

# Supplementary Materials

**Table S1.** Atom positions in the crystal structures of millerite, heazlewoodite, and polydymite under 0 GPa.

Mineral	Atom	<i>x</i>	<i>y</i>	<i>z</i>
Millerite	Ni	−0.088	0.088	0.088
	S	0.112	−0.112	0.616
Heazlewoodite	Ni	0.500	0.247	−0.247
	S	0.255	0.255	0.255
Polydymite	Ni	0	0	0
	S	−0.135	−0.135	−0.135

**Table S2.** Pressure dependence of parameters for millerite (NiS).

P (GPa)	<i>a</i> (Å)	<i>c</i> (Å)	<i>V</i> (Å <sup>3</sup> )	$\rho$ (g/cm <sup>3</sup> )	<i>C</i> <sub>11</sub> (GPa)	<i>C</i> <sub>33</sub> (GPa)	<i>C</i> <sub>44</sub> (GPa)	<i>C</i> <sub>12</sub> (GPa)	<i>C</i> <sub>13</sub> (GPa)	<i>C</i> <sub>14</sub> (GPa)
0	9.596	3.150	251.161	5.401	222.942	217.797	52.953	68.046	81.893	−11.855
1	9.569	3.142	249.177	5.444	230.736	231.835	54.808	72.350	86.613	−11.650
2	9.543	3.135	247.255	5.486	238.328	237.064	56.501	75.815	90.541	−11.916
3	9.520	3.128	245.460	5.527	246.238	244.025	58.780	79.748	95.168	−12.230
4	9.496	3.121	243.734	5.566	252.905	245.320	60.305	83.320	98.603	−12.117
5	9.474	3.114	242.049	5.604	258.679	251.776	62.543	85.661	101.413	−11.908
6	9.452	3.108	240.432	5.642	267.363	262.979	64.309	90.414	106.379	−12.625
7	9.432	3.101	238.924	5.678	269.377	267.327	65.985	90.226	110.258	−12.386
8	9.412	3.095	237.428	5.713	280.602	274.161	68.014	97.333	113.672	−12.917
9	9.391	3.090	236.000	5.748	282.999	277.197	69.050	100.323	114.368	−11.897
10	9.373	3.083	234.602	5.782	290.737	283.624	70.957	103.478	118.424	−12.493
11	9.355	3.078	233.262	5.816	298.009	292.130	72.262	107.573	123.019	−12.804
12	9.337	3.072	231.956	5.848	304.116	294.107	73.251	110.821	126.523	−13.026
13	9.320	3.067	230.700	5.880	309.791	298.572	75.600	115.059	130.753	−12.856
14	9.303	3.062	229.479	5.911	314.573	303.898	77.876	117.386	132.926	−13.038
15	9.287	3.056	228.279	5.942	323.044	312.058	78.131	123.579	139.168	−13.171
16	9.271	3.051	227.122	5.973	326.918	318.245	80.541	124.371	140.797	−13.512
17	9.255	3.047	226.006	6.002	333.401	323.352	81.039	129.301	145.029	−13.494
18	9.240	3.042	224.909	6.032	339.629	327.999	81.352	133.223	149.196	−13.689
19	9.225	3.037	223.861	6.060	345.519	332.881	84.193	137.104	152.915	−13.863
20	9.211	3.032	222.805	6.089	352.088	337.892	84.481	141.429	157.349	−14.044
21	9.197	3.028	221.796	6.116	356.850	346.134	84.854	144.101	160.169	−14.230
22	9.183	3.024	220.804	6.144	362.856	348.453	85.544	148.289	164.272	−14.369
23	9.169	3.019	219.834	6.171	369.203	351.566	86.817	152.606	168.669	−14.564
24	9.156	3.015	218.900	6.197	372.702	355.213	87.949	155.364	171.118	−14.510

**Table S3.** Pressure dependence of parameters for heazlewoodite (Ni<sub>3</sub>S<sub>2</sub>).

P (GPa)	a (Å)	$\alpha$ (°)	V (Å <sup>3</sup> )	$\rho$ (g/cm <sup>3</sup> )	C <sub>11</sub> (GPa)	C <sub>33</sub> (GPa)	C <sub>44</sub> (GPa)	C <sub>12</sub> (GPa)	C <sub>13</sub> (GPa)	C <sub>14</sub> (GPa)
0	4.082	89.318	68.003	5.867	213.496	214.748	52.093	109.815	73.865	3.400
1	4.071	89.344	67.479	5.912	220.498	222.813	52.565	115.500	76.963	3.700
2	4.061	89.371	66.976	5.957	224.276	227.831	53.582	121.512	78.446	3.975
3	4.052	89.396	66.499	5.999	234.103	236.440	54.234	130.642	84.828	4.156
4	4.042	89.421	66.039	6.041	240.183	241.019	55.076	134.269	86.634	5.027
5	4.033	89.446	65.597	6.082	246.592	255.420	56.492	140.020	89.624	5.365
6	4.024	89.471	65.173	6.121	253.527	257.484	57.185	146.545	93.263	5.734
7	4.016	89.496	64.763	6.160	255.237	259.942	57.840	149.924	92.774	5.306
8	4.008	89.521	64.367	6.198	266.615	268.866	58.484	155.872	99.549	5.615
9	4.000	89.545	63.987	6.235	272.316	274.551	59.219	164.571	102.926	6.883
10	3.992	89.569	63.619	6.271	276.871	287.150	59.795	169.011	104.635	6.635
11	3.985	89.593	63.259	6.307	282.864	288.752	60.397	174.528	107.525	6.787
12	3.977	89.616	62.911	6.341	289.704	295.766	60.998	179.707	110.687	7.571
13	3.970	89.640	62.574	6.376	293.931	304.325	61.425	184.299	112.199	7.604
14	3.963	89.663	62.246	6.409	303.792	314.110	62.536	189.239	117.858	7.880
15	3.956	89.687	61.928	6.442	307.451	320.124	62.192	196.688	119.563	8.454
16	3.950	89.709	61.618	6.475	314.226	326.867	63.095	201.759	123.543	8.670
17	3.943	89.733	61.315	6.507	318.967	329.171	64.103	207.325	125.139	9.170
18	3.937	89.755	61.021	6.538	324.522	331.253	64.059	211.844	128.195	9.606
19	3.931	89.777	60.734	6.569	330.787	337.913	65.041	217.288	130.664	9.640
20	3.925	89.800	60.454	6.599	335.100	338.381	65.519	223.893	133.164	9.936
21	3.919	89.822	60.181	6.629	340.204	350.908	66.152	228.255	135.286	9.909
22	3.913	89.844	59.913	6.659	347.132	350.686	66.741	234.619	139.179	10.843
23	3.907	89.865	59.652	6.688	354.160	362.260	66.814	238.741	142.219	11.078
24	3.902	89.886	59.397	6.717	363.919	373.958	67.149	246.264	148.880	9.859

**Table S4.** Pressure dependence of parameters for polydymite (Ni<sub>3</sub>S<sub>4</sub>).

P (GPa)	a (Å)	V (Å <sup>3</sup> )	ρ (g/cm <sup>3</sup> )	C <sub>11</sub> (GPa)	C <sub>44</sub> (GPa)	C <sub>12</sub> (GPa)
0	9.476	850.813	4.752	185.088	44.577	81.579
1	9.449	843.728	4.792	191.803	43.813	84.986
2	9.424	836.949	4.831	198.965	44.334	86.535
3	9.399	830.376	4.869	202.537	43.706	91.840
4	9.376	824.184	4.906	204.197	44.320	101.352
5	9.353	818.216	4.942	210.168	44.610	104.476
6	9.331	812.531	4.976	214.886	45.282	109.600
7	9.310	806.925	5.011	221.554	45.108	112.529
8	9.289	801.629	5.044	221.694	46.011	118.530
9	9.270	796.471	5.077	230.581	45.246	121.414
10	9.250	791.547	5.108	235.411	46.691	126.954
11	9.232	786.768	5.139	236.724	46.206	132.213
12	9.213	782.105	5.170	243.059	46.269	137.394
13	9.196	777.625	5.200	245.642	46.475	139.705
14	9.179	773.280	5.229	250.228	45.845	144.681
15	9.162	768.980	5.258	253.004	45.487	150.025
16	9.145	764.880	5.286	262.785	45.196	150.345
17	9.129	760.825	5.314	269.373	45.299	155.939
18	9.114	756.944	5.342	273.624	45.143	159.561
19	9.099	753.218	5.368	276.046	45.118	164.412
20	9.084	749.510	5.395	276.644	45.289	170.631
21	9.069	745.889	5.421	276.437	45.237	172.117
22	9.055	742.365	5.447	284.569	45.458	178.727
23	9.041	738.930	5.472	297.138	45.809	192.511
24	9.027	735.573	5.497	304.127	44.920	200.067



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