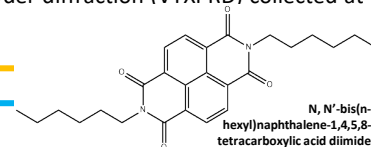


Introduction

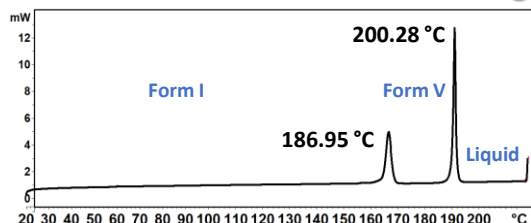
Polymorphism of organic semiconductors (OSCs) has become a topic of much interest since different polymorphs can have different properties being the main focus, in the area of semiconductors, the difference in charge mobility.

In this work, we studied N, N'-bis(n-hexyl)naphthalene-1,4,5,8-tetracarboxylic acid diimide (NDI-C6), a small molecule organic semiconductor, by performing an in deep analysis of the thermal behaviour using several characterization techniques such as hot stage optical microscopy (HSM), differential scanning calorimetry (DSC) and variable temperature x-ray powder diffraction (VTXRPD) collected at PSI synchrotron.



Results

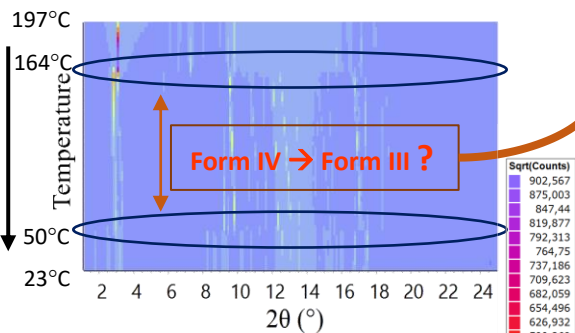
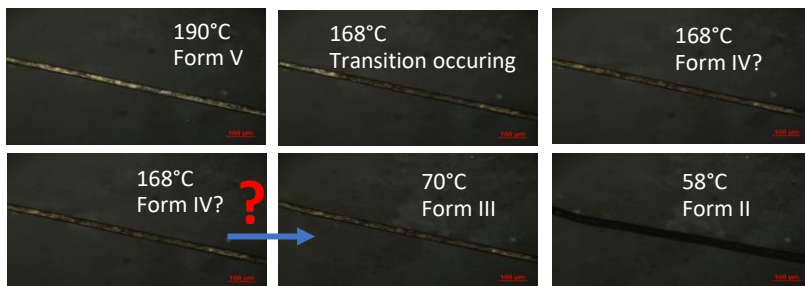
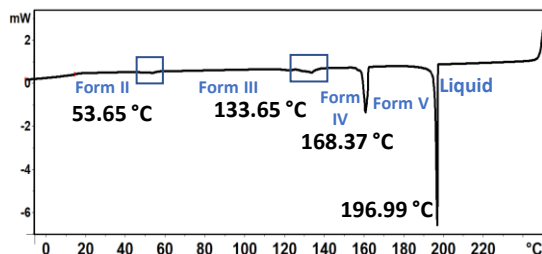
Heating – Transition Form I → Form V



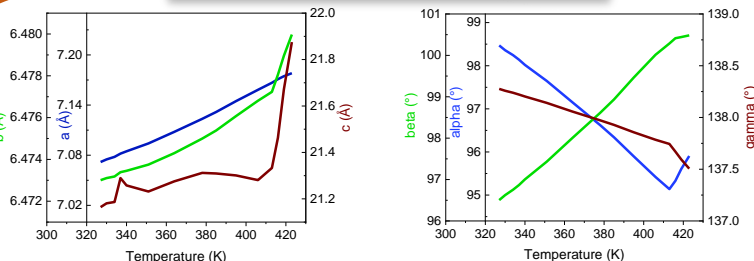
During the transition it can be observed one peak of Form III on the VTXRPD

This was not expected

Cooling – Several transitions observed



Pawley Refinement of the new cell



Around 406K (133°C) the trend of the curves change. At the same temperature, the Rwp increases

There is a FORM IV!

New cell obtained from peak indexing for Form III

a 7.0719 Å b 6.4717 Å c 21.2805 Å
α 98.47° β 96.50° γ 138.27°

Volume 603.150 Å³

Rwp 5.48

Conclusions

- NDI-C6 has proven to be a molecule really prompt to generate polymorphs as it can be observed by the thermal study of the molecule as bulk, where it was obtained 5 forms, one of which has not been reported previously (Form IV).
- The new elusive form IV is difficult to isolate and can easily be missed, being its presence only confirmed by Pawley refinement.