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Supporting Information

Kinetic and Experimental Study on the Reaction of 3,7-Dinitro-1,3,5,7-tetraazabicyclo[3.3.1]nonane in nitric acid

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1. Experimental data for the ^{1}H-NMR tracking

Table S1. Experimental data for the reaction of DPT in fuming HNO_3 under various temperatures.

Exp No.	T (℃) (± 1)	t (min)	sample volume (mL) (±0.01)	sample mass (mg) (±0.1)	n(HMX)/n(HMX)	Conc of HMX (M)	Conc of MNX (M)
1	-8	2	0.5	41.0	0.08	0.02159	0.2699
		4		41.1	0.22	0.05237	0.238
		6		41.3	0.50	0.09644	0.1929
		8		40.9	0.72	0.1194	0.1658
		10		40.7	0.91	0.1350	0.1485
		12		41.0	1.2	0.1548	0.129
		14		40.9	1.49	0.1694	0.1136
		16		40.6	2.05	0.1876	0.0915
		18		41.2	2.24	0.1959	0.08763
		20		41.5	2.50	0.2033	0.08132
		22		40.6	3.13	0.2102	0.06760
		24		41.9	3.8	0.2266	0.05966
		26		41.4	4.41	0.2300	0.05213
		28		40.5	5.16	0.2327	0.04509
		30		40.9	5.57	0.2361	0.04238
		32		41.2	6.2	0.2413	0.03893
		35		41.1	6.90	0.2441	0.03537
		36		40.9	7.5	0.2459	0.03260
		38		41.2	7.82	0.2482	0.03173
		40		41.0	8.51	0.2492	0.02929
		42		40.8	8.97	0.2504	0.02790
		44		41.0	9.8	0.2525	0.02577
$\Delta[MNX]_{2min-44min} = [MNX]_{2min} - [MNX]_{44min} = 0.2441\ (M)$ $\Delta[HMX]_{2min-44min} = [HMX]_{44min} - [HMX]_{2min} = 0.2309\ (M)$ $\Delta[byproduct]_{2min-44min} = \Delta[MNX]_{2min-44min} - \Delta[HMX]_{2min-44min} = 0.0132\ (M)$ $S^{[1,2]} = \frac{[HMX]}{[byproduct]} = \frac{\Delta[HMX]_{2min-44min}}{\Delta[byproduct]_{2min-44min}} = 17.5$							
2	-14	15	0.5	42.0	0.23	0.0545	0.2422
		19		42.1	0.39	0.08317	0.2132
		23		41.0	0.57	0.1037	0.1829
		29		42.1	0.8	0.13	0.1631
		33		42.0	1.09	0.1518	0.1393
		38		41.8	1.26	0.1616	0.1276
		43		41.9	1.57	0.1769	0.1126
		48		42.4	1.77	0.1866	0.1054
		53		42.1	2.22	0.1994	0.08965
		56		42.6	2.5	0.2087	0.08348

		62		42.0	3.15	0.2183	0.06929
		66		41.6	3.36	0.2192	0.06524
		70		41.7	4.07	0.2284	0.05614
		75		42.1	4.31	0.2325	0.05409
		79		42.0	4.45	0.2339	0.05256
		83		42.2	4.64	0.2365	0.05100
		90		42.0	5.7	0.2432	0.04273
		96		42.1	6.9	0.2492	0.03636
		101		41.9	7.11	0.2503	0.03522
$\Delta[MNX]_{15min-101min} = [MNX]_{15min} - [MNX]_{101min} = 0.2070\ (M)$ $\Delta[HMX]_{15min-101min} = [HMX]_{101min} - [HMX]_{15min} = 0.1958\ (M)$ $\Delta[byproduct]_{15min-101min} = \Delta[MNX]_{15min-101min} - \Delta[HMX]_{15min-101min} = 0.0112\ (M)$ $S^{[1,2]} = \frac{[HMX]}{[byproduct]} = \frac{\Delta[HMX]_{15min-101min}}{\Delta[byproduct]_{15min-101min}} = 17.5$							
3	-23	12	0.5	44.2	0.03	0.00843	0.3066
		26		44.1	0.11	0.03102	0.2820
		40		44.4	0.25	0.06265	0.2506
		54		44.3	0.38	0.08573	0.2256
		69		44.2	0.51	0.1041	0.2055
		84		44.0	0.67	0.1231	0.1839
		96		44.6	0.82	0.1398	0.1705
		108		44.2	1.00	0.1532	0.1536
		120		44.8	1.15	0.1660	0.1443
		132		44.1	1.33	0.1739	0.1312
		143		43.9	1.43	0.1784	0.1247
		155		44.2	1.62	0.1886	0.1162
		167		44.1	1.86	0.1979	0.1064
		181		44.7	2.03	0.2051	0.1012
		195		44.3	2.29	0.2117	0.09245
		207		44.4	2.58	0.2193	0.08504
		220		44.2	2.72	0.2215	0.08137
		233		44.1	3.07	0.2282	0.07427
		245		44.0	3.46	0.2332	0.06740
		257		44.2	3.81	0.2391	0.06283
$\Delta[MNX]_{12min-257min} = [MNX]_{12min} - [MNX]_{257min} = 0.2438\ (M)$ $\Delta[HMX]_{12min-257min} = [HMX]_{257min} - [HMX]_{12min} = 0.2307\ (M)$ $\Delta[byproduct]_{12min-257min} = \Delta[MNX]_{12min-257min} - \Delta[HMX]_{12min-257min} = 0.0131\ (M)$ $S^{[1,2]} = \frac{[HMX]}{[byproduct]} = \frac{\Delta[HMX]_{12min-257min}}{\Delta[byproduct]_{12min-257min}} = 17.6$							
4	-36	30	0.5	46.4	0.011	0.00346	0.3276
		60		46.3	0.020	0.00647	0.3236
		90		46.5	0.035	0.01120	0.3201
		120		46.4	0.058	0.01795	0.3123

		150		46.4	0.080	0.02443	0.3054
		180		46.2	0.103	0.03063	0.2974
		210		46.1	0.118	0.03453	0.2925
		240		46.6	0.138	0.04006	0.2903
		270		46.7	0.158	0.04513	0.2856
		300		46.4	0.168	0.04714	0.2814
		330		46.3	0.183	0.05068	0.2769
		360		46.3	0.200	0.05466	0.2733
		390		46.4	0.215	0.05798	0.27
		420		46.4	0.238	0.06288	0.2648
		450		46.4	0.245	0.06446	0.2631
		480		46.4	0.253	0.066	0.2614
		510		46.5	0.270	0.06973	0.2582
		540		46.6	0.283	0.07246	0.2560
		570		46.4	0.303	0.07592	0.251
		600		46.5	0.310	0.07750	0.2500
		630		46.4	0.318	0.07874	0.248
		660		46.6	0.325	0.08047	0.2475
		690		46.4	0.340	0.08285	0.2437

$\Delta[MNX]_{30min-690min} = [MNX]_{30min} - [MNX]_{690min} = 0.0839\ (M)$

$\Delta[HMX]_{30min-690min} = [HMX]_{690min} - [HMX]_{30min} = 0.0794\ (M)$

$\Delta[byproduct]_{30min-690min} = \Delta[MNX]_{30min-690min} - \Delta[HMX]_{30min-690min} = 0.0045\ (M)$

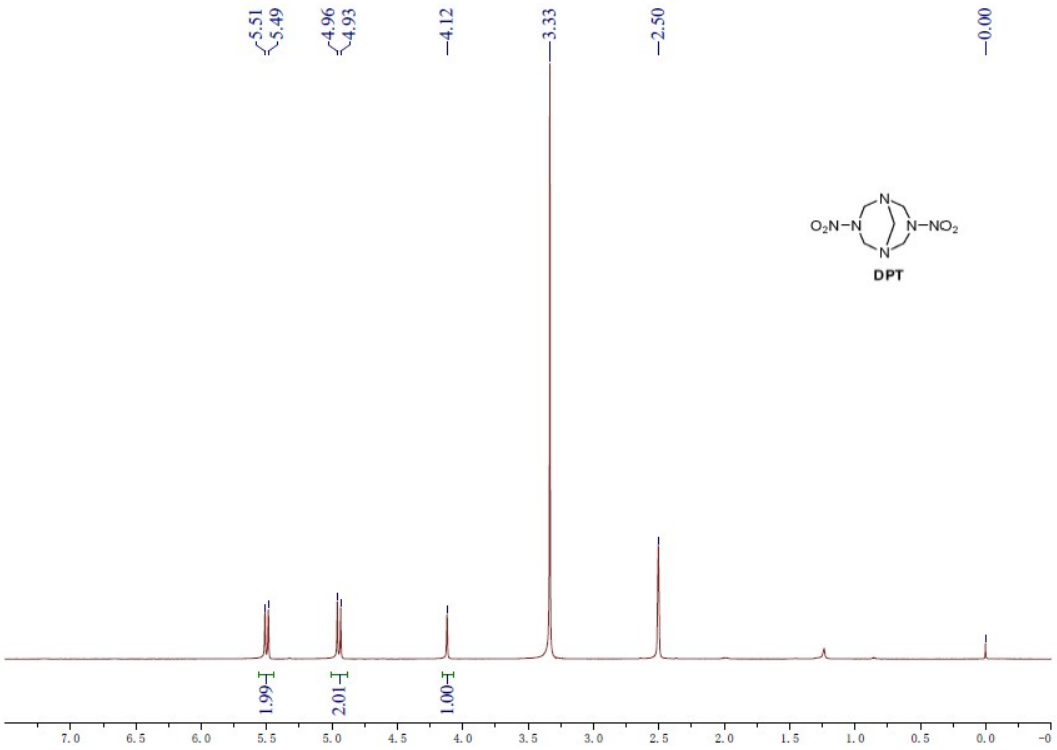
$$S^{[1,2]} = \frac{[HMX]}{[byproduct]} = \frac{\Delta[HMX]_{30min-690min}}{\Delta[byproduct]_{30min-690min}} = 17.6$$

[1] Levine, I. N. Physical Chemistry; 3 Ed. McGraw-Hill: New York, 1988; pp 512-572.

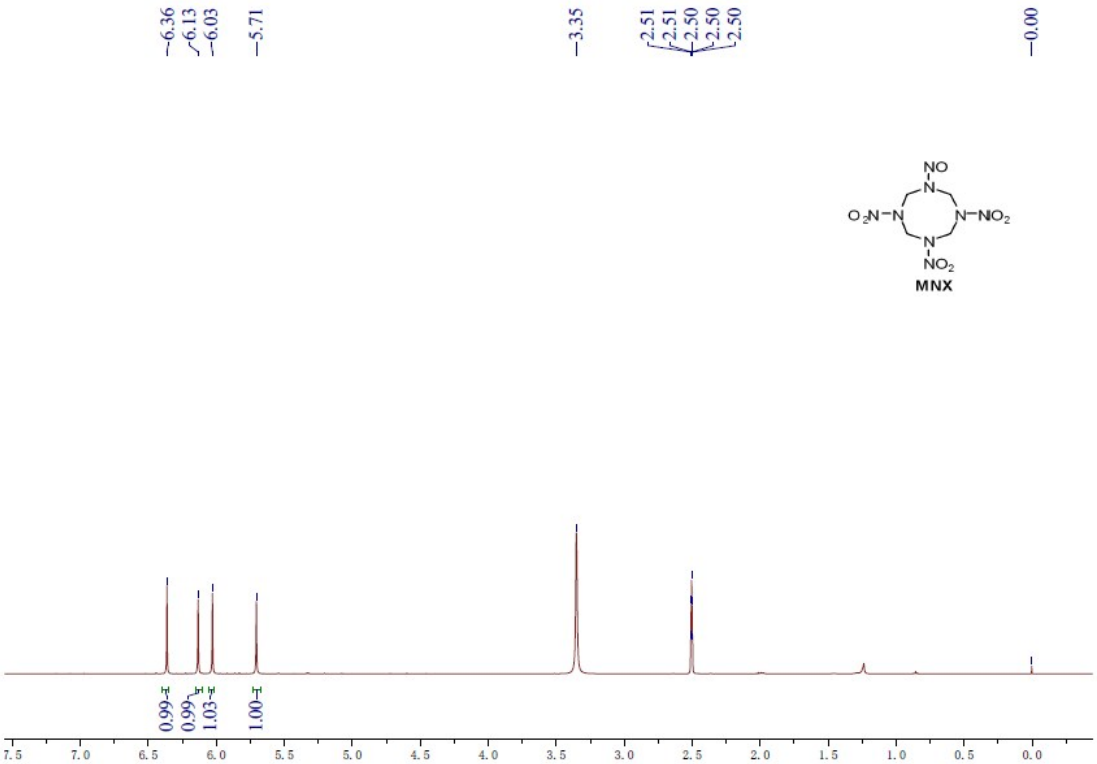
[2] Noggle, J. H. Physical Chemistry; Little Brown: Boston, 1985; pp 465-456.

2. Copies of identification spectra

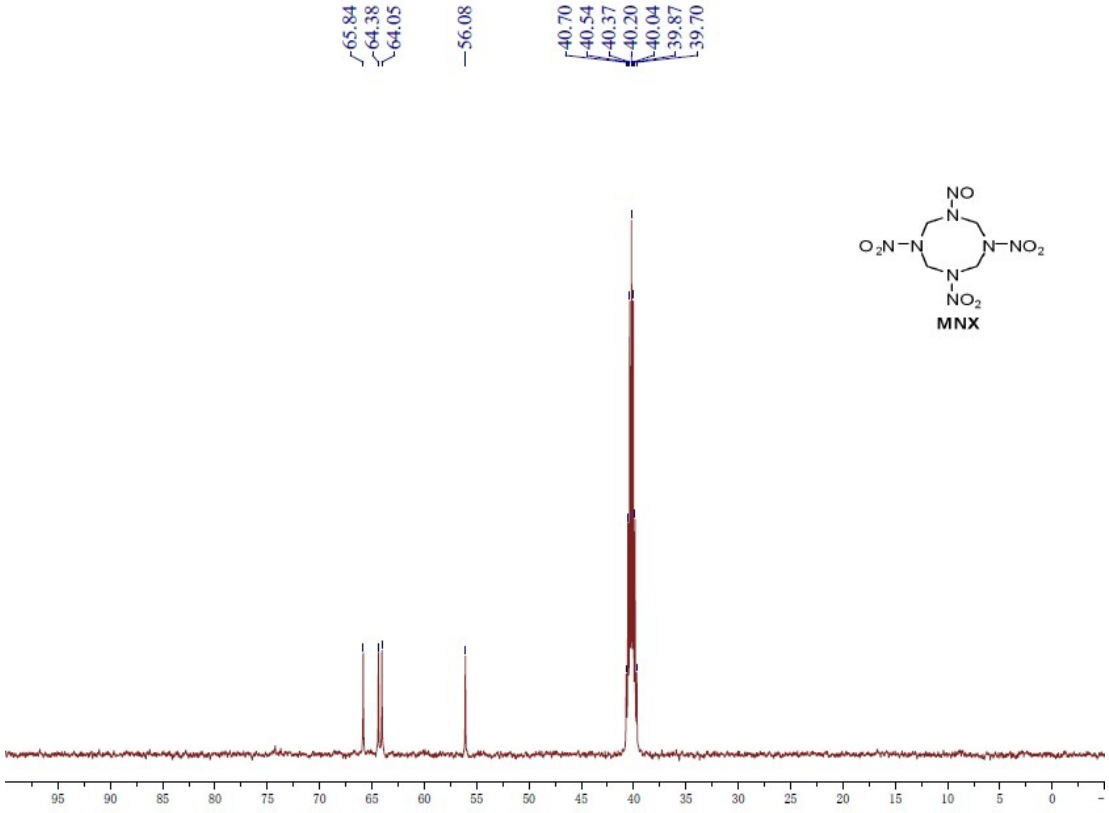
^{1}H NMR spectrum of DPT (DMSO-d_6, 500 MHz)



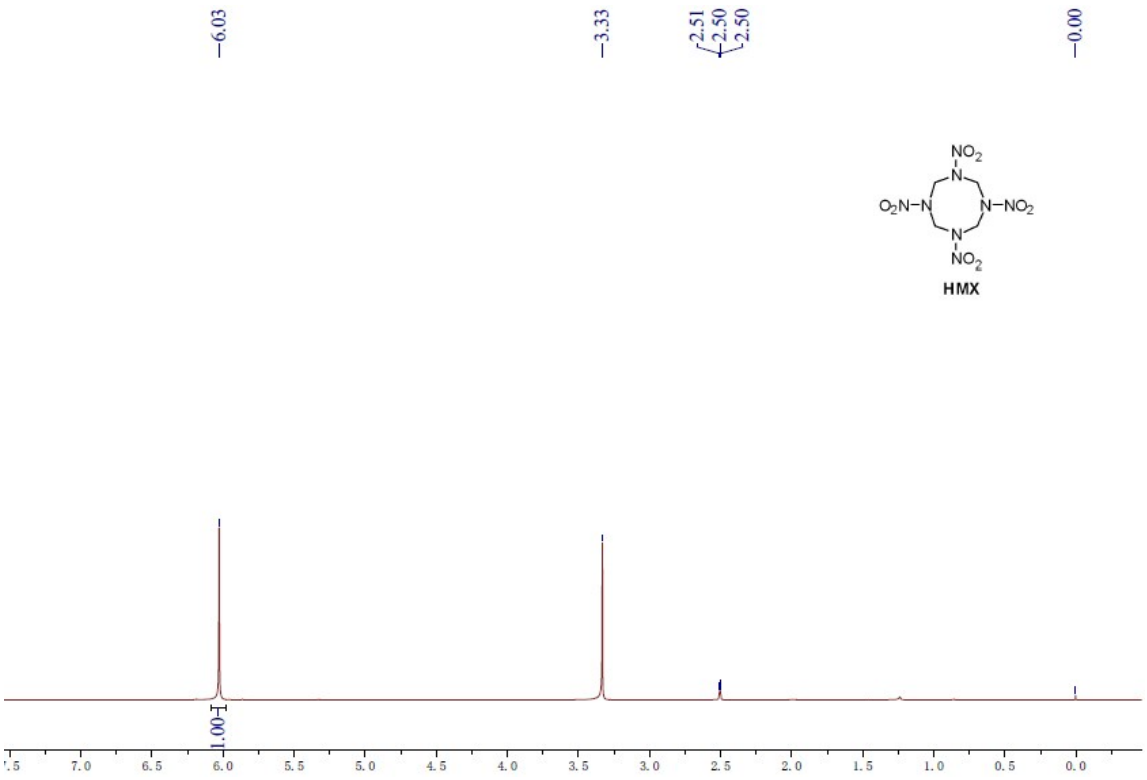
^{1}H NMR spectrum of MNX (DMSO-d_6, 500 MHz)



^{13}C NMR spectrum of MNX (DMSO-d_6, 126 MHz)



^{1}H NMR spectrum of HMX (DMSO-d_6, 500 MHz)



^{13}C NMR spectrum of HMX (DMSO-d_6, 126 MHz)