Supplementary Materials: Novel Polymer–Silica Composite-Based Bifunctional Catalysts for Hydrodeoxygenation of 4-(2-Furyl)-3-Buten-2-One as Model Substance for Furfural–Acetone Aldol Condensation Products

Michael Goepel, Ruben Ramos, Roger Gläser and David Kubička

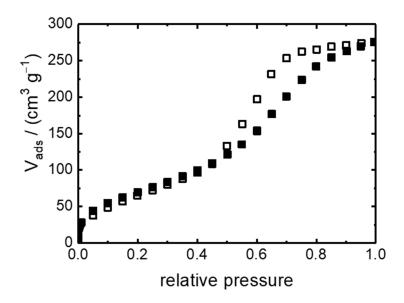


Figure S1. Volume adsorbed (V_{ads}) over relative pressure (p / p_0) from N_2 sorption for (1)Pt(13)PSC recorded at -196 °C.

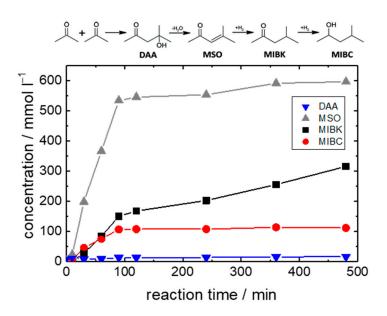


Figure S2. Reactant concentration of the self-condensation products of acetone over time for the HDO of FAc carried out using (1)Pt(13)PSC as a catalyst and acetone as a solvent (T = 250 °C, p_{H2} = 100 bar, $m_{catalyst}$ = 0.25 g, 0.5 g FAc (24.5 mmol l^{-1}) dissolved in 150 ml acetone, stirring speed = 1000 min⁻¹).

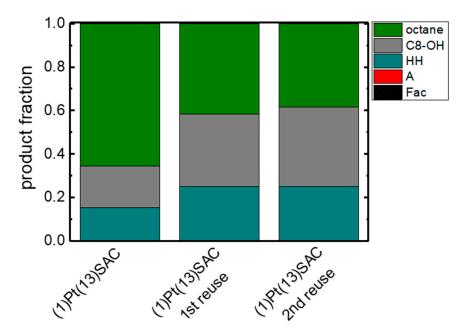


Figure S3. Product fractions obtained for the reusability studies of (1)Pt(13)PSC in the HDO of FAc (T = 250 °C, p_{H2} = 100 bar, $m_{catalyst}$: m_{FAc} = 2 : 1 , c_{FAc} = 24.5 mmol l^{-1} , solvent: cyclohexane, stirring speed = 1000 min⁻¹). The catalyst was washed five times with 50 ml cyclohexane and subsequently dried for 5 h at 200 °C in an air atmosphere between the experiments.

Table S1. Productivity (given as mmol octane produced per gram of noble metal and hour) and reaction conditions for the hydrodeoxygenation of 4-(2-furyl)-3-buten-2-one reported in literature and this work ((1)Ru(13)PSC)).

Catalyst	Productivity / (mmol g ⁻¹ h ⁻¹)	T/°C	рн2 / bar	Solvent
Ru/SILP [1] ^a	0.5	150	120	(EMIM)NTf2
Pt/Al-SBA15 [2]	0.0	200	50	Cyclohexane
Pd/Al-MCM-41 [3]	90.9	80	40^{b}	$scCO_2$
$Pd/Nb_2O_5[4]$	12.1	170	20	Cyclohexane
Pd/Nb2O5/SiO2 [5]	10.9	170	25	Cyclohexane
(1)Ru(13)PSC	165.3	250	200	Cyclohexane

^a using 4-(2-furyl)-butan-2-one (substance A, Figure 1) as reactant, ^b pco2 = 140 bar.

References

- 1. Luska, K.L.; Julis, J.; Stavitski, E.; Zakharov, D.N.; Adams, A.; Leitner, W. Bifunctional nanoparticle–SILP catalysts (NPs@ SILP) for the selective deoxygenation of biomass substrates. *Chem. Sci.* **2014**, *5*, 4895–4905.
- 2. Ramos, R.; Tišler, Z.; Kikhtyanin, O.; Kubička, D. Towards understanding the hydrodeoxygenation pathways of furfural–acetone aldol condensation products over supported Pt catalysts. *Catal. Sci. Technol.* **2016**, *6*, 1829–1841.
- 3. Chatterjee, M.; Matsushima, K.; Ikushima, Y.; Sato, M.; Yokoyama, T.; Kawanami, H.; Suzuki, T. Production of linear alkane via hydrogenative ring opening of a furfural-derived compound in supercritical carbon dioxide. *Green Chem.* **2010**, *12*, 779.
- 4. Xia, Q.N.; Cuan, Q.; Liu, X.H.; Gong, X.Q.; Lu, G.Z.; Wang, Y.Q. Pd/NbOPO4 Multifunctional Catalyst for the Direct Production of Liquid Alkanes from Aldol Adducts of Furans. *Angew. Chem. (International ed. in English)* **2014**, *53*, 9755–9760.
- Shao, Y.; Xia, Q.; Liu, X.; Lu, G.; Wang, Y. Pd/Nb2O5/SiO2 Catalyst for the Direct Hydrodeoxygenation of Biomass-Related Compounds to Liquid Alkanes under Mild Conditions. *ChemSusChem* 2015, 8, 1761– 1767.