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Supporting information for article:

Three polymorphs of a new *N,N'*-dipropylated isoindigo derivative

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S1. Characterization data of 1

3-(1,2-Dihydro-2-oxo-1-propyl-3*H*-indol-3-ylidene)-1,3-dihydro-1-propyl-2*H*-indol-2-one 1: m.p.: 402-405 K. ¹H-NMR (500 MHz, CDCl₃), δ[ppm]: 9.13 (*d*, *J* = 7.5 Hz, 2H), 7.44 (*t*, *J* = 7.8 Hz, 2H), 7.10(*d*, *J* = 8.0 Hz, 2H), 7.05 (*t*, *J* = 7.9 Hz, 2H), 3.76 (*t*, *J* = 7.3 Hz, 4H), 1.66 (*h*, *J* = 7.3 Hz, 4H), 0.92 (*t*, *J* = 7.5 Hz, 6H). ¹³C-NMR (500 MHz, CDCl₃), δ[ppm]: 11.472, 20.829, 41.594, 107.885, 121.687, 122.145, 129.919, 132.294, 133.543, 144.760, 167.929. HRMS (ESI) calc. for C₂₂H₂₃N₂O₂ ([M+H]⁺): 347.17541, found 347.17598.

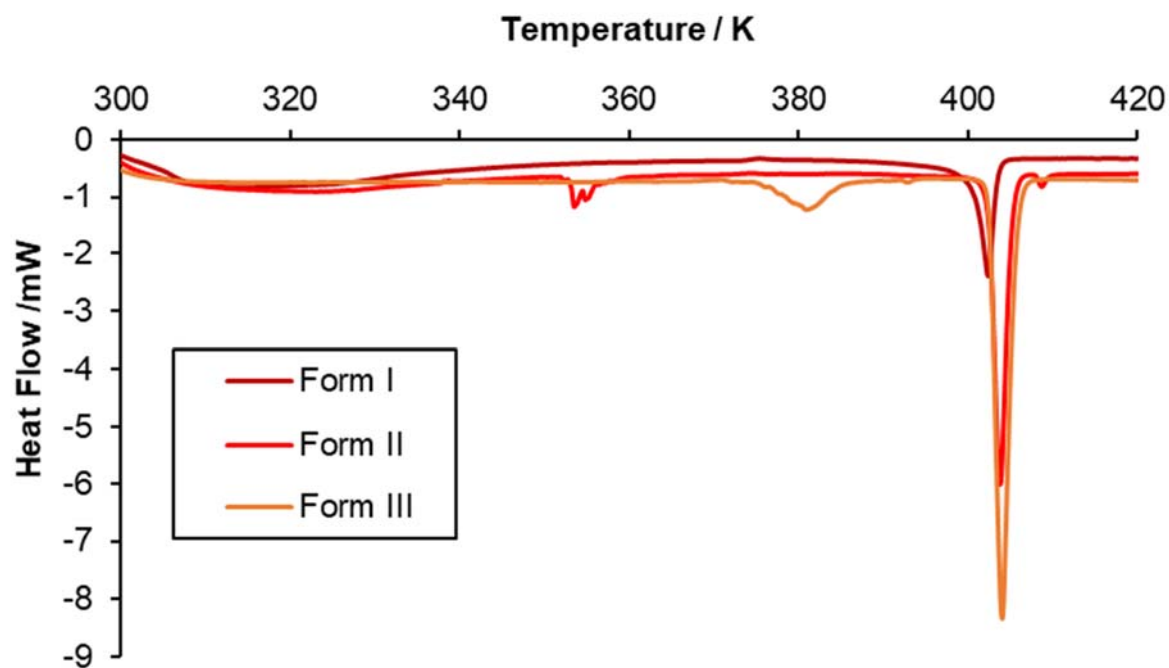


Figure S1 DSC profiles of Forms I, II and III.

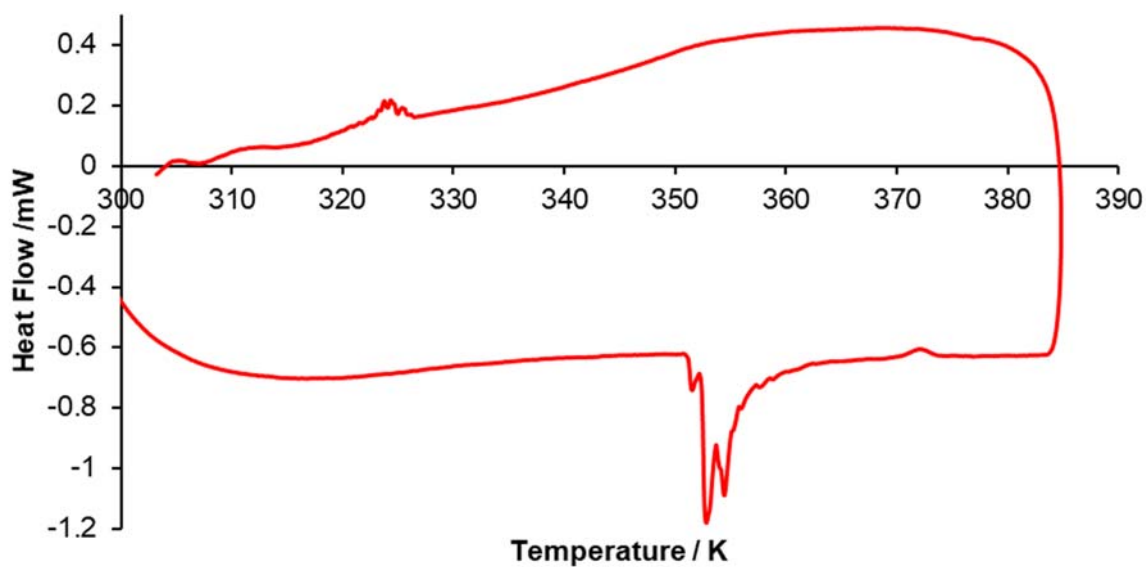


Figure S2 DSC profile of Form II in a heating-cooling cycle.

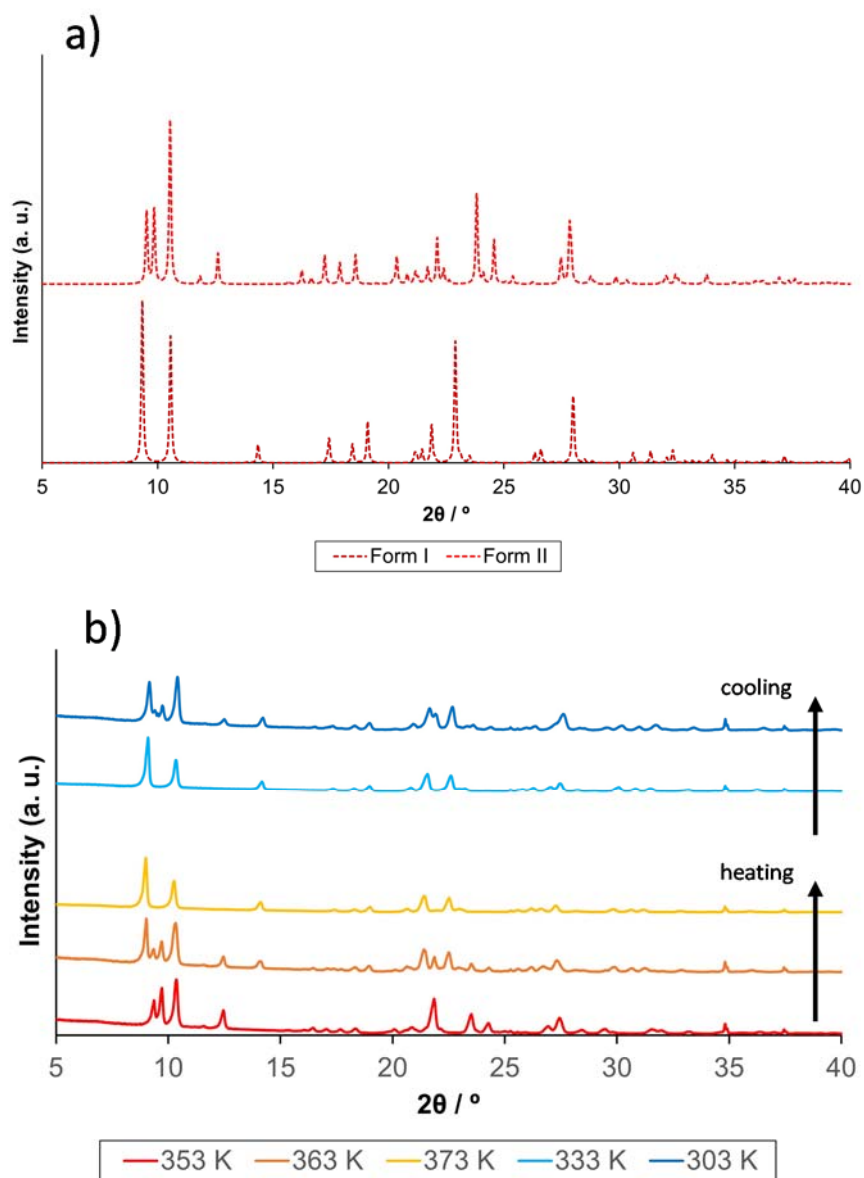


Figure S3 Variable-temperature PXRD profiles: a) Estimated PXRD profile from the X-ray data for Forms I, and II, and b) variable-temperature PXRD profiles of Form II.