

Heterogeneous Asymmetric Hydrogenation of Activated Ketones: Mechanistic Insight into the Role of Alcohol Products by in situ Modulation-Excitation IR Spectroscopy

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Supporting Information

Transient adsorption-desorption behavior of product alcohols on unmodified and CD-modified Pt/Al₂O₃

Figures S1, S2 and S3 show phase-domain and time-domain in situ ATR-IR spectra during transient adsorption-desorption of chiral product alcohols, (*R*)-PL, (*R*)-TFBA and (*R*)-EL, on CD-modified Pt/Al₂O₃, unmodified Pt/Al₂O₃ and ZnSe IRE crystal (blank test) at 283 K. To extract kinetic information for Figure 2, the peak of the absorption band assignable to C=O stretching vibration at around 1750 cm⁻¹ was selected for (*R*)-PL and (*R*)-EL while CF₃ deformation mode at around 1180 cm⁻¹ was used for (*R*)-TFBA profile.

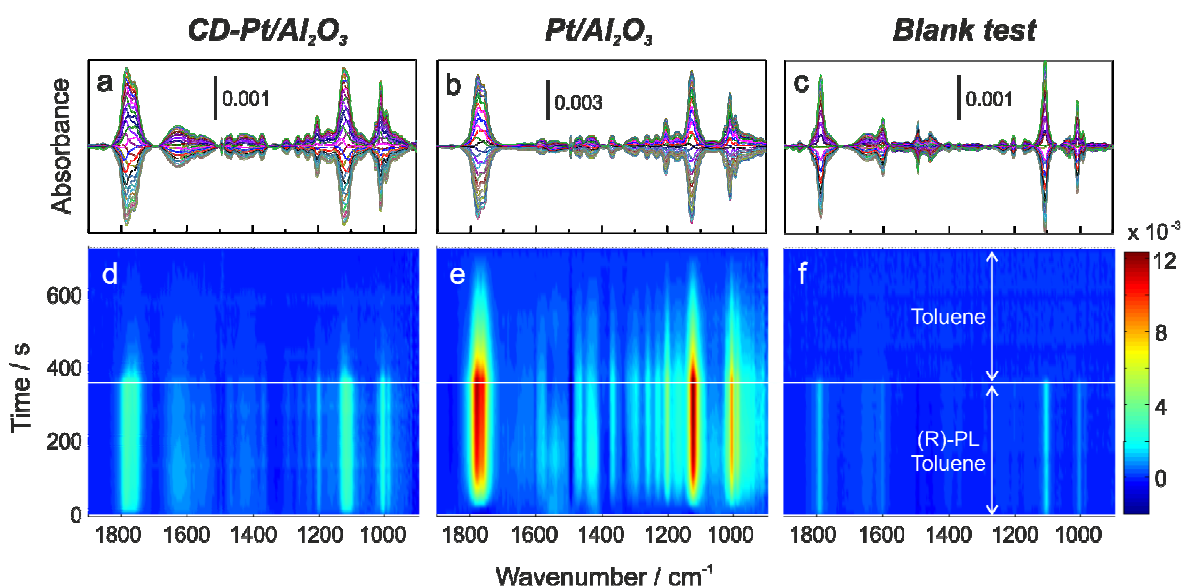


Figure S1. (a-c) phase-domain and (d-f) time-domain ATR-IR spectra of (*R*)-PL acquired from MES experiments by periodically changing between a 1 mM solution of (*R*)-PL in H₂-saturated toluene (0 – 375 s) and H₂-saturated toluene (375 – 750 s) on (a, d) CD-modified Pt/Al₂O₃, (b, e) Pt/Al₂O₃ and (c, f) ZnSe at 283 K. The last spectrum of the period at 750 s was used as the background.

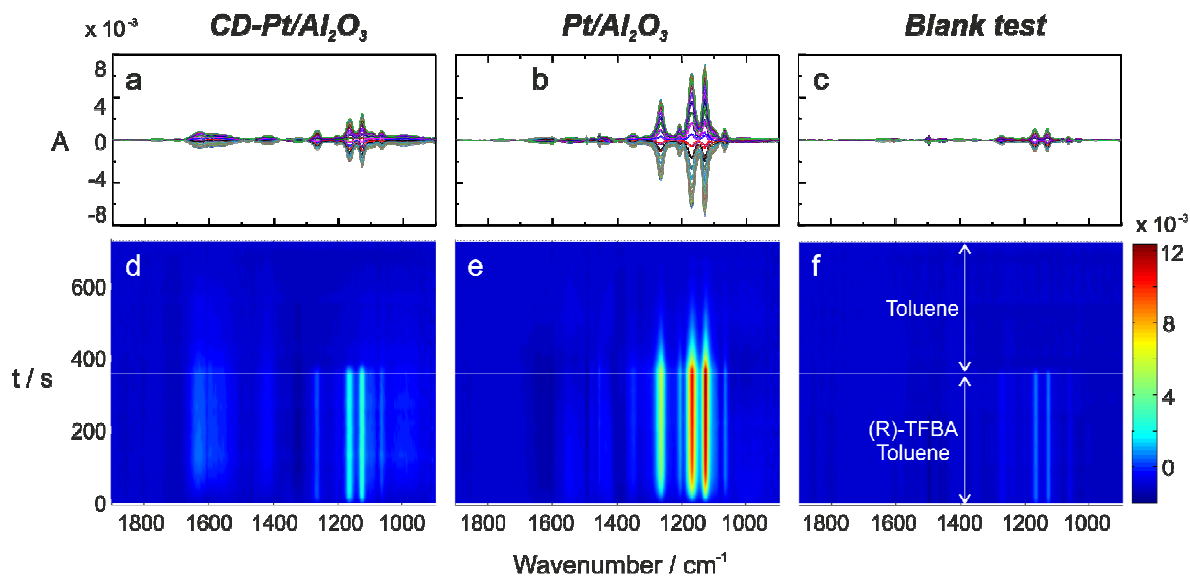


Figure S2. (a-c) phase-domain and (d-f) time-domain ATR-IR spectra of (R)-TFBA acquired from MES experiments using periodic changes between a 1 mM solution of (R)-TFBA in H₂-saturated toluene (0 – 375 s) and H₂-saturated toluene (375 – 750 s) on (a, d) CD-modified Pt/Al₂O₃, (b, e) Pt/Al₂O₃ and (c, f) ZnSe at 283 K. The last spectrum of the period at 750 s was used as the background.

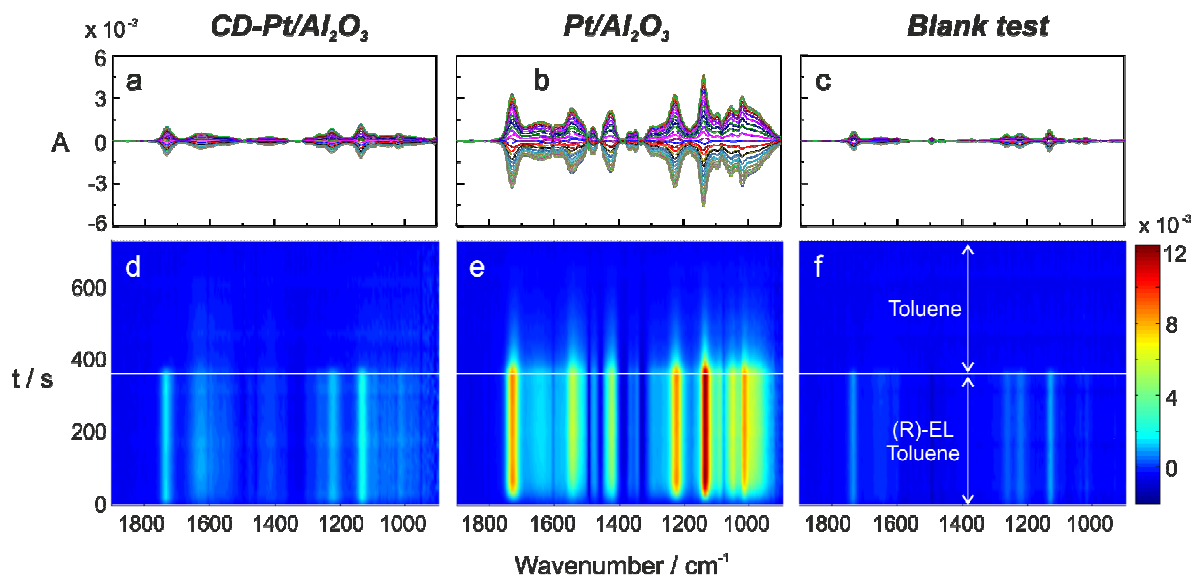


Figure S3. (a-c) phase-domain and (d-f) time-domain ATR-IR spectra of (*R*)-EL acquired from MES experiments using periodic changes between a 1 mM solution of (*R*)-EL in H₂-saturated toluene (0 – 375 s) and H₂-saturated toluene (375 – 750 s) on (a, d) CD-modified Pt/Al₂O₃, (b, e) Pt/Al₂O₃ and (c, f) ZnSe at 283 K. The last spectrum of the period at 750 s was used as the background.