SUPPLEMENTARY MATERIAL

Mechanical Characterization of Anhydrous Microporous Aluminophosphate Materials: Tridimensional Incompressibility, Ductility, Isotropy and Negative Linear Compressibility

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Table S.1. Material data and calculation parameters.

Compound	Framework topology	Structural formula	Crystal system	Space group	ε(eV)	k-mesh
VPI-5 [1-2]	VFI	$AlPO_4$	Hexagonal	$P6_3cm$ (no. 185)	1000	$2 \times 2 \times 4$
			Monoclinic	$C1m1$ (no. 8)	1000	$1 \times 1 \times 3$
ALPO-8 [3]	AET	$AlPO_4$	Orthorhombic	$Cmc2_1$ (no. 36)	1000	$1 \times 2 \times 3$
ALPO-5 [4-5]	AFI	$AlPO_4$	Orthorhombic	$Pcc2$ (no. 27)	1000	$2 \times 1 \times 3$
			Hexagonal	$P6cc$ (no. 184)	1000	$2 \times 2 \times 4$
ALPO-18 [6]	AEI	$AlPO_4$	Monoclinic	$C2/c$ (no. 15)	1000	$2 \times 2 \times 1$
ALPO-18W [7]	AEI	$AlPO_4 \cdot 2\ H_2O$	Triclinic	$P1$ (no. 1)	1000	$3 \times 3 \times 1$
ALPO-31 [8]	ATO	$AlPO_4$	Trigonal	$R\bar{3}$ (no. 148)	1000	$1 \times 1 \times 6$

Table S.2. Most intense reflections in the X-ray diffraction pattern of VPI-5 ($P6_3cm$): (a) X-ray pattern derived from the experimental crystal structure [1]; (b) X-ray pattern derived from the calculated crystal structure.

[$h\ k\ l$]	(a) Exp [1].			(b) Calc.		Δ (**2θ**)
	2θ (**deg**)	**d** (Å)	**I (%)**	**2θ** (**deg**)	**d** (Å)	
[0 1 0]	5.482	16.109	100.000	5.499	16.059	0.02
[0 2 0]	10.976	8.054	9.126	11.010	8.029	0.03
[0 0 2]	21.222	4.183	6.082	20.786	4.270	-0.44
[-2 4 1]	21.849	4.065	4.054	21.797	4.074	-0.05
[-1 4 1]	22.543	3.941	3.765	22.496	3.949	-0.05
[-2 4 0]	19.070	4.650	3.207	19.130	4.636	0.06
[0 1 2]	21.935	4.049	2.784	21.517	4.127	-0.42
[-2 5 0]	24.062	3.696	2.569	24.138	3.684	0.08
[-1 6 0]	30.882	2.893	1.484	30.980	2.884	0.10
[-3 6 0]	28.775	3.100	1.426	28.866	3.091	0.09
[-1 5 1]	27.501	3.241	1.195	27.490	3.242	-0.01
[-2 7 0]	34.751	2.579	1.093	34.862	2.572	0.11

Table S.3. Most intense reflections in the X-ray diffraction pattern of ALPO-8 ($Cmc2_1$): (a) X-ray pattern derived from the experimental crystal structure [3]; (b) X-ray pattern derived from the calculated crystal structure.

[$h\ k\ l$]	(a) Exp. [3]			(b) Calc.		Δ (2θ)
	2θ (deg)	d (Å)	I (%)	2θ (deg)	d (Å)	
[1 1 0]	6.545	13.493	100.000	6.552	13.479	0.01
[2 0 0]	5.305	16.645	78.476	5.269	16.759	-0.04
[0 0 2]	21.507	4.129	21.719	20.786	4.270	-0.72
[3 1 0]	9.964	8.870	13.583	9.930	8.900	-0.03
[4 2 0]	16.038	5.522	8.517	16.013	5.530	-0.02
[6 2 1]	22.742	3.907	7.237	22.512	3.946	-0.23
[3 3 1]	22.492	3.950	6.939	22.340	3.976	-0.15
[7 1 1]	22.380	3.969	5.820	22.106	4.018	-0.27
[9 1 0]	24.795	3.588	4.584	24.638	3.610	-0.16
[6 2 0]	20.005	4.435	4.449	19.937	4.450	-0.07
[0 4 0]	24.099	3.690	4.031	24.161	3.681	0.06
[1 3 1]	21.172	4.193	3.846	21.030	4.221	-0.14
[10 2 0]	29.410	3.035	3.784	29.254	3.050	-0.16
[4 4 0]	26.400	3.373	2.926	26.428	3.370	0.03
[6 2 3]	38.463	2.339	2.732	37.475	2.398	-0.99
[7 1 0]	19.596	4.527	2.648	19.479	4.553	-0.12
[2 0 2]	22.166	4.007	2.570	21.458	4.138	-0.71
[1 1 2]	22.503	3.948	2.503	21.817	4.071	-0.69
[1 3 0]	18.212	4.867	2.253	18.256	4.856	0.04
[5 1 0]	14.583	6.069	2.101	14.507	6.101	-0.08
[0 4 1]	26.435	3.369	2.070	26.347	3.380	-0.09

Table S.4. Most intense reflections in the X-ray diffraction pattern of ALPO-5 (*P*6*cc*): (a) X-ray pattern derived from the experimental crystal structure [5]; (b) X-ray pattern derived from the calculated crystal structure.

[***h k l***]	**(a) Exp. [5]**			**(b) Calc.**		Δ (**2θ**)
	2θ (**deg**)	**d** (Å)	**I (%)**	**2θ** (**deg**)	**d** (Å)	
[0 1 0]	7.435	11.880	100.000	7.357	12.007	-0.08
[-1 3 1]	22.402	3.966	25.962	22.165	4.007	-0.24
[0 0 2]	21.003	4.226	20.972	20.790	4.269	-0.21
[-1 3 0]	19.756	4.490	15.619	19.545	4.538	-0.21
[-1 2 0]	12.896	6.859	10.255	12.760	6.932	-0.14
[-2 4 0]	25.960	3.430	8.765	25.681	3.466	-0.28
[-1 5 0]	34.571	2.593	5.960	34.194	2.620	-0.38
[0 4 0]	30.064	2.970	5.470	29.739	3.002	-0.32
[-1 3 3]	37.660	2.387	5.151	37.262	2.411	-0.40
[0 1 2]	22.309	3.982	5.150	22.081	4.022	-0.23
[-1 3 5]	58.272	1.582	3.917	57.628	1.598	-0.64
[-1 3 2]	28.990	3.078	3.001	28.686	3.110	-0.30
[0 2 0]	14.902	5.940	2.707	14.744	6.004	-0.16
[-1 4 1]	29.063	3.070	2.311	28.752	3.103	-0.31

Table S.5. Most intense reflections in the X-ray diffraction pattern of ALPO-18 ($C2/c$): (a) X-ray pattern derived from the experimental crystal structure [6]; (b) X-ray pattern derived from the calculated crystal structure.

[$h\ k\ l$]	(a) Exp. [6]			(b) Calc.		Δ (**2θ**)
	2θ (**deg**)	**d** (Å)	**I (%)**	**2θ** (**deg**)	**d** (Å)	
[1 1 0]	9.472	9.330	100.000	9.539	9.264	0.07
[0 0 2]	9.517	9.285	57.941	9.575	9.230	0.06
[0 2 2]	16.873	5.250	19.281	16.961	5.223	0.09
[-1 -1 1]	10.603	8.337	14.788	10.676	8.280	0.07
[2 0 0]	12.903	6.856	13.341	13.029	6.789	0.13
[1 1 1]	10.604	8.336	13.173	10.677	8.279	0.07
[3 1 0]	20.631	4.302	12.080	20.823	4.263	0.19
[-1 1 3]	17.176	5.158	9.610	17.286	5.126	0.11
[1 1 3]	17.178	5.158	9.496	17.288	5.125	0.11
[0 2 3]	19.991	4.438	6.690	20.101	4.414	0.11
[2 0 2]	16.059	5.515	6.286	16.195	5.469	0.14
[0 2 5]	27.787	3.208	6.157	27.949	3.190	0.16
[-2 0 2]	16.056	5.516	6.150	16.193	5.469	0.14
[-2 -2 2]	21.298	4.169	5.628	21.446	4.140	0.15
[4 2 2]	31.136	2.870	5.122	31.404	2.846	0.27
[-2 2 3]	23.865	3.726	4.682	24.027	3.701	0.16
[2 2 3]	23.867	3.725	4.671	24.030	3.700	0.16
[0 2 6]	32.131	2.784	4.380	32.322	2.768	0.19
[1 1 4]	21.362	4.156	4.373	21.496	4.131	0.13
[-4 -2 2]	31.133	2.870	4.103	31.402	2.847	0.27
[4 0 0]	25.973	3.428	3.944	26.231	3.395	0.26
[-1 3 2]	23.931	3.715	3.655	24.062	3.696	0.13
[1 3 3]	26.257	3.391	3.325	26.403	3.373	0.15
[2 2 0]	19.009	4.665	3.129	19.146	4.632	0.14
[-1 3 3]	26.256	3.392	2.909	26.402	3.373	0.15
[2 4 0]	30.951	2.887	2.817	31.131	2.871	0.18
[-3 -1 1]	21.183	4.191	2.760	21.377	4.153	0.19
[-1 1 2]	13.442	6.582	2.721	13.531	6.539	0.09
[-1 3 5]	32.672	2.739	2.669	32.863	2.723	0.19
[1 1 2]	13.444	6.581	2.389	13.532	6.538	0.09
[-4 -2 1]	29.970	2.979	2.387	30.234	2.954	0.26

Table S.6. Most intense reflections in the X-ray diffraction pattern of ALPO-31 ($R\bar{3}$): (a) X-ray pattern derived from the experimental crystal structure [8]; (b) X-ray pattern derived from the calculated crystal structure.

[$h\ k\ l$]	(a) Exp. [8]			(b) Calc.		Δ (**2θ**)
	2θ (**deg**)	**d** (Å)	**I (%)**	**2θ** (**deg**)	**d** (Å)	
[-1 2 0]	8.484	10.414	100.000	8.429	10.482	-0.05
[-1 5 0]	22.572	3.936	32.779	22.423	3.962	-0.15
[0 2 1]	20.282	4.375	32.490	20.023	4.431	-0.26
[-2 3 1]	22.020	4.033	20.452	21.759	4.081	-0.26
[2 4 1]	31.739	2.817	15.750	31.445	2.843	-0.29
[-4 5 0]	22.572	3.936	15.539	22.423	3.962	-0.15
[-5 3 1]	27.959	3.189	11.108	27.681	3.220	-0.28
[-2 4 0]	17.015	5.207	10.333	16.904	5.241	-0.11
[0 3 0]	14.722	6.012	9.145	14.626	6.052	-0.10
[-4 7 1]	35.153	2.551	5.812	34.841	2.573	-0.31
[0 6 0]	29.695	3.006	5.228	29.497	3.026	-0.20
[-3 2 1]	22.020	4.033	4.664	21.759	4.081	-0.26
[-9 8 1]	46.662	1.945	4.658	46.281	1.960	-0.38
[0 1 2]	36.225	2.478	3.567	35.687	2.514	-0.54
[-1 4 1]	25.154	3.538	3.427	24.886	3.575	-0.27
[-7 14 0]	62.369	1.488	3.296	61.918	1.497	-0.45
[-3 6 0]	25.643	3.471	2.934	25.473	3.494	-0.17
[1 9 1]	51.637	1.769	2.705	51.221	1.782	-0.42
[-1 1 1]	18.388	4.821	2.456	18.130	4.889	-0.26
[-7 4 1]	35.153	2.551	2.349	34.841	2.573	-0.31
[-2 2 2]	37.273	2.411	2.197	36.734	2.445	-0.54
[-1 3 2]	38.296	2.348	2.184	37.757	2.381	-0.54
[4 8 2]	66.310	1.409	2.149	65.634	1.421	-0.68
[1 4 3]	60.219	1.536	2.072	59.337	1.556	-0.88
[-11 6 1]	51.637	1.769	2.060	51.221	1.782	-0.42

Table S.7. Interatomic distances for the $P6_3cm$ structure of VPI-5 (in Å).

Distance	Exp [1].	Calc.	Distance	Exp [1].	Calc.
P-O			**Al-O**		
P1-O1	1.459	1.507	Al1-O1	1.666	1.692
P1-O2	1.500	1.508	Al1-O2	1.650	1.692
P1-O4	1.568	1.516	Al1-O3	1.768	1.704
P1-O4′	1.568	1.516	Al1-O3′	1.768	1.704
<P1-O>	1.524	1.512	<Al1-O>	1.713	1.698
P2-O7	1.541	1.505	Al2-O7	1.733	1.692
P2-O5	1.466	1.507	Al2-O5	1.715	1.693
P2-O6	1.476	1.517	Al2-O6	1.722	1.704
P2-O3	1.546	1.522	Al2-O4	1.780	1.712
<P2-O>	1.507	1.513	<Al2-O>	1.738	1.700
<P-O>	1.52	1.51	<Al-O>	1.72	1.70

Table S.8. Interatomic distances in ALPO-8 (in Å).

Distance	Exp [3].	Calc.	Distance	Exp [3].	Calc.
P-O			**Al-O**		
P1-O5	1.499	1.505	Al1-O3	1.703	1.691
P1-O6	1.506	1.507	Al1-O2	1.725	1.701
P1-O4	1.525	1.520	Al1-O2′	1.725	1.701
P1-O2	1.529	1.522	Al1-O1	1.734	1.689
<P1-O>	1.515	1.514	<Al1-O>	1.722	1.696
P2-O11	1.511	1.510	Al2-O5	1.713	1.693
P2-O12	1.519	1.509	Al2-O7	1.726	1.693
P2-O10	1.521	1.515	Al2-O8	1.745	1.697
P2-O8	1.531	1.504	Al2-O9	1.749	1.703
<P2-O>	1.521	1.510	<Al2-O>	1.733	1.697
P3-O3	1.484	1.508	Al3-O14	1.714	1.694
P3-O15	1.516	1.517	Al3-O11	1.730	1.700
P3-O15′	1.516	1.517	Al3-O18	1.744	1.701
P3-O1	1.529	1.505	Al3-O3	1.748	1.703
<P3-O>	1.511	1.512	<Al3-O>	1.734	1.700
P4-O7	1.504	1.506	Al4-O6	1.708	1.694
P4-O16	1.513	1.509	Al4-O16	1.710	1.695
P4-O17	1.518	1.514	Al4-O4	1.726	1.708
P4-O18	1.534	1.516	Al4-O15	1.777	1.716
<P4-O>	1.517	1.511	<Al4-O>	1.730	1.703
P5-O14	1.506	1.507	Al5-O12	1.726	1.695
P5-O19	1.526	1.518	Al5-O10	1.731	1.700
P5-O9	1.530	1.513	Al5-O19	1.732	1.698
P5-O13	1.538	1.515	Al5-O17	1.739	1.692
<P5-O>	1.525	1.513	<Al5-O>	1.732	1.696
<P-O>	1.52	1.51	<Al-O>	1.73	1.70

Table S.9. Interatomic distances for the *P6cc* structure of ALPO-5 (in Å).

Distance	Exp [5].	Calc.	Distance	Exp [5].	Calc.
P-O			**Al-O**		
P1-O2	1.431	1.508	Al1-O4	1.672	1.693
P1-O3	1.480	1.514	Al1-O2	1.713	1.694
P1-O1	1.485	1.515	Al1-O1	1.718	1.701
P1-O4	1.533	1.508	Al1-O3	1.732	1.701
<P-O>	1.48	1.51	<Al-O>	1.71	1.70

Table S.10. Interatomic distances in ALPO-18 (in Å).

Distance	Exp [6].	Calc.	Distance	Exp [6].	Calc.
P-O			**Al-O**		
P1-O5	1.507	1.509	Al1-O5	1.712	1.696
P1-O12	1.510	1.516	Al1-O11	1.720	1.704
P1-O4	1.514	1.516	Al1-O6	1.729	1.702
P1-O10	1.518	1.510	Al1-O9	1.745	1.696
<P1-O>	1.512	1.513	<Al1-O>	1.727	1.700
P2-8	1.505	1.511	Al2-O3	1.635	1.697
P2-O2	1.510	1.517	Al2-O10	1.727	1.696
P2-O11	1.515	1.517	Al2-O7	1.764	1.702
P2-O3	1.583	1.510	Al2-O4	1.764	1.701
<P2-O>	1.528	1.514	<Al2-O>	1.723	1.699
P3-O1	1.496	1.511	Al3-O8	1.724	1.697
P3-O7	1.502	1.516	Al3-O2	1.735	1.703
P3-O9	1.504	1.510	Al3-O12	1.736	1.703
P3-O6	1.517	1.516	Al3-O1	1.740	1.698
<P3-O>	1.505	1.513	<Al3-O>	1.734	1.700
<P-O>	1.51	1.51	<Al-O>	1.73	1.70

Table S.11. Interatomic distances in ALPO-31 (in Å).

Distance	Exp [8].	Calc.	Distance	Exp [8].	Calc.
P-O			**Al-O**		
P-O3	1.568	1.509	Al1-O2	1.686	1.698
P-O1	1.580	1.513	Al1-O3	1.720	1.695
P-O2	1.583	1.513	Al1-O1	1.738	1.700
P-O4	1.633	1.513	Al1-O4	1.788	1.700
<P-O>	1.59	1.51	<Al1-O>	1.73	1.70

Table S.12. Unit cell volume and lattice parameters of VPI-5 ($P6_3cm$) under the effect of different external isotropic pressures.

P (GPa)	**Vol. (Å^3)**	$\boldsymbol{a}$ **(Å)**	$\boldsymbol{b}$ **(Å)**	$\boldsymbol{c}$ **(Å)**	$\boldsymbol{\alpha}$ **(deg)**	$\boldsymbol{\beta}$ **(deg)**	$\boldsymbol{\gamma}$**(deg)**
-0.5000	2564.3816	18.6095	18.6095	8.5503	90.00	90.00	120.00
-0.2502	2553.5546	18.5760	18.5760	8.5450	90.00	90.00	120.00
-0.0001	2542.9197	18.5431	18.5431	8.5396	90.00	90.00	120.00
0.2500	2532.4231	18.5105	18.5105	8.5343	90.00	90.00	120.00
0.4998	2522.0647	18.4781	18.4781	8.5293	90.00	90.00	120.00
1.0003	2501.2104	18.4123	18.4123	8.5193	90.00	90.00	120.00
2.0011	2460.4440	18.2820	18.2820	8.5003	90.00	90.00	120.00
3.0000	2421.2291	18.1635	18.1635	8.4743	90.00	90.00	120.00
4.0002	2374.3623	18.0309	18.0309	8.4330	90.00	90.00	120.00
5.0000	2307.8959	17.8764	17.8764	8.3392	90.00	90.00	120.00

Table S.13. Calculated volumetric compressibilities ($k_V = -1/V \cdot (\partial V/\partial P)_P$) of VPI-5 ($P6_3cm$) and compressibilities along a, b and c directions ($k_m = -1/m \cdot (\partial m/\partial P)_P$) for different external isotropic pressures. The computed bulk moduli (B) are given in the last column of the table.

P (GPa)	$\boldsymbol{k_V}$**(TPa^{-1})**	$\boldsymbol{k_a}$**(TPa^{-1})**	$\boldsymbol{k_b}$**(TPa^{-1})**	$\boldsymbol{k_c}$**(TPa^{-1})**	$\boldsymbol{B}$**(GPa)**
0.00	16.46	6.95	6.95	2.56	60.74
0.50	16.55	7.10	7.10	2.35	60.40
1.00	16.67	7.25	7.25	2.16	60.01
1.50	16.42	7.10	7.10	2.22	60.91
2.00	16.00	6.74	6.74	2.53	62.50
2.50	15.94	6.46	6.46	3.02	62.75
3.00	16.86	6.58	6.58	3.70	59.32
3.50	19.26	7.26	7.26	4.75	51.92
4.00	23.28	8.29	8.29	6.70	42.95

Table S.14. Unit cell volume and lattice parameters of ALPO-8 under the effect of different external isotropic pressures.

P (GPa)	**Vol. (Å^3)**	$\boldsymbol{a}$ **(Å)**	$\boldsymbol{b}$ **(Å)**	$\boldsymbol{c}$ **(Å)**	$\boldsymbol{\alpha}$ **(deg)**	$\boldsymbol{\beta}$ **(deg)**	$\boldsymbol{\gamma}$**(deg)**
-0.4998	4243.7090	33.6361	14.7582	8.5488	90.00	90.00	90.00
-0.2502	4228.6333	33.5636	14.7453	8.5443	90.00	90.00	90.00
-0.0004	4213.9746	33.5175	14.7223	8.5398	90.00	90.00	90.00
0.2498	4197.3731	33.4377	14.7072	8.5352	90.00	90.00	90.00
0.5002	4167.7665	33.3253	14.6755	8.5219	90.00	90.00	90.00
1.0001	4093.3425	33.1506	14.5813	8.4682	90.00	90.00	90.00
1.9997	3911.6747	32.8182	14.3298	8.3178	90.00	90.00	90.00
3.0005	3695.2847	32.6778	13.9605	8.1001	90.00	90.00	90.00
4.0005	3535.8598	32.4206	13.7281	7.9445	90.00	90.00	90.00
4.9998	3400.4830	31.9466	13.5530	7.8538	90.00	90.00	90.00

Table S.15. Calculated volumetric compressibilities ($k_V = -1/V \cdot (\partial V/\partial P)_P$) of ALPO-8 and compressibilities along a, b and c directions ($k_m = -1/m \cdot (\partial m/\partial P)_P$) for different external isotropic pressures. The computed bulk moduli (B) are given in the last column of the table.

P (GPa)	$\boldsymbol{k_V}$**(TPa^{-1})**	$\boldsymbol{k_a}$**(TPa^{-1})**	$\boldsymbol{k_b}$**(TPa^{-1})**	$\boldsymbol{k_c}$**(TPa^{-1})**	$\boldsymbol{B}$**(GPa)**
0.00	13.77	6.93	5.04	1.81	72.60
0.50	28.35	11.26	9.25	7.84	35.27
1.00	38.01	12.03	12.87	13.11	26.31
1.50	47.33	10.08	18.23	19.02	21.13
2.00	54.47	6.64	23.69	24.15	18.36
2.50	57.12	3.88	26.53	26.71	17.51
3.00	53.63	3.88	24.43	25.32	18.65
3.50	44.60	7.49	17.20	19.91	22.42
4.00	34.76	13.33	8.71	12.72	28.77

Table S.16. Unit cell volume and lattice parameters of ALPO-5 (*P*6*cc*) under the effect of different external isotropic pressures.

P (GPa)	**Vol. (Å^3)**	$\boldsymbol{a}$ **(Å)**	$\boldsymbol{b}$ **(Å)**	$\boldsymbol{c}$ **(Å)**	$\boldsymbol{\alpha}$ **(deg)**	$\boldsymbol{\beta}$ **(deg)**	$\boldsymbol{\gamma}$**(deg)**
-0.4989	1429.0148	13.8935	13.8935	8.5484	90.00	90.00	120.00
-0.2500	1424.9925	13.8779	13.8779	8.5435	90.00	90.00	120.00
0.0003	1421.3664	13.8645	13.8645	8.5382	90.00	90.00	120.00
0.2498	1417.0366	13.8470	13.8470	8.5337	90.00	90.00	120.00
0.5000	1413.4931	13.8341	13.8341	8.5283	90.00	90.00	120.00
1.0000	1404.6021	13.7983	13.7983	8.5187	90.00	90.00	120.00
1.9999	1384.0784	13.7114	13.7114	8.5010	90.00	90.00	120.00
3.0000	1354.9392	13.5744	13.5744	8.4908	90.00	90.00	120.00
3.9998	1327.3986	13.4447	13.4447	8.4795	90.00	90.00	120.00
5.0001	1301.7433	13.3217	13.3217	8.4699	90.00	90.00	120.00

Table S.17. Calculated volumetric compressibilities ($k_V = -1/V \cdot (\partial V/\partial P)_P$) of ALPO-5 ($P6cc$) and compressibilities along a, b and c directions ($k_m = -1/m \cdot (\partial m/\partial P)_P$) for different external isotropic pressures. The computed bulk moduli (B) are given in the last column of the table.

P (GPa)	$\boldsymbol{k_V}$**(TPa^{-1})**	$\boldsymbol{k_a}$**(TPa^{-1})**	$\boldsymbol{k_b}$**(TPa^{-1})**	$\boldsymbol{k_c}$**(TPa^{-1})**	$\boldsymbol{B}$**(GPa)**
0.00	11.45	4.61	4.61	2.25	87.27
0.50	11.38	4.50	4.50	2.36	87.97
1.00	12.26	4.94	4.94	2.36	81.64
1.50	14.87	6.40	6.40	2.07	67.21
2.00	18.45	8.44	8.44	1.59	54.15
2.50	21.48	10.16	10.16	1.17	46.55
3.00	22.47	10.70	10.70	1.04	44.55
3.50	20.84	9.77	9.77	1.29	48.01
4.00	17.86	8.12	8.12	1.67	55.83

Table S.18. Unit cell volume and lattice parameters of ALPO-31 under the effect of different external isotropic pressures.

P (GPa)	Vol. (Å^3)	a (Å)	b (Å)	c (Å)	α (deg)	β (deg)	γ(deg)
-0.5000	1944.7329	21.0150	21.0150	5.0848	90.00	90.00	120.00
-0.2504	1938.5988	20.9896	20.9896	5.0810	90.00	90.00	120.00
0.0000	1932.1567	20.9635	20.9635	5.0767	90.00	90.00	120.00
0.2503	1926.1653	20.9370	20.9370	5.0738	90.00	90.00	120.00
0.5000	1919.0519	20.9087	20.9087	5.0687	90.00	90.00	120.00
1.0001	1899.6773	20.8402	20.8402	5.0506	90.00	90.00	120.00
1.4997	1857.3030	20.7078	20.7078	5.0013	90.00	90.00	120.00
2.0001	1808.3281	20.5438	20.5438	4.9475	90.00	90.00	120.00
2.9996	1734.9453	20.2762	20.2762	4.8729	90.00	90.00	120.00
4.0011	1671.5079	20.0160	20.0160	4.8175	90.00	90.00	120.00
5.0004	1619.9759	19.7873	19.7873	4.7775	90.00	90.00	120.00

Table S.19. Calculated volumetric compressibilities ($k_V = -1/V \cdot (\partial V/\partial P)_P$) of ALPO-31 and compresibilities along a, b and c directions ($k_m = -1/m \cdot (\partial m/\partial P)_P$) for different external isotropic pressures. The computed bulk moduli (B) are given in the last column of the table.

P (GPa)	$\boldsymbol{k_V}$**(TPa^{-1})**	$\boldsymbol{k_a}$**(TPa^{-1})**	$\boldsymbol{k_b}$**(TPa^{-1})**	$\boldsymbol{k_c}$**(TPa^{-1})**	$\boldsymbol{B}$**(GPa)**
0.00	11.09	4.43	4.43	2.23	90.14
0.50	20.58	6.67	6.67	7.24	48.59
1.00	32.98	9.89	9.89	13.20	30.32
1.50	43.46	12.81	12.81	17.84	23.01
2.00	48.99	14.61	14.61	19.77	20.41
2.50	48.34	14.91	14.91	18.52	20.69
3.00	42.21	13.83	13.83	14.54	23.69
3.50	33.37	11.98	11.98	9.41	29.97
4.00	26.74	10.49	10.49	5.76	37.39

Table S.20. Unit cell volume and lattice parameters of ALPO-18 under the effect of different external isotropic pressures.

P (GPa)	**Vol. (Å^3)**	a **(Å)**	b **(Å)**	c **(Å)**	α **(deg)**	β **(deg)**	γ**(deg)**
-0.4999	3197.7568	13.6000	12.7052	18.5065	90.00	90.01	90.00
-0.2506	3186.8453	13.5887	12.6883	18.4833	90.00	90.01	90.00
-0.0004	3175.9001	13.5788	12.6705	18.4592	90.00	90.01	90.00
0.2494	3164.8470	13.5707	12.6512	18.4339	90.00	90.01	90.00
0.4994	3153.4940	13.5651	12.6299	18.4064	90.00	90.00	90.00
1.0000	3128.3061	13.5564	12.5810	18.3421	90.00	90.04	90.00
1.5001	3096.3524	13.5809	12.4818	18.2660	90.00	90.00	90.00
1.7500	3077.6167	13.5963	12.4237	18.2197	90.00	90.00	90.00
1.9995	3026.2831	13.7075	12.2421	18.0340	90.00	90.05	90.00
2.2503	2928.7204	13.8127	11.9483	17.7458	90.00	90.00	90.00
2.4998	2859.8113	13.8460	11.7527	17.5742	90.00	90.01	90.00

Table S.21. Calculated volumetric compressibilities ($k_V = -1/V \cdot (\partial V/\partial P)_P$) of ALPO-18 and compressibilities along a, b and c directions ($k_m = -1/m \cdot (\partial m/\partial P)_P$) for different external isotropic pressures. The computed bulk moduli (B) are given in the last column of the table.

P (GPa)	$\boldsymbol{k_V}$**(TPa^{-1})**	$\boldsymbol{k_a}$**(TPa^{-1})**	$\boldsymbol{k_b}$**(TPa^{-1})**	$\boldsymbol{k_c}$**(TPa^{-1})**	$\boldsymbol{B}$**(GPa)**
0.00	13.54	3.40	5.17	4.97	73.85
0.25	16.72	1.06	8.12	7.54	59.81
0.50	16.60	0.44	8.54	7.62	60.24
0.75	13.89	1.32	7.00	5.57	72.02
1.00	12.18	1.75	6.55	3.89	82.08
1.25	16.10	-0.72	11.01	5.81	62.12
1.50	29.35	-7.74	23.30	13.79	34.08
1.75	53.02	-18.93	43.81	28.14	18.86
2.00	83.69	-30.57	68.68	45.58	11.95
2.25	123.92	-21.02	87.51	57.43	8.07
2.38	136.65	-8.72	88.85	56.52	7.32
2.50	125.66	-1.88	80.16	47.37	7.96

Table S.22. Unit cell volume and lattice parameters of ALPO-18 under the effect of different external pressures applied along the direction of minimum compressibility.

P (GPa)	Vol. (Å^3)	a (Å)	b (Å)	c (Å)	α (deg)	β (deg)	γ(deg)
-1.4998	3164.2264	14.5821	12.0236	18.0475	90.00	89.79	90.00
-1.0000	3172.3018	14.3027	12.2131	18.1606	90.00	89.82	90.00
-0.6667	3177.7231	14.0973	12.3486	18.2543	90.00	89.84	90.00
-0.3330	3179.9498	13.8608	12.4987	18.3556	90.00	89.92	90.00
-0.2496	3180.0308	13.7913	12.5458	18.3793	90.00	89.95	90.00
-0.0005	3175.9121	13.5787	12.6706	18.4592	90.00	90.01	90.00
0.3334	3154.1855	13.2061	12.8474	18.5907	90.00	90.13	90.00
0.6670	3073.9803	12.5903	13.0452	18.7162	90.00	90.23	90.00
0.9999	2950.4856	11.8747	13.2099	18.8093	90.00	90.21	90.00

Table S.23. Calculated volumetric compressibilities ($k_V = -1/V \cdot (\partial V/\partial P)_P$) of ALPO-18 for different external anisotropic pressures applied along the direction of minimum compressibility.

P (GPa)	$\boldsymbol{k_V}$**(TPa^{-1})**
-1.00	-5.27
-0.75	-6.03
-0.50	-4.39
-0.25	1.52
0.00	13.59
0.25	33.87
0.50	64.80
0.63	85.23
0.75	109.63

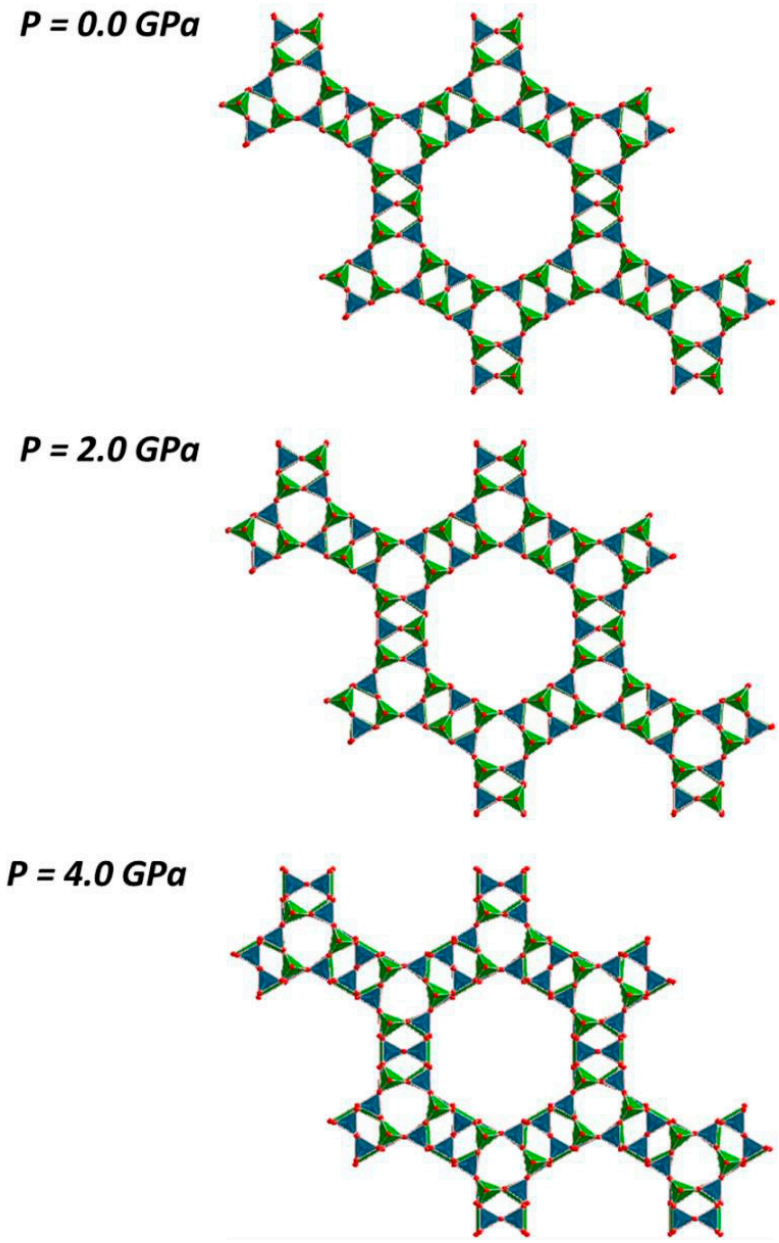

Figure S.1. View of a 2 × 2 × 2 supercell of VPI-5 from [001] under the effect of three different isotropic pressures (0.0, 2.0 and 4.0 GPa).

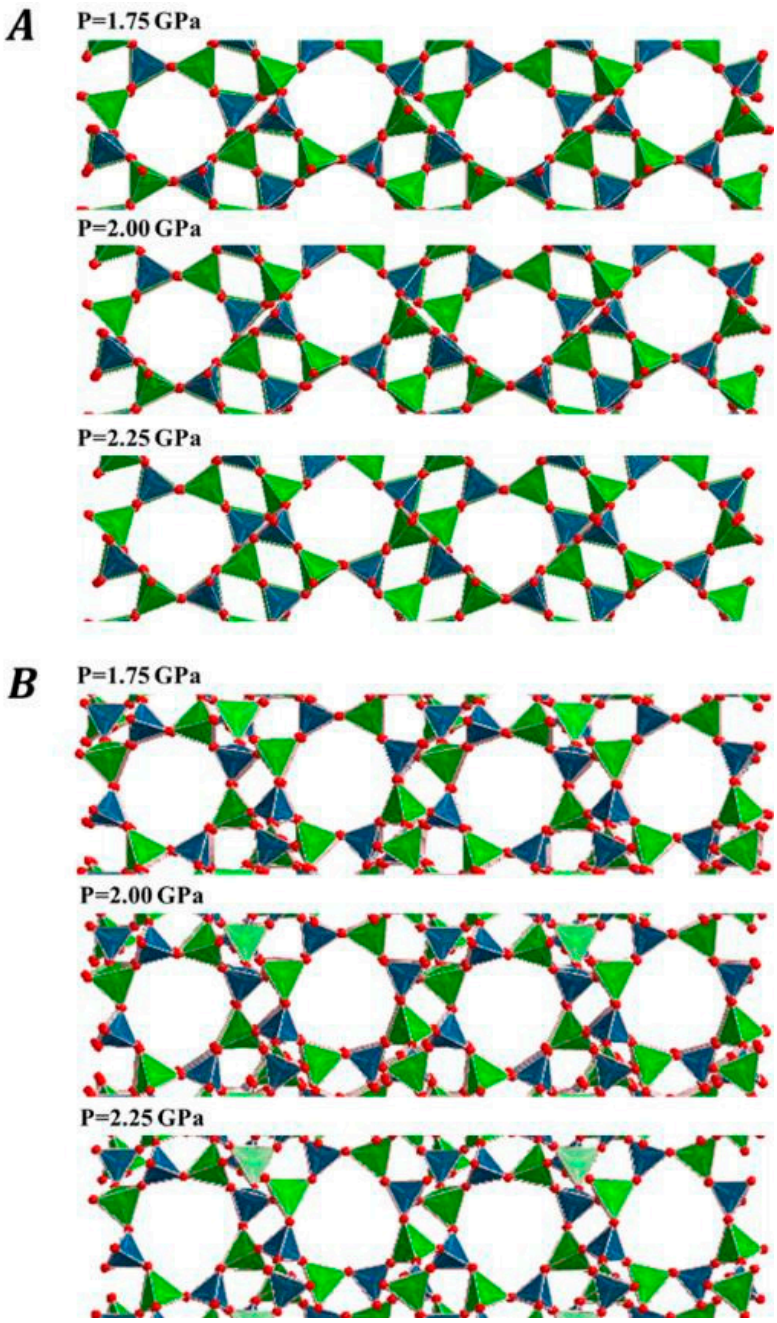

Figure S.2. The 8-MR structural channels expanding along (A) [1 0 0] and (B) [1 1 0] directions in the crystal structure of ALPO-18 under the effect of three different isotropic pressures, P = 1.75, 2.0 and 2.25 GPa.

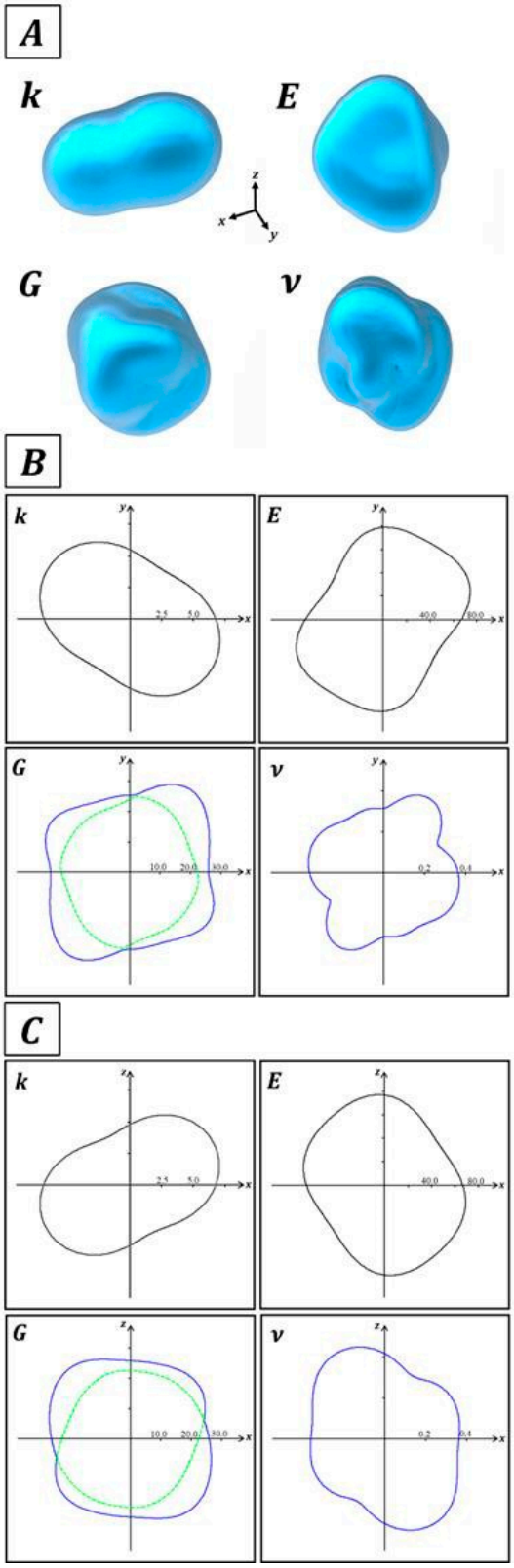

Figure S.3. (A) Mechanical properties of ALPO-18W ($P1$) as a function of the orientation of the applied strain: k − compressibility, E − Young modulus, G − Maximum shear modulus, ν − Maximum Poisson's ratio; (B) Bidimensional projections on the xy plane; (C) Bidimensional projections on the xz plane. The projections of the surface of minimum shear modulus are also displayed using green color in panels (B) and (C).

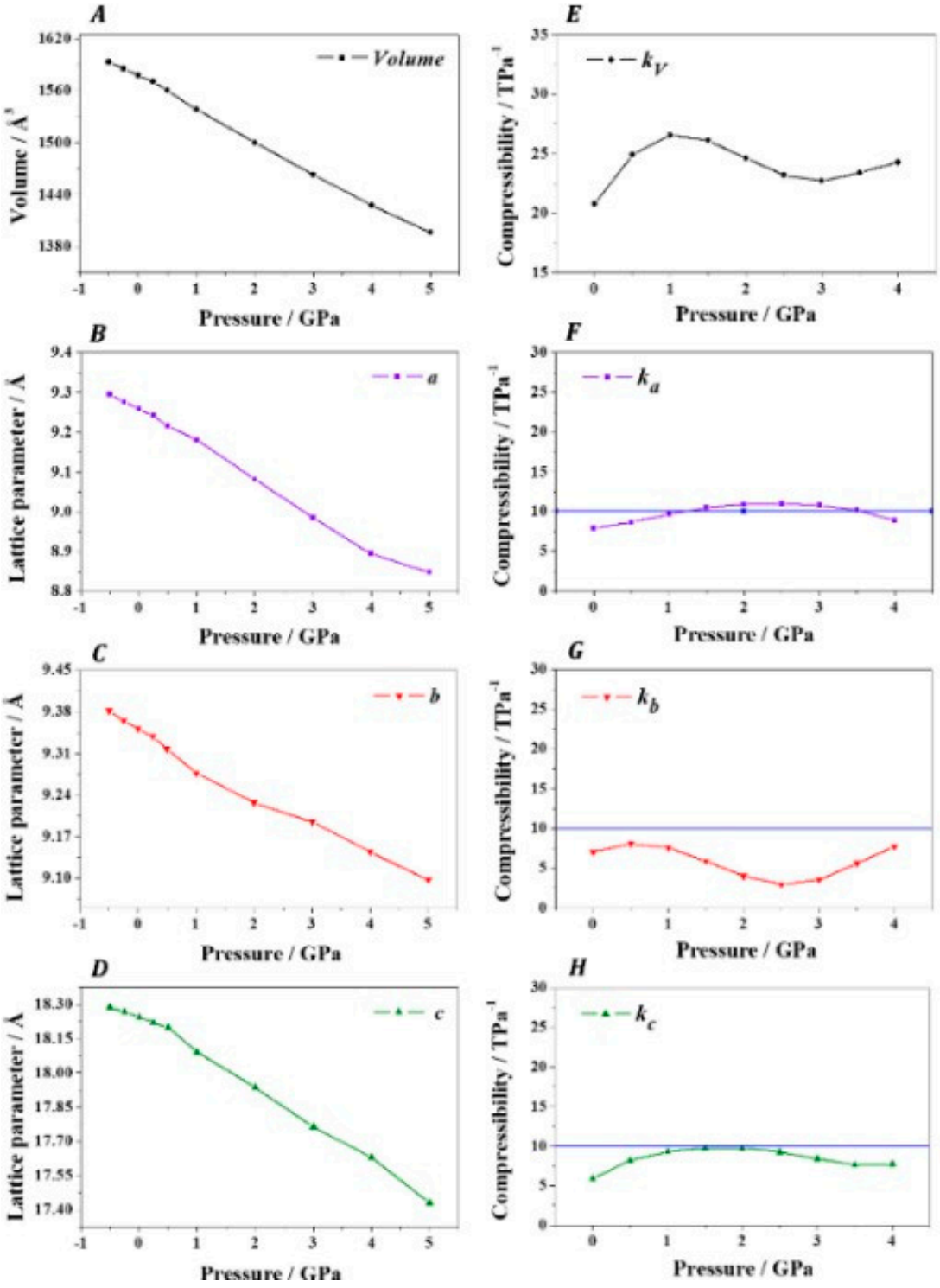

Figure S.4. Computed unit cell volume (A) and lattice parameters (B-D) of ALPO-18W under different external isotropic pressures. The volumetric compressibilities (E) and the linear compressibilities along a, b and c (F-H) directions are shown in the panels of the right-hand side. The blue horizontal lines in panels (F), (G) and (H) mark k_l = 10.0 TPa^{-1}.

Table S.24. Unit cell volume and lattice parameters of ALPO-18W under the effect of different external isotropic pressures.

P (GPa)	Vol. (Å^3)	a (Å)	b (Å)	c (Å)	α (deg)	β (deg)	γ(deg)
-0.5004	1593.0622	9.2950	9.3818	18.2868	88.06	91.60	89.46
-0.2500	1585.2300	9.2762	9.3654	18.2676	88.03	91.73	89.39
-0.0002	1577.6793	9.2582	9.3513	18.2448	87.99	91.81	89.32
0.2501	1570.6914	9.2421	9.3387	18.2212	87.98	91.87	89.27
0.4998	1560.3447	9.2149	9.3174	18.1991	88.53	91.91	88.19
1.0004	1538.2880	9.1809	9.2769	18.0900	88.43	91.88	87.95
2.0001	1499.8588	9.0819	9.2269	17.9365	88.63	92.08	87.28
3.0006	1462.8963	8.9848	9.1950	17.7636	88.83	93.17	87.00
4.0001	1427.7488	8.8944	9.1446	17.6296	88.70	93.88	86.71
4.9996	1396.4871	8.8484	9.0974	17.4285	88.73	94.51	87.24

Table S.25. Calculated volumetric compressibilities ($k_V = -1/V \cdot (\partial V/\partial P)_P$) of ALPO-18W and compressibilities along a , b and c directions ($k_m = -1/m \cdot (\partial m/\partial P)_P$) for different external isotropic pressures. The computed bulk moduli (B) are given in the last column of the table.

P (GPa)	$\boldsymbol{k_V}$**(TPa^{-1})**	$\boldsymbol{k_a}$**(TPa^{-1})**	$\boldsymbol{k_b}$**(TPa^{-1})**	$\boldsymbol{k_c}$**(TPa^{-1})**	$\boldsymbol{B}$**(GPa)**
0.00	17.01	6.51	5.05	5.27	58.80
0.13	18.64	9.02	5.98	5.98	53.66
0.25	23.01	8.46	7.60	7.60	43.46
0.38	26.06	8.20	8.65	8.65	38.37
0.50	27.90	8.18	9.18	9.18	35.84
0.63	28.80	8.35	9.29	9.29	34.72
0.75	29.00	8.64	9.07	9.07	34.49
0.88	28.70	9.01	8.63	8.63	34.84
1.00	28.08	9.40	8.03	8.03	35.61
1.50	24.90	10.76	5.19	5.19	40.16
2.00	23.74	11.19	3.35	3.35	42.13
2.50	24.95	10.84	3.27	3.27	40.08
3.00	26.17	10.36	4.41	4.41	38.21
3.50	24.80	10.14	5.65	5.65	40.32
4.00	20.76	9.61	5.98	5.98	48.16

Table S.26. Unit-cell parameters of the VPI-5 ($C1m1$) and ALPO-5 ($Pcc2$).

Parameter	α (Å)	b (Å)	c (Å)	α (deg)	β (deg)	γ(deg)	Vol. (Å^3)	ρ(g/cm^3)
VPI-5 ($C1m1$)								
PBE	18.5639	32.1132	8.5042	90.0	90.00	90.0	5069.7613	1.438
PBE+Disp	18.5014	32.0028	8.4502	90.0	90.05	90.0	5003.3578	1.457
PBEsol	18.5331	32.0688	8.4940	90.0	89.99	90.0	5048.3145	1.444
Exp. [2]	18.5218(1)	32.1247(2)	8.4003(2)	90.0	90.00	90.0	4998.2396	1.459
ALPO-5 ($Pcc2$)								
PBE	13.8543	24.0375	8.5339	90.0	90.0	90.0	2841.9699	1.710
PBE+Disp	13.8322	23.9860	8.5218	90.0	90.0	90.0	2827.3454	1.719
PBEsol	13.8602	24.0215	8.5382	90.0	90.0	90.0	2842.7340	1.710
Exp. [4]	13.794(3)	23.900(6)	8.4168(6)	90.0	90.0	90.0	2774.8220	1.752

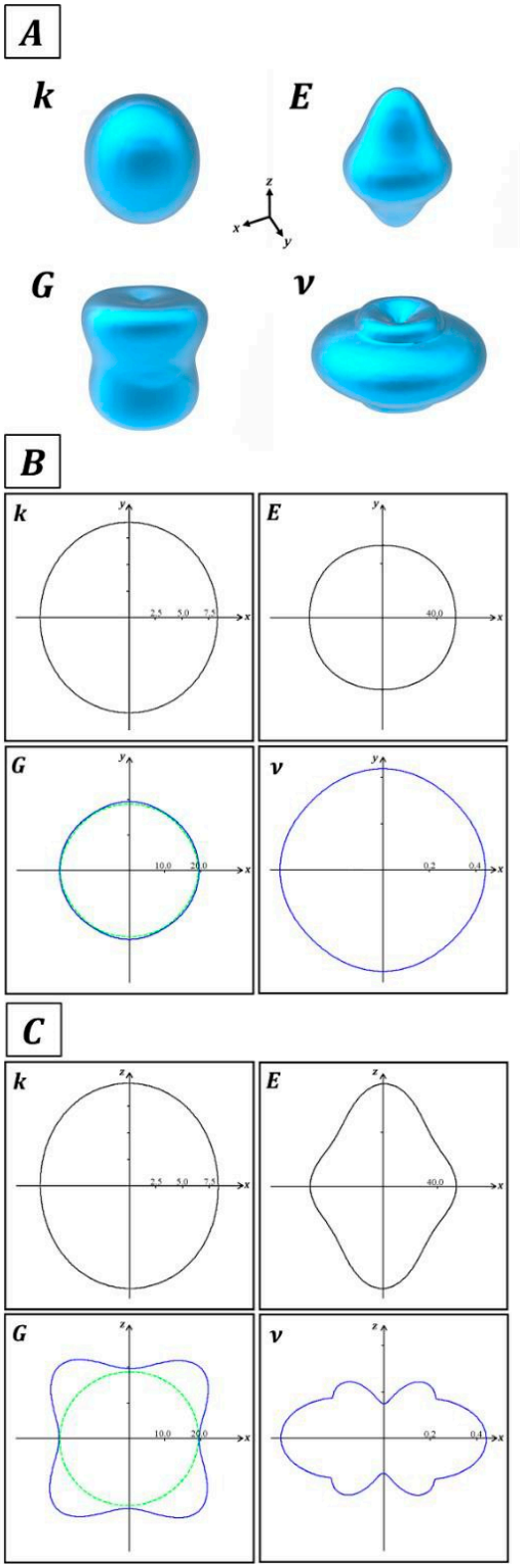

Figure S.5. (A) Mechanical properties of VPI-5 ($C1\mathrm{m}1$) as a function of the orientation of the applied strain: k − compressibility, E − Young modulus, G − Maximum shear modulus, ν − Maximum Poisson's ratio; (B) Bidimensional projections on the xy plane; (C) Bidimensional projections on the xz plane. The projections of the surface of minimum shear modulus are also displayed using green color in panels (B) and (C).

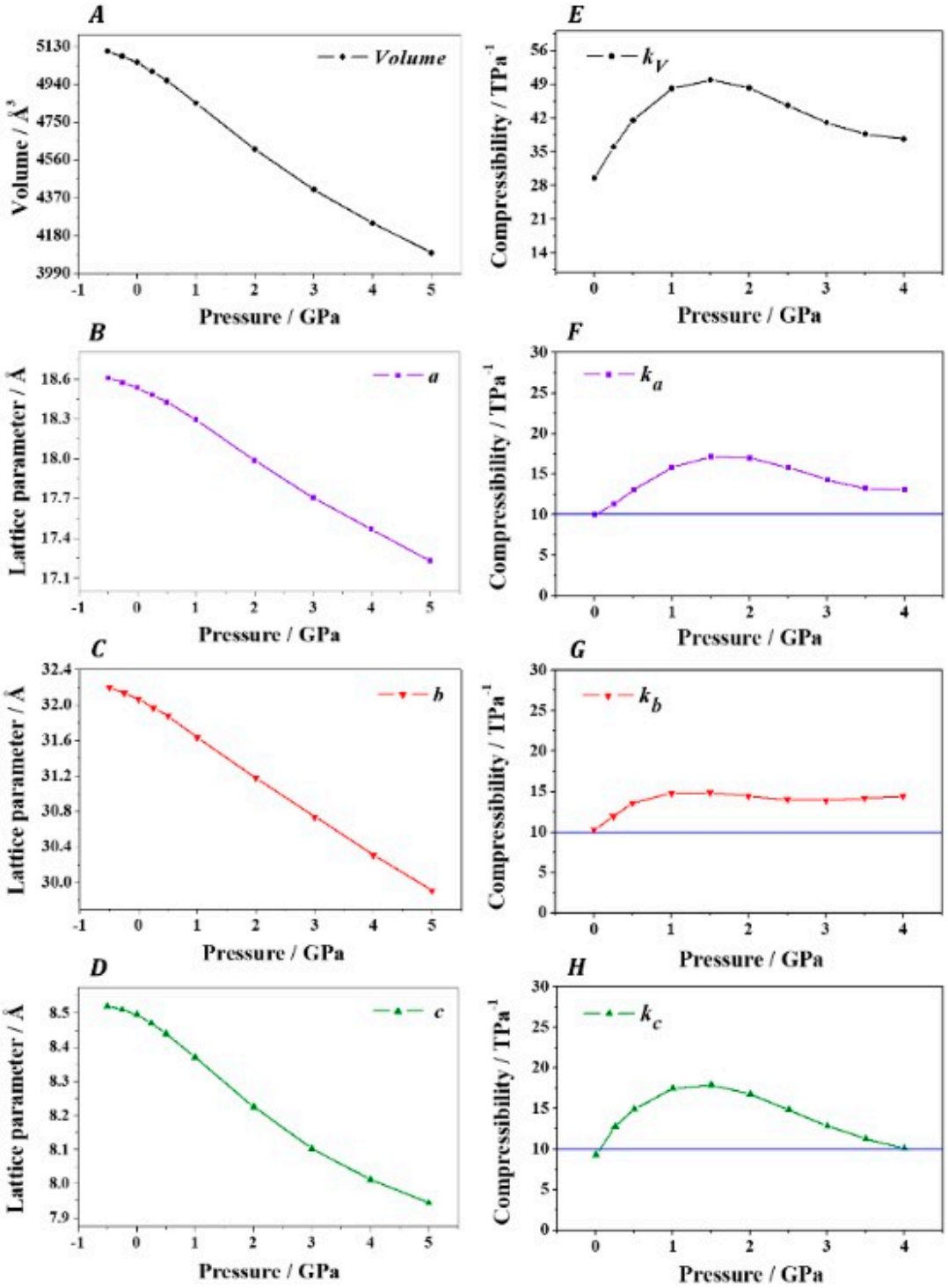

Figure S.6. Computed unit cell volume (A) and lattice parameters (B-D) of VPI-5 ($C1m1$) under different external isotropic pressures. The volumetric compressibilities (E) and the linear compressibilities along a, b and c (F-H) directions are shown in the panels of the right-hand side. The blue horizontal lines in panels (F), (G) and (H) mark k_l = 10.0 TPa^{-1}.

Table S.27. Unit cell volume and lattice parameters of VPI-5 ($C1m1$) under the effect of different external isotropic pressures.

P (GPa)	**Vol. (Å^3)**	$\boldsymbol{a}$ **(Å)**	$\boldsymbol{b}$ **(Å)**	$\boldsymbol{c}$ **(Å)**	$\boldsymbol{\alpha}$ **(deg)**	$\boldsymbol{\beta}$ **(deg)**	$\boldsymbol{\gamma}$**(deg)**
-0.5021	5105.1785	18.6052	32.2013	8.5213	90.00	90.01	90.00
-0.2499	5078.5879	18.5714	32.1359	8.5096	90.00	90.01	90.00
-0.0008	5048.3145	18.5331	32.0688	8.4940	90.00	89.99	90.00
0.2501	5003.1629	18.4778	31.9683	8.4698	90.00	90.00	90.00
0.5021	4957.4319	18.4265	31.8752	8.4404	90.00	90.01	90.00
0.9999	4843.9728	18.2937	31.6347	8.3702	90.00	90.00	90.00
1.9999	4612.1601	17.9848	31.1786	8.2251	90.00	90.00	90.00
3.0014	4409.8252	17.7043	30.7389	8.1031	90.00	89.99	90.00
4.0000	4242.0565	17.4684	30.3086	8.0123	90.00	89.98	90.00
4.9997	4093.2800	17.2294	29.9064	7.9440	90.00	89.96	90.00

Table S.28. Calculated volumetric compressibilities ($k_V = -1/V \cdot (\partial V/\partial P)_P$) of VPI-5 ($C1m1$) and compressibilities along a, b and c directions ($k_m = -1/m \cdot (\partial m/\partial P)_P$) for different external isotropic pressures. The computed bulk moduli (B) are given in the last column of the table.

P (GPa)	$\boldsymbol{k_V}$**(TPa^{-1})**	$\boldsymbol{k_a}$**(TPa^{-1})**	$\boldsymbol{k_b}$**(TPa^{-1})**	$\boldsymbol{k_c}$**(TPa^{-1})**	$\boldsymbol{B}$**(GPa)**
0.00	29.54	10.01	10.28	9.26	33.85
0.25	36.00	11.28	11.94	12.78	27.78
0.50	41.56	13.05	13.59	14.92	24.06
1.00	48.12	15.84	14.79	17.49	20.78
1.50	49.95	17.17	14.88	17.91	20.02
2.00	48.22	17.00	14.44	16.78	20.74
2.50	44.66	15.81	14.00	14.84	22.39
3.00	41.05	14.31	13.90	12.84	24.36
3.50	38.67	13.25	14.16	11.25	25.86
4.00	37.64	13.10	14.42	10.12	26.57

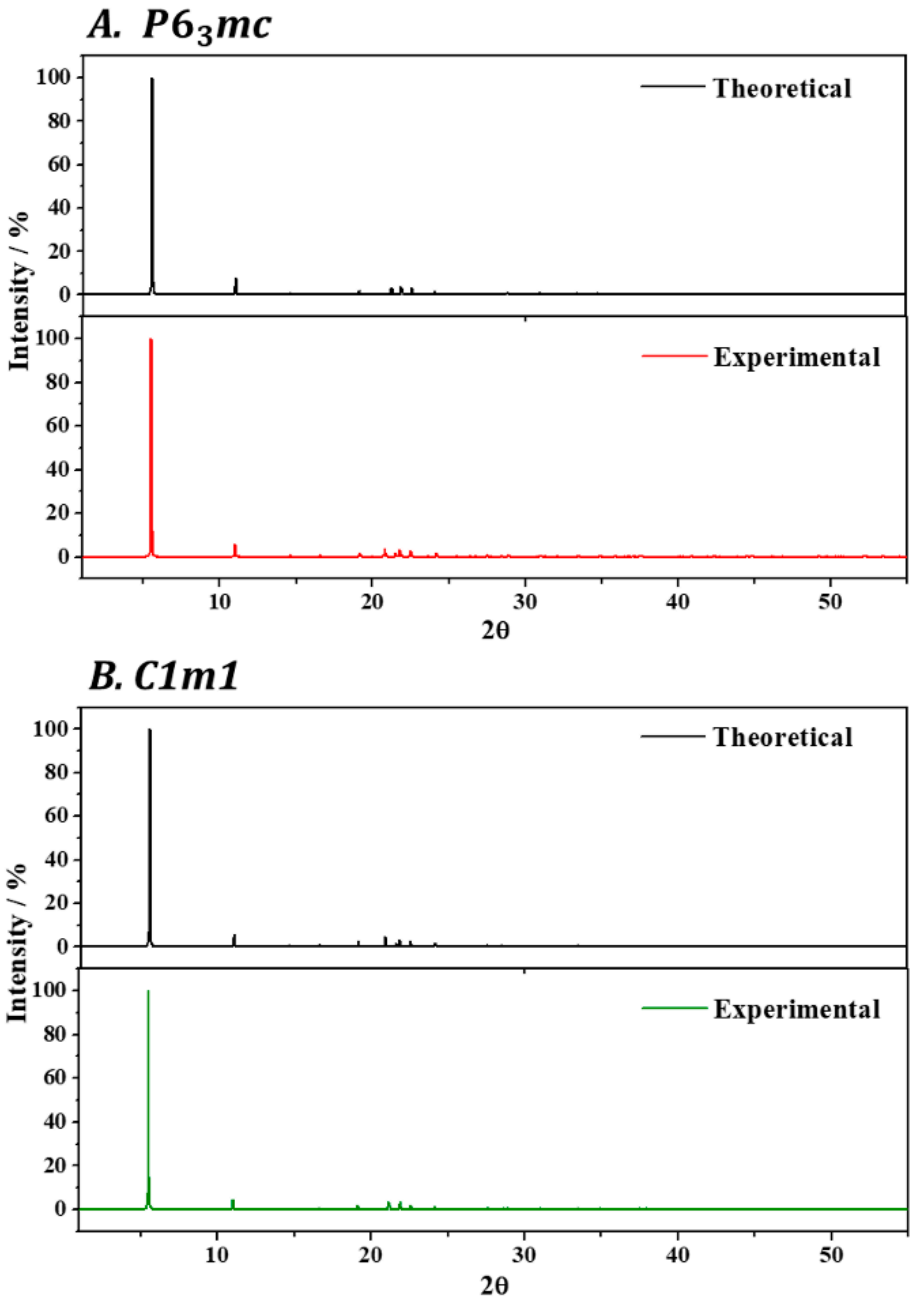

Figure S.7. Comparison of the X-ray diffraction patterns of VPI-5 derived from the computed and experimental [1-2] crystal structures: (A) $P63cm$ structure; (B) $C1m1$ structure.

Table S.29. Most intense reflections in the X-ray diffraction pattern of VPI-5 ($C1m1$): (a) X-ray pattern derived from the experimental crystal structure [2]; (b) X-ray pattern derived from the calculated crystal structure.

[$h\ k\ l$]	(a) Exp [2].			(b) Calc.		Δ (**2θ**)
	2θ (**deg**)	**d** (Å)	**I (%)**	**2θ** (**deg**)	**d** (Å)	
[1 1 0]	5.503	16.046	100.000	5.503	16.047	0.00
[0 2 0]	5.498	16.062	53.499	5.507	16.035	0.01
[0 0 2]	21.135	4.200	8.947	20.900	4.247	-0.24
[2 2 0]	11.019	8.023	8.691	11.019	8.023	0.00
[0 4 0]	11.008	8.031	4.170	11.027	8.018	0.02
[2 6 0]	19.132	4.635	3.389	19.154	4.630	0.02
[-2 6 1]	21.883	4.058	2.030	21.846	4.065	-0.04
[2 6 1]	21.883	4.058	1.919	21.844	4.065	-0.04
[4 0 0]	19.152	4.630	1.592	19.140	4.633	-0.01
[2 8 0]	24.137	3.684	1.501	24.170	3.679	0.03
[-1 1 2]	21.856	4.063	1.462	21.628	4.106	-0.23
[0 2 2]	21.855	4.064	1.406	21.629	4.105	-0.23
[1 1 2]	21.856	4.063	1.392	21.627	4.106	-0.23
[3 7 0]	24.144	3.683	1.362	24.165	3.680	0.02
[3 9 0]	28.869	3.090	1.342	28.902	3.087	0.03
[5 1 0]	24.165	3.680	1.298	24.151	3.682	-0.01
[4 0 1]	21.900	4.055	1.090	21.832	4.068	-0.07

Table S.30. Comparison of the most intense reflections in the X-ray diffraction patterns of VPI-5 derived from the experimental $C1m1$ crystal structures reported by Fabbiani *et al*. [9] and De Oñate Martínez *et al.* [2].

[$h\ k\ l$]	(a) Exp. [9]			(b) Exp [2].		Δ (**2θ**)
	2θ (**deg**)	**d** (Å)	**I (%)**	**2θ** (**deg**)	**d** (Å)	
[1 1 0]	5.518	16.002	100.000	5.503	16.046	-0.01
[0 2 0]	5.514	16.016	50.649	5.498	16.062	-0.02
[0 0 4]	21.204	4.187	8.546	21.135	4.200	-0.07
[2 2 0]	11.049	8.001	8.528	11.019	8.023	-0.03
[0 4 0]	11.040	8.008	4.360	11.008	8.031	-0.03
[2 6 0]	19.187	4.622	3.336	19.132	4.635	-0.05
[-2 6 2]	21.945	4.047	2.081	21.883	4.058	-0.06
[2 6 2]	21.950	4.046	2.013	21.883	4.058	-0.07
[4 0 0]	19.203	4.618	1.733	19.152	4.630	-0.05
[2 8 0]	24.208	3.674	1.388	24.137	3.684	-0.07
[0 2 4]	21.925	4.051	1.376	21.856	4.063	-0.07
[-1 1 4]	21.924	4.051	1.367	21.855	4.064	-0.07
[1 1 4]	21.929	4.050	1.362	21.855	4.064	-0.07
[5 1 0]	24.23	3.670	1.354	24.165	3.680	-0.07
[3 7 0]	24.213	3.673	1.350	24.144	3.683	-0.07
[3 9 0]	28.954	3.081	1.166	28.869	3.090	-0.09

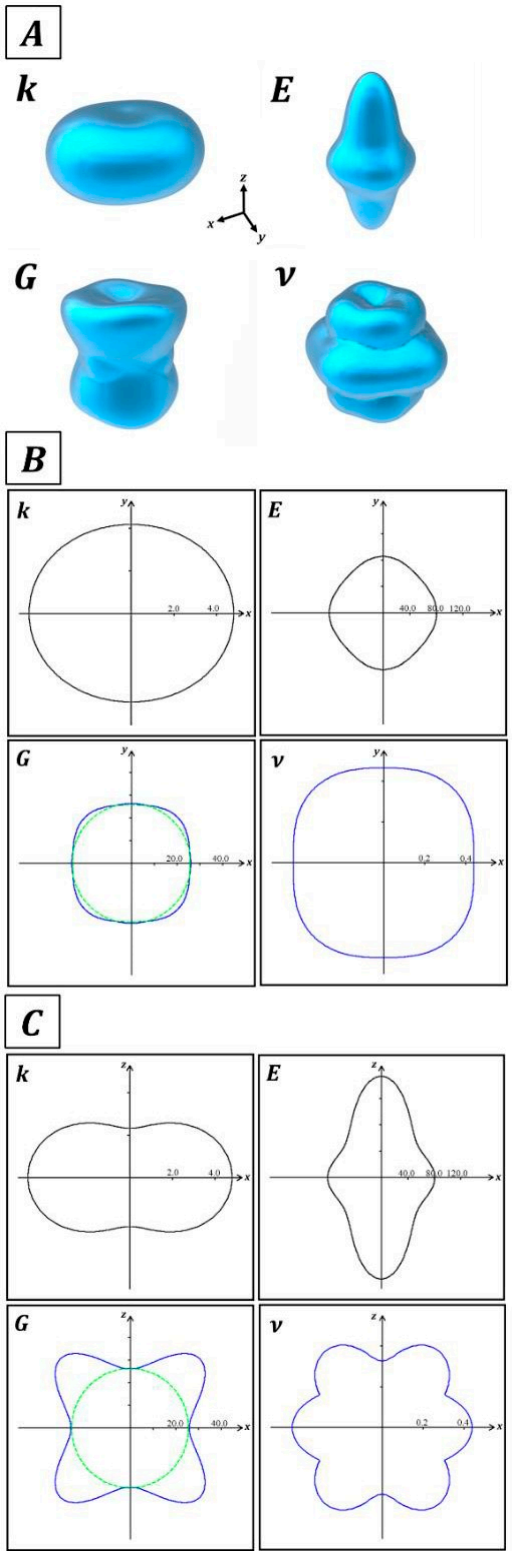

Figure S.8. (A) Mechanical properties of ALPO-5 ($Pcc2$) as a function of the orientation of the applied strain: k − compressibility, E − Young modulus, G − Maximum shear modulus, ν − Maximum Poisson's ratio; (B) Bidimensional projections on the xy plane; (C) Bidimensional projections on the xz plane. The projections of the surface of minimum shear modulus are also displayed using green color in panels (B) and (C).

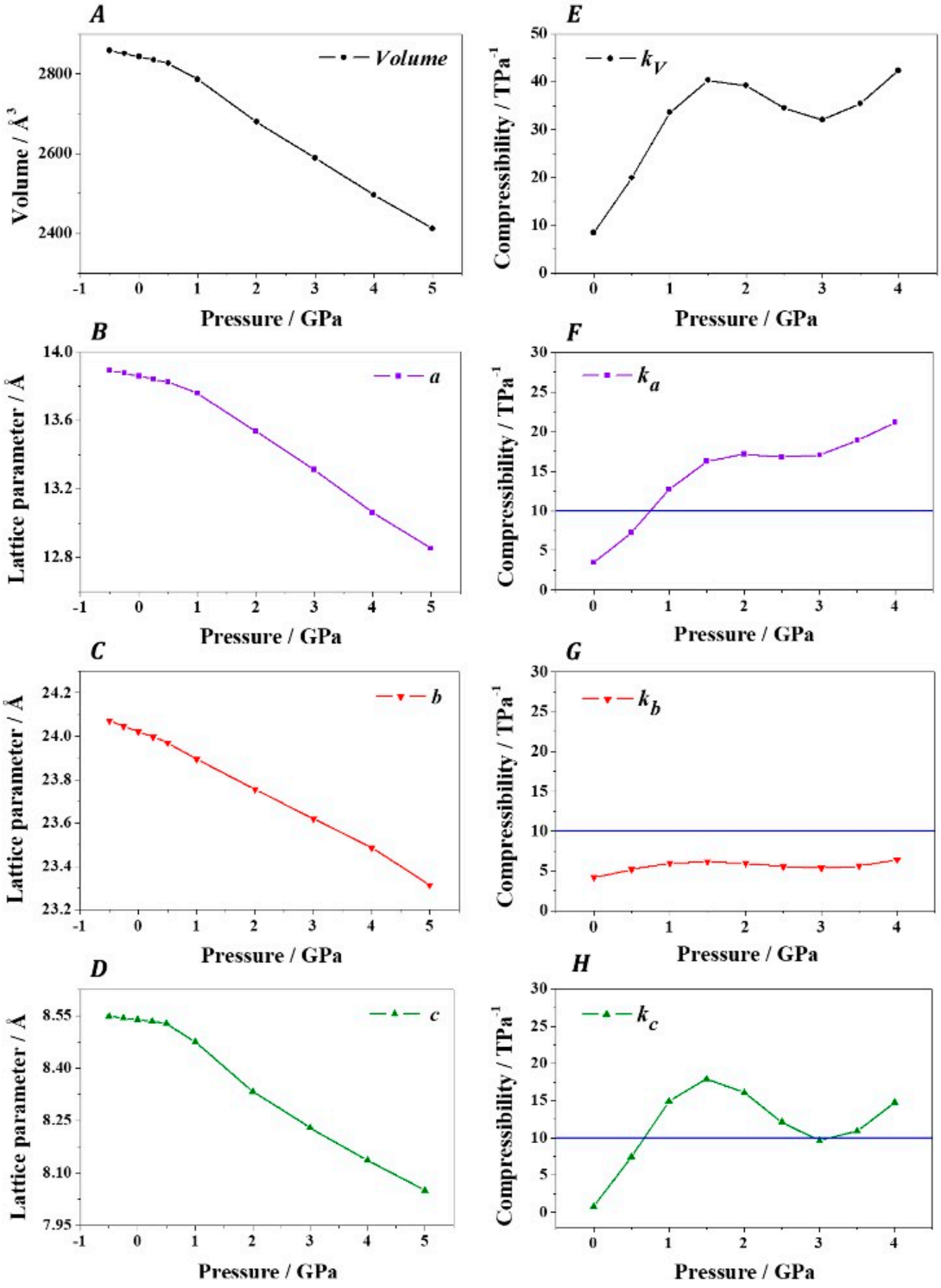

Figure S.9. Computed unit cell volume (A) and lattice parameters (B-D) of ALPO-5 ($Pcc2$) under different external isotropic pressures. The volumetric compressibilities (E) and the linear compressibilities along a, b and c (F-H) directions are shown in the panels of the right-hand side. The blue horizontal lines in panels (F), (G) and (H) mark k_l = 10.0 TPa^{-1}.

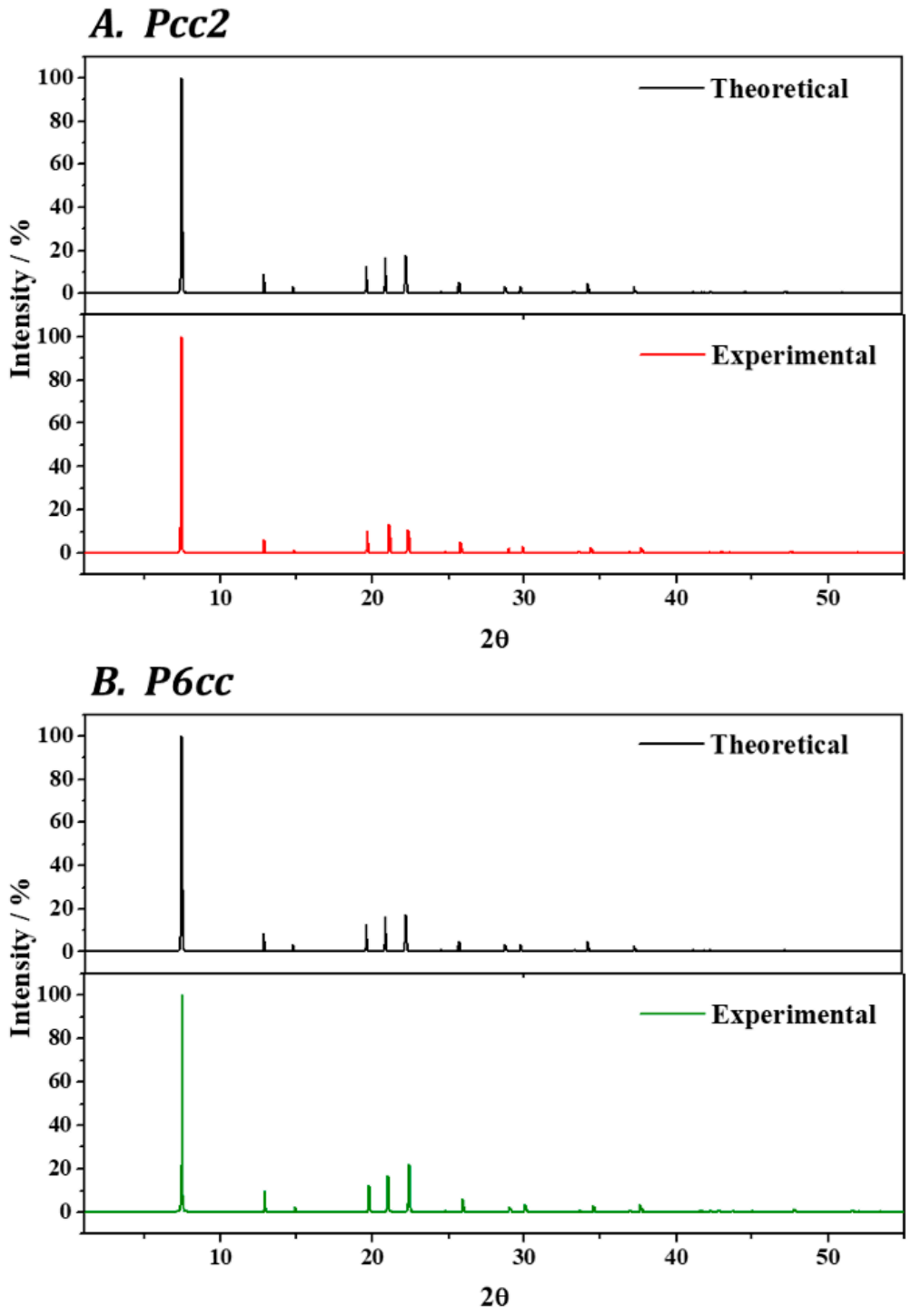

Figure S.10. Comparison of the X-ray diffraction patterns of ALPO-5 derived from the computed and experimental [4-5] crystal structures: (A) *Pcc*2 structure; (B) *P*6*cc* structure.

Table S.31. Most intense reflections in the X-ray diffraction pattern of ALPO-5 (*Pcc*2): (a) X-ray pattern derived from the experimental crystal structure [4]; (b) X-ray pattern derived from the calculated crystal structure.

[$h\ k\ l$]	(a) Exp [4].			(b) Calc.		Δ (2θ)
	2θ (deg)	d (Å)	I (%)	2θ (deg)	d (Å)	
[1 1 0]	7.394	11.947	100.000	7.358	12.005	-0.04
[0 2 0]	7.392	11.950	52.108	7.354	12.011	-0.04
[0 0 2]	21.094	4.208	28.725	20.790	4.269	-0.30
[2 4 1]	22.323	3.979	13.225	22.164	4.008	-0.16
[1 5 1]	22.321	3.980	11.418	22.161	4.008	-0.16
[3 1 1]	22.326	3.979	10.114	22.170	4.006	-0.16
[1 3 0]	12.822	6.899	8.580	12.758	6.933	-0.06
[3 1 0]	19.646	4.515	8.281	19.551	4.537	-0.10
[1 5 0]	19.640	4.517	7.921	19.540	4.539	-0.10
[2 6 0]	25.808	3.449	7.271	25.677	3.467	-0.13
[4 0 0]	25.814	3.449	5.855	25.689	3.465	-0.13
[2 4 0]	19.642	4.516	5.640	19.544	4.538	-0.10
[2 0 0]	12.825	6.897	5.608	12.764	6.930	-0.06
[1 1 2]	22.380	3.969	4.897	22.081	4.022	-0.30
[4 4 0]	29.892	2.987	4.341	29.743	3.001	-0.15
[2 2 0]	14.818	5.974	3.555	14.746	6.003	-0.07
[0 8 0]	29.884	2.988	3.502	29.729	3.003	-0.16
[5 3 0]	34.373	2.607	3.194	34.203	2.620	-0.17
[3 1 3]	37.718	2.383	3.116	37.265	2.411	-0.45
[1 5 3]	37.715	2.383	2.997	37.260	2.411	-0.46
[1 9 0]	34.363	2.608	2.906	34.184	2.621	-0.18
[0 2 2]	22.379	3.969	2.574	22.080	4.023	-0.30
[0 0 4]	42.948	2.104	2.026	42.307	2.135	-0.64

Table S.32. Unit cell volume and lattice parameters of ALPO-5 (*Pcc*2) under the effect different external isotropic pressures.

P (GPa)	**Vol. (Å^3)**	$\boldsymbol{a}$ **(Å)**	$\boldsymbol{b}$ **(Å)**	$\boldsymbol{c}$ **(Å)**	$\boldsymbol{\alpha}$ **(deg)**	$\boldsymbol{\beta}$ **(deg)**	$\boldsymbol{\gamma}$**(deg)**
-0.4996	2858.8735	13.8941	24.0709	8.5482	90.00	90.00	90.00
-0.2500	2850.8291	13.8775	24.0457	8.5432	90.00	90.00	90.00
0.0003	2842.7300	13.8602	24.0214	8.5382	90.00	90.00	90.00
0.2503	2834.6532	13.8420	23.9978	8.5335	90.00	90.00	90.00
0.5001	2825.8905	13.8247	23.9706	8.5275	90.00	90.00	90.00
0.9999	2786.5189	13.7601	23.8953	8.4748	90.00	90.00	90.00
2.0002	2679.7941	13.5384	23.7554	8.3325	90.00	90.00	90.00
3.0005	2588.0800	13.3142	23.6197	8.2298	90.00	90.00	90.00
3.9996	2496.2857	13.0627	23.4860	8.1368	90.00	90.00	90.00
5.0004	2412.1252	12.8524	23.3130	8.0504	90.00	90.00	90.00

Table S.33. Calculated volumetric compressibilities ($k_V = -1/V \cdot (\partial V/\partial P)_P$) of ALPO-5 ($Pcc2$) and compressibilities along a, b and c directions ($k_m = -1/m \cdot (\partial m/\partial P)_P$) for different external isotropic pressures. The computed bulk moduli (B) are given in the last column of the table.

P (GPa)	$\boldsymbol{k_V}$**(TPa^{-1})**	$\boldsymbol{k_a}$**(TPa^{-1})**	$\boldsymbol{k_b}$**(TPa^{-1})**	$\boldsymbol{k_c}$**(TPa^{-1})**	$\boldsymbol{B}$**(GPa)**
0.00	11.40	5.24	3.90	2.26	87.71
0.13	11.35	5.29	3.90	2.16	88.07
0.25	11.47	5.14	4.10	2.23	87.15
0.38	12.19	4.96	4.51	2.72	82.04
0.50	18.77	6.22	5.55	7.00	53.28
0.63	24.12	7.75	6.13	10.25	41.46
0.75	28.62	9.38	6.43	12.81	34.94
0.88	32.29	11.02	6.53	14.75	30.97
1.00	35.19	12.56	6.48	16.15	28.42
1.50	40.21	16.84	5.80	17.57	24.87
2.00	38.24	17.61	5.46	15.17	26.15
2.50	34.40	16.53	5.73	12.14	29.07
3.00	32.98	16.37	6.01	10.59	30.32
3.50	35.81	18.87	5.74	11.20	27.92
4.00	40.43	22.46	5.18	12.80	24.73

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