Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Information - Discovery and Recovery of delta *p*-aminobenzoic acid

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Table S1. Experimental details

For all structures: $C_7H_7NO_2$, M_r = 137.14, monoclinic, *Pn*, *Z* = 2. Refinement was with 71 restraints.

	δ-*p*ABA recovered from high pressure	δ-*p*ABA recovered from high pressure	δ-*p*ABA in ethanol at 0.49 GPa	δ-*p*ABA in water at 0.33 GPa
Crystal data				
Temperature (K)	295	100	296	296
a, *b*, *c* (Å)	6.5086 (5), 4.6661 (4), 10.7596 (8)	6.4551 (5), 4.6740 (4), 10.5470 (9)	6.4341 (11), 4.6151 (3), 10.5313 (7)	6.4342 (10), 4.6146 (4), 10.5397 (10)
β (°)	100.685 (1)	100.754 (3)	100.73 (1)	100.667 (9)
V (Å^3)	321.10 (4)	312.63 (4)	307.25 (6)	307.53 (6)
Radiation type	Mo *K*α	Cu *K*α	Mo *K*α	Mo *K*α
μ (mm^{-1})	0.11	0.91	0.11	0.11
Crystal size (mm)	0.2 × 0.15 × 0.02	0.2 × 0.18 × 0.02	0.15 × 0.08 × 0.08	0.15 × 0.08 × 0.05
Data collection				
Diffractometer	Bruker *APEX*-II CCD	Bruker *APEX*-II CCD	Bruker *SMART APEX2* area detector	Bruker *SMART APEX2* area detector
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.1202 before and 0.0619 after correction. The Ratio of minimum to maximum transmission is 0.8072. The λ/2 correction factor is Not present.	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.0715 before and 0.0460 after correction. The Ratio of minimum to maximum transmission is 0.8525. The λ/2 correction factor is Not present.	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.0921 before and 0.0409 after correction. The Ratio of minimum to maximum transmission is 0.9017. The λ/2 correction factor is Not present.	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.1150 before and 0.0458 after correction. The Ratio of minimum to maximum transmission is 0.8491. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.603, 0.746	0.643, 0.754	0.672, 0.745	0.633, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7461, 2326, 2079	3384, 1014, 991	1365, 357, 320	1444, 471, 396
R_{int}	0.040	0.035	0.030	0.043
θ_{max} (°)	32.6	74.2	23.3	23.2
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.758	0.624	0.556	0.554

Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.115, 1.05	0.029, 0.073, 1.11	0.034, 0.077, 1.17	0.041, 0.107, 1.11
No. of reflections	2326	1014	357	471
No. of parameters	93	100	81	81
H-atom treatment	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, -0.19	0.18, -0.24	0.11, -0.10	0.16, -0.16
Absolute structure	Flack x determined using 955 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).	Flack x determined using 350 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).	Flack x determined using 130 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).	Flack x determined using 156 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	-0.4 (6)	0.01 (12)	-0.6 (10)	1.3 (10)

	δ-*p*ABA in 50:50 ethanol:water at 0.8 GPa
Crystal data	
Temperature (K)	295
a, *b*, *c* (Å)	6.4003 (11), 4.5981 (4), 10.4452 (15)
β (°)	100.748 (14)
V (Å^3)	302.00 (7)
Radiation type	Mo *K*α
μ (mm^{-1})	0.11
Crystal size (mm)	0.2 × 0.15 × 0.02
Data collection	
Diffractometer	Bruker *SMART APEX2* area detector
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.0951 before and 0.0476 after correction. The Ratio of minimum to maximum transmission is 0.7098. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.529, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	1317, 333, 300

R_{int}	0.030
θ_{max} (°)	23.3
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.555
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.028, 0.064, 1.04
No. of reflections	333
No. of parameters	81
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.09, -0.07
Absolute structure	Flack x determined using 129 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	1.5 (10)

Computer programs: *SAINT* v8.37A (Bruker, 2015), XT (Sheldrick, 2015), XL (Sheldrick, 2008), Olex2 (Dolomanov *et al.*, 2009).

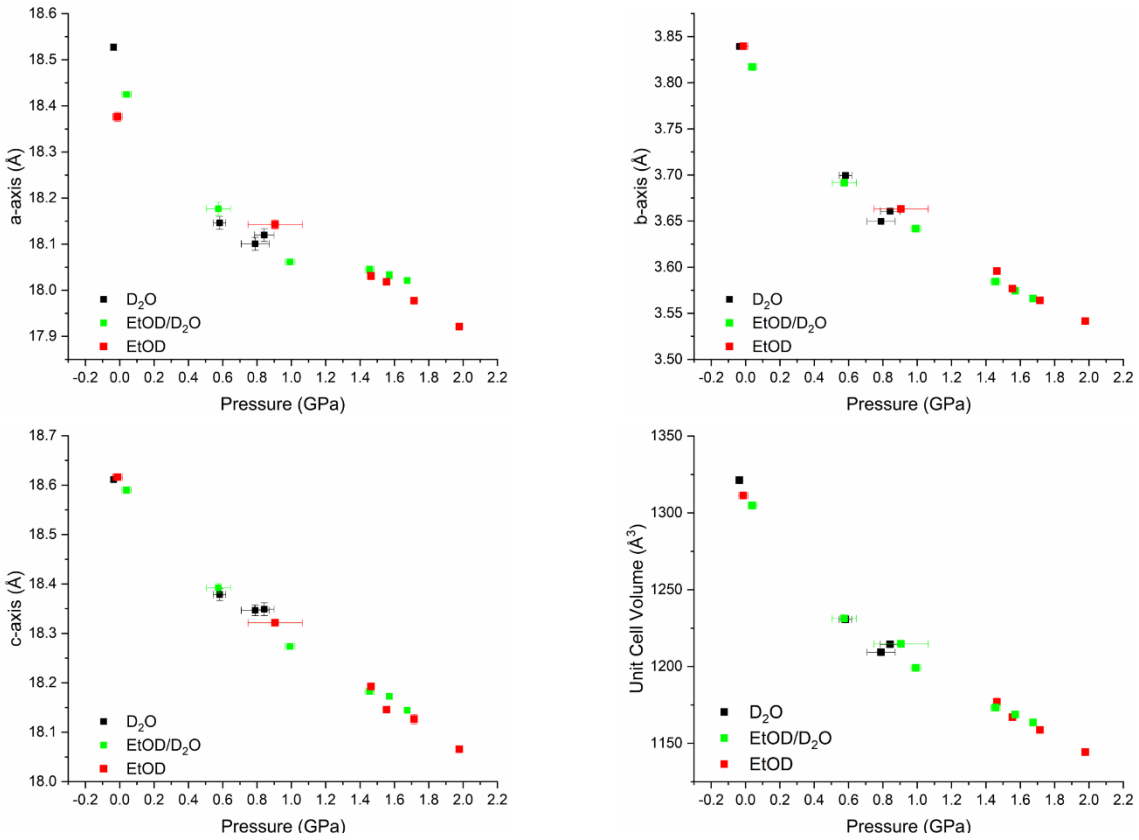

Figure S1: The refined unit cell parameters for α-form as a function of pressure. The parameters are consistent with one another from each of the media.

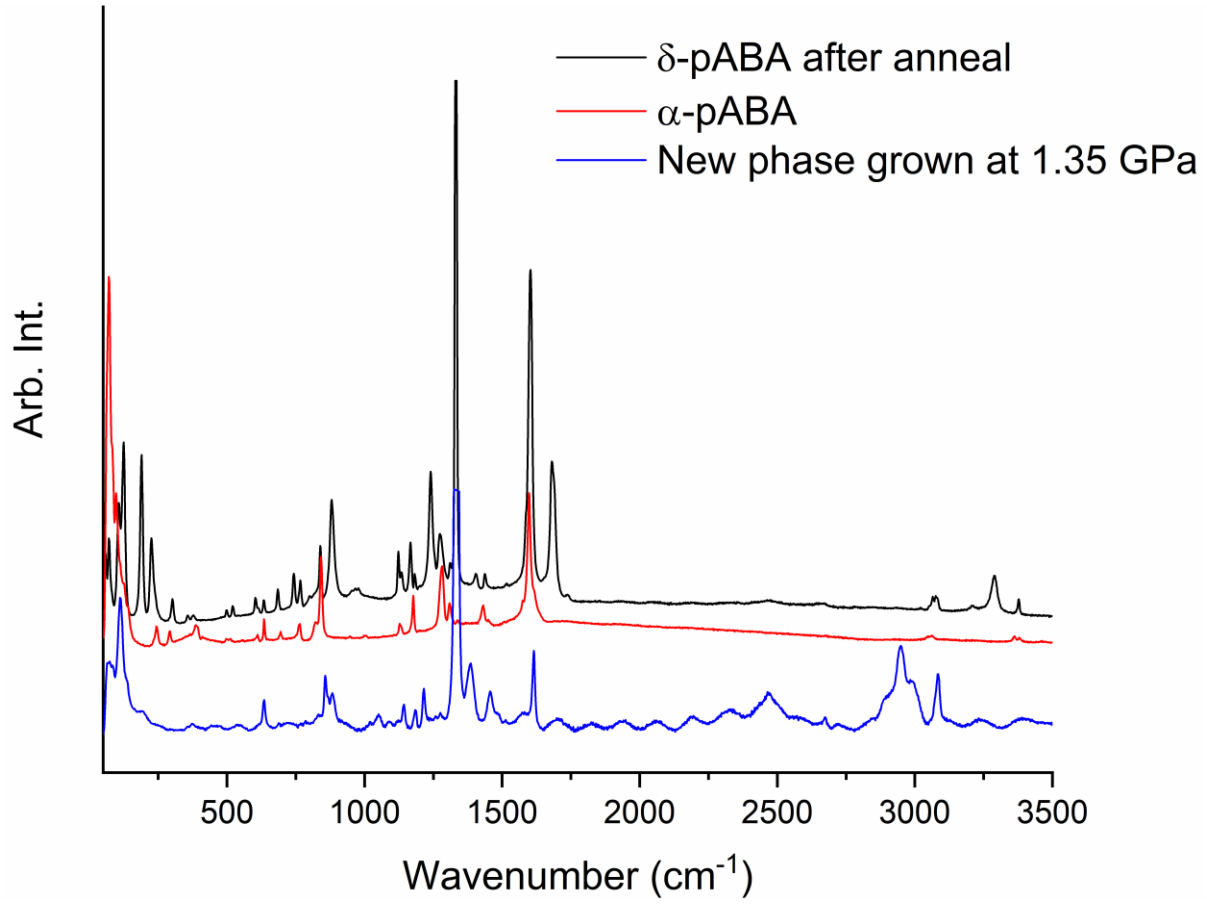

Figure S2: The Raman spectrum for the new phase that nucleated after 8 hours from a α-*p*ABA sample in 50:50 v/v water:ethanol at 1.35 GPa together with the spectrum for α-*p*ABA and the annealed sample which was identified at δ-*p*ABA by single crystal diffraction.

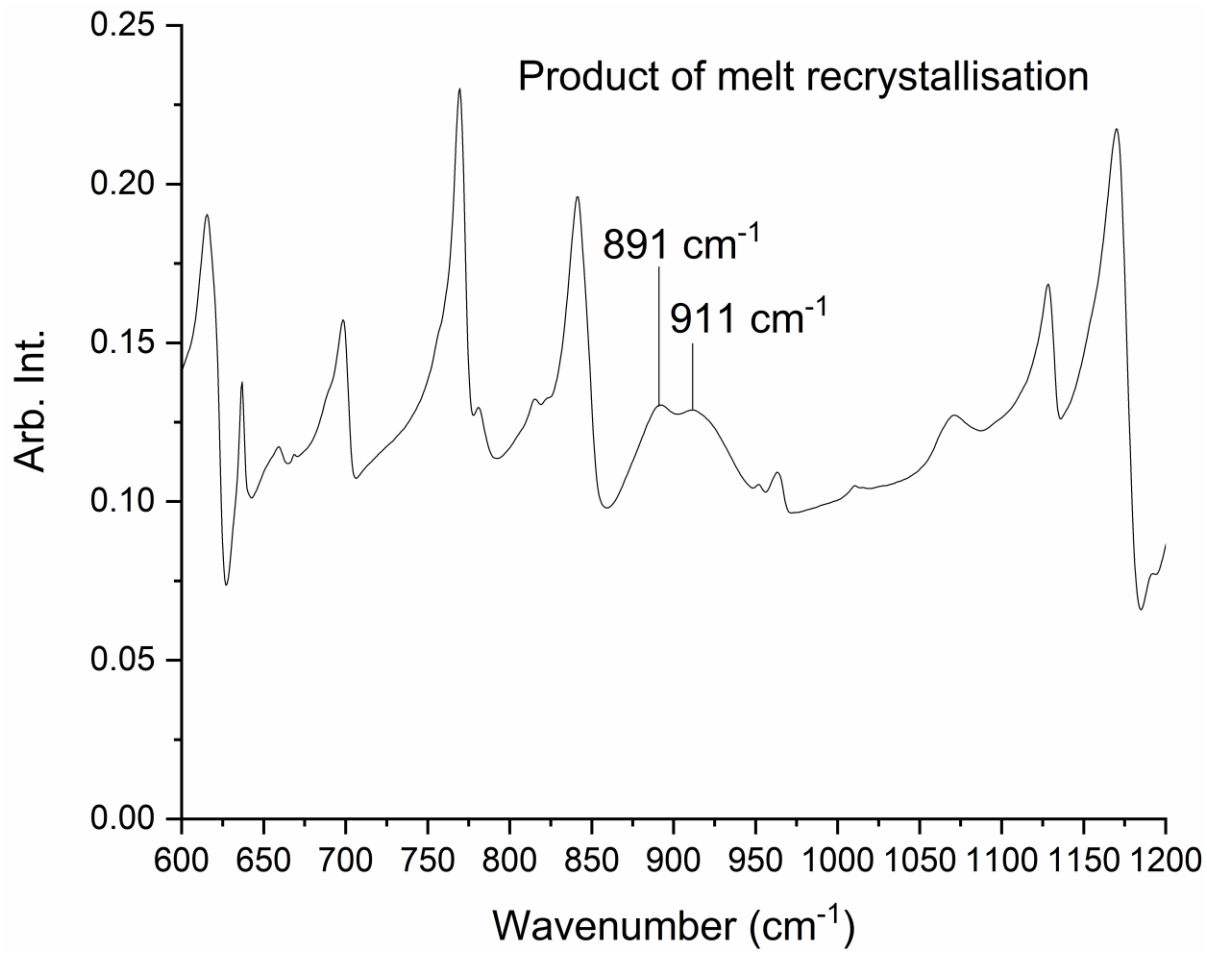

Figure S3: The FT-IR of the recrystallised material from the melt using the DSC sample. The peaks indicate that it is γ-*p*ABA.