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.

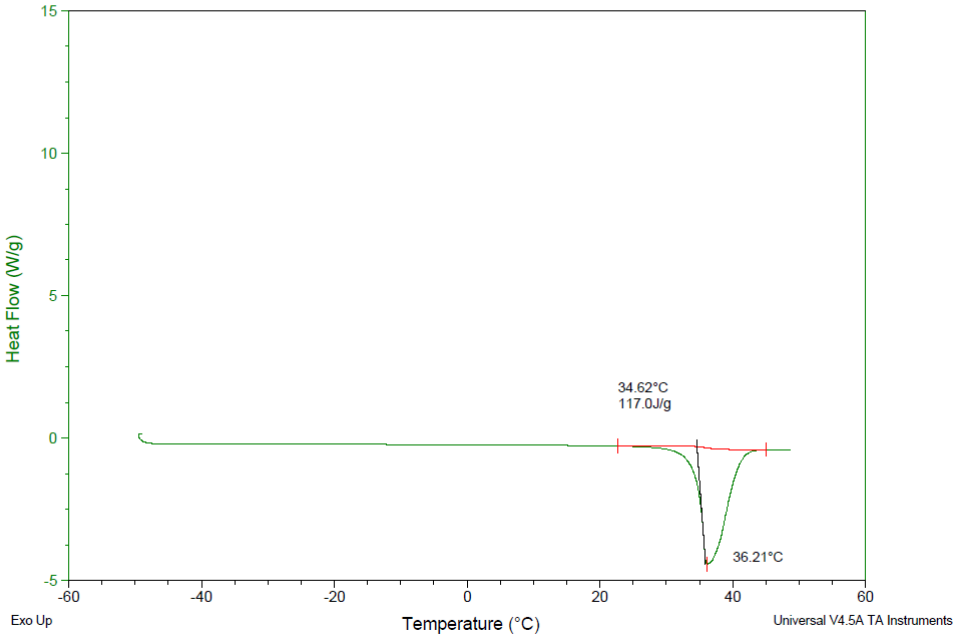

Figure S1 DSC curve of Form I crystals.

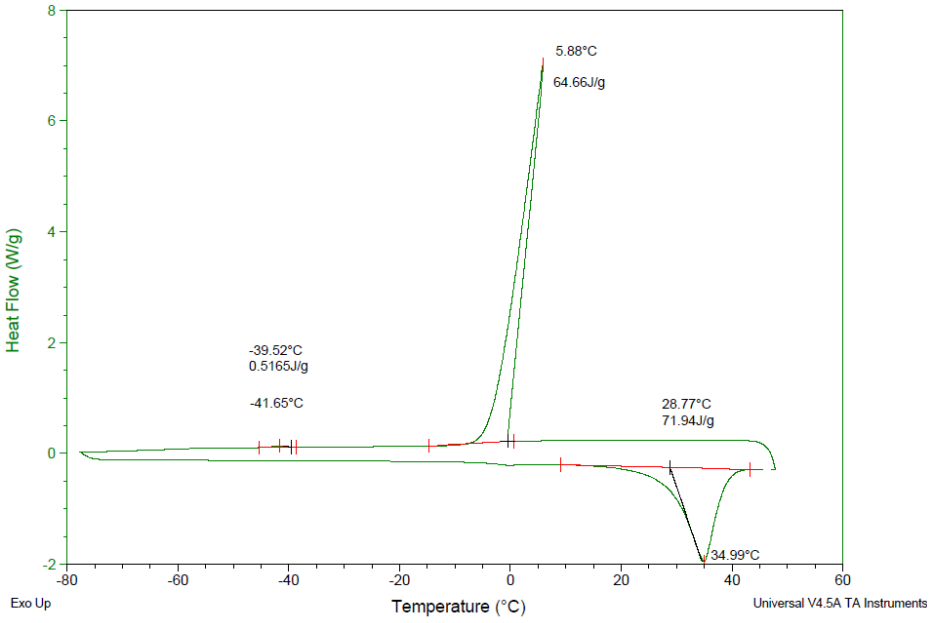

Figure S2 DSC curve of Form II.

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)

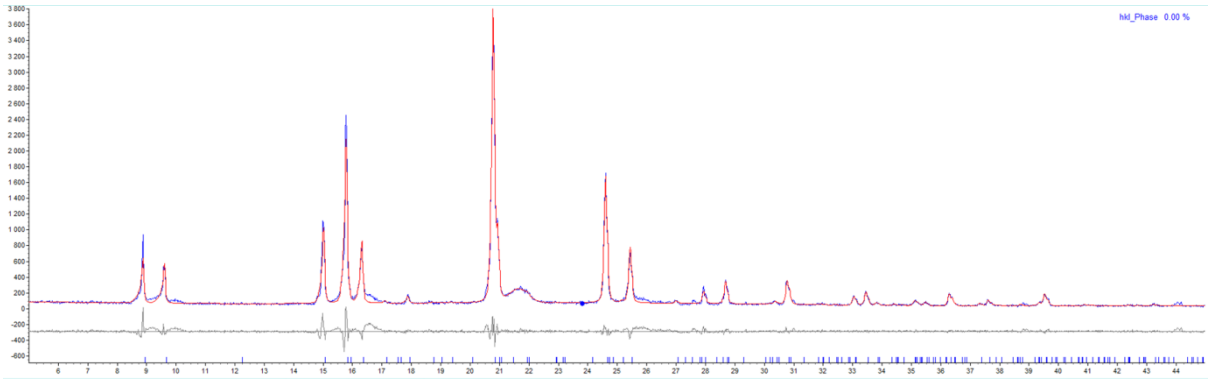

Figure S3. Pawley refinement results: experimental profile of Form I (blue), the calculated profile (red) and the difference curve (grey).

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.

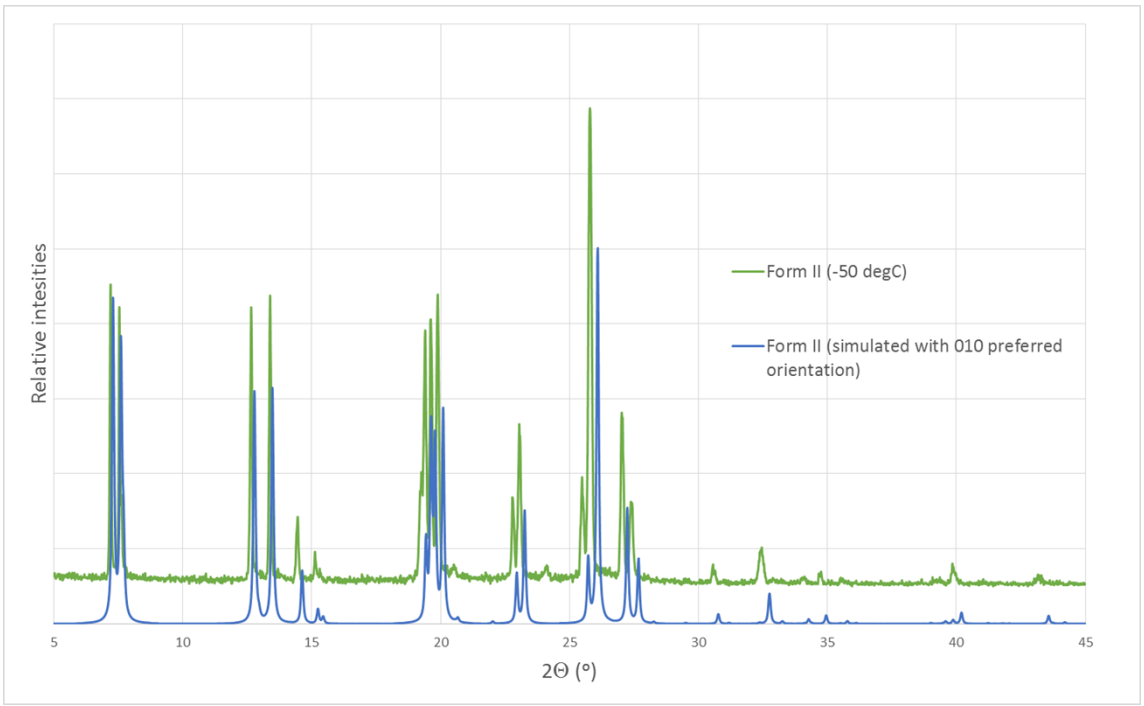

Figure S4. Computed profile for Form II with preferred orientation in 010 direction (blue) and the experimental profile recorded at -50°C (green).

3. Additional information to lattice energy calculations:

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