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

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### Table S1. Experimental details

For all structures: C$_7$H$_7$NO$_2$, $M_r = 137.14$, monoclinic, $Pn$, $Z = 2$. Refinement was with 71 restraints.

<table>
<thead>
<tr>
<th>Crystal data</th>
<th>δ-pABA recovered from high pressure</th>
<th>δ-pABA recovered from high pressure</th>
<th>δ-pABA in ethanol at 0.49 GPa</th>
<th>δ-pABA in water at 0.33 GPa</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Temperature (K)</strong></td>
<td>295</td>
<td>100</td>
<td>296</td>
<td>296</td>
</tr>
<tr>
<td><strong>$β$ (°)</strong></td>
<td>100.685 (1)</td>
<td>100.754 (3)</td>
<td>100.73 (1)</td>
<td>100.667 (9)</td>
</tr>
<tr>
<td><strong>V (Å$^3$)</strong></td>
<td>321.10 (4)</td>
<td>312.63 (4)</td>
<td>307.25 (6)</td>
<td>307.53 (6)</td>
</tr>
<tr>
<td><strong>Radiation type</strong></td>
<td>Mo $Kα$</td>
<td>Cu $Kα$</td>
<td>Mo $Kα$</td>
<td>Mo $Kα$</td>
</tr>
<tr>
<td><strong>$\mu$ (mm$^{-1}$)</strong></td>
<td>0.11</td>
<td>0.91</td>
<td>0.11</td>
<td>0.11</td>
</tr>
<tr>
<td><strong>Crystal size (mm)</strong></td>
<td>$0.2 \times 0.15 \times 0.02$</td>
<td>$0.2 \times 0.18 \times 0.02$</td>
<td>$0.15 \times 0.08 \times 0.08$</td>
<td>$0.15 \times 0.08 \times 0.05$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Data collection</th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Diffractometer</strong></td>
<td>Bruker APEX-II CCD</td>
<td>Bruker APEX-II CCD</td>
<td>Bruker SMART APEX2 area detector</td>
<td>Bruker SMART APEX2 area detector</td>
</tr>
<tr>
<td><strong>Absorption correction</strong></td>
<td>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 $\lambda/2$ correction factor is Not present.</td>
<td>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 $\lambda/2$ correction factor is Not present.</td>
<td>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 $\lambda/2$ correction factor is Not present.</td>
<td>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 $\lambda/2$ correction factor is Not present.</td>
</tr>
<tr>
<td><strong>$T_{min}$, $T_{max}$</strong></td>
<td>0.603, 0.746</td>
<td>0.643, 0.754</td>
<td>0.672, 0.745</td>
<td>0.633, 0.745</td>
</tr>
<tr>
<td><strong>No. of measured, independent and observed [$I &gt; 2\sigma(I)$] reflections</strong></td>
<td>7461, 2326, 2079</td>
<td>3384, 1014, 991</td>
<td>1365, 357, 320</td>
<td>1444, 471, 396</td>
</tr>
<tr>
<td><strong>$R_{int}$</strong></td>
<td>0.040</td>
<td>0.035</td>
<td>0.030</td>
<td>0.043</td>
</tr>
<tr>
<td><strong>$θ_{max}$ (°)</strong></td>
<td>32.6</td>
<td>74.2</td>
<td>23.3</td>
<td>23.2</td>
</tr>
<tr>
<td><strong>(sin $θ/\lambda$)$_{max}$ (Å$^{-1}$)</strong></td>
<td>0.758</td>
<td>0.624</td>
<td>0.556</td>
<td>0.554</td>
</tr>
</tbody>
</table>
### Refinement

<table>
<thead>
<tr>
<th>$R[F^2 &gt; 2\sigma(F^2)], \ wR(F^2), S$</th>
<th>0.041, 0.115, 1.05</th>
<th>0.029, 0.073, 1.11</th>
<th>0.034, 0.077, 1.17</th>
<th>0.041, 0.107, 1.11</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. of reflections</td>
<td>2326</td>
<td>1014</td>
<td>357</td>
<td>471</td>
</tr>
<tr>
<td>No. of parameters</td>
<td>93</td>
<td>100</td>
<td>81</td>
<td>81</td>
</tr>
<tr>
<td>H-atom treatment</td>
<td>H-atoms treated by a mixture of independent and constrained refinement</td>
<td>H-atoms constrained</td>
<td>H-atoms constrained</td>
<td>H-atoms constrained</td>
</tr>
<tr>
<td>$\Delta \rho_{\text{max}}, \Delta \rho_{\text{min}} (\text{e Å}^{-3})$</td>
<td>0.27, -0.19</td>
<td>0.18, -0.24</td>
<td>0.11, -0.10</td>
<td>0.16, -0.16</td>
</tr>
</tbody>
</table>

### Absolute structure

<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>Absolute structure parameter</td>
<td>-0.4 (6)</td>
<td>0.01 (12)</td>
<td>-0.6 (10)</td>
</tr>
</tbody>
</table>

### Crystal data

| $\delta$-pABA in 50:50 ethanol:water at 0.8 GPa |

| Temperature (K) | 295 |
| $a, b, c$ (Å) | 6.4003 (11), 4.5981 (4), 10.4452 (15) |
| $\beta$ (°) | 100.748 (14) |
| $V$ (Å$^3$) | 302.00 (7) |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.11 |
| Crystal size (mm) | $0.2 \times 0.15 \times 0.02$ |

### Data collection

| Bruker SMART APEX2 area detector |

<table>
<thead>
<tr>
<th>Absorption correction</th>
<th>Multi-scan SADAB2016/2 (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 $\lambda/2$ correction factor is Not present.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{\text{min}}, T_{\text{max}}$</td>
<td>0.529, 0.745</td>
</tr>
<tr>
<td>No. of measured, independent and observed ([I &gt; 2\sigma(I)]) reflections</td>
<td>1317, 333, 300</td>
</tr>
<tr>
<td>$R_{int}$</td>
<td>0.030</td>
</tr>
<tr>
<td>$\theta_{\text{max}}$ (°)</td>
<td>23.3</td>
</tr>
<tr>
<td>$(\sin \theta / \lambda)_{\text{max}}$ (Å$^{-1}$)</td>
<td>0.555</td>
</tr>
</tbody>
</table>

**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 |
| $\Delta \rho_{\text{max}}, \Delta \rho_{\text{min}}$ (e Å$^{-3}$) | 0.09, -0.07 |
| 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-pABA sample in 50:50 v/v water:ethanol at 1.35 GPa together with the spectrum for α-pABA and the annealed sample which was identified at δ-pABA 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 $\gamma$-pABA.