Electronic Supplementary Material

Theoretical study on the effect of H_2O on the formation mechanism of NO_x precursors during indole pyrolysis

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Table S1 Virtual frequencies of all transition states

TS	Frequency	TS	Frequency	TS	Frequency
A-TS1	-1794.23	B2-TS4	-1953.42	D2-TS4	-778.48
A1-TS2	-651.19	B3-TS4	-1927.96	E-TS1	-714.11
A1-TS3	-1896.88	C-TS1	-541.55	E-TS2	-335.59
A2-TS2	-461.00	C-TS2	-1013.61	E1-TS3	-1145.40
A2-TS3	-1679.67	D-TS1	-1002.92	E2-TS3	-1992.69
A2-TS4	-2589.19	D1-TS2	-1422.19	F-TS1	-641.77
B-TS1	-1700.73	D1-TS3	-436.06	F1-TS2	-1208.06
B-TS2	-342.70	D1-TS4	-1141.78	F2-TS2	-544.14
B1-TS3	-1903.82	D2-TS2	-1321.14	F3-TS2	-1345.17
B1-TS4	-181.65	D2-TS3	-1562.42	F3-TS3	-1478.46

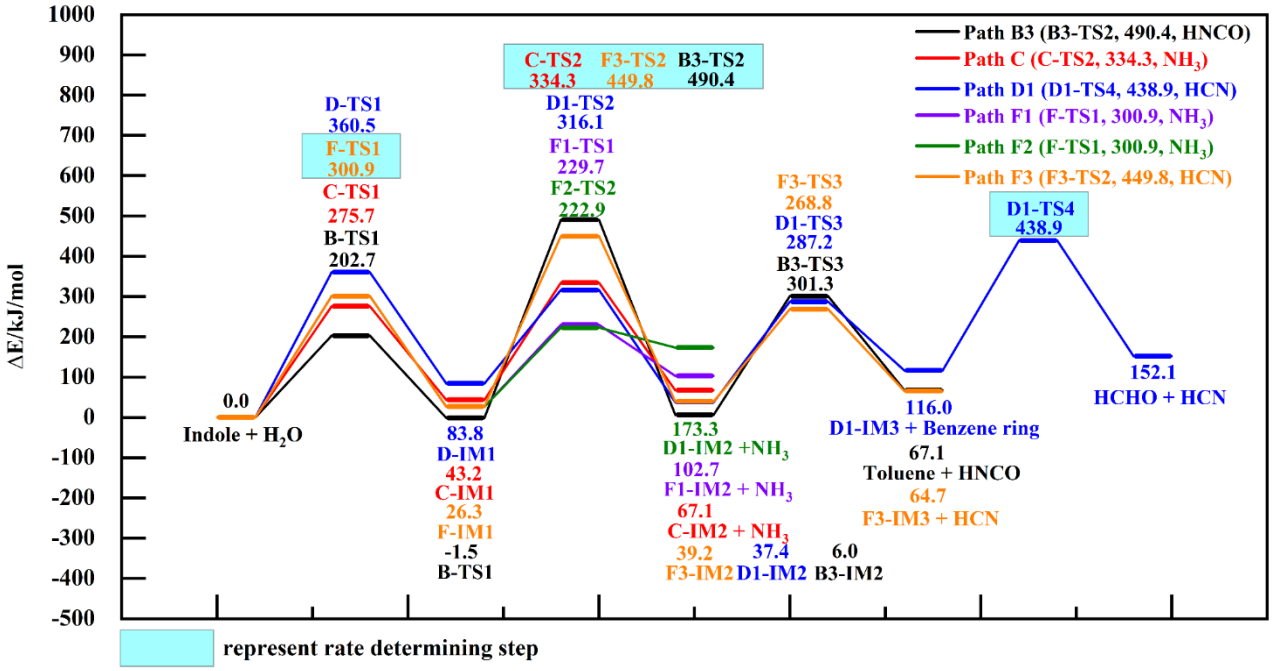

Fig. S1. Energy distribution of favorable paths (Blue highlighted indicates the rate determining step).

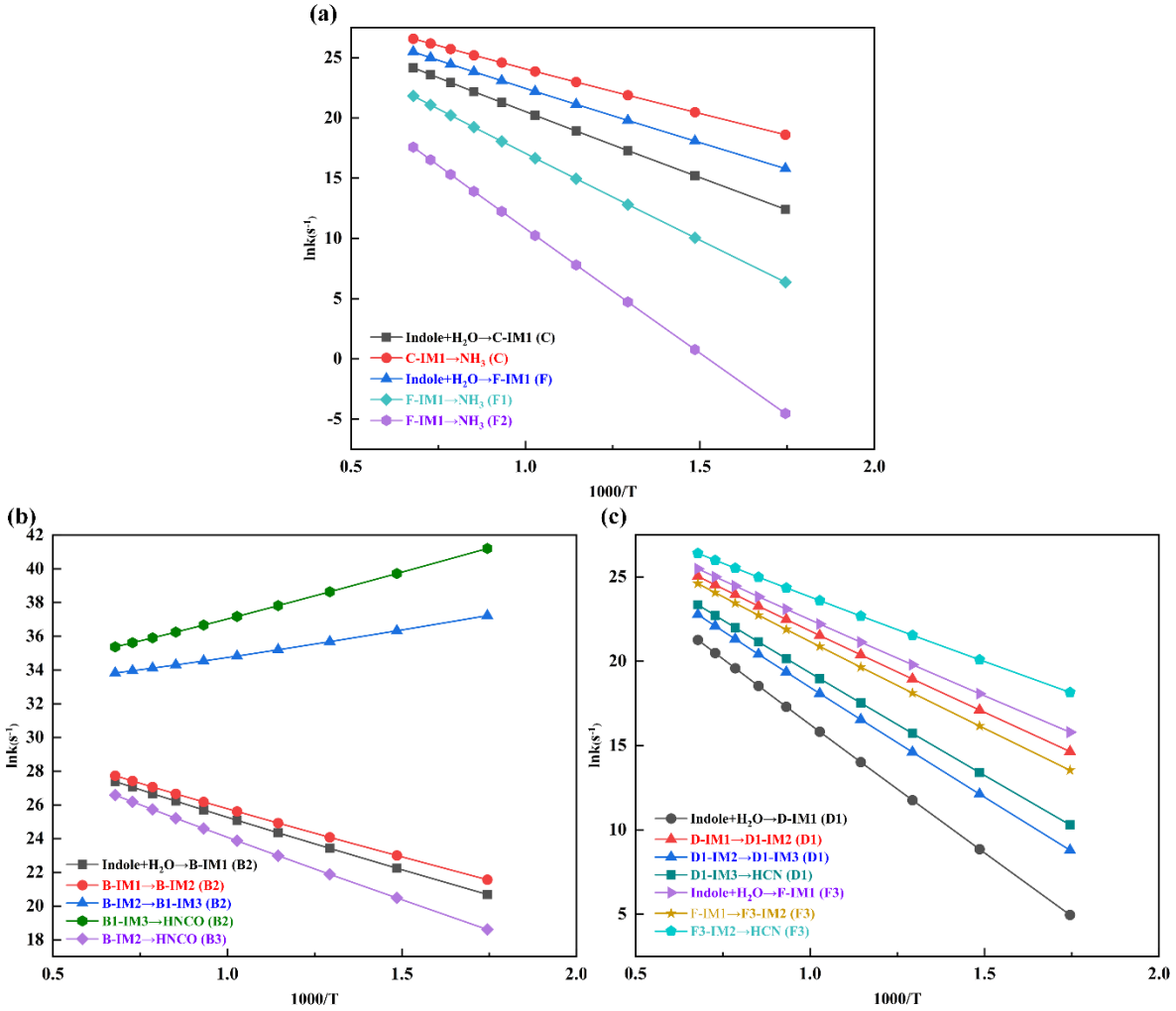

Fig. S2. The main formation pathways rate constant of NO_x precursors ranges from 300 to 1200 °C. (a) NH_3 (b) HNCO (c) HCN

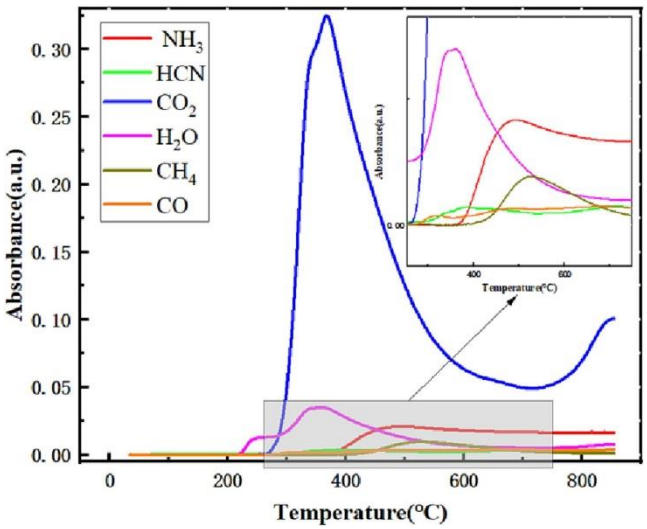

Fig. S3. Gas release curves of soybean protein after pyrolysis at different temperatures by TG-FTIR [15].