Table ES1: Crystallographic data for Form I and II of chlorothiazide at various pressures.

	0 GPa	0.5 GPa	1.3 GPa	2.1 GPa	3.5 GPa	4.0 GPa	4.4 GPa	5.1 GPa	5.9 GPa
Chemical formula	$C_7H_6ClN_3O_4S_2$	$C_7H_6ClN_3O_4S_2$	$C_7H_6ClN_3O_4S_2$	$C_7H_6ClN_3O_4S_2$	$C_7H_6ClN_3O_4S_2$	$C_7H_6ClN_3O_4S_2$	$C_7H_6ClN_3O_4S_2$	$C_7H_6ClN_3O_4S_2$	$C_7H_6ClN_3O_4S_2$
M_r	295.73	295.73	295.73	295.73	295.73	295.73	295.73	295.73	295.73
Radiation type	Mo *K*α	Mo *K*α	Mo *K*α	Mo *K*α	Mo *K*α	Mo *K*α	Mo *K*α	Mo *K*α	Mo *K*α
Cell setting, space group	Triclinic, *P*1	Triclinic, *P*1	Triclinic, *P*1	Triclinic, *P*1	Triclinic, *P*1	Triclinic, *P*1	Triclinic, *P*1	Triclinic, *P*1	Triclinic, *P*1
Temperature (K)	293	293	293	293	293	293	293	293	293
a, *b*, *c* (Å)	4.8746 (14), 6.4011 (10), 8.980 (3)	4.835 (3), 6.310 (2), 8.895 (7)	4.760 (2), 6.1455 (12), 8.737 (4)	4.728 (2), 6.0501 (14), 8.684 (5)	4.693 (2), 5.9013 (14), 8.599 (5)	4.676 (3), 5.8115 (17), 8.543 (6)	4.5100 (5), 5.9287(6), 8.503 (3)	4.4832(4), 5.8932(4), 8.465(2)	4.4609 (4), 5.8592 (5), 8.427 (2)
α, β, γ (°)	74.05 (2), 83.54 (2), 80.468 (18)	74.62 (4), 84.12 (5), 80.67 (4)	76.06 (3), 84.56 (3), 81.25 (2)	76.54 (3), 84.73 (4), 81.67 (3)	77.48 (3), 84.97 (4), 82.35 (3)	77.95 (4), 85.11 (5), 82.77 (4)	76.528 (16), 85.624 (17), 83.203 (8)	76.234 (13), 85.836 (13), 83.284 (6)	75.991 (15), 86.055 (14), 83.349(6)
V (Å^3)	265.03 (13)	257.7 (3)	244.75 (16)	238.57 (18)	229.99 (18)	224.8 (2)	219.26 (8)	215.49 (6)	212.08 (7)
Z	1	1	1	1	1	1	1	1	1
D_x (Mg m^{-3})	1.853	1.905	2.006	2.058	2.135	2.184	2.239	2.279	2.315
No. of reflns for cell	557	482	552	366	448	447	778	778	778
2θmax (°)	52.5	52.52	52.65	46.56	47.66	46.48	46.44	46.21	46.46
μ (mm^{-1})	0.76	0.78	0.82	0.85	0.876	0.896	0.919	0.935	0.950
Reflns collected	5860	5354	5000	3973	4121	4031	2095	2157	2115
Unique [Rint]	644 [0.0609]	619 [0.058]	602 [0.0638]	463 [0.0686]	410 [0.070]	454 [0.0678]	246 [0.0421]	447 [0.037]	243 [0.0384]
No. I>2u(I)	544	537	517	408	368	407	232	234	234
T_{min}, T_{max}	0.49, 0.96	0.16, 0.96	0.54, 0.96	0.24, 0.96	0.49, 0.96	0.08, 0.96	0.85, 0.96	0.88, 0.95	0.88, 0.95
Params	72	72	72	72	72	72	72	72	72
R1[F>4u(F)]	0.0657	0.0701	0.058	0.0564	0.0642	0.0625	0.0288	0.0256	0.0240
wR2 (F2, all data)	0.1653	0.1678	0.1350	0.1735	0.1755	0.1678	0.0693	0.0583	0.0584
S	1.05	1.071	1.03	1.21	1.095	1.135	1.2230	1.2151	1.1898
ρ_{max} (e Å^{-3})	0.50	0.49	0.345	0.41	0.39	0.37	0.19	0.15	0.15
ρ_{min} (e Å^{-3})	–0.35	–0.45	–0.33	–0.36	-0.43	-0.39	-0.17	-0.18	-0.20

Table ES2: The cell parameters with respect to pressure calculated from a Le Bail fit of the powder diffraction data.

Pressure (GPa)	Phase	*a*-axis	*b*-axis	*c*-axis	α	β	γ	Volume (Å^3)	R_{wp}
0.1	I	4.873(2)	6.413(2)	8.941(4)	74.066(6)	83.714(10)	80.588(11)	264.4(2)	0.76
0.8	I	4.8122(11)	6.27806(6)	8.829(3)	75.089(18)	84.071(18)	80.935(8)	253.99(11)	0.85
1.4	I	4.7679(7)	6.1847(6)	8.767(3)	75.657(19)	84.530(18)	81.236(8)	247.09(9)	0.79
2.2	I	4.7344(5)	6.0738(4)	8.6909(9)	76.298(8)	84.830(10)	81.701(9)	239.85(4)	0.83
2.8	I	4.7182(9)	5.9979(7)	8.656(2)	76.637(17)	84.89(2)	82.045(15)	235.62(8)	1.26
4.1	I	4.6807(9)	5.8950(8)	8.587(2)	77.336(19)	85.12(2)	82.362(15)	228.73(8)	1.45
5.1	I	4.695(5)	5.804(4)	8.538(19)	77.98(15)	84.85(13)	81.80(11)	224.8(6)	1.769
	II	4.524(2)	5.9333 (17)	8.523(5)	76.64(3)	85.54(4)	83.47(5)	220.84(19)	
6.2	I	4.666(4)	5.793 (7)	8.618(17)	77.62(2)	85.24(7)	82.03(13)	225.0(6)	1.64
	II	4.5099(17)	5.897 (2)	8.472(4)	76.31(3)	85.65(2)	83.29(5)	217.14(16)	
5.4	I	4.701(6)	5.796 (6)	8.502(11)	78.04(13)	84.84(8)	82.01(12)	224.0(5)	1.43
	II	4.5200(12)	5.9174 (13)	8.494(4)	76.336(15)	85.58(2)	83.19(4)	218.91(12)	
4.2	I	4.679(5)	5.848(3)	8.59(2)	77.62(8)	84.70(13)	81.76(7)	226.9(6)	1.48
	II	4.5285(17)	5.9569(17)	8.539(6)	76.519(2)	76.52(2)	83.27(4)	222.15(18)	
3.2	I	4.6781(14)	5.9104(13)	8.593(3)	77.223(3)	85.05(3)	82.54(3)	229.33(13)	2.20
0	I	8.985(2)	6.4049(7)	4.8860(10)	74.049(12)	83.56(2)	80.541(14)	266.01(10)	1.08

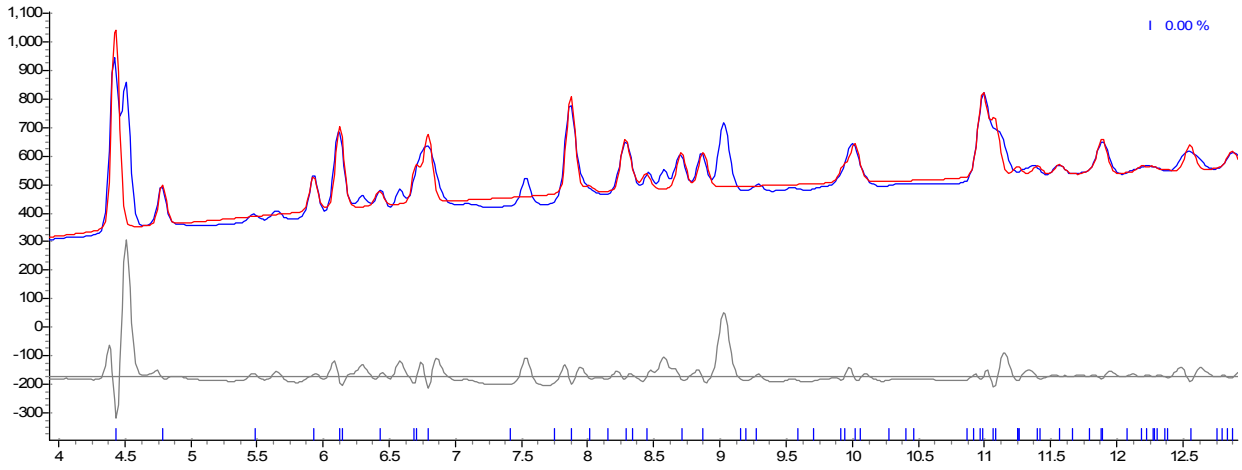

Figure ESI 0a. A single phase Pawley-type fit to the 5.1GPa data. Tick marks show reflection positions for form I (blue). The blue line shows the observed data, the red the fit to the data. The difference profile is shown in grey.

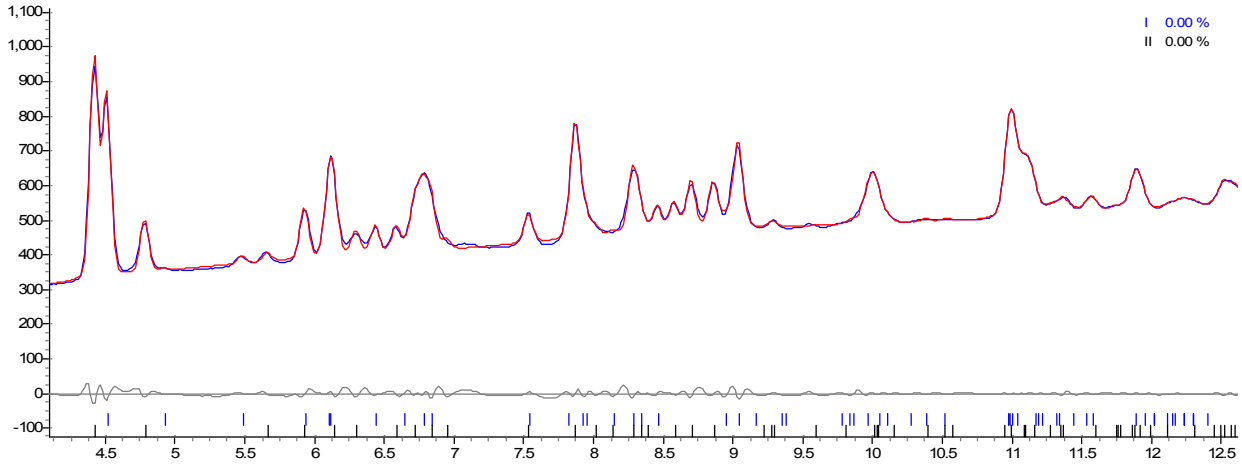

Figure ESI 0b. A two phase Pawley-type fit to the 5.1GPa data. Tick marks show reflection positions for form I (blue) and form II (black). The blue line shows the observed data, the red the fit to the data. The difference profile is shown in grey.

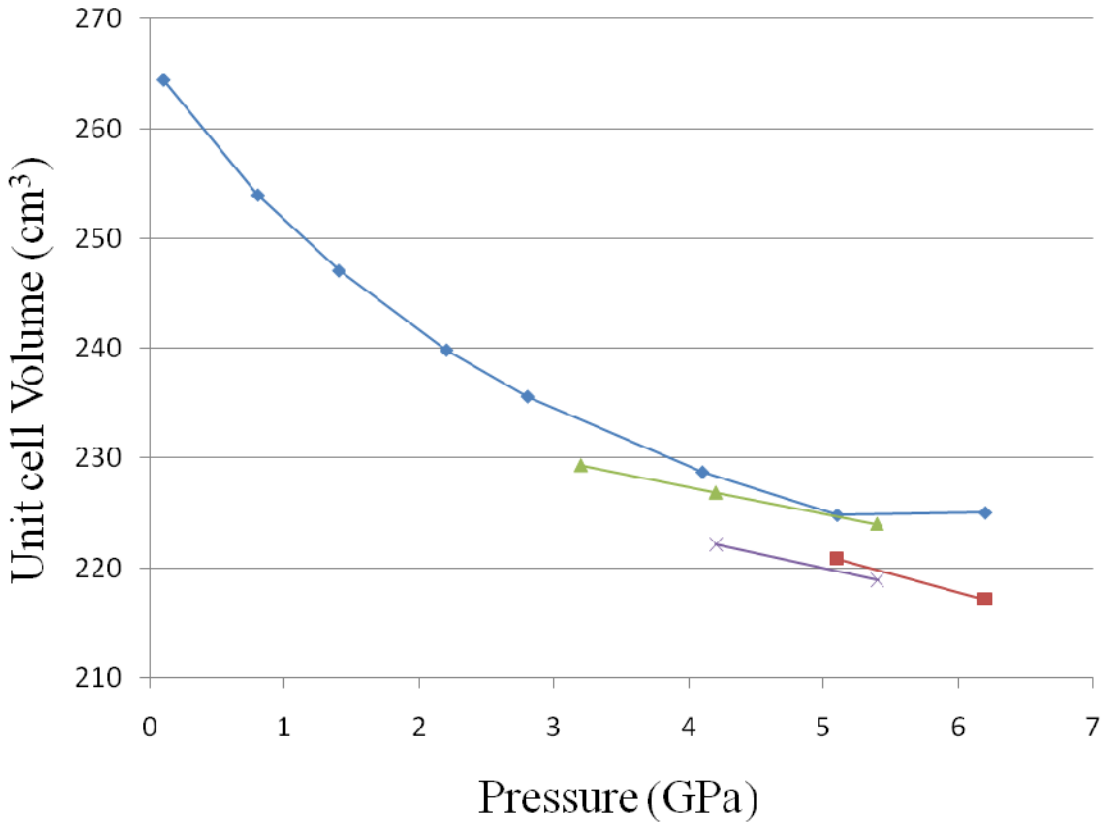

Figure ES1: Compression of the unit cell dimensions calculated from the X-ray powder diffraction measurements. The blue diamonds and green triangles represent the compression and decompression of Form I, respectively. The red squares and purple crosses represent the compression and decompression of Form II, respectively. The standard deviations on the unit cell volumes are smaller than the size of the data points. The lines have been added as a guide to the eye.