Supporting information

Advanced high-loaded Ni-Cu catalysts in transfer hydrogenation of anisole: unexpected effect of Cu addition

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In order to demonstrate stability of the catalysts used in this study the samples were analyzed by XRD after anisole treatment at 250 °C. As clearly seen in **Figure S1** the catalysts are presented by Ni^0 phase (PDF № 04-0850), at the same time, the mean crystallite size of metal nanoparticles does not exceed 7.0 nm (**Table S1**). The lattice parameter of Ni^0 phase is increased that shows the presence of Cu^0. This fact demonstrates the absence of the phase separation after treatment TH of anisole at 250 °C. Thus, we can conclude that the properties of the catalyst do not change dramatically during TH.

Table S1. D – mean crystallite size, a – lattice parameter, measured by XRD for the catalysts treated in TH of anisole at 250 °C.

Catalyst	D(Ni^0), nm	a(Ni^0), Å
Ni(36)-SiO_2	7.0	3.523
Ni(41)Cu(4)-SiO_2	5.5	3.528
Ni(36)Cu(14)-SiO_2	6.5	3.553

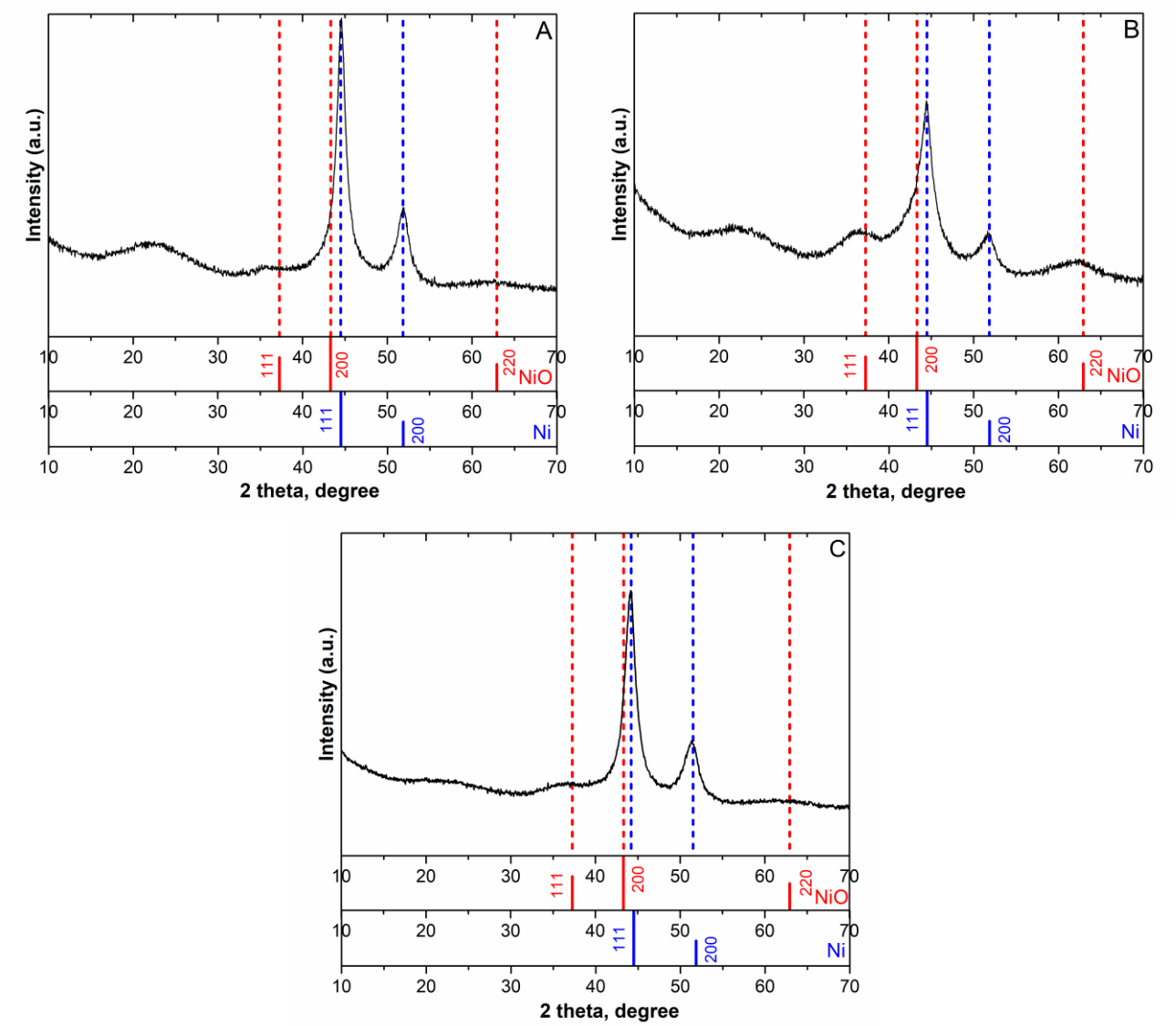

Figure S1. XRD data obtained for the catalysts after the 3 h treatment at 250 °C in anisole TH. A – Ni(36)-SiO_2, B – Ni(41)Cu(4)-SiO_2, C – Ni(36)Cu(14)-SiO_2.

The kinetic constants were calculated accordingly the equations presented in the main text. To take into account the negative influence of acetone the pseudo-equilibrium constant $K_{acetone}$ showing the ratio between acetone in the solution and on the catalyst surface was calculated (**Table S2**). Also, the rate constants of different pathways are provided. The same calculations were made for the experiments at 150 °C (**Table S3**).

Table S2. Rate constants of the product formation in the experiments at 250 °C. The constants were calculated using the least-square method with a kinetic model that would take into account the effect of acetone concentration on the rate of catalytic transformations, m(catalyst) = 0.10 – 0.11 g.

#	Catalyst	k_1^0 ×10^4, s^{-1}	k_2^0×10^4, s^{-1}	k_3^0×10^4, s^{-1}	k_4^0×10^4, s^{-1}	$K_{acetone}$×10^4, s^{-1}mol^{-1}
1	Ni(36)-SiO_2	-	-	-	-	-
2	Ni(41)Cu(4)-SiO_2	0.48	2.99	2.79	0.53	26.9
3	Ni(36)Cu(14)-SiO_2	1.21	7.04	2.32	-	140.0
4	Ni(36)-SiO_2*	-	-	-	-	-
5	Ni(41)Cu(4)-SiO_2*	0.23	1.63	0.99	0.16	51.2

* 15 ml of 2-PrOH was replaced with 15 ml of acetone.

Table S3. Rate constants of product formation in the experiments at 150 °C. The constants were calculated using the least-square method with a kinetic model that would take into account the effect of acetone concentration on the rate of catalytic transformations, m(catalyst) = 0.36 – 0.37 g.

#	Catalyst	k_1^0 ×10^4, s^{-1}	k_2^0×10^4, s^{-1}	k_3^0×10^4, s^{-1}	k_4^0×10^4, s^{-1}	$K_{acetone}$×10^4, s^{-1}*mol^{-1}*l
1	Ni-SiO_2	-	-	-	-	-
2	Ni10Cu-SiO_2	0.10	0.93	0.55	-	310
3	Ni2.5Cu-SiO_2	0.10	0.94	0.31	-	440

The reaction mixtures were analyzed by GC-MS and **Figure S2** shows the example of chromatogram obtained for the initial reaction mixture (A) and the final reaction mixture (B).

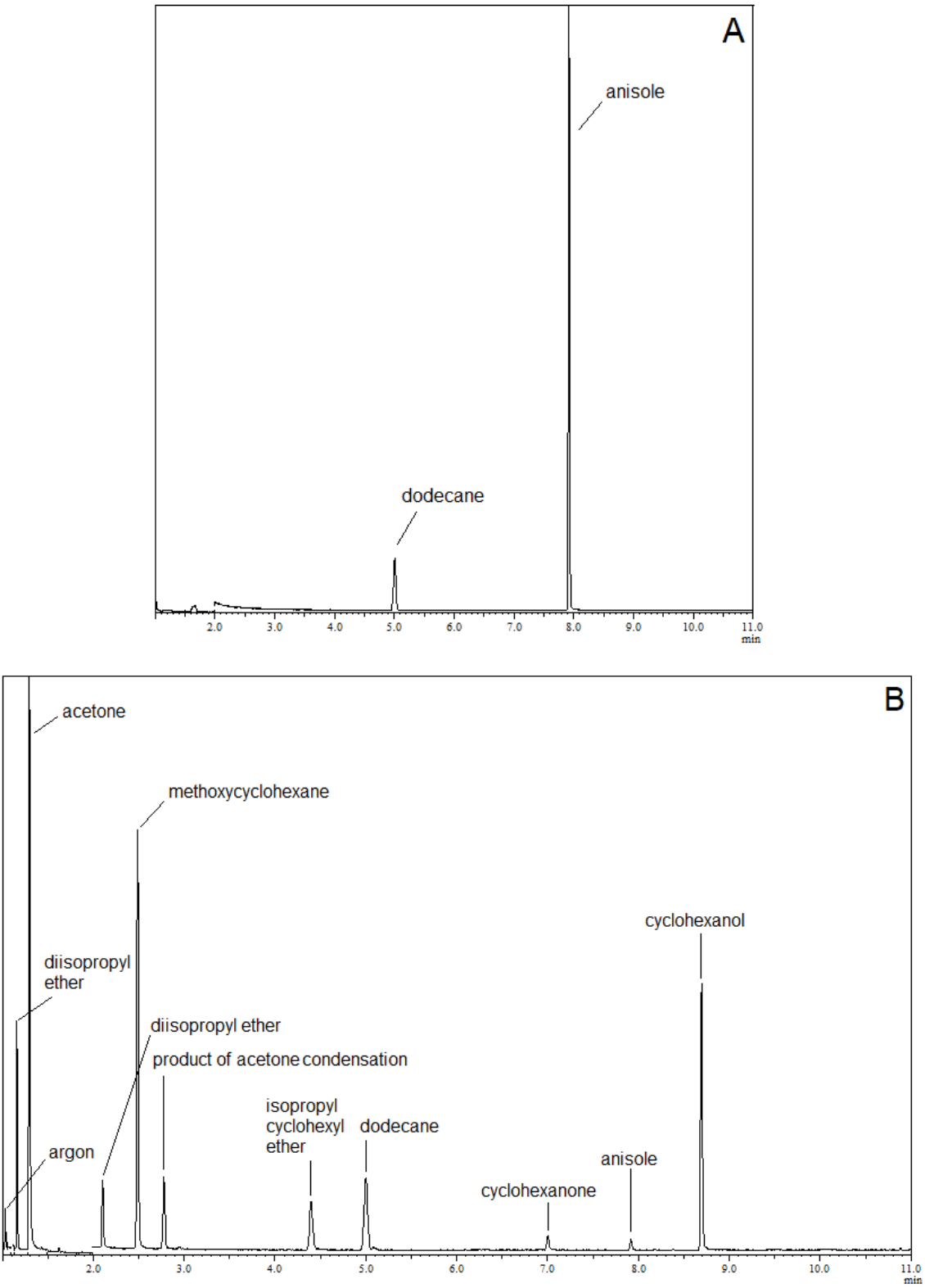

Figure S2. Examples of chromatograms of an initial reaction mixture (A) and a final reaction mixture (B).