

## Supporting Information

### Polymorphism, Phase Transformation and Energetic Properties of 3-Nitro-1,2,4-triazole

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**Table S1:** 3-Nitro-1,2,4-triazole crystallized from various solvents

Solvent	Solubility	Crystallization method	Crystal Form
methanol	Soluble	SE	Form I
acetone	Soluble	SE	Form I
ethanol	Soluble	SE	Form I
ethyl acetate	Soluble	SE	Form I
<b>Mixture of Solvents in a 1:1 ratio</b>			
Methanol & Ethyl acetate	Soluble	SE	Form I

SE – Slow Evaporation at room temperature

**Table S2:** 3-Nitro-1,2,4-triazole crystallized from various solvents and additive

Solvent	Component 2	Crystallization method	Crystal Form
methanol	hydrazine hydrate	SE	Form I
methanol	hydroxylamine	SE	Form I
acetone	dichloromethane	SE	Form I
methanol & ethyl acetate (1:1)	hydrazine hydrate	SE	Form I
methanol & ethyl acetate (1:1)	hydroxylamine	SE	<b>Form II</b>

**Table S3.** Hydrogen Bond Parameters (distances, Å and angles, deg)

	Form I		Form II	
	D...A	∠D-H...A	D...A	∠D-H...A
N-H...O	3.2385	114.979	3.3734	116.402
	3.4087	108.694	3.0887	118.364
	3.8411	111.549	3.0599	117.368
			3.2057	105.560
C-H...O	3.3945	130.188	3.5083	145.183
	3.2799	133.444	3.3483	116.837
	3.1501	121.667	3.1150	123.078
			3.3863	141.716
			3.4732	112.768
			3.0489	116.884

**Table S4.** Transition temperatures (°C) observed for the polymorphic transformation in different methods.

Crystal Forms	DSC	TG	Variable Temp PXRD	SCSC Reactivity
I	Not observed	Not observed	Not observed	Not observed
II → I	98	98	98-115	98-115

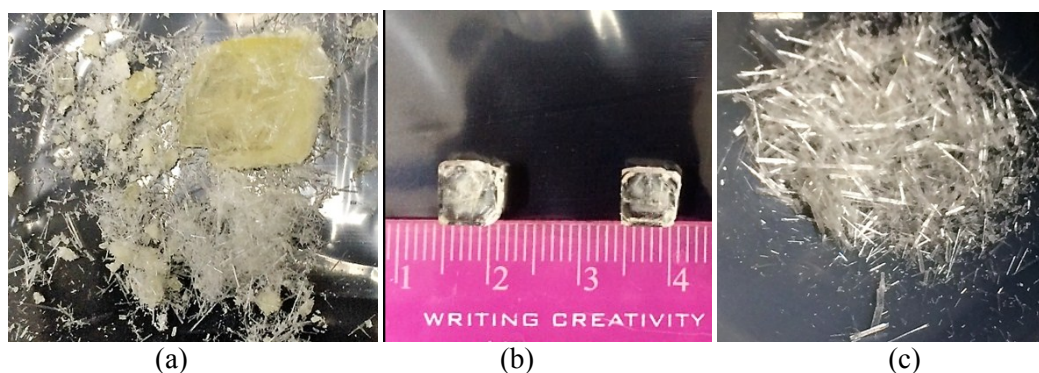


Figure S1: polymorphs of 3-Nitro-1,2,4-triazole (a) Forms I (tetragonal) and II (monoclinic); (b) isolated single crystals of Forms I of 3-Nitro-1,2,4-triazole. (c) isolated single crystals of Forms II of 3-Nitro-1,2,4-triazole.

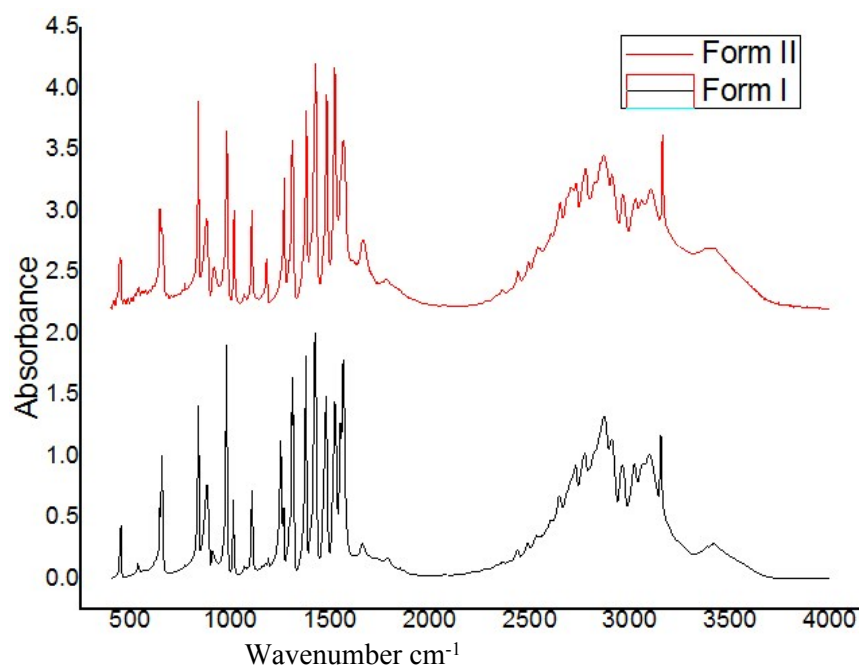


Figure S2: IR spectra of the 3-Nitro-1,2,4-triazole : Forms I and Forms II.