

Electronic Supplementary Information (ESI)

New polymorphs of the cocrystal formers isonicotinamide and nicotinamide
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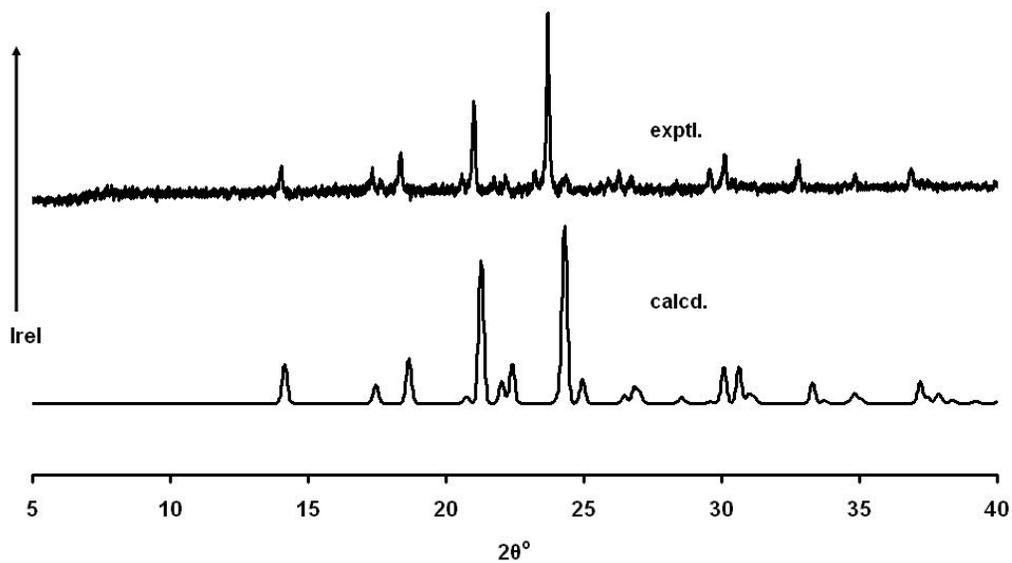


Fig. S1 Experimental (298 K) and computed (173 K) PXR D patterns for Iso3.

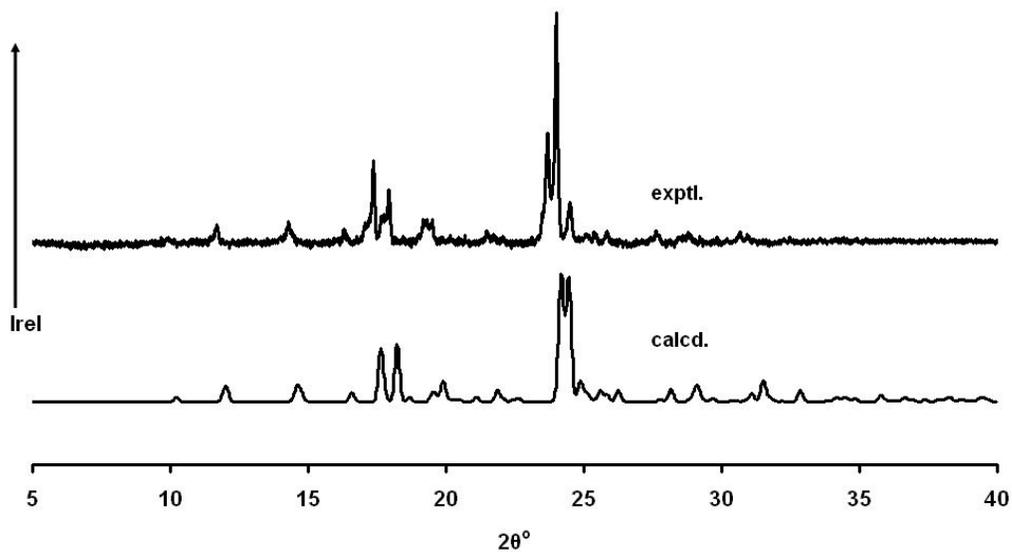


Fig. S2 Experimental (298 K) and computed (173 K) PXR D patterns for Nic2.

NOTES:

Powder X-ray diffraction patterns were measured using a Philips PW1120/00 X-ray generator with nickel-filtered $\text{CuK}\alpha_1$ radiation ($\lambda = 1.5406 \text{ \AA}$). The generator, which was fitted with a Huber long fine-focus tube PW2273/20 and a Huber Guinier Monochromator Series 611/15, produced X-rays at 20 mA and 40 kV. The PXRD patterns were then recorded using a Huber Imaging Plate Guinier Camera 670. Samples were very gently manually ground and packed into Markröhrchen non-diffracting glass capillaries supplied by Hilgenberg (Germany). In this study, samples were exposed to radiation for 20 min depending on the quantity and quality of the sample. A 2θ range of 5 to 40.0° was used with a step size of $0.005^\circ 2\theta$.

For each polymorph, there is reasonable correspondence between the relative peak intensities in the experimental and computed traces. In both cases, the computed peaks are generally shifted to slightly higher 2θ -angles owing to the low temperature of the single crystal X-ray diffraction data.