Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Origin Determination of Multistep Thermal Decomposition of 2,6-Diamino-3,5-dinitropyrazine-1-oxide (LLM-105)

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Supporting Information

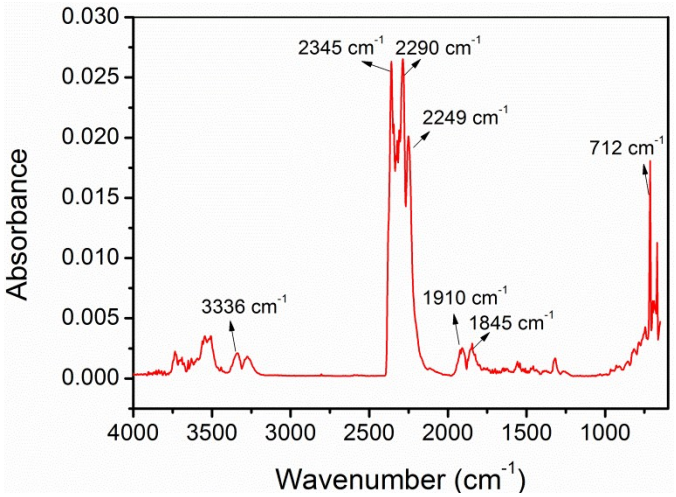
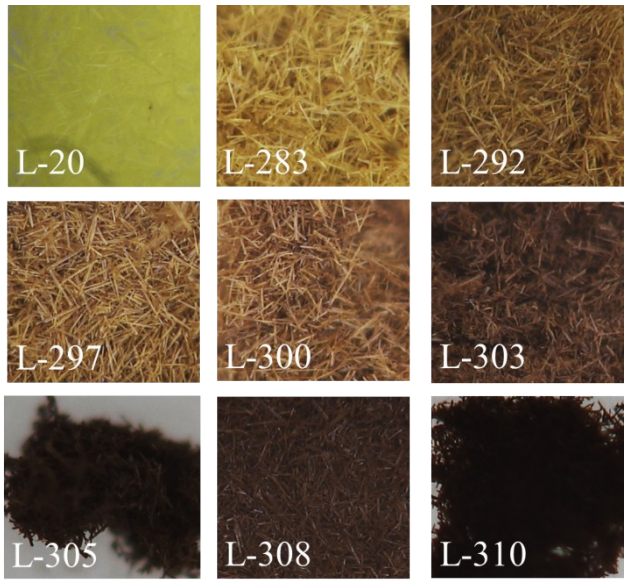


Fig. S1 IR spectra of evolved gaseous products of LLM-105 at 340 °C



* J. Li, email: ljs915@263.net.

Fig. S2 Photomicrographs of different quenched LLM-105 samples

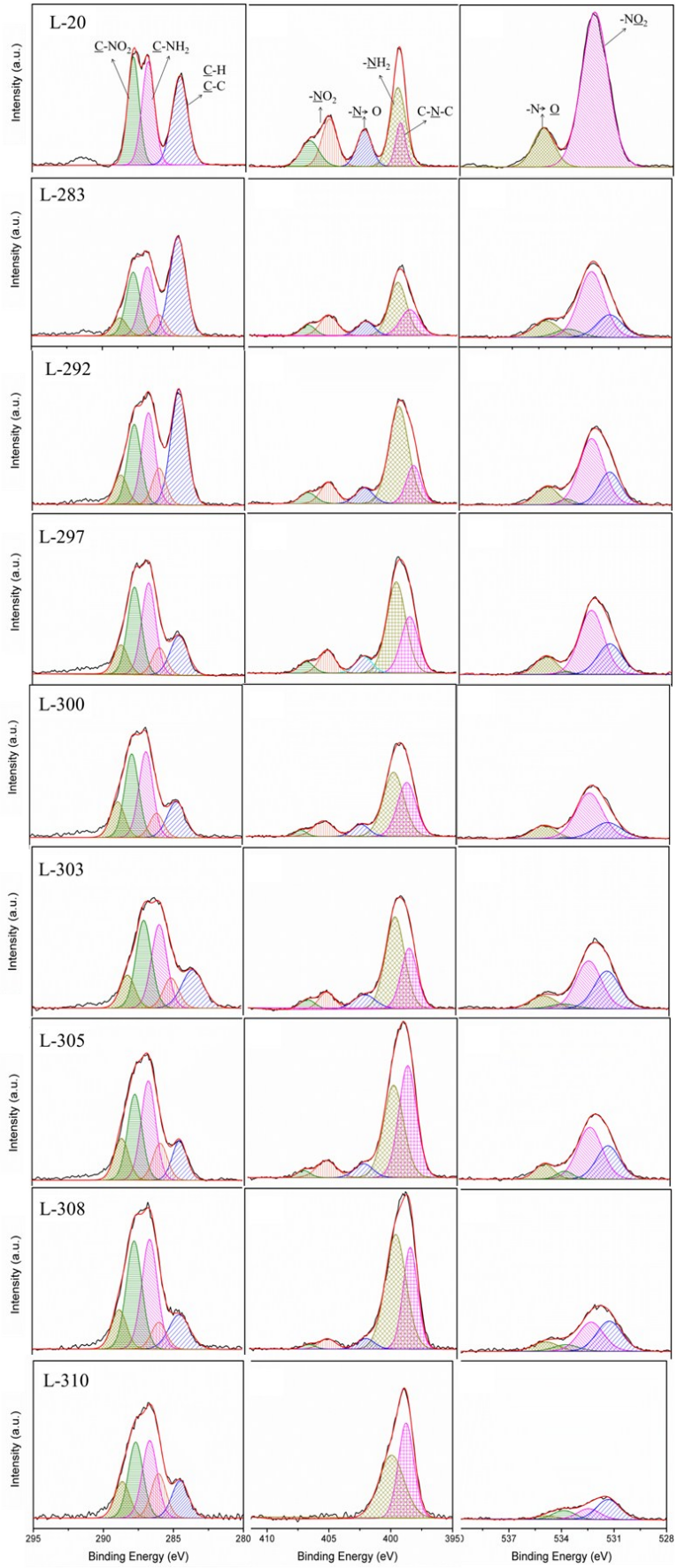


Fig. S3 XPS spectra of LLM-105 quenched at different temperatures

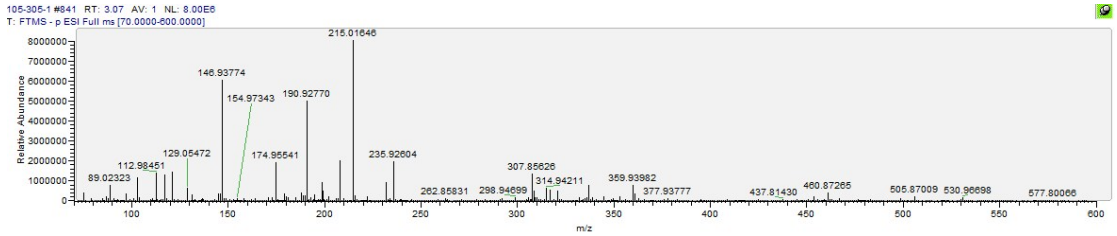


Fig. S4 Mass spectra of LLM-105 for the chromatographic peak at 3.07 minutes

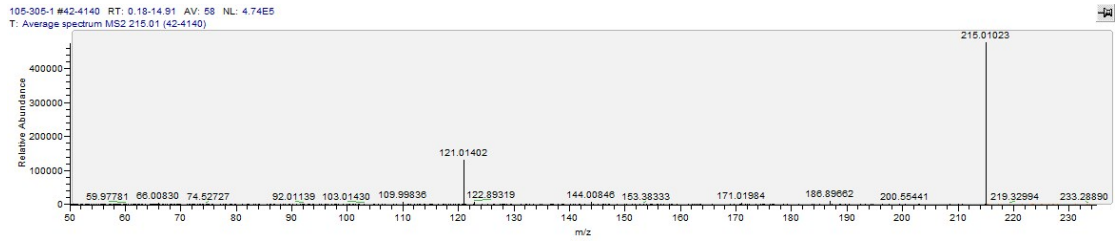


Fig. S5 MS/MS of LLM-105 adduct ion at *m/z* 215.01

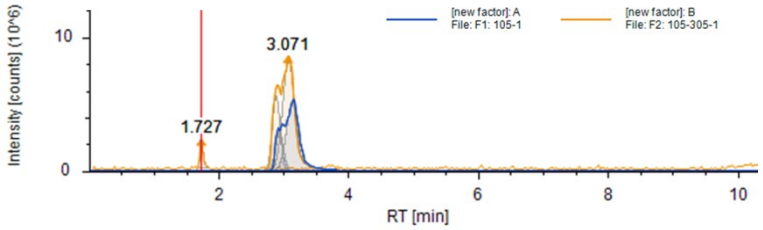


Fig. S6 LC spectra of LLM-105 and L-305

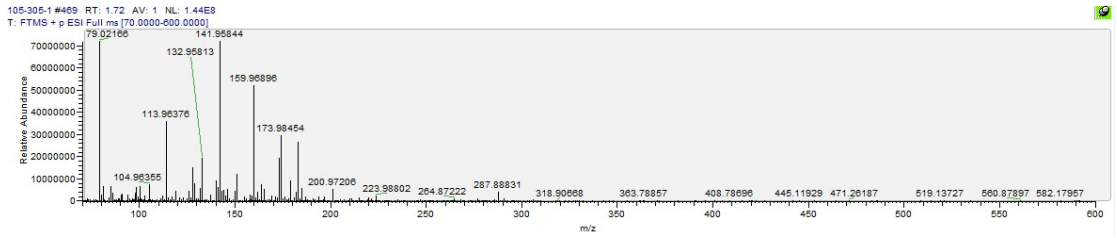


Fig. S7 Mass spectra of L-305 for the chromatographic peak at 1.72 minutes

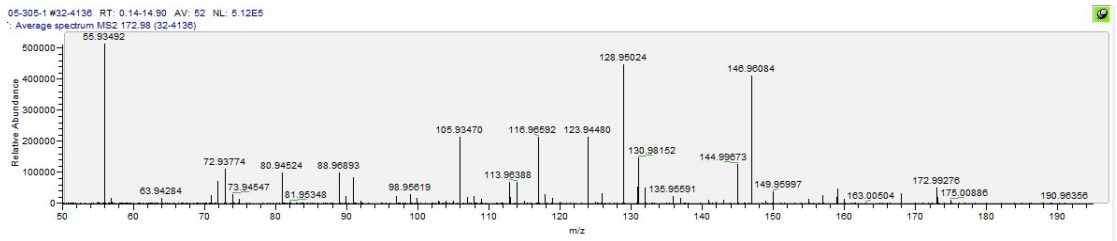


Fig. S8 MS/MS of L-305 adduct ion at *m/z* 172.98

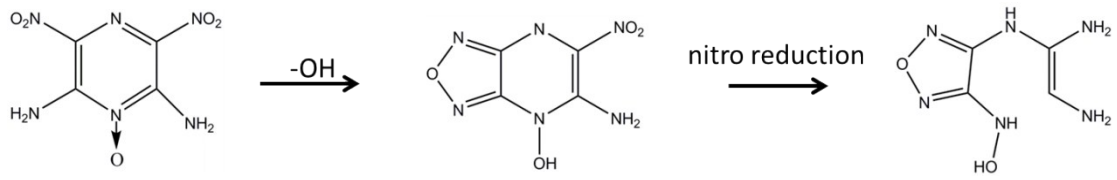


Fig. S9 Degradation pathway of LLM-105 to the intermediate

Table 1 Elemental contents of LLM-105 at different quenched time

Sample	C content / %	Deviation / %	N content / %	Deviation / %	O content/ %	Deviation / %
L-20	22.22	-	38.89	-	37.04	-
L-283	29.27	0.49	40.33	0.38	30.40	0.66
L-292	29.93	0.28	40.91	0.28	29.15	0.20
L-297	30.39	0.98	41.37	0.46	28.23	0.58
L-300	32.40	0.52	41.30	0.31	26.29	0.39
L-303	34.30	0.18	42.30	0.37	23.39	0.28
L-305	37.52	1.25	41.38	1.13	21.09	0.14
L-308	39.31	3.54	49.51	1.18	11.19	2.36
L-310	38.70	1.36	53.14	0.81	8.17	0.99