z; ^{2}1-Y+X,+X,-1/2+Z; ^{3}1-Y,+X-Y,-1+Z; ^{4}+X,+Y,1/2-Z; ^{5}1-Y,1+X-Y,+Z; ^{6}1-Y+X,1+X,-1/2+Z; ^{7}1-X,1-Y,1-Z; ^{8}-1+X,+Y,+Z; ^{9}+Y-X,1-X,+Z; ^{10}+Y,1-X+Y,1/2+Z; ^{11}-1+Y,-X+Y,1/2+Z; ^{12}1+Y-X,1-X,1+Z

Table S55 Bond Angles for AlPO$_4$-17 at 1.11 GPa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1^1	P1	O2^1	123(4)	O6^5	Al2	O1^4	100(5)
O3^2	P1	O1^1	109(4)	O6^5	Al2	O5	131(7)
O3^2	P1	O2^1	109(3)	O2^5	Al1	O1B	122(4)
O4^3	P1	O1^1	102(4)	O2^5	Al1	O3^6	98(3)
O4^3	P1	O2^1	107(3)	O2^5	Al1	O4^7	101(3)
O4^3	P1	O3^2	105(3)	O3^6	Al1	O1B	106(3)
O1B^4	P2	O1B	109(8)	O3^6	Al1	O4^7	112(2)
O5^5	P2	O1B^4	117(5)	O4^7	Al1	O1B	117(4)
O5^5	P2	O1B	117(5)	P1^8	O1	Al2	136(6)
O5^5	P2	O6	117(8)	P2	O1B	Al1	137(7)
O6	P2	O1B^4	97(6)	Al1^9	O2	P1^8	140(5)
O6	P2	O1B	97(6)	P1^{10}	O3	Al1^{11}	154(2)
O1^4	Al2	O1	98(7)	P1^{12}	O4	Al1^7	146(5)
O5	Al2	O1	112(4)	P2^9	O5	Al2	164(6)

Table S55 Bond Angles for $AlPO_4$-17 at 1.11 GPa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O5	Al2	O1[4]	112(4)	P2	O6	Al2[9]	156(10)
O6[5]	Al2	O1	100(5)				

[1]1+X,+Y,+Z; [2]1-Y+X,+X,-1/2+Z; [3]1-Y,+X-Y,-1+Z; [4]+X,+Y,1/2-Z; [5]1-Y,1+X-Y,+Z; [6]1-Y+X,1+X,-1/2+Z; [7]1-X,1-Y,1-Z; [8]-1+X,+Y,+Z; [9]+Y-X,1-X,+Z; [10]+Y,1-X+Y,1/2+Z; [11]-1+Y,-X+Y,1/2+Z; [12]1+Y-X,1-X,1+Z

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