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Supplementary Materials for the paper:

The pressure-temperature phase diagram of tetramorphic pyrazinamide

By

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Data of vapour pressure of four forms of pyrazinamide

Table S1. The vapor pressure of α, β, γ, and δ as a function of temperature

α		γ		β		δ	
T /K	*p* /Pa	*T* /K	*p* /Pa	*T* /K	*p* /Pa	*T* /K	*p* /Pa
293.15	0.00121(6)	323.15	0.0564(20)	293.15	0.00136(2)	301.15	0.00375(6)
295.15	0.00166(19)	333.15	0.167(9)	295.15	0.00187(15)	303.15	0.00504(20)
301.15	0.0036(1)	343.15	0.484(32)	297.15	0.00243(11)	305.15	0.0067(6)
313.15	0.01804(5)	363.16	2.88(6)	299.15	0.00322(13)	308.15	0.0095(4)
323.15	0.0492(9)	383.15	11.9(1.3)	301.15	0.00415(20)	313.15	0.0177(5)
333.15	0.162(4)					323.15	0.0560(14)
343.15	0.428(10)					343.15	0.535(49)
363.15	2.59(1)						
373.15	5.68(49)						
383.15	10.32(65)						

Data of phase transition of four forms of pyrazinamide

Table S2. DSC results measured by using δ form at different heating rate

measurement	Heating rate /K·min^{-1}	Transition temperature /K	Transition enthalpy /J·g^{-1}
	Transition of δ to γ		
1	2	400.09	14.69
2	2	402.24	14.59
3	4	401.76	16.68
4	4	402.63	12.81
5	4	405.84	14.47
6	5	402.61	16.33
7	5	402.15	15.70
8	6	406.36	15.01
9	6	405.95	15.71
10	8	406.23	16.17
11	8	404.89	16.58
12	10	405.65	16.58
13	10	406.21	16.38
14	10	405.98	16.44
15	10	407.11	16.51
16	10	406.20	15.68
17	10	406.97	16.92
18	10	404.26	17.57
19	10	404.96	17.92
20	10	404.99	17.37
21	10	406.07	16.88
22	10	404.94	17.06
23	10	405.37	17.10
24	10	406.40	16.93
25	10	405.49	18.36
26	10	405.03	18.10
27	10	405.54	17.70
28	10	407.97	17.03

measurement	Heating rate /K·min^{-1}	Transition temperature /K	Transition enthalpy /J·g^{-1}
	Transition of δ to α		
29	0.5	386.33	5.46
30	1	386.72	6.02

Table S3. DSC results obtained with form β (10 K min^{-1})

meas.	peak 1		peak 2		total[b]	fusion	
	T /K	ΔH / J·g^{-1}	T /K	ΔH / J·g^{-1}	ΔH / J·g^{-1}	T /K	ΔH / J·g^{-1}
1	367.75	7.81	393.65	7.20	15.01		
2	372.85	7.61	399.95	7.17	14.78		
3[a]	373.45	5.37	390.65	12.37	19.02[a]	461.55	233.6
4	373.95	6.54	378.55	8.78	15.32	461.65	226.6
5	374.35	7.40		11.93	19.33	461.55	
6	375.65	11.57		7.72	19.29	461.65	232.1
7	376.45	9.79		6.80	16.60	461.55	232.0
8	375.45	10.66		9.26	19.92	461.55	235.6
9	374.75	8.16	413.75	7.451	15.61	461.55	229.1
10	369.75	9.69	393.35	11.16	20.85	461.55	235.0
11	373.15	7.25	399.35	8.66	15.91	461.45	237.3
12	367.95	8.92	397.25	9.89	18.81	461.55	234.3
13	370.45				15.41	461.45	230.1
14[c]			392.25		20.17	462.15	238.0
15[c]			397.05		15.43	461.65	240.0
16[c]			387.95		21.62	461.65	233.6
17[c]			396.65		19.06	462.15	236.9

[a] Measurement 3 exhibited a small precursor peak starting at 350.25 K with 1.28 J·g^{-1}.
[b] Total enthalpy observed in the solid-solid transitions up to melting.
[c] single crystal(s) sample

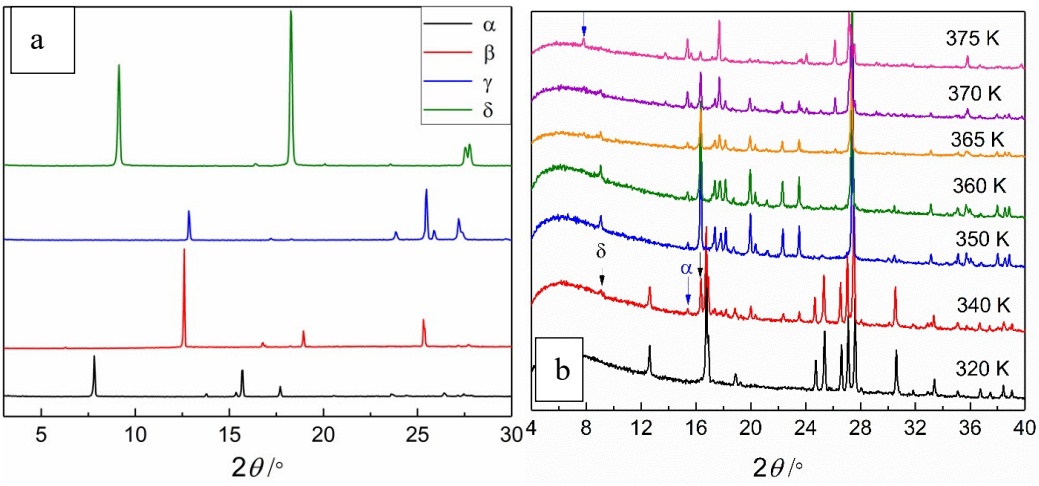

Figure S1. (a) Diffraction patterns (3-30° 2θ) of the four polymorphs used in this article. **(b)** X-ray diffraction starting with form β at 320 K as a function of the temperature. From 340 K peaks of forms α and δ can be observed demonstrating the complications to interpret the peaks in the DSC data. At around 370 K, the δ peaks have almost fully converted to α.

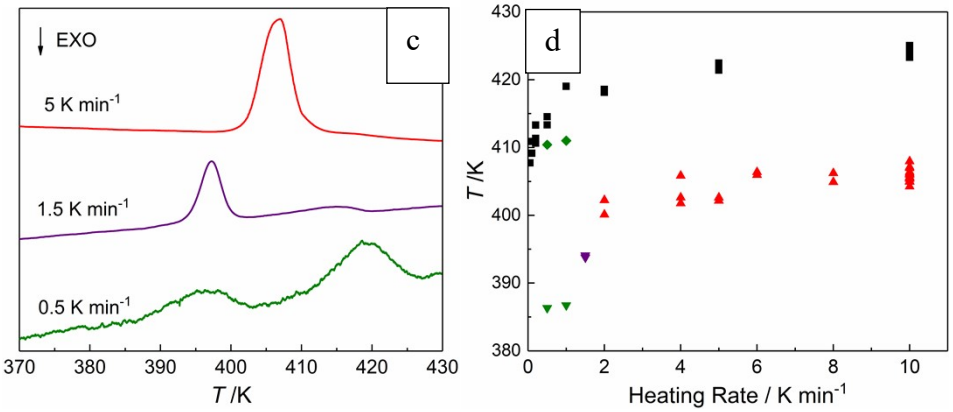

Figure S1. (c) DSC curves of the transition from form δ through form α to form γ (green curve) and directly to form γ (red curve) with **(d)** the evolution of the onset of the peaks with the heating rate. The purple curve shows intermediate behaviour. The black squares are α to γ conversions from a pure α sample for comparison.

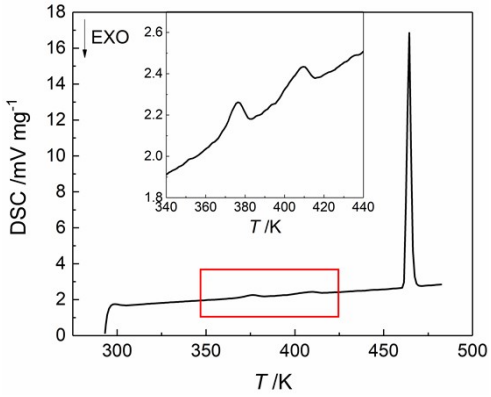

Figure S1. (e) A double transformation of polymorph β into another form followed by a transformation into γ demonstrated by its melting point. From the diffraction in Figure S1b, it follows that both α and δ are likely present during the transformations.

Unit cell parameters of α, β, γ and δ form of pyrazinamide as a function of temperature at ordinary pressure

Table S4. Unit cell parameters of α form of pyrazinamide as a function of temperature

T /K	*a* /Å	*b* /Å	*c* /Å	*β* /°	*V* /Å^3
100	3.6190(2)	6.7437(4)	22.473(2)	92.455(4)	547.97(13)
150	3.6404(2)	6.7380(4)	22.500(2)	92.248(4)	551.49(5)
200	3.6646(2)	6.7304(4)	22.540(2)	92.086(4)	555.59(5)
250	3.6919(2)	6.7171(3)	22.589(2)	91.912(5)	559.88(5)
300	3.7198(2)	6.7123(4)	22.618(2)	91.819(4)	564.45(6)
350	3.7511(2)	6.7078(6)	22.666(2)	91.745(3)	570.05(7)
377.91	3.7700(2)	6.6996(5)	22.681(2)	91.678(4)	572.64(6)
396.43	3.7811(2)	6.6981(5)	22.696(2)	91.661(4)	574.57(7)
405.69	3.7872(2)	6.6962(5)	22.709(2)	91.648(4)	575.69(7)
387.17	3.7757(2)	6.6977(6)	22.694(2)	91.676(4)	573.67(7)
387.17	3.7742(3)	6.6986(10)	22.679(4)	91.608(7)	573.14(12)
382.54	3.7727(2)	6.7018(5)	22.677(2)	91.632(4)	573.13(7)
396.43	3.7798(3)	6.6981(6)	22.689(2)	91.628(5)	574.21(8)
401.06	3.7852(3)	6.6993(7)	22.701(3)	91.635(6)	575.43(9)

Table S5. Unit cell parameters of β form of pyrazinamide as a function of temperature

T /K	*a* /Å	*b* /Å	*c* /Å	*β* /°	*V* /Å^3
125	14.351(1)	3.6415(2)	10.6463(7)	101.278(5)	545.62(6)
150	14.353(3)	3.6531(5)	10.6635(21)	101.332(15)	548.23(17)
175	14.355(1)	3.6608(2)	10.6668(8)	101.434(5)	549.44(7)
200	14.357(1)	3.6720(2)	10.6824(8)	101.543(5)	551.81(7)
250	14.368(1)	3.6932(3)	10.7086(8)	101.777(6)	556.30(7)
273	14.371(1)	3.7036(3)	10.7190(8)	101.867(6)	558.34(7)
295	14.376(2)	3.7157(3)	10.7331(10)	102.006(6)	560.80(8)
320	14.378(2)	3.7257(3)	10.7425(9)	102.091(6)	562.72(7)

Table S6. Unit cell parameters of γ form of pyrazinamide as a function of temperature

T /K	a /Å	b /Å	c /Å	β /°	V /Å^3
100	7.1884(4)	3.6515(2)	10.6922(6)	106.580(4)	268.99(2)
125	7.1933(5)	3.6582(3)	10.7066(9)	106.654(6)	269.93(4)
150	7.1883(4)	3.6698(2)	10.7062(6)	106.626(4)	270.63(2)
175	7.1931(5)	3.6767(3)	10.7174(9)	106.699(6)	271.50(4)
200	7.1848(5)	3.6915(2)	10.7226(7)	106.656(5)	272.46(3)
225	7.1934(6)	3.6990(3)	10.7363(10)	106.740(6)	273.58(4)
250	7.1862(4)	3.7157(2)	10.7439(7)	106.716(4)	274.76(3)
275	7.1955(5)	3.7232(3)	10.7582(9)	106.792(6)	275.93(4)
297	7.1947(5)	3.7361(3)	10.7672(10)	106.804(6)	277.07(4)
300	7.1872(5)	3.7373(2)	10.7626(8)	106.778(5)	276.79(3)
325	7.1934(6)	3.7483(3)	10.7784(10)	106.870(6)	278.12(4)
350	7.1913(6)	3.7638(3)	10.7873(10)	106.834(6)	279.47(4)
373.28	7.1901(5)	3.7794(2)	10.7975(8)	106.903(5)	280.74(3)
396.43	7.1970(6)	3.7918(3)	10.8127(9)	106.970(5)	282.23(4)
419.58	7.2000(5)	3.8028(3)	10.8291(9)	107.014(5)	283.53(4)
419.58	7.2061(5)	3.8035(3)	10.8320(9)	107.035(5)	283.87(4)
424.21	7.2066(5)	3.8062(2)	10.8339(9)	107.059(5)	284.10(4)
428.84	7.2022(5)	3.8076(3)	10.8340(9)	107.051(5)	284.05(3)
433.47	7.2097(5)	3.8126(2)	10.8432(9)	107.111(5)	284.87(3)
442.73	7.2082(5)	3.8149(3)	10.8428(10)	107.129(5)	284.94(4)
461.25	7.2153(6)	3.8261(3)	10.8529(10)	107.201(5)	286.22(4)

Table S7. Unit cell parameters of δ form of pyrazinamide as a function of temperature

T /K	a /Å	b /Å	c /Å	α /°	β /°	γ /°	V /Å^3
100	5.1262(3)	5.7101(3)	9.8561(8)	97.471(5)	98.183(4)	106.477(4)	269.39(3)
150	5.1453(3)	5.7135(3)	9.8710(7)	97.409(5)	97.871(4)	106.444(4)	271.37(3)

200	5.1668(3)	5.7163(3)	9.8855(8)	97.348(5)	97.525(4)	106.389(4)	273.50(3)
250	5.1910(3)	5.7198(4)	9.9078(9)	97.244(6)	97.129(5)	106.314(4)	276.12(3)
295	5.2156(3)	5.7229(4)	9.9260(9)	97.176(6)	96.753(4)	106.232(5)	278.60(3)
300	5.2167(3)	5.7229(3)	9.9266(8)	97.192(6)	96.734(4)	106.238(4)	278.67(3)
315	5.2254(3)	5.7231(4)	9.9339(9)	97.171(6)	96.601(4)	106.207(5)	279.53(4)
325	5.2313(3)	5.7243(4)	9.9384(8)	97.112(6)	96.526(4)	106.177(5)	280.18(3)
335	5.2384(3)	5.7253(4)	9.9397(8)	97.105(6)	96.424(5)	106.164(4)	280.76(3)
350	5.2471(3)	5.7268(4)	9.9526(8)	97.070(6)	96.285(5)	106.136(5)	281.85(3)
364.02	5.2585(3)	5.7270(4)	9.9638(9)	97.046(6)	96.092(8)	106.104(4)	283.01(4)
368.65	5.2613(4)	5.7248(5)	9.9608(9)	96.942(5)	96.112(6)	106.131(6)	282.99(4)

Unit cell parameters of polymorphs α, β, γ, and δ of pyrazinamide as a function of pressure for various temperatures

Table S8a. Unit cell parameters of form α at 295 K as a function of pressure

P /MPa	a /Å	b /Å	c /Å	β /°	V /Å^3
17	3.7128(3)	6.7125(5)	22.610(3)	91.848(10)	563.18(8)
16	3.7120(2)	6.7109(5)	22.604(3)	91.851(9)	562.78(7)
19	3.7114(2)	6.7107(4)	22.601(3)	91.851(9)	562.60(7)
22	3.7103(2)	6.7108(4)	22.597(2)	91.859(9)	562.36(7)
26	3.7091(2)	6.7108(5)	22.595(3)	91.865(9)	562.10(7)
31	3.7079(3)	6.7107(5)	22.593(3)	91.864(10)	561.87(8)
36	3.7062(3)	6.7109(5)	22.592(3)	91.886(10)	561.59(7)
41	3.7050(3)	6.7109(5)	22.589(3)	91.884(11)	561.35(8)
47	3.7032(3)	6.7110(3)	22.587(2)	91.889(11)	561.05(7)
60	3.7007(3)	6.7096(6)	22.583(3)	91.865(14)	560.44(9)
70	3.6979(3)	6.7093(6)	22.580(3)	91.878(15)	559.92(9)
80	3.6953(4)	6.7091(6)	22.576(3)	91.882(16)	559.41(10)
93	3.6921(4)	6.7094(6)	22.571(3)	91.894(18)	558.81(11)
108	3.6889(3)	6.7100(6)	22.563(3)	91.891(16)	558.18(10)
124	3.6841(3)	6.7102(6)	22.556(3)	91.856(16)	557.30(9)
139	3.6798(4)	6.7092(6)	22.552(3)	91.870(15)	556.47(10)
155	3.6759(4)	6.7091(6)	22.545(3)	91.885(14)	555.70(10)
174	3.6722(4)	6.7085(7)	22.541(3)	91.903(14)	554.98(11)
193	3.6688(4)	6.7081(7)	22.535(3)	91.924(15)	554.29(11)
222	3.6616(4)	6.7073(8)	22.529(4)	91.967(16)	552.99(12)
255	3.6552(4)	6.7087(7)	22.517(4)	92.023(17)	551.79(11)
286	3.6499(4)	6.7088(8)	22.506(4)	92.040(17)	550.74(12)
318	3.6440(4)	6.7074(8)	22.498(4)	92.073(16)	549.54(12)
341	3.6400(5)	6.7072(8)	22.490(4)	92.092(15)	548.71(13)
363	3.6332(5)	6.7119(8)	22.466(4)	92.050(19)	547.51(12)
386	3.6296(5)	6.7112(8)	22.460(4)	92.074(19)	546.74(13)
407	3.6257(5)	6.7110(8)	22.455(4)	92.099(19)	546.00(13)
428	3.6222(5)	6.7108(8)	22.448(4)	92.143(18)	545.27(13)
451	3.6182(5)	6.7108(8)	22.439(4)	92.171(20)	544.46(13)
471	3.6146(5)	6.7105(8)	22.437(4)	92.212(19)	543.81(13)
492	3.6115(5)	6.7104(9)	22.430(4)	92.252(21)	543.15(14)
512	3.6081(5)	6.7104(9)	22.425(5)	92.282(21)	542.52(14)
533	3.6049(5)	6.7099(9)	22.422(5)	92.313(21)	541.90(15)
554	3.6016(5)	6.7094(9)	22.416(5)	92.339(21)	541.21(15)

573	3.5986(5)	6.7095(9)	22.407(5)	92.342(20)	540.55(15)
594	3.5955(5)	6.7089(9)	22.403(4)	92.359(21)	539.94(14)
613	3.5923(6)	6.7086(9)	22.396(5)	92.352(23)	539.27(15)
633	3.5894(6)	6.7084(9)	22.390(5)	92.357(23)	538.69(15)
654	3.5867(5)	6.7077(10)	22.385(5)	92.359(24)	538.07(15)
673	3.5835(6)	6.7065(10)	22.384(5)	92.358(21)	537.49(15)
691	3.5811(6)	6.7061(10)	22.380(5)	92.370(26)	536.99(16)
708	3.5788(5)	6.7053(10)	22.375(5)	92.375(27)	536.48(16)
728	3.5756(6)	6.7047(10)	22.370(5)	92.390(24)	535.82(16)
747	3.5706(7)	6.7073(10)	22.351(5)	92.561(30)	534.76(17)
764	3.5681(6)	6.7066(10)	22.348(5)	92.564(28)	534.25(16)
782	3.5659(7)	6.7061(10)	22.340(5)	92.562(26)	533.69(17)
799	3.5640(6)	6.7055(10)	22.336(5)	92.576(25)	533.25(17)
817	3.5618(8)	6.7051(11)	22.326(6)	92.581(34)	532.66(19)
835	3.5591(8)	6.7042(11)	22.321(5)	92.612(34)	532.04(19)
852	3.5563(8)	6.7037(11)	22.313(6)	92.636(33)	531.39(19)
871	3.5532(9)	6.7043(12)	22.304(6)	92.687(33)	530.72(20)
887	3.5509(8)	6.7041(11)	22.295(6)	92.713(33)	530.16(19)
903	3.5495(9)	6.7032(12)	22.291(6)	92.735(33)	529.77(21)
939	3.5464(10)	6.7010(12)	22.281(6)	92.753(35)	528.89(21)
979	3.5387(11)	6.6986(12)	22.267(6)	92.821(34)	527.17(22)
1018	3.5359(11)	6.6960(13)	22.256(6)	92.841(35)	526.28(22)
1059	3.5333(12)	6.6932(13)	22.251(6)	92.879(42)	525.53(24)
1135	3.5273(14)	6.6882(14)	22.232(7)	92.950(56)	523.79(28)
1209	3.5227(16)	6.6837(15)	22.207(8)	92.925(69)	522.17(31)
1317	3.5067(17)	6.6751(16)	22.187(8)	92.751(72)	518.73(33)
1420	3.4981(18)	6.6698(16)	22.161(8)	92.620(80)	516.50(33)
1514	3.4921(20)	6.6656(17)	22.136(8)	92.663(88)	514.69(37)
1603	3.4870(21)	6.6614(17)	22.109(9)	92.648(94)	513.02(38)
1688	3.4813(25)	6.6551(18)	22.093(9)	92.59(11)	511.32(44)
1776	3.4777(26)	6.6507(18)	22.062(9)	92.51(12)	509.78(45)
1864	3.4697(26)	6.6419(19)	22.051(9)	92.52(12)	507.67(45)
1950	3.4662(27)	6.6362(19)	22.038(10)	92.53(14)	506.44(47)
2065	3.4609(26)	6.6220(20)	22.037(9)	92.59(15)	504.52(46)

Table S8b. Unit cell parameters of form α at 367 K as a function of pressure

P /MPa	a /Å	b /Å	c /Å	β /°	V /Å^3
1(1)	3.73840(16)	6.7318(4)	22.707(2)	91.810(7)	571.18(7)
2(1)	3.73886(16)	6.7314(4)	22.707(2)	91.807(7)	571.21(7)
18(1)	3.73464(15)	6.7305(4)	22.702(2)	91.814(7)	570.36(7)
33(1)	3.73099(16)	6.7294(4)	22.696(2)	91.809(7)	569.55(7)
53(1)	3.72609(17)	6.7281(4)	22.689(2)	91.814(8)	568.52(7)
72(1)	3.7209(2)	6.7275(5)	22.678(3)	91.823(9)	567.41(8)
97(2)	3.7144(3)	6.7262(5)	22.670(3)	91.817(11)	566.12(8)

120(1)	3.7081(3)	6.7260(5)	22.658(3)	91.798(14)	564.83(8)
146(2)	3.7021(3)	6.7257(5)	22.646(3)	91.790(16)	563.61(9)
178(1)	3.6917(3)	6.7264(5)	22.627(4)	91.652(15)	561.65(9)
203(2)	3.6876(5)	6.7258(7)	22.617(4)	91.692(19)	560.71(12)
233(2)	3.6824(5)	6.7250(8)	22.607(4)	91.739(19)	559.58(13)
260(2)	3.6780(5)	6.7237(8)	22.601(4)	91.759(18)	558.66(13)
296(2)	3.6685(4)	6.7229(8)	22.594(4)	91.797(19)	556.95(14)
323(2)	3.6636(5)	6.7227(8)	22.583(5)	91.86(2)	555.90(15)
347(2)	3.6590(5)	6.7224(10)	22.573(5)	91.88(2)	554.94(16)
365(2)	3.6559(5)	6.7218(10)	22.570(5)	91.87(2)	554.33(17)
392(3)	3.6514(6)	6.7226(12)	22.560(6)	91.92(3)	553.47(18)
417(3)	3.6452(5)	6.7255(9)	22.539(5)	91.84(3)	552.26(15)
439(2)	3.6406(6)	6.7256(10)	22.525(5)	91.74(3)	551.27(17)
457(2)	3.6365(6)	6.7252(9)	22.518(5)	91.68(3)	550.48(16)
479(3)	3.6333(6)	6.7247(11)	22.514(6)	91.77(3)	549.83(18)
496(3)	3.6302(7)	6.7240(12)	22.512(6)	91.77(3)	549.25(20)
511(2)	3.6286(6)	6.7234(11)	22.508(6)	91.80(3)	548.82(18)
525(3)	3.6261(6)	6.7230(12)	22.503(6)	91.81(3)	548.31(20)
541(3)	3.6246(6)	6.7247(12)	22.490(6)	92.03(3)	547.84(19)
557(3)	3.6225(6)	6.7244(12)	22.487(6)	92.08(3)	547.40(19)
574(3)	3.6196(5)	6.7241(12)	22.482(6)	92.093(19)	546.82(18)
588(3)	3.6164(5)	6.7217(13)	22.479(6)	92.06(3)	546.08(19)
601(3)	3.6144(6)	6.7214(13)	22.476(6)	92.07(3)	545.67(20)
616(3)	3.6123(6)	6.7212(13)	22.475(7)	92.10(3)	545.3(2)
631(2)	3.6105(6)	6.7222(13)	22.464(7)	92.18(3)	544.8(2)
646(3)	3.6082(6)	6.7218(13)	22.458(6)	92.20(3)	544.30(20)
665(3)	3.6058(6)	6.7219(13)	22.452(6)	92.23(3)	543.77(20)
697(3)	3.6000(6)	6.7196(12)	22.450(6)	92.22(3)	542.66(20)
713(3)	3.5982(6)	6.7192(13)	22.446(7)	92.25(3)	542.3(2)
726(3)	3.5947(6)	6.7199(13)	22.440(7)	92.26(3)	541.6(2)
743(3)	3.5936(7)	6.7187(14)	22.438(6)	92.26(3)	541.3(2)
757(3)	3.5909(5)	6.7180(14)	22.433(7)	92.25(3)	540.8(2)
769(3)	3.5889(7)	6.7194(14)	22.422(7)	92.28(4)	540.3(2)
783(3)	3.5867(7)	6.7179(13)	22.419(7)	92.28(3)	539.8(2)
804(3)	3.5824(6)	6.7182(11)	22.408(6)	92.26(4)	538.88(18)
827(3)	3.5798(8)	6.7178(15)	22.398(7)	92.23(4)	538.2(3)
846(3)	3.5770(8)	6.7169(15)	22.388(7)	92.27(4)	537.5(3)
871(3)	3.5699(11)	6.7186(15)	22.364(8)	92.36(5)	535.9(3)
924(3)	3.5622(13)	6.7154(13)	22.338(7)	92.39(6)	533.9(3)
982(3)	3.5579(13)	6.7131(16)	22.315(8)	92.58(6)	532.6(3)
1039(3)	3.5537(13)	6.7089(17)	22.298(9)	92.70(5)	531.0(3)
94(2)[a]	3.7124(3)	6.7262(7)	22.656(3)	91.818(13)	565.46(10)

[a] Obtained on releasing the pressure.

Table S8c. Unit cell parameters of form α at 427 K as a function of pressure

P /MPa	a /Å	b /Å	c /Å	β /°	V /Å^3
19(2)	3.78835(19)	6.7206(5)	22.7705(20)	91.708(8)	579.48(7)
4(1)	3.78694(19)	6.7220(5)	22.768(3)	91.715(7)	579.32(8)
2(1)	3.78767(18)	6.7221(5)	22.769(3)	91.718(7)	579.46(8)
2(1)	3.78771(19)	6.7217(5)	22.771(3)	91.716(7)	579.48(9)
2(1)	3.78784(18)	6.7219(5)	22.769(3)	91.719(7)	579.47(8)
2(1)	3.78789(19)	6.7219(5)	22.769(3)	91.719(7)	579.49(8)
3(1)	3.78784(18)	6.7219(5)	22.770(3)	91.720(7)	579.49(8)
2(1)	3.78796(18)	6.7219(5)	22.771(3)	91.720(7)	579.53(8)
5(1)	3.78723(18)	6.7228(5)	22.772(3)	91.725(7)	579.54(8)
5(1)	3.78701(15)	6.7228(5)	22.774(3)	91.728(7)	579.56(8)
11(1)	3.7854(18)	6.7232(5)	22.771(3)	91.736(7)	579.25(8)
12(1)	3.78487(18)	6.7228(5)	22.772(3)	91.738(7)	579.16(8)
19(1)	3.78202(14)	6.7221(5)	22.770(3)	91.733(7)	578.62(8)
21(1)	3.78113(18)	6.7218(5)	22.768(3)	91.734(7)	578.41(9)
34(1)	3.77666(16)	6.7207(4)	22.763(3)	91.718(8)	577.50(7)
46(1)	3.7718(2)	6.7198(5)	22.754(3)	91.702(8)	576.46(9)
61(1)	3.7671(2)	6.7190(5)	22.746(3)	91.678(8)	575.48(9)
76(1)	3.7622(3)	6.7186(6)	22.737(3)	91.656(9)	574.46(9)
102(1)	3.7526(3)	6.7174(6)	22.726(3)	91.633(10)	572.63(9)
136(1)	3.7419(3)	6.7178(6)	22.707(3)	91.643(11)	570.55(10)
179(1)	3.7302(3)	6.7175(6)	22.686(4)	91.650(14)	568.21(11)
227(1)	3.7188(5)	6.7154(7)	22.669(4)	91.656(19)	565.87(13)
286(1)	3.7061(6)	6.7121(8)	22.652(4)	91.66(3)	563.26(15)
340(1)	3.6953(8)	6.7100(8)	22.632(4)	91.64(2)	560.94(17)
398(1)	3.6820(8)	6.7071(10)	22.614(5)	91.61(3)	558.26(19)
460(1)	3.6717(9)	6.7044(11)	22.590(5)	91.63(3)	555.9(2)
523(2)	3.6582(8)	6.7032(12)	22.571(6)	91.66(3)	553.2(2)
590(2)	3.6472(6)	6.7040(10)	22.545(5)	91.69(4)	551.0(2)
656(2)	3.6364(9)	6.7039(15)	22.523(8)	91.67(4)	548.8(3)
740(2)	3.6215(6)	6.7059(15)	22.491(8)	91.67(4)	546.0(3)
838(2)	3.6062(10)	6.7026(16)	22.472(8)	91.76(5)	542.9(3)
953(2)	3.5875(12)	6.6989(18)	22.439(9)	91.88(6)	539.0(3)
1060(2)	3.5636(18)	6.7002(18)	22.374(8)	92.13(6)	533.9(4)
1202(2)	3.5349(16)	6.6936(19)	22.338(10)	92.65(8)	528.0(4)
1371(2)	3.5214(20)	6.681(3)	22.292(12)	92.87(10)	523.8(5)

Table S8d. Unit cell parameters of form α at 460 K as a function of pressure

P /MPa	a /Å	b /Å	c /Å	β /°	V /Å^3
2(1)	3.8169(3)	6.7274(6)	22.834(3)	91.742(10)	586.06(11)
1(1)	3.8172(3)	6.7275(6)	22.834(3)	91.741(9)	586.12(10)
1(1)	3.8173(3)	6.7274(6)	22.834(3)	91.741(10)	586.12(11)

1(1)	3.8174(3)	6.7274(6)	22.835(3)	91.737(9)	586.14(10)
2(1)	3.8173(3)	6.7273(6)	22.834(3)	91.732(9)	586.10(10)
3(1)	3.8172(3)	6.7273(6)	22.833(3)	91.734(9)	586.08(10)
5(1)	3.8172(3)	6.7275(6)	22.834(3)	91.746(9)	586.12(10)
9(1)	3.8149(3)	6.7284(6)	22.827(3)	91.736(10)	585.67(10)
18(1)	3.8084(3)	6.7265(7)	22.826(4)	91.711(11)	584.49(12)
35(1)	3.7991(3)	6.7271(7)	22.808(4)	91.772(12)	582.63(12)
54(1)	3.7936(4)	6.7254(8)	22.802(4)	91.776(12)	581.47(13)
57(1)	3.7948(3)	6.7239(7)	22.798(4)	91.760(11)	581.45(12)
117(1)	3.7804(4)	6.7202(8)	22.770(4)	91.748(13)	578.20(13)
188(1)	3.7625(4)	6.7152(8)	22.744(4)	91.680(13)	574.40(12)
269(1)	3.7424(4)	6.7099(7)	22.714(4)	91.656(12)	570.14(12)
330(1)	3.7274(3)	6.7074(7)	22.688(4)	91.659(15)	566.99(12)
2(1)	3.8148(3)	6.7288(7)	22.832(4)	91.748(10)	585.81(11)
2(1)	3.8156(3)	6.7287(7)	22.833(4)	91.744(10)	585.95(11)
6(1)	3.8142(3)	6.7277(6)	22.830(3)	91.725(9)	585.57(10)
11(1)	3.8071(3)	6.7242(7)	22.827(3)	91.708(10)	584.09(11)
200(1)	3.7594(3)	6.7117(6)	22.740(4)	91.598(12)	573.56(11)
262(1)	3.7452(3)	6.7087(7)	22.713(4)	91.615(12)	570.44(12)
318(1)	3.7340(4)	6.7070(7)	22.684(4)	91.616(14)	567.86(13)
359(1)	3.7226(5)	6.7055(8)	22.666(4)	91.638(16)	565.55(14)
400(1)	3.7136(5)	6.7038(8)	22.650(4)	91.639(16)	563.64(14)
445(1)	3.7034(7)	6.7011(8)	22.632(5)	91.65(3)	561.44(16)
486(1)	3.6940(9)	6.6984(9)	22.621(5)	91.66(3)	559.49(19)
529(2)	3.6854(10)	6.6939(11)	22.611(6)	91.66(3)	557.6(3)
578(2)	3.6760(9)	6.6959(13)	22.575(7)	91.63(3)	555.4(3)
628(2)	3.6684(10)	6.6927(14)	22.559(7)	91.66(4)	553.6(3)
674(2)	3.6582(12)	6.6880(15)	22.549(8)	91.66(4)	551.5(3)
769(2)	3.6386(9)	6.6917(16)	22.509(8)	91.70(5)	547.8(3)
857(2)	3.6263(14)	6.6901(16)	22.484(9)	91.66(5)	545.2(3)
928(2)	3.6126(16)	6.6912(17)	22.449(9)	91.70(7)	542.4(4)
1012(2)	3.6045(18)	6.6897(19)	22.412(9)	91.75(9)	540.2(4)
1091(2)	3.5970(8)	6.6870(20)	22.391(9)	91.74(9)	538.3(3)
1249(2)	3.5829(17)	6.6804(19)	22.340(10)	92.00(9)	534.4(4)
3(1)[a]	3.8146(4)	6.7276(7)	22.830(4)	91.777(12)	585.62(12)

[a] Obtained on releasing the pressure.

Table S9a. Unit cell parameters of form β at 295 K as a function of pressure[a]

P /MPa	a /Å	b /Å	c /Å	β /°	V /Å^3
24(8)	14.360(3)	3.7102(3)	10.7225(9)	101.927(10)	558.94(13)
84(9)	14.356(4)	3.7086(4)	10.7229(11)	101.949(12)	558.53(16)
85(11)	14.375(5)	3.7055(5)	10.720(2)	101.94(3)	558.7(3)
144(8)	14.373(5)	3.6995(4)	10.722(3)	101.91(3)	557.8(3)
147(9)	14.370(5)	3.6937(6)	10.724(2)	101.96(3)	556.9(3)
206(9)	14.358(5)	3.6858(8)	10.719(3)	101.94(3)	555.0(3)

208(9)	14.347(6)	3.6770(13)	10.703(3)	101.73(4)	552.8(4)
271(10)	14.326(6)	3.6662(13)	10.708(5)	101.70(6)	550.7(4)
334(12)	14.329(9)	3.6478(13)	10.676(13)	101.36(10)	547.1(8)
403(22)	14.318(9)	3.6313(12)	10.661(7)	101.41(4)	543.3(5)
530(16)	14.298(9)	3.6183(9)	10.648(11)	101.30(9)	540.2(7)
598(20)	14.282(9)	3.6047(11)	10.637(15)	101.22(10)	537.2(9)
700(21)	14.280(8)	3.5904(13)	10.617(16)	101.12(9)	534.1(9)
802(27)	14.274(7)	3.5786(15)	10.589(9)	101.06(9)	530.9(6)
877(28)	14.262(7)	3.5684(14)	10.570(10)	100.95(10)	528.1(6)
943(38)	14.240(11)	3.560(2)	10.564(17)	100.8(2)	526.0(1.0)
1019(60)	14.239(9)	3.5544(12)	10.55(2)	100.84(16)	524.6(1.2)
1233(37)	14.24(2)	3.531(3)	10.54(4)	100.7(4)	521(2)
1622(27)	14.223(13)	3.521(4)	10.50(3)	100.9(3)	516.6(1.4)

[a] The interpretation of the unit-cell parameters of the β form have been more complicated due to the presence of the γ form.

Table S9b. Unit cell parameters of form β at 348 K as a function of pressure[a]

P /MPa	a /Å	b /Å	c /Å	β /°	V /Å^3
206(23)	14.454(6)	3.677(3)	10.710(5)	101.71(7)	557.4(6)
236(18)	14.443(6)	3.671(3)	10.708(5)	101.59(7)	556.2(6)
329(15)	14.420(5)	3.661(4)	10.689(5)	101.45(7)	553.1(6)
430(17)	14.404(7)	3.654(4)	10.672(7)	101.45(11)	550.5(8)
524(18)	14.394(7)	3.6383(19)	10.658(8)	101.39(9)	547.2(6)
590(17)	14.392(9)	3.632(6)	10.651(10)	101.38(14)	545.8(1.1)
657(19)	14.379(7)	3.620(4)	10.642(8)	101.36(9)	543.0(7)
793(23)	14.336(6)	3.5900(14)	10.627(8)	101.29(8)	536.4(5)
869(17)	14.318(6)	3.5816(16)	10.618(6)	101.32(7)	533.9(5)
1003(20)	14.278(7)	3.572(2)	10.601(10)	101.21(9)	530.4(7)
1079(18)	14.290(11)	3.560(4)	10.585(12)	101.0(2)	528.4(1.0)
1219(19)	14.288(7)	3.5532(12)	10.576(12)	101.08(10)	526.9(7)
332(12)[b]	14.412(6)	3.660(3)	10.676(6)	101.39(8)	552.1(6)

[a] The interpretation of the unit-cell parameters of the β form have been more complicated due to the presence of form γ.
[b] Obtained on releasing the pressure.

Table S9c. Unit cell parameters of form β at 396 K as a function of pressure[a]

P /MPa	a /Å	b /Å	c /Å	β /°	V /Å^3
173(3)	14.504(7)	3.6882(19)	10.758(5)	101.71(7)	563.5(5)
295(4)	14.479(6)	3.6778(13)	10.735(5)	101.66(7)	559.8(5)
424(5)	14.458(7)	3.660(3)	10.716(6)	101.68(9)	555.4(6)
554(4)	14.456(7)	3.647(4)	10.697(7)	101.59(9)	552.4(7)
620(4)	14.452(4)	3.620(2)	10.682(5)	101.55(6)	547.5(5)
687(6)	14.428(4)	3.609(2)	10.674(6)	101.57(7)	544.4(4)

754(5)	14.405(5)	3.601(2)	10.665(6)	101.56(7)	542.0(4)
826(5)	14.357(6)	3.590(3)	10.643(8)	101.38(8)	537.8(7)
962(5)	14.324(6)	3.581(5)	10.630(7)	101.40(7)	534.5(8)
1036(5)	14.298(8)	3.574(7)	10.621(11)	101.48(11)	531.8(1.2)
1250(6)	14.273(14)	3.565(3)	10.601(16)	101.39(18)	528.8(1.1)
1402(5)	14.298(12)	3.563(4)	10.597(8)	101.66(8)	528.6(8)

[a] The interpretation of the unit-cell parameters of the β form have been more complicated due to the presence of the γ form.

Table S10a. Unit cell parameters of form γ at 295 K as a function of pressure

P /MPa	*a* /Å	*b* /Å	*c* /Å	*β* /°	*V* /Å^3
209(6)	7.1858(8)	3.6998(3)	10.7220(6)	106.649(8)	273.10(4)
223(7)	7.1847(8)	3.6986(3)	10.7203(6)	106.638(9)	272.95(4)
403(8)	7.1738(13)	3.6689(4)	10.6949(8)	106.650(12)	269.68(6)
516(9)	7.1778(13)	3.6461(6)	10.6780(8)	106.656(13)	267.73(7)
604(9)	7.1797(12)	3.6294(6)	10.6662(9)	106.623(13)	266.33(7)
684(8)	7.1747(10)	3.6168(5)	10.6580(8)	106.678(12)	264.94(6)
812(8)	7.1615(9)	3.5978(5)	10.6439(8)	106.719(8)	262.66(5)
924(8)	7.1544(9)	3.5839(4)	10.6306(8)	106.717(12)	261.06(5)
1027(9)	7.1497(10)	3.5710(4)	10.6171(9)	106.715(12)	259.62(5)
1124(9)	7.1433(11)	3.5600(4)	10.6049(9)	106.698(13)	258.32(6)
1271(9)	7.1414(13)	3.5437(5)	10.5850(10)	106.648(15)	256.64(7)
1434(10)	7.1424(13)	3.5263(5)	10.5640(10)	106.557(15)	255.03(7)
1620(10	7.1509(17)	3.5048(7)	10.5440(11)	106.557(18)	253.30(9)
1849(10	7.1529(17)	3.4796(7)	10.5213(11)	106.548(18)	251.03(9)

Table S10b. Unit cell parameters of form γ at 324 K as a function of pressure

P /MPa	*a* /Å	*b* /Å	*c* /Å	*β* /°	*V* /Å^3
307(8)	7.1836(10)	3.6796(5)	10.7187(7)	106.722(10)	271.35(6)
438(8)	7.1796(10)	3.6628(4)	10.7033(6)	106.720(9)	269.57(5)
652(8)	7.1803(8)	3.6308(3)	10.6775(6)	106.703(9)	266.62(4)
788(9)	7.1727(8)	3.6134(3)	10.6627(6)	106.718(9)	264.68(4)
889(17)	7.1679(12)	3.6013(4)	10.6515(18)	106.718(9)	263.33(7)
972(9)	7.1635(8)	3.5913(3)	10.6417(7)	106.722(9)	262.19(4)
1048(10)	7.1584(9)	3.5816(3)	10.6321(7)	106.734(10)	261.05(4)
1170(10)	7.1506(10)	3.5676(3)	10.6188(8)	106.735(11)	259.42(5)
1279(11)	7.1444(12)	3.5550(4)	10.6042(8)	106.724(12)	257.94(6)
1387(12)	7.1400(12)	3.5440(4)	10.5912(9)	106.695(13)	256.71(6)
1491(13)	7.1414(13)	3.5326(4)	10.5780(9)	106.671(13)	255.64(6)
1595(14)	7.1461(15)	3.5217(5)	10.5652(10)	106.615(16)	254.79(8)
1751(14)	7.1528(18)	3.5042(7)	10.5477(11)	106.608(17)	253.35(9)
1917(14)	7.1585(9)	3.4844(6)	10.5323(11)	106.614(16)	251.74(6)

Table S10c. Unit cell parameters of form γ at 381 K as a function of pressure

P /MPa	a /Å	b /Å	c /Å	β /°	V /Å^3
190(8)	7.1939(9)	3.7451(3)	10.7751(8)	106.775(10)	277.94(5)
310(7)	7.1940(9)	3.7229(3)	10.7543(6)	106.751(9)	275.80(5)
609(7)	7.1785(12)	3.6738(5)	10.7091(8)	106.728(12)	270.48(6)
762(7)	7.1851(13)	3.6438(6)	10.6860(8)	106.733(13)	267.92(7)
867(7)	7.1814(11)	3.6244(6)	10.6721(8)	106.737(13)	266.01(7)
953(7)	7.1732(10)	3.6110(4)	10.6604(8)	106.737(12)	264.44(6)
1022(7)	7.1678(9)	3.6011(5)	10.6504(8)	106.763(12)	263.23(6)
1093(8)	7.1619(11)	3.5920(5)	10.6411(8)	106.783(12)	262.08(6)
1214(8)	7.1500(11)	3.5759(5)	10.625(9)	106.790(13)	260.08(6)
1326(9)	7.1421(13)	3.5625(5)	10.6101(10)	106.776(14)	258.47(6)
1429(9)	7.1376(13)	3.5515(5)	10.5954(10)	106.732(14)	257.21(7)
1531(10)	7.1352(15)	3.5400(4)	10.5799(11)	106.702(16)	255.96(7)
1628(10)	7.1412(17)	3.5295(5)	10.5654(11)	106.634(17)	255.16(8)

Table S10d. Unit cell parameters of form γ at 428 K as a function of pressure

P /MPa	a /Å	b /Å	c /Å	β /°	V /Å^3
89(6)	7.1999(7)	3.7945(2)	10.8208(5)	106.977(7)	282.75(4)
88(6)	7.2016(7)	3.7928(2)	10.8187(5)	106.971(6)	282.64(4)
153(7)	7.1996(7)	3.7749(2)	10.8029(5)	106.941(7)	280.86(4)
375(9)	7.1972(9)	3.7301(3)	10.7632(7)	106.866(9)	276.52(5)
499(9)	7.1935(9)	3.7069(4)	10.7404(8)	106.831(9)	274.13(5)
580(9)	7.1872(11)	3.6927(4)	10.7274(8)	106.828(12)	272.51(6)
647(9)	7.1838(11)	3.6808(5)	10.7166(8)	106.845(11)	271.20(6)
739(9)	7.1849(15)	3.6611(7)	10.7010(9)	106.859(14)	269.39(8)
816(10)	7.1915(14)	3.6416(6)	10.6891(9)	106.852(14)	267.91(7)
885(10)	7.1869(14)	3.6305(8)	10.6780(10)	106.860(15)	266.64(8)
1012(9)	7.1778(11)	3.6086(6)	10.6607(9)	106.858(12)	264.26(7)
1121(9)	7.1695(12)	3.5934(6)	10.6454(10)	106.874(14)	262.45(7)
1231(10)	7.1590(11)	3.5796(5)	10.6310(9)	106.874(13)	260.71(6)
1335(10)	7.1482(14)	3.5667(5)	10.6186(10)	106.872(15)	259.07(7)
1436(10)	7.1396(12)	3.5549(4)	10.6041(10)	106.856(15)	257.58(6)
1556(11)	7.1358(17)	3.5434(5)	10.5877(11)	106.798(17)	256.28(8)

Table S11a. Unit cell parameters of form δ at 295 K as a function of pressure

P /MPa	a /Å	b /Å	c /Å	α /°	β /°	γ /°	V /Å^3
13(3)	5.2132(5)	5.7186(4)	9.9296(14)	97.175(12)	96.683(12)	106.251(11)	278.39(6)
18(3)	5.2124(5)	5.7184(4)	9.9277(13)	97.164(12)	96.706(10)	106.249(10)	278.28(5)
16(3)	5.2119(5)	5.7181(4)	9.9276(13)	97.153(13)	96.710(11)	106.252(11)	278.23(6)
17(3)	5.2112(5)	5.7184(4)	9.9283(12)	97.177(11)	96.710(9)	106.250(10)	278.21(5)
17(3)	5.2110(5)	5.7184(4)	9.9280(12)	97.178(11)	96.713(9)	106.249(9)	278.19(5)
22(3)	5.2110(5)	5.7182(4)	9.9281(12)	97.174(11)	96.715(9)	106.251(10)	278.18(5)

29(3)	5.2102(5)	5.7178(4)	9.9282(13)	97.172(11)	96.722(10)	106.254(10)	278.12(5)
16(3)	5.2117(6)	5.7172(4)	9.9235(15)	97.158(13)	96.728(12)	106.251(11)	278.05(6)
15(3)	5.2112(6)	5.7163(5)	9.9213(18)	97.159(15)	96.713(15)	106.253(13)	277.93(7)
16(3)	5.2114(7)	5.7152(5)	9.9188(18)	97.167(17)	96.714(15)	106.249(15)	277.81(8)
22(3)	5.2096(8)	5.7143(5)	9.917(2)	97.153(16)	96.723(17)	106.261(15)	277.60(8)
29(3)	5.2090(8)	5.7134(6)	9.913(3)	97.146(18)	96.73(2)	106.270(17)	277.40(9)
32(3)	5.2077(9)	5.7119(6)	9.908(3)	97.150(19)	96.74(2)	106.271(16)	277.11(10)
50(3)	5.2045(8)	5.7093(6)	9.898(3)	97.12(2)	96.83(2)	106.277(17)	276.49(10)
79(3)	5.1972(9)	5.7071(7)	9.876(4)	97.098(19)	97.01(3)	106.323(18)	275.16(12)
117(2)	5.1860(9)	5.7028(7)	9.865(4)	97.07(2)	97.17(3)	106.390(19)	273.84(13)
164(2)	5.1776(9)	5.6960(7)	9.835(4)	97.09(2)	97.40(3)	106.306(19)	272.15(12)
218(2)	5.1668(9)	5.6899(7)	9.817(3)	97.063(18)	97.57(2)	106.335(19)	270.64(11)
274(2)	5.1562(10)	5.6838(7)	9.796(3)	97.04(2)	97.74(2)	106.362(19)	269.06(11)
327(3)	5.1473(10)	5.6781(7)	9.781(3)	97.02(2)	97.896(18)	106.377(19)	267.73(11)
382(3)	5.1383(10)	5.6722(7)	9.762(3)	97.02(2)	98.036(16)	106.39(2)	266.34(10)
440(3)	5.1278(10)	5.6675(7)	9.751(3)	97.03(2)	98.184(15)	106.443(19)	265.05(10)
500(4)	5.1196(10)	5.6622(7)	9.737(3)	97.02(2)	98.302(14)	106.451(18)	263.88(10)
631(4)	5.1045(11)	5.6499(8)	9.706(3)	97.01(3)	98.530(14)	106.38(2)	261.59(11)
785(5)	5.0887(12)	5.6402(8)	9.675(3)	97.06(3)	98.762(15)	106.38(3)	259.24(12)
1079(5)	5.0622(15)	5.6213(9)	9.616(3)	97.10(3)	99.187(15)	106.39(3)	255.02(13)
1079(5)	5.0624(15)	5.6213(9)	9.616(3)	97.10(3)	99.184(14)	106.39(3)	255.03(13)
1216(4)	5.0498(17)	5.6127(10)	9.593(4)	97.16(4)	99.371(15)	106.37(3)	253.17(15)
1369(4)	5.0347(16)	5.6034(10)	9.576(3)	97.25(3)	99.540(15)	106.30(3)	251.42(14)
1511(6)	5.022(2)	5.5952(11)	9.559(4)	97.24(3)	99.721(15)	106.29(3)	249.79(17)
1647(4)	5.006(3)	5.5878(11)	9.545(4)	97.25(3)	99.875(16)	106.28(3)	248.18(18)

Table S11b. Unit cell parameters of form δ at 323 K as a function of pressure

P /MPa	a /Å	b /Å	c /Å	α /°	β /°	γ /°	V /Å^3
26(4)	5.2270(10)	5.7105(9)	9.939(3)	97.42(3)	96.430(18)	106.10(3)	279.21(12)
28(4)	5.2287(10)	5.7106(8)	9.934(4)	97.46(3)	96.41(2)	106.08(3)	279.18(12)
37(4)	5.2280(9)	5.7110(9)	9.920(3)	97.48(2)	96.494(19)	106.11(3)	278.65(12)
54(4)	5.2271(10)	5.7074(7)	9.924(2)	97.474(19)	96.451(13)	106.09(2)	278.62(9)
104(4)	5.2165(9)	5.7005(7)	9.900(3)	97.38(2)	96.613(16)	106.15(2)	276.90(10)
220(5)	5.1912(17)	5.6886(15)	9.845(2)	97.41(3)	97.10(2)	106.15(5)	273.01(16)
323(4)	5.1745(14)	5.6769(13)	9.804(3)	97.37(3)	97.406(17)	106.12(5)	270.28(15)
407(5)	5.1624(17)	5.6716(16)	9.775(3)	97.18(3)	97.670(17)	106.25(6)	268.32(17)
471(5)	5.1525(18)	5.6632(16)	9.749(3)	97.29(3)	97.811(15)	106.14(5)	266.65(17)
530(5)	5.1448(19)	5.6591(17)	9.731(4)	97.28(3)	97.942(16)	106.17(5)	265.41(18)
576(5)	5.1380(16)	5.6548(14)	9.721(3)	97.28(3)	98.042(14)	106.18(5)	264.48(15)
664(5)	5.1284(19)	5.6498(16)	9.698(4)	97.07(3)	98.270(17)	106.35(6)	262.86(18)
743(5)	5.116(2)	5.642(2)	9.682(3)	97.26(3)	98.378(19)	106.23(7)	261.3(2)
899(5)	5.097(2)	5.6322(16)	9.652(4)	97.11(3)	98.688(18)	106.35(6)	258.77(19)
1069(5)	5.0798(19)	5.6212(16)	9.620(4)	97.14(3)	98.961(14)	106.36(6)	256.23(18)
1465(5)	5.043(3)	5.5993(11)	9.562(6)	97.20(3)	99.462(13)	106.38(3)	251.3(2)

1575(5)	5.028(3)	5.5940(15)	9.555(5)	97.19(3)	99.606(12)	106.39(6)	249.9(2)
34(4)[a]	5.2273(11)	5.7097(7)	9.939(4)	97.37(3)	96.45(2)	106.18(2)	279.09(13)

[a] Obtained on releasing the pressure.

Table S11c. Unit cell parameters of form δ at 428 K as a function of pressure

P /MPa	a /Å	b /Å	c /Å	α /°	β /°	γ /°	V /Å^3
86(5)	5.2726(17)	5.7135(12)	9.968(6)	97.37(4)	95.64(5)	106.01(4)	283.4(2)
87(5)	5.2725(16)	5.7139(11)	9.976(6)	97.34(3)	95.63(5)	106.02(3)	283.7(2)
98(5)	5.273(3)	5.7129(12)	9.982(7)	97.37(4)	95.58(7)	106.00(3)	283.9(3)
103(4)	5.2758(19)	5.7127(12)	9.982(6)	97.39(4)	95.52(6)	105.95(4)	284.1(2)
439(4)	5.1923(19)	5.6757(13)	9.817(7)	97.13(4)	97.03(6)	106.29(4)	271.8(3)
757(5)	5.154(2)	5.6452(17)	9.704(8)	97.13(5)	97.82(5)	106.20(6)	264.7(3)
770(5)	5.157(3)	5.6451(18)	9.693(9)	97.10(5)	97.87(6)	106.27(6)	264.4(3)
988(4)	5.125(3)	5.6281(18)	9.640(6)	97.21(5)	98.37(3)	106.22(7)	260.1(3)
1196(4)	5.103(3)	5.6087(14)	9.583(6)	97.20(6)	98.79(3)	106.12(6)	256.3(3)
744(5)[a]	5.147(2)	5.6450(16)	9.725(7)	97.10(5)	97.90(4)	106.29(6)	264.7(3)
626(5)[a]	5.165(3)	5.6550(17)	9.737(5)	97.13(5)	97.68(4)	106.28(6)	266.6(3)
507(4)[a]	5.179(2)	5.6688(15)	9.767(8)	97.21(5)	97.45(4)	106.29(5)	268.9(3)
353(4)[a]	5.210(2)	5.6804(15)	9.864(7)	97.25(4)	96.63(6)	106.17(5)	274.6(3)
345(4)[a]	5.209(2)	5.6796(15)	9.893(6)	97.21(4)	96.52(6)	106.15(5)	275.5(3)
199(4)[a]	5.247(3)	5.6980(15)	9.921(5)	97.42(4)	95.92(6)	106.09(5)	279.6(2)
155(4)[a]	5.2586(15)	5.7039(12)	9.948(5)	97.41(4)	95.75(4)	106.05(4)	281.46(19)
109(4)[a]	5.2665(14)	5.7110(13)	9.969(6)	97.41(4)	95.65(5)	106.03(4)	283.0(2)
86(5)[a]	5.2683(18)	5.7138(11)	9.968(5)	97.43(3)	95.64(5)	105.99(3)	283.18(19)
66(4)[a]	5.281(3)	5.7138(15)	9.992(6)	97.40(4)	95.36(7)	105.98(5)	284.8(3)
60(4)[a]	5.288(2)	5.7133(12)	9.995(6)	97.40(4)	95.23(5)	105.94(4)	285.4(2)
29(4)[a]	5.2922(2)	5.7145(10)	9.989(5)	97.38(4)	95.23(4)	105.91(3)	285.57(18)
25(4)[a]	5.291(3)	5.7158(16)	10.009(6)	97.34(4)	95.21(6)	105.95(5)	286.1(3)
5(4)[a]	5.297(3)	5.7160(13)	10.014(6)	97.33(4)	95.12(6)	105.91(4)	286.8(3)
1(4)[a]	5.303(3)	5.7188(16)	10.004(9)	97.37(5)	95.17(7)	105.94(5)	286.8(4)

[a] Obtained on releasing the pressure.

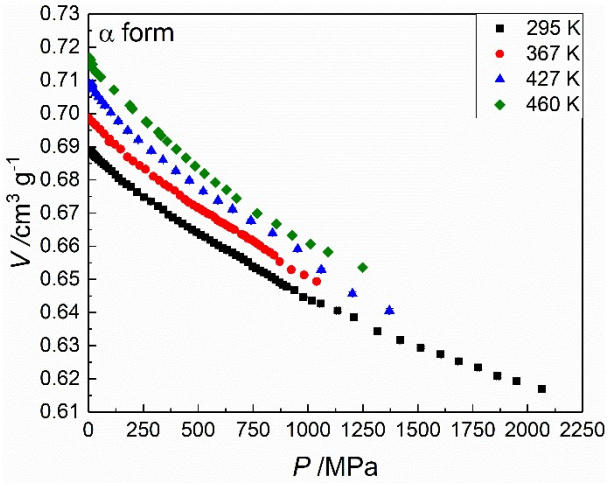

Figure S2. The specific volume of pyrazinamide form α as a function of pressure at 295 K (black squares), 367 K (red circles), 427 K (blue triangles), and 460 K (green diamonds)

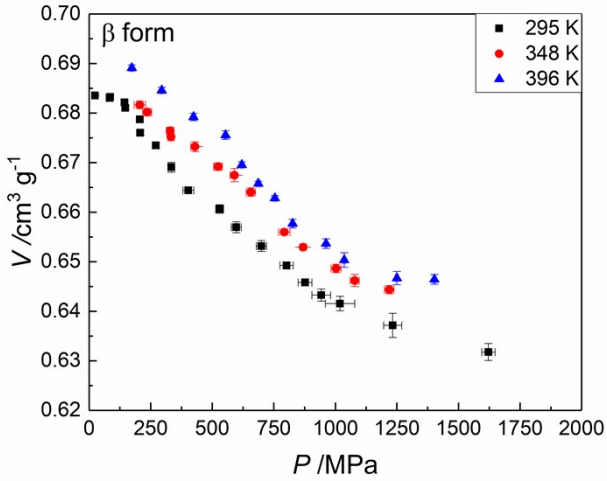

Figure S3. The specific volume of pyrazinamide form β as a function of pressure at 295 K (black squares), 348 K (red circles), and 396 K (blue triangles)

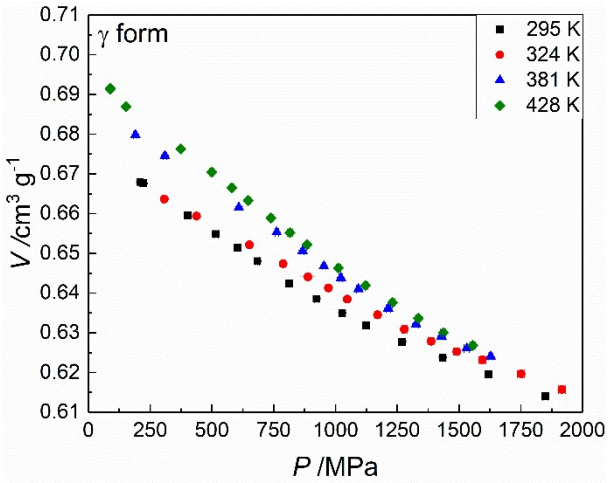

Figure S4. The specific volume of pyrazinamide form γ as a function of pressure at 295 K (black squares), 324 K (red circles), 381 K (blue triangles), and 428 K (green diamonds)

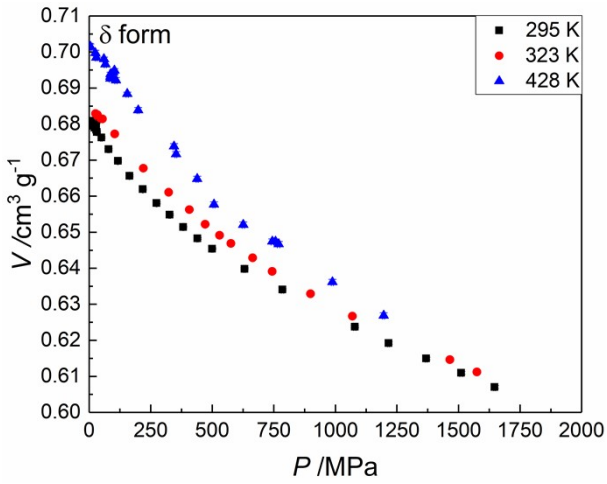

Figure S5. The specific volume of pyrazinamide form δ as a function of pressure at 295 K (black squares), 323 K (red circles), and 428 K (blue triangles)

Table S12. Principal coefficients of the isobaric thermal expansion tensor and the corresponding principal axes for form α

Principal axis, *i*	α_I (MK^{-1})	Component of x_i along the crystallographic axes		
		a	*b*	*c*
1	-23.1(6)	0.0000	1.0000	0.0000
2	31 (2)	0.7588	0.0000	-0.6514
3	161(3)	-0.9993	0.0000	-0.0368
V	170(4)			

Table S13. Principal coefficients of the isobaric thermal expansion tensor and the corresponding principal axes for form β

Principal axis, *i*	α_I (MK^{-1})	Component of x_i along the crystallographic axes		
		a	*b*	*c*
1	-22.1(10)	-0.7464	0.0000	-0.6655
2	64(2)	-0.3690	0.0000	0.9294
3	119(2)	0.0000	-1.0000	0.0000
V	161(3)			

Table S14. Principal coefficients of the isobaric thermal expansion tensor and the corresponding principal axes for form γ

Principal axis, *i*	α_I (MK^{-1})	Component of x_i along the crystallographic axes		
		a	*b*	*c*
1	-1.86(7)	-0.09593	0.0000	-0.2823
2	44(2)	-0.2507	0.0000	0.9681
3	137(3)	0.0000	-1.0000	0.0000
V	183(5)			

Table S15. Principal coefficients of the isobaric thermal expansion tensor and the corresponding principal axes for form δ

Principal axis, i	α_1 (MK^{-1})	Component of x_i along the crystallographic axes		
		a	b	c
1	-6.1(9)	0.5860	0.6391	-0.4981
2	17.1(7)	0.3459	-0.9099	-0.2290
3	178(6)	0.8848	0.3337	0.3252
V	192(7)			

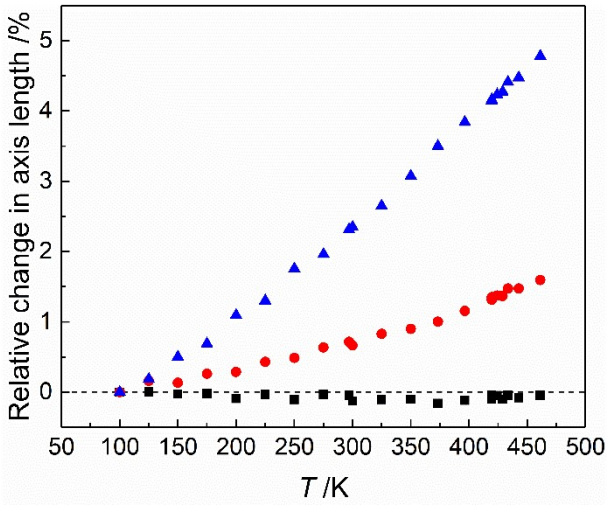

Figure S6. Thermal expansion tensor: relative change in the principal axes (x_1: ■, x_2: ●, and x_3: ▲) of form α as a function of temperature

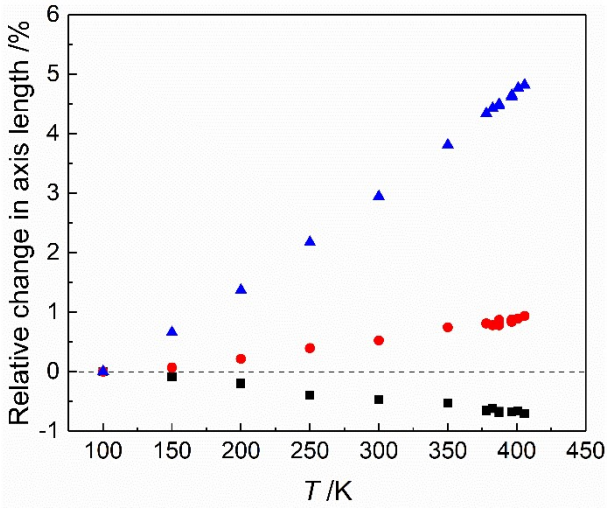

Figure S7. Thermal expansion tensor: relative change in the principal axes (x_1: ■, x_2: ●, and x_3: ▲) of form β as a function of temperature

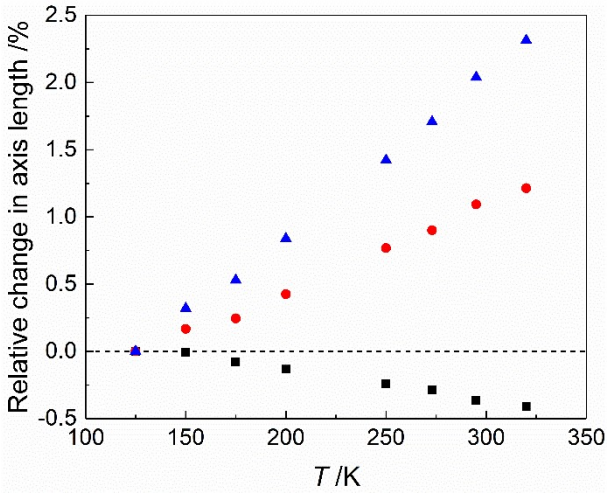

Figure S8. Thermal expansion tensor: relative change in the principal axes (x_1: ■, x_2: ●, and x_3: ▲) of form γ as a function of temperature

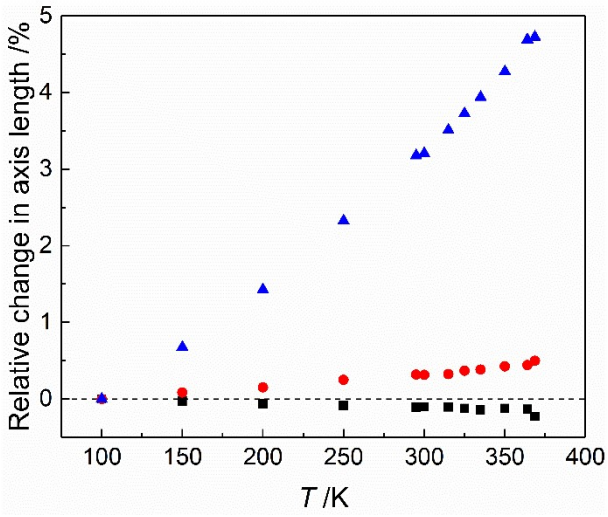

Figure S9. Thermal expansion tensor: relative change in the principal axes (x_1: ■, x_2: ●, and x_3: ▲) of form δ as a function of temperature

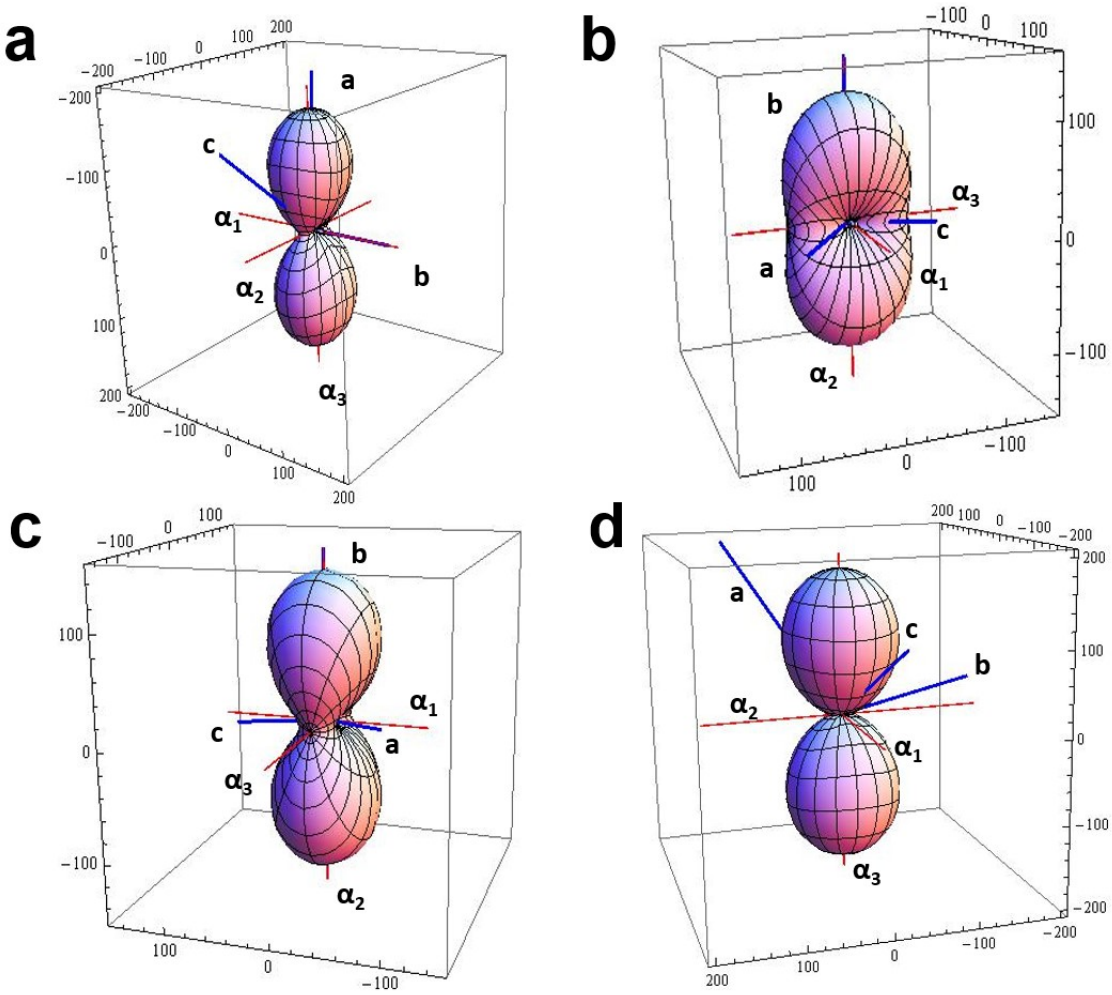

Figure S10. Graphic representations of the isobaric thermal expansion tensors of forms α (a), β (b), γ (c), and δ (d). The numbers on the axes represent the value of the respective tensor component α_1, α_2, and α_3 as indicated by the respective red lines (see also Tables S12-S15). The negative tensor parts are relatively small in comparison with the positive parts and therefore very hard to distinguish.

Table S16. Principal coefficients of the isothermal compression tensor and the corresponding principal axes for form *α*

Principal axis, *i*	K_I (TPa^{-1})	Component of x_i along the crystallographic axes		
		a	*b*	*c*
1	40.9(8)	-0.9994	0.0000	-0.0333
2	13.2(2)	0.7227	0.0000	-0.6911
3	2.7(2)	0.0000	1.0000	0.0000
V	55(2)			

Table S17. Principal coefficients of the isothermal compression tensor and the corresponding principal axes for form *β*

Principal axis,	K_I (TPa^{-1})	Component of x_i along the crystallographic axes

i		*a*	*b*	*c*
1	29(5)	0.0000	-1.0000	0.0000
2	8(5)	-0.4514	0.0000	0.8923
3	0.0(7)	-0.6936	0.0000	-0.7204
V	60(5)			

Table S18. Principal coefficients of the isothermal compression tensor and the corresponding principal axes for form γ

Principal axis, *i*	K_I (TPa^{-1})	Component of x_i along the crystallographic axes		
		a	*b*	*c*
1	34.6(7)	0.0000	-1.0000	0.0000
2	11.3(2)	0.3839	0.0000	0.9234
3	3(2)	-1.0000	0.0000	-0.0058
V	51(3)			

Table S19. Principal coefficients of the isothermal compression tensor and the corresponding principal axes for form δ

Principal axis, *i*	K_I (TPa^{-1})	Component of x_i along the crystallographic axes		
		a	*b*	*c*
1	82.0(8)	-0.8460	-0.2871	-0.4493
2	15(2)	-0.5175	-0.8242	0.2301
3	13.4(4)	0.6627	-0.6701	-0.3343
V	73(4)			

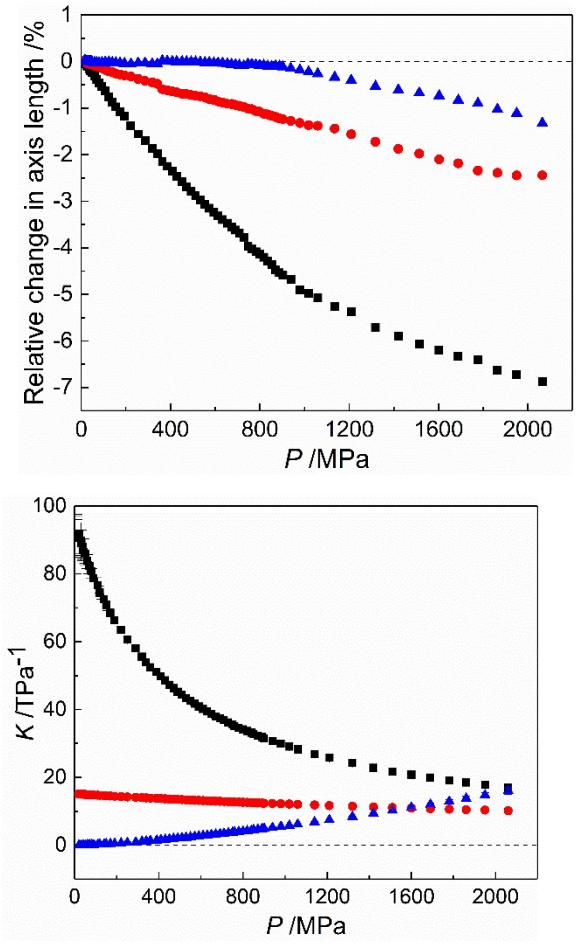

Figure S11. Compression tensor form α left-hand side: relative change in the principal axes (x_1: ■, x_2: ●, and x_3: ▲) and, right-hand side, the principal compressibility (K_1: ■, K_2: ●, and K_3: ▲) as a function of pressure

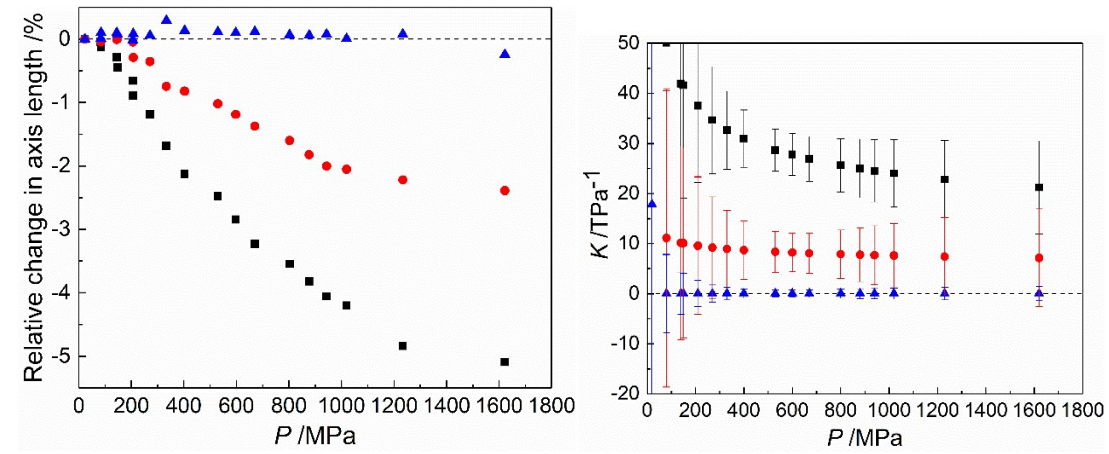

Figure S12. Compression tensor form β left-hand side: relative change in the principal axes (x_1: ■, x_2: ●, and x_3: ▲) and, right-hand side, the principal compressibility (K_1: ■, K_2: ●, and K_3: ▲) as a function of pressure

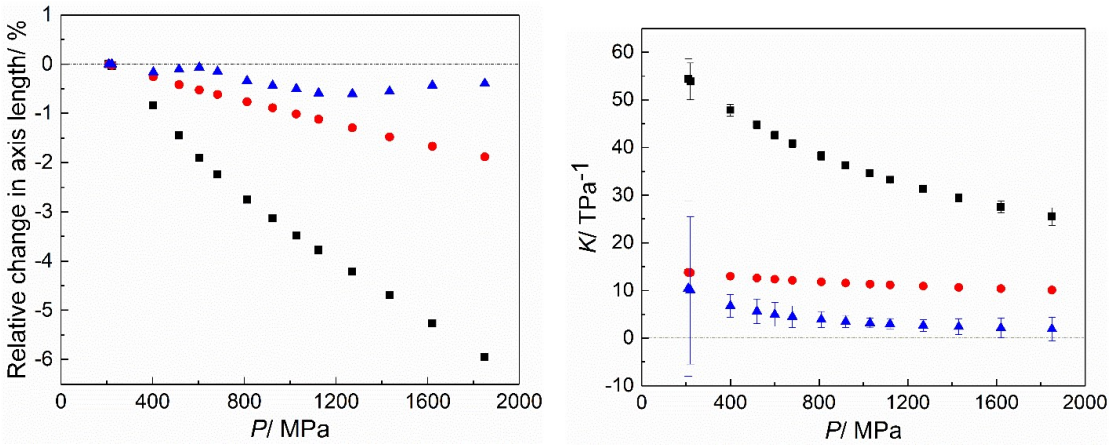

Figure S13. Compression tensor form γ left-hand side: relative change in the principal axes (x_1: ■, x_2: ●, and x_3: ▲) and, right-hand side, the principal compressibility (K_1: ■, K_2: ●, and K_3: ▲) as a function of pressure

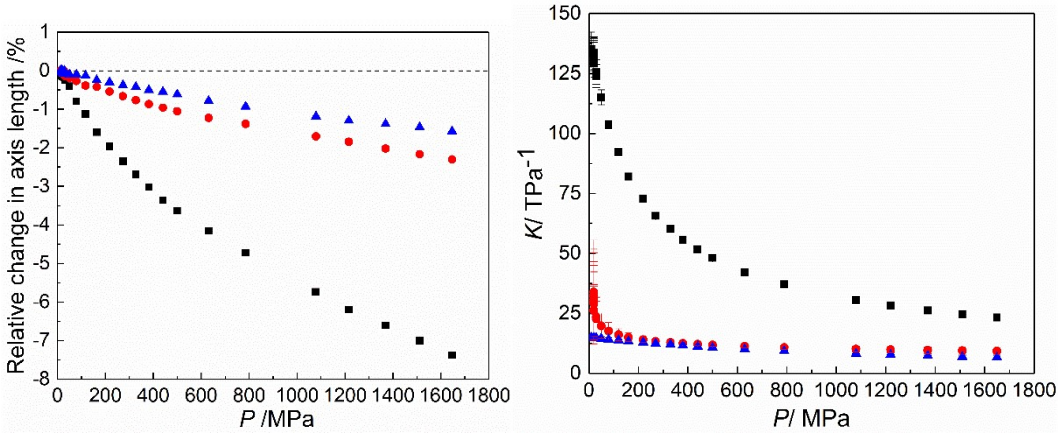

Figure S14. Compression tensor form δ left-hand side: relative change in the principal axes (x_1: ■, x_2: ●, and x_3: ▲) and, right-hand side, the principal compressibility (K_1: ■, K_2: ●, and K_3: ▲) as a function of pressure

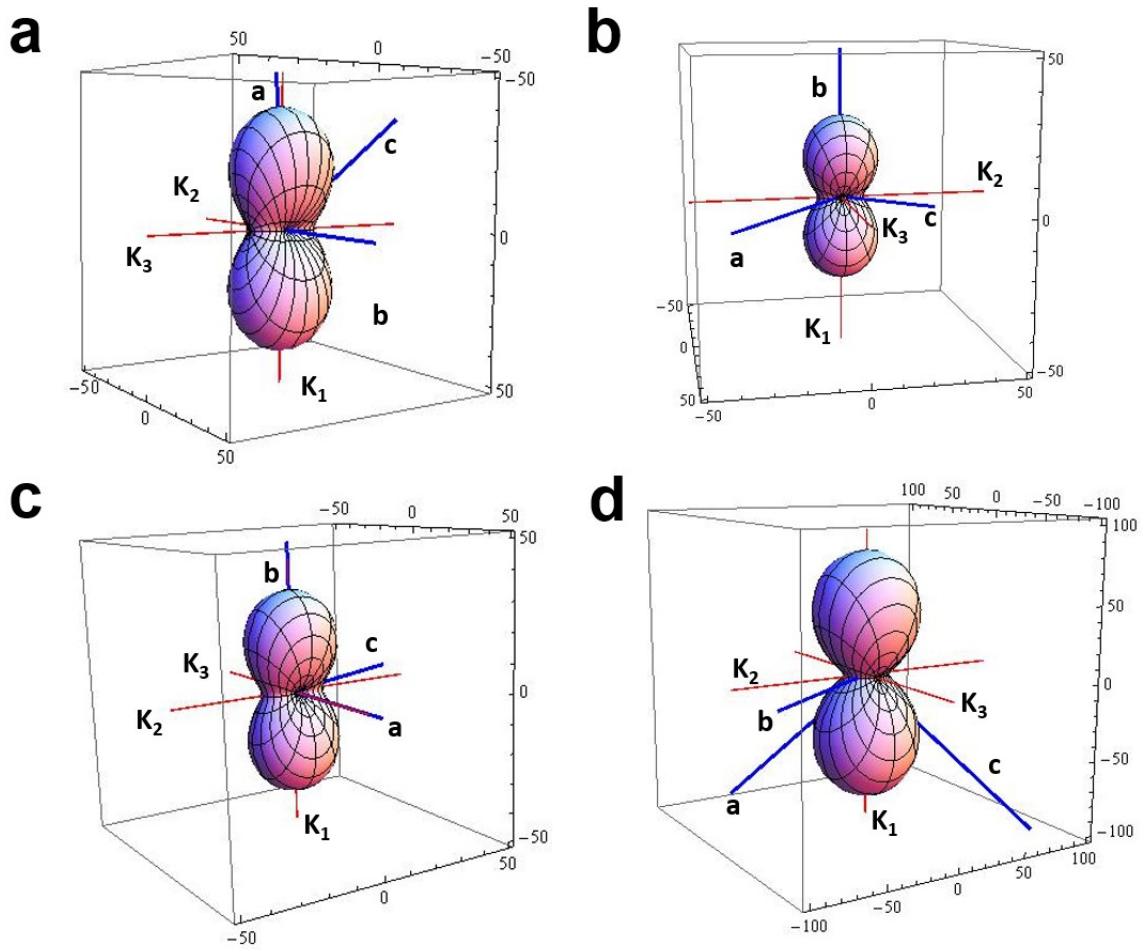

Figure S15. Graphic representations of the isothermal compression tensors of forms α (a), β (b), γ (c), and δ (d). The numbers on the axes represent the value of the respective tensor component K_1, K_2, and K_3 as indicated by the respective red lines (see also Tables S16-S19).

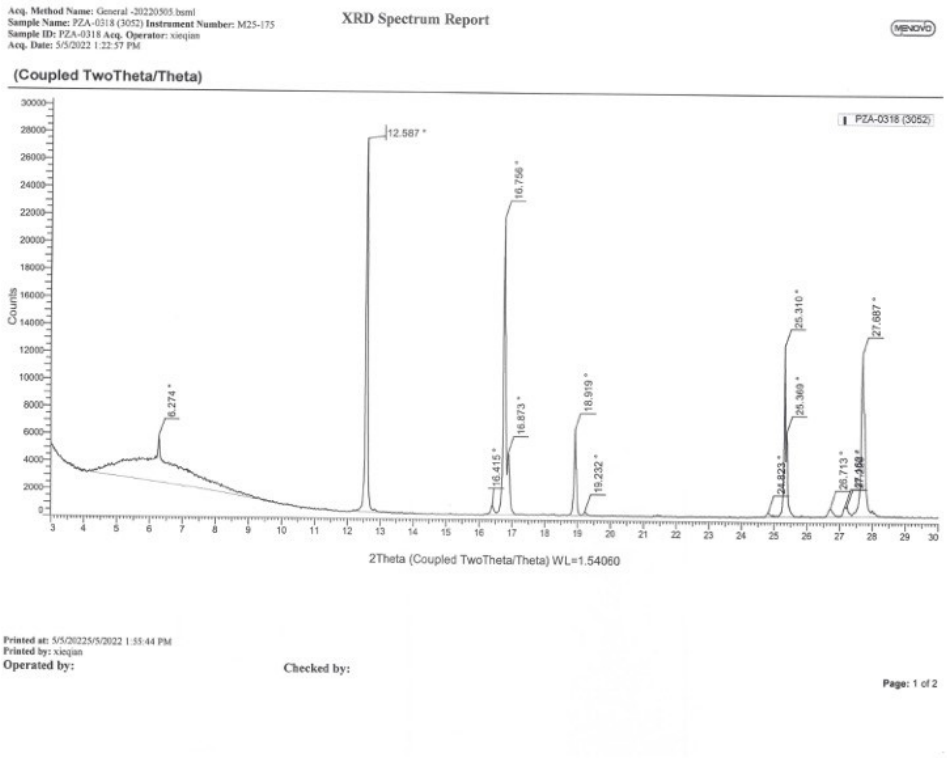

Figure S16. X-ray diffraction pattern of pyrazinamide crystallized at 252 K from acetonitrile. The pattern is fully equivalent to that of form β. Only the peak at 16.415° 2θ may be ascribed to form δ.

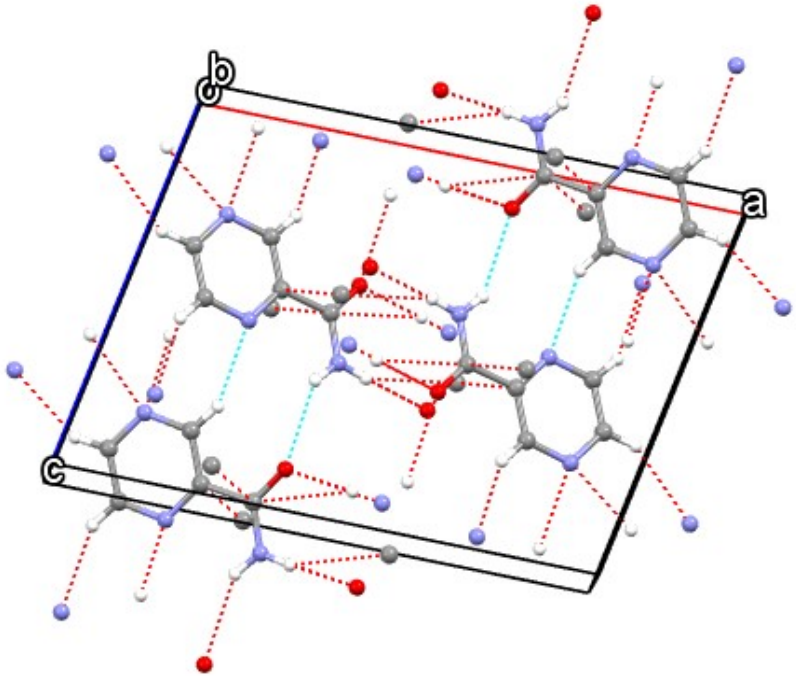

Figure S17. Global hydrogen bond network in form β.