

Supporting Information

Better Through Oxygen Functionality? The Benzophenone/Dicyclohexylmethanol LOHC-System

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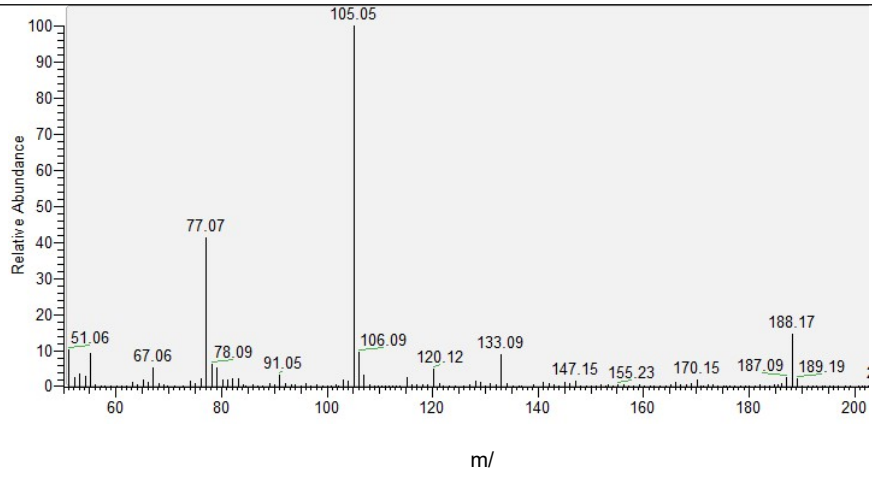
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Table SI-1: Acquired mass spectra and retention times of the reaction intermediates and (side) products during dehydrogenation of H14-BP.

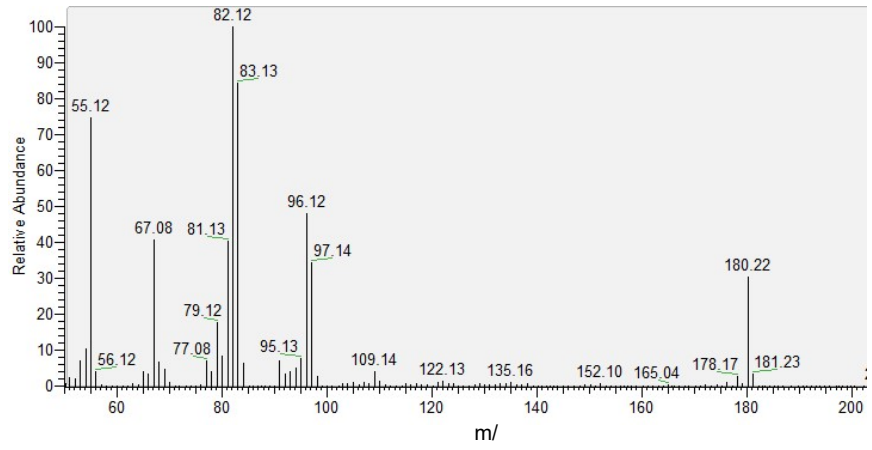
Compound	Acquired mass spectrum	Retention time [min]
H14-BP	<p>Mass spectrum of H14-BP. The x-axis represents m/z from 60 to 200, and the y-axis represents Relative Abundance from 0 to 100. The base peak is at m/z 95.13. Other labeled peaks include 55.08, 57.08, 67.10, 68.12, 81.12, 93.11, 96.15, 98.15, 113.11, 114.13, 135.13, 149.15, 165.11, 178.18, and 194.16.</p>	22.7-23.5
H12-BP	<p>Mass spectrum of H12-BP. The x-axis represents m/z from 60 to 200, and the y-axis represents Relative Abundance from 0 to 100. The base peak is at m/z 83.13. Other labeled peaks include 55.10, 56.12, 67.09, 68.12, 79.09, 84.15, 96.14, 110.10, 111.09, 112.11, 129.08, 139.19, 147.01, 163.14, 174.16, 192.16, and 194.18.</p>	21.5-22.2
H8-BP	<p>Mass spectrum of H8-BP. The x-axis represents m/z from 60 to 200, and the y-axis represents Relative Abundance from 0 to 100. The base peak is at m/z 107.07. Other labeled peaks include 55.09, 63.10, 67.12, 77.06, 79.11, 81.10, 82.17, 91.07, 104.16, 105.06, 108.11, 121.16, 141.04, 155.23, 172.19, 190.21, and 191.30.</p>	28.0-28.1

H6-BP



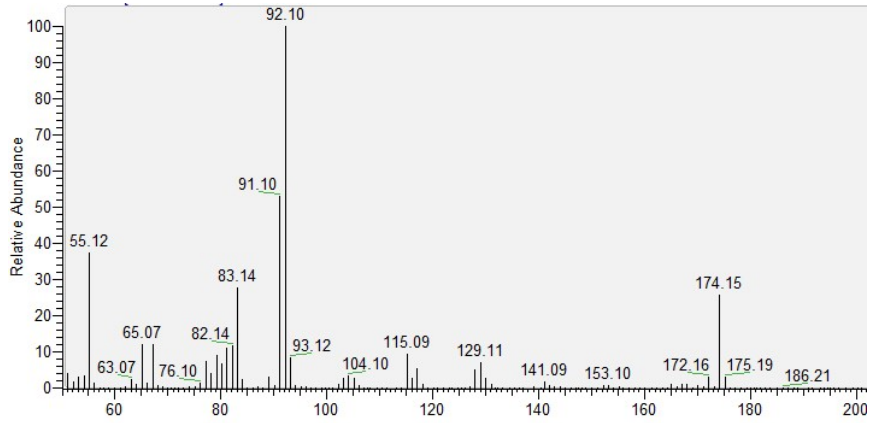
28.2-28.5

H12-DPM



9.7-10.0

H6-DPM



13.6-13.8

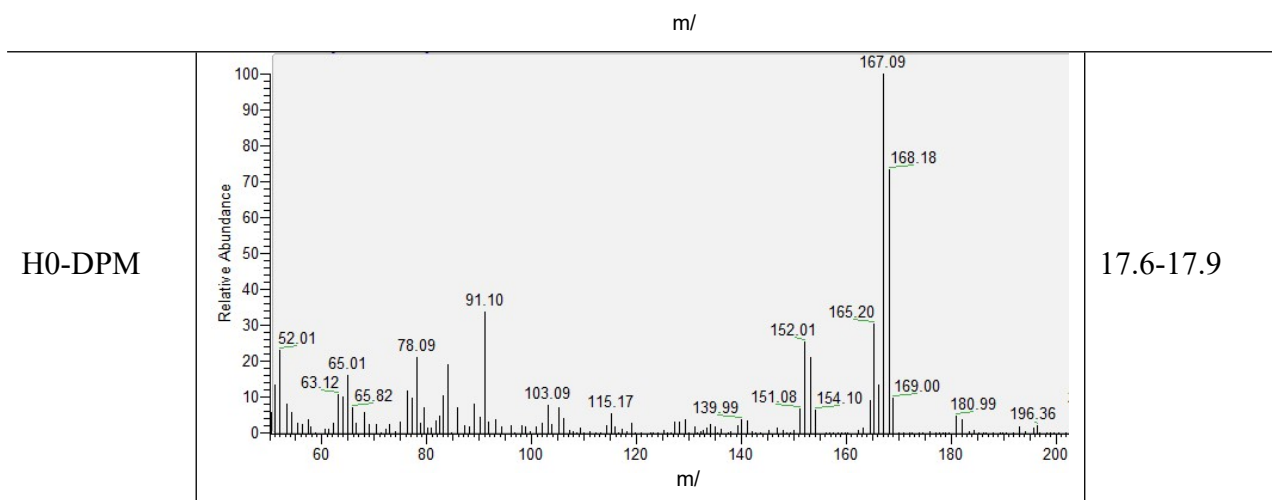
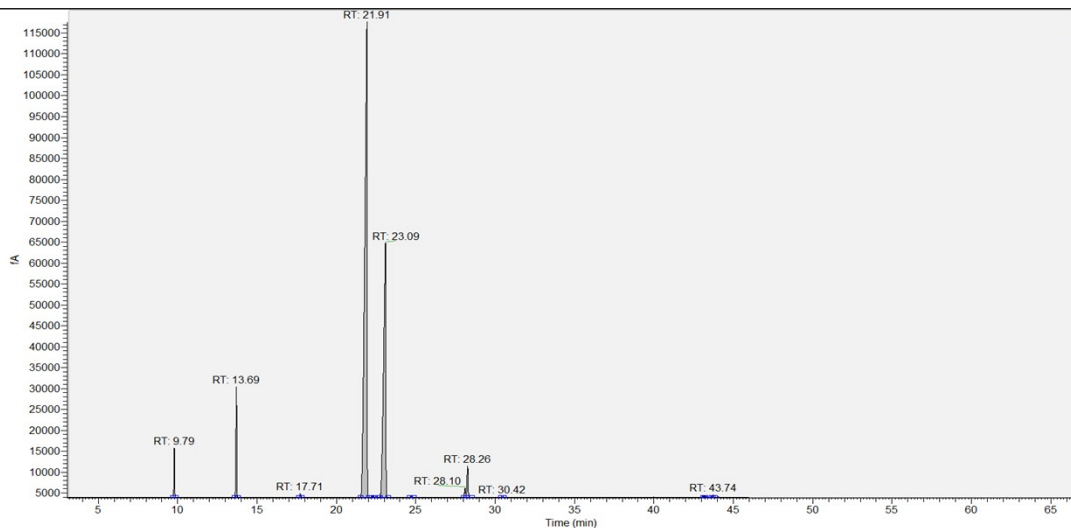


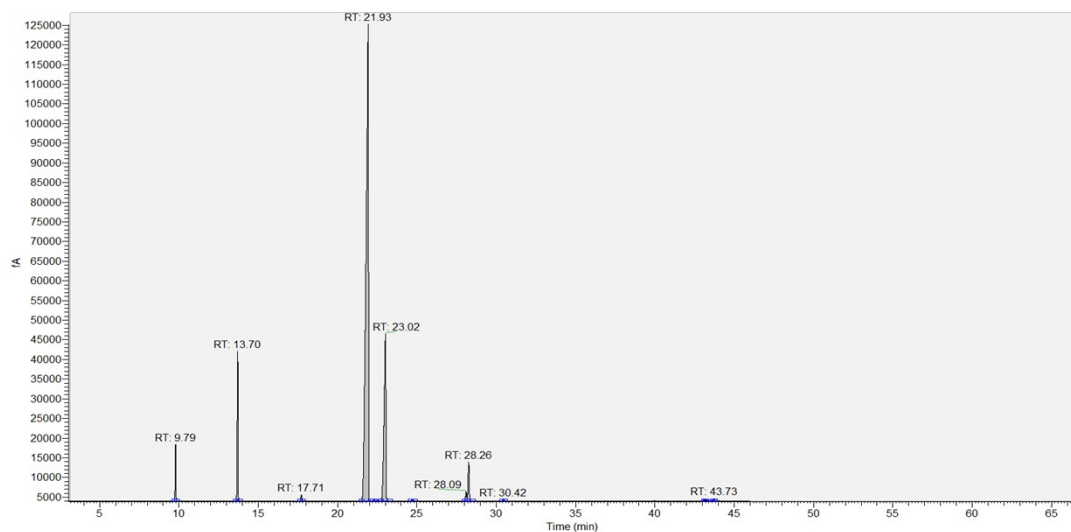
Table SI-2: GC spectra over the course of the dehydrogenation of H14-BP with a Pt/Al₂O₃ catalyst.

Reaction time [min]	GC spectrum
0	
30	

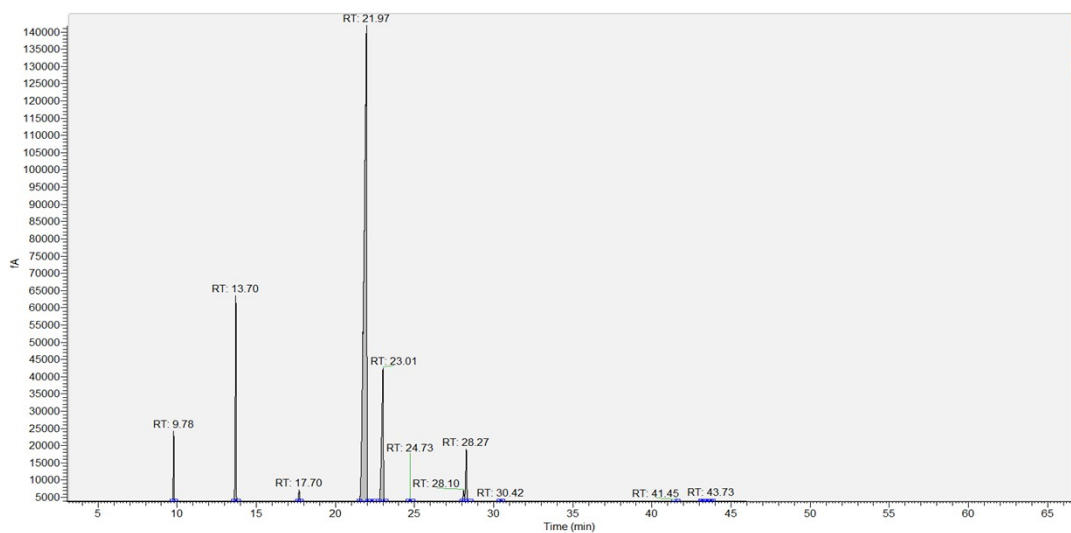
60



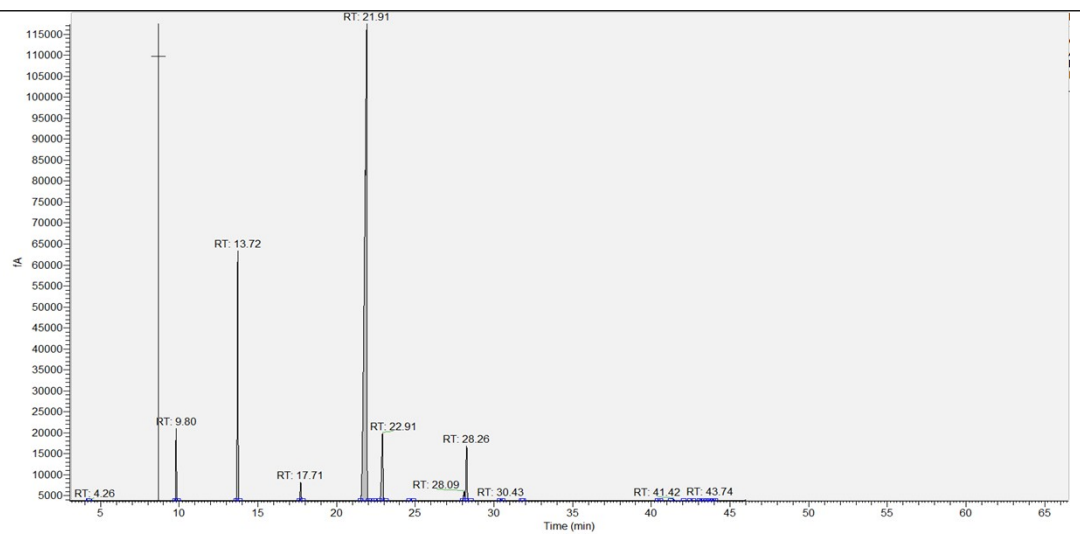
90



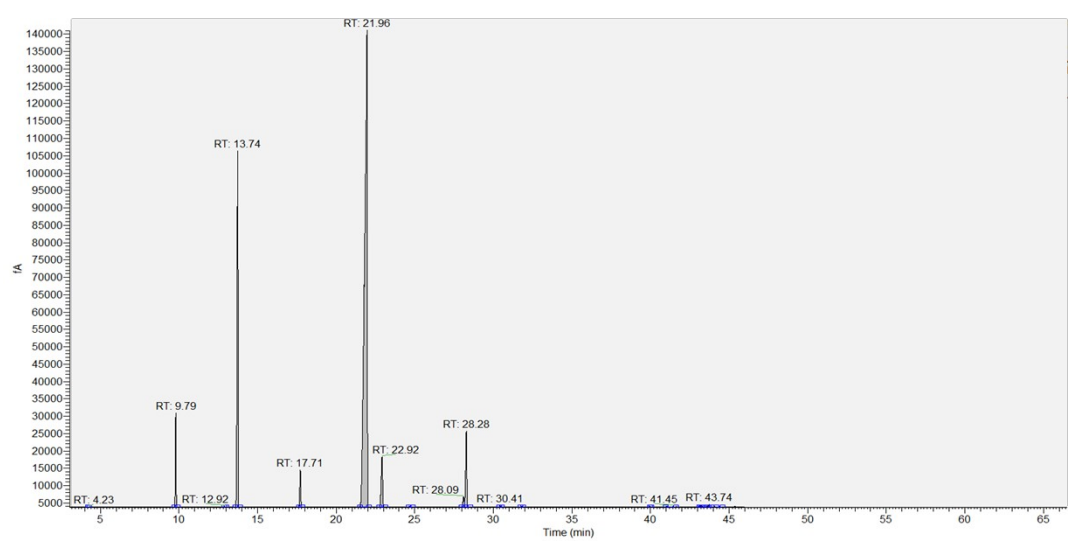
120



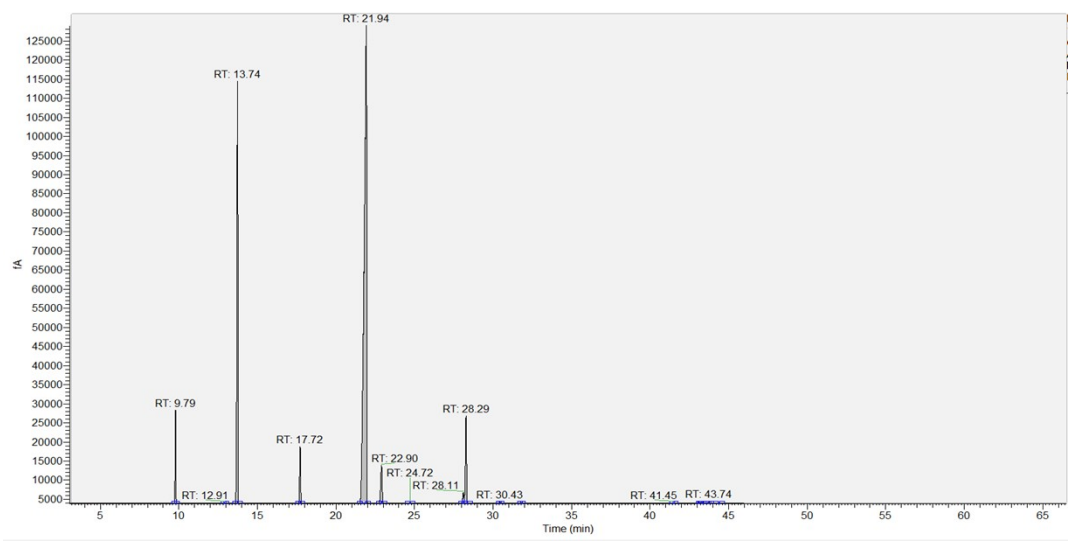
180



240



300



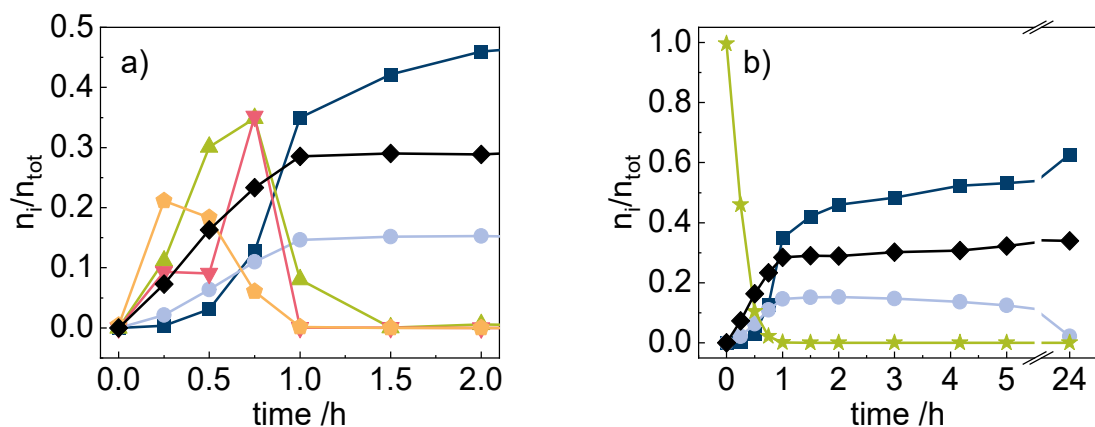


Figure SI-1: Liquid-phase molar reactant and product concentration in the hydrogenation of H0-BP with 5 mass% Ru/Al₂O₃ at 180 °C and 50 bar H₂, a) desired product H14-BP (■) and intermediate species H2-BP (◆), H6-BP (▼), H8-BP (▲), H12-BP (●) as well as the sum of all Hx-DPM side products (◆) in the first 2 h of reaction time, b) reactant H0-BP (★) and main products H14-BP (■) and H12-BP (●) as well as the sum of all Hx-DPM side products (◆) over the course of 24 h reaction time.

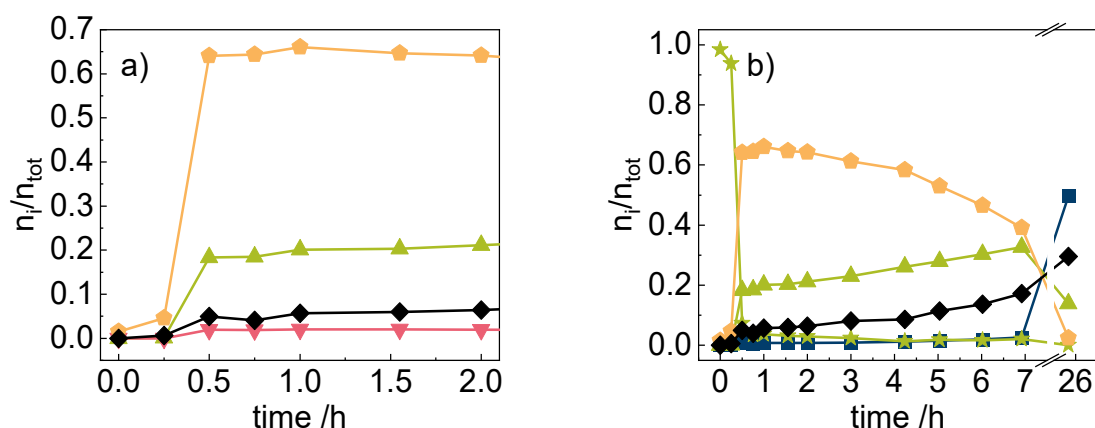


Figure SI-2: Liquid-phase molar reactant and product concentration in the hydrogenation of H0-BP with 0.3 mass% Pt/Al₂O₃ at 180 °C and 50 bar H₂, a) intermediate species H2-BP (◆), H6-BP (▼) and H8-BP (▲) as well as the sum of all Hx-DPM side products (◆) in the first 2 h of reaction time, b) reactant H0-BP (★) and main products H14-BP (■), H2-BP (◆) and H8-BP (▲), as well as the sum of all Hx-DPM side products (◆) over the course of 26 h reaction time.

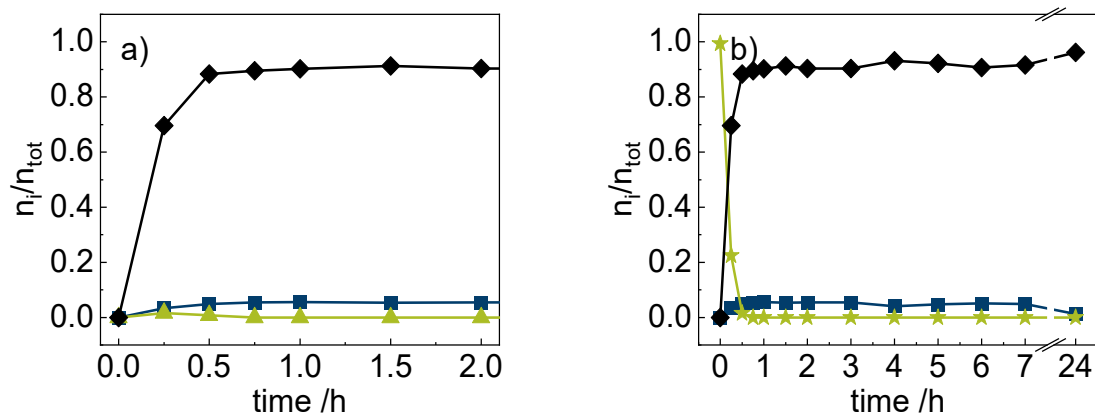


Figure SI-3: Liquid-phase molar reactant and product concentration in the hydrogenation of H0-BP with 5 mass% Pt/C at 180 °C and 50 bar H₂, a) desired product H14-BP (■) and intermediate species H8-BP (▲) as well as the sum of all Hx-DPM side products (◆) in the first 2 h of reaction time, b) reactant H0-BP (★) and product H14-BP (■) as well as the sum of all Hx-DPM side products (◆) over the course of 24 h reaction time.

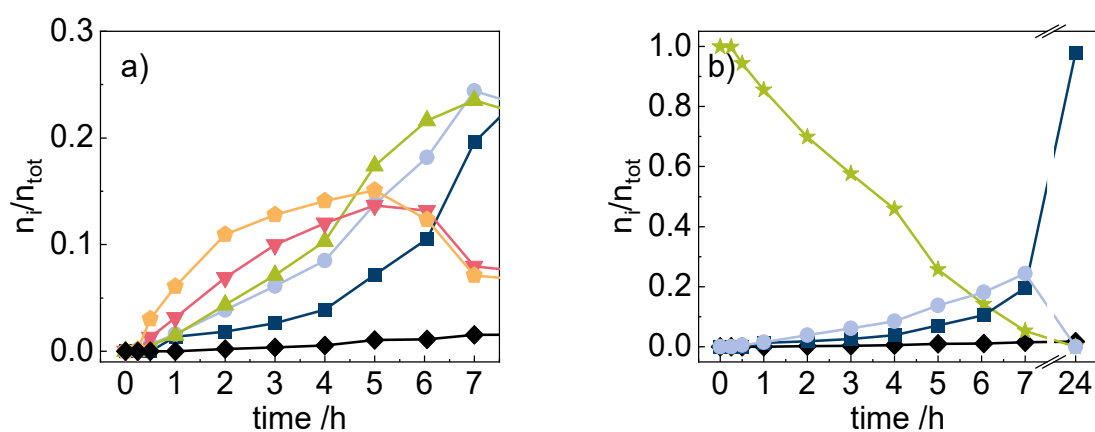


Figure SI-4: Liquid-phase molar reactant and product concentration in the hydrogenation of H0-BP with 5 mass% Ru/Al₂O₃ at 90 °C and 50 bar H₂, a) desired product H14-BP (■) and intermediate species H2-BP (◆), H6-BP (▼), H8-BP (▲), H12-BP (●) as well as the sum of all Hx-DPM side products (◆) in the first 7 h of reaction time, b) reactant H0-BP (★) and main products H14-BP (■) and H12-BP (●) as well as the sum of all Hx-DPM side products (◆) over the course of 24 h reaction time.

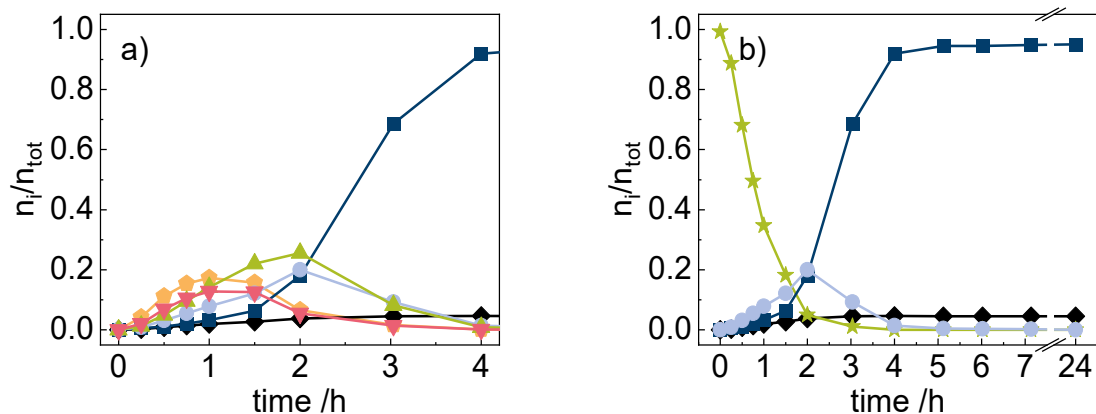


Figure SI-5: Liquid-phase molar reactant and product concentration in the hydrogenation of H0-BP with 5 mass% Ru/Al₂O₃ at 120 °C and 50 bar H₂, a) desired product H14-BP (■) and intermediate species H2-BP (◆), H6-BP (▼), H8-BP (▲), H12-BP (●) as well as the sum of all Hx-DPM side products (◆) in the first 4 h of reaction time, b) reactant H0-BP (★) and main products H14-BP (■) and H12-BP (●) as well as the sum of all Hx-DPM side products (◆) over the course of 24 h reaction time.

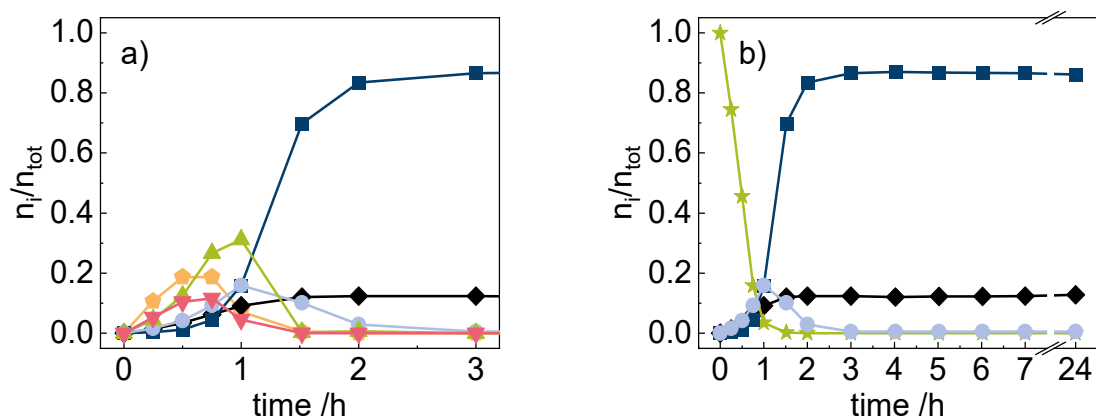


Figure SI-6: Liquid-phase molar reactant and product concentration in the hydrogenation of H0-BP with 5 mass% Ru/Al₂O₃ at 150 °C and 50 bar H₂, a) desired product H14-BP (■) and intermediate species H2-BP (◆), H6-BP (▼), H8-BP (▲), H12-BP (●) as well as the sum of all Hx-DPM side products (◆) in the first 3 h of reaction time, b) reactant H0-BP (★) and main products H14-BP (■) and H12-BP (●) as well as the sum of all Hx-DPM side products (◆) over the course of 24 h reaction time.

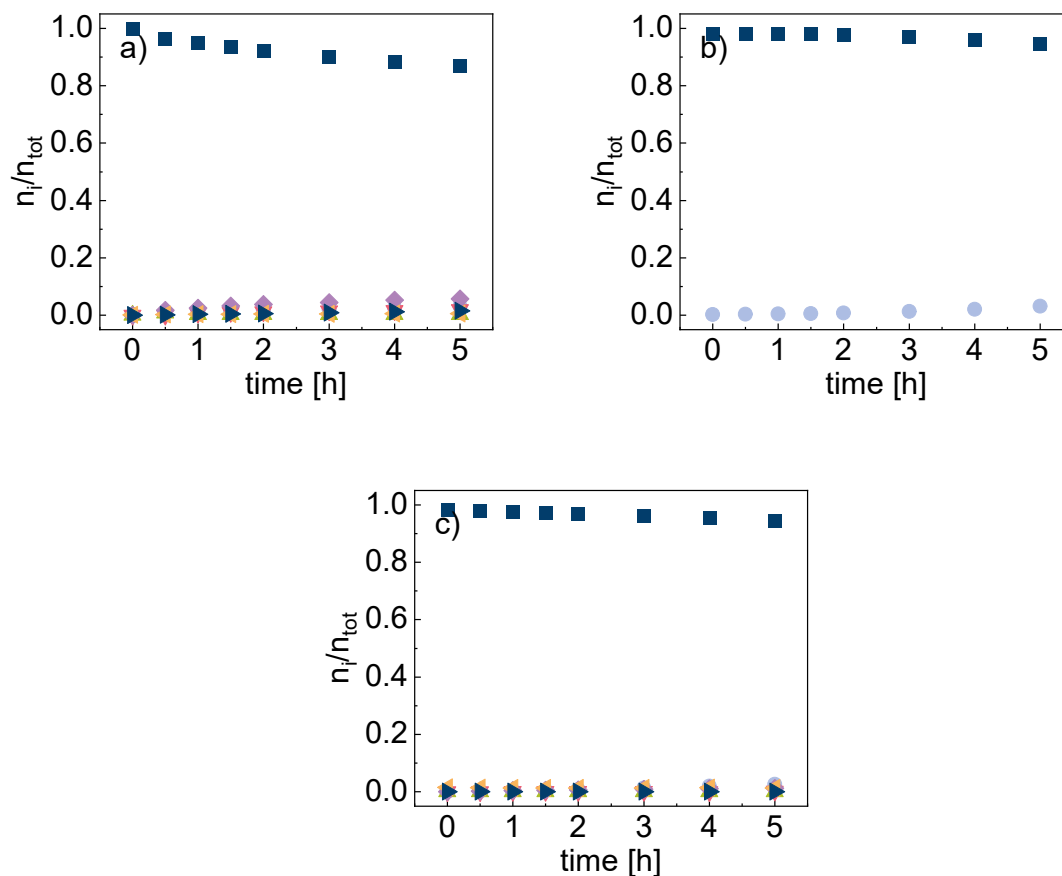


Figure SI-7: Liquid phase molar concentration of reactant and products in the dehydrogenation of 0.15 mol H14-BP at 230 °C with 200 mL min⁻¹ argon overflow over a) Pd/C, 5 mass%, b) Ir/C, 5 mass%, or c) Rh/C, 5 mass%: H14-BP (■), H12-BP (●), H8-BP (▲), H6-BP (▼), H12-DPM (◀), H6-DPM (◆), H0-DPM (▶). Pd/C: Sigma Aldrich, 75992; Ir/C: Fuelcellstore, 6091601; Rh/C: Alfa Aesar, A15965.

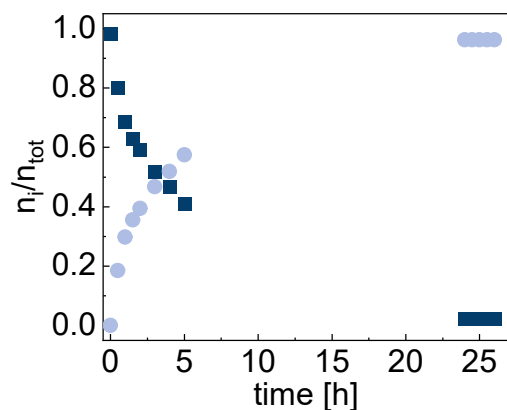


Figure SI-8: Liquid phase molar concentrations of reactant H14-BP (■) and only product H12-BP (●) in the dehydrogenation of 0.15 mol H14-BP at 170 °C with 200 mL min⁻¹ argon overflow over CuO/ZnO/Al₂O₃.

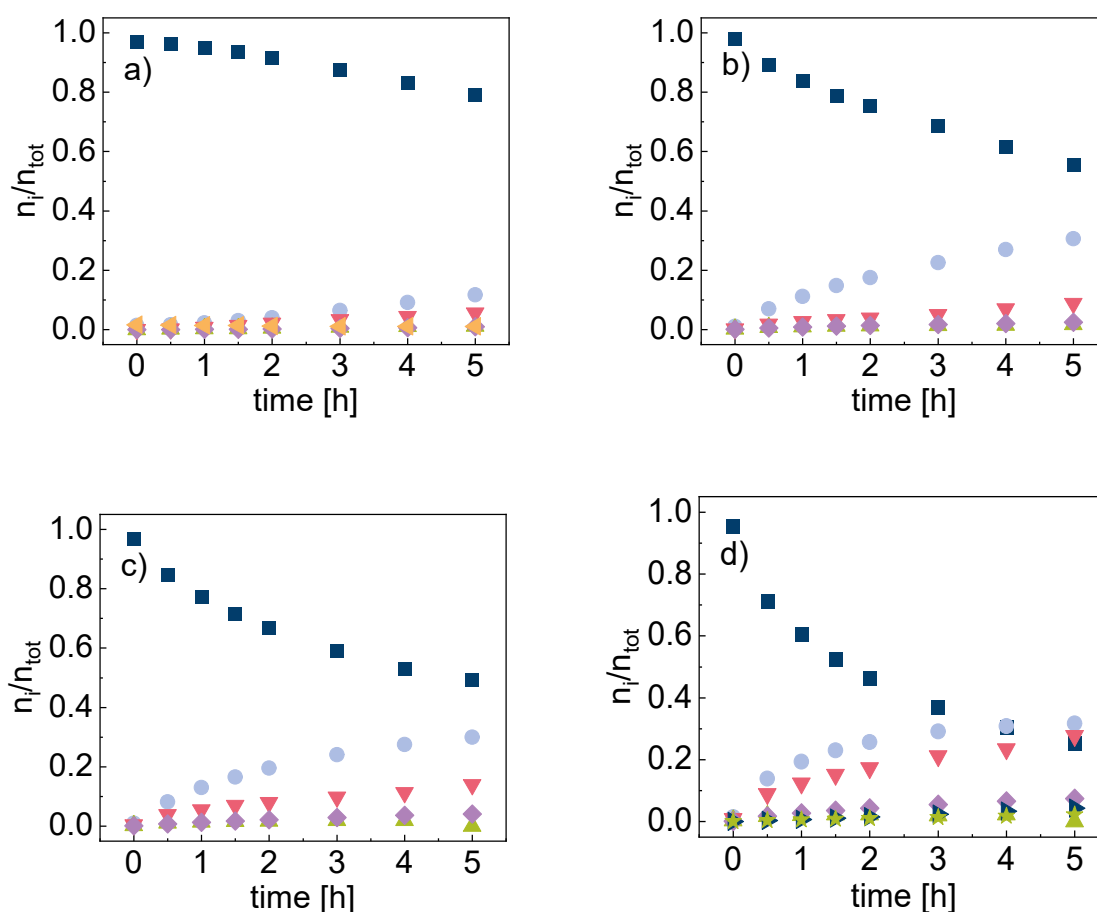


Figure SI-9: Liquid phase molar concentration of reactant and products in the dehydrogenation of 0.15 mol H14-BP at a) 220 °C, b) 230 °C, c) 240 °C, and d) 250 °C, with 200 mL min⁻¹ argon overflow over Pt/C, 5 mass%: H14-BP (■), H12-BP (●), H8-BP (▲), H6-BP (▼), H0-BP (★), H6-DPM (◆), H0-DPM (▶).