

Supporting Information

for

C-N bond hydrogenolysis of aniline and cyclohexylamine over TaO_x-Al₂O₃

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Table S1. Product Distribution for the Denitrogenation of Cyclohexylamine

| T (°C) | Product Distribution | | | | | Benzene/cyclohexane | | |
|--------------|----------------------|--------------|-------------|-------------|------------------|---------------------------------|------|----------------------|
| | Benzene | Cyclohexene | Cyclohexane | Aniline | Cyclohexyl-amine | HC/NH ₂ ^a | Obs. | Equil. ^b |
| 150 | 4.7% | 2.4% | 0.1% | 0.3% | 1.1% | 5 | 65 | 7.1x10 ⁻⁷ |
| 200 | 4.5% | 6.9% | 0.1% | 0.1% | 0.7% | 14 | 31 | 4.4x10 ⁻⁴ |
| 250 | 10.1% | 30.3% | 0.4% | 0.2% | 0.4% | 67 | 25 | 8.1x10 ⁻² |
| 300 | 7.4% | 28.9% | 0.1% | 0.0% | 0.1% | 274 | 51 | 6.0 |
| 350 | 0.5% | 0.0% | 0.0% | 0.0% | 0.0% | 11 | n/a | 220 |
| 400 | 0.6% | 0.0% | 0.0% | 0.0% | 0.0% | 20 | n/a | 4700 |
| Total | 27.7% | 68.5% | 0.8% | 0.7% | 2.3% | 32 | 36 | 23 |

^aMoles C-N bond cleavage products (cyclohexane, cyclohexene, benzene) detected per mole cyclohexylamine and aniline desorbed in a given temperature range.

^bEquilibrium ratios at a given temperature were calculated based on the thermodynamic data for the hydrogenation of benzene to cyclohexene and cyclohexane by G. G. Janz, *J. Chem. Phys.*, **1954**, 22, 751.

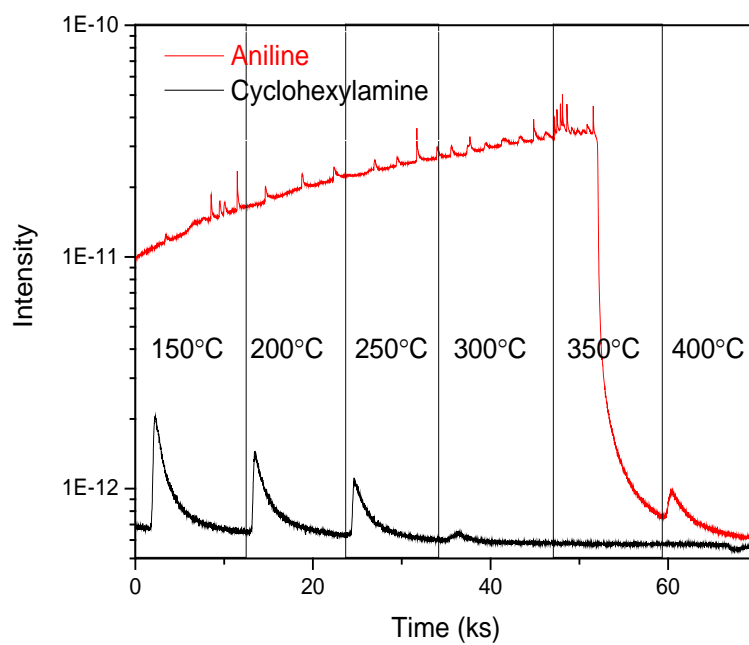


Figure S1. Signals from process mass spectrometry for aniline ($m/z = 93$) and cyclohexylamine ($m/z = 99$) desorbing **intact** from $\text{TaO}_x\text{-Al}_2\text{O}_3$ surfaces saturated in the respective amines.