**Electronic Supplementary Information**

# Direct production of indoles via thermo-catalytic conversion of bio-derived furans with ammonia over zeolites

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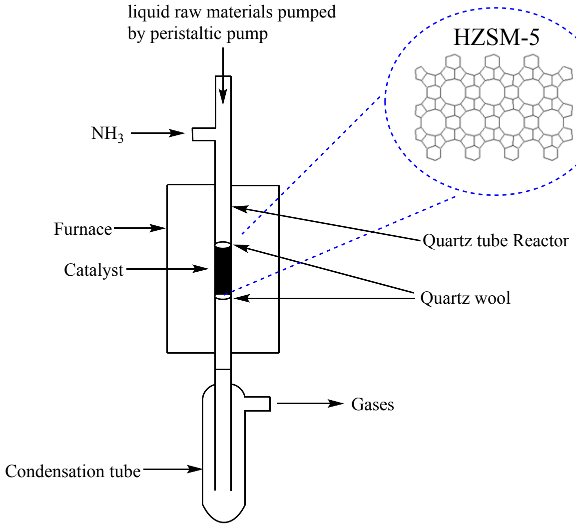


Fig. S1: The scheme of the apparatus for thermo-catalytic conversion of furans with ammonia.

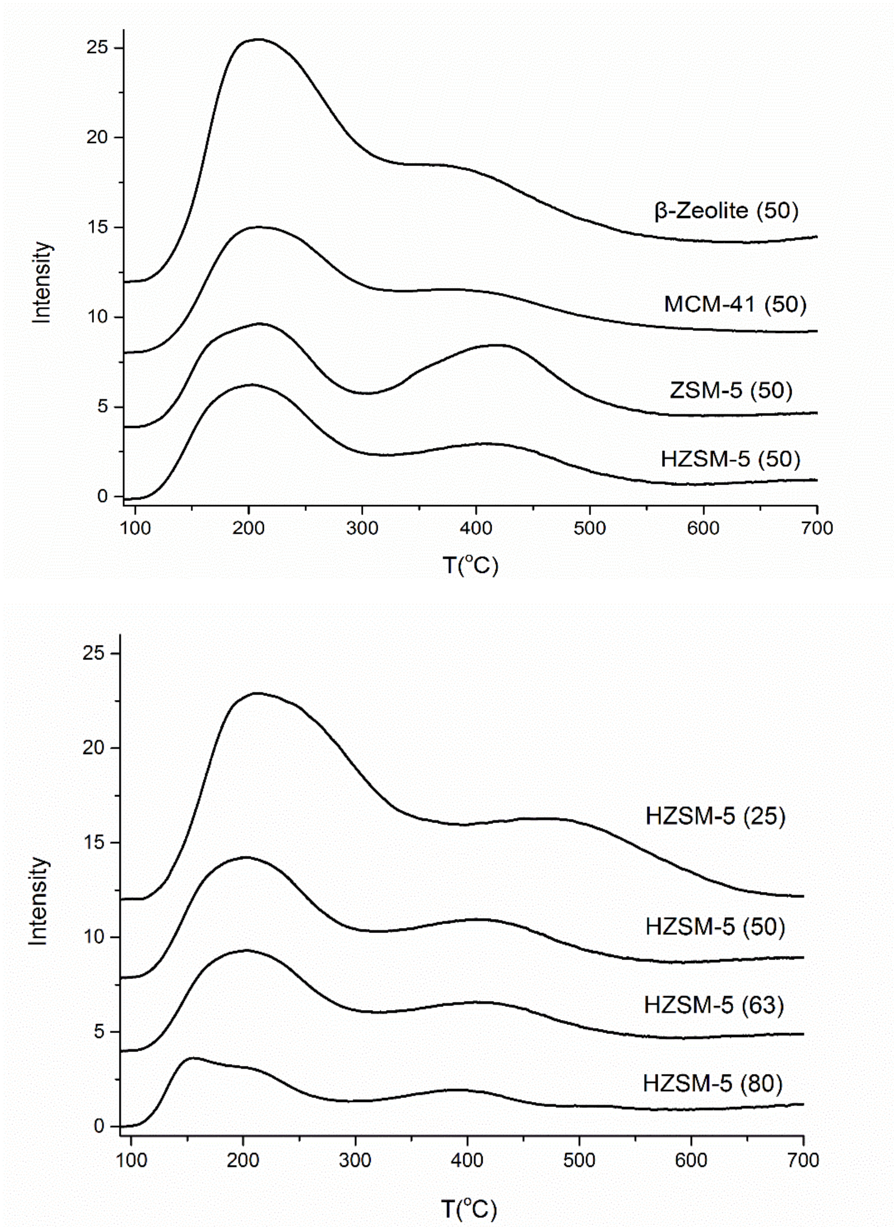


Fig. S2: The detailed information of the $NH_3$-TPD spectra of different zeolites with different pore structure and HZSM-5 with different Si/Al ratio.

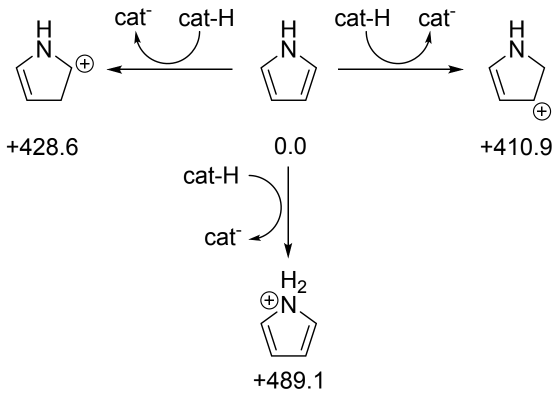


Figure S3. The geometry-optimized structures and ground state electronic energies of the three protonated pyrrole

**Table S1.** The detailed product distribution from thermo-catalytic conversion of furan with ammonia at different temperatures.

| Entry | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| Tem. (°C) | 450 | 500 | 550 | 600 | 650 |
| The overall carbon selectivity of products (C %) | | | | | |
| Total carbon | 94.5 | 91.5 | 90 | 92.4 | 91.6 |
| Coke | 25.8 | 21.0 | 18.7 | 13.6 | 9.5 |
| Gases | 18.2 | 23.4 | 30.6 | 35.8 | 46.7 |
| N-containing chemicals | 50.0 | 45.7 | 37.9 | 37.8 | 26.3 |
| Aromatics | 0.5 | 1.4 | 2.8 | 5.2 | 9.1 |
| The overall carbon yield of N-containing chemicals (C %) | | | | | |
| Pyridines | 0.5 | 2.0 | 4.9 | 9.9 | 10.5 |
| Pyrroles | 20.2 | 9.9 | 4.0 | 0.8 | 0 |
| Aniline | 2.1 | 2.1 | 2.3 | 2.7 | 3.2 |
| Indoles | 27.2 | 31.7 | 26.7 | 24.4 | 12.7 |
| The selectivity of indoles (%) | | | | | |
| Indole | 68.7 | 74.2 | 72.5 | 80.9 | 90.9 |
| Methylindole | 31.3 | 25.8 | 27.5 | 19.1 | 9.7 |
| The selectivity of Gases (%) | | | | | |
| CO | 79.3 | 73.9 | 65.3 | 66.0 | 72.0 |
| $CH_4$ | 1.1 | 5.6 | 6.3 | 12.1 | 18.8 |
| $C_2H_4$ | 4.6 | 8.3 | 17.6 | 13.9 | 7.3 |
| $C_3H_6$ | 15.0 | 12.2 | 10.8 | 8.0 | 1.8 |

a. Reaction Condition: Catalyst=HZSM-5, Si/Al=25, Catalyst usage=2g, WHSV = 0.5 $h^{-1}$, and the ammonia to furan molar ratio = 8:1.

**Table S2.** The detailed product distribution from thermo-catalytic conversion of furan with ammonia at different WHSV

| Entry | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| WHSV | 0.25 | 0.5 | 0.75 | 1 |
| The overall carbon selectivity of products (C %) | | | | |
| Total carbon | 87.4 | 91.5 | 98.2 | 99.7 |
| Coke | 24.2 | 21.0 | 10.5 | 7.7 |
| Gases | 29.7 | 23.4 | 12.7 | 11.2 |
| N-containing chemicals | 31.8 | 45.7 | 75.0 | 80.3 |
| Aromatics | 1.7 | 1.4 | 1.0 | 0.5 |
| The overall carbon yield of N-containing chemicals (C %) | | | | |
| Pyridines | 3.0 | 2.0 | 2.8 | 2.6 |
| Pyrroles | 9.0 | 10.0 | 31.7 | 40.4 |
| Aniline | 3.5 | 2.1 | 4.8 | 5.4 |
| Indoles | 19.3 | 31.7 | 35.7 | 31.9 |
| The selectivity of indoles (%) | | | | |
| Indole | 72.1 | 74.2 | 75.7 | 79.5 |
| Methylindole | 27.9 | 25.8 | 24.3 | 20.5 |
| The selectivity of Gases (%) | | | | |
| CO | 66.1 | 73.9 | 74.4 | 72.2 |
| $CH_4$ | 4.6 | 5.6 | 4.4 | 4.4 |
| $C_2H_4$ | 16.8 | 14.3 | 13.0 | 12.7 |
| $C_3H_6$ | 12.9 | 6.2 | 8.2 | 10.7 |

a. Reaction Condition: T=500°C,Catalyst=HZSM-5, Si/Al=25, Catalyst usage=2g ,and the ammonia to furan molar ratio = 8:1.

**Table S3.** The detailed product distribution from thermo-catalytic conversion of furan with ammonia at different ammonia to furan molar ratio

| Entry | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| Mole ration of $NH_3$ to furan | 2 | 4 | 8 | 12 |
| The overall carbon selectivity of products (C %) | | | | |
| Total carbon | 96.6 | 93.8 | 91.5 | 91.0 |
| Coke | 19.4 | 20.3 | 21.0 | 24.9 |
| Gases | 27.3 | 24.8 | 23.4 | 22.5 |
| N-containing chemicals | 49.3 | 47.9 | 45.7 | 42.8 |
| Aromatics | 0.6 | 0.8 | 1.4 | 0.8 |
| The overall carbon yield of N-containing chemicals (C %) | | | | |
| Pyridines | 3.1 | 2.8 | 2.0 | 1.6 |
| Pyrroles | 8.2 | 9.3 | 10.0 | 17.9 |
| Aniline | 5.5 | 3.7 | 2.1 | 1.9 |
| Indoles | 32.5 | 32.1 | 31.7 | 21.4 |
| The selectivity of indoles (%) | | | | |
| Indole | 79.8 | 74.5 | 74.2 | 72.5 |
| Methylindole | 20.1 | 25.5 | 25.8 | 27.5 |
| The selectivity of Gases (%) | | | | |
| CO | 69.9 | 70.4 | 73.9 | 67.6 |
| $CH_4$ | 4.0 | 4.0 | 5.6 | 3.9 |
| $C_2H_4$ | 11.2 | 12.5 | 14.3 | 17.2 |
| $C_3H_6$ | 14.8 | 13.0 | 6.2 | 11.4 |

a. Reaction Condition: T=500°C, Catalyst=HZSM-5, Si/Al=25, Catalyst usage=2g, and WHSV = 0.5 $h^{-1}$.