Supporting Information:

In situ investigation of molecular kinetics and particle formation of water-dispersible titania nanocrystals

G. Garnweitner* and C. Grote

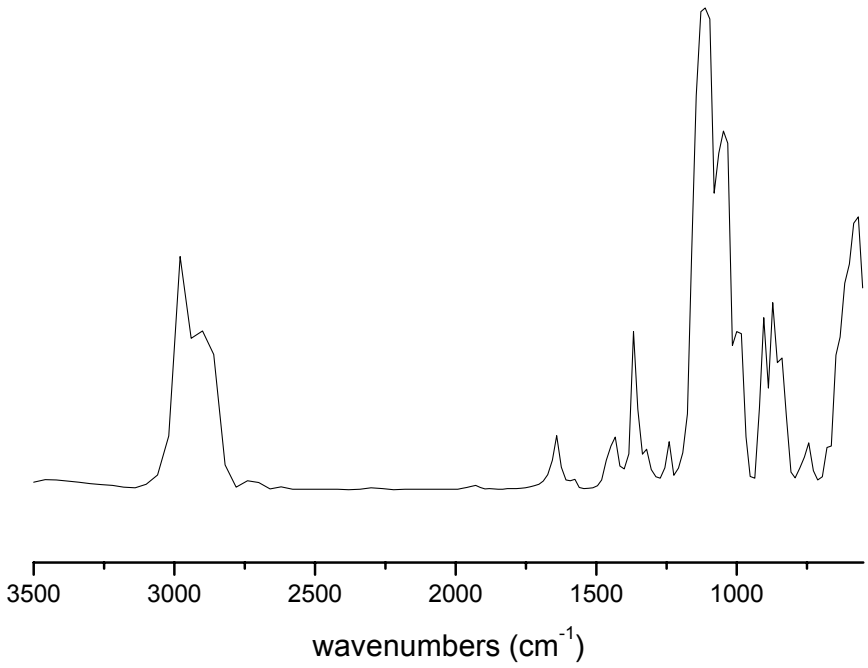

Fig. SI_1: Simulated IR spectrum of $Ti(OEt)_2Cl_2$.[1]

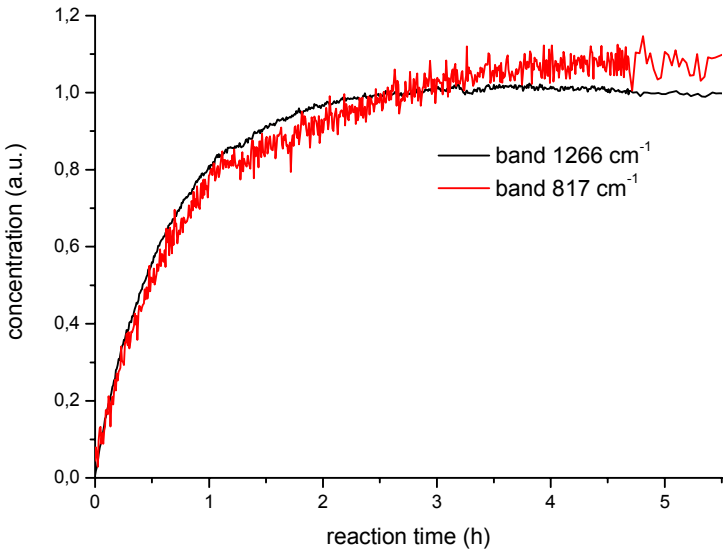

Fig. SI_2: Comparison of the normalized kinetics of benzyl chloride, as obtained from the baseline-corrected IR band at 1266 cm^{-1} and 817 cm^{-1} (black line), respectively.

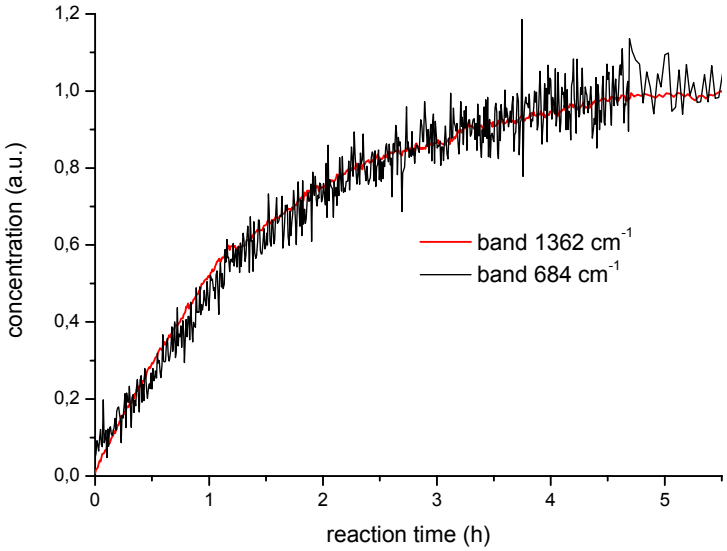

Fig. SI_3: Comparison of the normalized kinetics of benzyl ether, as obtained from the baseline-corrected IR band at 1362 cm^{-1} and 684 cm^{-1} (black line), respectively.

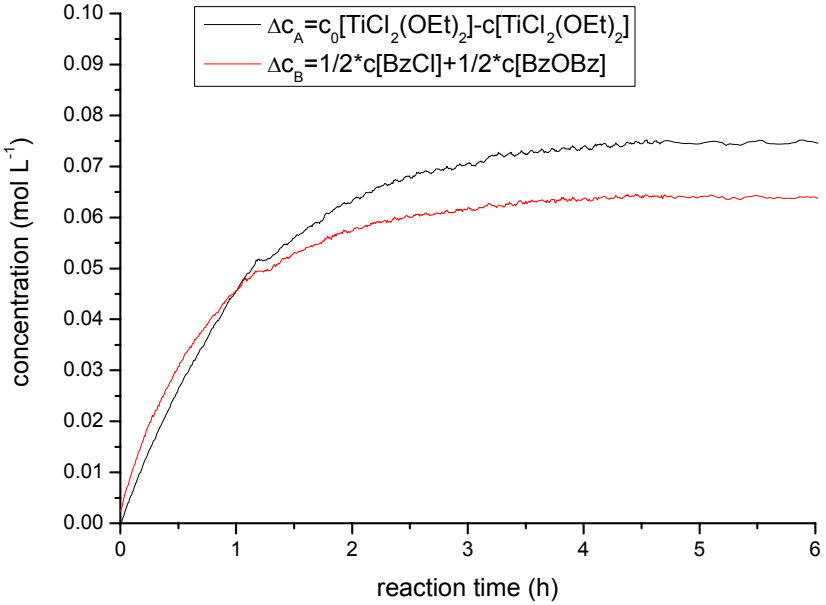

Fig. SI_4: Comparison of the consumption of the $TiCl_2(OEt)_2$ species with the formation of organic side products (as determined from the in-situ FTIR measurements).

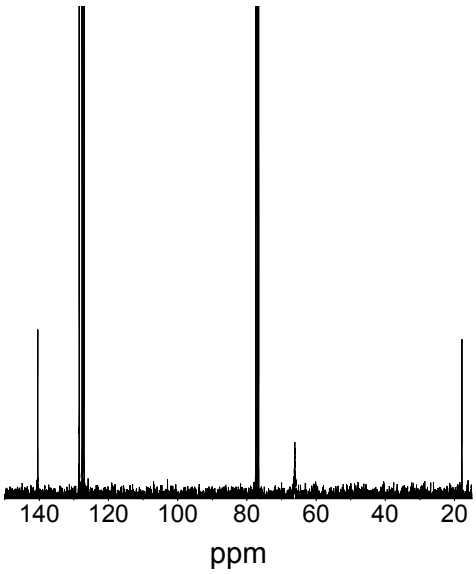

Fig. SI_5: ^{13}C NMR spectrum of the reaction solution after 0.5 h:
δ_C (75 MHz; $CDCl_3$; TMS) 65.4 ppm, (-CH_2-, benzyl alcohol).

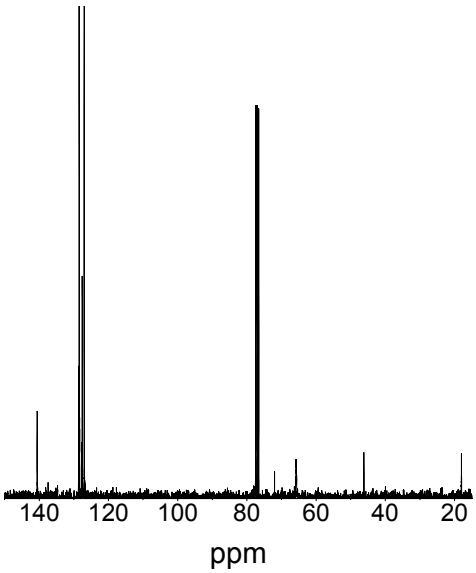

Fig. SI_6: ^{13}C NMR spectrum of the reaction solution after 8 h:
δ_C (75 MHz; $CDCl_3$; TMS) 65.4 ppm, (-CH_2-, benzyl alcohol), 46.2 ppm, (-CH_2-, benzyl chloride), 72.0 ppm (-CH_2-, benzyl ether).

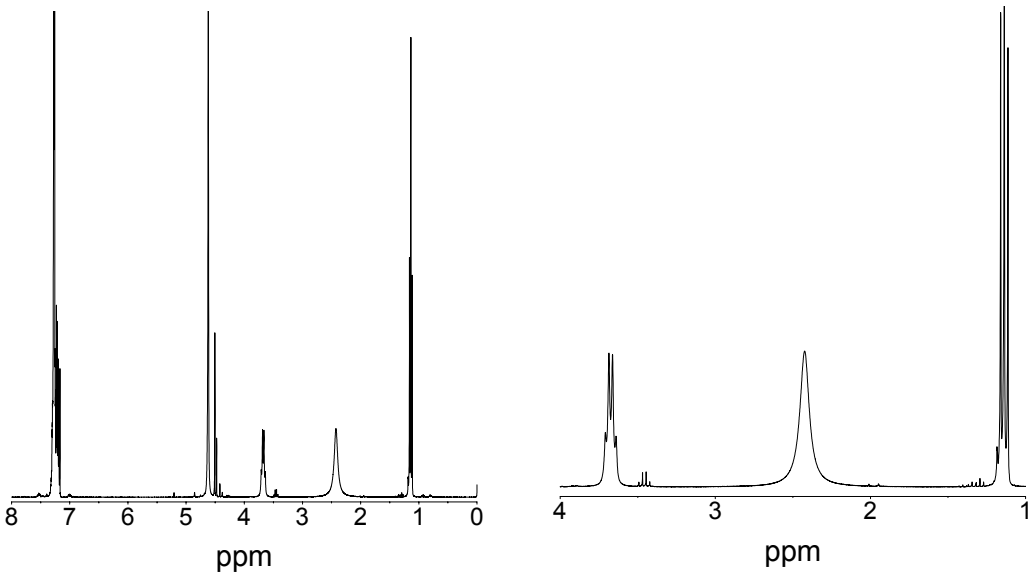

Fig. SI_7a, b: ^{1}H NMR spectrum of the reaction solution (left: overview, right: magnified region 1-4 ppm):
δ_H (300 MHz; $CDCl_3$; TMS) 1.12 ppm (-CH_3-, ethanol), 3.64 ppm (-CH_2-, ethanol).

References

1. M. C. Hemmer, J. Gasteiger, *TeleSpec Simulation Tool*, www.chemie.uni-erlangen.de/services/telespec.