

## Supporting Information

# Nickel catalysts in the hydrogenation of benzyltoluene using impure hydrogen streams

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*KEYWORDS Hydrogenation, Hydrogen purification, Nickel catalyst, Liquid organic hydrogen carrier*

### S1 Equations

Selectivity

$$S_{Hx-BT, t_i} = \frac{A_{total, formed Hx-BT \text{ until } t_i}}{A_{total, consumed H0-BT \text{ until } t_i}} \quad (1)$$

Conversion

$$X_{t_i} = \frac{A_{H0-BT, total} - A_{H0-BT, t_i}}{A_{H0-BT, total}} \quad (2)$$

Degree of hydrogenation

$$DoH = \frac{A_{H12-BT} + A_{H6-BT}}{A_{H12-BT} + A_{H6-BT} + A_{H0-BT}} \quad (3)$$

Hydrogen utilization

$$Utilization = \frac{mol_{H_2, H0-BT \text{ hydrogenation}}}{mol_{H_2, total \text{ consumption}}} \quad (4)$$

*Table S 1 liquid and gas sampling intervals for the hydrogenation experiments*

REACTION TIME [min]	LIQUID SAMPLE [-]	GAS SAMPLE [-]
0	X	X
10	X	-
20	X	-
30	X	X
45	X	-

60	X	X
90	X	X
120	X	X
150	-	-
180	X	X
240	X	X
300	X	X
360	X	X

## S2 Discussion and Results

### TEMPERATUR VARIATION

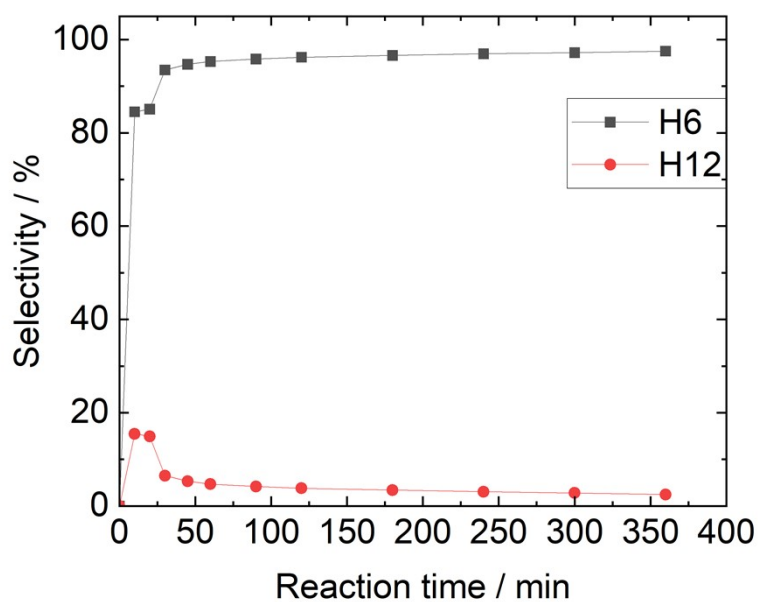


Figure S 1 Selectivity for H6-Benzyltoluene (black) and H12 Benzyltoluene (red) of Benzyltoluene hydrogenation using a commercial Nickel catalyst (reaction conditions:  $m_{BT} = 100g$ ,  $p = 50bar$ ,  $T = 170^{\circ}C$ ,  $t = 6h$ , **CO-gas fraction 6%**)

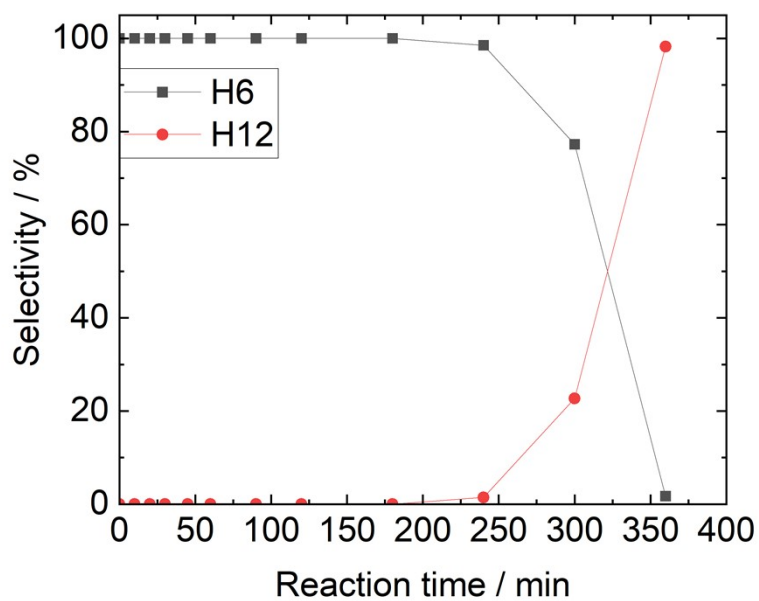


Figure S 2 Selectivity for H6-Benzyltoluene (black) and H12 Benzyltoluene (red) of Benzyltoluene hydrogenation using a commercial Nickel catalyst (reaction conditions:  $m_{BT} = 100g$ ,  $p = 50bar$ ,  $T = 200^{\circ}C$ ,  $t = 6h$ , **CO-gas fraction 6%**)

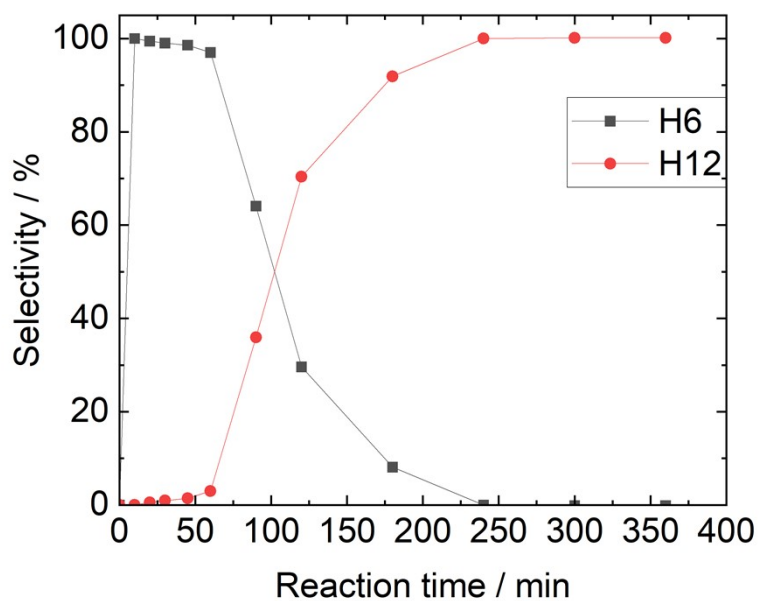


Figure S 3 Selectivity for H6-Benzyltoluene (black) and H12 Benzyltoluene (red) of Benzyltoluene hydrogenation using a commercial Nickel catalyst (reaction conditions:  $m_{BT} = 100g$ ,  $p = 50bar$ ,  $T = 230^{\circ}C$ ,  $t = 6h$ , **CO-gas fraction 6%**)

## VARIATION OF TOAL PRESSURE

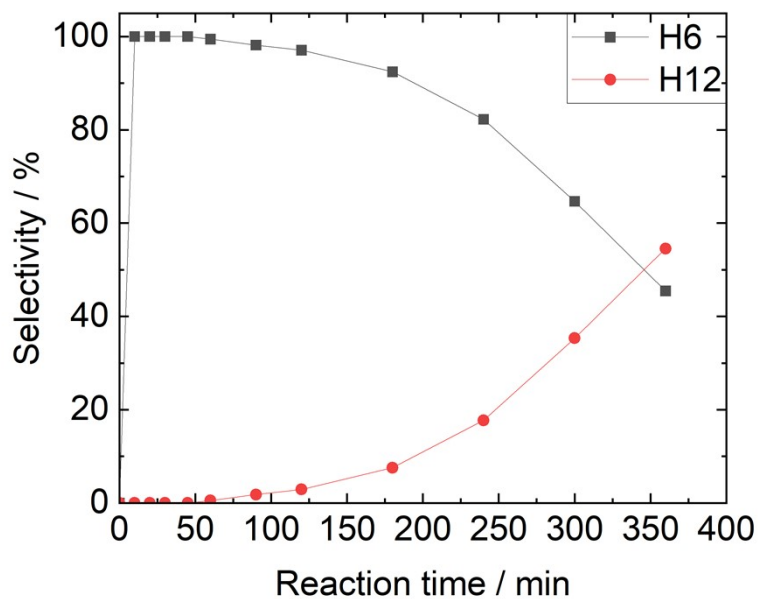


Figure S 4 Selectivity for H6-Benzyltoluene (black) and H12 Benzyltoluene (red) of Benzyltoluene hydrogenation using a commercial Nickel catalyst at 10 bar (reaction condition:  $m_{BT} = 100g$ ,  $T = 200^{\circ}C$ ,  $t = 6h$ , CO-gas fraction 1.2%)

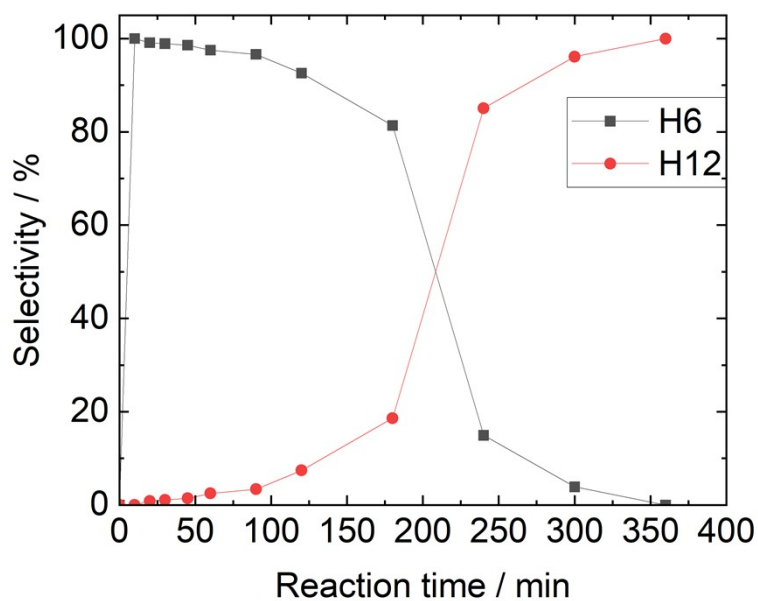


Figure S 5 Selectivity for H6-Benzyltoluene (black) and H12 Benzyltoluene (red) of Benzyltoluene hydrogenation using a commercial Nickel catalyst at 30 bar (reaction conditions:  $m_{BT} = 100g$ ,  $T = 200^{\circ}C$ ,  $t = 6h$ , CO-gas fraction 1.2%)

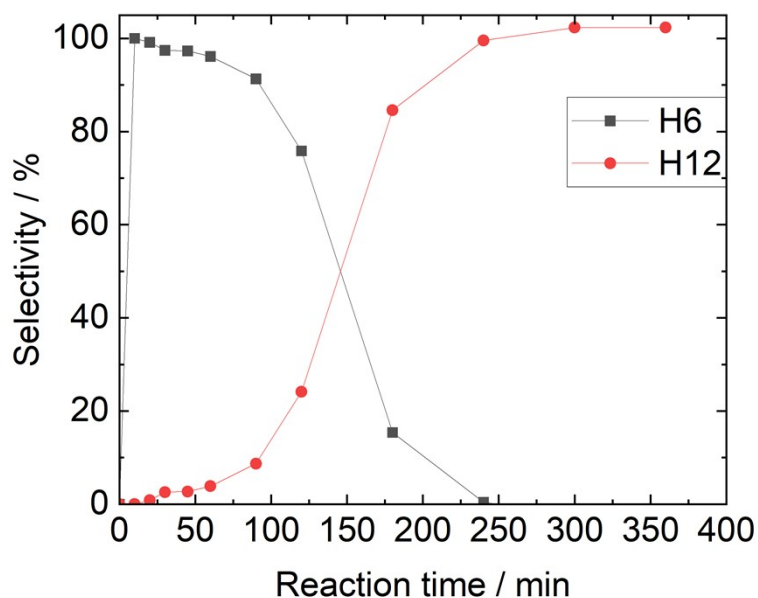


Figure S 6 Selectivity for H6-Benzyltoluene (black) and H12 Benzyltoluene (red) of Benzyltoluene hydrogenation using a commercial Nickel catalyst at 50 bar (reaction conditions:  $m_{BT} = 100g$ ,  $T = 200^{\circ}C$ ,  $t = 6h$ , CO-gas fraction 1.2%)

#### GAS VARIATION

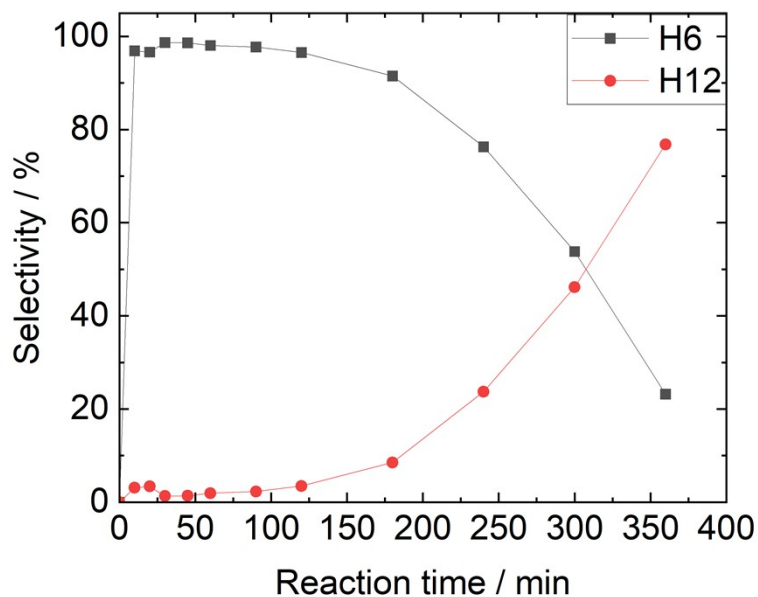


Figure S 7 Selectivity for H6-Benzyltoluene (black) and H12 Benzyltoluene (red) of Benzyltoluene hydrogenation using a commercial Nickel catalyst (reaction conditions:  $m_{BT} = 100g$ ,  $p = 50bar$ ,  $T = 170^{\circ}C$ ,  $t = 6h$ , CO-gas fraction 0.6%)

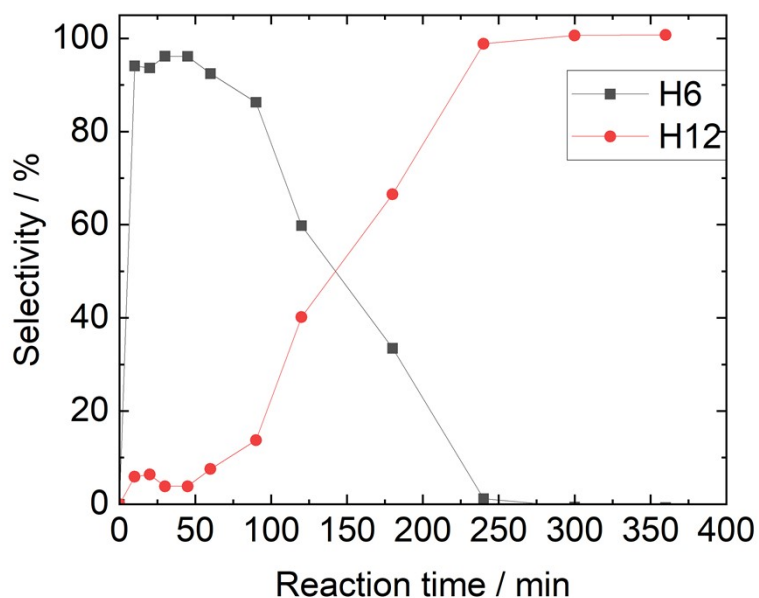


Figure S 8 Selectivity for H6-Benzyltoluene (black) and H12 Benzyltoluene (red) of Benzyltoluene hydrogenation using a commercial Nickel catalyst (reaction conditions:  $m_{BT} = 100g$ ,  $p = 50bar$ ,  $T = 200^{\circ}C$ ,  $t = 6h$ , **CO-gas fraction 0.6%**)

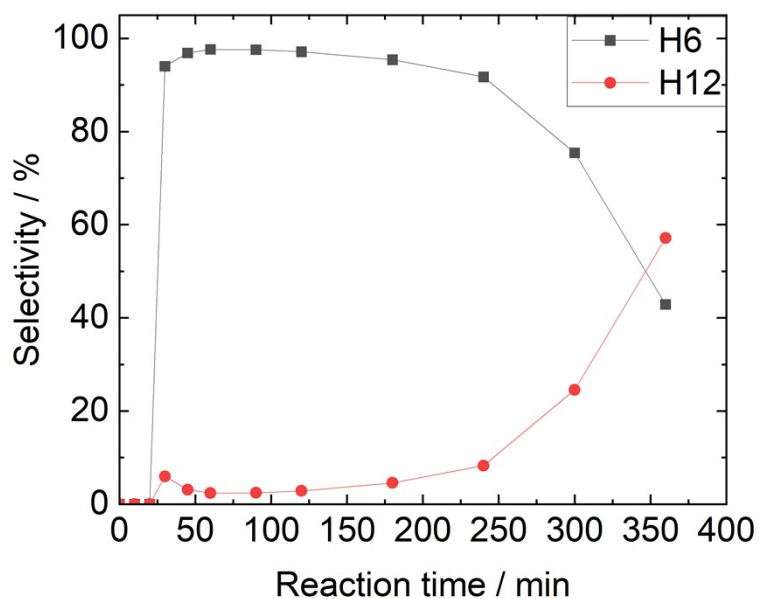


Figure S 9 Selectivity for H6-Benzyltoluene (black) and H12 Benzyltoluene (red) of Benzyltoluene hydrogenation using a commercial Nickel catalyst with **15 bar  $N_2$ -partial pressure** (reaction conditions:  $m_{BT} = 100g$ ,  $p = 50bar$ ,  $T = 170^{\circ}C$ ,  $t = 6h$ , **CO-gas fraction 0.6%**)

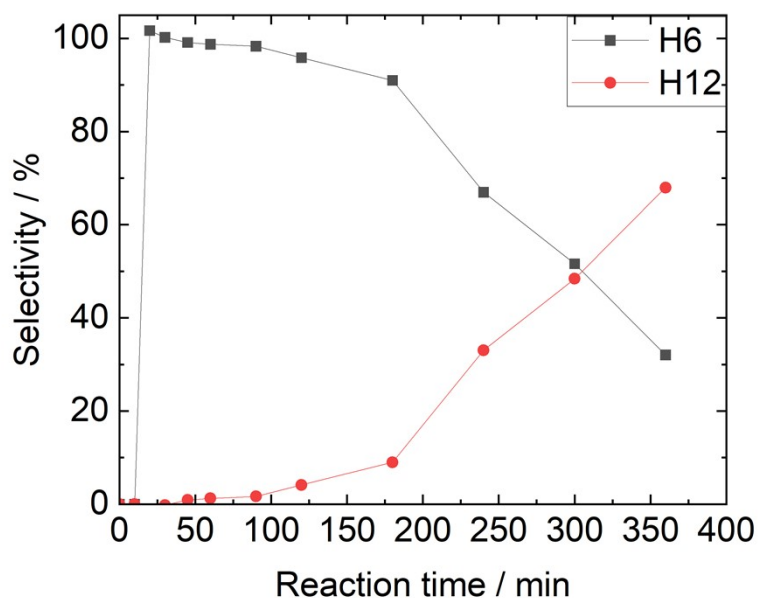


Figure S 10 Selectivity for H6-Benzyltoluene (black) and H12 Benzyltoluene (red) of Benzyltoluene hydrogenation using a commercial Nickel catalyst with **15 bar N<sub>2</sub>-partial pressure** (reaction conditions:  $m_{BT} = 100g$ ,  $p = 50bar$ ,  $T = 200^{\circ}C$ ,  $t = 6h$ , **CO-gas fraction 0.6%**)

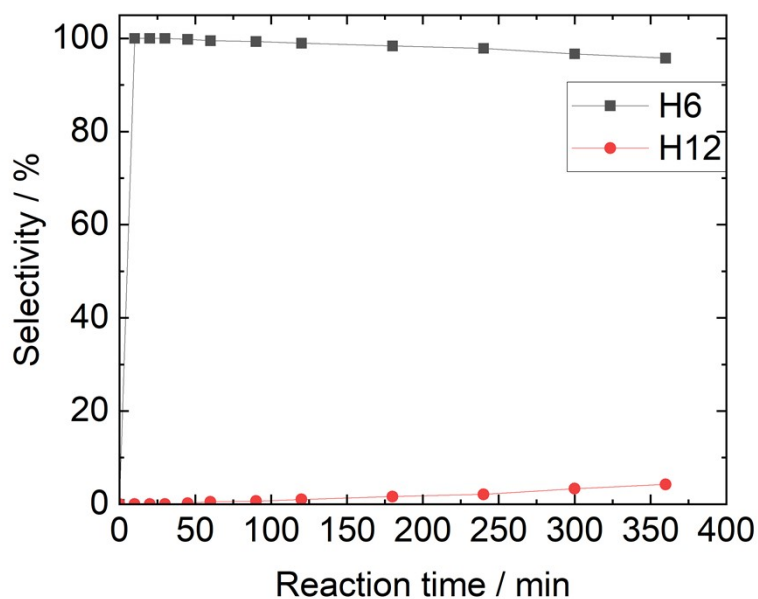


Figure S 11 Selectivity for H6-Benzyltoluene (black) and H12 Benzyltoluene (red) of Benzyltoluene hydrogenation using a commercial Nickel catalyst with **15 bar CO<sub>2</sub>-partial pressure** (reaction conditions:  $Ru/BT$  ratio: 1/2000;  $m_{BT} = 100g$ ,  $p = 50bar$ ,  $T = 170^{\circ}C$ ,  $t = 6h$ , **CO-gas fraction 0.6%**)



Figure S 12 Selectivity for H6-Benzyltoluene (black) and H12 Benzyltoluene (red) of Benzyltoluene hydrogenation using a commercial Nickel catalyst with 15 bar CO<sub>2</sub>-partial pressure (reaction conditions: Ru/BT ratio: 1/2000; m<sub>BT</sub> = 100g, p = 50bar, T= 200°C, t = 6h, CO-gas fraction 0.6%)

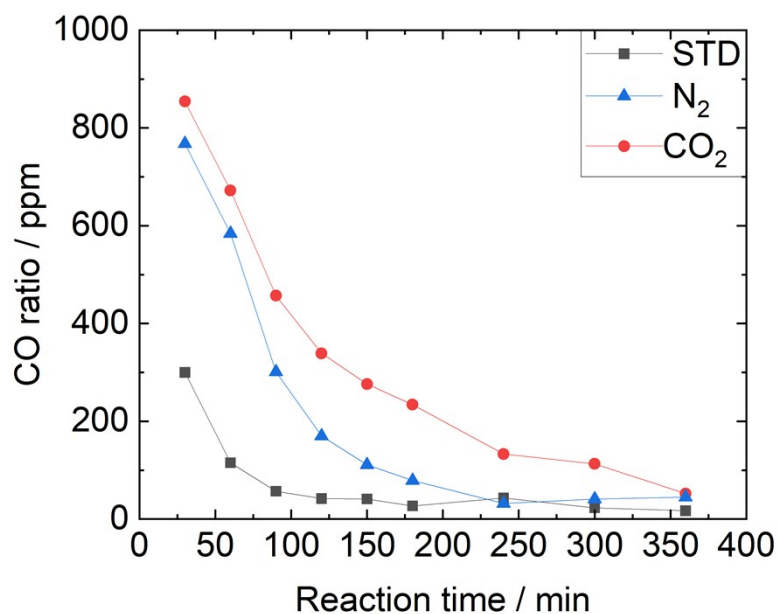


Figure S 13 CO ratio in ppm over reaction time for the Benzyltoluene hydrogenation using a commercial Nickel catalyst and N<sub>2</sub> and CO<sub>2</sub> as additional gases, compared to a hydrogenation experiment with CO as only impurity (STD), (reaction conditions: Ni/BT ratio 0.045; m<sub>BT</sub> = 100 g, p = 50 bar, p<sub>N<sub>2</sub>/CO<sub>2</sub></sub> = 15 bar, T = 200 °C, t = 6 h, CO-gas fraction 0,6 %)

## S3 Catalyst stability

XRD results

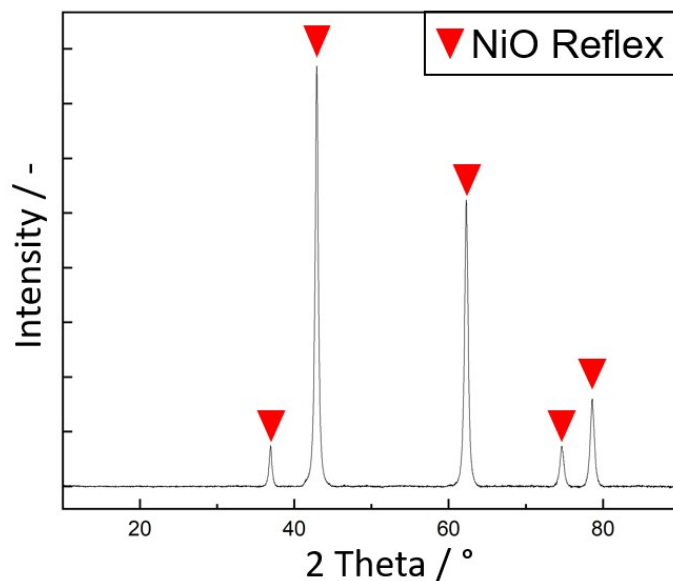


Figure S 14 XRD-pattern for an unused Ni catalyst (black) compared to simulated NiO reflexes (Red; ICSD reference code: 98-016-6112)

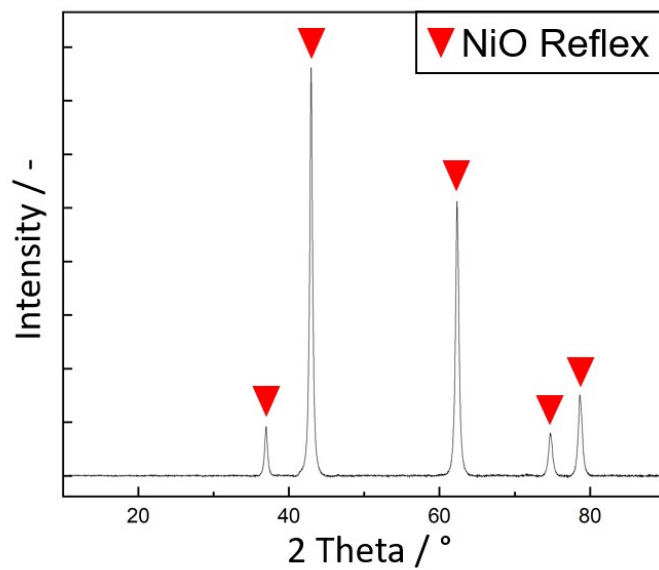


Figure S 15 XRD-pattern for a spent Ni catalyst (black, reaction conditions:  $m_{BT} = 100g$ ,  $p = 50bar$ ,  $T = 200^{\circ}C$ ,  $t = 6h$ , CO-gas fraction 1.2%) compared to simulated NiO reflexes (Red; ICSD reference code: 98-016-6112)

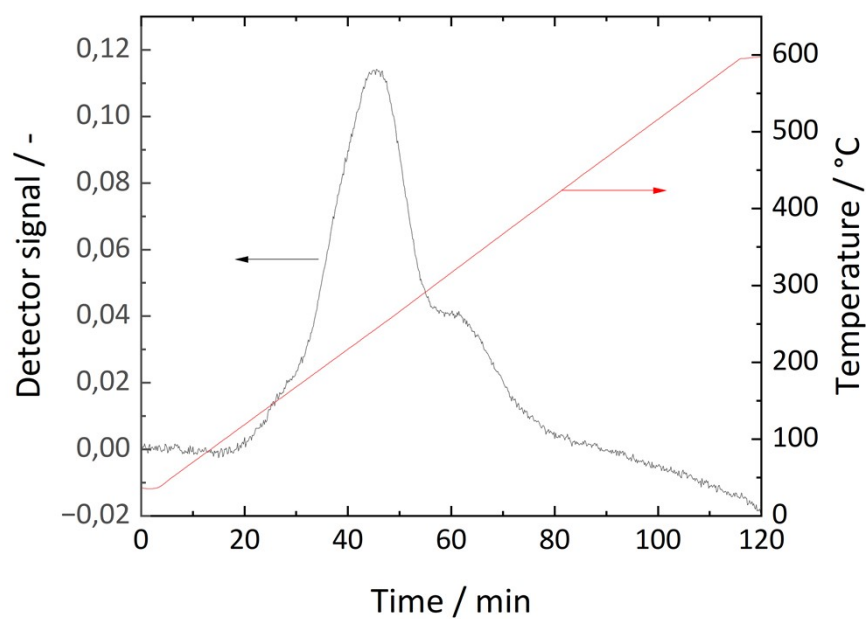


Figure S 16 H<sub>2</sub>-TPR Measurement of the commercial Ni catalyst (H<sub>2</sub>-flow = 20 cm<sup>3</sup> min<sup>-1</sup>, Temperature ramp = 5 °C min<sup>-1</sup>)

Table S2 Nickel content determined with ICP-OES, Surface area and pore volume determined with nitrogen physisorption for fresh and spent Ni catalyst (reaction conditions:  $m_{BT} = 100\text{g}$ ,  $p = 50\text{bar}$ ,  $T = 200^\circ\text{C}$ ,  $t = 6\text{h}$ , CO-gas fraction 1.2%)

<b>MATERIAL</b>	<b>NI CONTENT [WT%]</b>	<b>SURFACE AREA [m<sup>2</sup>/g]</b>	<b>PORE VOLUME [cc/g]</b>
<b>NI CATALYST BEFORE REACTION</b>	50,2	2.232x10 <sup>2</sup>	2.798x10 <sup>-1</sup>
<b>NI CATALYST AFTER REACTION</b>	52,0	2.367 x10 <sup>2</sup>	3.278x10 <sup>-1</sup>