

# Three Insensitive Energetic Cocrystals: Cocrystals of 1-Nitronaphthalene

## Supplementary Information (SI)

### SI 1. Infrared Spectroscopy (IR)

IR Spectra were recorded on a IR Prestige-21 infrared Spectrophotometer, using KRS-5 pellets. The IR spectra were collected for 64 scans at  $4\text{cm}^{-1}$  resolution.

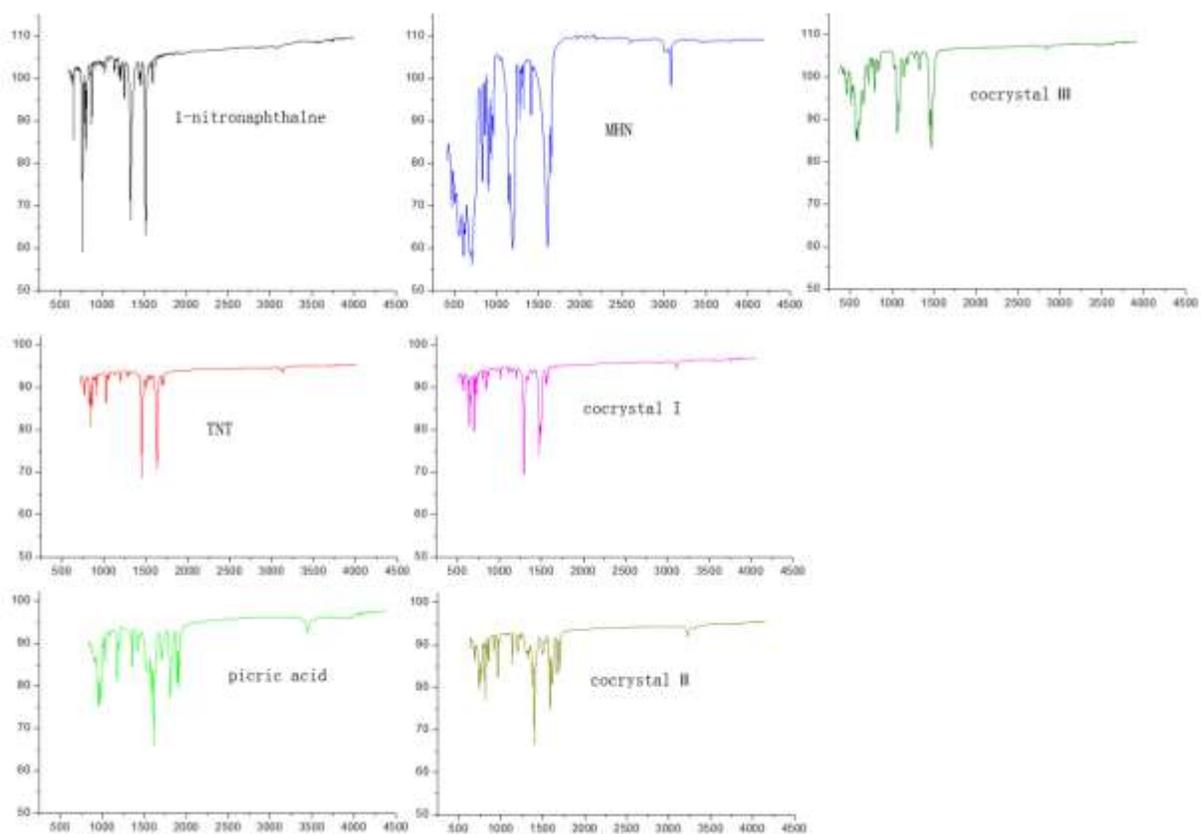


Figure S1. IR spectra for 1-nitronaphthalene, TNT, picric acid, MHN, cocrystal I, cocrystal II, cocrystal III

Table S1. Experimental IR peak positions and transmittance (%) for 1-nitronaphthalene, TNT, picric acid, MHN, cocrystall, cocrystalllland cocrystalllll

1-nitronaphthalene		TNT		Picric acid		MHN		cocrystall		cocrystallll		cocrystalllll	
Wavenu mber	Transmit tance	Wavenu mber	Transmit tance	Wavenu mber	Transmit tance	Wavenu mber	Transmit tance	Wavenu mber	Transmit tance	Wavenu mber	Transmit tance	Wavenu mber	Transmit tance
(cm <sup>-1</sup> )	(%)	(cm <sup>-1</sup> )	(%)	(cm <sup>-1</sup> )	(%)	(cm <sup>-1</sup> )	(%)	(cm <sup>-1</sup> )	(%)	(cm <sup>-1</sup> )	(%)	(cm <sup>-1</sup> )	(%)
661.0	86.2	646.7	90.7	700.9	68.4	598.4	40.4	648.4	92.6	648.4	91.3	681.5	84.3
774.1	59.5	719.1	73.1	915.1	79.1	725.3	24.6	714.6	77.4	692.2	80.0	726.3	80.9
809.8	83.4	804.8	92.4	1082.6	87.0	830.2	21.6	781.8	76.1	771.0	73.9	804.1	64.3
875.2	89.1	910.0	85.38	1160.5	92.2	924.9	49.1	915.1	94.4	871.3	95.3	1004.7	86.5
1330.9	67.3	1081.3	98.6	1350.3	52.6	999.4	46.1	1350.3	56.5	915.1	84.8	1260.8	67.8
1465.1	99.1	1357.8	43.0	1428.2	89.6	1272.5	26.7	1517.8	65.2	1082.6	91.3	1528.5	95.3
1517.7	63.2	1417.0	94.9	1540.2	72.2	1346.0	71.5	1618.1	97.4	1138.1	95.72	1662.9	60.0
1599.3	99.1	1529.1	51.0	1618.1	77.4	1472.9	73.2	3111.6	103.1	1350.3	53.9		
		1614.8	96.4	3111.6	100.0	1651.3	27.0			1439.9	94.8		
		3108.8	104.0			2988.3	82.6			1517.8	69.1		
										1550.9	81.3		
										1606.4	87.8		
										3100.9	102.2		