Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting information

Determining the Kinetics of Desolvation of a TNT/Aniline Solvate

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Table S1. Crystal data and structure of TNT and TNT/aniline solvates

	Monoclinic TNT[1]	Orthorhombic TNT[1]	TNT/aniline[2]
Formula weight	227.14	227.14	320.27
Crystal system	monoclinic	orthorhombic	orthorhombic
Space group	$P2_1/a$	$Pca2_1$	Pnma
a/Å	14.9113(1)	14.910(2)	18.726(2)
b/Å	6.0340(1)	6.034(2)	10.9375(13)
c/Å	20.8815(3)	19.680(4)	6.7023(8)
α, β, γ /°	α = γ = 90°, β = 110.365(1)	α = β = γ = 90°	α = β = γ = 90°
V/Å^3	1761.37(4)	1770.6(7)	1372.3(3)
Z	8	8	4
ρ/g cm^{-3}	1.654	1.654	1.550

1. R. M. Vrcelj, J. N. Sherwood, A. R. Kennedy, H. G. Gallagher and T. Gelbrich, *Cryst. Growth Des.*, 2003, ***3***, 1027–1032.
2. CCDC 1919306. CCDC 1919306 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S2. Mean Statistical parameters calculated by model-fitting method

		Integral form of rate equation	26 °C		35 °C		45 °C		60 °C	
		$g(\alpha) = kt$	S_K	R_K^2	S_K	R_K^2	S_K	R_K^2	S_K	R_K^2
Geometrical contraction models	Contracting cylindrical (R2)	$1-(1-\alpha)^{\frac{1}{2}} = kt$	5.80×10^{-9}	0.9998	3.59×10^{-8}.	0.9978	2.00×10^{-8}	0.9999	1.59×10^{-7}	0.9998
	Contracting spherical (R3)	$1-(1-\alpha)^{\frac{1}{3}} = kt$	1.73×10^{-8}	0.9980	5.22×10^{-8}	0.9921	4.72×10^{-8}	0.9986	4.10×10^{-7}	0.9990
Diffusion models	1-D diffusion (D1)	$\alpha^2 = kt$	5.55×10^{-8}	0.9856	1.27×10^{-7}	0.9781	1.90×10^{-7}	0.9899	1.17×10^{-6}	0.9938
	2-D diffusion (D2)	$[(1-\alpha)\ln(1-\alpha)] + a = kt$	7.24×10^{-8}	0.9607	1.62×10^{-7}	0.9417	2.64×10^{-7}	0.9684	1.75×10^{-6}	0.9779
	3-D diffusion-Jander (D3)	$\left(1-(1-\alpha)^{\frac{1}{3}}\right)^2 = kt$	4.89×10^{-8}	0.8970	1.04×10^{-7}	0.8589	1.83×10^{-7}	0.9102	1.33×10^{-6}	0.9269
	Ginstling-Brounshtein (D4)	$1-\frac{2}{3}\alpha-(1-\alpha)^{\frac{2}{3}} = kt$	2.37×10^{-8}	0.9431	5.20×10^{-8}	0.9179	8.74×10^{-8}	0.9526	6.02×10^{-7}	0.9647
Reaction-order models	First-order (F1)	$-ln(1-\alpha) = kt$	2.02×10^{-7}	0.9757	4.67×10^{-7}	0.9620	7.08×10^{-7}	0.9817	$4..74 \times 10^{-6}$	0.9935
	Second-order (F2)	$[1(1-\alpha)] - 1 = kt$	2.63×10^{-6}	0.7531	5.23×10^{-6}	0.7011	9.74×10^{-6}	0.7735	7.84×10^{-5}	0.7885
	Third-order (F3)	$\frac{1}{2}[(1-\alpha)]^{-2} - 1 = kt$	2.95×10^{-5}	0.4845	5.53×10^{-5}	0.4307	1.07×10^{-4}	0.4943	9.30×10^{-4}	0.5121

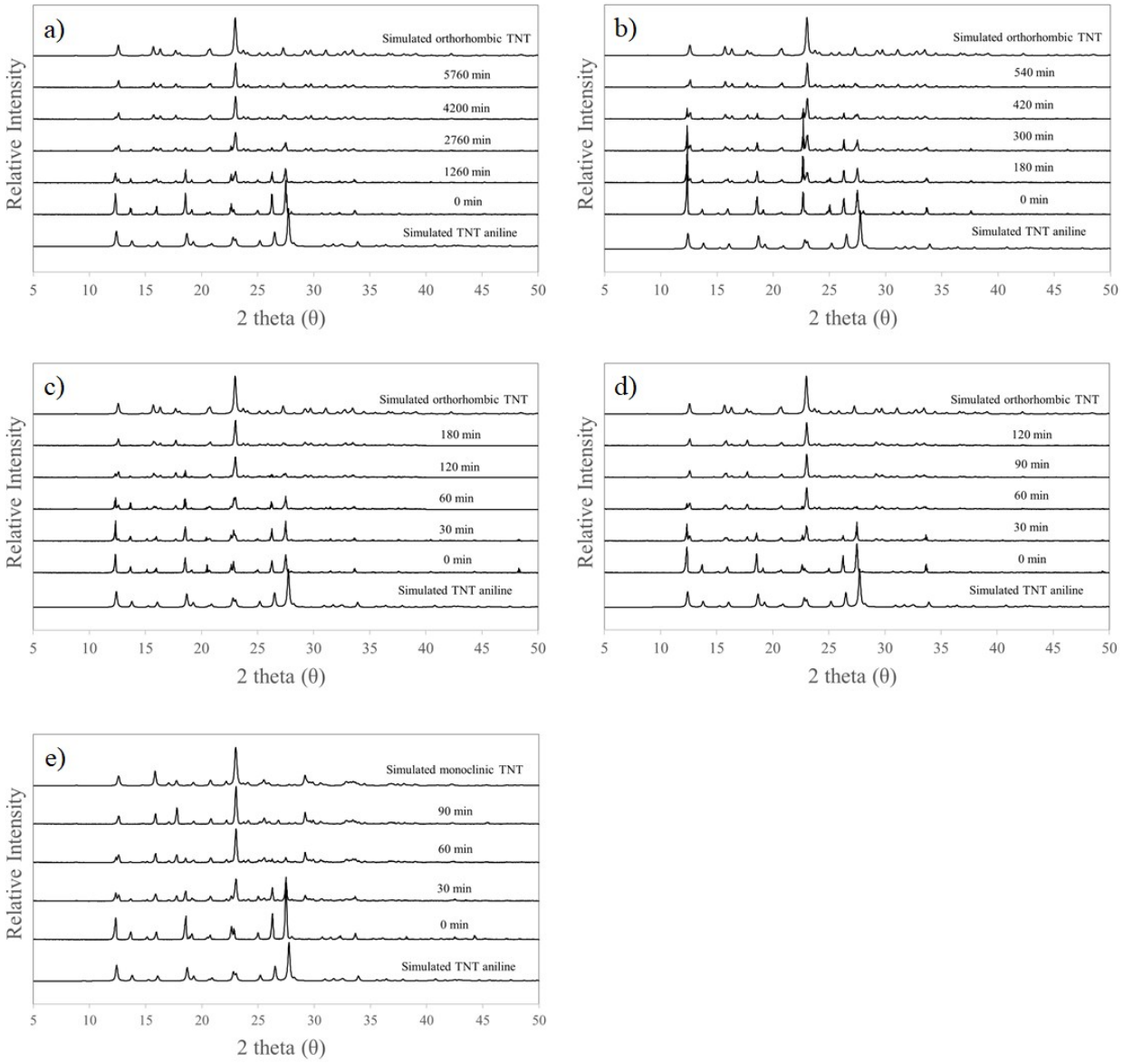

Figure S1. The changes of PXRD Patterns with time at a) RT; b) 45 °C; c) 60 °C; d) 65 °C; e) 70 °C. Simulated PXRD patterns for two polymorphic forms of TNT (monoclinic and orthorhombic) and TNT aniline are also displayed together.

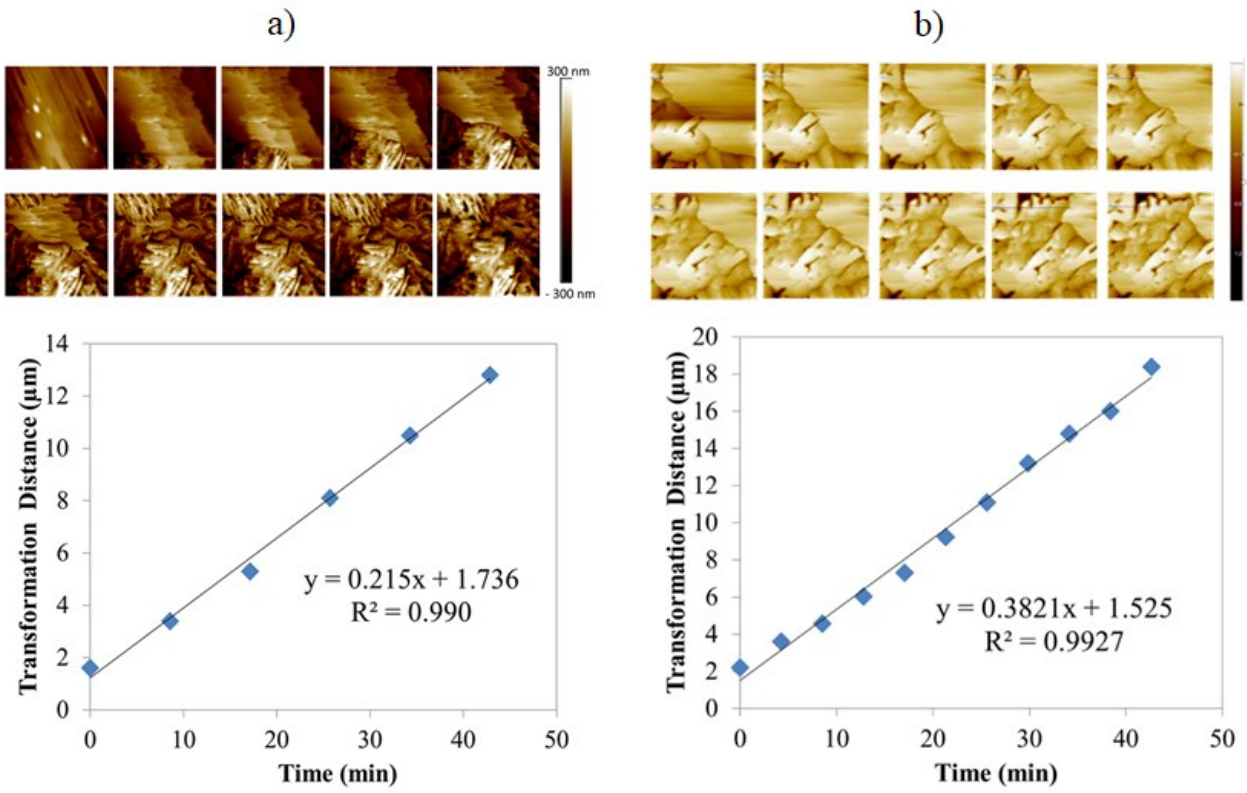

Figure S2. AFM measurement of growth of new crystalline phase at a) 26 °C and b) 45 °C.