Temperature-mediated polymorphism: impact on packing motifs and charge transport

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We report a novel synthesis to ultra high purity 7,14-bis((trimethylsilyl)ethynyl)dibenzo[b,def]-chrysene (TMS-DBC). Single crystals of this material were grown by solution and vapor deposition techniques and structural determination by single crystal X-ray crystallography was then carried out at the Microfocus Crystallography beamline at the Australian Synchrotron. Two polymorphs of TMS-DBC were observed; low temperature (LT) fine red needles and high temperature (HT) large yellow platelets. These polymorphs represent a rare example where both are extremely stable and do not interconvert to the other crystal structure upon solvent or thermal annealing. Single crystal X-ray crystallographic studies identified two distinct packing structures where the LT crystals form a 1D slipped-stack structure, while the HT crystals adopt a 2D brickwork motif. Single crystal organic field-effect transistors of the LT and HT crystals showed the impact of packing motif on charge transport.

[1] Stevens, L. A. et al. (2015). Chem. Mater., 27, 112-118 **Keywords:** polymorphism, crystal packing, charge transport