

Three Insensitive Energetic Cocrytals: Cocrytals 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 4cm^{-1} resolution.

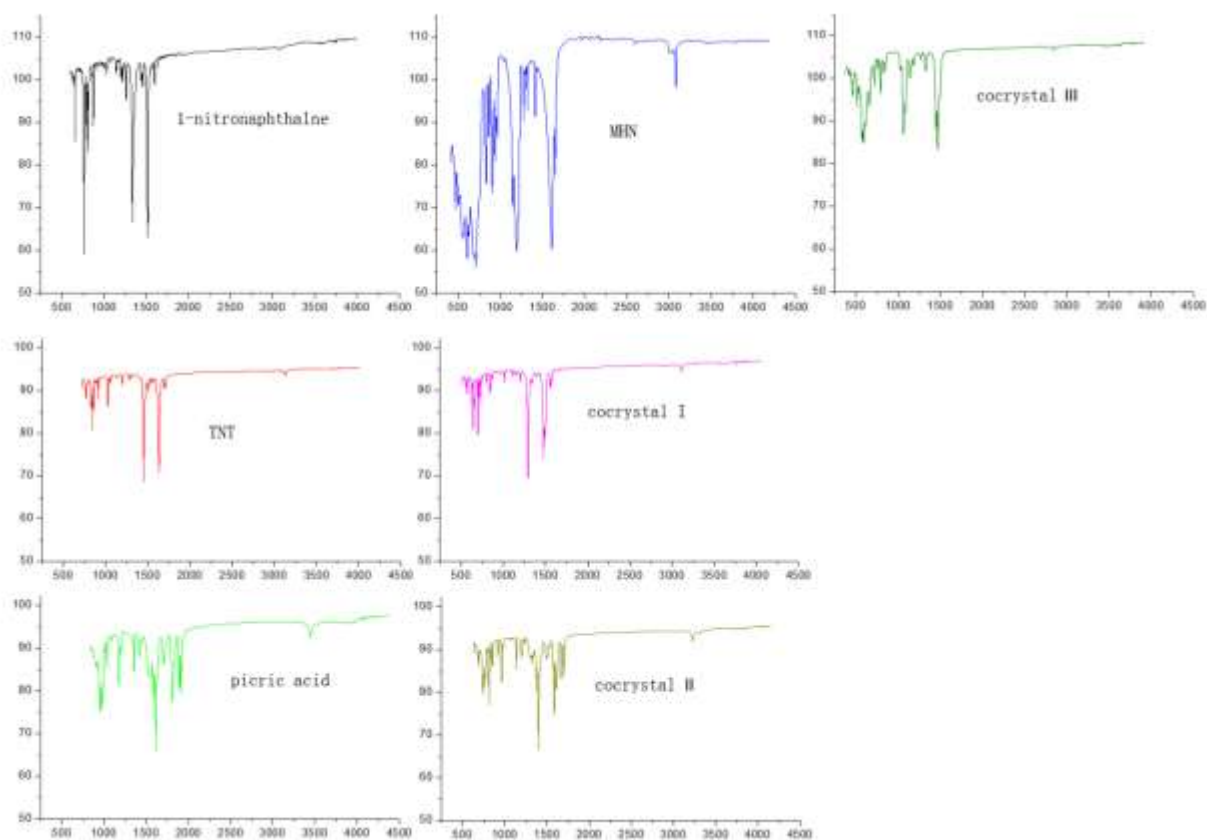


Figure S1. IR spectra for 1-nitronaphthalene, TNT, picric acid, MHN, cocrytalI, cocrytalII, cocrytalIII

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

1-nitronaphthalene		TNT		Picric acid		MHN		cocrystall		cocrystallII		cocrystallIII	
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 ⁻¹)	(%)	(cm ⁻¹)	(%)	(cm ⁻¹)	(%)	(cm ⁻¹)	(%)	(cm ⁻¹)	(%)	(cm ⁻¹)	(%)	(cm ⁻¹)	(%)
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		