

Supporting Information

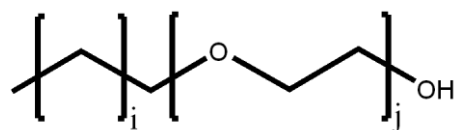
Palladium-Catalyzed Hydroxycarbonylation of 1-Dodecene in Microemulsion Systems: Does Reaction Performance Care about Phase Behavior?

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S1 Chemical structure of the applied surfactants



i=11-13

j=2 (Marlipal 24/20)

j=3 (Marlipal 24/30)

j=4 (Marlipal 24/40)

j=5 (Marlipal 24/50)

j=6 (Marlipal 24/60)

j=7 (Marlipal 24/70)

j=8 (Marlipal 24/80)

Figure S1. Chemical structure of the applied surfactants.

S2 Variation of the ionic strength

We investigated the effect on the initial rate of hydroxycarbonylation, the l:b regioselectivity and the chemoselectivity with different amounts of sodium sulfate as shown in Figure S1. In general, the initial rate of hydroxycarbonylation decreases significantly from 18 mmol/(L·h) for no added salt to 1.5 mmol/(L·h) for 6 wt % sodium sulfate. We have to mention that it was found that the ligand SulfoXantPhos precipitates at salt concentrations above 6 wt % due to a salting out effect. The increase of the ionic strength leads to a lower solubility of SulfoXantPhos in water which results in its precipitation.

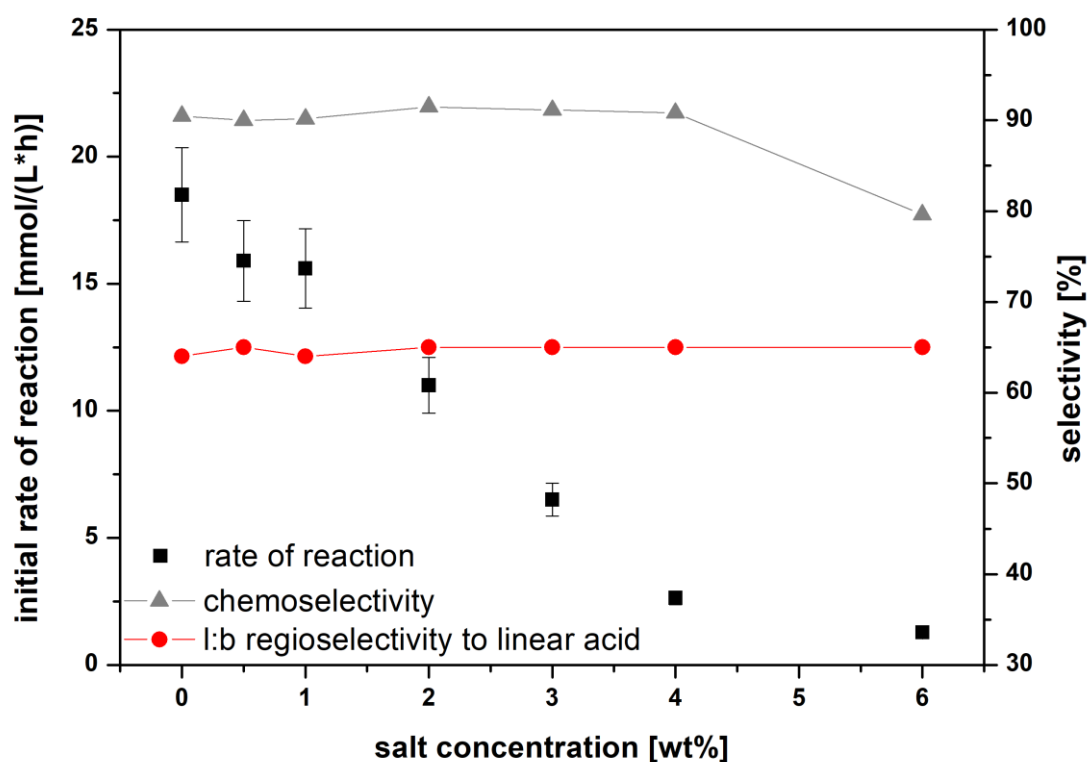


Figure S2. Effect of salt concentration on the hydroxycarbonylation of 1-dodecene. Experimental conditions: $\text{Pd}_2(\text{allyl})_2\text{Cl}_2$ (0.08 mmol), $\text{Pd}/\text{SX}/\text{MSA}/1\text{-dodecene}$ (1:4:40:110), $\alpha=0.5$, tetradecane as the cosolvent (9 g), water (12 g), Marlupal 24/70 as the surfactant, $\gamma=9\%$, Na_2SO_4 as salt, $p(\text{CO})=30$ bar, $T=85^\circ\text{C}$, $n=1200$ rpm, $t=20$ h, $V_R=0.03$ L.

Besides the reaction rate, the 1:b selectivity remains constant at 65:35 and the chemoselectivity at a value of 90% for salt concentrations of up to 4wt%. The chemoselectivity drops to 80% with 6 wt% sodium sulfate in the reaction mixture. Apparently, the precipitation of the catalyst complex leads to a higher isomerization of 1-dodecene. For all experiments 1wt% sodium sulfate was chosen because of an accelerated phase separation.