Supporting Information

for

Mechanochemical Knoevenagel condensation

investigated in situ

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Raman spectra and XRPD data
Figure S1: Time-resolved Raman spectra measured simultaneously. The progress of the reaction can be detected from the decreasing signal of the C=O-stretching band of 1 at 1706 cm\(^{-1}\) (green) and the increasing signal of the C=C-stretching band at 1581 cm\(^{-1}\) (blue). The band attributed to the C≡N-stretching shifts from 2266 cm\(^{-1}\) (yellow) in 2 to 2233 cm\(^{-1}\) (red) in the product.
Figure S2: Quantitative evaluation of the PXRD reflections intensities of selected reactant (red (11-2) reflection of 1) and product reflections (blue (002) reflection of 3).

The PXRD data are representative measurements of repeated sets measured at two different beam times (intensive colour November 2016 and light colour August 2017). The data indicate a high reproducibility of the results. The cause of the reaction can be divided in three steps. First a fast consumption of the reactant 1 is observed. After 11 minutes a decelerated consumption is observed. The formation of the product 3 starts after approx. 35 minutes and is characterized by a slow (until approx. 48 min.) and finally a very fast conversion.