

Supporting Information (SI)

A Novel Insensitive Cocrystal Explosive Composed of BTF and the Non-Energetic 2-Nitroaniline

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SI 1. HPLC Data

Figure S1. Chromatogram.

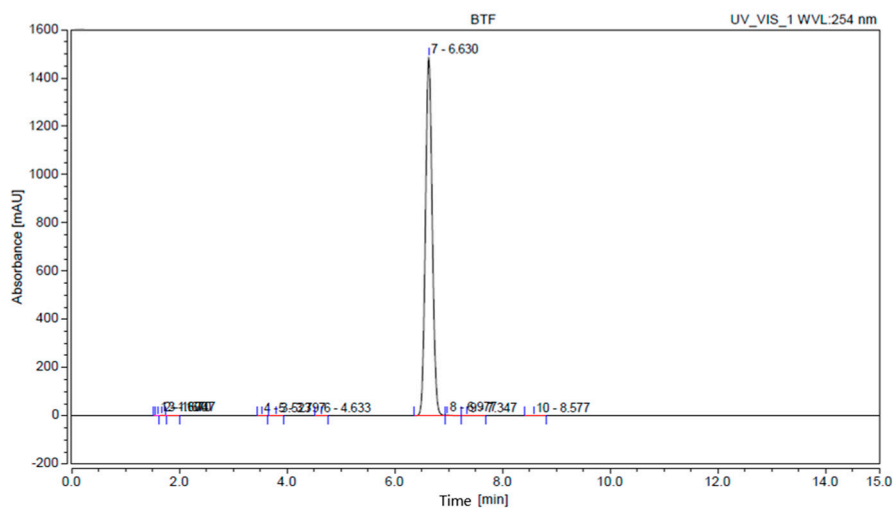


Table S1. Accumulated points of chromatogram.

Number	Time (min)	Peak area (mAU*min)	Peak height (mAU)	Relative peak area (%)	Relative peak height (%)
1	1.600	0.001	0.024	0.00	0.00
2	1.670	0.159	1.737	0.07	0.12
3	1.747	0.000	0.008	0.00	0.00
4	3.523	0.011	0.143	0.01	0.01
5	3.797	0.017	0.192	0.01	0.01
6	4.633	0.012	0.115	0.01	0.01
7	6.630	216.864	1487.489	99.73	99.69
8	6.977	0.318	2.049	0.15	0.14
9	7.347	0.052	0.255	0.02	0.02
10	8.577	0.010	0.060	0.00	0.00

SI 2. Crystallographic Data

Table S2. Crystallographic data and refinement parameters for BTF/ONA cocrystal.

BTF/ONA cocrystal			
Formula	C ₁₂ N ₈ O ₁₂ H ₆	α (°)	90
MW (g/mol)	390.263	β (°)	101.786 (3)
Stoichiometry	1:1	γ (°)	90
CCDC number	2053697	V (Å ³)	1493.5 (14)
Crystal system	monoclinic	cell volume (Å ³)	2962.53 (13)
Color	light yellow	Z	4
Space group	P2 ₁ /n	ρ_{calc} (g/cm ³)	1.750
Temperature (K)	2	$h_{\text{min, max}}$	−14, 16
a (Å)	13.6285 (4)	$k_{\text{min, max}}$	−16, 15
b (Å)	13.8193 (3)	$l_{\text{min, max}}$	−16, 18
c (Å)	16.0688 (4)	ωR_2 [all data]	0.3066

SI 3. Powder X-ray Diffraction (PXRD)

Table S3. Characteristic peaks in XRD patterns of BTF/ONA, BTF, and ONA

Component	Characteristic peaks (°)
BTF	19.17, 23.11, 26.06, 29.50
ONA	12.02, 14.90, 25.52, 27.26, 29.96
BTF/ONA	10.88, 16.50, 25.55, 26.49, 30.94

Figure S3. XRD patterns of other BTF cocrystals.

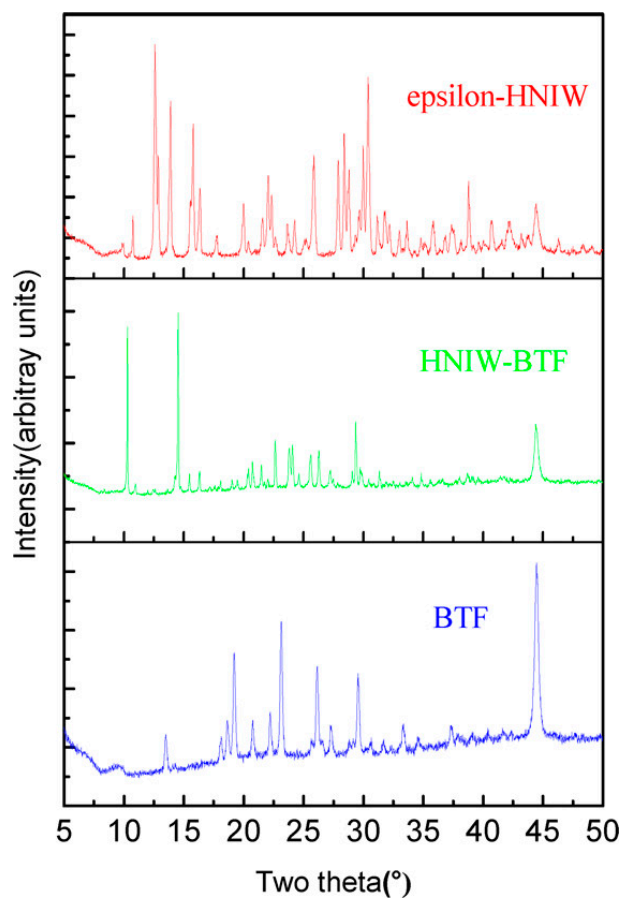


Figure S3. XRD patterns of BTF/CL–20 cocrystal. The characteristic peaks of the BTF/CL–20 cocrystal are near 10° and 14.9°.

SI 4. Infrared Spectroscopy (IR)

Table S4. Experimental IR peak positions and transmittance (%) for BTF/ONA, BTF, and ONA.

BTF		BTF/ONA		ONA	
Wavenumber	Transmittance	Wavenumber	Transmittance	Wavenumber	Transmittance
(cm ⁻¹)	(%)	(cm ⁻¹)	(%)	(cm ⁻¹)	(%)
1650.7	4.2	3495.4	55.7	3102.9	43.5
1567.8	8.7	3384.5	49.1	1633.4	39.5

1417.4	38.5	1652.7	10.7	1610.3	32.2
1290.1	57.6	1621.8	34.7	1529.3	31.1
1078.0	48.5	1569.8	18.7	1342.2	25.4
962.3	24.8	1502.3	38.2	1270.9	33.1
806.1	40.3	1346.1	44.3	1085.8	38.0
647.9	45.4	1284.4	55.1	917.9	40.0
439.7	56.2	964.2	41.1	730.9	39.4
		806.1	55.1	703.9	37.7
		750.2	56.0		
		646.0	60.4		

SI 5. Differential Scanning Calorimetry (DSC)

Figure S5. DSC curves of BTF/CL–20 cocrystal.

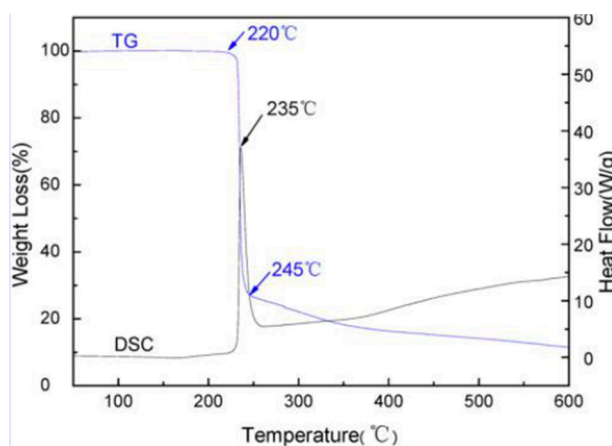


Figure S5. DSC curves of BTF/CL–20 cocrystal. A strong exothermic peak at 235 °C is attributed to the decomposing event of the cocrystal.

References

1. Yang, Z.; Li, H.; Zhou, X.; Zhang, C.; Huang, H.; Li, J.; Nie, F. Characterization and Properties of a Novel Energetic–Energetic Cocrystal Explosive Composed of HNIW and BTF. *Crystal Growth & Design*