

Probing the reaction mechanisms of 3,5-difluoro-2,4,6-trinitroanisole (DFTNAN) through a comparative study with trinitroanisole (TNAN)

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Figures

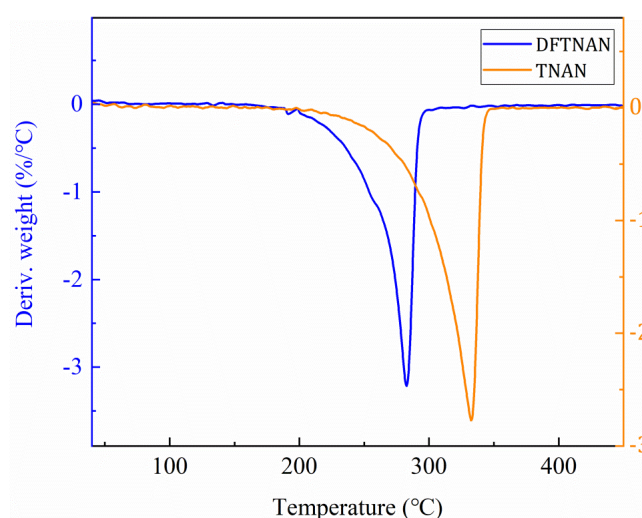


Figure S1. DTG curves of DFTNAN and TNAN.

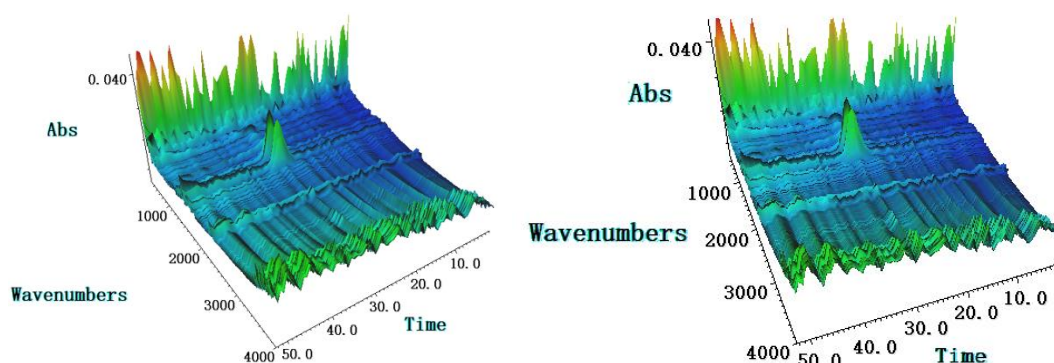


Figure S2. 3D FTIR spectrum of the pyrolysis gaseous products of DFTNAN and TNAN.

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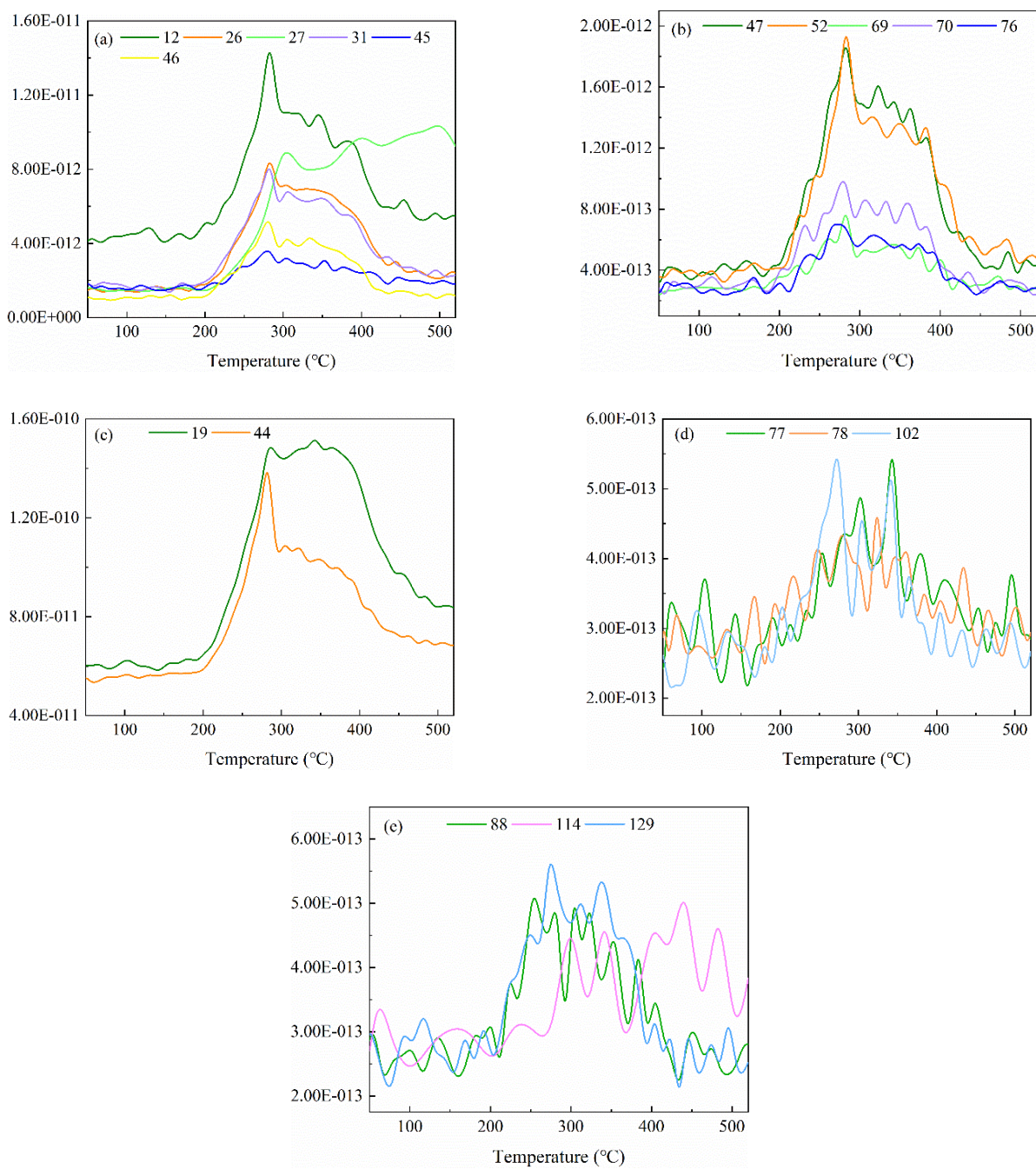


Figure S3. MS curves of the pyrolysis gaseous products of DFTNAN.

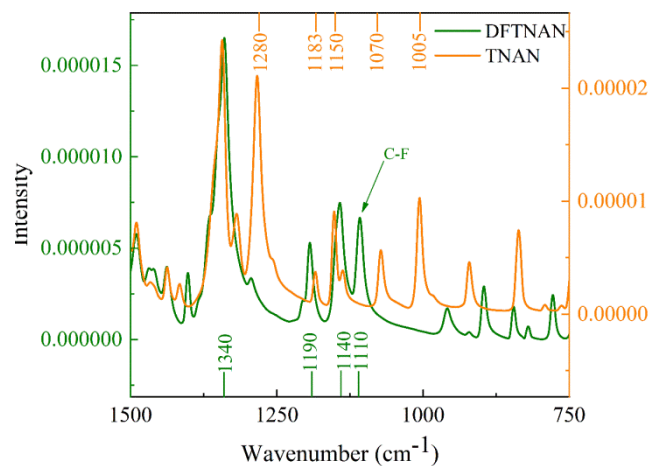


Figure S4. FTIR spectrum of the DFTNAN and TNAN

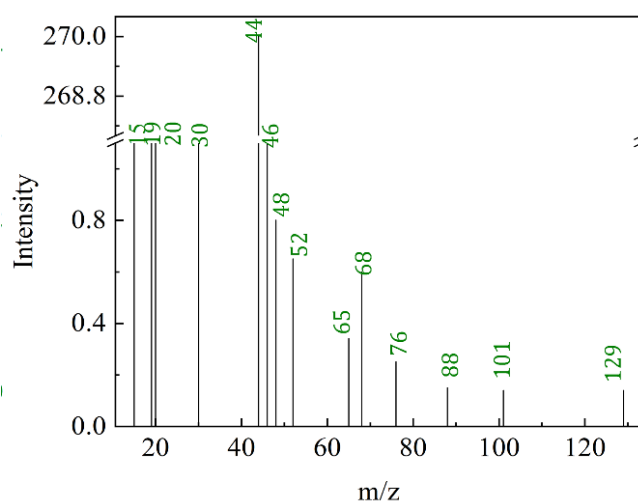


Figure S5. MS curves of the pyrolysis gaseous products of TNAN.


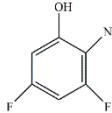
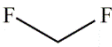
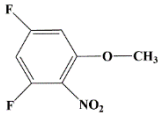
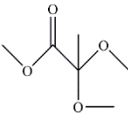
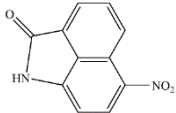
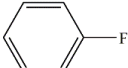
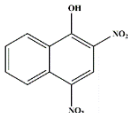
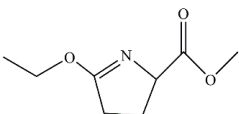
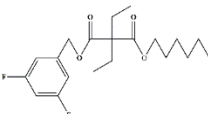
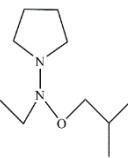
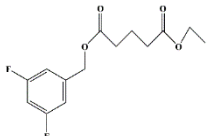
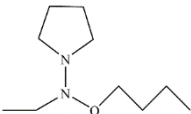
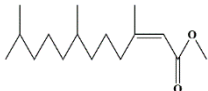
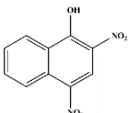
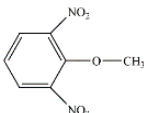
Tables

Table S1. The m/z of Py-MS and possible assignments

m/z	Possible assignments	m/z	Possible assignments
1	H	44	CO ₂ 、N ₂ O
2	H ₂	45	COOH
12	C	46	HCOOH,NO ₂ ,C ₂ FH, C ₂ H ₆ O
14	N	47	C ₂ FH ₂
15	CH ₃	48	C ₂ FH ₅
16	O, CH ₄	50	CF ₂

17	OH, NH ₃	52	CH ₂ F ₂
18	H ₂ O, NH ₄	64	C ₂ H ₂ F ₂
19	F	66	CF ₂ O
20	HF	68	NOF ₂
26	C ₂ H ₂	69	CF ₃
27	HCN	70	CHF ₃
28	CO, N ₂	76	C ₃ H ₂ F ₂
30	NO	77	C ₃ F ₂ H ₃
31	CF	78	C ₃ F ₂ H ₄
32	CH ₃ OH	88	CF ₄ 、C ₅ H ₁₂ O
33	NF	102	C ₅ H ₄ F ₂
34	CFH ₃	114	C ₆ H ₄ F ₂
38	F ₂	129	C ₆ H ₃ F ₂ O

Table S2. Gaseous products of DFTNAN after T-jump pyrolysis identified by GC-MS (Retention time with corresponding molecular structures).

RT _{DFTNAN}	m/z	Chemical	Structure	RT _{DFTNAN}	m/z	Chemical	Structure
1.5	86	C ₅ H ₁₀ O		14.7	175	C ₆ H ₃ F ₂ NO ₃	
1.6	52	CH ₂ F ₂		15.3	189	C ₇ H ₅ F ₂ NO ₃	
2.2	148	C ₆ H ₁₂ O ₄		15.7	214	C ₁₁ H ₆ N ₂ O ₃	
3.1	96	C ₆ H ₅ F		15.8	234	C ₁₀ H ₆ N ₂ O ₅	
3.4	171	C ₈ H ₁₃ NO ₃		15.9	370	C ₂₀ H ₂₈ F ₂ O ₄	
9.5	186	C ₁₀ H ₂₂ N ₂ O		16.3	286	C ₁₄ H ₁₆ F ₂ O ₄	
9.6	186	C ₁₀ H ₂₂ N ₂ O		16.6	254	C ₁₆ H ₃₀ O ₂	
13.6	234	C ₁₀ H ₆ N ₂ O ₅		17.1	198	C ₇ H ₆ N ₂ O ₅	

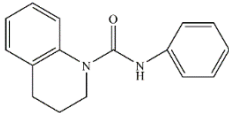
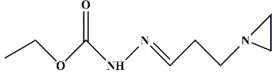
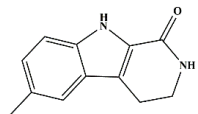
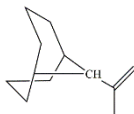
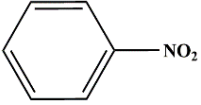
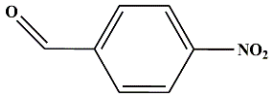
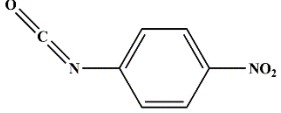
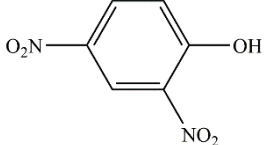
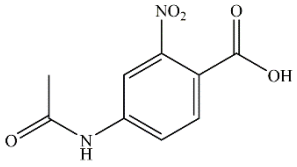
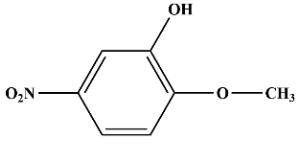
13.8	252	$C_{16}H_{16}N_2O$		18.5	185	$C_8H_{15}N_3O_2$	
13.9	200	$C_{12}H_{12}N_2O$		20.9	164	$C_{12}H_{20}$	

Table S3. Gaseous products of TNAN after T-jump pyrolysis identified by GC-MS (Retention time with corresponding molecular structures).

RT_{TNAN}	m/z	Chemical	Structure
10.9	123	$C_6H_5NO_2$	
13.7	151	$C_7H_5NO_3$	
14.6	164	$C_7H_4N_2O_3$	
15.2	184	$C_6H_4N_2O_5$	
15.7	224	$C_9H_8N_2O_5$	
16.8	169	$C_7H_7NO_4$	
17.4	243	$C_7H_5N_3O_7$	