

Supplementary information

Exploring the pressure-temperature behaviour of crystalline and plastic crystalline phases of *N*-isopropylpropionamide

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Table S1 – Cell parameters and volume estimated in the refinement of X-ray diffraction data collected from the crystalline phase of NiPPA up to 10.3 GPa.

Pressure (GPa)	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	β (°)	Volume (Å ³)
0.1	16.73(2)	8.88(3)	4.92(2)	97.7(7)	724.8
0.5	16.25(9)	8.83(9)	4.89(1)	98.0(0)	696.1
1.1	15.76(0)	8.79(2)	4.86(1)	98.2(0)	666.7
2	15.26(3)	8.70(1)	4.81(0)	98.3(8)	632.0
3	14.92(7)	8.62(3)	4.76(7)	98.5(4)	606.8
4	14.69(8)	8.56(5)	4.73(8)	98.7(9)	589.5
5	14.50(0)	8.51(8)	4.71(1)	98.9(7)	574.8
6	14.24(8)	8.46(6)	4.67(1)	99.1(0)	556.3
7.2	14.03(8)	8.41(8)	4.64(4)	99.3(9)	541.4
8	13.90(2)	8.39(8)	4.63(3)	99.5(9)	533.4
9	13.71(2)	8.37(6)	4.62(3)	99.9(1)	523.1
10.3	13.52(9)	8.33(6)	4.61(4)	100.2(7)	512.0

Table S2 – Crystallographic data of the NiPPA structure up to 10.3 GPa.

P (GPa)	Bond Length (Å)							
	C1C2	C2C3	C2N4	N4C5	C5C6	C5O8	C6C7	
0.1	1.4788(5)	1.4346(3)	1.5013(5)	1.4068(3)	1.4890(4)	1.2907(3)	1.4838(6)	
0.5	1.4654(3)	1.4054(4)	1.4835(3)	1.3883(3)	1.4642(3)	1.2820(3)	1.4758(3)	
1.1	1.4512(3)	1.3743(4)	1.4652(4)	1.3687(3)	1.4386(3)	1.2735(3)	1.4675(3)	
2	1.4312(4)	1.3414(5)	1.4418(4)	1.3451(4)	1.4095(4)	1.2596(4)	1.4520(4)	
3	1.4155(4)	1.3188(5)	1.4239(4)	1.3280(4)	1.3882(4)	1.2480(4)	1.4388(4)	
4	1.4044(4)	1.3046(6)	1.4105(4)	1.3171(4)	1.3726(4)	1.2396(4)	1.4290(4)	
5	1.61(2)	1.45(2)	1.55(2)	1.37(2)	1.49(2)	1.33(1)	1.54(2)	
6	1.5997(2)	1.4383(3)	1.5306(2)	1.3583(2)	1.4738(2)	1.3200(2)	1.5279(2)	
7.2	1.5888(2)	1.4243(3)	1.5156(2)	1.3466(3)	1.4552(3)	1.3116(2)	1.5178(2)	
8	1.5836(2)	1.4163(4)	1.5073(3)	1.3402(3)	1.4438(4)	1.3082(2)	1.5133(3)	
9	1.5774(2)	1.4058(3)	1.4964(2)	1.3320(3)	1.4281(3)	1.3046(2)	1.5078(2)	
10.3	1.5691(3)	1.3964(5)	1.4835(3)	1.3240(4)	1.4117(4)	1.3009(3)	1.4994(3)	
	Bond Angle (°)							
	C1C2C3	C1C2N4	C3C2N4	C2N4C5	N4C5C6	N4C5O8	C6C5O8	C5C6C7
0.1	127.19	122.9	97.76	123.06	126.86	118.28	114.76	117.22
0.5	126.89	124.04	96.77	122.65	126.38	118.79	114.74	117.83
1.1	126.57	125.26	95.69	122.2	125.83	119.31	114.77	118.14
2	126.31	126.27	94.77	121.81	125.36	119.77	114.78	118.93
3	126.16	126.89	94.21	121.57	125.07	120.07	114.77	119.25
4	126.07	127.32	93.82	121.4	124.89	120.35	114.68	119.52
5	120	120	106	121	135	112	112	106
6	119.41	120.09	105.92	120.24	135	111.88	112.46	106.71
7.2	119.3	120.55	105.56	120	134.83	112.17	112.35	107.15
8	119.2	120.93	105.26	119.8	134.67	112.39	112.29	107.49
9	119.07	121.5	104.8	119.49	134.43	112.74	112.18	108.01
10.3	119.02	121.97	104.35	119.14	134.17	113.16	112.02	108.44
	Torsion Angle (°)							
	C1C2N4C5	C3C2N4C5	C2N4C5C6	C2N4C5O8	N4C5C6C7	O8C5C6C7		
0.1	72.7	-143.24	-166	17.75	-123	53.36		
0.5	72.64	-143.3	-166.13	17.6	-123.5	52.9		
1.1	73.17	-143.36	-166.28	17.43	-124.09	52.35		
2	73.62	-143.42	-166.42	17.27	-124.61	51.86		
3	73.87	-143.49	-166.5	17.17	-124.93	51.57		
4	73.94	-143.61	-166.56	17.11	-125.11	51.41		
5	59.2	-161.1	-162.2	8.2	-102.2	88.1		
6	59.59	-161.34	-161.91	7.81	-102.52	87.8		
7.2	59.64	-161.41	-161.94	7.78	-102.53	87.76		
8	59.69	-161.45	-161.97	7.77	-102.55	87.71		
9	59.77	-161.53	-162.01	7.73	-102.58	87.63		
10.3	59.78	-161.63	-162.07	7.7	-102.59	87.55		

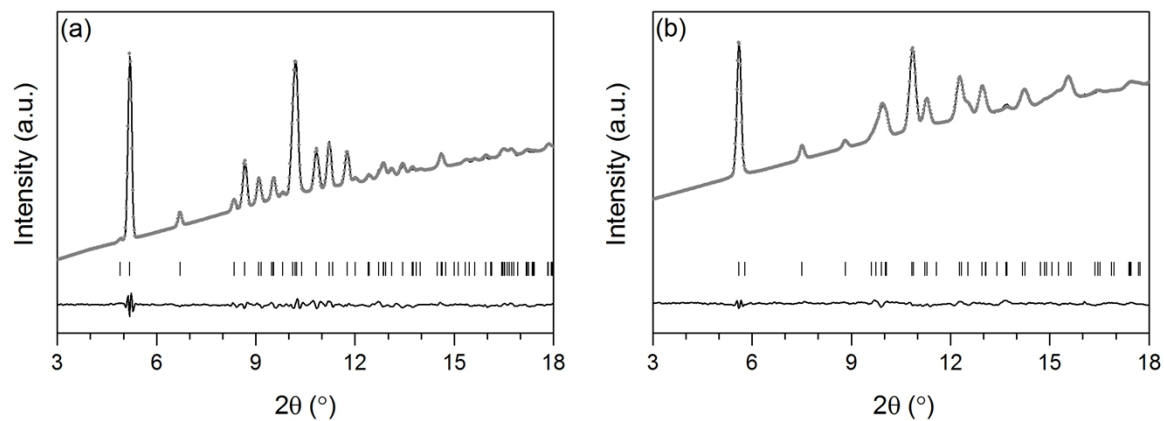


Figure S1 - Rietveld refinement profiles for the crystalline phase at (a) 0.1 MPa and (b) 6 GPa at ambient temperature ($\lambda = 0.71171 \text{ \AA}$).

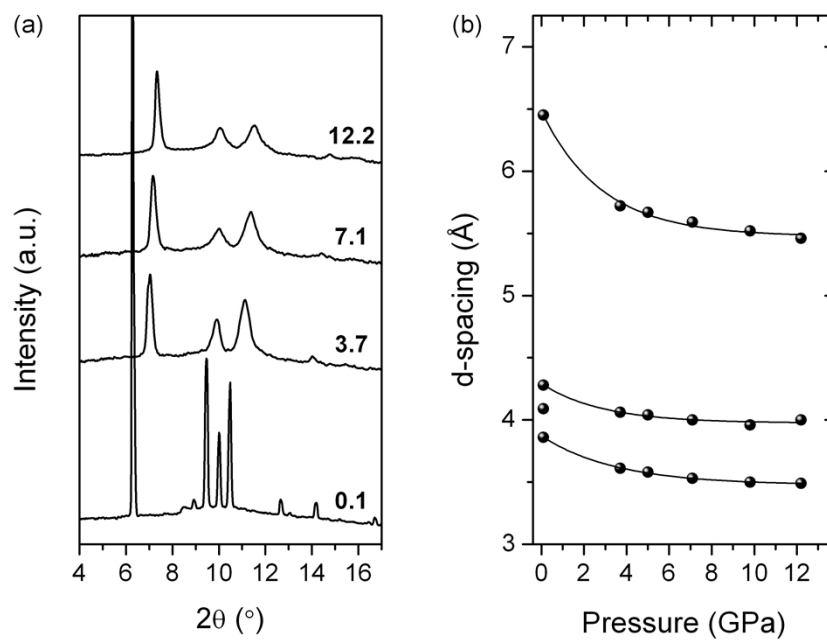


Figure S2 – (a) Selected X-ray diffraction patterns of the plastic crystalline phase of NiPPA and (b) peak shifts upon compression at 293 K (b). Pressure values in (a) are given in GPa.