Solid state structures of p-cresol revisited

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1. Original DSC curves of Form I and II

The energy difference between the two polymorphs is ca. 1.1 kcal/mol based on the DSC results.

![Figure S1 DSC curve of Form I crystals.](image1)

![Figure S2 DSC curve of Form II.](image2)
2. Additional information to VTPXRD experiments

Form I:

A Pawley refinement was carried out on the profile of Form I recorded at -50 °C. We found that this phase consists of mainly Form I having $R_{wp} = 14.479$. and an additional unknown form appears that has limited crystallinity. Thus, it explains the slight mismatch between the calculated and experimental profiles. (Figure S3)

![Figure S3. Pawley refinement results: experimental profile of Form I (blue), the calculated profile (red) and the difference curve (grey).](image)

Form II:

Due to the severe preferred orientation present in the sample recorded at -50 °C we were unable to perform a successful Pawley refinement of the profile. However, we used the program Mercury to compute the preferred orientation in 010, shown here in Figure S4.

![Figure S4. Computed profile for Form II with preferred orientation in 010 direction (blue) and the experimental profile recorded at -50°C (green).](image)

3. Additional information to lattice energy calculations:

The program GRACE (Neumann, M. A. 2013. Version 2.1. [http://www.avmatsim.eu](http://www.avmatsim.eu)) was used to calculate lattice energies. The calculated $\Delta U$ is 0.34 kcal/mol and the error on the calculations is about 0.5 kcal/mol.