Negative linear compressibility

SUPPLEMENTARY INFORMATION

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Contents

1 Lattice parameter data

Lattice parameter data are reported here as previously published in tabular form or as extracted from published figures. Data extraction was carried out using WebPlotDigitizer[S1] and standard errors were estimated in pressure measurements. In all cases lattice parameters are presented in a standard form which is suitable for direct input into PASCAL for calculation of compressibilities along principal directions.[S2] No standard errors in lattice parameters are used in the calculation using PASCAL as the inherent experimental scatter is assumed to be the main source of error in the final compressibility calculation; it is also the case that errors on values are not available for published work where data were not reported in raw form.

1.1 Ferroelastic systems

Table S1: Variable pressure lattice parameters of TeO_2 as reported in Ref. S3 (Worlton *et al.*, Cs_2 medium and D-methanol medium) and Ref. S4 (Liu *et al.*).

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
Ref. S3, Cs_2 medium							
1.01	0.02	4.7283	4.8234	7.5808	90	90	90
1.13	0.02	4.6978	4.8355	7.5704	90	90	90
1.39	0.02	4.6616	4.8492	7.5483	90	90	90
1.93	0.03	4.6024	4.8669	7.5418	90	90	90
2.42	0.03	4.568	4.874	7.5435	90	90	90
3.03	0.03	4.5321	4.8822	7.5366	90	90	90
3.25	0.04	4.5247	4.8832	7.5374	90	90	90
Ref. S3, D-methanol medium							
0.98	0.02	4.7418	4.8051	7.5632	90	90	90
1.14	0.02	4.7085	4.8234	7.5525	90	90	90
1.36	0.02	4.6753	4.8366	7.5468	90	90	90
1.66	0.02	4.641	4.8504	7.5364	90	90	90
1.98	0.02	4.6053	4.8557	7.53	90	90	90
Ref. S4							
2.1	0.1	4.603	4.875	7.558	90	90	90
7.6	0.1	4.333	4.89	7.434	90	90	90
8.5	0.1	4.281	4.884	7.414	90	90	90
11	0.1	4.225	4.85	7.333	90	90	90
13.2	0.1	4.161	4.856	7.292	90	90	90
17	0.1	4.084	4.831	7.214	90	90	90
21.5	0.1	3.986	4.833	7.132	90	90	90
24.9	0.1	3.958	4.821	7.104	90	90	90

Compressibilities:

K_1	$-5.1(6)$ TPa^{-1}
K_2	2.1(7) TPa^{-1}
K_3	18.4(6) TPa^{-1}
K_V	16.7(15) TPa^{-1}

Birch-Murnaghan Coefficients:

B_0	52(4) GPa
B'	$\equiv 4$
V_0	175.3(5) Å^3
p_c	0.9 GPa

Table S2: Variable pressure lattice parameters of NiF_2 extracted from Ref. S5.

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
2.145	0.2	4.605	4.633	3.072	90	90	90
2.50	0.2	4.596	4.635	3.072	90	90	90
2.89	0.2	4.588	4.637	3.071	90	90	90
3.24	0.2	4.580	4.638	3.070	90	90	90

Compressibilities:

K_1	-0.48(-) TPa^{-1}
K_2	0.61(-) TPa^{-1}
K_3	4.42(-) TPa^{-1}
K_V	4.57(3) TPa^{-1}

Birch-Murnaghan Coefficients:

B_0	226(-) GPa
B'	-8(-)
V_0	66(-) Å^3
p_c	1.8 GPa

Table S3: Variable pressure lattice parameters of β-MnO_2 extracted from Ref. S6

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
2.036	0.2	4.43	4.366	2.821	90	90	90
2.032	0.2	4.43	4.357	2.821	90	90	90
3.119	0.2	4.432	4.352	2.821	90	90	90
4.202	0.2	4.441	4.34	2.822	90	90	90
5.749	0.2	4.436	4.321	2.821	90	90	90
7.456	0.2	4.44	4.313	2.82	90	90	90
9.546	0.2	4.439	4.291	2.816	90	90	90
12.409	0.2	4.447	4.259	2.814	90	90	90
14.112	0.2	4.442	4.241	2.814	90	90	90
15.424	0.2	4.446	4.218	2.811	90	90	90
19.305	0.2	4.444	4.206	2.811	90	90	90
20.078	0.2	4.454	4.186	2.808	90	90	90
25.35	0.2	4.454	4.161	2.805	90	90	90
29.309	0.2	4.451	4.148	2.802	90	90	90

Compressibilities:

K_1	$-0.16(7)$ TPa^{-1}
K_2	0.269(17) TPa^{-1}
K_3	1.82(10) TPa^{-1}
K_V	2.06(9) TPa^{-1}

Birch-Murnaghan Coefficients:

B_0	280(80) GPa
B'	19(11)
V_0	54.97(17) Å^3
p_c	0.3 GPa

Table S4: Variable pressure lattice parameters of MgF_2 as reported in Ref. S7

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
9.4	0.1	4.5164	4.4768	2.9845	90	90	90
9.8	0.1	4.5223	4.4634	2.9815	90	90	90
10.4	0.1	4.5227	4.4409	2.977	90	90	90

Compressibilities (linear):

K_1	$-1.3(3)\,\mathrm{TPa}^{-1}$
K_2	$2.51(2)\,\mathrm{TPa}^{-1}$
K_3	$8.05(10)\,\mathrm{TPa}^{-1}$
K_V	$9.4(5)\,\mathrm{TPa}^{-1}$

Birch-Murnaghan Coefficients:

B_0	68(13) GPa
B'	$\equiv 4$
V_0	67.4(12) $\mathrm{Å}^3$
p_c	9.1 GPa

Table S5: Variable pressure lattice parameters of PbO_2-I′ extracted from Ref. S8. NLC found up to 6.1 GPa.

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
4.297	0.2	4.920	4.877	3.398	90	90	90
5.415	0.2	4.932	4.855	3.391	90	90	90
6.095	0.2	4.936	4.842	3.387	90	90	90
7.311	0.2	4.928	4.814	3.381	90	90	90
8.818	0.2	4.923	4.796	3.377	90	90	90
11.443	0.2	4.927	4.740	3.368	90	90	90
12.367	0.2	4.908	4.745	3.364	90	90	90

Compressibilities (linear):

K_1	−1.83(15)) TPa^{-1}
K_2	1.76(7) TPa^{-1}
K_3	4.00(3) TPa^{-1}
K_V	3.94(5) TPa^{-1}

Table S6: Variable pressure lattice parameters of GeO_2 as reported in Ref. S9. NLC found up to 32 GPa.

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
28	1	4.2841	4.2098	2.8089	90	90	90
29	1	4.2852	4.1959	2.8062	90	90	90
32	1	4.2866	4.1742	2.7995	90	90	90
35	1	4.2834	4.1508	2.7941	90	90	90
36	1	4.2814	4.1424	2.7919	90	90	90

Compressibilities (linear):

K_1	−0.137(12) TPa^{-1}
K_2	0.827(14) TPa^{-1}
K_3	2.02(13) TPa^{-1}
K_V	2.74(13) TPa^{-1}

Table S7: Variable pressure lattice parameters of SnO_2-II as reported in Refs. S 10, S11. NLC calculated from lattice parameters reported in Haines *et al.* (only two reported, but strain calculated over many more points in publication but not reported).

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
Ref. 10							
12.6	0.4	4.6533	4.6313	3.155	90	90	90
15.5	0.5	4.6558	4.5998	3.1514	90	90	90
Ref. 11							
17.2	0.2	4.609	5.528	5.079	90	90	90
18.4	0.2	4.607	5.523	5.07	90	90	90
19.5	0.2	4.599	5.504	5.067	90	90	90
20.8	0.2	4.592	5.507	5.077	90	90	90
21.8	0.2	4.598	5.505	5.065	90	90	90
22.8	0.2	4.591	5.504	5.041	90	90	90
23.6	0.2	4.596	5.498	5.06	90	90	90

Compressibilities (linear):

K_1	-0.185(-) TPa^{-1}
K_2	0.394(-) TPa^{-1}
K_3	2.345(-) TPa^{-1}
K_V	2.552(-) TPa^{-1}

Table S8: Variable pressure lattice parameters of $Zn(CN)_2$ as reported in Ref. S12

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
1.95	0.1	12.504	7.4438	7.2983	90	90	90
2.77	0.1	12.627	7.2315	7.0525	90	90	90
3.57	0.1	12.624	7.137	6.9219	90	90	90
4.44	0.1	12.625	7.0572	6.8064	90	90	90
5.47	0.1	12.589	7.0085	6.7299	90	90	90
7.5	0.1	12.492	6.9195	6.5848	90	90	90
12.2	0.1	12.413	6.83	6.3832	90	90	90
9.61	0.1	12.437	6.8743	6.5322	90	90	90

Table S9: Variable pressure lattice parameters of $Pb_3(PO_4)_2$ as reported in Ref. S13.

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
0.000	0.1	13.809	5.695	9.431	90	102.367	90
0.158	0.1	13.804	5.673	9.432	90	102.467	90
0.387	0.1	13.798	5.642	9.436	90	102.603	90
0.581	0.1	13.790	5.618	9.438	90	102.688	90
0.799	0.1	13.785	5.590	9.444	90	102.819	90
1.217	0.1	13.773	5.540	9.451	90	102.994	90
1.434	0.1	13.766	5.515	9.458	90	103.082	90
1.594	0.1	13.767	5.495	9.467	90	103.17	90

Compressibilities:

K_1	−4.3(4) TPa^{-1}
K_2	5.0(2) TPa^{-1}
K_3	20.98(18) TPa^{-1}
K_V	23.5(5) TPa^{-1}

Birch-Murnaghan Coefficients:

B_0	38.7(5) GPa
B'	$\equiv 4$
V_0	724.1(2) $Å^3$

Table S10: Variable pressure lattice parameters of InS as reported in Refs. S14, S15. NLC calculated from more recent study of Schwartz *et al.*

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
Ref. 14							
0.1	0.1	3.9457	4.453	10.65	90	90	90
0.2	0.1	3.943	4.401	10.654	90	90	90
2.1	0.1	3.924	4.188	10.706	90	90	90
3.6	0.1	3.906	4.059	10.743	90	90	90
4.3	0.1	3.899	4.016	10.763	90	90	90
Ref. 15							
0	0.1	3.944	4.447	10.648	90	90	90
1	0.1	3.94	4.32	10.78	90	90	90
2.7	0.1	3.92	4.12	10.8	90	90	90
3.7	0.1	3.88	4.06	10.8	90	90	90

Compressibilities:

K_1	$-2.41(13)$ TPa^{-1}
K_2	2.9(4) TPa^{-1}
K_3	15(2) TPa^{-1}
K_V	23.6(13) TPa^{-1}

Birch-Murnaghan Coefficients:

B_0	33.2(18) GPa
B'	$\equiv 4$
V_0	186.7(7) Å^3

Table S11: Variable pressure lattice parameters of silimanite calculated by DFT as reported in Ref. S16.

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
29.922	0.2	7.062	7.253	5.669	90	90	90
32.603	0.2	6.973	7.231	5.673	90	90	90
34.97	0.2	6.878	7.202	5.692	90	90	90
37.503	0.2	6.671	7.18	5.728	90	90	90

Compressibilities:

K_1	-3.30(-) TPa^{-1}
K_2	1.45(-) TPa^{-1}
K_3	10.81(-) TPa^{-1}
K_V	7.3(5) TPa^{-1}

1.2 Tilting polyhedra

Table S12: Variable pressure lattice parameters of BPO_4 extracted from Ref. S17.

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
0.000	0.2	4.339	4.339	6.647	90	90	90
3.687	0.2	4.224	4.224	6.632	90	90	90
6.089	0.2	4.159	4.159	6.632	90	90	90
9.162	0.2	4.081	4.081	6.641	90	90	90
11.676	0.2	4.042	4.042	6.648	90	90	90
15.251	0.2	3.985	3.985	6.652	90	90	90
18.827	0.2	3.915	3.915	6.711	90	90	90
24.302	0.2	3.834	3.834	6.744	90	90	90
24.469	0.2	3.807	3.807	6.782	90	90	90
29.274	0.2	3.733	3.733	6.781	90	90	90
31.061	0.2	3.716	3.716	6.794	90	90	90
33.352	0.2	3.660	3.660	6.901	90	90	90
36.034	0.2	3.649	3.649	6.881	90	90	90
41.061	0.2	3.597	3.597	6.907	90	90	90
43.799	0.2	3.597	3.597	6.896	90	90	90
48.939	0.2	3.551	3.551	6.916	90	90	90
49.721	0.2	3.535	3.535	6.901	90	90	90
53.464	0.2	3.527	3.527	6.912	90	90	90
55.810	0.2	3.500	3.500	6.906	90	90	90

Compressibilities:

K_a	2.83(12) TPa^{-1}
K_c	$-0.92(10)$ TPa^{-1}
K_V	5.6(5) TPa^{-1}

Birch-Murnaghan Coefficients:

B_0	52(9) GPa	(reported 56(3) GPa)
B'	4.9(6)	(reported 4.7(3))
V_0	135.7(10) $Å^3$	

Table S13: Variable pressure lattice parameters of $BAsO_4$ extracted from Ref. S17.

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
0.000	0.2	4.465	4.465	6.815	90	90	90
2.775	0.2	4.354	4.354	6.797	90	90	90
3.676	0.2	4.331	4.331	6.798	90	90	90
5.768	0.2	4.258	4.258	6.788	90	90	90
6.597	0.2	4.235	4.235	6.794	90	90	90
7.498	0.2	4.212	4.212	6.798	90	90	90
9.588	0.2	4.150	4.150	6.854	90	90	90
11.788	0.2	4.123	4.123	6.866	90	90	90
14.094	0.2	4.073	4.073	6.892	90	90	90
16.005	0.2	4.023	4.023	6.867	90	90	90
20.006	0.2	3.935	3.935	7.030	90	90	90
27.504	0.2	3.788	3.788	7.154	90	90	90
32.010	0.2	3.727	3.727	7.202	90	90	90
37.020	0.2	3.673	3.673	7.247	90	90	90
40.013	0.2	3.658	3.658	7.227	90	90	90
44.013	0.2	3.619	3.619	7.237	90	90	90
49.024	0.2	3.596	3.596	7.217	90	90	90
51.007	0.2	3.585	3.585	7.181	90	90	90

Compressibilities:

K_a	3.64(11) TPa^{-1}
K_c	$-1.48(15)$ TPa^{-1}
K_V	6.0(5) TPa^{-1}

Birch-Murnaghan Coefficients:

B_0	49(5) GPa	(reported 49(2) GPa)
B'	5.1(4)	(reported 5.0(5))
V_0	126.2(19) $Å^3$	

1.3 Spiral systems

Table S14: Variable pressure lattice parameters of trigonal selenium as reported in Refs. S18, S19.

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
Ref. S18, *Neutron data*							
0.58	0.1	4.281	4.281	4.993	90	90	120
0.58	0.1	4.286	4.286	4.976	90	90	120
2.4	0.1	4.058	4.058	5.061	90	90	120
2.5	0.1	4.069	4.069	5.031	90	90	120
4.3	0.1	3.937	3.937	5.064	90	90	120
4.3	0.1	3.912	3.912	5.096	90	90	120
6.2	0.1	3.869	3.869	5.085	90	90	120
7.3	0.1	3.767	3.767	5.112	90	90	120
Ref. S18, *X-ray data*							
1.4	0.1	4.169	4.169	5.056	90	90	120
1.8	0.1	4.162	4.162	5.055	90	90	120
1.8	0.1	4.154	4.154	5.072	90	90	120
2.6	0.1	4.027	4.027	5.108	90	90	120
2.9	0.1	4.046	4.046	5.091	90	90	120
3.1	0.1	4.027	4.027	5.122	90	90	120
3.9	0.1	3.937	3.937	5.136	90	90	120
4.4	0.1	3.944	3.944	5.122	90	90	120
4.4	0.1	3.931	3.931	5.139	90	90	120
5.2	0.1	3.878	3.878	5.139	90	90	120
3.3	0.1	4.035	4.035	5.094	90	90	120
6	0.1	3.894	3.894	5.128	90	90	120
10.3	0.1	3.731	3.731	5.178	90	90	120
14	0.1	3.642	3.642	5.147	90	90	120
Ref. S19							
0	0.1	4.368	4.368	4.958	90	90	120
0.12	0.1	4.343	4.343	4.964	90	90	120
2.58	0.1	4.052	4.052	5.038	90	90	120
4.15	0.1	3.956	3.956	5.069	90	90	120
4.99	0.1	3.91	3.91	5.08	90	90	120
6.57	0.1	3.846	3.846	5.095	90	90	120
7.7	0.1	3.81	3.81	5.11	90	90	120
8.64	0.1	3.779	3.779	5.109	90	90	120
9.98	0.1	3.745	3.745	5.119	90	90	120

Compressibilities:

K_a	12.0(4) TPa^{-1}
K_c	$-2.5(4)$ TPa^{-1}
K_V	23(2) TPa^{-1}

Birch-Murnaghan Coefficients:

B_0	23.0(14) GPa
B'	$\equiv 4$
V_0	79.7(7) Å^3

Table S15: Variable pressure lattice parameters of trigonal tellurium as reported in Ref. S20.

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
0	0.1	4.451	4.451	5.926	90	90	120
0.38	0.1	4.411	4.411	5.934	90	90	120
0.6	0.1	4.398	4.398	5.941	90	90	120
1.26	0.1	4.331	4.331	5.951	90	90	120
1.48	0.1	4.312	4.312	5.957	90	90	120
1.88	0.1	4.28	4.28	5.967	90	90	120
2.26	0.1	4.258	4.258	5.966	90	90	120
2.62	0.1	4.238	4.238	5.969	90	90	120
2.94	0.1	4.225	4.225	5.975	90	90	120
3.41	0.1	4.204	4.204	5.972	90	90	120
3.82	0.1	4.191	4.191	5.981	90	90	120

Compressibilities:

K_a	13.6(9) TPa^{-1}
K_c	$-1.8(3)$ TPa^{-1}
K_V	29.0(17) TPa^{-1}

Birch-Murnaghan Coefficients:

B_0	26.6(13) GPa
B'	$\equiv 4$
V_0	101.2(3) Å^3

1.4 Hinged systems

Table S16: Variable pressure lattice parameters of Ag(mim) as reported in Ref. S21.

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
0	0.01	7.8926	5.9767	10.8739	90	92.47	90
0.305	0.005	7.726	5.9233	10.888	90	92.73	90
1.08	0.08	7.433	5.8092	10.9101	90	93.736	90
2.17	0.14	7.2027	5.6926	10.9057	90	94.504	90
3.27	0.08	7.0544	5.6024	10.8873	90	95.062	90
3.8	0.16	6.992	5.559	10.875	90	95.344	90
4.85	0.04	6.9259	5.5072	10.8549	90	95.667	90
5.6	0.3	6.871	5.467	10.8393	90	95.878	90
6.4	0.4	6.828	5.4298	10.8209	90	96.076	90

Table S17: Variable pressure lattice parameters of $KMn[Ag(CN)_2]_3$ as reported in Ref. S22.

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
0.22	0.12	6.82042	6.82042	8.1961	90	90	120
0.5	0.15	6.73777	6.73777	8.2387	90	90	120
0.86	0.12	6.64413	6.64413	8.2842	90	90	120
1.2	0.17	6.56392	6.56392	8.3215	90	90	120
1.52	0.17	6.4973	6.4973	8.3543	90	90	120
1.78	0.15	6.4543	6.4543	8.3722	90	90	120
1.98	0.15	6.427	6.427	8.377	90	90	120
1.95	0.18	6.4227	6.4227	8.382	90	90	120
2.15	0.15	6.3888	6.3888	8.387	90	90	120

Table S18: Variable pressure lattice parameters of ZAG-4 as reported in Ref. S23.

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
0	0.1	18.515	8.291	8.265	90	113.837	90
1.65	0.1	17.991	8.000	8.0643	90	117.609	90
2.81	0.09	17.685	8.147	7.7557	90	119.697	90
5.69	0.03	17.1996	8.139	7.4651	90	122.431	90
7.32	0.07	17.023	8.066	7.4078	90	123.227	90

Compressibilities:

K_1	$-2.6(15)\,\mathrm{TPa}^{-1}$
K_2	$7.8(5)\,\mathrm{TPa}^{-1}$
K_3	$29(3)\,\mathrm{TPa}^{-1}$
K_V	$55(3)\,\mathrm{TPa}^{-1}$

Birch-Murnaghan Coefficients:

B_0	13.4(10) GPa
B'	$\equiv 4$
V_0	1163(10) Å^3

Table S19: Variable pressure lattice parameters of [Fe(dpp)$_2$(NCS)$_2$]·py as reported in Ref. S24.

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
0	0.1	13.379	8.7384	16.3583	90	104.247	90
0.48	0.1	13.585	8.236	16.306	90	103.3	90
1.82	0.1	13.614	7.741	16.059	90	102.55	90
2.48	0.1	13.562	7.541	15.878	90	101.57	90
0	0.1	13.3756	8.6951	16.3247	90	104.261	90
0.2	0.1	13.44	8.548	16.2728	90	103.8	90
0.3	0.1	13.511	8.349	16.23	90	103.663	90
0.85	0.1	13.59	8.07	16.21	90	103.33	90

Compressibilities:

K_1	$-10(2)$ TPa^{-1}
K_2	12(3) TPa^{-1}
K_3	53(4) TPa^{-1}
K_V	55(3) TPa^{-1}

Birch-Murnaghan Coefficients:

B_0	12.9(6) GPa
B'	$\equiv 4$
V_0	1842(9) Å^3

Table S20: Variable pressure lattice parameters of methanol monohydrate as reported in Ref. S25.

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
0.0106	0.1	4.6422	14.0303	4.6823	90	90	90
0.052	0.1	4.6437	13.9422	4.6739	90	90	90
0.102	0.1	4.6437	13.8503	4.6642	90	90	90
0.1545	0.1	4.6446	13.7542	4.6545	90	90	90
0.202	0.1	4.6457	13.673	4.646	90	90	90
0.255	0.1	4.6476	13.5853	4.6364	90	90	90
0.302	0.1	4.6493	13.5131	4.6293	90	90	90
0.35	0.1	4.6507	13.4347	4.6228	90	90	90
0.4015	0.1	4.6516	13.3658	4.6162	90	90	90
0.453	0.1	4.6545	13.2947	4.609	90	90	90
0.5	0.1	4.6554	13.2392	4.6035	90	90	90

Compressibilities:

K_1	$-2.7(18)$ TPa^{-1}
K_2	31.9(4) TPa^{-1}
K_3	108.0(9) TPa^{-1}
K_V	143(4) TPa^{-1}

1.5 NAC Systems

Table S21: Variable pressure lattice parameters of $PbTiO_3$ as reported in Ref. S26.

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
0	0.05	3.8977	3.8977	4.1526	90	90	90
0.32	0.05	3.8977	3.8977	4.132	90	90	90
1.41	0.05	3.9000	3.9000	4.0682	90	90	90
1.7	0.05	3.9006	3.9006	4.0513	90	90	90
2.05	0.05	3.8985	3.8985	4.0409	90	90	90
2.6	0.05	3.8968	3.8968	4.0252	90	90	90
3.0	0.05	3.8956	3.8956	4.0123	90	90	90
3.25	0.05	3.8955	3.8955	4.0056	90	90	90
3.6	0.05	3.8933	3.8933	3.9954	90	90	90
4.05	0.05	3.8896	3.8896	3.9818	90	90	90
4.8	0.05	3.8881	3.8881	3.9656	90	90	90
5.63	0.05	3.8843	3.8843	3.9498	90	90	90
5.94	0.05	3.8829	3.8829	3.9454	90	90	90
6.2	0.05	3.8818	3.8818	3.9399	90	90	90
6.35	0.05	3.8805	3.8805	3.9370	90	90	90

Table S22: Variable pressure lattice parameters of NaV_2O_5 extracted from Ref. S27.

p (GPa)	σ_p (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)
0	0.1	11.32978	3.61335	4.79150	90	90	90
0.57377	0.1	11.29585	3.61749	4.68632	90	90	90
1.88525	0.1	11.27901	3.61766	4.54885	90	90	90
2.78689	0.1	11.27489	3.62183	4.45183	90	90	90
4.01639	0.1	11.27930	3.62605	4.35076	90	90	90
5.32787	0.1	11.28801	3.63432	4.24162	90	90	90
6.88525	0.1	11.30524	3.65073	4.13251	90	90	90
9.42623	0.1	11.31411	3.65107	4.00330	90	90	90
12.86885	0.1	11.28908	3.65558	3.90255	90	90	90
15.40984	0.1	11.25964	3.65593	3.85432	90	90	90
18.77049	0.1	11.22182	3.65233	3.80213	90	90	90
21.47541	0.1	11.18816	3.64460	3.75391	90	90	90
29.26230	0.1	11.04885	3.62136	3.66589	90	90	90

Compressibilities:

K_1	$-1.2(5)$ TPa^{-1}
K_2	$-0.48(16)$ TPa^{-1}
K_3	14.3(11) TPa^{-1}
K_V	14.5(9) TPa^{-1}

Birch-Murnaghan Coefficients:

B_0	23(6) GPa
B'	14(3)
V_0	196(2) Å^3

2 Elastic data

Table S23: Elastic stiffness data in GPa for CsH_2PO_4 determined from ultrasonic velocity measurements from Ref. S28.

$C_{11} = 28.83$	$C_{12} = 11.4$	$C_{35} = 7.50$
$C_{22} = 26.67$	$C_{13} = 42.87$	$C_{46} = -2.25$
$C_{33} = 65.45$	$C_{15} = 5.13$	
$C_{44} = 8.10$	$C_{23} = 14.5$	
$C_{55} = 5.20$	$C_{25} = 8.4$	
$C_{66} = 9.17$		

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