Supporting Information

Ultraviolet-Initiated Decomposition of Solid 1,1-Diamino-2,2-Dinitroethylene (FOX-7)

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Table S1. Experimental infrared band positions of FOX-7 compared to previous values.

Mode	This work (cm^{-1})	Thin Layer[a] (cm^{-1})	Powder[a] (cm^{-1})	Assignment[a]
1	3425	3425		$\nu_{as}(NH_2)$
2	3396	3406	3402	$\nu_{as}(NH_2)$
3	3333	3333	3329	$\nu_{s}(NH_2)$
4	3292	3298	3295	$\nu_{s}(NH_2)$
5	1635	1633	1632	$\nu_{s}(C–NH_2)$
6	1608	1608	1605	$\delta_{s}(NH_2)$
7	1529	1523	1520	$\delta_{s}(NH_2)$
8	1506	1503		$\nu(C–C)$
	1474	1470	1470	$\nu_{17} + \nu_{24}$
	1457			
9	1391	1392	1390	$\nu(C–C)$
10	1358	1352	1350	$\nu_{as}(NO_2)$
11		1312		$\rho(NH_2)$, $\nu_{s}(C–NO_2)$
	1258			$\rho(NH_2)$, $\nu_{as}(C–NO_2)$
12	1221	1221	1212	
13	1167	1169	1166	$\rho(NH_2)$, $\nu_{s}(NO_2)$
14	1141 1127	1141	1140	$\rho(NH_2)$, $\nu_{s}(NO_2)$
15	1064	1063		$\rho(NH_2)$
16	1022	1025	1022	$\rho(NH_2)$
17	858	858	857	$\delta_{s}(NO_2)$
18	786 775	790	789	$\tau(NH_2)$
19	750	751	749	$\delta_{s}(NO_2)$
20	738	739	738	$\delta(C−NO_2)$, $\tau(NH_2)$
21	678	674	673	$\delta(C−NO_2)$, $\tau(NH_2)$
22		644		$\omega(NH_2)$
23	633	635	636	$\tau(NH_2)$
24		620	617	$\tau(NH_2)$

Notes:
[a] Data and assignments from Turner et al. 2022.[1] Thin layer solid sample recorded under UHV conditions and powdered sample spectrum obtained at ambient conditions

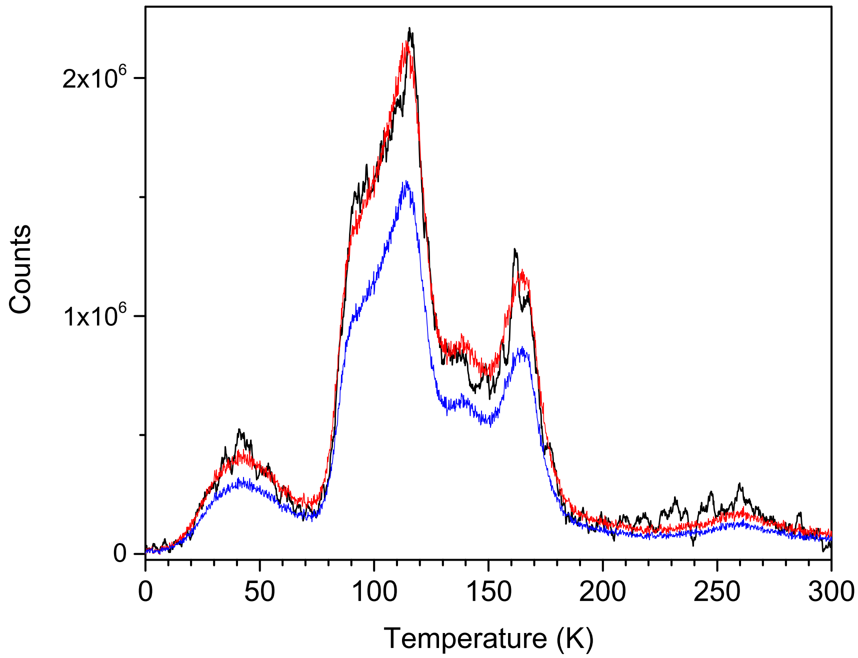

Figure S1. TPD profile of FOX-7 recorded using QMS of m/z = 45 (black) compared to the adjusted signal of m/z = 44 assuming natural isotopic abundances of CO_2 (i.e., $^{13}CO_2$, in red) and N_2O ($^{14,15}N_2O$, blue). Oxygen-17 also provided an insignificant contribution to each. The profile at m/z = 45 closely matches the expected $^{13}CO_2$ signal.

Table S2. Energetics of reactions displayed in Figure 7 including the change in free energy of the reaction (Δ_rG) and any known positive reaction barriers (E_a). Species in red are products with observed mass spectral signals.

	Reaction	E_a (kJ mol^{-1})	Δ_rG (kJ mol^{-1})	Ref.
R1	$(NH_2)_2CC(NO_2)_2 \rightarrow (NH_2)_2CC(NO_2)(ONO)$	273	−18	1
R2	$(NH_2)_2CC(NO_2)(ONO) \rightarrow (NH_2)_2CC(O)(NO_2)$ + **NO**		−15	1
R3	$(NH_2)_2CC(O)(NO_2) \rightarrow (NH_2)_2CCO$ + **NO_2**		169	2
R4	$(NH_2)_2CCO \rightarrow C(NH_2)_2$ + **CO**	52	−12	2
R5	$(NH_2)_2CC(O)(NO_2) \rightarrow (NH_2)_2CO_2$ + **NO**	151	−133	2
R6	$(NH_2)_2CO_2 \rightarrow C(NH_2)_2$ + **CO_2**	55	45	2
R7	$(NH_2)_2CC(NO_2)_2 \rightarrow (NH_2)_2CC(NO_2)(NO) + O$	385	346	1
R8	$CO + O \rightarrow$ **CO_2**		526	3, 4
R9	$(NH_2)_2CC(O)(NO_2) \rightarrow (NH_2)C(NH)CO + HONO$		125	2
R10	$(NH_2)C(NH)CO \rightarrow HNCNH_2$ + **CO**	59	37	2
R11	$HONO \rightarrow OH$ + **NO**		198	2
R12	$OH + H \rightarrow$ **H_2O**		−492	5
R13	$(NH_2)_2CC(NO_2)_2 \rightarrow (NH_2)_2CCNO_2$ + **NO_2**		300	1
R14 R15	$(NH_2)_2CCNO_2 \rightarrow (NH_2)C(NH)CHONO$ $(NH_2)C(NH)CHONO \rightarrow (NH_2)C(NH)CHO$ + **NO**	131	−359	1, 2
R16	$(NH_2)C(NH)CHO \rightarrow NHCNH_2 + HCO$		−386	2, 6
R17	$C(NH_2)_2 + O \rightarrow$ **$(NH_2)_2CO$**		468	7-9
R18	$C(NH_2)_2 \rightarrow$ **HNCNH** + H_2	221	−7	2
R19	$NHCNH_2 \rightarrow HNC + NH_2$		−33	9, 10
R20	$NH_2 + H \rightarrow$ **NH_3**		−444	11
R21	$NH_2 + HCO \rightarrow$ **NH_2CHO**		−409	12
R22	$CN + CN \rightarrow$ **NCCN**		−565	13
R23	$NH_2 + CN \rightarrow$ **NH_2CN**		−485	12
R24	$(NH_2)_2CC(NO_2)_2 \rightarrow NH_2CC(NO_2)_2 + NH_2$		461	1
R25	$NH_2 + H \rightarrow$ **NH_3**		−444	11
R26	$NH_2CC(NO_2)_2 \rightarrow C(NO_2)_2 + CNH_2$		−142	2, 9
R27	$CNH_2 + CNH_2 \rightarrow$ **NH_2CCNH_2**		−439	9
R28	$NH_2 + OH \rightarrow$ **NH_2OH**		−259	12
R29	$NH_2 + NO \rightarrow$ **NH_2NO**		195	12
R30	$(NH_2)_2CO + O \rightarrow$ **$NH_2C(O)NHOH$**		−222	13

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